Contributions to geometric inference on manifolds and to the statistical study of persistence diagrams

Quelques contributions à l'inférence géométrique pour les variétés et à l'étude statistique des diagrammes de persistance

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À mon père.

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Chapter 1

Introduction (français)

Ce travail s'inscrit dans le cadre de l'Analyse Topologique des Données (ou TDA, pour *Topological Data Analysis*), qui est ici abordée selon deux points de vue différents : celui de l'inférence géométrique et celui de la théorie de l'homologie persistante. Ces deux approches visent toutes deux à extraire (dans des cadres différents) des informations pertinentes de nature géométrique et topologique sur des jeux de données complexes possédant des structures *a priori* non linéaires.

1 Les enjeux de l'inférence géométrique

La théorie statistique classique développée dans les années 1930 par Fisher fait les hypothèses suivantes : on observe des données en basse dimension, et on possède un modèle génératif simple expliquant ces données (gaussien, exponentiel, etc.). On s'intéresse alors à des estimateurs de paramètres caractérisant la loi des données, pour lesquels on est capable de donner des garanties fortes d'optimalité. À l'inverse, les jeux de données modernes se présentent typiquement sous la forme de nuages de points en grande dimension. Si les méthodes classiques peuvent s'appliquer dans ce cadre, leurs performances théorique et pratique deviennent médiocres. Ce phénomène, couramment appelé *fléau de la dimension*, montre la nécessité d'un changement de paradigme. Il s'agit tout d'abord, dans une phase de modélisation, de développer des jeux d'hypothèses raisonnables que vérifient une large classe de données acquises en grande dimension. Dans un second temps, il s'agira de développer des méthodes statistiques adaptées à ces nouveaux jeux d'hypothèses.

Ainsi, certaines méthodes, telle le LASSO [Tib96], ont des bonnes performances sous une hypothèse de parcimonie sur les jeux de données. Des méthodes de régression, telle la régression ridge [HK70], s'adaptent à la grande dimension en pénalisant la complexité de la fonction de régression proposée. On peut aussi mentionner d'autres méthodes standard, telle l'analyse en composante principale [Pea01; Hot33], dont l'utilisation suppose que les données sont proches d'un espace vectoriel de basse dimension en un sens L_2. Les hypothèses que nous venons de mentionner reposent toutes sur l'existence d'une structure linéaire de basse dimension pertinente pour expliquer le jeu de données. En particulier, elles nécessitent d'avoir une grande confiance en la paramétrisation des données utilisées, et toute reparamétrisation peut briser cette structure linéaire (voir la figure 1.1). L'idée clé de l'inférence géométrique est de relaxer cette hypothèse en supposant que les données en grande dimension se concentrent autour d'une forme de basse dimension, *a priori* non linéaire. Mathématiquement, on suppose alors que *les données observées sont proches d'une variété M de dimension d petite dans un espace de dimension ambiante D possiblement grande.*

D'un point de vue statistique, ce type d'hypothèses a d'abord été étudié dans le cas où la variété M est connue [Hen90; Pel05]. C'est notamment le cas pour des problèmes de géolocalisation [IPT19], où les données sont des éléments de $\mathbb{S}^2$, ou

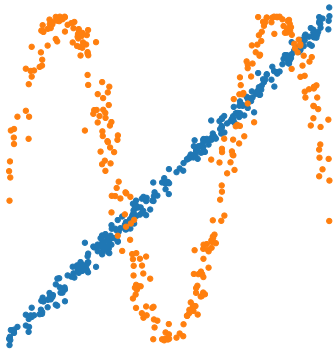


FIGURE 1.1: La structure linéaire du jeu de données bleu disparaît lorsque l'axe vertical est reparamétrisé par une fonction non-linéaire (ici sinusoïdale). Le jeu de données orange reste cependant près d'une variété.

lors de l'étude d'images de visages se présentant sous différents éclairages [Cha+07] dans laquelle les jeux de données présents se trouvent être sur une Grassmannienne $G(k, d)$. Connaître la variété M est le plus souvent trop exigeant, et, au cours des années 2000, une autre famille de techniques, que l'on peut regrouper sous le terme de méthodes de réduction de dimension non-linéaire, est apparue [RS00; ZZ03; WSS04] (on pourrait aussi mentionner des techniques proposées antérieurement comme les cartes autoadaptatives [Koh89] ou les surfaces principales adaptatives [LT94]). Ces méthodes, ne nécessitant pas une connaissance *a priori* de la variété M, cherchent à plonger de la manière la plus fidèle possible un nuage de points proche d'une forme "non-linéaire" dans un espace euclidien $\mathbb{R}^d$ pour d petit. Par exemple, la méthode ISOMAP [TDSL00] est basée sur le plongement dans $\mathbb{R}^d$, à l'aide d'un positionnement multidimensionnel (ou MDS pour *multidimensional scaling*), d'un graphe de voisinage construit sur les observations. Elle permet ainsi de "déplier" des jeux de données qui se trouveraient sur des objets difféomorphes à un ouvert convexe (voir la figure 1.2). On peut ensuite appliquer des techniques standard de classification ou de régression aux données "dépliées". Notons tout de même que ces approches ne possèdent des garanties théoriques que dans un cadre restreint, qui nécessite au moins que le jeu de données soit difféomorphe à $\mathbb{R}^d$. Il est ainsi par exemple impossible de plonger continûment une sphère dans $\mathbb{R}^2$.

Parallèlement à cette ligne de travaux, se sont développées dans le domaine de la géométrie algorithmique des méthodes de reconstruction d'une variété $M \subset \mathbb{R}^D$ à partir d'un échantillon fini $\mathcal{X}$, avec une attention toute particulière portée aux courbes et aux surfaces [BTG95; AB99]. Ainsi, l'algorithme COCONE [Ame+00] permet la reconstruction d'une surface lisse M à partir d'une approximation finie, si le taux d'approximation $\varepsilon(\mathcal{X}) := \sup\{d(x, \mathcal{X}) : \ x \in M\}$ de l'échantillon $\mathcal{X}$ est suffisamment petit, tandis que le *Tangential Delaunay Complex* de Boissonnat et Ghosh [BG14] permet une telle reconstruction en dimension supérieure. On peut aussi se poser des questions sur la reconstruction d'invariants topologiques ou géométriques de M, comme son axe médian [ABE09] ou ses groupes d'homologie ou d'homotopie [CO08]. Encore une fois, ces travaux requièrent uniquement une échantillon fini $\mathcal{X}$ se trouvant sur la variété M et ayant un bon taux d'échantillonnage. Un autre point de vue consiste à supposer que l'approximation $\mathcal{X}$ est la réalisation d'un processus aléatoire, de n observations indépendantes d'une certaine loi μ concentrée autour de la variété M : on peut alors espérer que les méthodes de reconstruction fonctionnent avec grande probabilité, sur des échantillons "typiques". Cette approche statistique des problèmes

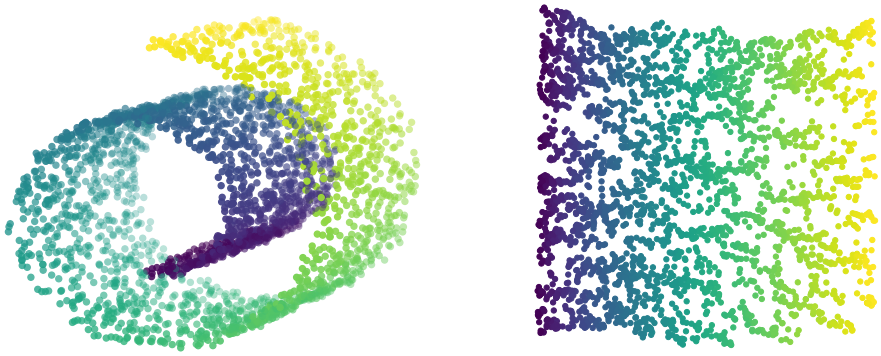


FIGURE 1.2: À gauche : un ensemble $\mathcal{X}$ de 3000 points échantillonnés sur un *swiss roll*. À droite : sortie de l'algorithme ISOMAP appliqué à $\mathcal{X}$ (implémenté sur `scikit-learn` [Bui+13]).

de géométrie algorithmique a pour la première fois été adoptée dans un article de Niyogi, Smale et Weinberger [NSW08], où les auteurs montrent que l'homologie d'une variété M est reconstruite avec grande probabilité à partir du complexe de Čech (un objet combinatoire défini dans le chapitre 3) d'un n-échantillon aléatoire $\mathcal{X}_n$. Dans les années 2010, a ensuite été abordée l'estimation au sens statistique du terme de plusieurs descripteurs de M, comme sa dimension [HA05; LJM09; KRW19], ses espaces tangents [AL19; CC16], son reach [Aam+19; Ber+21], sa courbure [AL19], ses distances géodésiques [ACC20], ou la variété M elle-même [Gen+12a; Gen+12b; MMS16; AL18; AL19].

Ce point de vue statistique sur les problèmes de reconstruction géométrique a l'avantage de permettre de poser simplement la question de l'optimalité des procédures envisagées. Ceci est rendu possible grâce à la théorie statistique minimax. Considérons par exemple le problème de l'estimation d'une variété M à partir d'un n-échantillon aléatoire $\mathcal{X}_n$. Un estimateur $\hat{M}$ de M est alors n'importe quel sous-ensemble compact de $\mathbb{R}^D$, fonction (mesurable) de l'échantillon. La qualité de l'estimateur $\hat{M}$ sous loi μ, appelée son *μ-risque*, est donnée par sa distance de Hausdorff d_H moyenne à M, c'est-à-dire

$$R_n(\hat{M}, \mu, d_H) := \mathbb{E}[d_H(\hat{M}, M)], \tag{1.1}$$

où il est sous-entendu que $\hat{M} = \hat{M}(\mathcal{X}_n)$ et $\mathcal{X}_n$ est un n-échantillon de loi μ. En pratique, la loi μ générant les données est inconnue, et il est plus intéressant de contrôler ce risque uniformément sur tout un ensemble $\mathcal{Q}$ de lois μ, que l'on appelle un *modèle statistique*. En inférence géométrique, plusieurs modèles statistiques ont été introduits, prenant en compte différents modèles de bruits et de régularité pour M. Le risque uniforme de l'estimateur $\hat{M}$ sur une classe $\mathcal{Q}$ est alors donné par

$$R_n(\hat{M}, \mathcal{Q}, d_H) := \sup\{R_n(\hat{M}, \mu, d_H) : \ \mu \in \mathcal{Q}\}, \tag{1.2}$$

tandis qu'un estimateur sera dit *minimax* si il atteint (à une constante multiplicative près) le *risque minimax* défini par

$$\mathcal{R}_n(M, \mathcal{Q}, d_H) := \inf\{R_n(\hat{M}, \mathcal{Q}, d_H) : \ \hat{M} \text{ est un estimateur}\}. \tag{1.3}$$

Mentionnons par exemple la famille de modèles $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$ introduite par Genovese *et al.* dans [Gen+12a], comprenant les lois μ supportées sur une variété M de dimension d satisfaisant certaines propriétés. Tout d'abord, on suppose que μ a une densité f sur M comprise entre deux bornes $f_{\min}$ et $f_{\max} > 0$. Cela permet d'assurer que toutes

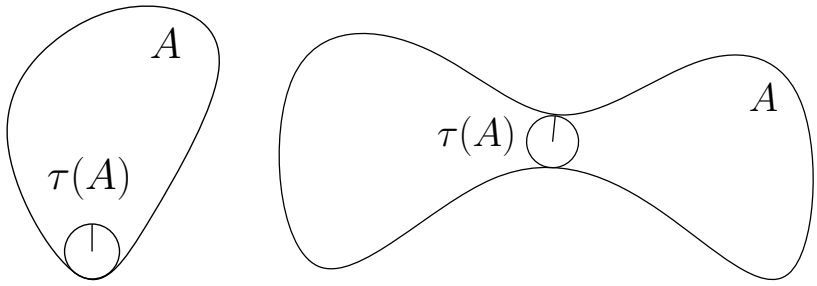


FIGURE 1.3: Si le reach de la courbe M est grand, alors la courbe ne peut pas être trop courbée (gauche) et ne peut pas présenter une structure fine en goulot d'étranglement (droite)

les régions de la variété sont à peu près autant échantillonnées : on parle alors de lois presque-uniformes sur M. Le paramètre $\tau_{\min}$ impose une borne inférieure sur le reach $\tau(M)$ de la variété. Ce dernier est une notion centrale en inférence géométrique. Le reach $\tau(M)$ est défini comme le plus grand rayon r tel que, si $d(x, M) \leq r$, alors il existe une unique projection y de x sur M, c'est-à-dire un point $y \in M$ satisfaisant $|x - y| = d(x, M)$. D'un point de vue plus géométrique, avoir un reach $\tau(M)$ plus grand que r implique qu'il est possible de faire "rouler" une boule le long de M sans "se cogner" à une autre partie de M [PL08, Lemma A.0.6]. Ainsi, le reach $\tau(M)$ contrôle deux quantités différentes, d'une part le rayon de courbure de la variété M (donc une régularité locale), et d'autre part une régularité globale, contrôlant la présence de structure en goulot d'étranglement dans la variété (voir la figure 1.3). Sur le modèle $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$, la vitesse minimax satisfait

$$c_0 \left(\frac{\ln n}{n}\right)^{2/d} \leq \mathcal{R}_n(M, \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}, d_H) \leq c_1 \left(\frac{\ln n}{n}\right)^{2/d} \tag{1.4}$$

pour deux constantes $c_0, c_1 > 0$ dépendant de $\tau_{\min}$, $f_{\min}$, $f_{\max}$ et d. La borne inférieure dans cette inégalité a été montrée par Kim et Zhou [KZ15], tandis que la borne supérieure est obtenue en fournissant un estimateur ayant un risque uniforme de l'ordre de $(\ln n/n)^{2/d}$. Un tel estimateur (non calculable en pratique) a tout d'abord été proposé par Genovese *et al.* dans [Gen+12a], tandis qu'un autre estimateur, cette fois-ci calculable, atteignant cette même vitesse, basé sur le *Tangential Delaunay Complex*, a été introduit par Aamari et Levrard [AL18].

1.1 Le problème de l'adaptivité

Notons que le *Tangential Delaunay Complex* dépend de plusieurs paramètres, comme par exemple d'un rayon quantifiant la taille des voisinages utilisés pour calculer des analyses en composantes principales locales. Pour que le *Tangential Delaunay Complex* soit minimax, ces paramètres doivent être calibrés d'une certaine manière par rapport aux variables $\tau_{\min}$, $f_{\min}$ et $f_{\max}$ définissant le modèle. Or, ces quantités sont *a priori* inconnues. Se pose alors la question du choix en pratique des paramètres définissant l'estimateur. Cette question du calibrage pratique des paramètres définissant un estimateur n'est pas restreint à l'estimation de variétés, mais est un problème classique en statistique.

Citons par exemple la question du choix de la largeur de bande dans l'estimation à noyaux. Soit $X_1, \ldots, X_n$ un n-échantillon d'une certaine loi μ ayant une densité f sur $\mathbb{R}$, et supposons que l'on souhaite reconstruire la valeur de la densité $f(x_0)$ en un point fixé $x_0 \in \mathbb{R}$. Une méthode standard pour réaliser cet objectif est de convoler la mesure

empirique $\mu_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ par un certain noyau K_h, où $K_h = h^{-1}K(\cdot/h)$ et K vérifie $\int K = 1$. On obtient alors une fonction $\hat{f}_h = K_h * \mu_n$. Supposons que la densité f soit de régularité s, c'est-à-dire que $f \in \mathcal{C}^s(\mathbb{R})$, l'ensemble des fonctions dérivables $\lfloor s \rfloor$ fois, dont la dérivée $\lfloor s \rfloor$ième est $(s - \lfloor s \rfloor)$-Hölder. Alors, en choisissant bien le noyau K, on sait qu'il est optimal de choisir la largeur de bande h_{opt} de l'ordre de $c \cdot n^{-1/(2s+1)}$, où c dépend de la norme $\mathcal{C}^s$ de f [Tsy08, Chapitre 1]. Le risque associé est alors de l'ordre de $n^{-s/(2s+1)}$, ce qui est la vitesse minimax d'estimation sur les densités de régularité s. En pratique, il est impossible de connaître exactement s, de sorte que nous devons trouver une autre stratégie pour choisir h. Les méthodes adaptatives consistent à choisir une largeur de bande $\hat{h}$ *en fonction des données*, de sorte que l'estimateur $\hat{f}_{\hat{h}}$ ait un μ-risque presque aussi bon que l'estimateur optimal $\hat{f}_{h_{\text{opt}}}$ sous des hypothèses faibles sur μ. En particulier, la méthode PCO (pour *Penalized Comparison to Overfitting*) introduite par Lacour, Massart et Rivoirard [LMR17] consiste à comparer chaque estimateur $\hat{f}_h$ à un estimateur dégénéré $\hat{f}_{h_{\min}}$ pour un certain $h_{\min}$ très petit. La largeur de bande $\hat{h}$ sélectionnée est choisie parmi une famille $\mathcal{H}$ de largeurs de bande (toutes supérieures à $h_{\min}$), en minimisant un critère qui dépend de la distance $\|\hat{f}_h - \hat{f}_{h_{\min}}\|_{L_2(\mathbb{R})}$ et qui pénalise les petites valeurs de h. Lacour, Massart et Rivoirard montrent alors une *inégalité oracle* pour leur estimateur, c'est-à-dire une inégalité du type

$$\mathbb{E}\|\hat{f}_{\hat{h}} - f\|^2_{L_2(\mathbb{R})} \leq C \min\{\mathbb{E}\|\hat{f}_h - f\|^2_{L_2(\mathbb{R})} : \ h \in \mathcal{H}\} + C(n, |\mathcal{H}|), \tag{1.5}$$

où $C(n, |\mathcal{H}|)$ est un terme de reste négligeable devant le risque optimal. On obtient ainsi que $\hat{f}_{\hat{h}}$ a un risque presque aussi bon que le meilleur estimateur $\hat{f}_{h_{\text{opt}}}$, sans jamais avoir eu à estimer les paramètres définissant le modèle (ici la régularité de la densité ainsi que sa norme).

Dans le chapitre 4, nous nous inspirons de la philosophie de la méthode PCO pour créer un estimateur adaptatif de variété. Une première étape consiste à créer une famille d'estimateurs $(\hat{M}_t)_{t\geq 0}$, analogue des estimateurs à noyaux pour l'estimation de variété. Ceci est permis par la notion de t-enveloppe convexe. Pour $t \geq 0$, la t-enveloppe convexe $\text{Conv}(t, A)$ d'un ensemble A interpole entre A ($t = 0$) et son enveloppe convexe $\text{Conv}(A)$ ($t = \infty$). Elle est définie par

$$\text{Conv}(t, A) := \bigcup_{\substack{\sigma \subset A \\ r(\sigma) \leq t}} \text{Conv}(\sigma), \tag{1.6}$$

où $r(\sigma)$ est le rayon de l'ensemble σ, à savoir le rayon de la plus petite boule contenant σ. On montre dans un premier temps que pour $t = c \cdot (\ln n/n)^{1/d}$, où c dépend de d et des paramètres $\tau_{\min}$ et $f_{\min}$, la t-enveloppe convexe $\text{Conv}(t, \mathcal{X}_n)$ d'un n-échantillon aléatoire de points fournit un estimateur de variétés qui est minimax sur le modèle $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$. Dans un deuxième temps, nous considérons le problème de la sélection adaptative du paramètre t. Un analogue de l'estimateur dégénérée $\hat{f}_{h_{\min}}$ est ici donné par le choix de $t = 0$: on trouve alors l'estimateur $\text{Conv}(0, \mathcal{X}_n) = \mathcal{X}_n$. Si on croît en la méthode PCO, il s'agira donc de comparer les estimateurs $\text{Conv}(t, \mathcal{X}_n)$ à $\mathcal{X}_n$, c'est-à-dire d'étudier la fonction $t \mapsto h(t, \mathcal{X}_n) := d_H(\text{Conv}(t, \mathcal{X}_n), \mathcal{X}_n)$. Il se trouve que cette fonction a été précédemment introduite sous le nom de *défaut de convexité de l'ensemble* $\mathcal{X}_n$ dans un papier d'Attali, Lieutier et Salinas [ALS13], où elle était utilisée pour étudier le type d'homotopie des complexes de Rips. Nous montrons que le défaut de convexité de l'échantillon aléatoire $\mathcal{X}_n$ exhibe des comportements différents dans deux régimes : avant une certaine valeur seuil $t^*(\mathcal{X}_n)$, elle a un comportement globalement linéaire, tandis qu'après cette valeur seuil, elle possède un comportement (sous-)quadratique. Le défaut de convexité est calculable uniquement à partir des

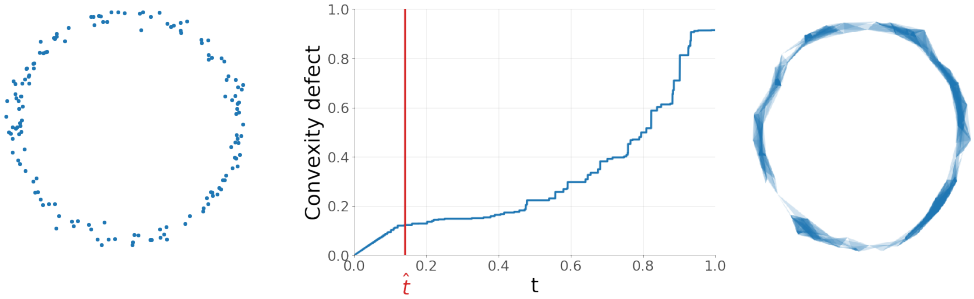


FIGURE 1.4: Gauche. Échantillon $\mathcal{X}_n$. Centre. Défaut de convexité de $\mathcal{X}_n$ et échelle sélectionnée $\hat{t}_\lambda$. Droite. L'ensemble $\mathrm{Conv}(\hat{t}_\lambda, \mathcal{X}_n)$.

données, et on peut donc en pratique observer ces deux phases. On peut alors montrer que les valeurs de t juste au-dessus de la valeur seuil $t^*(\mathcal{X}_n)$ fournissent un risque minimax de l'ordre de $(\ln n/n)^{2/d}$. En pratique, nous fixons deux hyperparamètres $0 < \lambda < 1$ et $t_{\max}$, posons

$$\hat{t}_\lambda := \sup\{t < t_{\max} : \ h(t, \mathcal{X}_n) > \lambda t\}, \tag{1.7}$$

et montrons que, si $t_{\max}$ est assez petit par rapport à $\tau_{\min}$, alors $\mathrm{Conv}(\hat{t}_\lambda, \mathcal{X}_n)$ fournit un estimateur minimax adaptatif de variétés, voir la figure 1.4. Notons que nous n'obtenons pas le caractère adaptatif de notre estimateur en montrant une inégalité oracle du type (1.5), mais en montrant que $\hat{t}_\lambda$ est plus grand que la valeur seuil $t^*(\mathcal{X}_n)$ (tout en restant du bon ordre de grandeur) avec grande probabilité, ce qui suffit à montrer le caractère minimax de l'estimateur correspondant. On peut aussi montrer que le paramètre $\hat{t}_\lambda$ est en fait proche du taux d'approximation $\varepsilon(\mathcal{X}_n)$. Comme mentionné précédemment, un certain nombre d'algorithmes en géométrie algorithmique nécessitent la connaissance du taux d'échantillonnage (ou plutôt d'un encadrement du taux d'échantillonnage), et peuvent donc être utilisés en utilisant le paramètre $\hat{t}_\lambda$.

1.2 Reconstruire la mesure plutôt que la variété

La deuxième contribution proposée ici est motivée par les problématiques d'estimation de densité. En inférence géométrique, la possibilité de reconstruire la densité f de la mesure μ générant les observations $\mathcal{X}_n$ a d'abord été considérée dans le cas où M est connue. Hendriks [Hen90] propose d'utiliser les fonctions propres de l'opérateur de Laplace-Beltrami sur la variété pour reconstruire la densité, tandis que Pelletier [Pel05] propose un estimateur à noyaux utilisant la distance géodésique sur la variété. Dans le cadre de l'inférence géométrique, où la variété M est supposée inconnue, les travaux d'estimation de densité sont plus récents. Soit un point x_0 que l'on suppose appartenir à M. L'estimation de de $f(x_0)$, la densité de f en x_0, a été abordée dans [BS17; WW20], où des vitesses de convergence des estimateurs à noyaux sont exhibées, respectivement dans le cas où la variété est à bord et dans le cas où la densité est supposée Hölder. Berenfeld et Hoffmann [BH19] exhibent des vitesses minimax d'estimation pour ce problème, et montrent que deux régularités entrent en jeu dans la vitesse optimale : d'une part la régularité s de la densité f, et d'autre part la régularité k de la variété M. De plus, les auteurs montrent que la méthode de sélection de Goldenshluger-Lepski [GL13] s'applique dans ce cadre pour sélectionner la largeur de bande du noyau et permet d'obtenir des estimateurs adaptatifs de $f(x_0)$.

Pour aller au-delà de l'estimation ponctuelle de f (ou de manière équivalente de la mesure associée μ), le choix de la fonction de perte est un problème délicat. En effet,

les choix standard en estimation de densité comprennent la distance L_p, la distance de Hellinger ou encore la divergence de Kullback-Leibler. Toutes ces fonctions de perte deviennent dégénérées pour la comparaison de deux mesures mutuellement singulières. Or, si le support M de la mesure μ est inconnu, il sera impossible de construire à partir d'un n-échantillon une mesure non-singulière par rapport à la mesure volume vol_M sur M, quand bien même son support serait très proche de M pour la distance de Hausdorff. Au contraire, les distances de Wasserstein W_p ($1 \leq p \leq \infty$) sont par construction robustes aux perturbations métriques du support d'une mesure, et sont donc particulièrement adaptées à notre problème. Elles sont définies de la manière suivante. Étant données deux mesures de probabilité μ et ν, nous définissons un plan de transport π entre μ et ν comme une mesure sur $\mathbb{R}^D \times \mathbb{R}^D$ ayant pour première marginale μ et seconde marginale ν. Informellement, au point $x \in \mathbb{R}^D$, une fraction $\mathrm{d}\pi(x,y)$ de la masse $\mathrm{d}\mu(x)$ présente en x est envoyée en y. Le coût d'un tel plan de transport est donné par $C_p(\pi) = \iint d(x,y)^p \mathrm{d}\pi(x,y)$, tandis que la distance Wasserstein W_p est donné par le coût du plus petit plan de transport :

$$W_p(\mu,\nu) := \inf\{C_p^{1/p}(\pi) : \ \pi \in \Pi(\mu,\nu)\}, \tag{1.8}$$

où $\Pi(\mu,\nu)$ est l'ensemble des plans de transport entre μ et ν.

L'utilisation des distances de Wasserstein, et plus généralement de la théorie du transport optimal, a montré son efficacité dans une large gamme de problèmes récents d'apprentissage automatique, avec des algorithmes efficaces et des garanties théoriques fortes (voir par exemple le livre de Peyré et Cuturi [PC19]). D'un intérêt tout particulier pour nous, Niles-Weed et Berthet ont abordé le problème de l'estimation d'une densité f supportée sur le cube $[0,1]^d$ pour les distances de Wasserstein [WB19b]. Supposons que f appartienne à l'espace de Besov $B^s_{p,q}([0,1]^d)$ de régularité s sur le cube (pour $s \geq 0$, et $1 \leq p < \infty$ et $1 \leq q \leq \infty$, voir le chapitre 5 pour une définition précise). Alors, Niles-Weed et Berthet montrent qu'une modification d'un estimateur par ondelettes classique atteint la vitesse de convergence de $n^{-(s+1)/(2s+d)}$ pour $d \geq 3$ en distance Wasserstein W_p (à comparer avec la vitesse de convergence $n^{-s/(2s+d)}$ pour l'estimation ponctuelle de densité). De plus, cette vitesse est la vitesse minimax.

Notre contribution principale, décrite dans le chapitre 5, est d'étendre ce résultat minimax en remplaçant le cube par n'importe quelle sous-variété M de régularité k pour $k \geq s+1$. Nous montrons alors qu'une mesure ayant pour densité par rapport à vol_M un estimateur à noyaux pondéré atteint la même vitesse minimax $n^{-(s+1)/(2s+d)}$. Dans le cas d'intérêt où la variété M est inconnue, nous ne pouvons pas utiliser vol_M, de sorte que l'estimateur précédent n'est pas calculable. Nous proposons donc dans un premier temps d'estimer la mesure volume. Nous exhibons ainsi un estimateur $\widehat{\mathrm{vol}}_M$ et montrons que $\hat{U}_M := \widehat{\mathrm{vol}}_M / |\widehat{\mathrm{vol}}_M|$ est un estimateur minimax de la mesure uniforme sur M. La reconstruction de la mesure volume est basée sur les procédures d'estimation de paramétrisations $\mathcal{C}^k$ locales de la variété M introduites par Aamari et Levrard [AL19].

2 Un point de vue multi-échelle : la persistance des données

Les travaux que nous avons mentionné jusqu'à maintenant font tous l'hypothèse forte de l'existence d'une variété de basse dimension interpolant les données. Il est légitime de s'intéresser à des questions de nature topologique dans un cadre beaucoup plus général. Par exemple, on peut imaginer qu'une information pertinente est présente dans la structure topologique fine de processus spatiaux, information pouvant servir dans

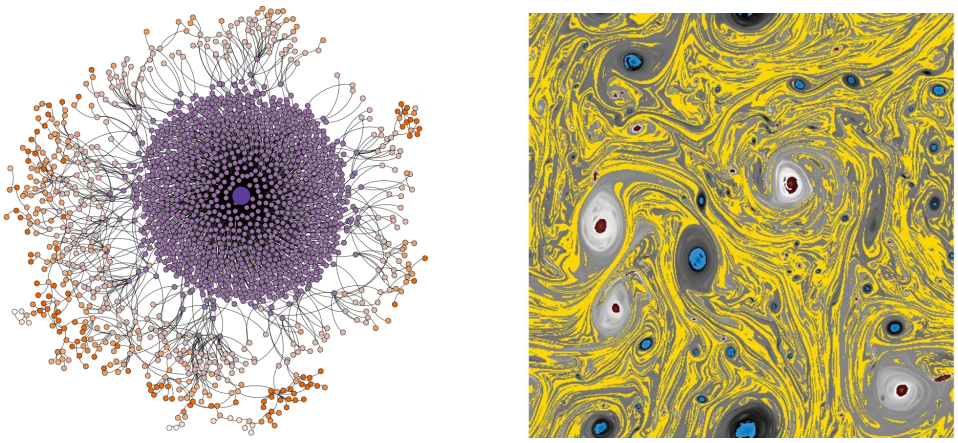


FIGURE 1.5: Gauche : un graphe d'interactions entre utilisateurs de Reddit provenant du jeu de données `REDDIT-5K`, présenté dans [YV15]. Droite : simulation d'un flot de turbulence donné par l'équation de Navier-Stokes [Sch+06].

un objectif de classification [Bro+20]. Dans certains problèmes, les données observées ne se présentent pas sous la forme de nuages de points, alors qu'une "topologie" reste présente. C'est le cas notamment lorsque l'on observe une famille de graphes, où la topologie est alors décrite par l'existence de cycles ou de plusieurs composantes connexes [AMA07; Hof+17; ZW19; Car+20], voir aussi la figure 1.5. La théorie de l'homologie persistante en TDA se propose de quantifier en un sens précis ce qu'est la "topologie" sous-jacente à un jeu de données de façon très générale. Pour cela, nous adoptons une approche multi-échelle.

Considérons tout d'abord un exemple simple. Soit $\mathcal{X}_n$ un ensemble fini de n points dans $\mathbb{R}^D$. D'un point de vue topologique, l'ensemble $\mathcal{X}_n$ est particulièrement peu intéressant : il comporte n composantes connexes, chacune réduite à un point. Une possibilité pour obtenir un ensemble plus riche topologiquement est de choisir une échelle t à laquelle regarder les données, dans la veine des t-enveloppes convexes du chapitre 4, ou plus simplement en considérant le t-voisinage de $\mathcal{X}_n$:

$$\mathcal{X}_n^t := \bigcup_{x \in \mathcal{X}_n} \mathcal{B}(x, t). \tag{1.9}$$

Comme expliqué précédemment, choisir une "bonne" échelle t est alors un problème délicat, bien que nous ayons proposé dans le chapitre 4 un algorithme dans le cas où l'échantillon $\mathcal{X}_n$ est suffisamment proche d'une variété M. La théorie de l'homologie persistante propose d'éviter ce choix du paramètre t en regardant comment évoluent les groupes d'homologie de $\mathcal{X}_n^t$ lorsque t grandit de 0 à $+\infty$. Si on s'intéresse par exemple à l'homologie de dimension 1 (c'est-à-dire à la présence de "boucles" dans un espace), on peut observer que des boucles apparaîtront à certains instants dans le processus, avant d'être bouchées par la suite lorsque le paramètre t du rayon des boules deviendra plus grand (voir la figure 1.6). Lorsque t devient très grand, nous obtenons un ensemble homotopiquement équivalent à une boule, qui ne possède plus de cycles. Cette évolution peut être résumée par un ensemble d'intervalles, chaque intervalle $[b, d)$ représentant une boucle apparue à l'échelle b, et ayant disparue à l'échelle d. De manière équivalente, nous pouvons considérer la collection de points $(b, d) \in \mathbb{R}^2$, que nous appelons le *diagramme de persistance* associé au processus. Notons que l'on a forcément $d > b$, de sorte qu'un diagramme de persistance est une liste de points dans $\Omega := \{u = (u_1, u_2) \in \mathbb{R}^2 : \ u_2 > u_1\}$, ou de manière équivalente

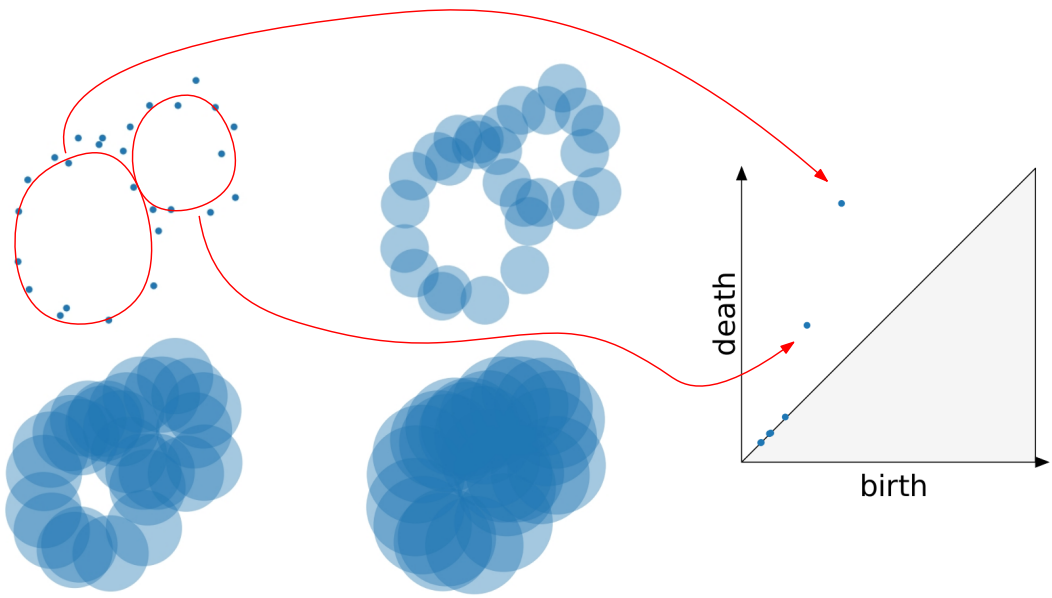


FIGURE 1.6: Le diagramme de persistance de dimension 1 associé à la filtration $(\mathcal{X}_n^t)_{t\geq 0}$.

une mesure de la forme $\sum_{i\in I} \delta_{u_i}$ sur Ω. Plus un cycle sera resté longtemps dans le processus $(\mathcal{X}_n^t)_{t\geq 0}$, plus il aura de l'importance. On appelle *persistance* du cycle la durée de vie $d-b$ de l'intervalle associé. Ainsi, dans un diagramme de persistance, les points loin de la diagonale $\partial\Omega := \{(t,t) : \ t \in \mathbb{R}\}$ correspondent à des caractéristiques topologiques importantes du processus sous-jacent. De manière plus générale, la théorie de l'homologie persistante peut s'appliquer à n'importe quelle *filtration* d'espaces topologiques, c'est-à-dire à une suite croissante d'espaces topologiques $(\mathcal{X}^t)_{t\in\mathbb{R}}$. Ceci inclut donc notamment les sous-niveaux d'une fonction $f : \mathcal{X} \to \mathbb{R}$, où $\mathcal{X}$ peut être un graphe, une image, ou un espace métrique quelconque. Quand la fonction f est la distance à un ensemble $\mathcal{X}_n$, nous retrouvons le processus décrit précédemment, tandis que le diagramme de persistance associé est appelé diagramme de Čech de l'ensemble $\mathcal{X}_n$. De plus, on peut s'intéresser à différentes dimensions d'homologie : composantes connexes (dimension 0), boucles (dimension 1), cavités (dimension 2), etc.

La théorie de l'homologie persistante et la notion de diagramme de persistance se sont construites progressivement durant la première moitié des années 2000, voir par exemple [Rob99; ELZ00; Car+04], tandis que le concept de persistance a aussi été introduit de manière indépendante par Barannikov dans le domaine de la théorie de Morse [Bar94]. Un des premiers résultats majeurs de la TDA a consisté à montrer que les diagrammes de persistance sont en un sens fort stables vis-à-vis des objets sur lesquels ils sont construits [CSEH07]. Cette propriété, couramment appelée "théorème de stabilité", repose sur un résultat puissant de stabilité algébrique énoncé précisément dans le chapitre 3. Ce théorème de stabilité est basé sur une notion de distance entre diagrammes, appelée la distance *bottleneck* d_∞. Par la suite, les distances d_p pour $1 \leq p \leq \infty$ ont été introduites, généralisant la distance bottleneck, et pour lesquelles des résultats de stabilité plus faibles existent (découlant de la stabilité en distance bottleneck) [CS+10]. Soient a et b deux diagrammes de persistance, où a est donné par la liste de points $x_1, \ldots, x_n \in \Omega$ et b par la liste de points $y_1, \ldots, y_m \in \Omega$. On appelle un appariement entre a et b une bijection entre $a \cup \partial\Omega$ et $b \cup \partial\Omega$: chaque point x_i est envoyé par γ soit sur un certain y_j, soit sur un point quelconque de la diagonale, et les y_j non atteints sont l'image par γ d'un certain point de la diagonale.

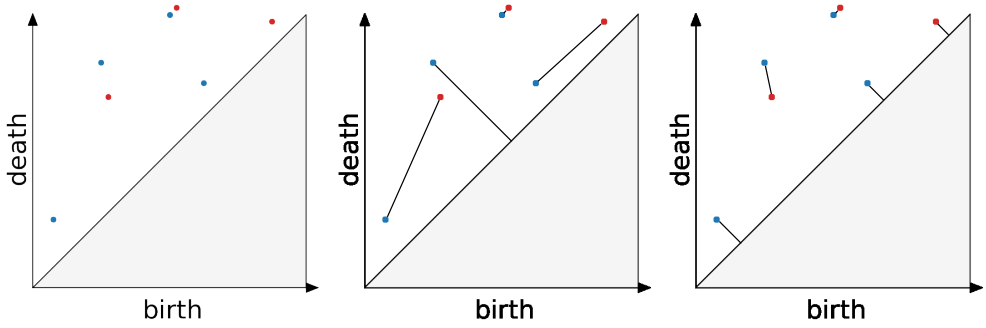


FIGURE 1.7: Gauche : deux diagrammes de persistance. Centre : un appariement γ entre les deux diagrammes. Le coût $C_p(\gamma)$ est donné par la somme des longueurs à la puissance p des segments apparaissant dans l'appariement, tandis que le coût *bottleneck* $C_\infty(\gamma)$ est donné par la longueur du plus long segment. Droite : un appariement optimal pour tout $p \in [1, +\infty]$.

Le coût $C_p(\gamma)$ de l'appariement γ est donné par

$$C_p(\gamma) := \sum_{x \in a \cup \partial\Omega} \|x - \gamma(x)\|^p, \tag{1.10}$$

où $\|\cdot\|$ représente une norme quelconque sur $\mathbb{R}^2$. Un appariement de coût minimal est dit *optimal*, et on pose

$$d_p(a, b) := \inf\{C_p(\gamma)^{1/p} : \ \gamma \in \Gamma(a, b)\}, \tag{1.11}$$

où $\Gamma(a, b)$ est l'ensemble des appariements entre a et b (voir la figure 1.7). On peut par ailleurs noter que dans un appariement optimal, tout point envoyé sur la diagonale $\partial\Omega$ est en fait envoyé sur son projeté orthogonal sur la diagonale. Intuitivement, on est en train d'apparier les différents cycles correspondant à chaque point des deux diagrammes, tandis qu'apparier un point à la diagonale, revient à l'apparier à un cycle "n'ayant par persisté", de la forme $[b, d)$ avec $b = d$. D'intérêt tout particulier en TDA est la distance *bottleneck* d_∞, obtenue comme limite des distances d_p pour $p \to \infty$. De manière équivalente, on peut définir le coût $C_\infty(\gamma)$ d'un appariement γ par $\sup\{\|x - \gamma(x)\| : \ x \in a \cup \partial\Omega\}$ et définir

$$d_\infty(a, b) := \inf\{C_\infty(\gamma) : \gamma \in \Gamma(a, b)\}. \tag{1.12}$$

Les diagrammes de persistance encodent une information topologique riche sur les données qu'ils résument, et souvent complémentaires d'autres méthodes plus classiques. N'étant pas naturellement des éléments d'un espace vectoriel, il est cependant délicat de les incorporer directement dans des algorithmes d'apprentissage automatique. Deux approches ont été proposées dans la littérature. La première consiste en l'utilisation de *feature maps* (ou représentations) sur l'espace des diagrammes, qui permettent de transformer les diagrammes de persistance en vecteurs, qui peuvent alors être facilement inclus dans des algorithmes standard d'apprentissage automatique. La seconde est de travailler malgré tout directement dans l'espace des diagrammes $\mathcal{D}$, par exemple en utilisant des méthodes nécessitant uniquement des distances en entrée (comme le *multidimensional scaling* précédemment mentionné). Nous étudierons ici ces deux approches.

2.1 L'espace des diagrammes de persistance étudié à travers le transport optimal partiel

Pour ce qui est de la deuxième approche, il est capital de tout d'abord comprendre de manière fine la structure de l'espace des diagrammes de persistance, vu en tant qu'espace métrique. Cette étude a été initiée par Mileyko, Mukherjee et Harer [MMH11], qui montrent des propriétés de l'espace métrique

$$\mathcal{D}^p := \{a \in \mathcal{D} : \ d_p(a, 0) < \infty\}, \quad \text{muni de la distance } d_p, \tag{1.13}$$

où 0 est le diagramme vide, de sorte que $d_p(a,0)^p = \sum_{u \in a}(u_2 - u_1)^p$, quantité appelée la *p-persistance totale* du diagramme a, et notée $\mathrm{Pers}_p(a)$. Notons que nous nous autorisons ici à avoir des diagrammes possédant un nombre infini de points, de sorte qu'il est possible d'avoir $d_p(a,0) = \infty$.

Nous proposons dans le chapitre 6 de participer à l'étude de la structure de l'espace des diagrammes de persistance en adoptant un point de vue différent de celui de [MMH11]. Nous avons déjà mentionné qu'un diagramme de persistance peut de manière équivalente être défini soit comme une liste de points dans Ω, soit comme une mesure ponctuelle $\sum_{i \in I} \delta_{u_i}$. Bien que l'approche "liste" semble être favorisée dans la littérature, le point de vue mesure s'avère plus riche. D'une part, ce point de vue permet de définir sans effort la somme, ou la moyenne de plusieurs diagrammes, qui sera alors une mesure quelconque (et non plus une mesure ponctuelle). D'autre part, cela permet d'appliquer la théorie du transport optimal aux diagrammes de persistance. En effet, la théorie du transport optimal, et plus précisément les distances de Wasserstein déjà mentionnées précédemment, permettent de comparer des mesures. Les distances d_p et W_p partagent des points communs : elles sont toutes deux définies comme étant le coût minimal de transport (ou d'appariement) entre deux mesures. De par ces similitudes, les distances d_p sont couramment appelées distances de Wasserstein dans la littérature en TDA. Cette appellation est cependant trompeuse, puisqu'il existe une différence fondamentale entre les distances d_p et W_p : les distances W_p ne sont définies que pour des mesures de probabilité (ou ayant la même masse), tandis que les distances d_p ne sont définies que pour des mesures ponctuelles, mais de masses potentiellement différentes.

Nous établissons dans le chapitre 6 un lien précis entre la structure métrique de l'espace des diagrammes de persistance et le transport optimal, en faisant le lien entre les distances d_p et des distances de transport optimal partiel introduites par Figalli et Gigli [FG10]. Établir ce lien permet d'une part d'obtenir certaines propriétés métriques de l'espace $\mathcal{D}^p$ (telle sa complétude, ou l'existence de barycentres), mais aussi d'étendre l'espace $\mathcal{D}^p$ à un espace plus grand $\mathcal{M}^p$, que nous appelons l'espace des *mesures persistantes*, et que nous munissons de la distance de Figalli-Gigli FG_p étendant la distance d_p. L'espace des mesures persistantes a l'avantage d'être "linéairement" convexe, ce qui nous permet de définir des moyennes de diagrammes, le diagramme de persistance moyen $E(P)$ d'une loi P sur l'espace des diagrammes de persistance étant au centre du chapitre 8. De plus, exhiber ce lien justifie l'adaptation d'algorithmes utilisés en transport optimal pour les diagrammes de persistances, une approche qui peut se révéler fructueuse [LCO18]. Le chapitre 6 est tiré de l'article [DL20], écrit en collaboration avec Théo Lacombe.

2.2 Représentations linéaires sur l'espace des diagrammes et le choix de la fonction de poids

La première approche que nous avions évoquée pour effectuer des procédures statistiques à l'aide de diagrammes de persistance consiste à utiliser une application $\Psi : \mathcal{D} \to B$,

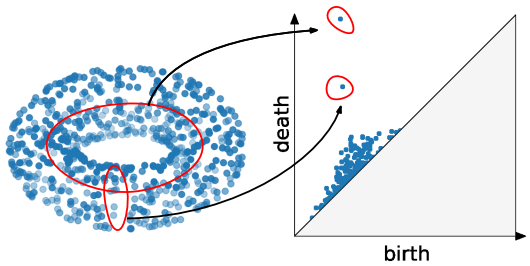


FIGURE 1.8: Le diagramme de persistance a_n de $n = 700$ points aléatoires sur le tore (pour l'homologie de dimension 1). Les deux points de haute persistance dans le diagramme donne des informations sur la géométrie du tore (ses deux trous), tandis que les points proches de la diagonale $\partial\Omega$ représentent du bruit topologique.

où $\mathcal{D}$ est l'espace des diagrammes de persistance et B est un espace de Banach. Une telle application, appelée *feature map* ou *représentation*, permet de transformer un échantillon de diagrammes de persistance en échantillon de vecteurs, qui peut ensuite s'incorporer facilement dans un algorithme d'apprentissage automatique. De nombreuses représentations ont été proposées dans la littérature. On peut en identifier une grande classe, que nous appelons représentations *linéaires*, et qui inclut par exemple la surface persistante [Ada+17] (et ses variantes [Che+15; KHF16; Rei+15]), la fonction d'accumulation persistante [BM19] ou la silhouette persistante [Cha+15a].

Definition 2.1 (Représentation linéaire)**.** *Soit $f : \Omega \to B$ une application, où B est un espace de Banach. L'application $\Psi_f : \mathcal{D} \to B$ définie par $\Psi_f(a) := \sum_{u \in a} f(u)$ est appelée la* représentation linéaire *associée à f.*

Un premier critère pour évaluer la pertinence d'une représentation Ψ est sa stabilité : est-ce que Ψ est Lipschitz (ou Hölder) pour une certaine distance d_p ? Nous donnons dans le chapitre 8 des critères sur la fonction f qui permettent d'établir la continuité de la fonction Ψ_f, puis son caractère Lipschitz (ou Hölder) pour les distances d_p. Il apparaît alors, que pour obtenir des représentations stables, il est primordial de pondérer la fonction f par une fonction de poids w qui s'écrase suffisamment proche de la diagonale. Nous donnons des conditions suffisantes sur la fonction w permettant d'assurer la stabilité de toute représentation de la forme Ψ_{wf} avec f Lipschiz bornée. En particulier, une fonction de poids de la forme $w : u \mapsto (u_2 - u_1)^p$ permet la création de représentations Hölder sur l'ensemble des diagrammes construits sur une variété de dimension $d < p$.

Nous nous proposons ensuite d'éclairer le choix de la fonction de poids w en prenant un point de vue asymptotique. Nous avons mentionné précédemment que les points de haute persistance dans un diagramme de persistance ont "plus d'importance" et représentent des caractéristiques topologiques importantes de l'objet sous-jacent. Dans le cas où un ensemble de n points $\mathcal{X}_n$ est échantillonné sur une variété M, on observe ainsi dans le diagramme de persistance a_n de $\mathcal{X}_n$ (par exemple de Čech) deux types de points : des points de haute persistance correspondant au diagramme de persistance de la variété, et un grand nombre de points de basse persistance mesurant le "bruit topologique" de l'échantillonnage, voir par exemple la figure 1.8 pour un exemple sur le tore. Nous nous intéressons alors à la structure du bruit topologique dans un cadre simplifié, où des points sont tirés aléatoirement dans le cube $[0, 1]^d$. Nous montrons que la taille du bruit topologique a_n, mesurée par sa persistance totale $\mathrm{Pers}_p(a_n) := \sum_{u \in a_n} (u_2 - u_1)^p$, est d'ordre $c \cdot n^{1-p/d}$, avec une constante c dépendant de la densité d'échantillonnage. Ceci suggère que si les points de haute persistance

dans le diagramme d'un nuage de points donnent des informations sur la structure macroscopique de l'ensemble, le bruit topologique fournit d'autres types d'information, telle la dimension intrinsèque de l'échantillonnage. Ces remarques ont par la suite été utilisées par Adams *et al.* [Ada+20] pour définir une notion de dimension persistante d'un ensemble. De manière plus générale, nous montrons que le diagramme normalisé $n^{-1/d}a_n$ (qui est une mesure persistante) converge pour les métriques FG_p vers une certaine mesure persistante limite dépendant de la densité d'échantillonnage. D'autre part, ceci implique que les représentations de la forme $\Psi_{wf}(a_n)$ convergent pour w de la forme $u \mapsto (u_2 - u_1)^p$ et $p > d$. Nous retrouvons dans les deux cas la même heuristique : une fonction de poids de la forme $u \mapsto (u_2 - u_1)^p$ est légitime pour $p > d$ si les diagrammes sont construits sur un objet de dimension d.

Le contenu du chapitre 7 est basé sur une collaboration avec Wolfgang Polonik [DP19].

2.3 Le diagramme de persistence moyen

Dans un cadre statistique, nous serons souvent en présence d'un échantillon de n diagrammes de persistance $a_1, \dots, a_n$, provenant par exemple d'une collection de graphes [Car+20], de séries temporelles [SDB16], ou de formes 3D [COO15b]. On peut alors considérer leur représentation associée $\Psi(a_1), \dots, \Psi(a_n)$. Si l'on souhaite obtenir des résultats statistiques sur l'échantillon $\Psi(a_1), \dots, \Psi(a_n)$, il est sans doute pertinent de commencer par s'intéresser à des quantités simples, telles leur moyenne $\frac{1}{n}(\Psi(a_1) + \cdots + \Psi(a_n))$. Si la loi des grands nombres implique directement que cette moyenne converge vers $\mathbb{E}_{a\sim P}[\Psi(a)]$, où P est la loi générant les a_i, rien ne nous dit à quoi ressemble cette espérance, et quelles sont ses propriétés. Nous nous proposons de répondre à cette question dans le cas des représentations linéaires Ψ_f. Dans ce cas là, si on note

$$\overline{a}_n := \frac{1}{n}\left(a_1 + \cdots + a_n\right) \tag{1.14}$$

la moyenne empirique des a_i, qui est une mesure persistante, nous avons

$$\frac{1}{n}(\Psi_f(a_1) + \cdots + \Psi_f(a_n)) = \Psi_f(\overline{a_n}). \tag{1.15}$$

Cette quantité converge vers $\Psi_f(E(P)) = \int f(u)\mathrm{d}E(P)(u)$, où $E(P) = \mathbb{E}_{a\sim P}[a]$ est le diagramme moyen de P, défini précisément dans le chapitre 8 et initialement défini dans une publication écrite en collaboration avec Frédéric Chazal [DC19]. Le diagramme moyen est une mesure sur Ω, qui donne l'intensité moyenne de points d'un diagramme aléatoire $a \sim P$ dans une région donnée. Nous montrons dans le chapitre 8 des propriétés variées des diagrammes moyens : leur stabilité par rapport à la loi P, des vitesses d'estimation du diagramme moyen empirique $\overline{a}_n$ vers $E(P)$ (pour les distances de Figalli-Gigli FG_p), ou encore l'existence d'une densité λ_P pour $E(P)$ dans un cadre très général. Ce dernier résultat décrit en particulier de manière précise ce vers quoi converge $\frac{1}{n}(\Psi_f(a_1) + \cdots + \Psi_f(a_n))$: la limite est égale à $\int f(u)\lambda_P(u)\mathrm{d}u$, et la connaissance de λ_P (qui est possible à travers des procédures d'estimation) permet une connaissance précise de cette limite. Un des inconvénients du diagramme de persistance empirique $\overline{a}_n$ est qu'il contient potentiellement un très grand nombre de points, ce qui peut limiter son utilisation en pratique. Nous étudions ainsi le problème de la *quantization* d'une telle mesure, c'est-à-dire de celui de trouver une mesure de petit support qui va approcher $\overline{a}_n$. Le chapitre 8 compile des résultats sur le diagramme de persistance moyen obtenus en collaboration avec Théo Lacombe [DL20; DL21] et Frédéric Chazal [DC19].

Chapter 2

Introduction (English)

This thesis fits within the framework of Topological Data Analysis (or TDA), which is here tackled from two different perspectives, namely geometric inference, and persistent homology theory. These two approaches both aim at extracting, in different contexts, relevant information of a geometric and topological nature from complex datasets exhibiting nonlinear structures.

1 Challenges in geometric inference

The classical statistical theory developed in the 30s by Fischer relies on the following hypothesis: we observe a low-dimensional dataset, for which we possess a simple generative model (gaussian, exponential, etc.). The goal is then to find estimators of parameters characterizing the law of the dataset, for which we are able to give strong optimality guarantees. In contrast, modern datasets are typically high-dimensional point clouds. If classical methods can still be applied to such datasets, their performance (both in theory and in practice) becomes poor. This phenomenon, called the *curse of dimensionality*, shows the need of a paradigm shift. First, in a modelization step, sets of hypotheses tailored to a large class of high-dimensional datasets must be designed. Second, it is necessary to develop statistical methods adapted to those new sets of hypotheses.

For instance, some methods, such as the LASSO [Tib96], are effective under a sparsity assumption on the dataset. Some regression methods, such as ridge regression [HK70], penalize the complexity of the proposed regression function to adapt to the high-dimensional setting. Let us also mention the PCA method (for Principal Component Analysis [Pea01; Hot33]), which aims at finding the subspace fitting the best the dataset with respect to the L_2-norm. All the methods we have mentioned rely on the existence of a low-dimensional linear structure being relevant to explain the dataset. In particular, they require to have a high level of trust in the parametrization of the dataset, while any reparametrization can break this linear structure (see Figure 2.1). The key idea of geometric inference consists in relaxing this hypothesis by supposing that the dataset in high dimension lies around a low-dimensional shape, *a priori* non-linear. Mathematically, we suppose that *the observed dataset is close to a manifold M of dimension d small in an ambient space of dimension D, possibly large.*

From a statistical point of view, this type of hypotheses was first studied in the case where one has access to the manifold M [Hen90; Pel05]. This is for instance the case for geolocalization problems [IPT19], where datasets are located on the sphere $\mathbb{S}^2$, or for studying images of faces under different lightings, the dataset then lying on a Grassmannian $G(k, d)$ [Cha+07]. Having access to the manifold is however most of the time too demanding. During the 2000s, another family of techniques was developed, that may be aggregated under the name of non-linear dimensionality reduction methods [RS00; ZZ03; WSS04] (let us also mention earlier attempts like

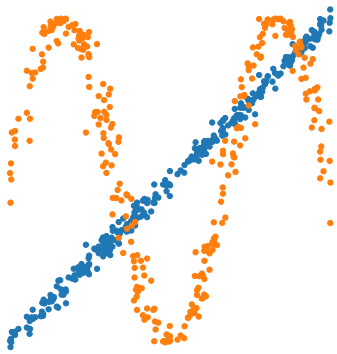


FIGURE 2.1: The linear structure of the blue dataset disappears when the vertical axis is reparametrized by a non-linear function (here sinusoidal). The orange dataset is however still close to a manifold.

self-organizing maps [Koh89] or adaptive principal surfaces [LT94]). Those methods, which do not require the knowledge of the manifold M, aim at embedding in the most faithful way possible a point cloud close to a "non-linear" shape in the Euclidean space $\mathbb{R}^d$ for some small d. For instance, the ISOMAP method [TDSL00], relies on the embedding in $\mathbb{R}^d$, thanks to a multidimensional scaling (or MDS), of a neighborhood graph built on top of the observations. It allows the "unfolding" of datasets lying on objects which are diffeomorphic to an open convex set (see Figure 2.2). We may then apply standard classification or regression techniques to the "unfolded" dataset. However, those techniques possess theoretical guarantees only in a restricted setting: the dataset must be close to a shape at least diffeomorph to $\mathbb{R}^d$, while it is for instance impossible to embed continuously a sphere in $\mathbb{R}^2$.

Around the same time, the field of computational geometry has witnessed the development of algorithms allowing the reconstruction of a manifold $M \subset \mathbb{R}^D$ based on a finite sample $\mathcal{X}$, with the emphasis being put on the reconstruction of curves and surfaces [BTG95; AB99]. For example, the COCONE algorithm [Ame+00] reconstructs a smooth surface M thanks to a finite approximation, under the condition that the approximation rate $\varepsilon(\mathcal{X}) := \sup\{d(x, \mathcal{X}) : \ x \in M\}$ of the sample $\mathcal{X}$ is small enough, while the Tangential Delaunay Complex [BG14] allows such a reconstruction in higher dimension. The reconstruction of topological or geometric invariants of M, like its medial axis [ABE09] or its homology and homotopy groups [CO08] has also been addressed. Once again, those results only require a finite sample $\mathcal{X}$ of the manifold M having a good approximation rate. Another point of view consists in assuming that $\mathcal{X}$ is the realization of a random process of n independent observations from some law μ concentrated around M. One can then hope that methods of interest have a good performance with high probability, on "typical" samples. This statistical approach on computational geometry problems was first proposed in a seminal paper by Niyogi, Smale and Weinberger [NSW08], where the authors show that the homology of a manifold M is recovered with high probability by the Čech complex (a combinatorial object defined in Chapter 3) of the n-sample $\mathcal{X}_n$. In the 2010s, the estimation of other descriptors of M was proposed: its dimension [HA05; LJM09; KRW19], its tangent spaces [AL19; CC16], its reach [Aam+19; Ber+21], its curvature [AL19], its geodesic distances [ACC20], or the manifold M itself [Gen+12a; Gen+12b; MMS16; AL18; AL19].

This statistical point of view on computational geometry allows us to define in a simple manner what it means for a procedure to be optimal. This is made

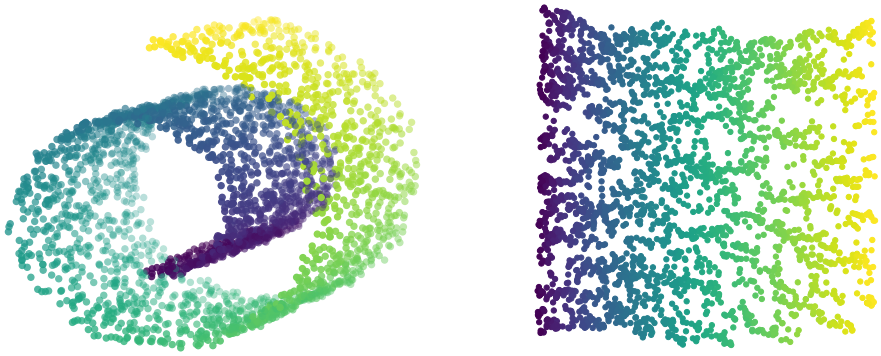


FIGURE 2.2: Left: a set $\mathcal{X}$ of 3000 points sampled on a swiss roll. Right: output of the ISOMAP algorithm with input $\mathcal{X}$ (implemented with `scikit-learn` [Bui+13]).

possible thanks to the minimax statistical theory. Consider for instance the problem of estimating a manifold M thanks to a random n-sample $\mathcal{X}_n$. An estimator $\hat{M}$ of M is by definition any compact subset of $\mathbb{R}^D$, being a measurable function of the sample. The quality of the estimator $\hat{M}$ with respect to the law μ, called its *μ-risk*, is given by the average Hausdorff distance d_H between the estimator and M:

$$R_n(\hat{M}, \mu, d_H) := \mathbb{E}[d_H(\hat{M}, M)], \tag{2.1}$$

where $\hat{M} = \hat{M}(\mathcal{X}_n)$ and $\mathcal{X}_n$ is a n-sample of law μ. In reality, the law μ generating the dataset is unknown, and it is more interesting to control the μ-risk over a set $\mathcal{Q}$ of laws μ, that we call a *statistical model*. In geometric inference, several statistical models were introduced, which take into account different noise models and regularities of the manifold M. The uniform risk of the estimator $\hat{M}$ on the class $\mathcal{Q}$ is given by

$$R_n(\hat{M}, \mathcal{Q}, d_H) := \sup\{R_n(\hat{M}, \mu, d_H) : \ \mu \in \mathcal{Q}\}, \tag{2.2}$$

while we say that an estimator is *minimax* if it attains (up to a multiplicative constant as n goes to ∞) the *minimax risk*

$$\mathcal{R}_n(M, \mathcal{Q}, d_H) := \inf\{R_n(\hat{M}, \mathcal{Q}, d_H) : \ \hat{M} \text{ is an estimator}\}. \tag{2.3}$$

Let us mention for instance the family of models $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$ introduced by Genovese *et al.* in [Gen+12a], consisting of the laws μ supported on a d-dimensional manifold M satisfying some additional properties. First, we assume that μ has a density f on M, lower bounded by some constant $f_{\min} > 0$ and upper bounded by another constant $f_{\max}$. This ensures that all the parts of the manifold M are approximately evenly sampled: we then say that the law is "almost-uniform" on M. The parameter $\tau_{\min}$ gives a lower bound on the reach $\tau(M)$ of the manifold. The reach is a central notion in geometric inference, defined as the largest radius r such that, if some point x is at distance less than r to M, then there exists a unique projection y of x on M. More geometrically, having a reach larger than r implies that it is possible to make a ball "roll" along the manifold M without "bumping" into another part of M [PL08, Lemma A.0.6]. Therefore, the reach $\tau(M)$ controls two different quantities: the curvature radius of M (that is a local regularity), and a global regularity parameter, indicating the presence of a bottleneck structure in the manifold (see Figure 2.3). On the statistical model $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$, the minimax rate of convergence satisfies

$$c_0 \left(\frac{\ln n}{n}\right)^{2/d} \leq \mathcal{R}_n(M, \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}, d_H) \leq c_1 \left(\frac{\ln n}{n}\right)^{2/d} \tag{2.4}$$

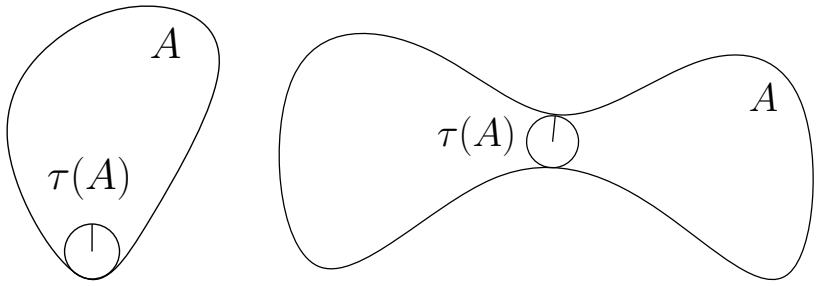


FIGURE 2.3: If the reach of the curve M is too large, then the curve cannot be too pinched (left) and cannot present a tight bottleneck structure (right).

for two positive constants c_0, c_1 depending on $\tau_{\min}$, $f_{\min}$, $f_{\max}$ and d. The lower bound in this inequality was shown by Kim and Zhou [KZ15], while the upper bound is obtained by exhibiting an estimator having a uniform risk of order $(\ln n/n)^{2/d}$. Such an estimator (although not computable in practice) was first proposed by Genovese *et al.* in [Gen+12a], while another estimator attaining this same minimax rate (computable in practice), and based on the Tangential Delaunay Complex, was proposed by Aamari and Levrard [AL18].

1.1 The adaptivity problem

The Tangential Delaunay Complex depends on several parameters, like for instance a radius quantifying the size of the neighborhoods used to compute local PCAs. For the Tangential Delaunay Complex to be minimax, those parameters have to be calibrated in a precise manner with respect to the quantities $\tau_{\min}$, $f_{\min}$ and $f_{\max}$ defining the model. However, those quantities are *a priori* unknown. The question of the practical choice of the parameters defining the estimator is then raised. This question of the tuning of parameters defining an estimator is not restricted to the framework of manifold estimation, but is a classical problem in statistics.

Let us cite for instance the question of the choice of the bandwidth for kernel density estimation. Let $X_1, \dots, X_n$ be a n-sample of some law μ having a density f on $\mathbb{R}$, and suppose that we want to recover the value $f(x_0)$ of the density at some fixed point $x_0 \in \mathbb{R}$. A standard method to achieve this goal is to consider the convolution of the empirical measure $\mu_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ by some kernel K_h, where $K_h = h^{-1}K(\cdot/h)$ and K satisfies $\int K = 1$. We then obtain a function $\hat{f}_h = K_h * \mu_n$. Assume that the density f is of regularity s, that is $f \in \mathcal{C}^s(\mathbb{R})$, the set of $\lfloor s \rfloor$-times differentiable functions, whose $\lfloor s \rfloor$th derivative is $(s - \lfloor s \rfloor)$-Hölder continuous. Then, for a good choice of kernel K, it is optimal to choose the bandwidth h_{opt} of order $c \cdot n^{-1/(2s+1)}$, where c depends of the $\mathcal{C}^s$-norm of f [Tsy08, Chapter 1]. The associated risk is then of order $n^{-s/(2s+1)}$, which is the minimax rate of estimation on the class of densities of regularity s. In practice, it is impossible to know exactly the value of s, so that we must find another strategy to choose the bandwidth h. Adaptive methods consist in choosing a bandwidth $\hat{h}$ in a data-dependent way, such that the estimator $\hat{f}_{\hat{h}}$ has a μ-risk almost as good as the optimal estimator $\hat{f}_{h_{\text{opt}}}$ under weak hypotheses on μ. One of such method, the PCO method (for Penalized Comparison to Overfitting) introduced by Lacour, Massart and Rivoirard [LMR17] consists in comparing each estimator $\hat{f}_h$ to some degenerate estimator $\hat{f}_{h_{\min}}$ for some very small $h_{\min}$. The selected bandwidth $\hat{h}$ is chosen among a family $\mathcal{H}$ of bandwidths (all larger than $h_{\min}$), by minimizing a criterion depending on the distance $\|\hat{f}_h - \hat{f}_{h_{\min}}\|_{L_2(\mathbb{R})}$, while penalizing

small values of h. Lacour, Massart and Rivoirard then show an *oracle inequality* for their estimator, that is an inequality of the form

$$\mathbb{E}\|\hat{f}_{\hat{h}} - f\|^2_{L_2(\mathbb{R})} \leq C \min\{\mathbb{E}\|\hat{f}_h - f\|^2_{L_2(\mathbb{R})} : \ h \in \mathcal{H}\} + C(n, |\mathcal{H}|), \tag{2.5}$$

where $C(n, |\mathcal{H}|)$ is a reminder term negligible in front of the optimal risk. Thus, we obtain that $\hat{f}_{\hat{h}}$ has a risk almost as good as the best estimator $\hat{f}_{h_{\text{opt}}}$, while we never had to estimate the parameters defining the statistical model (that is the regularity s of the density and the $\mathcal{C}^s$-norm of f).

In Chapter 4, we draw inspiration from the PCO method to create an adaptive manifold estimator. A first step consists in creating a family of estimators $(\hat{M}_t)_{t\geq 0}$, similar to kernel density estimators for manifold estimation. This is made possible with t-convex hulls. For $t \geq 0$, the t-convex hull $\text{Conv}(t, A)$ of a set A is an interpolation between the set A ($t = 0$) and its convex hull $\text{Conv}(A)$ ($t = \infty$). It is defined by

$$\text{Conv}(t, A) := \bigcup_{\substack{\sigma \subset A \\ r(\sigma) \leq t}} \text{Conv}(\sigma), \tag{2.6}$$

where $r(\sigma)$ is the radius of the set σ, that is the radius of the smallest enclosing ball of σ. We first show that for $t = c \cdot (\ln n/n)^{1/d}$, where c depends on d and on the parameters $\tau_{\min}$, $f_{\min}$ and $f_{\max}$, the t-convex hull $\text{Conv}(t, \mathcal{X}_n)$ of a n-sample is a manifold estimator which is minimax on the statistical model $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$. We then consider the problem of selecting the parameter t. An analog of the degenerate estimator $\hat{f}_{h_{\min}}$ is given by the choice $t = 0$, with $\text{Conv}(0, \mathcal{X}_n) = \mathcal{X}_n$. The PCO method therefore suggests comparing the estimators $\text{Conv}(t, \mathcal{X}_n)$ with $\mathcal{X}_n$, that is to study the function $t \mapsto h(t, \mathcal{X}_n) := d_H(\text{Conv}(t, \mathcal{X}_n), \mathcal{X}_n)$. This function was actually already introduced under the name of "convexity defect function of the set $\mathcal{X}_n$" in a paper by Attali, Lieutier and Salinas [ALS13], where it was used to study the homotopy type of Rips complexes. We show that the convexity defect function of $\mathcal{X}_n$ exhibits different behaviors in two different regimes: before a certain threshold value $t^*(\mathcal{X}_n)$, it has a globally linear behavior, whereas after this threshold value, it has a (sub)quadratic behavior. The convexity defect function is computable based on the dataset, so that we may in practice observe those two regimes. We are then able to show that values of t just above the threshold value $t^*(\mathcal{X}_n)$ provide a minimax risk of order $(\ln n/n)^{2/d}$. More precisely, we fix two hyperparameters $0 < \lambda < 1$ and $t_{\max}$, and let

$$\hat{t}_\lambda := \sup\{t < t_{\max} : \ h(t, \mathcal{X}_n) > \lambda t\}. \tag{2.7}$$

Our main result states that if $t_{\max}$ is small enough with respect to $\tau_{\min}$, then $\text{Conv}(\hat{t}_\lambda, \mathcal{X}_n)$ is a minimax adaptive manifold estimator (see Figure 2.4). Note that we do not obtain the adaptive property of the estimator by providing an oracle inequality of the type (2.5), but by showing that $\hat{t}_\lambda$ is larger than the threshold value $t^*(\mathcal{X}_n)$ (while being of the right order of magnitude) with high probability, this property being enough to ensure the minimax behavior of the corresponding estimator. We also are able to show that the parameter $\hat{t}_\lambda$ is actually close to the approximation rate $\varepsilon(\mathcal{X}_n)$. As mentioned earlier, some algorithms in computational geometry require the knowledge of the approximation rate (or rather of bounds on the approximation rate), and may therefore be used with plugging in the parameter $\hat{t}_\lambda$.

1.2 Reconstructing the measure rather than the manifold

The second contribution proposed here is motivated by the density estimation problem. In geometric inference, the issue of reconstructing the density f of the measure μ

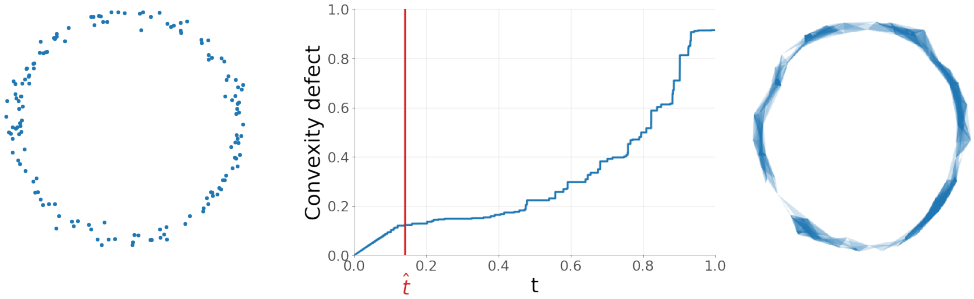


FIGURE 2.4: Left. Sample $\mathcal{X}_n$. Center. Convexity defect function of $\mathcal{X}_n$ and selected scale $\hat{t}_\lambda$. Right. The set $\mathrm{Conv}(\hat{t}_\lambda, \mathcal{X}_n)$.

generating the observations $\mathcal{X}_n$ was first addressed in the case where one has access to the manifold M. Hendriks [Hen90] proposes to use the eigenfunctions of the Laplace-Beltrami operator on the manifold to estimate the density, whereas Pelletier [Pel05] introduces a kernel density estimator using the geodesic distance on the manifold. In the setting of manifold inference, where the manifold M is supposed to be unknown, papers addressing density estimation are more recent. Let x_0 be a point that we assume belongs to M. The estimation of $f(x_0)$, the density of f at x_0, was first tackled in [BS17; WW20], where estimation rates of kernel density estimators are given, respectively in the case where the manifold has a boundary and in the case where the density is supposed to be Hölder continuous. Berenfeld and Hoffmann [BH19] exhibit minimax rates of convergence for this problem, and show that two regularities come into play in the optimal rate: on one hand the regularity s of the density f, and on the other hand the regularity k of the manifold M. Moreover, authors show that the Goldenshluger-Lepski method [GL13] can be applied in this setting to select a kernel bandwidth, producing a minimax adaptive estimator of $f(x_0)$.

To go beyond the pointwise estimation of f (or equivalently of the associated measure μ), the choice of the loss function is a delicate issue. Indeed, standard choices in density estimation include the L_p distance, the Hellinger distance, or the Kullback-Leibler divergence. All those loss functions become degenerate for the comparison of two mutually singular measures. If the support M of the measure μ is unknown, it will be impossible to build, thanks to a finite sample, a measure which is non-singular with respect to the volume measure vol_M on M, even though we may be able to build measures whose supports are very close to M for the Haussdorf distance. On the contrary, Wasserstein distances W_p ($1 \leq p \leq \infty$) are by design robust to metric perturbations of the support of a measure, and are therefore particularly adapted to our problem. They are defined in the following way. Given two probability measures μ and ν, we define a transport plan π between μ and ν as a measure on $\mathbb{R}^D \times \mathbb{R}^D$ having first marginal μ and second marginal ν. Informally, at the point $x \in \mathbb{R}^D$, a fraction $\mathrm{d}\pi(x, y)$ of the mass $\mathrm{d}\mu(x)$ located at x is sent to y. The cost of such a plan is given by $C_p(\pi) = \iint d(x, y)^p \mathrm{d}\pi(x, y)$, whereas the Wasserstein distance W_p is given by the optimal cost of a transport plan:

$$W_p(\mu, \nu) := \inf\{C_p^{1/p}(\pi) : \ \pi \in \Pi(\mu, \nu)\}, \tag{2.8}$$

where $\Pi(\mu, \nu)$ is the set of transport plans between μ and ν.

Using Wasserstein distances, and more generally the theory of optimal transport, has shown its efficiency in a wide class of modern machine learning problems (see e.g. [PC19]). In particular, Niles-Weed and Berthet have tackled the problem of estimating the density f supported on the cube $[0, 1]^d$ using Wasserstein distances as

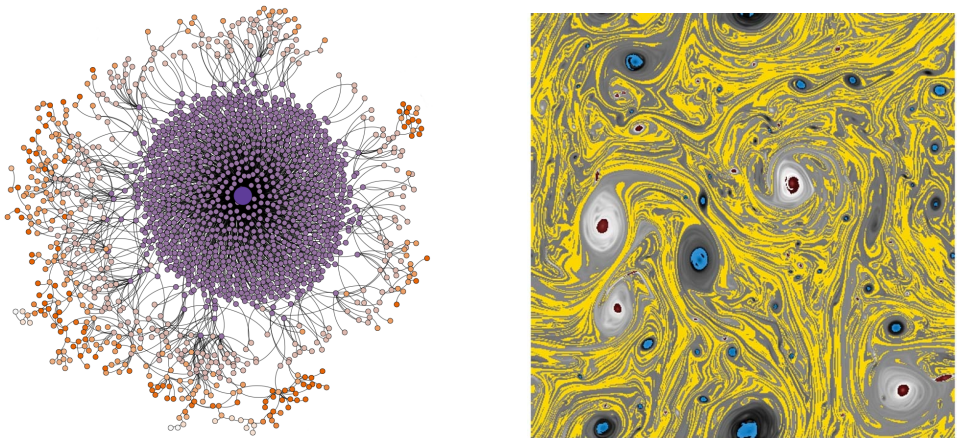


FIGURE 2.5: Left: an interaction graph between Reddit users, from the dataset REDDIT-5K, presented in [YV15]. Right: simulation of turbulent flows given by Navier-Stokes equation [Sch+06].

loss functions [WB19b]. Assume that f belongs to the Besov space $B^s_{p,q}$ (see Chapter 5 for details). Then, they show that a modification of a classical wavelet density estimator attains the rate of convergence $n^{-(s+1)/(2s+d)}$ for $d \geq 3$ with respect to the Wasserstein distance W_p (whereas the rate of convergence for the pointwise estimation of the density is of order $n^{-s/(2s+d)}$). Moreover, this rate is the minimax rate.

Our contribution, presented in Chapter 5, consists in extending this minimax result by replacing the cube by any submanifold M of regularity k for $k \geq s+1$. We show that a measure having a density with respect to vol_M given by a weighted kernel density estimator, attains the same minimax rate of $n^{-(s+1)/(2s+d)}$. In the case of interest where the manifold M is unknown, we cannot use vol_M, such that the previous estimator cannot be computed. We therefore propose in a first step to estimate the volume measure, thanks to some estimator $\widehat{\mathrm{vol}}_M$, and show that $\hat{U}_M := \widehat{\mathrm{vol}}_M / |\widehat{\mathrm{vol}}_M|$ is a minimax estimator of the uniform measure on M. The reconstruction of the volume measure is based on the estimation of local $\mathcal{C}^k$ parametrizations of the manifold M introduced by Aamari and Levrard [AL19].

2 A multiscale perspective: persistent homology theory

Works we have mentioned so far all rely on the strong hypothesis of the existence of a low-dimensional manifold interpolating the dataset. It is however reasonable to ask questions of a topological nature in a much more general framework. For instance, one can imagine that relevant information is present in the fine topological structure of a spatial process, information which can be used for a classification task [Bro+20]. In certain problems, the observed dataset is not a point cloud, whereas a notion of topology is still relevant. This is for instance the case if a family of graphs is observed, where topology is then described by the presence of cycles or connected components [AMA07; Hof+17; ZW19; Car+20], see also Figure 2.5. Persistent homology theory in TDA aims at quantifying in a precise sense what is the underlying topology of a dataset in a very general way. To do so, we adopt a multiscale approach.

Consider first a simple example. Let $\mathcal{X}_n$ be a finite set of n points in $\mathbb{R}^D$. From a topological perspective, the set $\mathcal{X}_n$ is trivial: it consists of n connected components, each of them being reduced to a point. A possibility to obtain a topologically more

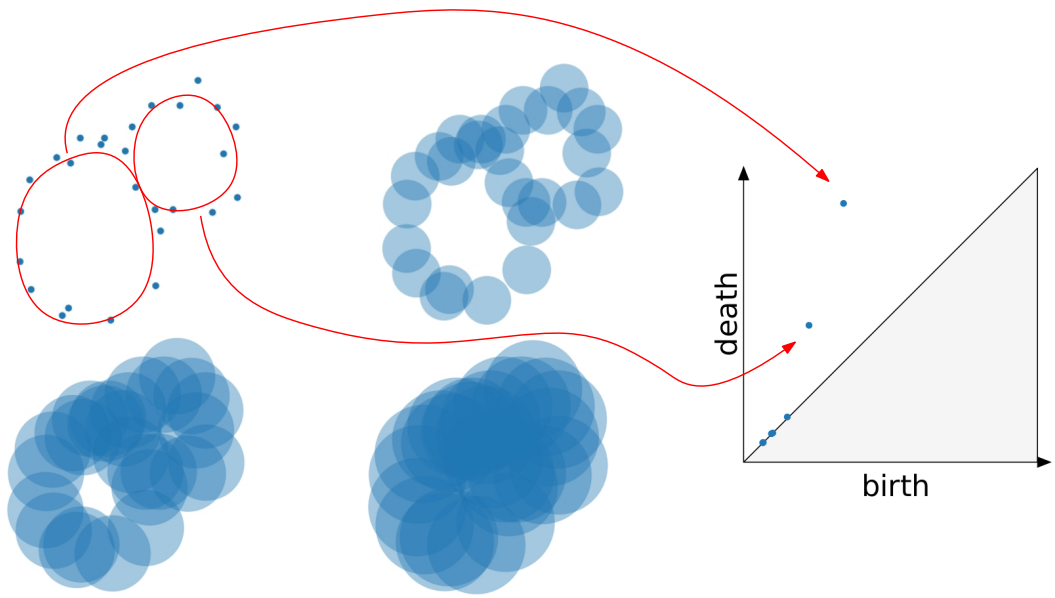


FIGURE 2.6: The one-dimensional persistence diagram associated with the filtration $(\mathcal{X}_n^t)_{t\geq 0}$.

complex set is to choose a scale t and to consider the t-neihborhood of $\mathcal{X}_n$:

$$\mathcal{X}_n^t := \bigcup_{x\in\mathcal{X}_n} \mathcal{B}(x,t). \tag{2.9}$$

As explained previously, choosing a "right" scale t is then a delicate issue, although we proposed in Chapter 4 an algorithm to select such a scale in the case where the sample $\mathcal{X}_n$ is close enough to a manifold M. Persistent homology theory proposes to avoid the choice of the parameter t by tracking the evolution of the homology groups of $\mathcal{X}_n^t$ as t grows from 0 to $+\infty$. If for instance one is interested in 1-dimensional homology (that is the presence of "loops" in a shape), one can observe that loops will appear at certain times in the process, before being filled when the radius t of the balls becomes larger. When t becomes very large, the set becomes homotopy equivalent to a ball, and does not possess any non-trivial cycle. This process can be summarized by a set of intervals, each interval $[b,d)$ representing a loop appearing at scale b, and disappearing at scale d. An equivalent point of view is to consider the collection of points $(b,d)\in\mathbb{R}^2$, that we call the *persistence diagram* associated with the process, see Figure 2.6). Note that we always have $d>b$, so that a persistence diagram is a list of points in $\Omega := \{u=(u_1,u_2)\in\mathbb{R}^2 : \ u_2>u_1\}$, or equivalently a measure of the form $\sum_{i\in I}\delta_{u_i}$ on Ω. The longer a loop was present in the process $(\mathcal{X}_n^t)_{t\geq 0}$, the more important it is. We call persistence of the loop the lifetime $d-b$ of the associated interval. Therefore, in a persistence diagram, points far away from the diagonal $\partial\Omega := \{(t,t) : \ t\in\mathbb{R}\}$ correspond to important topological features of the underlying process. More generally, persistent homology theory can be applied to any *filtration* of topological spaces, that is any increasing sequence of topological spaces $(\mathcal{X}^t)_{t\in\mathbb{R}}$. This includes in particular the sublevel sets of a function $f:\mathcal{X}\to\mathbb{R}$, where $\mathcal{X}$ can be a graph, an image, or any metric space. When the function f is the distance to a set $\mathcal{X}_n\subset\mathcal{X}$, we recover the process mentioned before, while the persistence diagram is called the Čech persistence diagram of the set $\mathcal{X}_n$. Moreover, different homology dimensions may be considered: connected components (dimension 0), loops (dimension 1), cavities (dimension 2), etc.

Persistent homology theory and the notion of persistence diagram were progressively introduced in the early 2000s [Rob99; ELZ00; Car+04], while the concept of persistence was also introduced independently by Barannikov in the field of Morse theory [Bar94]. One of the first major results in TDA consisted in showing that persistence diagrams are in a strong sense stable with respect to the object on top of which they are built [CSEH07]. This property, commonly called the stability theorem, relies on a powerful algebraic stability result which is precisely stated in Chapter 3. This stability theorem is based on a notion of distance between diagrams, called the bottleneck distance d_∞. Subsequently, distances d_p for $1 \leq p \leq \infty$ were introduced. These generalizations of the bottleneck distance are known to satisfy weaker stability results (stemming from the bottleneck stability result) [CS+10]. Let a and b be two persistence diagrams, with a being given by the list of points $x_1, \ldots, x_n \in \Omega$ and b by the list $y_1, \ldots, y_m \in \Omega$. A matching γ between a and b is given by a bijection between $a \cup \partial\Omega$ and $b \cup \partial\Omega$. Precisely, each point x_i is sent by γ either towards some y_j, or to some point of the diagonal, while the y_js that are not the image of some x_i are the image by γ of some point of the diagonal. The cost $C_p(\gamma)$ of the matching γ is given by

$$C_p(\gamma) := \sum_{x \in a \cup \partial\Omega} \|x - \gamma(x)\|^p, \tag{2.10}$$

where $\|\cdot\|$ represents any norm on $\mathbb{R}^2$. A matching with minimal cost is said to be *optimal*, while we let

$$d_p(a, b) := \inf\{C_p(\gamma)^{1/p} : \ \gamma \in \Gamma(a, b)\}, \tag{2.11}$$

with $\Gamma(a, b)$ being the set of matchings between a and b (see Figure 2.7). We may moreover remark that in an optimal matching, every point sent towards the diagonal is actually sent towards its orthogonal projection on the diagonal. Intuitively, we are matching the different cycles corresponding to each point of the two diagrams, whereas matching a point to the diagonal corresponds to matching a cycle to a "non-persistent" cycle, with an interval of the form $[b, d)$ with $b = d$. Of particular interest in TDA is the bottleneck distance d_∞, obtained as the limit of the d_p distances for $p \to \infty$. Equivalently, the cost $C_\infty(\gamma)$ of a matching γ is given by $\sup\{\|x - \gamma(x)\| : \ x \in a \cup \partial\Omega\}$ whereas the bottleneck distance is given by

$$d_\infty(a, b) := \inf\{C_\infty(\gamma) : \gamma \in \Gamma(a, b)\}. \tag{2.12}$$

Persistence diagrams encode rich topological information of the dataset they summarize, and often complementary to more classical methods. However, they do not naturally belong to a vector space, so that it is unclear how to use them directly in standard machine learning algorithms. Two approaches have been proposed in the literature. The first one consists in using feature maps (also called representations) on the space of persistence diagrams, which allow the transformation of persistence diagrams into vectors, which can then be easily plugged in standard machine learning pipelines. The second one is to work directly in the space of diagrams $\mathcal{D}$, by example by using methods requiring only distances in entry (like the multidimensional scaling previously mentioned). We will study those two approaches.

2.1 The space of persistence diagrams studied through partial optimal transport

Concerning the second approach, it is first necessary to understand precisely the structure of the space of persistence diagrams, seen as a metric space. This study

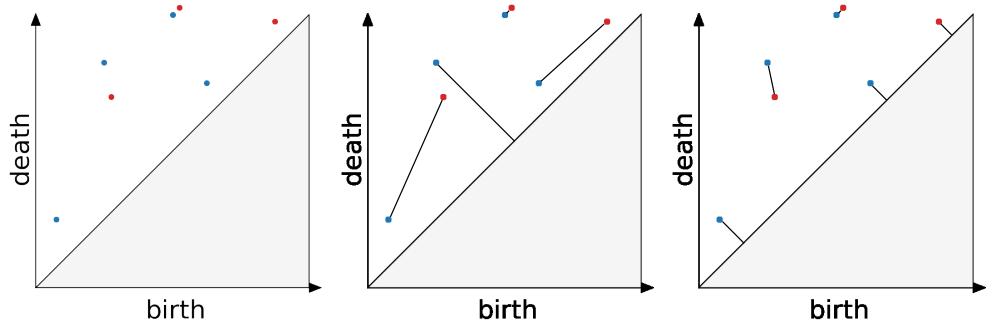


FIGURE 2.7: Left: two persistence diagrams. Center: a matching γ between the two diagrams. The cost $C_p(\gamma)$ is given by the sum of the lengths to the power p of the edges appearing in the matching, while the bottleneck cost $C_\infty(\gamma)$ is given by the length of the longest edge. Right: an optimal matching for every $1 \leq p \leq \infty$.

was initiated by Mileyko, Mukherjee and Harer [MMH11], who show properties of the metric space

$$\mathcal{D}^p := \{a \in \mathcal{D} : \ d_p(a, 0) < \infty\}, \quad \text{endowed with the distance } d_p, \tag{2.13}$$

where 0 is the empty diagram, so that $d_p(a,0)^p = \sum_{u \in a}(u_2 - u_1)^p$, a quantity called the *p-total persistence* of the diagram a, and denoted by $\mathrm{Pers}_p(a)$. Note that we allow here diagrams with infinitely many points, so that it is possible to have $d_p(a,0) = \infty$.

We propose in Chapter 6 to participate in the study of the structure of the space of persistence diagrams by adopting a different point of view than in [MMH11]. We have already mentioned that a persistence diagram can be seen either as a list of points in Ω, or as a point measure on $\sum_{i \in I} \delta_{u_i}$. Although the "list" approach appears to be favored in the literature, the measure point of view turns out to be more fruitful. On the one hand, this point of view allows us to define in an effortless manner the sum, or the average of several diagrams, which would then be a general measure (and not a point measure). On the other hand, this allows us to apply the theory of optimal transport to study persistence diagrams. Indeed, the Wasserstein distances W_p used in optimal transport, that we have already mentionned, allow for the comparison of measures, while the distances d_p and W_p share common aspects: they are both defined as some minimal transport/matching cost between two measures. Because of this similarity, distances d_p are commonly called Wasserstein distances in TDA literature. This name is however misleading, as there is a fundamental difference between the d_p and W_p distances: the W_p distances are only defined for probability measures (or measures having the same mass), while d_p distances are defined for measures having possibly different masses, but that have to be point measures.

We establish in Chapter 6 a precise link between the metric structure of the space of persistence diagrams and optimal transport, by leveraging partial optimal transport distances introduced by Figalli and Gigli [FG10]. By establishing this link, we are able to obtain metric properties of the space $\mathcal{D}^p$ (such as its completeness, or the existence of barycenters), but also to extend the space $\mathcal{D}^p$ to some larger space $\mathcal{M}^p$, that we call the space of *persistence measures*, and that we endow with the Figalli-Gigli distance FG_p, extending the distance d_p. The space of persistence measures benefits from being "linearly" convex, so that averages of diagrams are easily defined, the expected persistence diagram $E(P)$ of a law P on the space of diagrams being at the core of Chapter 8. Furthermore, exhibiting this link justifies the adaptation of algorithms used in optimal transport for persistence diagrams, an approach which can be fruitful

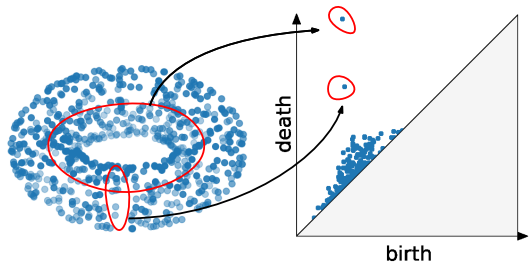


FIGURE 2.8: The persistence diagram a_n of $n = 700$ random points on the torus (for 1-dimensional homology). The two topmost points in the diagram give information on the geometry of the torus (its two holes), whereas points close to the diagonal represent topological noise.

[LCO18]. Chapter 6 is taken from the paper [DL20], written in collaboration with Théo Lacombe.

2.2 Linear representations on the space of persistence diagrams and the choice of the weight function

The first approach we have mentioned to perform statistical procedures using persistence diagrams consists in using a map $\Psi : \mathcal{D} \to B$, where $\mathcal{D}$ is the space of persistence diagrams and B is a Banach space. Such an application, that is called a *feature map* or a *representation* allows the transformation of a sample of persistence diagrams into a sample of vectors, which can then be plugged easily in a machine learning algorithm. Numerous representations were introduced in the literature. We may identify a large subclass of representations, that we call *linear representations*, and that includes for instance the persistence surface [Ada+17] (and its variants [Che+15; KHF16; Rei+15]), the accumulated persistence function [BM19] or the persistence silhouette [Cha+15a].

Definition 2.1 (Linear representation)**.** *Let $f : \Omega \to B$ be any map, where B is a Banach space. The application $\Psi_f : \mathcal{D} \to B$ defined by $\Psi_f(a) := \sum_{u \in a} f(u)$ is called the* linear representation *associated with f.*

A first criterion to evaluate the relevance of a representation Ψ is its stability: is Ψ Lipschitz-continuous (or Hölder continuous) for a certain distance d_p? We give in Chapter 8 criteria on the function f which ensure the continuity of the function Ψ_f, then its Lipschitz (or Hölder) behavior with respect to the d_p distances. It appears that, to obtain stable representations, it is fundamental to weight the function f by some weight function w which is sufficiently small close to the diagonal. We give sufficient conditions on w to ensure that representations of the form Ψ_{wf} for f Lipschitz continuous and bounded are stable. In particular, a weight function of the form $u \mapsto (u_2 - u_1)^p$ produces Hölder continuous linear representations on Čech persistence diagrams built on top of d-dimensional manifolds, as long as $p > d$.

We then address the question of the choice of the weight function w by taking an asymptotic point of view. We have mentioned earlier that points of high persistence in a persistence diagram are "more important" and represent important topological features of the underlying object. In the case where n points $\mathcal{X}_n$ are sampled on a manifold M, we observe that the persistence diagram a_n of $\mathcal{X}_n$ (for the filtration $(\mathcal{X}_n^t)_{t \geq 0}$) contains two types of points: points with high persistence corresponding to the persistence diagram of the manifold, and a large number of points with low persistence measuring the "topological noise" of the sample, see Figure 2.8 for an example on the torus. We explore the behavior of the structure of the topological noise

in a simplified framework, where points are randomly sampled on the cube $[0,1]^d$. We show that the size of the topological noise of a_n, measured by its total persistence $\mathrm{Pers}_p(a_n) := \sum_{u \in a_n} (u_2 - u_1)^p$, is of order $c \cdot n^{1-p/d}$, with a constant c depending on the sampling density. This suggests that if points with high persistence in the diagram of a point cloud informs us on the macroscopic structure of the shape, the topological noise contains other types of information, such as the intrinsic dimension of the sample. These remarks were then used by Adams *et al.* [Ada+20] to define a notion of persistent dimension of a set. More generally, we show that the rescaled diagram $n^{-1/d} a_n$ (which is a persistence measure) converges with respect to the metric FG_p towards some limit persistence measure depending on the sampling density. This implies in particular that representations of the form $\Psi_{wf}(a_n)$ converge for w of the form $u \mapsto (u_2 - u_1)^p$ for $p > d$. We find in the two cases the same heuristic: a weight function of the form $u \mapsto (u_2 - u_1)^p$ for $p > d$ should be chosen if the persistence diagrams are built on top of a d-dimensional object.

Chapter 7 is based on a collaboration with Wolfgang Polonik [DP19].

2.3 The expected persistence diagram

In a statistical context, we are often in presence of a n-sample of persistence diagrams $a_1, \dots, a_n$ arising from e.g. a collection of graphs [Car+20], of time series [SDB16], or of 3D shapes [COO15b]. We may then consider their associated representations $\Psi(a_1), \dots, \Psi(a_n)$. To obtain statistical results on the sample $\Psi(a_1), \dots, \Psi(a_n)$, it is best to start by considering simple quantities such as their average $\frac{1}{n}(\Psi(a_1) + \cdots + \Psi(a_n))$. The law of large numbers implies that the average converges towards $\mathbb{E}_{a \sim P}[\Psi(a)]$, where P is the law generating the diagrams a_i. However, it is not clear *a priori* what are the properties of this limit. We propose to describe this expectation for linear representations Ψ_f. In this case, if we denote by

$$\overline{a}_n := \frac{1}{n}(a_1 + \cdots + a_n) \tag{2.14}$$

the average of the a_is, which is a persistence measure, we have

$$\frac{1}{n}(\Psi_f(a_1) + \cdots + \Psi_f(a_n)) = \Psi_f(\overline{a_n}). \tag{2.15}$$

This quantity converges towards $\Psi_f(E(P)) = \int f(u) \mathrm{d}E(P)(u)$, where $E(P) = \mathbb{E}_{a \sim P}[a]$ is the expected persistence diagram of P, defined precisely in Chapter 8 and first defined in a publication written in collaboration with Frédéric Chazal [DC19]. The expected persistence diagram is a measure on Ω, which gives the average intensity of the number of points of a random diagram $a \sim P$ in a given zone. We establish in Chapter 8 various properties of expected persistence diagrams: their stability with respect to the law P, rates of convergence of the empirical expected persistence diagram $\overline{a}_n$ towards $E(P)$ (with respect to Figalli-Gigli distances FG_p), or the existence of a density λ_P for $E(P)$ in a very general framework. This last result implies in particular a precise description of the limit of $\frac{1}{n}(\Psi_f(a_1) + \cdots + \Psi_f(a_n))$: it is equal to $\int f(u) \lambda_P(u) \mathrm{d}u$, and the knowledge of λ_P (which is possible through estimation procedures) allows us to have a precise knowledge of the limit. One of the drawbacks of the empirical expected persistence diagram $\overline{a}_n$ is that it potentially contains a very large number of points, which may hinder its use in practice. We therefore also study the problem of the quantization of such a measure, that is the problem of finding a measure with small support which approximates it. Chapter 8 gathers results on the expected persistence diagram obtained in collaboration with Théo Lacombe [DL20; DL21] and Frédéric Chazal [DC19].

Chapter 3

Background

3.1 Elements of measure theory

Let $(\mathcal{X}, \mathcal{G})$ be a measurable space. We denote by $\mathcal{P}^{\pm}(\mathcal{X})$ the set of signed measures on $\mathcal{X}$, while $\mathcal{P}(\mathcal{X})$ is the set of finite measures on the space $(\mathcal{X}, \mathcal{G})$. By the Jordan decomposition theorem [Fol13, Proposition 3.4], every measure $\mu \in \mathcal{P}^{\pm}(\mathcal{X})$ can be decomposed into two positive mutually singular measures μ^+ and μ^-, such that $\mu = \mu^+ - \mu^-$. For $m > 0$, we let $\mathcal{P}_m(\mathcal{X})$ be the set of measures in $\mathcal{P}(\mathcal{X})$ having mass m, i.e. such that $\mu(\mathcal{X}) = m$.

We will focus on the case where $\mathcal{X}$ is endowed with some metric d and $\mathcal{G} = \mathcal{B}(\mathcal{X})$ is the associated Borel σ-algebra. In that case, we let $\mathcal{C}_b(\mathcal{X})$ be the space of continuous bounded functions on $\mathcal{X}$, which is a Banach space when endowed with the ∞-norm $\|\cdot\|_\infty$. Every $\mu \in \mathcal{P}(\mathcal{X})$ then induces a linear functional on $\mathcal{C}_b(\mathcal{X})$, defined by

$$f \in \mathcal{C}_b(\mathcal{X}) \mapsto \mu(f). \tag{3.1}$$

As $|\mu(f)| \leq \mu(\mathcal{X})\|f\|_\infty$, this linear functional is continuous, so that $\mathcal{P}(\mathcal{X})$ can be identified with a subset of $\mathcal{C}_b(\mathcal{X})^*$, the topological dual of $\mathcal{C}_b(\mathcal{X})$. The *weak topology* on $\mathcal{P}(\mathcal{X})$ is the topology induced by the weak-* topology on $\mathcal{C}_b(\mathcal{X})^*$. Concretely, a sequence $(\mu_n)_n$ in $\mathcal{P}(\mathcal{X})$ weakly converges towards μ in $\mathcal{P}(\mathcal{X})$ if for all $f \in \mathcal{C}_b(\mathcal{X})$ we have $\mu_n(f) \to \mu(f)$. We then write $\mu_n \xrightarrow{w} \mu$. A stronger topology on $\mathcal{P}(\mathcal{X})$ is given by the dual norm on $\mathcal{C}_b(\mathcal{X})^*$, that we call the *total variation norm*: for $\mu, \nu \in \mathcal{P}(\mathcal{X})$,

$$|\mu - \nu| := \frac{1}{2}\sup\{|\mu(f) - \nu(f)| : \ f \in \mathcal{C}_b(\mathcal{X}), \ \|f\|_\infty \leq 1\}. \tag{3.2}$$

When $(\mathcal{X}, d)$ is locally compact and separable [AFP00, Proposition 1.47], this formula coincides with more common definitions of the total variation:

$$\begin{aligned} |\mu - \nu| &= \sup\{|\mu(A) - \nu(A)| : \ A \in \mathcal{B}(\mathcal{X})\} \\ &= \frac{1}{2}\int \left|\frac{d\mu}{d\lambda} - \frac{d\nu}{d\lambda}\right| \mathrm{d}\lambda, \end{aligned} \tag{3.3}$$

where λ is any measure dominating μ and ν.

We now state elementary topological properties of $\mathcal{P}(\mathcal{X})$. We make the distinction between a Polish *metric* space, that is a complete separable metric space, and a Polish space, the latter being a *topological space* $\mathcal{X}$ (not necessarily associated with a metric) for which there exists a distance d metrizing the topology such that $(\mathcal{X}, d)$ is a Polish metric space. The following proposition appears for instance in [Var58].

Proposition 3.1.1. *Let $m > 0$. We endow $\mathcal{P}_m(\mathcal{X})$ with the weak topology.*

1. *The space $\mathcal{X}$ is separable if and only if $\mathcal{P}_m(\mathcal{X})$ is separable.*
2. *The space $\mathcal{X}$ is compact if and only if $\mathcal{P}_m(\mathcal{X})$ is compact.*

3. *The space $\mathcal{X}$ is a Polish space if and only if $\mathcal{P}_m(\mathcal{X})$ is a Polish space.*

Persistence diagrams, that are defined rigorously in Section 3.8, are not finite measures in general, but may have infinite masses. The space $\mathcal{P}(\mathcal{X})$ is therefore not suited to study them, while the larger space of Radon measures provides a satisfactory framework to handle such non-finite measures. We assume for the remainder of the section that $(\mathcal{X}, d)$ *is a locally compact Polish metric space.*

Definition 3.1.2 (Radon measures)**.** *A Radon measure μ on $\mathcal{X}$ is a locally finite measure, that is such that for every point $x \in \mathcal{X}$, there exists a neighborhood U of x with $\mu(U) < \infty$. We denote by $\mathcal{M}(\mathcal{X})$ the set of Radon measures on $\mathcal{X}$.*

Remark 3.1.3. It is common in the literature to define Radon measures by imposing further regularity conditions on μ (namely inner regularity on open sets and outer regularity on Borel sets). When $\mathcal{X}$ is a locally compact Polish metric space, those regularity conditions are automatically satisfied, and the definition of a Radon measure becomes more straightforward, see [Fol13, Theorem 7.8].

The Riesz–Markov–Kakutani representation theorem asserts that Radon measures correspond exactly to nonnegative elements of the dual space of $\mathcal{C}_c(\mathcal{X})$, the space of continuous functions with compact support on $\mathcal{X}$. Before stating the theorem, we need to endow $\mathcal{C}_c(\mathcal{X})$ with a topology. Let A_n be a sequence of relatively compact open subsets such that $\bigcup_{n\geq 0} A_n = \mathcal{X}$. We let $\mathcal{C}_0(A_n)$ be the completion of $\mathcal{C}_c(A_n)$ for the $\|\cdot\|_\infty$-norm (the space of functions which vanish on the boundary of A_n). We then endow $\mathcal{C}_c(\mathcal{X})$ with the strongest locally convex topology such that all the inclusions $\mathcal{C}_0(A_n) \hookrightarrow \mathcal{C}_c(\mathcal{X})$ are continuous, and which makes $\mathcal{C}_c(\mathcal{X})$ a complete topological vector space. More concretely, endowed with this topology, a sequence $(f_n)_n$ in $\mathcal{C}_c(\mathcal{X})$ converges towards some function $f \in \mathcal{C}_c(\mathcal{X})$ if and only if there exists a compact set containing the supports of all the functions and we have uniform convergence of $(f_n)_n$ towards f.

Definition 3.1.4. *Let $\mathcal{C}_c(\mathcal{X})^*$ be the topological dual of $\mathcal{C}_c(\mathcal{X})$. We say that $\phi \in \mathcal{C}_c(\mathcal{X})^*$ is nonnegative if $\phi(f) \geq 0$ for any $f \in \mathcal{C}_c(\mathcal{X})$ which is nonnegative.*

The following theorem is for instance found in [AFP00, Theorem 1.54].

Theorem 3.1.5 (Riesz–Markov–Kakutani representation theorem)**.**

1. *Let $\mu \in \mathcal{M}(\mathcal{X})$. Then, the application $f \in \mathcal{C}_c(\mathcal{X}) \mapsto \mu(f)$ is continuous.*
2. *If $\phi \in \mathcal{C}_c(\mathcal{X})^*$ is nonnegative, then there exists a unique Radon measure $\mu \in \mathcal{M}(\mathcal{X})$ such that $\phi(f) = \mu(f)$ for every $f \in \mathcal{C}_c(\mathcal{X})$.*

As such, $\mathcal{M}(\mathcal{X})$ can be identified with a subset of $\mathcal{C}_c(\mathcal{X})^*$. We endow $\mathcal{M}(\mathcal{X})$ with the topology induced by the weak-* topology on $\mathcal{C}_c(\mathcal{X})^*$, that we call the *vague topology*. Concretely, a sequence of Radon measures $(\mu_n)_n$ converges vaguely towards some Radon measure μ if, for all $f \in \mathcal{C}_c(\mathcal{X})$, we have $\mu_n(f) \to \mu(f)$. We then write $\mu_n \xrightarrow{v} \mu$.

The following propositions are standard results. Corresponding proofs can be found for instance [Kal83, Section 15.7].

Proposition 3.1.6. *The space $\mathcal{M}(\mathcal{X})$ is a Polish space.*

Also, $\mathcal{P}(\mathcal{X}) \subset \mathcal{M}(\mathcal{X})$, with the injection being continuous: if a sequence of finite measures converges weakly to some finite measure, then the vague convergence also holds.

Definition 3.1.7. *A set $F \subset \mathcal{M}(\mathcal{X})$ is said to be* tight *if, for every $\varepsilon > 0$, there exists a compact set K with $\mu(\mathcal{X} \backslash K) \leq \varepsilon$ for every $\mu \in F$.*

Proposition 3.1.8. *A set $F \subset \mathcal{M}(\mathcal{X})$ is relatively compact for the vague topology if and only if for every compact set K included in $\mathcal{X}$,*

$$\sup\{\mu(K) : \ \mu \in F\} < \infty.$$

Proposition 3.1.9 (Prokhorov's theorem)**.** *A set $F \subset \mathcal{P}(\mathcal{X})$ is relatively compact for the weak topology if and only if F is tight and* $\sup\{|\mu| : \ \mu \in F\} < \infty$.

Proposition 3.1.10. *Let $\mu, \mu_1, \mu_2, \ldots$ be measures in $\mathcal{P}(\mathcal{X})$. Then, $\mu_n \xrightarrow{w} \mu$ if and only if $|\mu_n| \to |\mu|$ and $\mu_n \xrightarrow{v} \mu$.*

Proposition 3.1.11 (The Portmanteau theorem)**.** *Let $\mu, \mu_1, \mu_2, \ldots$ be measures in $\mathcal{M}(\mathcal{X})$. Then, $\mu_n \xrightarrow{v} \mu$ if and only if one of the following propositions holds:*

- *for all open sets $U \subset \mathcal{X}$ and all* bounded *closed sets $F \subset \mathcal{X}$,*

$$\limsup_{n\to\infty} \mu_n(F) \leq \mu(F) \ \textit{and} \ \liminf_{n\to\infty} \mu_n(U) \geq \mu(U).$$

- *for all* bounded *Borel sets A with $\mu(\partial A) = 0$, $\lim\limits_{n\to\infty} \mu_n(A) = \mu(A)$.*

Finally, we define $\mathcal{D}(\mathcal{X})$ the set of integer measures on $\mathcal{X}$, that is Radon measures of the form $\sum_{i\in\mathcal{I}} \delta_{x_i}$ for some index set $\mathcal{I}$. Integer measures will be particularly important in the following, as they will be identified with persistence diagrams.

Proposition 3.1.12. *The set $\mathcal{D}(\mathcal{X})$ is closed in $\mathcal{M}(\mathcal{X})$ for the vague topology.*

3.2 Optimal transport

Optimal transport is a widely developed theory providing tools to study and compare probability measures supported on some metric space $\mathcal{X}$ [Vil03; Vil08; San15], that is, up to a renormalization factor, non-negative measures with same mass. The optimal transport problem was first introduced by Gaspard Monge in 1781 in its "Mémoire sur la théorie des déblais et des remblais" [Mon81]. Consider a distribution of dirt (or "remblais") μ and a distribution of holes (or "déblais") ν, see Figure 3.1. A transport plan π between μ and ν is a strategy for moving the dirt to fill the holes: at each point x, a fraction $\mathrm{d}\pi(x, y)$ of the mass $\mathrm{d}\mu(x)$ is moved to y. The quantity of mass moved from x, which could be written as $\int_y \mathrm{d}\pi(x, y)$ should be exactly equal to $\mathrm{d}\mu(x)$, the total mass originally present at x. Likewise, the quantity of mass $\int_x \mathrm{d}\pi(x, y)$ arriving to y should be equal to $\mathrm{d}\nu(y)$. Mathematically, if ν and μ are measures on some metric space $(\mathcal{X}, d)$, then a transport plan is a measure on $\mathcal{X} \times \mathcal{X}$, which must satisfy the marginal constraints $\pi^1 = \mu$ and $\pi^2 = \nu$ (the first and second marginals of π). Remark that for a transport plan to exist, μ and ν must necessarily have the same mass. For $p = 1$, the cost of the transport plan π is then given by $\iint d(x, y)\mathrm{d}\pi(x, y)$, that is we consider the total distance covered by the dirt through the transport plan π. The 1-Wasserstein distance $W_1(\mu, \nu)$ between μ and ν (also called earthmover distance) is then given by the smallest cost possible of a transport plan. More generally, we introduce the following problem.

Given a metric space $(\mathcal{X}, d)$, $1 \leq p < \infty$ and $m > 0$, we let $\mathcal{P}_m^p(\mathcal{X})$ be the set of distributions $\mu \in \mathcal{P}_m(\mathcal{X})$ such that there exists $x_0 \in \mathcal{X}$ with $\int d(x, x_0)^p \mathrm{d}\mu(x) < \infty$. Remark that if $\mu \in \mathcal{P}_m^p(\mathcal{X})$, then the previous integral is actually finite for every $x_0 \in \mathcal{X}$. For $p = \infty$, we let $\mathcal{P}_m^\infty(\mathcal{X})$ be the set of distributions $\mu \in \mathcal{P}_m(\mathcal{X})$ with bounded support. We write $\Pi(\mu, \nu)$ for the set of transport plans between μ and ν.

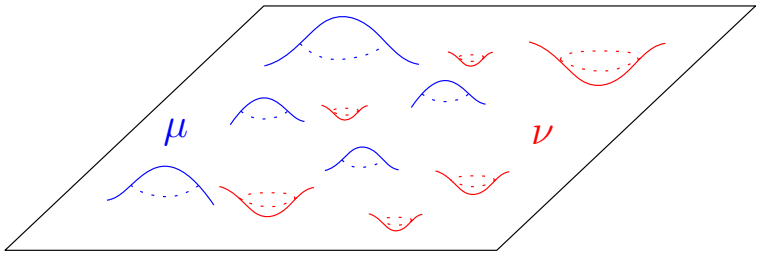


FIGURE 3.1: A distribution μ of "remblais" (in blue) and a distribution ν of "déblais" (in red).

Definition 3.2.1 (Wasserstein distances)**.** *Let $1 \leq p \leq \infty$ and let $\mu, \nu \in \mathcal{P}_m^p(\mathcal{X})$. Let $\pi \in \Pi(\mu, \nu)$. For $p < \infty$, the p-cost of π is equal to*

$$C_p(\pi) := \iint_{\mathcal{X}\times\mathcal{X}} d(x,y)^p \mathrm{d}\pi(x,y), \tag{3.4}$$

while $C_\infty(\pi) := \pi - \operatorname{ess\,sup} d(\cdot,\cdot)$. The Wasserstein distance $W_{p,d}(\mu,\nu)$ between μ and ν is given by

$$W_{p,d}(\mu,\nu) := \inf\{C_p(\pi)^{1/p} : \ \pi \in \Pi(\mu,\nu)\} \tag{3.5}$$

for $p < \infty$, and $C_p(\pi)^{1/p}$ should be replaced by $C_\infty(\pi)$ for $p = \infty$.

When there is no ambiguity on the distance d used, we simply write W_p instead of $W_{p,d}$. We refer to [Vil08, Chapter 6] for the following proposition.

Proposition 3.2.2. *For $1 \leq p \leq \infty$, the Wasserstein distance W_p is a distance on $\mathcal{P}_m^p(\mathcal{X})$. Furthermore, there exist transport plans attaining the infimum in (3.5), that we call* optimal *transport plans. If $p < \infty$ and $(\mathcal{X}, d)$ is a Polish metric space, then the following propositions hold.*

1. *The space $(\mathcal{P}_m^p(\mathcal{X}), W_p)$ is a Polish metric space.*
2. *If $\mathcal{X}$ is compact, then $\mathcal{P}_m^p(\mathcal{X}) = \mathcal{P}_m(\mathcal{X})$ and W_p metricizes the weak topology.*
3. *Let $\mu, \mu_1, \mu_2, \ldots$ be measures in $\mathcal{P}_m^p(\mathcal{X})$. Then, $W_p(\mu_n, \mu) \to 0$ if and only if $\mu_n \xrightarrow{w} \mu$ and $\int d(x,x_0)^p \mathrm{d}\mu_n(x) \to \int d(x,x_0)^p \mathrm{d}\mu(x)$.*

We will denote by $\mathrm{Opt}_{W_p}(\mu,\nu)$ the set of optimal transport plans between μ and ν. One of the key specificities of optimal transport distances with respect to other distances between measures lies in that they are closely linked to the geometry of the underlying metric space $(\mathcal{X}, d)$. For instance the embedding $x \in \mathcal{X} \mapsto \delta_x \in \mathcal{P}_1^p(\mathcal{X})$ is an isometry when $\mathcal{P}_1^p(\mathcal{X})$ is endowed with the Wasserstein distance. Also, metric properties of $(\mathcal{X}, d)$ (e.g. compactness, completeness or separability) are inherited by the space $(\mathcal{P}_1^p(\mathcal{X}), W_p)$. More profound results indicate that studying the space $(\mathcal{P}_1^p(\mathcal{X}), W_p)$ can in turn give insights on the geometry of the space $(\mathcal{X}, d)$, and more precisely on its curvature, see [Vil08, Part II].

For $p = 1$, the Wasserstein distance satisfies a duality formula, known as the Kantorovitch-Rubinstein duality formula [Vil08, Chapter 5].

Proposition 3.2.3. *Let $\mu, \nu \in \mathcal{P}_m^1(\mathcal{X})$. Then,*

$$W_1(\mu,\nu) = \sup\{|\mu(f) - \nu(f)| : \ f : \mathcal{X} \to \mathbb{R} \text{ is 1-Lipschitz continuous}\}. \tag{3.6}$$

Note that the above formula shows that W_1 acts as a norm on the space of signed measures with zero mass.

In this thesis, the theory of optimal transport will have two different uses. First, it will be used in Chapter 5 where we propose estimators to reconstruct measures supported on unknown manifolds. The quality of the reconstruction will be measured thanks to Wasserstein distances. Second, metrics used in Topological Data Analysis (see Section 3.8) share key ideas with metrics used in optimal transport. Making this connection precise will be at the core of Chapter 6, and will in particular allow us to introduce generalizations of persistence diagrams, that we call persistence measures. Persistence measures will then be studied in the remainder of Part II, while optimal transport will be a key technical tool to analyze their behaviors.

3.3 Statistical models and minimax rates

We end the prerequisites on measure theory by defining minimax rates in statistical theory, which will be at the core of Part I.

Let $(\mathcal{X}, \mathcal{G})$ be a measurable space. A *statistical model* is given by the data of $(\mathcal{X}, \mathcal{G}, \mathcal{Q})$, where $\mathcal{Q}$ is a subset of $\mathcal{P}_1(\mathcal{X})$. Let $(E, \mathcal{E})$ be another measurable space and let $\theta : \mathcal{Q} \to (E, \mathcal{E})$ be a functional to be estimated. Given a number n of observations, an estimator of θ is a measurable function $\hat{\theta} : \mathcal{X}^n \to E$, whereas the quality of the estimator is measured through a measurable loss function $\mathcal{L} : E \times E \to [0, +\infty]$. The *risk* of the estimator $\hat{\theta}$ in $\mu \in \mathcal{Q}$ is equal to

$$R_n(\hat{\theta}, \mu, \mathcal{L}) := \mathbb{E}_{(X_1,\dots,X_n)\sim\mu^{\otimes n}}[\mathcal{L}(\hat{\theta}(X_1, \dots, X_n), \theta(\mu))], \tag{3.7}$$

and the smaller the risk, the better the estimator. The *minimax risk* for the estimation of θ on the model $\mathcal{Q}$ with respect to the loss $\mathcal{L}$ is given by

$$\mathcal{R}_n(\theta, \mathcal{Q}, \mathcal{L}) := \inf_{\hat{\theta}} \sup_{\mu\in\mathcal{Q}} R_n(\hat{\theta}, \mu, \mathcal{L}), \tag{3.8}$$

where the infimum is taken over all estimators $\hat{\theta}$ of θ. An estimator attaining the minimax rate (up to a constant) as n goes to $+\infty$ is called a *minimax estimator*.

It will be sometimes necessary to allow for $\mathcal{Q}$ to vary with n (for instance if the model $\mathcal{Q}$ includes a noise which we assume is small with respect to some function of n). Also, there will sometimes be latent variables in the model. For instance, in the *deconvolution problem*, we observe some random variables $X_i = Y_i + \varepsilon_i$, where ε_i is a small noise, and the goal is to recover some information $\theta(\mu)$ about the distribution μ of Y_i (e.g. its support). Depending on what is assumed on the noise ε_i, the quantity $\theta(\mu)$ may not be characterized by the distribution ν of X_i, so that we have to extend slightly the previous definition. Let $\iota : (\mathcal{Y}, \mathcal{H}) \to (\mathcal{X}, \mathcal{G})$ be a measurable function. We now consider a subset $\mathcal{Q}$ of $\mathcal{P}_1(\mathcal{Y})$ and assume that we do not observe a n-sample of distribution $\mu \in \mathcal{Q}$, but of distribution $\iota_\#\mu$ (the pushforward of μ by ι). The minimax risk is then defined by

$$R_n(\hat{\theta}, \mu, \mathcal{L}) := \mathbb{E}_{(X_1,\dots,X_n)\sim(\iota_\#\mu)^{\otimes n}}[\mathcal{L}(\hat{\theta}(X_1, \dots, X_n), \theta(\mu))]. \tag{3.9}$$

For instance, in the deconvolution problem, $\mathcal{Q}$ would be a (strict) subset of the possible distributions of the couple (Y_i, ε_i), whereas ι would be the addition. This generalization will be useful to deal with noise in a rigorous manner when the model is not completely *identifiable*.

Statistical models of interest in this thesis describe strong geometrical hypotheses on the way the observations are distributed, and are detailed in Section 3.5.

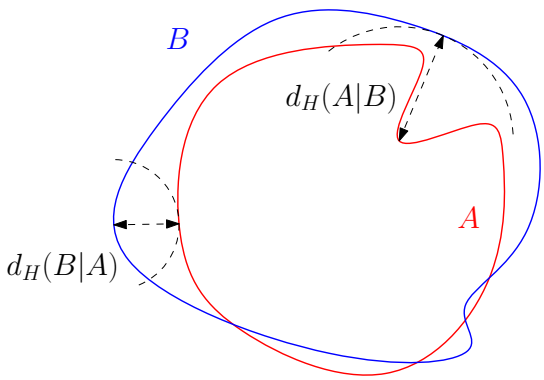


FIGURE 3.2: The Hausdorff distance between the two closed sets A and B is given by $d_H(A|B)$.

3.4 Elements of metric geometry

We now introduce basic concepts of metric geometry.

Hausdorff distance. The Hausdorff distance is a measure of proximity between subsets of some metric space $(\mathcal{X}, d)$. Let $A, B \subset \mathcal{X}$ be two sets. We define the asymmetric Hausdorff distance $d_H(A|B) := \sup\{d(x, B) : x \in A\}$, and the Hausdorff distance $d_H(A, B) = d_H(A|B) \vee d_H(B|A)$, see Figure 3.2. When comparing general subsets A and B, the Hausdorff distance is not very well-behaved: it may be equal to $+\infty$, or be equal to 0 for two different sets. It becomes a proper distance when we restrict to compact sets of $\mathcal{X}$. We let $\mathcal{K}(\mathcal{X})$ be the space of nonempty compact subsets of $\mathcal{X}$.

Proposition 3.4.1 (Proposition III.6 in [Aam17]). *Let $(\mathcal{X}, d)$ be a metric space. Then, d_H is a distance on $\mathcal{K}(\mathcal{X})$. Furthermore, endowed with this metric:*

1. *$\mathcal{K}(\mathcal{X})$ is separable if and only if $\mathcal{X}$ is separable.*
2. *$\mathcal{K}(\mathcal{X})$ is compact if and only if $\mathcal{X}$ is compact.*
3. *$\mathcal{K}(\mathcal{X})$ is complete if and only if $\mathcal{X}$ is complete.*

Note that the asymmetric Hausdorff distance also verifies the following pseudo triangle inequality: for $A, B, C \subset \mathbb{R}^D$,

$$d_H(A|C) \leq d_H(A|B) + d_H(B|C). \tag{3.10}$$

An equivalent formulation of the Hausdorff distance is given by the ∞-norm between the distance functions to a set.

Proposition 3.4.2 (Example 4.13 in [RW09]). *Let $A, B \in \mathcal{K}(\mathcal{X})$. Then,*

$$d_H(A, B) = \|d(\cdot, A) - d(\cdot, B)\|_\infty. \tag{3.11}$$

It will also be useful to compare objects up to isometry: for instance, two segments of comparable lengths are in some sense close to each others, even if they live in different spaces. The *Gromov-Hausdorff distance* allows us to formalize this concept, see also Figure 3.3.

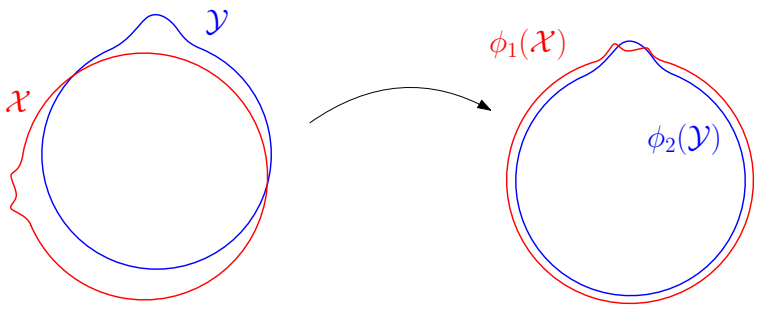


FIGURE 3.3: The Gromov-Hausdorff distance between the two curves $\mathcal{X}$ and $\mathcal{Y}$ is obtained as the Hausdorff distance between $\phi_1(\mathcal{X})$ and $\phi_2(\mathcal{Y})$.

Definition 3.4.3. *Let $(\mathcal{X}, d_1)$ and $(\mathcal{Y}, d_2)$ be two metric spaces. We let $d_{GH}(\mathcal{X}, \mathcal{Y})$ be the infimum of the numbers $r > 0$ such that there exists a metric space $(\mathcal{Z}, d_3)$ and isometries $\phi_1 : (\mathcal{X}, d_1) \to (\mathcal{Z}, d_3)$, $\phi_2 : (\mathcal{Y}, d_2) \to (\mathcal{Z}, d_3)$ such that $d_H(\phi_1(\mathcal{X}), \phi_2(\mathcal{Y})) \leq r$.*

The set $\mathcal{Z}$ in the previous definition can actually be chosen equal to $\mathcal{X} \sqcup \mathcal{Y}$, with d_3 being any distance extending d_1 on $\mathcal{X}$ and d_2 on $\mathcal{Y}$. Furthermore, two compact metric spaces are at distance 0 for the Gromov-Hausdorff distance if and only if they are isometric, and the distance d_{GH} becomes a proper distance on the set of classes of isometric compact spaces [Mém08].

Of particular interest for us will be the space $(\mathcal{K}(\mathbb{R}^D), d_H)$, as the estimators built in Chapter 4 will take their values in this space. We will show that our estimators are measurable as composition of elementary operations on the space $\mathcal{K}(\mathbb{R}^D)$.

Proposition 3.4.4. *1. The function $x \in \mathbb{R}^D \mapsto \{x\} \in \mathcal{K}(\mathbb{R}^D)$ is an isometry.*

2. The "union" function $(A, B) \in \mathcal{K}(\mathbb{R}^D) \times \mathcal{K}(\mathbb{R}^D) \mapsto A \cup B \in \mathcal{K}(\mathbb{R}^D)$ is continuous.

3. The "convex hull" function $A \in \mathcal{K}(\mathbb{R}^D) \mapsto \mathrm{Conv}(A) \in \mathcal{K}(\mathbb{R}^D)$ is continuous.

4. Let $E \in \mathcal{B}(\mathcal{K}(\mathbb{R}^D))$ be a measurable event. Then, the function

$$G_E : (A, B) \in \mathcal{K}(\mathbb{R}^D) \times \mathcal{K}(\mathbb{R}^D) \mapsto \begin{cases} A & \text{if } A \in E \\ B & \text{else.} \end{cases}$$

is measurable.

Proof. For the first three functions, see the proof of Proposition III.7 in [Aam17]. For the last function, let F be any measurable set in $\mathcal{K}(\mathbb{R}^D)$. Then, the preimage of F is given by

$$((F \cap E) \times \mathcal{K}(\mathbb{R}^D)) \cup (E^c \times F),$$

which is measurable. Therefore, the function is measurable. □

We end this paragraph by introducing two different quantities measuring the size of a compact set $A \in \mathcal{K}(\mathbb{R}^D)$. The first one is the *diameter* $\mathrm{diam}(A) := \sup\{|x - y| : x, y \in A\}$. The second is the *radius* of A. It is by definition the radius of the smallest ball B such that $A \subset B$. We denote by $r(A)$ this radius.

Proposition 3.4.5. *The function* diam *is 2-Lipschitz continuous and the function r is 1-Lipschitz continuous.*

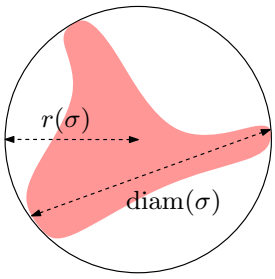


FIGURE 3.4: The radius and diameter of a set $A \subset \mathbb{R}^2$.

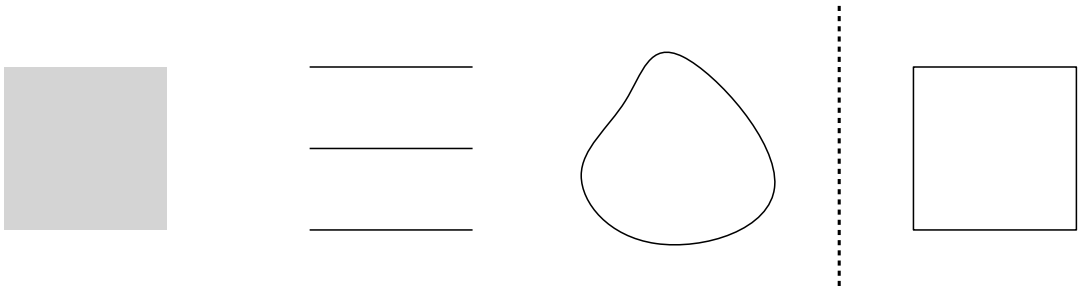


FIGURE 3.5: The three first shapes have positive reach, whereas the square (boundary of $[0,1]^2$) has zero reach.

Proof. For the 1-Lipschitz continuity of the radius, see [ALS13, Lemma 16]. For the diameter, let $x_1, x_2 \in A$ such that $|x_1 - x_2| = \text{diam}(A)$. Let $y_1 \in B$ be such that $|x_1 - y_1| = d(x_1, B)$ and $y_2 \in B$ with $|x_2 - y_2| = d(x_2, B)$. Then,

$$\begin{aligned}\text{diam}(A) &= |x_1 - x_2| \leq |x_1 - y_1| + |y_1 - y_2| + |y_2 - x_2| \\ &\leq d(x_1, B) + \text{diam}(B) + d(x_2, B) \leq \text{diam}(B) + 2d_H(A|B).\end{aligned}$$

We conclude by exchanging the roles of A and B. □

Reach of a set. Let $A \subset \mathbb{R}^D$ be a closed subset. Given $x \in \mathbb{R}^D$, we denote by $\pi_A(x)$ the set of points realizing the distance from x to A:

$$y \in \pi_A(x) \iff (|x - y| = d(x, A) \text{ and } y \in A).$$

Two situations may arise: either $\pi_A(x)$ is a singleton (and we then identify the set with its unique element) or it is not. In the latter case, we say that x is in the *medial axis* $\text{Med}(A)$ of A.

Definition 3.4.6. *The reach of a non-empty closed set $A \subset \mathbb{R}^D$ is given by*

$$\tau(A) := \inf\{d(x, \text{Med}(A)) : \ x \in A\}. \tag{3.12}$$

By definition, for every $r < \tau(A)$, if $d(x, A) \leq r$, then there exists a unique point $\pi_A(x) \in A$ such that $d(x, A) = |x - \pi_A(x)|$. In particular, the projection π_A on A is a well-defined map on $A^r := \{x \in \mathbb{R}^D : \ d(x, A) \leq r\}$, the r-tubular neighborhood of A. A more visual way to understand the reach is given by the "rolling-ball condition": if a set A has reach larger than r, then it is possible to make a ball of radius r roll freely around A without ever bumping into another part of A [CFPL12]. See Figure 3.5 for examples of sets A having positive (and zero) reach.

Examples of sets with positive reach include convex sets (for which $\tau(A) = +\infty$) and compact submanifolds without boundary. More generally, having a large reach

imposes both a local regularity condition on A (it cannot be too "curved") and a global regularity condition (it cannot have a "bottleneck structure"), ideas which can be made mathematically precise [Aam+19], see also Figure 2.3 in the introduction. The reach was originally introduced by Fereder [Fed59] when studying generalizations of Steiner formula for convex sets [Ste40] and Weyl's tube formula for submanifolds [Wey39]. He proved that such a formula relating the volume of tubular neighborhoods of a set A to some notion of curvature also holds for the large class of sets with positive reach. Considering sets with positive reach is often considered as a minimal requirement in computational geometry. For instance, minimax rates of estimation in manifold inference are known to break down when no assumptions on the reach of the underlying sets are made [AL18; AL19].

The positivity of the reach is actually linked to the regularity of the distance function to a set. We say that a function $f : \mathbb{R}^D \to \mathbb{R}^l$ is $\mathcal{C}^{1,1}$ if it is differentiable and its differential is Lipschitz continuous.

Proposition 3.4.7 (Theorem 6.3 in [DZ01])**.** *Let $A \subset \mathbb{R}^D$ be a non-empty closed set. Then, $\tau(A) > 0$ if and only if the function $x \in \mathbb{R}^D \mapsto d^2(x, A)$ is of class $\mathcal{C}^{1,1}$ in some tubular neighborhood of A.*

Remark that the distance function $d(\cdot, A)$ is in general not differentiable on a tubular neighborhood of A, even if A is a smooth object (think of a circle for instance), so that considering the squared distance in the above proposition is required. From a statistical perspective, the estimation of the reach of a manifold has been tackled in [Aam+19] and [Ber+21].

Another point of view consists in seeing the reach as a function $\tau : \mathcal{K}(\mathbb{R}^D) \to [0, +\infty]$. It is clear that this function is not continuous: take a set $A = \{x, y\}$. If $x \neq y$, then $\tau(A)$ is given by the half-distance between x and y, whereas when $x \to y$, we obtain a singleton at the limit, whose reach is infinite. However, such a discontinuity may only happen with an increase of the reach, that is the reach is upper semi-continuous.

Proposition 3.4.8 (Remark 4.14 in [Fed59])**.** *The function τ is upper semi-continuous.*

Hausdorff measure. The d-dimensional Hausdorff measure is a generalization of the d-dimensional Lebesgue measure to arbitrary subsets of $\mathbb{R}^D$. For instance, the 1-dimensional Hausdorff measure of a curve is given by its length, the 2-dimensional Hausdorff of a surface is given by its area, etc.

Definition 3.4.9. *Let $d \geq 0$ be an integer. For $A \subset \mathbb{R}^D$, and $\delta > 0$, consider*

$$\mathcal{H}_d^\delta(A) := \inf \left\{ \sum_{i \geq 0} \omega_d \left(\frac{\operatorname{diam}(U_i)}{2} \right)^d : \; A \subset \bigcup_{i \geq 0} U_i \text{ and } \operatorname{diam}(U_i) < \delta \right\}, \tag{3.13}$$

*where $\omega_d = \pi^{d/2}/\Gamma\left(\frac{d}{2} + 1\right)$ is the volume of the d-dimensional unit ball. The d-*dimensional Hausdorff measure *of A is defined by $\mathcal{H}_d(A) := \lim_{\delta \to 0} \mathcal{H}_d^\delta(A)$.*

3.5 Elements of differential geometry

The goal of this section is twofold. First, we introduce succinctly the language of differential geometry to fix notation that will be used throughout Part I. Second, we explore in more detail the geometry of submanifolds of $\mathbb{R}^D$. In particular, we introduce statistical models tailored to the estimation of geometric quantities related to $\mathcal{C}^k$

submanifolds, introduced in [AL19] and [BH19]. We refer to do Carmo's book [Car92] for a more thorough introduction to Riemannian geometry. Due to their primary importance in manifold inference, we will focus on *submanifolds* in this presentation. This simplifies most definitions, while Nash's embedding theorem actually ensures that this is not restrictive [Nas56]. We begin with preliminary definitions.

- Let $G(d, D)$ be the Grassmannian manifold of all d-dimensional subspaces of $\mathbb{R}^D$. For $E \in G(d, D)$, we denote by π_E the orthogonal projection on E and $\pi_E^\perp := \mathrm{id} - \pi_E$ the orthogonal projection on $E^\perp$, the orthogonal complement of E. The angle $\angle(E, F)$ between two subspaces $E, F \in G(d, D)$ is defined as the distance $\|\pi_E - \pi_F\|_{\mathrm{op}}$, the operator norm between the orthogonal projections on E and F.

- Let $U \subset \mathbb{R}^D$ be an open set and $f : U \to \mathbb{R}$ be a $\mathcal{C}^k$ function. We denote by $d^k f(x) : (\mathbb{R}^D)^k \to \mathbb{R}$ the k-th differential of f at $x \in U$. The $\mathcal{C}^k$-norm of f is equal to
$$\|f\|_{\mathcal{C}^k} := \sup_{x \in U} \left\| d^k f(x) \right\|_{\mathrm{op}}. \tag{3.14}$$
The $\mathcal{C}^0$-norm is equal to the L_∞-norm, and we will often write $\|\cdot\|_\infty$ instead of $\|\cdot\|_{\mathcal{C}^0}$.

Definition 3.5.1. *A* topological d-dimensional (sub)manifold M *of* $\mathbb{R}^D$ *is a subset of* $\mathbb{R}^D$ *(endowed with the subspace topology) such that every* $x \in M$ *has a neighborhood homeomorphic to* $\mathbb{R}^d$.

This definition has the advantage of being very simple. It is however not restrictive enough for our purposes. Indeed, every graph of a continuous function $\mathbb{R}^d \to \mathbb{R}^D$ is a topological submanifold, including wild objects such as the Koch snowflake.

Definition 3.5.2 (see Chapter 8 in [Lee13])**.** *Let* $k \geq 1$. *A* $\mathcal{C}^k$ d-dimensional (sub)manifold M *of* $\mathbb{R}^D$ *is a set such that, for every* $x \in M$, *there exists a* $\mathcal{C}^k$ *diffeomorphism* $\phi : V_x \to \mathbb{R}^D$, *where* $V_x \subset \mathbb{R}^D$ *is a neighborhood of* x, *such that* $\phi(V_x \cap M)$ *is the intersection of a* d*-dimensional plane with* $\phi(V_x)$.

If M is a submanifold (that is $\mathcal{C}^k$ for some $k \geq 1$), we define the *tangent space* $T_x M$ of $x \in M$ as the set

$$T_x M := \left\{ u \in \mathbb{R}^D : \ \forall \varepsilon > 0, \exists y \in M, \ |x - y| \leq \varepsilon \text{ and } \left| \frac{x - y}{|x - y|} - \frac{u}{|u|} \right| \leq \varepsilon \right\}. \tag{3.15}$$

In particular, the tangent spaces are elements of the Grassmannian manifold $G(d, D)$, and we write π_x for $\pi_{T_x M}$. If U is a neighborhood of 0 in $T_x M$, we say that a $\mathcal{C}^k$ function $\Psi : U \to M \subset \mathbb{R}^D$ is a *local parametrization* of M at x if it is a one-to-one function such that $\Psi(0) = x$, $d\Psi(0)$ is the inclusion $T_x M \hookrightarrow \mathbb{R}^D$, and $d\Psi(u)$ is of full rank for every $u \in U$. One can show that a manifold M is $\mathcal{C}^k$ if and only if there are $\mathcal{C}^k$ local parametrizations at every $x \in M$.

Proposition 3.4.7 states that the positivity of the reach of a set is equivalent to the $\mathcal{C}^{1,1}$ regularity of the squared distance to the set. When the set is assumed to be a manifold, this is in turn equivalent to the manifold being of regularity $\mathcal{C}^{1,1}$ (that is the diffeomorphisms are of regularity $\mathcal{C}^{1,1}$ in the previous definition).

Proposition 3.5.3. *Let* $M \subset \mathbb{R}^D$ *be a compact topological submanifold. Then,* $\tau(M) > 0$ *if and only if* M *is of regularity* $\mathcal{C}^{1,1}$.

Proof. The direct implication is proved in [RZ17]. For the converse implication, we first show that given a point $y \in \mathbb{R}^D$, if $z \in \pi_M(y)$, then $y - z$ is orthogonal to $T_z M$. Indeed, let Ψ be a local parametrization in z. Then, 0 is a local minimum of the function $u \in T_z M \mapsto |y - \Psi(u)|^2$. The gradient of this function at 0 is null, and is given by $-2\pi_z(y - z)$, implying that $y - z$ is orthogonal to $T_z M$.

We now show that for every $x \in M$, there is a small neighborhood of x in $\mathbb{R}^D$ on which there is a unique projection on M. The compactness of M then implies the conclusion. Let Ψ be a local $\mathcal{C}^{1,1}$ parametrization of M at x, defined on a neighborhood U of 0 in $T_x M$. Let $F : U \times \mathbb{R}^D \to T_x M$ be defined by $F(u, y) = d\Psi(u)^\top(\Psi(u) - y)$. The function F is Lipschitz continuous in u and linear in y. We apply a version of the implicit function theorem for Lipschitz continuous maps [Kum91], which holds under the condition that, for any sequences $\lambda_k \to 0$, $u^k \to 0$, $y^k \to y$ and $v \in T_x M \backslash \{0\}$, we have

$$\lim_k \frac{F(u^k + \lambda_k v, y^k) - F(u^k, y^k)}{\lambda_k} \neq 0$$

whenever the limit exists. One can check directly that this limit always exist, and is given by $d\Psi(0)^* d\Psi(0)[v] = v \neq 0$. Therefore, by [Kum91, Theorem 1], as F is Lipschitz continuous, there exists, for $\varepsilon, \varepsilon' > 0$ small enough, a unique map $\phi : \mathcal{B}(x, \varepsilon) \to T_x M$ such that, for $y \in \mathcal{B}(x, \varepsilon)$ and $u \in \mathcal{B}_{T_x M}(0, \varepsilon')$,

$$F(u, y) = 0 \text{ if and only if } u = \phi(y).$$

Fix $y \in \mathcal{B}(x, \varepsilon'')$ for some $\varepsilon'' > 0$ to fix. If $z \in M$ belongs to $\pi_M(y)$, then $y - z$ is orthogonal to $T_z M$, that is $F(\Psi^{-1}(z), y) = 0$. Furthermore,

$$|z - x| \leq |z - y| + |y - x| \leq 2|y - x| \leq 2\varepsilon'',$$

which implies that $\Psi^{-1}(z) \in \Psi^{-1}(\mathcal{B}_M(x, 2\varepsilon'')) \subset \mathcal{B}_{T_x M}(0, \varepsilon')$ for ε'' small enough. Therefore, we have that $\Psi^{-1}(z) = \phi(y)$, that is $z = \Psi(\phi(y))$ is uniquely determined by y. Hence, there is a unique projection on M on $\mathcal{B}(x, \varepsilon'')$, proving that the reach $\tau(M)$ is positive. □

We will consider in the following a slightly stronger requirement: all manifolds are now assumed to be at least $\mathcal{C}^2$. This ensures that the *second fundamental form* of the manifold M (that we define below) is well-defined.

Definition 3.5.4. *Let $\tau_{\min} > 0$ and $1 \leq d < D$. We let $\mathcal{M}^{2,d}_{\tau_{\min}}$ be the set of closed $\mathcal{C}^2$ d-dimensional submanifolds without boundary, with reach larger than $\tau_{\min}$ and let furthermore $\mathcal{M}^{2,d} := \bigcup_{\tau_{\min} > 0} \mathcal{M}^{2,d}_{\tau_{\min}}$ be the set of closed $\mathcal{C}^2$ d-dimensional submanifolds without boundary with positive reach.*

Let $M \in \mathcal{M}^{2,d}$. A *geodesic* is the analogue of a straight line on M. It is a $\mathcal{C}^2$ curve $\gamma : I \to M \subset \mathbb{R}^D$ defined on some interval I satisfying that $\gamma''(t) \in T_{\gamma(t)} M^\perp$ for every $t \in I$ (where γ is seen as taking its values in $\mathbb{R}^D$). The *geodesic distance* $d_g(x, y)$ between two points x and y in M is defined as the infimum over all geodesics γ joining x and y of the length of the geodesic, defined as

$$L(\gamma) := \int_I |\gamma'(t)| \mathrm{d}t. \tag{3.16}$$

Also, we denote by vol_M the d-dimensional Hausdorff measure restricted to M.

Definition 3.5.5. *Let $M \in \mathcal{M}^{2,d}$. Let $x \in M$ and $\eta \in T_xM^\perp$. Let N be a local extension of η normal to M, that is $N : U_x \to \mathbb{R}^D$ is defined on a neighborhood $U_x \subset \mathbb{R}^D$ of x, is of class $\mathcal{C}^2$ and satisfies $N(x) = \eta$ and $N(y) \in T_yM^\perp$ for $y \in M$. The second fundamental form $S_M(x,\eta) : T_xM \to T_xM$ of M at x along the normal η is the operator given by*

$$S_M(x,\eta)[u] = -\pi_x(d_xN[u]) \qquad \forall u \in T_xM. \tag{3.17}$$

One can check that the second fundamental form does not depend on the extension N. Furthermore, for each $x \in M$ and $\eta \in T_xM^\perp$, the operator $S_M(x,\eta)$ is a linear self-adjoint operator on T_xM. Given a normal direction η and a tangent vector u, the second fundamental form describes how the normal direction η varies as x is moved in the direction u. As such, it gives a description of the extrinsic curvature of the manifold M.

Proposition 3.5.6 (Proposition 6.1 in [NSW08])**.** *Let $M \in \mathcal{M}^{2,d}$, $x \in M$ and $\eta \in T_xM^\perp$. Then,*

$$\|S_M(x,\eta)\|_{\mathrm{op}} \leq \frac{1}{\tau(M)}. \tag{3.18}$$

We now give further geometric constraints given by the reach.

Proposition 3.5.7. *Let $M \in \mathcal{M}^{2,d}$ and $x, y \in M$.*

1. *If some point z is at distance less than $\tau(M)$ from M with $\pi_M(z) = x$, then $\pi_x(z - x) = 0$.*
2. *We have $|\mathrm{vol}_M| \geq \omega_d \tau(M)^d$, where ω_d is the volume of the d-dimensional sphere. Furthermore, the equality is attained only if M is a d-dimensional sphere of radius $\tau(M)$.*
3. *We have $\mathrm{diam}(M) \leq C_d \frac{|\mathrm{vol}_M|}{\tau(M)^{d-1}}$ for some positive constant C_d. Furthermore, $\tau(M) \leq \sqrt{\frac{D}{2(D+1)}}\,\mathrm{diam}(M)$.*
4. *We have $|\pi_x^\perp(y - x)| \leq \frac{|x-y|^2}{2\tau(M)}$.*
5. *We have $\angle(T_xM, T_yM) \leq 2\frac{|x-y|}{\tau(M)}$.*
6. *If $d_g(x,y) \leq \pi\tau(M)$ (or if $|x - y| \leq \tau(M)/2$), then $|x - y| \leq d_g(x,y) \leq |x - y| \min\left(\frac{\pi}{2}, 1 + \frac{c_0}{\tau(M)^2}|x - y|\right)$, where $c_0 = \pi^2/50$.*
7. *If $h \leq \tau(M)/4$, then $8^{-d}\omega_d h^d \leq \mathrm{vol}_M(\mathcal{B}_M(x,h)) \leq 8^d \omega_d h^d$.*

Proof. Point 1 was already shown in the proof of Proposition 3.5.3. Point 2 is stated in [Alm86], whereas Point 3 is proved in [Aam17, Section III.3.4]. Point 4 is proved in Federer's article [Fed59, Theorem 4.18]. Point 5 is stated in [BSW09, Lemma 3.4]. For Point 6, see the proof of [ACLG19, Lemma 3.12]. Also, having $|x - y| \leq \tau(M)/2$ implies that $d_g(x,y) \leq \pi\tau(M)$ is a consequence of [NSW08, Proposition 6.3]. Finally we prove Point 7. Proposition 8.7 in [AL18] states that for $h \leq \tau(M)/4$,

$$2^{-d}\alpha_d h^d \leq \mathrm{vol}_M(\mathcal{B}_M(x,h)) \leq 2^d \alpha_d h^d,$$

where α_d is the volume of the d-dimensional ball. It remains to show that $2^d\alpha_d \leq 8^d\omega_d$ and that $2^d\omega_d \leq 8^d\alpha_d$. One can check by recursion on d that those inequalities hold for any $d \geq 1$, concluding the proof. □

In particular, if $|\mathrm{vol}_M| < \infty$ and $\tau(M) > 0$, then M is automatically compact. Among all local parametrizations of a manifold M, a particularly natural one is given by the inverse of the projection on the tangent space. We let $\tilde{\pi}_x$ be defined by $\tilde{\pi}_x(y) = x + \pi_x(y - x)$ (so that $\tilde{\pi}_x(x) = x$) and let $\tilde{T}_x M = x + T_x M$ be the image of $\tilde{\pi}_x$.

Proposition 3.5.8. *Let $x \in M$. For $r \leq \tau(M)/3$, the application $\tilde{\pi}_x$ is a diffeormorphism from $\mathcal{B}_M(x, r)$ on its image. Moreover, its image $\tilde{\pi}_x(\mathcal{B}_M(x, r))$ contains $\mathcal{B}_{\tilde{T}_x M}(x, 7r/8)$. In particular, if $y \in \mathcal{B}_M(x, \tau(M)/4)$, then*

$$|\tilde{\pi}_x(y) - x| \geq \frac{7}{8}|y - x|. \tag{3.19}$$

Proof. We first show that $\tilde{\pi}_x$ is injective on $\mathcal{B}_M(x, \tau(M)/3)$. Assume that $\tilde{\pi}_x(y) = \tilde{\pi}_x(y')$ for some $y \neq y' \in M$. Consider without loss of generality that $|x - y| \geq |x - y'|$. The goal is to show that $|x-y| > \tau(M)/3$. If $|x-y| > \tau(M)/2$, the conclusion obviously holds. Proposition 3.5.7.5 states that if it is not the case then, $\angle(T_x M, T_y M) < 2\frac{|x-y|}{\tau(M)}$. Also, by definition,

$$\begin{aligned}
\angle(T_x M, T_y M) &\geq \frac{|(\pi_x - \pi_y)(y - y')|}{|y - y'|} \\
&= \frac{|\pi_y(y - y')|}{|y - y'|} \geq \frac{|y - y'| - |\pi_y^{\perp}(y - y')|}{|y - y'|} \\
&\geq 1 - \frac{|y - y'|}{2\tau(M)} \text{ by Proposition 3.5.7.4} \\
&\geq 1 - \frac{|x - y|}{\tau(M)} \text{ by the triangle inequality.}
\end{aligned}$$

Therefore, we have $3|x - y|/\tau(M) > 1$, i.e. $|x - y| > \tau(M)/3$ and $\tilde{\pi}_x$ is injective on $\mathcal{B}_M(x, \tau(M)/3)$. To conclude that $\tilde{\pi}_x$ is a diffeomorphism, it suffices to show that its differential is always invertible. As $\tilde{\pi}_x$ is an affine application, the differential $d\tilde{\pi}_x(y)$ is equal to π_x. Therefore, the Jacobian $J\tilde{\pi}_x(y)$ of the function $\tilde{\pi}_x : M \to T_x M$ in y is given by the determinant of the projection π_x restricted to $T_y M$. In particular, it is larger than the smallest singular value of $\pi_x \circ \pi_y$ to the power d, which is larger than

$$(1 - \angle(T_x M, T_y M))^d \geq \left(1 - 2\frac{|x - y|}{\tau(M)}\right)^d \geq \left(\frac{1}{3}\right)^d,$$

thanks to Proposition 3.5.7.5 and using that $|x - y| \leq \tau(M)/3$. In particular, the Jacobian is positive, and $\tilde{\pi}_x$ is a diffeormorphism from $\mathcal{B}_M(x, \tau(M)/3)$ to its image. The second statement is stated in [AL19, Lemma A.2]. The last statement is a consequence of the two first, using that if $|y - x| \leq \tau(M)/4$, then $8|\tilde{\pi}_x(y) - x|/7 \leq \tau(M)/3$. □

Note that this proposition was already proven in [ACLZ17, Lemma 5], but with a slightly worse constant of $\tau(M)/12$. We write Ψ_x for the inverse of the map $y \in M \mapsto \pi_x(y - x) \in T_x M$, which is defined according to the previous lemma on $\mathcal{B}_{T_x M}(0, 7r/8)$ for $r \leq \tau(M)/3$ (in particular it is defined on $\mathcal{B}_{T_x M}(0, \tau(M)/4)$). The parametrizations Ψ_x will be used in the following to quantify the regularity of the manifold M.

Proposition 3.5.9. *Let M be a $\mathcal{C}^k$ submanifold for $k \geq 2$ and let $x \in M$. Then, Ψ_x is a local $\mathcal{C}^k$ parametrization of M.*

Proof. Let Ψ be a $\mathcal{C}^k$ parametrization at x. We may write $\Psi_x = \Psi \circ (\Psi^{-1} \circ \Psi_x)$ on a small neighborhood of 0. As Ψ is $\mathcal{C}^k$, it suffices to show $G = \Psi^{-1} \circ \Psi_x : T_xM \to T_xM$ is $\mathcal{C}^k$ on a neighborhood of 0. Given $u \in T_xM$ small enough, $v = G(u)$ is characterized by the equation $\pi_x(\Psi(v) - x) = u$. This expression is $\mathcal{C}^k$ in (u, v) and, by the implicit function theorem, using that $d\Psi(0)$ is the inclusion $T_xM \hookrightarrow \mathbb{R}^D$, we obtain that G is indeed $\mathcal{C}^k$. □

We denote by $\mathcal{M}^{k,d}$ the set of $\mathcal{C}^k$ closed d-dimensional submanifolds without boundary with positive reach.

Definition 3.5.10 (Class of regular manifolds)**.** *Let $d \geq 1, k \geq 2$ and $L, \tau_{\min} > 0$. Let $r_0 = (\tau_{\min} \wedge L)/4$. We say that $M \in \mathcal{M}^{k,d}_{\tau_{\min},L}$ if M is in $\mathcal{M}^{k,d}$ with $\tau(M) \geq \tau_{\min}$ and if, for all $x \in M$, Ψ_x is defined on $\mathcal{B}_{T_xM}(0, r_0)$ and the function $u \in \mathcal{B}_{T_xM}(0, r_0) \mapsto \Psi_x(u) - x$ has a $\mathcal{C}^k$norm smaller than L.*

The second differential of Ψ_x can be expressed thanks to the second fundamental form of M. In particular, one can obtain using Proposition 3.5.6 an inequality of the form $\|\Psi_x - x\|_{\mathcal{C}^2} \leq L_{d,\tau(M)}$, implying that the parameter L is not relevant to quantify the $\mathcal{C}^2$-regularity of a manifold. For $k \geq 3$, there are no constraints on the $\mathcal{C}^k$-norm of the local parametrizations based on the reach, and the parameter L becomes useful.

We say that a function $f : M \to \mathbb{R}^l$ is $\mathcal{C}^k$ if $f \circ \Psi_x$ is $\mathcal{C}^k$ for every $x \in M$. We define the norm $\left\|d^k f(x)\right\|_{\text{op}}$ at x as $\left\|d^k(f \circ \Psi_x)(0)\right\|_{\text{op}}$. Defining rigorously what is the kth differential of the function f is more delicate and would require introducing concepts such as the Levi-Civita connection, whereas only defining a notion of $\mathcal{C}^k$-norm of a function is of interest for us. If $l \leq d$, the Jacobian of f is defined by $Jf = \sqrt{\det((df)(df)^*)}$.

We compare our definition with other models of $\mathcal{C}^k$ manifolds appearing in the manifold inference literature. In [BH19], a similar approach is taken to measure the regularity of manifolds, but with exponential maps used as local parametrizations. However, exponential maps may only be $\mathcal{C}^{k-2}$ on a $\mathcal{C}^k$ manifold [Har51] so that we prefer to use the inverse projections Ψ_x as parametrizations. In [AL19], Aamari and Levrard assume the existence of a local parametrization $\tilde{\Psi}_x$ at $x \in M$ with $\mathcal{C}^k$ norm smaller than L, not necessarily equal to the inverse Ψ_x of the projection $\tilde{\pi}_x$. However, the choice of Ψ_x as a local parametrization is not restrictive. Indeed, one can write $\Psi_x = \tilde{\Psi}_x \circ (\pi_x \circ \tilde{\Psi}_x)^{-1}$, so that, by the inverse function theorem, the $\mathcal{C}^k$ norm of Ψ_x is controlled by the $\mathcal{C}^k$ norm of $\tilde{\Psi}_x$.

Statistical models for measures supported on manifolds Statistical models of interest in the following correspond to sampling "almost-uniformly" points on (or close to) a manifold which is regular enough.

Definition 3.5.11. *Let $1 \leq d < D$, $k \geq 2$, $\tau_{\min}, L > 0$ and $0 < f_{\min} \leq f_{\max} \leq \infty$. The set $\mathcal{Q}^{k,d}_{\tau_{\min},L,f_{\min},f_{\max}}$ is the set of all probability measures μ, whose support M belongs to $\mathcal{M}^{k,d}_{\tau_{\min},L}$, and which have a density f with respect to the volume measure on M, satisfying $f_{\min} \leq f \leq f_{\max}$.*

We also consider sampling with a bounded additive noise: each observation X_i is of the form $Y_i + Z_i$, where the law of Y_i is supported on a manifold and $|Z_i| \leq \gamma$, whereas Y_i and Z_i are not necessarily independent.

Definition 3.5.12. *Let $1 \leq d < D$, $k \geq 2$, $\tau_{\min}, L, \gamma > 0$ and $0 < f_{\min} \leq f_{\max} \leq \infty$. The set $\mathcal{Q}^{k,d}_{\tau_{\min},L,f_{\min},f_{\max}}(\gamma)$ is the set of all probability measures ξ on $\mathbb{R}^D \times \mathbb{R}^D$, such that the first marginal of ξ belongs to $\mathcal{Q}^{k,d}_{\tau_{\min},L,f_{\min},f_{\max}}$ and the second marginal of ξ is supported on $\mathcal{B}(0, \gamma)$.*

We then assume that we observe samples having distribution $\iota_\# \xi$, where $\iota : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^D$ is the addition. As explained in Section 3.3, this slightly more technical definition allows us to define the function $\theta(\xi) = M$ as the support of the first marginal of ξ, whereas M cannot be recovered solely thanks to the law of the observation $X = Y + Z$, where $(Y, Z) \sim \xi$.

For $k = 2$, the parameter L has no impact on the statistical rates of convergence, and we only consider $\mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}(\gamma) := \mathcal{Q}^{2,d}_{\tau_{\min}, +\infty, f_{\min}, f_{\max}}(\gamma)$. The minimax rates for the estimation of the manifold M are known to satisfy:

$$c_0 \left(\frac{\ln n}{n}\right)^{2/d} \leq \mathcal{R}_n(M, \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}(\gamma), d_H) \leq c_1 \left(\left(\frac{\ln n}{n}\right)^{2/d} \vee \gamma\right) \tag{3.20}$$

$$c_2 \left(\frac{1}{n}\right)^{k/d} \leq \mathcal{R}_n(M, \mathcal{Q}^{k,d}_{\tau_{\min}, L, f_{\min}, f_{\max}}(\gamma), d_H) \leq c_1 \left(\left(\frac{\ln n}{n}\right)^{k/d} \vee \gamma\right). \tag{3.21}$$

The lower bound in (3.20) is provided in [KZ15] while the upper bound was first given in [Gen+12a]. The statistical models $\mathcal{Q}^{k,d}_{\tau_{\min}, L, f_{\min}, f_{\max}}(\gamma)$ were introduced in [AL19], where (3.21) is also shown. The upper bound follows from exhibiting a minimax estimator, obtained by using a local polynomial estimator around every observation point. In particular, these estimators will be used in Chapter 5 to estimate the volume measure of M.

The coarea formula Finally, we introduce the coarea formula, which is a far-reaching generalization of the change of variables formula for integrals on manifolds.

Theorem 3.5.13 (Coarea formula [Mor16])**.** *Let M (resp. N) be a submanifold of dimension m (resp. n). Assume that $m \geq n$ and let $\phi : M \to N$ be a differentiable map. For $f : M \to [0, +\infty)$ a measurable function, the following equality holds:*

$$\int_M f(x) J\phi(x) \mathrm{dvol}_M(x) = \int_N \left(\int_{x \in \phi^{-1}(\{y\})} f(x) \mathrm{d}\mathcal{H}_{m-n}(x) \right) \mathrm{dvol}_N(y). \tag{3.22}$$

In particular, if $J\phi > 0$ almost everywhere, one can apply the coarea formula to $f \cdot (J\phi)^{-1}$ to compute $\int_M f$, while having $J\phi > 0$ is equivalent to $d\phi$ being of full rank.

3.6 Simplicial complexes

Simplicial complexes are higher dimensional analogs of graphs. Their simple combinatorial structure makes their use particularly appealing in computational geometry, as they can be easily stored on a computer. We refer to [EH10] for results in this section.

Definition 3.6.1 (Simplicial complex)**.** *Let S be a set. A* simplicial complex *with vertex set S is a family of finite subsets of S containing all the singletons and such that, if $\sigma \subset \sigma'$ is nonempty and if $\sigma' \in K$, then $\sigma \in K$.*

Let K be a simplicial complex with vertex set S and K' be a simplicial complex with vertex set S'. We say that a map $f : S \to S'$ is a simplicial map *between K and K' if for every $\sigma \in K$ the image of σ by f belongs to K'.*

A subset $\sigma \in K$ is called a *simplex*, and its *dimension* $|\sigma|$ is equal to $\#\sigma - 1$ (where $\#\sigma$ denotes the cardinality of the set σ). The dimension of K is the maximal dimension of its simplexes (possibly $+\infty$). The *q-skeleton* $\mathcal{S}_q(K)$ of K is the set of simplexes of K of dimension q.

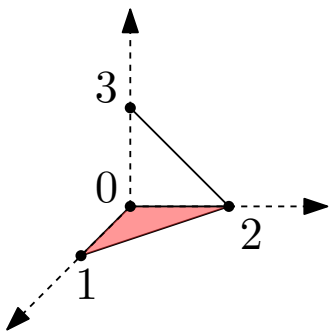


FIGURE 3.6: The geometric realization of K_0 as a subset of $\mathbb{R}^3$.

A simplicial complex is a purely combinatorial object and does not possess any geometric structure. It is however possible to associate with each simplicial complex K a topological space $\tilde{K}$, called its *geometric realization*. As a set, $\tilde{K}$ is the set of functions $\alpha \in [0,1]^S$ with $\sum_{s\in S} \alpha(s) = 1$ and such that the set $\mathrm{spt}(\alpha) := \{s \in S : \alpha(s) > 0\} \in K$. For $\sigma \in K$ of dimension q, let $\tilde{\sigma} := \{\alpha \in [0,1]^S : \mathrm{spt}(\alpha) \subset \sigma\}$. This is a topological subspace of $[0,1]^S$ endowed with the product topology (the space $\tilde{\sigma}$ is actually homeomorphic to $\tilde{\Delta}_q = \{(x_0, x_1, \ldots, x_q) \in [0,1]^{q+1} : \sum_{i=0}^{q} x_i = 1\}$, the *standard q-dimensional simplex*). We then endow the set $\tilde{K}$ with the final topology associated with the inclusions $\tilde{\sigma} \hookrightarrow \tilde{K}$ for $\sigma \in K$.

Example 3.6.2. The geometric realization of very simplicial complex with vertex set $\{0,1,2,3\}$ has its geometric realization that is homeomorphic to a subset of $\mathbb{R}^3$. In Figure 3.6, we display the geometric realization of the 2-dimensional simplicial complex

$$K_0 = \{0,1,2,3,\{0,1\},\{0,2\},\{1,2\},\{2,3\},\{0,1,2\}\}.$$

Example 3.6.3. Let $S \subset \mathbb{R}^D$ and $t > 0$. We review different simplicial complexes of geometric interest that can be built on top of S.

1. The *Rips complex* $\mathrm{Rips}(t,S)$ of S at scale t is the simplicial complex with vertex set S, and such that $\sigma \in \mathrm{Rips}(t,S)$ if σ is finite and of diameter $\mathrm{diam}(\sigma)$ smaller than t.

2. Given a compact set $\sigma \subset \mathbb{R}^D$, there exists a unique ball $\mathcal{B}(\sigma)$ with minimal radius such that $\sigma \subset \mathcal{B}(\sigma)$ [ALS13]. The radius of this ball is called the *radius* of σ and is denoted by $r(\sigma)$. The *Čech complex* $\mathrm{Cech}(t,S)$ of S at scale t is the simplicial complex with vertex set S, and such that $\sigma \in \mathrm{Cech}(t,S)$ if σ is finite and $r(\sigma) \leq t$. The *nerve theorem* asserts that (the geometric realization of) $\mathrm{Cech}(t,S)$ is homotopy equivalent to S^t, the t-neighborhood of S [Hat02, Corollary 4G.3].

3. If S is finite, a *triangulation* of S is a simplicial complex T of dimension D with vertex set S such that

   (a) every simplex of T is included in a D-simplex of T.

   (b) for $\sigma \neq \sigma' \in T$ the interior of $\mathrm{Conv}(\sigma)$ is disjoint from the interior of $\mathrm{Conv}(\sigma')$.

   (c) $\bigcup_{\sigma\in T} \mathrm{Conv}(\sigma) = \mathrm{Conv}(S)$.

   (d) if $\sigma \in \mathcal{S}_D(T)$, then $\mathrm{Conv}(\sigma) \cap S = \sigma$.

   In particular, a triangulation is uniquely determined by its D-skeleton.

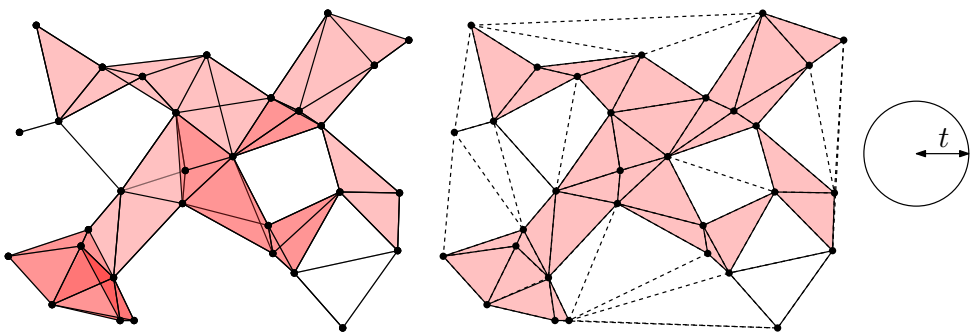


FIGURE 3.7: Left. The Čech complex $\mathrm{Cech}(S,t)$ of a finite set $S \subset \mathbb{R}^2$. A simplex is in the Čech complex only if it fits in a circle of radius t. Brighter colors indicate that a simplex of dimension larger than 3 is present. Right. The Delaunay triangulation of S (dashed), and its α-shape $\mathrm{Alpha}(S,t)$ for a certain value of t.

4. Assume that S is finite and does not lie on a hyperplane of $\mathbb{R}^D$. Then, for each D-simplex of S, there exists a unique $(D-1)$-dimensional sphere containing σ, called the *circumsphere* of σ. A *Delaunay triangulation* of S is a triangulation $\mathrm{Del}(S)$ of S such that the interior of every circumsphere of $\sigma \in \mathcal{S}_D(\mathrm{Del}(S))$ does not contain any point of S [EH10, Chapter III.3]. It is unique when S is in general position, in the sense that no set of $D+2$ points of S lies on a sphere.

5. Under the same assumptions, the *α-complex* $\mathrm{Alpha}(S,t)$ of S is equal to set of simplices $\sigma \subset \mathrm{Del}(S)$ such that there exists a point x that is equidistant to all the points of σ, at distance less than t from each point, see [EH10, Chapter III.4]. The Čech complex and the α-complex are homotopy equivalent, see Figure 3.7.

Both the Rips and the Čech complex of a set S capture the geometry of the set at scale t. Note however that such objects may be very wild. For instance, there exists a compact set $S \subset \mathbb{R}^4$ with $\mathrm{Rips}(t,S)$ having singular homology (see below) with uncountable dimension for every t in some interval [Dro12]. From a computational point of view, their sizes may become prohibitively large for $|S|$ even of moderate size if t is too large. Although computing the radius of a set σ is possible in quasi-linear time in $\mathbb{R}^2$, such a computation becomes a non-trivial task in moderate dimensions, which may be a serious issue to compute the Čech complex of a set in practice. Algorithms with $O(|S|\log|S|)$ complexity exist to compute the Delaunay triangulation for $D \leq 3$, whereas algorithms with $O(|S|^{\lfloor D/2 \rfloor})$ time complexity exist for larger D. In practice, computing a Delaunay triangulation becomes prohibitive for $D > 6$ [HB08]. Unlike the Čech and the Rips complexes, the size of the Delaunay triangulation does not explode, as it is of order $O(|S|^{\lfloor D/2 \rfloor})$. In practice, the α-complex is therefore often computed instead of the Čech complex.

3.7 Simplicial and singular homologies

Homological algebra is a general theory which gives a mathematically precise meaning to the presence of topological features in an object. Different versions of homologies exist and are defined for different mathematical structures. We will focus on simplicial homology, defined for simplicial complexes and which has the benefit of being easily computable, and then on singular homology, which is defined for any topological space. We first define homology groups in an abstract setting. An introduction to homology theory may be found in [Hat02].

3.7.1 Homological algebra

Let G be an abelian group (only the cases $G = \mathbb{Z}$ and G a finite field will be relevant for us). A *chain complex* $C_\bullet$ is a sequence of abelian G-modules $(C_q)_{q\geq -1}$ together with homomorphisms $\partial_q : C_q \to C_{q-1}$ for $q \geq 0$, such that $\partial_q\partial_{q+1} = 0$ and $C_{-1} = \{0\}$. The map ∂_q is called a *boundary map*. Elements of $Z_q := \ker \partial_q$ are called *q-cycles* whereas elements of $B_q := \operatorname{im} \partial_{q+1}$ are called *q-boundaries*. The relation $\partial_q\partial_{q+1} = 0$ implies that $B_q \subset Z_q$, i.e. every boundary is a cycle. Two cycles are called *homologous* if they differ by a boundary, and we refer to $H_q(C) = Z_q/B_q$ as the qth *homology group* of $C_\bullet$. The dimension of $H_q(C)$ (should it be finite) is called the *Betti number* $\beta_q(C)$ of the chain complex.

If $C_\bullet$ and $C'_\bullet$ are two chain complexes, a *chain map* is a collection of morphisms $\varphi_q : C_q \to C'_q$ such that the following diagram commutes.

$$\begin{tikzcd} C_q \arrow[r, "\partial_q"] \arrow[d, "\varphi_q"'] & C_{q-1} \arrow[d, "\varphi_{q-1}"] \\ C'_q \arrow[r, "\partial'_q"] & C'_{q-1} \end{tikzcd}$$

This commutation property ensures that the morphisms φ_q induces morphisms at the homology level $H_q(\varphi) : H_q(C) \to H_q(C')$. Two chain complexes C and C' are said to be isomorphic if there exist two chain maps $\varphi : C \to C'$ and $\varphi' : C' \to C$ with $\varphi_q\varphi'_q = \mathrm{id}_{C'_q}$ and $\varphi'_q\varphi_q = \mathrm{id}_{C_q}$ for every $q \geq 0$.

3.7.2 Simplicial homology

Let K be a simplicial complex. An ordering of a simplex $\sigma = \{x_0, \ldots, x_q\}$ is an enumeration of $x_0, \ldots, x_q$. We say that two orderings of a simplex σ have the same orientation if they differ by an even permutation. This defines an equivalence relation on the set of orderings of σ, with two equivalence classes, that we call oriented simplexes and denote by $\vec{\sigma}$ and $-\vec{\sigma}$. The chain complex $C_\bullet(K) = C_\bullet(K, G)$ is defined by letting $C_q(K)$ be the free group generated by the oriented q-simplexes of K with coefficients in G. Given $\vec{\sigma}$ an oriented q-simplex, we denote by $\vec{\sigma}^i$ the oriented $(q-1)$-simplex obtained from $\vec{\sigma}$, with ith entry omitted. The boundary operator is defined by

$$\partial_q\vec{\sigma} = \sum_{i=0}^{q} (-1)^i \vec{\sigma}^i, \tag{3.23}$$

and is then extended by linearity to $C_q(K)$. One can check that $\partial_q\partial_{q+1} = 0$, so that $C_\bullet(K)$ is indeed a chain complex. The corresponding homology groups are called the *simplicial homology groups* of K (with coefficients in G), and are denoted by $H_\bullet(K) = H_\bullet(K, G)$.

3.7.3 Singular homology

Let X be a topological space. A singular simplex is a continuous map $\sigma : \tilde{\Delta}_q \to X$. We let σ^i be the map $(x_0, \ldots, x_{q-1}) \in \tilde{\Delta}_{q-1} \mapsto \sigma(x_0, \ldots, 0, \ldots, x_{q-1})$, where 0 is at the ith position. The chain complex $C_\bullet(X, G)$ is defined by letting $C_q(X)$ be the free group generated by the q-dimensional singular simplexes of X with coefficients in G. The boundary operator is defined by

$$\partial_q\sigma = \sum_{i=0}^{q} (-1)^i \sigma^i, \tag{3.24}$$

and is then extended by linearity to $C_q(X)$. The corresponding homology groups are called the *singular homology groups* of X (with coefficients in G), and are denoted by $H_\bullet(X) = H_\bullet(X, G)$.

Simplicial homology can be seen as a particular case of singular homology. Indeed, the singular chain complex $C_\bullet(\tilde{K})$ of the geometric realization of K can be shown to be isomorphic to the simplicial chain complex $C_\bullet(K)$, so that in particular the homology groups are also isomorphic [Spa12, Section 4.4].

For both homologies, maps between objects (simplicial complexes or topological spaces) induce maps between chain complexes, and therefore also maps between homology groups. Precisely, if $f : X \to Y$ is a continuous map, then there exists a chain map $C_\bullet(f) : C_\bullet(X) \to C_\bullet(Y)$, obtained by defining $C_\bullet(f)(\sigma) = f \circ \sigma$ for σ a singular simplex in X (and extended by linearity). The map $f_* := H_\bullet(C_\bullet(f))$ is then defined between the homology groups $H_\bullet(X)$ and $H_\bullet(Y)$. A similar statement holds for simplicial homology, with continuous maps replaced by simplicial maps. We will drop the C in the notation when the context is clear, e.g. $\beta_q(X)$ for $\beta_q(C(X))$, $Z_q(X)$ for $Z_q(C(X))$, etc.

Remark 3.7.1. The *universal coefficient theorem* asserts that the integral homology groups $H_\bullet(C, \mathbb{Z})$ completely determines the homology groups $H_\bullet(C, G)$ for any abelian group G [Hat02, Chapter 3.A]. However, the theory of persistence homology is developed for vector spaces over some field $\mathbf{k}$ (having a field is in particular required for the decomposition theorem to hold, see Theorem 3.8.4 below). We will therefore choose G to be a finite field. This has an impact on the homology groups only if the underlying space has non-null torsion, whereas in practice, the choice of the field for which persistent homology is computed seems to have very little impact [OY20].

3.8 Theoretical foundations of Topological Data Analysis

The fundamental object of persistent homology theory is the persistence module. We fix a field $\mathbf{k}$ and a homology dimension $q \geq 0$ in the following. We refer to the book [Cha+16] for a thorough presentation of the content of this section.

Definition 3.8.1 (Persistence modules)**.** *A* persistence module $\mathbb{V}$ *is a family of* $\mathbf{k}$-*vector spaces* $(V_t)_{t\in\mathbb{R}}$ *together with linear maps* $v_{s,t} : V_s \to V_t$ *for all* $s \leq t$*, satisfying the conditions* $v_{t,t} = \mathrm{id}_{V_t}$ *and* $v_{t,r}v_{s,t} = v_{s,r}$ *for all* $s \leq t \leq r$*.*

Persistence modules are typically induced by a filtration of some topological space $\mathcal{X}$. Let $\phi : \mathcal{X} \to \mathbb{R}$ be a function and $\phi^t := \{x \in \mathcal{X} : \ \phi(x) \leq t\}$ be the sublevel sets of ϕ. The collection $(\phi^t)_{t\in\mathbb{R}}$ forms an increasing sequence of spaces that we call a filtration. Letting $V(\phi)_{q,t} = H_q(\phi^t, \mathbf{k})$ be the q-dimensional singular homology group of ϕ^t with coefficients in $\mathbf{k}$, we obtain a persistent module $\mathbb{V}_q(\phi)$, with maps $v(\phi)_{s,t}$ being induced by the inclusion maps $\phi^s \hookrightarrow \phi^t$ for $s \leq t$. The persistent module $\mathbb{V}_q(\phi)$ describes the evolution of the homology of ϕ through different scales t. A similar class of persistence modules is given by the simplicial homology of filtrations of simplicial complexes. A filtration K of simplicial complexes is an increasing sequence of simplicial complexes $(K^t)_{t\geq 0}$ sharing the same vertex set. One can define the persistence module $\mathbb{V}_q(K)$ with $V(K)_{q,t} = H_q(K^t, \mathbf{k})$ being the simplicial homology group of K^t. Of particular interest are the Rips filtration $\mathrm{Rips}(A) = (\mathrm{Rips}(t, A))_{t\geq 0}$ of a set A and its Čech filtration $\mathrm{Cech}(A) = (\mathrm{Cech}(t, A))_{t\geq 0}$.

3.8.1 The interleaving distance

Two persistence modules $\mathbb{V}$ and $\mathbb{W}$ are close if for every $t \in \mathbb{R}$, V_t is similar to $W_{t'}$ for some t' close to t. This idea is made precise by the *interleaving distance*. Let $\varepsilon \geq 0$. An *ε-morphism* between two persistence modules $\mathbb{V}$ and $\mathbb{W}$ is a collection of linear maps $\varphi_t : V_t \to W_{t+\varepsilon}$ for $t \geq 0$ such that the following diagram commutes.

$$\begin{tikzcd} V_s \arrow[r, "v_{s,t}"] \arrow[d, "\varphi_t"'] & V_t \arrow[d, "\varphi_t"] \\ W_{s+\varepsilon} \arrow[r, "w_{s+\varepsilon,t+\varepsilon}"] & W_{t+\varepsilon} \end{tikzcd}$$

The persistence modules $\mathbb{V}$ and $\mathbb{W}$ are ε-interleaved if there exists two ε-morphisms $\varphi : \mathbb{V} \to \mathbb{W}$ and $\varphi' : \mathbb{W} \to \mathbb{V}$ such that the following diagrams commute for every $t \in \mathbb{R}$.

$$\begin{tikzcd} V_t \arrow[rr, "v_{t,t+2\varepsilon}"] \arrow[dr, "\varphi_t"] & & V_{t+2\varepsilon} \\ & W_{t+\varepsilon} \arrow[ur, "\varphi'_{t+\varepsilon}"'] & \end{tikzcd} \qquad \begin{tikzcd} & V_{t+\varepsilon} \arrow[dr, "\varphi_{t+\varepsilon}"] & \\ W_t \arrow[ur, "\varphi'_t"] \arrow[rr, "w_{t,t+2\varepsilon}"] & & W_{t+2\varepsilon} \end{tikzcd}$$

The interleaving distance d_i between $\mathbb{V}$ and $\mathbb{W}$ is equal to

$$d_i(\mathbb{V}, \mathbb{W}) := \inf\{\varepsilon \geq 0 : \ \mathbb{V} \text{ and } \mathbb{W} \text{ are } \varepsilon\text{-interleaved}\}. \tag{3.25}$$

The interleaving distance can be bounded efficiently in different settings.

Theorem 3.8.2 (Stability theorem)**.**

1. *Let $f, g : X \to \mathbb{R}$ be two functions. Then,*

$$d_i(\mathbb{V}_q(f), \mathbb{V}_q(g)) \leq \|f - g\|_\infty. \tag{3.26}$$

2. *Let A, B be two compact sets in $\mathbb{R}^D$. Then,*

$$\begin{aligned} d_i(\mathbb{V}_q(\mathrm{Cech}(A)), \mathbb{V}_q(\mathrm{Cech}(B)) &\leq d_{GH}(A, B), \\ d_i(\mathbb{V}_q(\mathrm{Rips}(A)), \mathbb{V}_q(\mathrm{Rips}(B)) &\leq d_{GH}(A, B). \end{aligned} \tag{3.27}$$

3.8.2 The decomposition theorem

In general, a persistence module is a complex object that may be cumbersome to work with. However, it turns out that under finiteness assumptions, persistence modules enjoy a simple combinatorial description given by the so-called *decomposition theorem*. Before stating the result, we explicit what it means for two persistence modules to be isomorphic (see also Figure 3.8).

Definition 3.8.3. *An* (observable) morphism $\varphi : \mathbb{V} \to \mathbb{W}$ *between persistence modules is a collection of linear maps $\varphi_{s,t} : V_s \to W_t$ for $s < t$, such that for every $s \leq u < v \leq t$, the following diagram commutes.*

$$\begin{tikzcd} V_s \arrow[r, "v_{s,u}"] \arrow[d, "\varphi_{s,t}"'] & V_u \arrow[d, "\varphi_{u,v}"] \\ W_t & W_v \arrow[l, "w_{v,t}"] \end{tikzcd}$$

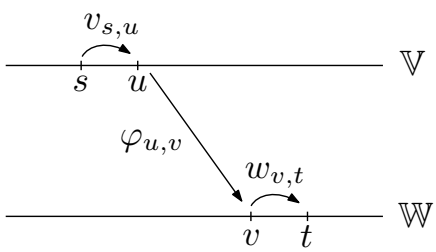


FIGURE 3.8: A morphism φ between persistence modules is a collection of maps which satisfy some coherence properties.

If $\varphi : \mathbb{V} \to \mathbb{W}$ and $\varphi' : \mathbb{W} \to \mathbb{U}$ are two observable morphisms, the composition $\varphi\varphi'$ is defined by $(\varphi\varphi')_{s,t} = \varphi_{u,t} \circ \varphi'_{s,u}$ for any $u \in (t, s)$. The identity morphism $\mathrm{id}_{\mathbb{V}} : \mathbb{V} \to \mathbb{V}$ is defined by $\varphi_{s,t} = v_{s,t}$ for all $s < t$. A morphism $\varphi : \mathbb{V} \to \mathbb{W}$ is an isomorphism if there exists another morphism $\varphi' : \mathbb{W} \to \mathbb{V}$ with $\varphi\varphi' = \mathrm{id}_{\mathbb{W}}$ and $\varphi'\varphi = \mathrm{id}_{\mathbb{V}}$. The persistence modules $\mathbb{V}$ and $\mathbb{W}$ are then said to be isomorphic*, and we write $\mathbb{V} \overset{\mathrm{ob}}{\simeq} \mathbb{W}$.*

It can be shown that two persistence modules $\mathbb{V}$ and $\mathbb{W}$ are at distance 0 for the interleaving distance if and only if $\mathbb{V} \overset{\mathrm{ob}}{\simeq} \mathbb{W}$, while being 0-interleaved is a slightly stronger notion [CCBS16].

The direct sum $\mathbb{V} \oplus \mathbb{W}$ between two persistence modules $\mathbb{V}$ and $\mathbb{W}$ is defined by $(V_t \oplus W_t)_{t\in\mathbb{R}}$, with linear maps $v_{t,s} \oplus w_{t,s}$. Let $\Omega^\infty := \{u = (u_1, u_2) \in [-\infty, +\infty]^2 : u_1 < u_2\}$. Given a point $u \in \Omega^\infty$, we let $\mathbf{k}^u$ be the persistence module with $\mathbf{k}^u_t = \mathbf{k}$ if $u_1 \leq t \leq u_2$ and $\{0\}$ otherwise, with arrows given by $v_{s,t} = \mathrm{id}_{\mathbf{k}}$ if $u_1 \leq s \leq t \leq u_2$ and 0 otherwise. Those persistence modules, that we call *interval modules*, serve as building blocks for more complex persistence modules. We call a persistence module tame (or q-tame) if, for all $s < t$, the rank of the map $v_{s,t}$ is finite. We call this quantity the persistent Betti number $\beta_{s,t}(\mathbb{V})$ of the persistence module $\mathbb{V}$.

Theorem 3.8.4 (Decomposition theorem)**.** *Let $\mathbb{V}$ be a tame persistence module. Then, there exists a unique multiset* $\mathrm{dgm}(\mathbb{V})$ *in Ω^∞ such that $\mathbb{V}$ is isomorphic to*

$$\mathbb{V} \overset{\mathrm{ob}}{\simeq} \bigoplus_{u\in\mathrm{dgm}(\mathbb{V})} \mathbf{k}^u. \tag{3.28}$$

The multiset $\mathrm{dgm}(\mathbb{V})$ *is called the* persistence diagram *of $\mathbb{V}$.*

There are two types of points u appearing in the decomposition (3.28): those which contain infinite coordinates, called *essential points*, and the others. It can be shown that if two persistence modules $\mathbb{V}$ and $\mathbb{W}$ possess a different number of essential points, then $d_i(\mathbb{V}, \mathbb{W}) = +\infty$, while the distance is finite otherwise. To simplify the exposition, **we will only consider persistence modules with no essential points**, so that the interleaving distance is always finite. Properties of persistence diagrams with a fixed number $n > 0$ of essential points can then be easily inferred from this case.

With this assumption in mind, a persistence diagram is actually a multiset of points in $\Omega := \{u = (u_1, u_2) \in \mathbb{R}^2 : \ u_1 < u_2\}$. Equivalently, it can be considered as a discrete measure on Ω, by identifying a multiset a with the measure $\sum_{u\in a} \delta_u$. Both perspectives are relevant, and we will often switch between the two without mentioning it. Each point $u = (u_1, u_2)$ of a persistence diagram corresponds to some interval in the decomposition (3.28), which informally represents a topological feature of the associated persistence module, which appeared at $\mathbb{V}_{u_1}$ and disappeared at $\mathbb{V}_{u_2}$. The *persistence* $\mathrm{pers}(u) := u_2 - u_1$ of the point u represents the length of the corresponding

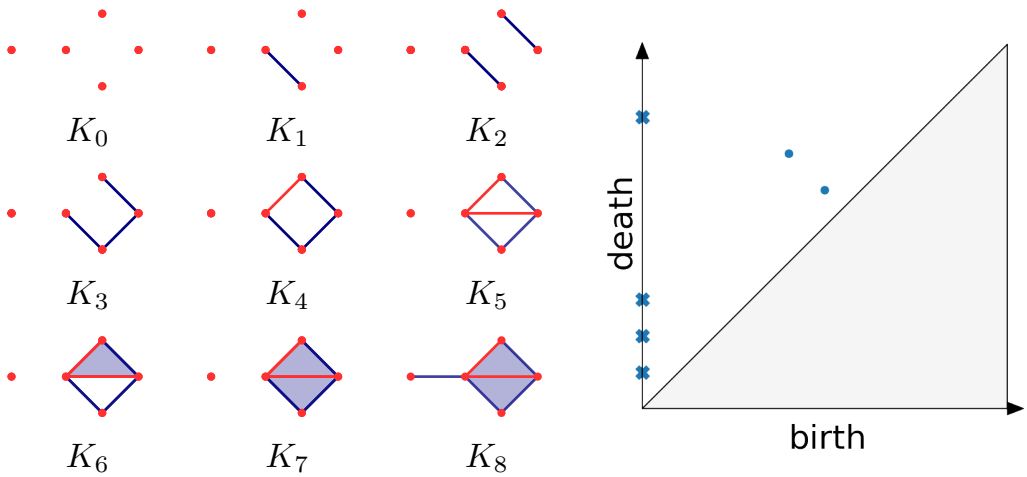


FIGURE 3.9: Left. A filtration of simplicial complexes. Positive simplexes are displayed in red, whereas negative simplexes are displayed in blue. Right. The corresponding persistence diagrams for $q = 0$ (crosses) and $q = 1$ (dots).

interval, while the associated topological feature is considered relevant if $\mathrm{pers}(u)$ is large. As such, points close to the diagonal $\partial\Omega := \{(u_1, u_2),\ u_1 = u_2\}$ in a persistence diagram are often thought of as representing topological noise whereas points with large persistence are considered to contain relevant topological information.

The "q" in q-tame is for quadrant: a persistence module is q-tame if the associated persistence diagram, seen as a measure, gives finite mass to every quadrant $\lrcorner_u = \{v \in \Omega :\ v_1 \leq u_1 < u_2 \leq v_2\}$, with the relation

$$\beta_{u_1,u_2}(\mathbb{V}) = \mathrm{dgm}(\mathbb{V})(\lrcorner_u), \quad \forall u = (u_1, u_2) \in \Omega. \tag{3.29}$$

Proposition 3.8.5 (Theorem 3.37 in [Cha+16]). *Fix an integer $q \geq 0$.*

1. *Let $\mathcal{X}$ be a topological space homeomorphic to a locally finite simplicial complex, and let $\phi : \mathcal{X} \to \mathbb{R}$ be a proper continuous function bounded below. Then, $\mathbb{V}_q(\phi)$ is tame.*

2. *Let S be a compact subset of $\mathbb{R}^D$. Then, $\mathbb{V}_q(\mathrm{Cech}(S))$ and $\mathbb{V}_q(\mathrm{Rips}(S))$ are tame.*

In particular, under such assumptions, by Theorem 3.8.4, the persistence diagram $\mathrm{dgm}_q(\phi) := \mathrm{dgm}(\mathbb{V}_q(\phi))$ of ϕ is well-defined, and so are the Čech and Rips persistence diagrams of S, denoted respectively by $\mathrm{dgm}_q^C(S) := \mathrm{dgm}(\mathbb{V}_q(\mathrm{Cech}(S)))$ and $\mathrm{dgm}_q^R(S) := \mathrm{dgm}(\mathbb{V}_q(\mathrm{Rips}(S)))$.

Definition 3.8.6 (Space of persistence diagrams). *The space $\mathcal{D}$ of persistence diagrams is the space of all discrete Radon measures on Ω with integer masses.*

Note that by the decomposition theorem, the space $\mathcal{D}$ contains the set of persistence diagrams of q-tame persistence modules $\mathbb{V}$. It however also contains more general persistence diagrams, such as the measure $a = \sum_{n\geq 1} \delta_{(0,n)}$ that would correspond to the non-tame persistence module $\bigoplus_{n\geq 1} \mathbf{k}^{(0,n)}$. We introduce also the space $\mathcal{D}_f$ of finite persistence diagrams.

3.8.3 Persistence diagrams in the finite setting

In practice, persistence modules will be obtained through the simplicial homology of some finite filtration $K = (K_{t_i})_{0\leq i\leq N}$ of simplicial complexes with $t_0 \leq \cdots \leq t_N$ and

finite vertex set S:

$$K_{t_0} \subset K_{t_1} \subset \cdots \subset K_{t_N}.$$

We may assume without loss of generality that at each step only one simplex is added, so that $K_{t_{i+1}} = K_{t_i} \cup \{\sigma_i\}$. If σ_i is of dimension $q+1$, then two different situations may arise:

1. Either σ_i is contained in a cycle $c \in Z_{q+1}(K_{t_{i+1}})$. In that case, one can show that c cannot be homologous to a cycle in K_{t_i}, and that

$$H_{q+1}(K_{t_{i+1}}) \simeq H_{q+1}(K_{t_i}) \oplus [c]_{t_{i+1}},$$

   where $[c]_{t_{i+1}}$ represents the class of cycles homologous to c in $K_{t_{i+1}}$. The simplex σ_i is then called *positive*.

2. Either $\sigma_i \notin Z_{q+1}(K_{t_{i+1}})$. In that case, it holds that $\partial_{q+1}\sigma_i \in B_q(K_{t_i})$ and we have

$$H_q(K_{t_{i+1}}) \simeq H_q(K_{t_i})/[\partial_{q+1}\sigma_i]_{t_i}.$$

   where $[\partial_{q+1}\sigma_i]_{t_i}$ represents the class of cycles homologous to σ_i in K_{t_i}. The simplex σ_i is then called *negative*.

When a negative simplex σ_i appears, then the "hole" corresponding to the class $[\partial_{q+1}\sigma_i]_{t_i}$ in $H_q(K_{t_i})$ is "filled". The class $[\partial_{q+1}\sigma_i]_{t_i}$ appeared with some positive q-dimensional simplex σ_j: informally, the "hole" was born with σ_j. Those two simplexes (one positive and one negative) form a *q-simplex pair*. The persistence diagram $\mathrm{dgm}(\mathbb{V}(K))$ of the filtration for q-dimensional homology is given by the collection of the pairs (t_j, t_i) for (σ_i, σ_j) a q-simplex pair (if $t_i = t_j$, we discard the pair). Those pairings can be efficiently computed by a Gaussian elimination algorithm on the boundary matrix operator, see [EH10] for details.

3.8.4 The bottleneck distance

The stability theorem (Theorem 3.8.2) justifies the use of the interleaving distance as a meaningful distance between persistence modules. However, detecting if two persistence modules are ε-interleaved is *a priori* a nontrivial task, so that it is not clear how the interleaving distance can be computed. The *isometry theorem* states that the interleaving distance is actually equal to a distance between persistence diagrams, called the *bottleneck distance*, which is defined as the optimum of some matching problem. As such, the bottleneck distance can be computed efficiently on a computer, opening the door to the use of persistence diagrams in real-life applications. We fix an arbitrary norm $\|\cdot\|$ on $\mathbb{R}^2$.

Definition 3.8.7 (Bottleneck distances)**.** *Let $a, b \in \mathcal{D}$. The set of partial matchings $\Gamma(a,b)$ between a and b is the set of bijections $\gamma : a \cup \partial\Omega \to b \cup \partial\Omega$. For $1 \leq p < \infty$, the p-bottleneck distance is defined as*

$$d_p(a,b) := \inf_{\gamma \in \Gamma(a,b)} \left(\sum_{x \in a \cup \partial\Omega} \|x - \gamma(x)\|^p \right)^{1/p}. \tag{3.30}$$

while the bottleneck distance is equal to $d_\infty(a,b) := \inf_{\gamma\in\Gamma(a,b)} \sup_{x\in a\cup\partial\Omega} \|x - \gamma(x)\|$.

Given two persistence diagrams a and b, a partial matching is a way to transport the points of a towards the points of b. However, the total masses of a and b may differ. Therefore, the diagonal is used as an infinite reservoir of mass, and one can

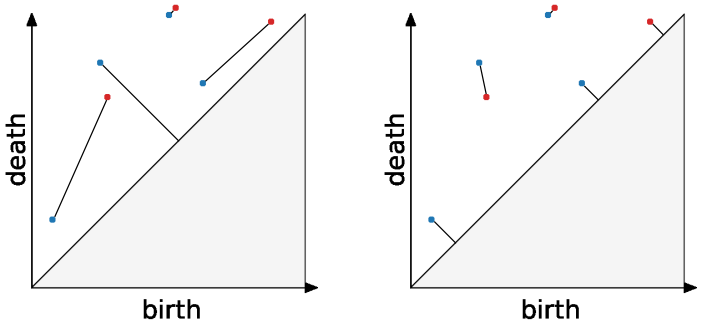


FIGURE 3.10: Two matchings between a blue persistence diagram and a red persistence diagram. The rightmost matching is optimal, i.e. it attains the minimum in Definition 3.8.7.

freely map points from a or b towards the diagonal with cost given by the distance to the diagonal. In the persistence module decomposition $\bigoplus_{u\in a}\mathbf{k}^u$ associated with a diagram a, points on the diagonal represent interval modules $\mathbf{k}^u$ with length 0, and one can indeed show that for any finite set $c \subset \partial\Omega$,

$$\bigoplus_{u\in a\cup c}\mathbf{k}^u \overset{\text{ob}}{\simeq} \bigoplus_{u\in a}\mathbf{k}^u, \tag{3.31}$$

justifying the use of $\partial\Omega$ as a reservoir. The bottleneck distance is then given by the longest edge in an optimal matching between two diagrams a and b. The distance is then not changed if we add an arbitrary number of points in the two diagrams at distance less than $d_\infty(a,b)$ from the diagonal. On the contrary, the p-bottleneck distance for p finite is not blind to points close to the diagonal, as every edge is taken into account when computing the cost of a matching.

Remark 3.8.8. The p-bottleneck distance for $p < \infty$ was originally introduced in [CS+10] as a generalization of the bottleneck distance. Due to its similarities with optimal transport metrics, it was then called the Wasserstein distance between persistence diagrams. There are however key differences between the metrics d_p and classical Wasserstein distances between W_p. Exploring the differences (and the similarities) between the two notions will be at the core of Chapter 6. To avoid confusion, we therefore choose the name of p-bottleneck distance for the d_p distance, although it is not standard in the literature.

Theorem 3.8.9 (Isometry theorem)**.** *Let $\|\cdot\|$ be the ∞-norm on $\mathbb{R}^2$. Let $\mathbb{V}$, $\mathbb{W}$ be q-tame persistence modules. Then,*

$$d_i(\mathbb{V},\mathbb{W}) = d_\infty(\mathrm{dgm}(\mathbb{V}),\mathrm{dgm}(\mathbb{W})). \tag{3.32}$$

The three theorems we have introduced (the stability theorem, the decomposition theorem and the isometry theorem) lay the theoretical foundations of TDA. They ensure that persistence diagrams exist in a large variety of settings (decomposition theorem), while a meaningful distance between them exists (stability theorem), which can be efficiently computed (isometry theorem).

Remark that for persistence diagrams having an infinite number of points, the p-bottleneck distance d_p ($p < \infty$) can be infinite. For $p \leq \infty$, we introduce the class $\mathcal{D}^p$ of persistence diagrams which are at finite d_p-distance from the empty diagram 0. Precisely, for $a \in \mathcal{D}$, we call the quantity $\mathrm{Pers}_p(a) := d_p^p(a,0) = \sum_{u\in a}\mathrm{pers}(u)^p$ the total p-persistence of a, and let

$$\mathcal{D}^p := \{a \in \mathcal{D},\ \mathrm{Pers}_p(a) < \infty\}. \tag{3.33}$$

For $p = \infty$, we let $\mathcal{D}^\infty$ be the set of $a \in \mathcal{D}$ with $d_\infty(a, 0) < \infty$. Although smaller than $\mathcal{D}^\infty$, the metric space $(\mathcal{D}^p, d_p)$ possesses better properties than $(\mathcal{D}^\infty, d_\infty)$ from a geometric and topological perspective (see Chapter 6). However, the fundamental isometry theorem does not hold for $p < \infty$. A weaker form of stability is still satisfied by the p-bottleneck distance for $p < \infty$, proven in [CS+10]. We say that a function $\phi : \mathcal{X} \to \mathbb{R}$ is tame if $\mathbb{V}_q(\phi)$ is tame for every $q \geq 0$.

Definition 3.8.10. *Let $(\mathcal{X}, d)$ be a metric space and $1 \leq p < \infty$. We say that $(\mathcal{X}, d)$ implies bounded degree-p total persistence if there exists a positive constant C such that, for every 1-Lipschitz tame function $\phi : \mathcal{X} \to \mathbb{R}$, we have $\mathrm{Pers}_p(\mathrm{dgm}_q(\phi)) \leq C$ for every $q \geq 0$.*

Spaces implying bounded degree-p total persistence include d-dimensional Riemannian compact manifolds for $p > d$, but also bilipschitz images of (geometric realizations of) finite simplicial complexes. In particular, a d-dimensional Riemannian compact manifold M implies bounded degree-p total persistence with constant $C_M \operatorname{diam}(M)^{p-d} \frac{p}{p-d}$.

Theorem 3.8.11 (p-bottleneck stability theorem)**.** *Let $(\mathcal{X}, d)$ be a space which implies bounded degree-p total persistence with associated constant C. Let $\phi_1, \phi_2 : \mathcal{X} \to \mathbb{R}$ be two L-Lipschitz tame functions. Then, for all $p' > p$,*

$$d_{p'}(\mathrm{dgm}(\phi_1), \mathrm{dgm}(\phi_2)) \leq (CL^p)^{\frac{1}{p'}} \|\phi_1 - \phi_2\|_\infty^{1-\frac{p}{p'}}. \tag{3.34}$$

We end this section by mentioning some basic results on the topological properties of $\mathcal{D}^p$, see [MMH11] for details.

Theorem 3.8.12. *For $1 \leq p \leq \infty$, the space $(\mathcal{D}^p, d_p)$ is complete. If $p < \infty$, it is also separable, so that $(\mathcal{D}^p, d_p)$ is a Polish metric space. The space $(\mathcal{D}^\infty, d_\infty)$ is not separable.*

Considering the space $\mathcal{D}^p$ instead of the set $\mathcal{D}_f$ of finite persistence diagrams is required to have a complete space. Indeed, the sequence $(a_n)_n$ in $\mathcal{D}_f$ given by $a_n = \sum_{i=0}^n \delta_{u_i}$, where $u_i = (0, 2^{-i})$ converges towards $a = \sum_{i \geq 0} \delta_{u_i} \in \mathcal{D}^p$. Actually, we have the following result.

Proposition 3.8.13. *For $1 \leq p < \infty$, the space $\mathcal{D}^p$ is the completion of $\mathcal{D}_f$ for the d_p metric.*

3.9 Statistical methods in Topological Data Analysis

The standard pipeline in TDA goes as follows. We observe a collection $X_1, \ldots, X_n$ of complex objects with some task in mind (e.g. classification or regression). Those objects can for instance be graphs, point clouds, 3D shapes, time series, images, etc. A first step consists in building filtrations $K_1, \ldots, K_n$ on top of them, which will then be used in a second step to obtain a collection of persistence diagrams $a_1, \ldots, a_n$. We think of this set of persistence diagrams as containing the relevant topological information to explain the underlying phenomenon generating the dataset. The goal is then to treat efficiently this topological information, either to directly use it for the learning task at stake or by plugging it in a larger pipeline (for instance by using persistence diagrams as a layer in a neural network).

A first approach consists in performing the statistical analysis directly in the space of persistence diagrams. As the space of persistence diagrams is only a metric space

and lacks additional structure, this is not a trivial task, and even simple objects like the expected value or the variance are not trivially defined. The metric analogue of the expected value is the Fréchet mean of a distribution. Fréchet means for persistence diagrams were introduced in a seminal paper by Mileyko, Mukherjee and Harer [MMH11], where authors study the metric properties of the space $\mathcal{D}^p$.

Definition 3.9.1. *Let $(\mathcal{X}, d)$ be a metric space and $P \in \mathcal{P}_1^p(\mathcal{X})$. Define the energy of $y \in \mathcal{X}$ as*

$$\mathcal{E}(y) := \mathbb{E}_{x\sim P}[d^p(x, y)]. \tag{3.35}$$

A p-Fréchet mean of P is an element $y^* \in \mathcal{X}$ such that

$$\mathcal{E}(y^*) = \inf\{\mathcal{E}(x) : \ x \in \mathcal{X}\}. \tag{3.36}$$

We denote by $\text{Fréchet}_p(P)$ *the set of p-Fréchet means of P.*

In particular, if $(\mathcal{X}, d)$ is the Euclidean space and $p = 2$, then there exists a unique barycenter, given by the expected value. The condition $\mathbb{E}_{x\sim P}[d(x, x_0)^p] < \infty$ (that is $P \in \mathcal{P}_1^p(\mathcal{X})$) ensures the finiteness of the energy functional. In general, the set of p-Fréchet means may either be empty or contain several elements. Mileyko, Mukherjee and Harer show that there exist 2-Fréchet means for distributions P with compact support.

Theorem 3.9.2 (Theorem 24 in [MMH11])**.** *Let $P \in \mathcal{P}_1^2(\mathcal{D}^p)$. Assume that P has compact support. Then,* $\text{Fréchet}_2(P)$ *is non-empty.*

The space $\mathcal{D}^p$ is not locally compact, so that the condition in the above theorem is strong. It can actually be replaced by a weaker tail condition on the random variable $\text{Pers}_p(a)$ for $a \sim P$ [MMH11, Theorem 28]. In Chapter 6, we will show that $\text{Fréchet}_p(P)$ is non-empty for the d_p distance for any $1 \leq p < \infty$, without any further assumptions on P.

From a computational perspective, several algorithms exist to compute Fréchet means of a set of persistence diagrams. A first algorithm, based on the Hungarian algorithm used in optimal transport, was proposed in [Tur+14]. Although it runs in polynomial time, it only converges to a local minimum of the energy functional, so that it may not output a Fréchet mean with a bad initialization. A faster version of the algorithm was then proposed in [KVT19; VBT19], without still any guarantees on the convergence towards a Fréchet mean. Another approach, developed by Lacombe, Cuturi and Oudot [LCO18], consists in relaxing the problem to make it convex, using an Eulerian approach. The output of their algorithm is provably close to a Fréchet mean, although it is not a persistence diagram, but a more general *persistence measure*. Persistence measures are natural generalizations of persistence diagrams in random settings and will be studied in detail in Chapter 6.

A second possibility to perform statistical tasks with persistence diagrams consists in creating easier to handle statistics by mapping the diagrams to a vector space thanks to a feature map Ψ, also called a representation or a vectorization.

Definition 3.9.3 (Representation of persistence diagrams)**.** *A* representation *of a persistence diagram is a map $\Psi : \mathcal{D}^p \to B$, where B is a Banach space.*

Numerous representations have been introduced in the literature (see, e.g., [Ada+17; BM19; Bub15; Cha+15a; Che+15; KHF16; Rei+15]). Let us give several examples, see also Figure 3.11.

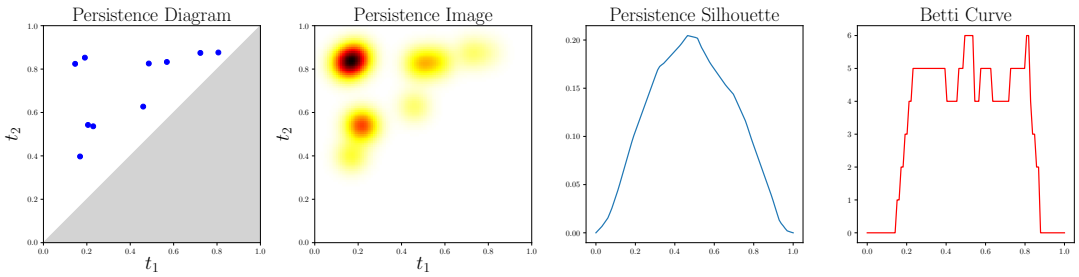


FIGURE 3.11: Some common representations of persistence diagrams. From left to right: A persistence diagram. Its persistence surface (also called persistence image) [Ada+17], which is a persistence measure. The corresponding persistence silhouette [Cha+15a]. The corresponding Betti Curve [Ume17].

- Let $K : \mathbb{R}^2 \to \mathbb{R}$ be a nonnegative Lipschitz continuous bounded function (e.g. $K(x,y) = \exp\left(-\frac{\|x-y\|^2}{2}\right)$) and define $f : x \in \Omega \mapsto d(x, \partial\Omega)^p \cdot K(x, \cdot)$, so that $f(x) : \mathbb{R}^2 \to \mathbb{R}$ is a real-valued function. The representation $\Psi : a \mapsto \sum_{x \in a} f(x)$ takes its values in $(C_b(\mathbb{R}^2), \|\cdot\|_\infty)$, the (Banach) space of continuous bounded functions. This representation is called the persistence surface and has been introduced with slight variations in different works [Ada+17; Che+15; KHF16; Rei+15].

- Let $u = (u_1, u_2) \in \Omega$. We let $f_u : t \in \mathbb{R} \mapsto \max(0, \min(u_1 + t, u_2 - t)$ be the tent function in u. The *persistence landscape* of a persistence diagram a is a sequence of functions $(\lambda_k)_{k \geq 1}$, where $\lambda_k(t)$ is the kth largest value among the $f_u(t)$ for $u \in a$ [Bub15]. A related representation is given by the persistence silhouette [Cha+15a]. Given a weight function $w : \Omega \to [0, +\infty)$, the *persistence silhouette* of a is obtained as the weighted average of the tent functions:

$$\text{Silhouette}_w(a) = \sum_{u \in a} w(u) f_u. \tag{3.37}$$

- The *Betti curve* associated to a persistence diagram a is the curve $\beta : t \in \mathbb{R} \mapsto a(\lrcorner_{t,t})$. If a is obtained as the persistence diagram of some filtration K for q-dimensional homology, then we indeed have $\beta(t)$ which is equal to the Betti number of the q-dimensional homology group of K_t.

- A kernel on the space of persistence diagrams is a map $k : \mathcal{D}^p \times \mathcal{D}^p \to \mathbb{R}$ such that, for every persistence diagrams $a_1, \ldots, a_n$ and real numbers $c_1, \ldots, c_n$, we have

$$\sum_{1 \leq i,j \leq n} k(a_i, a_j) c_i c_j \geq 0. \tag{3.38}$$

  Mercer's theorem asserts that for such a kernel there exists a Hilbert space $(H, \langle \cdot, \cdot \rangle)$, called a Reproducing Kernel Hilbert Space (or RKHS) such that $k(a,b) = \langle \Psi(a), \Psi(b) \rangle$ for some map $\Psi : \mathcal{D}^p \to H$. Kernel methods are typically used to perform non-linear classifications using SVMs. Kernels on the space of persistence diagrams can be seen as special instances of representations, although the map Ψ is never computed in practice (only the numbers $k(a_i, a_j)$ are computed). An example of a kernel on the space of persistence diagrams is given by the *sliced Wasserstein kernel* [CCO17].

Let us also mention that more recent approaches propose to use representations of persistence diagrams as a layer in a neural network architecture [Hof+17; Car+20; Kim+20]. The representations are then parametrized by some set $\Theta \subset \mathbb{R}^d$ (e.g. we consider a parametrized family of weight functions in the persistence silhouette) and the parameter $\theta \in \Theta$ is optimized to solve the learning task at stake.

In Chapter 8, we will propose a systemic study of representations on $\mathcal{D}^p$, by giving characterization of continuity for representations and by identifying a subclass of feature maps having particularly pleasant properties, that we will call *linear*.

Part I

Contributions to manifold inference

Chapter 4

Adaptive estimation in manifold inference

Given $\mathcal{X}_n = \{X_1, \dots, X_n\}$ a set of i.i.d. observations from some law μ on $\mathbb{R}^D$ supported on (or concentrated around) a d-dimensional manifold M, the goal of manifold inference is to design estimators $\hat{\theta}$ which approximate accurately some quantity $\theta(M)$ related to the geometry of M (e.g. its dimension d, its homology groups, its tangent spaces, or M itself). As explained in the introductory chapter (Chapter 2), the emphasis has mostly been put on designing estimators attaining minimax rates on a variety of models, which take into account different regularities of the manifold and noise models. We focus in this chapter on the problem of estimating a manifold in the models $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},f_{\max}}(\gamma)$ introduced in Chapter 3. The estimators introduced in the literature all rely on the knowledge of the quantities d, $\tau_{\min}$, $f_{\min}$ and $f_{\max}$, whereas those quantities are unknown in practice. One possibility to overcome this issue is to estimate in a preprocessing step those parameters. This may however become the main bottleneck in the estimating process, as regularity parameters are typically harder to estimate than the manifold itself. This is for instance the case of the reach $\tau(M)$ [Aam+19], while no procedures with theoretical guarantees exist to estimate $f_{\min}$ and $f_{\max}$.

Another approach, to which this chapter is dedicated, consists in designing *adaptive* estimators of $\theta(M)$. An estimator is called adaptive if it attains optimal rates of convergence on a large class of models (see Section 4.1 for a precise definition). Our main contribution consists in introducing a manifold estimator $\hat{M}$ which is minimax (with respect to the Hausdorff distance d_H) simultaneously on all the statistical models $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},f_{\max}}(\gamma)$. Our adaptive estimator, is built by selecting an estimator in a family of estimators defined in Section 4.2. The latter is based on the t-convex hull $\mathrm{Conv}(t, \mathcal{X}_n)$ of the set of observations $\mathcal{X}_n$. For a given set $A \subset \mathbb{R}^D$, the t-convex hull $\mathrm{Conv}(t, A)$ is defined by

$$\mathrm{Conv}(t, A) := \bigcup_{\sigma \subset A,\ r(\sigma) \leq t} \mathrm{Conv}(\sigma), \tag{4.1}$$

where $r(\sigma)$ is the *radius* of a set σ, i.e. the radius of the smallest enclosing ball of σ and $\mathrm{Conv}(\sigma)$ is its convex hull. The t-convex hull is an interpolation between the convex hull $\mathrm{Conv}(A)$ of A ($t = +\infty$) and the set A itself ($t = 0$): it gives a "local convex hull" of A at scale t. See Figure 4.1 for an example.

The loss $d_H(\mathrm{Conv}(t, \mathcal{X}_n), M)$ of the t-convex hull $\mathrm{Conv}(t, \mathcal{X}_n)$ can be efficiently controlled for t larger than some threshold $t^*(\mathcal{X}_n)$ (see Definition 4.2.2). As the threshold $t^*(\mathcal{X}_n)$ is very close to the approximation rate $\varepsilon(\mathcal{X}_n) := d_H(\mathcal{X}_n, M)$ of the point cloud, it is known to be of the order $(\log n/n)^{1/d}$ (see e.g. [RC07, Theorem 2]), and one obtains a minimax estimator on the C^2-models by taking the parameter t of

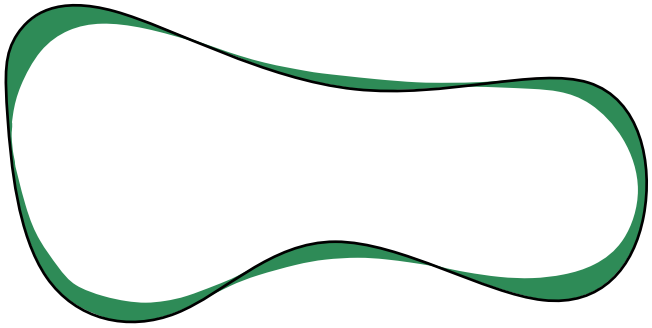


FIGURE 4.1: The t-convex hull $\mathrm{Conv}_t(A)$ (in green) of a curve A (in black).

this order (see Theorem 4.2.8). The exact value of t depends crucially on the parameter $f_{\min}$ which is unknown, so that it is unclear how the parameter t should be chosen in practice.

In Section 4.3, we build an adaptive estimator by selecting a parameter $t_\lambda(\mathcal{X}_n)$ (depending on some hyperparameter $\lambda \in (0,1)$), which is chosen solely based on the observations $\mathcal{X}_n$. More precisely, we consider the convexity defect function of a set A, originally introduced in [ALS13], and defined by

$$h(t, A) = d_H(\mathrm{Conv}(t, A), A) \in [0, t]. \tag{4.2}$$

As its name indicates, the convexity defect function measures how far a set is from being convex at a given scale. For instance, the convexity defect function of a convex set is null, whereas for a manifold M with positive reach $\tau(M)$, we have $h(t, M) \leq t^2/\tau(M)$ for $t > 0$, so that a manifold M is "locally almost convex" (see Proposition 4.3.2). We show that the convexity defect function of $\mathcal{X}_n$ exhibits a sharp change of behavior around the threshold $t^*(\mathcal{X}_n)$. Namely, for values t which are smaller than a fraction of $t^*(\mathcal{X}_n)$, the convexity defect function $h(t, \mathcal{X}_n)$ has a linear behavior, with a slope approximately equal to 1 (see Proposition 4.4.1), whereas for $t \geq t^*(\mathcal{X}_n)$, the convexity defect function exhibits the same quadratic behavior than the convexity defect of a manifold (see Proposition 4.3.3). In particular, its slope is much smaller than 1 as long as $t \geq t^*(\mathcal{X}_n)$ is significantly smaller than the reach $\tau(M)$. This change of behavior at the value $t^*(\mathcal{X}_n)$ suggests selecting the parameter

$$t_\lambda(\mathcal{X}_n) := \sup\{t < t_{\max},\ h(t, \mathcal{X}_n) > \lambda t\},$$

where $\lambda \in (0,1)$ and $t_{\max}$ is a parameter which has to be smaller than the reach $\tau(M)$ of the manifold (see Definition 4.3.4). We show (see Proposition 4.3.5) that with high probability, in the case where the sample $\mathcal{X}_n$ is exactly on the manifold M, we have

$$t^*(\mathcal{X}_n) \leq t_\lambda(\mathcal{X}_n) \leq \frac{2t^*(\mathcal{X}_n)}{\lambda}\left(1 + \frac{t^*(\mathcal{X}_n)}{\tau(M)}\right). \tag{4.3}$$

In particular, we are able to control the loss of $\mathrm{Conv}(t_\lambda(\mathcal{X}_n), \mathcal{X}_n)$ with high probability. By choosing $t_{\max}$ as a slowly decreasing function of n (for instance, $t_{\max} = (\log n)^{-1}$), we obtain an estimator

$$\hat{M} := \mathrm{Conv}(t_\lambda(\mathcal{X}_n), \mathcal{X}_n)$$

which is adaptive on the whole collection of C^2-models (see Corollary 4.3.6).

The estimator $\hat{M}$ is to our knowledge the first minimax adaptive manifold estimator. Our procedure allows us to actually estimate the approximation rate $\varepsilon(\mathcal{X}_n)$. The

parameter $t_\lambda(\mathcal{X}_n)$ can therefore be used as a hyperparameter in different settings. To illustrate this general idea, we show how to create an adaptive estimator of the homology groups (see Corollary 4.3.9) and of the tangent spaces (see Corollary 4.3.10) of a manifold.

Related work

"Localized" versions of convex hulls such as the t-convex hulls have already been introduced in the support estimation literature. For instance, slightly modified versions of the t-convex hull have been used as estimators in [AB16] under the assumption that the support has a smooth boundary and in [RC07] under reach constraints on the support, with different rates obtained in those models. Selection procedures were not designed in those two papers, and whether our selection procedure leads to an adaptive estimator in those frameworks is an interesting question.

The statistical models we study in this article were introduced in [Gen+12a] and [AL18], in which manifold estimators were also proposed. If the estimator in [Gen+12a] is of purely theoretical interest, the estimator proposed by Aamari and Levrard in [AL18], based on the Tangential Delaunay complex, is computable in polynomial time in the number of inputs and linear in the ambient dimension D. Furthermore, it is a simplicial complex which is known to be ambient isotopic to the underlying manifold M with high probability. It however requires the tuning of several hyperparameters in order to be minimax, which may make its use delicate in practice. In contrast, the t-convex hull estimator with parameter $t_\lambda(\mathcal{X}_n)$ is completely data-driven, while keeping the minimax property. In Section 4.5, we propose to select some parameter $\tilde{t}_\lambda(\mathcal{X}_n)$ which shares some properties with $t_\lambda(\mathcal{X}_n)$—although with less optimal constants—while being efficiently computable. However, unlike in the case of the Tangential Delaunay complex, we have no guarantees on the homotopy type of the corresponding estimator.

4.1 Preliminaries

Before going further, let us note that there are implicit constraints on the different parameters of the model $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},f_{\max}}$. Indeed, by Proposition 3.5.7.2, if $M \in \mathcal{M}^{2,d}$, we have $|\mathrm{vol}_M| \geq \omega_d \tau(M)^d$, with equality if and only if M is a d-dimensional sphere of radius $\tau(M)$. Hence, if μ has a density f on M lower bounded by $f_{\min}$, we have

$$1 = \int_M f(x)\mathrm{d}x \geq f_{\min}|\mathrm{vol}_M| \geq f_{\min}\omega_d \tau(M)^d,$$

with equality if and only if μ is the uniform distribution on a d-sphere of radius $\tau(M)$. We therefore have the following lemma.

Lemma 4.1.1. *Let d be an integer smaller than D and $\tau_{\min}$, $f_{\min}$ be positive constants. Let ω_d be the volume of the unit d-sphere. Then, $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},+\infty}$ is empty for $f_{\min}\omega_d\tau_{\min}^d > 1$ and contains only uniform distributions on d-sphere of radius $\tau_{\min}$ if $f_{\min}\omega_d\tau_{\min}^d = 1$.*

A model containing only spheres is degenerate from a minimax perspective, as laws in the model are then characterized by only $d+1$ observations. To discard such a model, we will assume in the following that there exists a constant $\kappa < 1$ such that $f_{\min}\omega_d\tau_{\min}^d \leq \kappa^d$. Note that this is not restrictive as any $\mu \in \mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},+\infty}$ also belongs to $\mathcal{Q}^{2,d}_{\tau'_{\min},f'_{\min},+\infty}$ for $\tau'_{\min} \leq \tau_{\min}$ and $f'_{\min} \leq f_{\min}$.

We let $\mathcal{Q}^{2,d}$ be the union of the $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},f_{\max}}(\gamma)$ for $\tau_{\min}$, $f_{\min}$, $f_{\max}$, $\gamma > 0$ with $f_{\min}\omega_d\tau^d_{\min} \leq \kappa^d$. For $\xi \in \mathcal{Q}^{2,d}$, let $M(\xi)$ be equal to the support of its first marginal ξ_1 (recall that the first marginal corresponds to the distribution supported on a manifold, whereas ξ_2 corresponds to the noise, see Chapter 3). Then M takes its values in the metric space $(\mathcal{K}(\mathbb{R}^D), d_H)$. We use the following parametrization of the set $\mathcal{Q}^{2,d}$: let Θ^d be the set of tuples $q = (\tau_{\min}, f_{\min}, f_{\max}, \eta)$, with $\tau_{\min}, f_{\min}, f_{\max}, \eta > 0$ and $f_{\min}\omega_d\tau^d_{\min} \leq \kappa^d$. We let $\mathcal{Q}^{2,d}_{q,n} = \mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},f_{\max}}(\gamma_n)$ for $\gamma_n = \eta(\log n/n)^{2/d}$.

Theorem 4.1.2. *Let $\kappa \in (0,1)$. For any $1 \leq d < D$ and $q = (\tau_{\min}, f_{\min}, f_{\max}, \eta) \in \Theta^d$ with $f_{\max} < \infty$, we have for n large enough,*

$$\left(\frac{C(1-\kappa)}{(\omega_d f_{\min})^{2/d}\tau_{\min}} + \frac{\eta}{2}\right) \leq \liminf_n \frac{\mathcal{R}_n(M, \mathcal{Q}^{2,d}_{q,n}, d_H)}{(\log n/n)^{2/d}} \leq \limsup_n \frac{\mathcal{R}_n(M, \mathcal{Q}_{q,n}, d_H)}{(\log n/n)^{2/d}} \leq C_{q,d} \tag{4.4}$$

where C is an absolute constant and $C_{q,d}$ is a constant which depends on q and d.

The upper bound in the previous theorem was already stated in Chapter 3, whereas the constant in the lower bound follows from a careful adaptation of the proof of Theorem 1 in [KZ15], detailed in Section 4.7.

Note that the statistical model $\mathcal{Q}^{2,d}_{q,n}$ is not identifiable because of the presence of noise. It however becomes identifiable "at the limit", as the size of the noise is assumed to converge to 0 at a certain rate. Changing the model by adding a small proportion of outliers would not change the minimax rates, as explained in [Gen+12a] or [AL18]. However, the t-convex hull estimators proposed in the next section are very sensible to this addition and some decluttering preprocessing would be needed to obtain better estimators on such models. Note also that the t-convex hull estimators will be minimax on the model $\mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},+\infty}(\gamma_n)$, that is without any upper bound needed on f, while the minimax rate is also equal to $(\log n/n)^{2/d}$ (the lower bound is clear, and the next section will show the upper bound).

The goal of the chapter is to design an estimator $\hat{M}$ which is minimax adaptive on the scale of models $\mathcal{Q}^{2,d}_{q,n}$, $1 \leq d < D$ and $q \in \Theta^d$, i.e. such that

$$\sup_{1\leq d<D} \sup_{q\in\Theta^d} \limsup_{n\to\infty} \frac{R_n(\hat{M}, \mathcal{Q}^{2,d}_{q,n}, d_H)}{\mathcal{R}_n(M; \mathcal{Q}^{2,d}_{q,n}, d_H)} < C, \tag{4.5}$$

for some constant C.

4.2 Minimax manifold estimation with t-convex hulls

Let $\mathcal{X}_n$ be a n-sample from law μ, where $\mu \in \mathcal{Q}^{2,d}_{q,n}$. In this section, we derive rates of convergence for $\mathrm{Conv}(t, \mathcal{X}_n)$. First, we note that $\mathrm{Conv}(t, \mathcal{X}_n)$ is indeed an estimator, that is the application

$$(x_1, \ldots, x_n) \in (\mathbb{R}^D)^n \mapsto \mathrm{Conv}(t, \{x_1, \ldots, x_n\})$$

is measurable. Indeed, using notation from Proposition 3.4.4, it can be written as

$$\bigcup_{I\subset\{1,\ldots,n\}} G_E(\mathrm{Conv}(\{x_i\}_{i\in I}), \{x_i\}_{i\in I})$$

where E is the closed set of $\mathcal{K}(\mathbb{R}^D)$ given by $\{K \in \mathcal{K}(\mathbb{R}^D) : r(K) \leq t\}$. As the function r is continuous and the functions $\cup$, Conv and G_E are measurable, the measurability

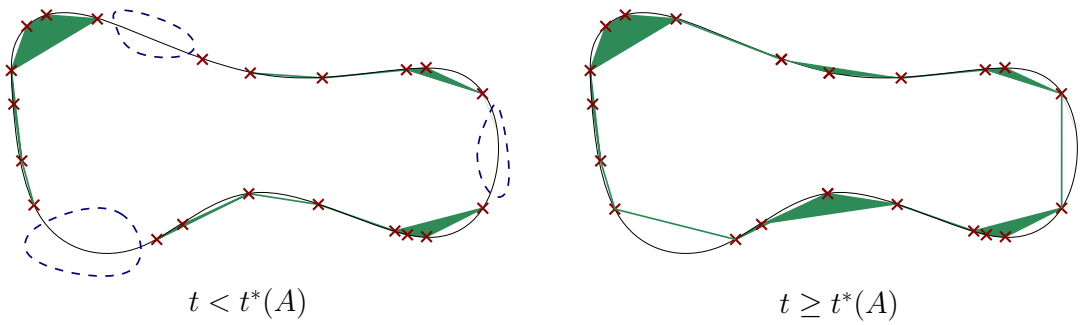


FIGURE 4.2: The t-convex hull of the finite set A (red crosses) is displayed (in green) for two values of t. The black curve represents the (one dimensional) manifold M. On the first display, the value of t is smaller than $t^*(A)$, as there are regions of the manifold (circled in blue) which are not attained by the projection π_M restricted to the t-convex hull. The value of t is larger than $t^*(A)$ on the second display.

follows. In order to obtain rates of convergence, we bound the Hausdorff distance $d_H(\mathrm{Conv}(t, A), M)$ for a general subset $A \subset M$. First, [ALS13, Lemma 12] gives a bound on the asymmetric Hausdorff distance between the convex hull of a subset of M and the manifold M.

Lemma 4.2.1. *Let $\sigma \subset M$ with $r(\sigma) < \tau(M)$ and let $y \in \mathrm{Conv}(\sigma)$. Then,*

$$d(y, M) \leq \frac{r(\sigma)^2}{\tau(M)}. \tag{4.6}$$

Proof. Lemma 12 in [ALS13] states that if $\sigma \subset M$ satisfies $r(\sigma) < \tau(M)$ and $y \in \mathrm{Conv}(\sigma)$, then,

$$d(y, M) \leq \tau(M) \left(1 - \sqrt{1 - \frac{r(\sigma)^2}{\tau(M)^2}}\right).$$

As $\sqrt{u} \geq u$ for $u \in [0, 1]$, one obtains the conclusion. □

This lemma directly implies that $d_H(\mathrm{Conv}(t, A)|M) \leq t^2/\tau(M)$ if $t < \tau(M)$, so that the set $\mathrm{Conv}(t, A)$ is included in the t-neighborhood of M. Therefore, the projection π_M is well-defined on the t-convex hull of A for such a t. We introduce a scale parameter $t^*(A)$, which has to be thought of as the "best" scale parameter t for approximating M with $\mathrm{Conv}(t, A)$.

Definition 4.2.2. *For $A \subset M$, let*

$$t^*(A) := \inf\{t < \tau(M) : \ \pi_M(\mathrm{Conv}(t, A)) = M\}. \tag{4.7}$$

See Figure 4.2 for an illustration. For $t^*(A) < t < \tau(M)$, and for any point $x \in M$, there exists $y \in \mathrm{Conv}(t, A)$ with $\pi_M(y) = x$. Therefore,

$$d(x, \mathrm{Conv}(t, A)) \leq |y - x| = d(y, M) \leq d_H(\mathrm{Conv}(t, A)|M).$$

By taking the supremum over $x \in M$, we obtain that for any $t^*(A) < t < \tau(M)$.

$$\begin{aligned} d_H(\mathrm{Conv}(t, A), M) &= \max\{d_H(\mathrm{Conv}(t, A)|M), d_H(M|\,\mathrm{Conv}(t, A)) \\ &= d_H(\mathrm{Conv}(t, A)|M) \leq \frac{t^2}{\tau(M)}. \end{aligned} \tag{4.8}$$

The minimax rate is now obtained thanks to two observations: (i) $t^*(A)$ is close to the approximation rate $\varepsilon(A) := d_H(A, M)$ and (ii) the approximation rate of a random sample can be very well controlled.

Proposition 4.2.3. *There exist absolute constants C_1 and C_2 such that the following holds. Let $A \subset M$ be a finite set. If $\varepsilon(A) \leq \tau(M)/8$, then*

$$\varepsilon(A)\left(1 - C_1\frac{\varepsilon(A)}{\tau(M)}\right) \leq t^*(A) \leq \varepsilon(A)\left(1 + C_2\frac{\varepsilon(A)}{\tau(M)}\right). \tag{4.9}$$

The proof of Proposition 4.2.3 relies on considering Delaunay triangulations. Given $d+1$ points σ in $\mathbb{R}^d$ that do not lie on a hyperplane, there exists a unique ball that contains the points on its boundary. It is called the circumball of σ, and its radius is called the circumradius $\mathrm{circ}(\sigma)$ of σ. Given a finite set $A \subset \mathbb{R}^d$ that does not lie on a hyperplane, there exists a triangulation of A, called the Delaunay triangulation, such that for each simplex σ in the triangulation, the circumball of σ contains no point of A in its interior. Note that there may exist several Delaunay triangulations of a set A, should the set A not be in general position. With a slight abuse, we will still refer to "the" Delaunay triangulation of A, by simply choosing a Delaunay triangulation among the possible ones should several exist. If the set A lies on lower dimensional subspace, we consider the Delaunay triangulation of A in the affine vector space spanned by A. Therefore, for every set A, the Delaunay triangulation is well defined (for instance, the Delaunay triangulation of three points aligned in the plane is the 1-dimensional triangulation obtained by joining the middle point with the two others).

Proof. Let $x \in M$ be such that $d(x, A) = \varepsilon(A)$. By definition, there exists a simplex $\sigma \subset A$ of radius smaller than $t^*(A)$ with $x = \pi_M(y)$ for some point $y \in \mathrm{Conv}(\sigma)$. We have, using Lemma 4.2.1,

$$\varepsilon(A) = d(x, A) \leq |x - y| + d(y, A) \leq \frac{t^*(A)^2}{\tau(M)} + d(y, A).$$

Furthermore, $d(y, A) \leq d(y, \sigma) \leq r(\sigma) \leq t^*(A)$ by [ALS13, Lemma 1]. Therefore,

$$\varepsilon(A) \leq t^*(A)\left(1 + \frac{t^*(A)}{\tau(M)}\right). \tag{4.10}$$

If we prove the upper bound in Proposition 4.2.3, then the previous equation is enough to imply the lower bound in Proposition 4.2.3. Let us show the upper bound. Without loss of generality, we assume that $0 \in M$ and we show that $0 \in \pi_M(\mathrm{Conv}(t, A))$ for $t = \varepsilon(A)(1 + 6\varepsilon(A)/\tau(M))$. This implies that $t^*(A) \leq \varepsilon(A)(1 + 6\varepsilon(A)/\tau(M))$. Let $\tilde{A} = \pi_0(A \cap \mathcal{B}(0, R))$ for $R = \varepsilon(A)(2 + c_0\varepsilon(A)/\tau(M))$ and $c_0 = 32/49$. Note that the condition $\varepsilon(A) \leq \tau(M)/8$ implies that $R < 7\tau(M)/24$. We first state two lemmas.

Lemma 4.2.4. *Assume that $\varepsilon(A) \leq 7\tau(M)/24$. Let $\tilde{x} \in T_0M$ with $|\tilde{x}| \leq \varepsilon(A)$. Then $d(\tilde{x}, \tilde{A}) \leq \varepsilon(A)$.*

Proof. By continuity, it suffices to prove the claim for $|\tilde{x}| < \varepsilon(A)$. In this case, according to Proposition 3.5.8, if $\varepsilon(A) \leq 7\tau(M)/24$, then there exists $x \in \mathcal{B}_M(0, 8\varepsilon(A)/7)$ with $\pi_0(x) = \tilde{x}$. Furthermore, by Proposition 3.5.7.4,

$$|x| \leq |\tilde{x}| + |x - \tilde{x}| \leq \varepsilon(A) + \frac{|x|^2}{2\tau(M)} \leq \varepsilon(A)\left(1 + \frac{32\varepsilon(A)}{49\tau(M)}\right).$$

We have $d(x, A) = |x - a|$ for some point $a \in A$, and $|a| \leq |x - a| + |x| \leq \varepsilon(A)(2 + c_0\varepsilon(A)/\tau(M))$. As $\pi_0(a) \in \tilde{A}$, we have $d(\tilde{x}, \tilde{A}) \leq |\tilde{x} - \pi_0(a)| \leq |x - a| = d(x, A) \leq \varepsilon(A)$. □

Lemma 4.2.5. *Let $V \subset \mathbb{R}^d$ be a finite set and $t > 0$. If $d_H(\mathcal{B}(0,t)|V) \leq t$, then $0 \in \mathrm{Conv}(V)$.*

Proof. We prove the contrapositive. If $0 \notin \mathrm{Conv}(V)$, then there exists an open half space which contains V. Let x be the unit vector orthogonal to this halfspace. Then, $d(tx, V) > t$. □

Apply Lemma 4.2.5 to $V = \tilde{A}$ and $t = \varepsilon(A)$. For $\tilde{x} \in \mathcal{B}_{T_0M}(0, \varepsilon(A))$, we have $d(\tilde{x}, \tilde{A}) \leq \varepsilon(A)$ according to Lemma 4.2.4. Therefore, we have $0 \in \mathrm{Conv}(\tilde{A})$. Consider the Delaunay triangulation of $\tilde{A}$. The point 0 belongs to the convex hull of some simplex $\tilde{\sigma}$ of the triangulation, with circumradius $\mathrm{circ}(\tilde{\sigma})$ and center of the circumball $\tilde{q}$. The simplex $\tilde{\sigma}$ corresponds to some simplex σ in A, and the point 0 is equal to $\pi_0(y)$ for some point $y \in \mathrm{Conv}(\sigma)$. By Proposition 3.5.7.1, we actually have $\pi_M(y) = 0$, and to conclude, it suffices to show that $r(\sigma) \leq \varepsilon(A)\left(1 + 6\frac{\varepsilon(A)}{\tau(M)}\right)$. To do so, we use the next lemma (recall that $\sigma \subset \mathcal{B}_M(0, R)$ with $R < 7\tau(M)/24$).

Lemma 4.2.6. *Let $\sigma \subset \mathcal{B}_M(0, 7\tau(M)/24)$ and $\tilde{\sigma} = \tilde{\pi}_0(\sigma)$. Assume that $0 \in \mathrm{Conv}(\tilde{\sigma})$. Then,*

$$r(\tilde{\sigma}) \leq r(\sigma) \leq r(\tilde{\sigma})\left(1 + 6\frac{r(\tilde{\sigma})}{\tau(M)}\right). \tag{4.11}$$

Proof. As the projection is 1-Lipschitz, it is clear that $r(\tilde{\sigma}) \leq r(\sigma)$. Let us prove the other inequality. Let $\sigma = \{y_0, \ldots, y_k\}$, $\tilde{\sigma} = \{\tilde{y}_0, \ldots, \tilde{y}_k\}$ and fix $0 \leq i \leq k$. As $y_i \in \mathcal{B}_M(0, 7\tau(M)/24)$, we have by Proposition 3.5.8

$$|y_i| \leq \frac{8}{7}|\tilde{y}_i| \leq \frac{16}{7}r(\tilde{\sigma}), \tag{4.12}$$

where we used that $|\tilde{y}_i| \leq 2r(\tilde{\sigma})$ as $0 \in \mathrm{Conv}(\tilde{\sigma})$. Let $\tilde{z}$ be the center of the minimum enclosing ball of $\tilde{\sigma}$. Write $\tilde{z} = \sum_{j=0}^k \lambda_j \tilde{y}_j$ and let $z = \sum_{j=0}^k \lambda_j y_j \in \mathrm{Conv}(\sigma)$. Then, we have

$$\begin{aligned}
|z - y_i| &\leq |z - \tilde{z}| + |\tilde{z} - \tilde{y}_i| + |\tilde{y}_i - y_i| \\
&\leq \sum_{j=0}^k \lambda_j |y_j - \tilde{y}_j| + r(\tilde{\sigma}) + \frac{|y_i|^2}{2\tau(M)} \text{ using Proposition 3.5.7.4} \\
&\leq \sum_{j=0}^k \lambda_j \frac{|y_j|^2}{2\tau(M)} + r(\tilde{\sigma}) + \frac{128}{49}\frac{r(\tilde{\sigma})^2}{\tau(M)} \text{ using Proposition 3.5.7.4 and (4.12)} \\
&\leq r(\tilde{\sigma}) + \frac{256}{49}\frac{r(\tilde{\sigma})^2}{\tau(M)} \leq r(\tilde{\sigma}) + 6\frac{r(\tilde{\sigma})^2}{\tau(M)} \text{ using (4.12)}.
\end{aligned}$$

We obtain the conclusion as σ is included in the ball of radius $\max_i |z - y_i|$ and center z. □

Using the previous lemma, we are left with showing that $r(\tilde{\sigma}) \leq \varepsilon(A)$. We will actually show the stronger inequality $\mathrm{circ}(\tilde{\sigma}) \leq \varepsilon(A)$ (the radius of a set is always smaller than its circumradius). As 0 is in the circumball (that is centered at $\tilde{q}$), the ball centered at $\tilde{q}$ of radius $|\tilde{q}|$ does not intersect $\tilde{A}$. This enforces $|\tilde{q}| \leq \varepsilon(A)$: otherwise, there would exist a ball of radius $\varepsilon(A)$ and at distance less than $\varepsilon(A)$ from 0 not intersecting $\tilde{A}$, a contradiction with Lemma 4.2.4 (see Figure 4.3). As $|\tilde{q}| \leq \varepsilon(A)$, we obtain, once again according to Lemma 4.2.4, that $\mathrm{circ}(\tilde{\sigma}) = d(\tilde{q}, \tilde{A}) \leq \varepsilon(A)$ concluding the proof. □

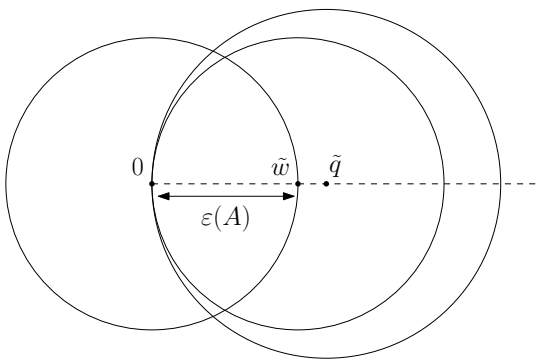


FIGURE 4.3: If $|\tilde{q}| > \varepsilon(A)$, then the ball $\mathcal{B}_{T_0M}(\tilde{q}, |\tilde{q}|)$ contains a ball of radius $\varepsilon(A)$ centered at a point at distance less than $\varepsilon(A)$ from 0 (here denoted by $\tilde{w}$).

Proposition 4.2.7. *Let $\mu \in \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, +\infty}$ and let $\mathcal{X}_n = \{X_1, \dots, X_n\}$ be a n-sample of law μ. If $r \leq \tau_{\min}/2$, then*

$$\mathbb{P}(\varepsilon(\mathcal{X}_n) > r) \leq \frac{32^d}{\omega_d f_{\min} r^d} \exp(-n 8^{-d} \omega_d f_{\min} r^d). \tag{4.13}$$

In particular, for n large enough

$$\mathbb{E}[\varepsilon(\mathcal{X}_n)^2] \leq 16 \left(\frac{\log n}{\omega_d f_{\min} n} \right)^{2/d}. \tag{4.14}$$

Proof. The inequality (4.13) follows from Proposition 3.5.7.2, which implies that the measure μ is (a, d)-standard with $a = 8^{-d}\omega_d f_{\min}$: Proposition III.14 in [Aam17] then yields the result. To prove the second inequality, we let $r = 8(3 \log n/(n\omega_d f_{\min}))^{1/d}$. Then, $\varepsilon(\mathcal{X}_n) \leq r$ with probability of order $(\log n)n^{-2}$. If this event is not satisfied, we bound $\varepsilon(\mathcal{X}_n)$ by $\operatorname{diam}(M)$, that is bounded by a constant depending on $d, f_{\min}, \tau_{\min}$ (see Proposition 3.5.7.3 and the fact that $|\mathrm{vol}_M| \leq f_{\min}^{-1}$). Therefore, for n large enough, $\mathbb{E}[\varepsilon(\mathcal{X}_n)^2] \leq 16 \left(\frac{\log n}{\omega_d f_{\min} n} \right)^{2/d}$. □

By gathering those different observations (Proposition 4.2.3 and Proposition 4.2.7) and by using stability properties of t-convex hulls with respect to noise, we show that t-convex hulls are minimax estimators on C^2-models.

Theorem 4.2.8. *Let $0 < d < D$, $n > 0$ and $q = (\tau_{\min}, f_{\min}, +\infty, \eta) \in \Theta^d$. If $t_n = C_0 \left(\log n/(\omega_d f_{\min} n)\right)^{1/d}$ (for some absolute constant C_0), then we have for n large enough, and some absolute constant C_1,*

$$R_n(\mathrm{Conv}(t_n, \mathcal{X}_n), \mathcal{Q}^{2,d}_{q,n}, d_H) \leq \left(\frac{\log n}{n} \right)^{2/d} \left(\eta + \frac{C_1}{\tau_{\min}(\omega_d f_{\min})^{2/d}} \right) \tag{4.15}$$

i.e. $\mathrm{Conv}(t_n, \mathcal{X}_n)$ *is a minimax estimator of M on $\mathcal{Q}^{2,d}_{q,n}$.*

Proof. We first state a lemma which shows that the t-convex hull is stable under small perturbations with respect to the Hausdorff distance.

Lemma 4.2.9. *Let $t, \gamma > 0$ and $A, B \subset \mathbb{R}^D$ with $d_H(A, B) \leq \gamma$. Then,*

$$d_H(\mathrm{Conv}(t, B) | \mathrm{Conv}(t + \gamma, A)) \leq \gamma. \tag{4.16}$$

Proof. Let $\sigma \subset B$ be a simplex with $r(\sigma) \leq t$. For each $y \in \sigma$, let $x \in A$ with $d(x,y) \leq \gamma$. By doing so, we create a non-empty simplex $\xi \subset A$ with $d_H(\sigma|\xi) \leq \gamma$. One has $r(\xi) \leq t+\gamma$ (see [ALS13, Lemma 16]) and $d_H(\mathrm{Conv}(\sigma)|\,\mathrm{Conv}(\xi)) \leq d_H(\sigma|\xi) \leq \gamma$. This implies the conclusion. □

Let $A \subset M$ and $B \subset \mathbb{R}^D$ with $d_H(A,B) \leq \gamma$. Then, if $t^*(A) < t+\gamma < \tau(M)$, using (3.10), Lemma 4.2.9 and (4.8),

$$\begin{aligned} d_H(\mathrm{Conv}(t,B)|M) &\leq d_H(\mathrm{Conv}(t,B)|\,\mathrm{Conv}(t+\gamma,A)) + d_H(\mathrm{Conv}(t+\gamma,A),M) \\ &\leq \gamma + \frac{(t+\gamma)^2}{\tau(M)}. \end{aligned} \tag{4.17}$$

Let $q \in \Theta^d$, let $\xi \in \mathcal{Q}^{2,d}_{q,n}$ with underlying manifold M and let $\mathcal{X}_n = \{X_1,\dots,X_n\}$ be a n-sample of law $\iota_\# \xi$, with $\mathcal{Y}_n = \{Y_1,\dots,Y_n\}$ the corresponding sample of law μ, the first marginal of ξ (that is $X_i = Y_i + Z_i$ with $Y_i \sim \mu$ and $|Z_i| \leq \gamma$). Then, for $0 \leq t < \tau(M) - \gamma$,

$$\begin{aligned} \mathbb{E}d_H(\mathrm{Conv}(t,\mathcal{X}_n),M) &= \mathbb{E}d_H(\mathrm{Conv}(t,\mathcal{X}_n),M)\mathbf{1}\{t+\gamma > t^*(\mathcal{Y}_n)\} \\ &\quad + \mathbb{E}d_H(\mathrm{Conv}(t,\mathcal{X}_n),M)\mathbf{1}\{t+\gamma \leq t^*(\mathcal{Y}_n)\} \\ &\leq \gamma + \frac{(t+\gamma)^2}{\tau(M)} + (\mathrm{diam}(M)+\gamma)\mathbb{P}(t^*(\mathcal{Y}_n) \geq t). \end{aligned}$$

By Proposition 4.2.3, if $\varepsilon(\mathcal{Y}_n) \leq C_0\tau(M)$, then $t^*(\mathcal{Y}_n) \geq t$ implies that

$$\varepsilon(\mathcal{Y}_n) \geq t\left(1 + C_1\frac{\varepsilon(\mathcal{Y}_n)}{\tau(M)}\right)^{-1} \geq C_2 t$$

for some absolute constant C_2. Therefore, $t^*(\mathcal{Y}_n) \geq t$ implies

$$\varepsilon(\mathcal{Y}_n) \geq \min\left(C_0\tau(M), C_2 t\right) = C_2 t \tag{4.18}$$

if $t \leq C_0\tau(M)/C_2$. By using Proposition 4.2.7, and by noting that $\mathrm{diam}(M)$ is bounded by a constant depending on $d, f_{\min}, \tau_{\min}$ (see Proposition 3.5.7.3), we obtain that, if $t \leq C_0\tau(M)/C_2$,

$$\mathbb{E}d_H(\mathrm{Conv}(t,\mathcal{X}_n),M) \leq \gamma + \frac{(t+\gamma)^2}{\tau(M)} + c_{d,\tau_{\min},f_{\min}}\frac{\exp(-8^{-d}\omega_d f_{\min} n (C_2 t)^d)}{(C_2 t)^d}. \tag{4.19}$$

In particular, we obtain the desired control for n large enough by letting $t = C_3\left(\log n/(\omega_d f_{\min} n)\right)^{1/d}$ for some constant C_3 large enough, if $\gamma \leq \eta\left(\log n/n\right)^{2/d}$. □

4.3 Selection procedure for the t-convex hulls

Assuming that we have observed a n-sample $\mathcal{X}_n$, we were able in the previous section to build a minimax estimator of the underlying manifold M. The tuning of this estimator requires the knowledge of $f_{\min}$, whereas this quantity will likely not be accessible in practice. A powerful idea to overcome this issue is to design a selection procedure for the family of estimators $(\mathrm{Conv}(t,\mathcal{X}_n))_{t\geq 0}$. Assume first for the sake of simplicity that *the noise level η is null*. As the loss of the estimator $\mathrm{Conv}(t,\mathcal{X}_n)$ is controlled efficiently for $t \geq t^*(\mathcal{X}_n)$ (see (4.8)), a good idea is to select the parameter t larger than $t^*(\mathcal{X}_n)$. We however do not have access to this quantity based on the observations $\mathcal{X}_n$, as the manifold M is unknown. To select a scale close to $t^*(\mathcal{X}_n)$, we monitor how the estimators $\mathrm{Conv}(t,\mathcal{X}_n)$ deviate from $\mathcal{X}_n$ as t increases. Namely, we use the convexity defect function introduced in [ALS13].

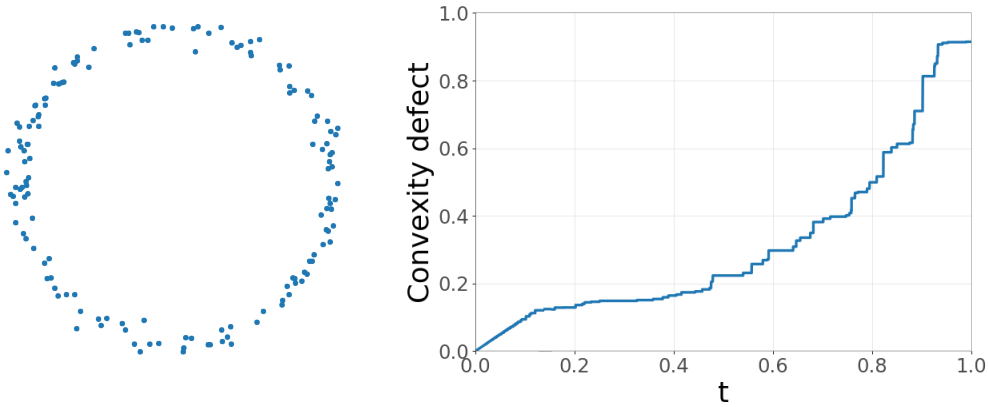


FIGURE 4.4: Left. n-sample $\mathcal{X}_n$ close to a circle. Right. Convexity defect function of $\mathcal{X}_n$.

Definition 4.3.1. *Let $A \subset \mathbb{R}^D$ and $t > 0$. The d-dimensional convexity defect function at scale t of A is defined as*

$$h(t, A) := d_H(\mathrm{Conv}(t, A), A). \tag{4.20}$$

As its name indicates, the convexity defect function measures the (lack of) convexity of a set A at a given scale t. The next proposition states preliminary results on the convexity defect function.

Proposition 4.3.2. *Let $A \subset \mathbb{R}^D$ be a closed set and $t \geq 0$.*

1. *We have $0 \leq h(t, A) \leq t$.*
2. *If A is convex then $h(\cdot, A) \equiv 0$.*
3. *If M is a manifold of reach $\tau(M)$ and $t < \tau(M)$, then*

$$h(t, M) \leq t^2/\tau(M). \tag{4.21}$$

Proof. Point 1 is stated in [ALS13, Section 3.1], Point 2 is clear and Point 3 is a consequence of Lemma 4.2.1. □

As expected, the convexity defect of a convex set is null, whereas for small values of t, the convexity defect of a manifold $h(t, M)$ is very small (compared to the maximum value possible, which is t): when looked at locally, M is "almost flat" (and thus almost convex). We first show that the convexity defect function $h(\cdot, \mathcal{X}_n)$ also has a subquadratic behavior for $t \geq t^*(\mathcal{X}_n)$.

Proposition 4.3.3 (Long-scale behavior)**.** *Let $A \subset M$. For $t^*(A) < t < \tau(M)$,*

$$h(t, A) \leq \frac{t^2}{\tau(M)} + t^*(A)\left(1 + \frac{t^*(A)}{\tau(M)}\right). \tag{4.22}$$

Proof. By using that $h(t, A) \leq t$ and (4.8), for any $t^*(A) < s < t$,

$$\begin{aligned} h(t, A) &= d_H(\mathrm{Conv}(t, A), A) \\ &\leq d_H(\mathrm{Conv}(t, A), M) + d_H(M, \mathrm{Conv}(s, A)) + d_H(\mathrm{Conv}(s, A), A) \\ &\leq \frac{t^2}{\tau(M)} + \frac{s^2}{\tau(M)} + s. \end{aligned}$$

The conclusion is obtained by letting s go to $t^*(A)$. □

Proposition 4.3.3 indicates that, for $t^*(\mathcal{X}_n) \ll t \ll \tau(M)$, the ratio $h(t, \mathcal{X}_n)/t$ is very small, while it might be of order 1 at the value $t^*(\mathcal{X}_n)$. This suggests the following strategy to obtain a scale t which is larger than $t^*(\mathcal{X}_n)$: choose the largest scale t such that $h(t, \mathcal{X}_n)$ is of order t.

Definition 4.3.4. *Let $A \subset M$, $\lambda > 0$ and $t_{\max} > 0$. We define*

$$t_\lambda(A) := \sup\{t < t_{\max} : \ h(t, A) \geq \lambda t\}. \tag{4.23}$$

The following theorem ensures that the scale $t_\lambda(A)$ is as expected, close to $t^*(A)$, as long as the approximation rate of A is small enough.

Theorem 4.3.5. *Let $0 < \lambda < 1$, $\gamma \geq 0$ and $M \in \mathcal{M}^{2,d}$. Let $A \subset M$ be a finite set with $\varepsilon(A) \leq C_1\tau(M)$ and $B \subset \mathbb{R}^D$ with $d_H(A, B) \leq \gamma$. Assume that*

1. $t^*(A) + \gamma < t_{\max} < \tau(M)\lambda/2 - \gamma$,
2. $t^*(A) < C_2(1-\lambda)\tau(M)$ *and* $t^*(A) \leq C_3\lambda^2\tau(M)$,
3. $\gamma \leq C_4(1-\lambda)t^*(A)$.

Then,

$$t^*(A) + \gamma \leq t_\lambda(B) \leq \frac{2t^*(A)}{\lambda}\left(1 + \frac{t^*(A)}{\tau(M)}\right) + \frac{6\gamma}{\lambda}. \tag{4.24}$$

Proof. **Upper bound on $t_\lambda(B)$:**

By [ALS13, Lemma 5] for any $t \geq 0$, we have $h(B, t) \leq h(A, t+\gamma) + 2\gamma$. Therefore, according to Proposition 4.3.3, we have for $t^*(A) \leq t + \gamma < \tau(M)$,

$$h(t, B) \leq \frac{(t+\gamma)^2}{\tau(M)} + t^*(A)\left(1 + \frac{t^*(A)}{\tau(M)}\right) + 2\gamma.$$

Therefore, $h(t, B) < \lambda t$ if $\frac{(t+\gamma)^2}{\tau(M)} + t^*(A)\left(1 + \frac{t^*(A)}{\tau(M)}\right) + 2\gamma < \lambda t$. A straightforward computation shows that this is the case if $\gamma \leq t^*(A) \leq C_0\lambda^2\tau(M)$ for some absolute constant C_0 and $t_0 < t + \gamma < t_1$ with (using $\sqrt{1-u} \geq 1 - u$ for $u \in [0, 1]$),

$$\begin{aligned} t_0 &:= \frac{\tau(M)\lambda}{2}\left(1 - \sqrt{1 - \frac{4}{\lambda^2\tau(M)}\left(t^*(A)\left(1 + \frac{t^*(A)}{\tau(M)}\right) + (2+\lambda)\gamma\right)}\right) \\ &\leq \frac{2t^*(A)}{\lambda}\left(1 + \frac{t^*(A)}{\tau(M)}\right) + \frac{6\gamma}{\lambda} \end{aligned}$$

and $t_1 \geq \tau(M)\lambda/2$. Therefore, $t_\lambda(B) \leq \frac{2t^*(A)}{\lambda}\left(1 + \frac{t^*(A)}{\tau(M)}\right) + \frac{6\gamma}{\lambda}$, as long as $t_{\max} < \tau(M)\lambda/2 - \gamma$.

Lower bound on $t_\lambda(A)$ in the noise-free case:

Assume that $\varepsilon(A)$ is sufficiently small so that Proposition 4.2.3 holds. Let $q \in M$ with $\varepsilon(A) = d(q, A)$. One has $q = \pi_M(x)$ for some $x \in \mathrm{Conv}(t^*(A), A)$, so that, by Proposition 4.2.3 and Lemma 4.2.1,

$$\begin{aligned} d(x, A) \geq d(q, A) - |x - q| &\geq \frac{t^*(A)}{\left(1 + C_0\frac{\varepsilon(A)}{\tau(M)}\right)} - \frac{t^*(A)^2}{\tau(M)} \\ &\geq t^*(A)\left(1 - C_0\frac{\varepsilon(A)}{\tau(M)} - \frac{t^*(A)}{\tau(M)}\right) \\ &\geq t^*(A)\left(1 - C_0\frac{2t^*(A)}{\tau(M)} - \frac{t^*(A)}{\tau(M)}\right) \geq t^*(A)\left(1 - C_1\frac{t^*(A)}{\tau(M)}\right), \end{aligned}$$

where we used at the last line that $\varepsilon(A) \leq 2t^*(A)$ is $\varepsilon(A)/\tau(M)$ is sufficiently small by Proposition 4.2.3. As $x \in \mathrm{Conv}(t^*(A), A)$, we have,

$$h(t^*(A), A) \geq t^*(A)\left(1 - C_1\frac{t^*(A)}{\tau(M)}\right). \tag{4.25}$$

Therefore, if $\lambda \leq 1 - C_1 t^*(A)/\tau(M)$ and $t^*(A) < t_{\max}$, then $t_\lambda(A) \geq t^*(A)$.

Lower bound on $t_\lambda(A)$ in the tubular noise case:
By [ALS13, Lemma 5] for any $t \geq \gamma$,

$$h(B, t) \geq h(A, t - \gamma) - 2\gamma. \tag{4.26}$$

Plugging $t = t^*(A) + \gamma$, and using (4.25),

$$h(B, t^*(A) + \gamma) \geq t^*(A)\left(1 - C_1\frac{t^*(A)}{\tau(M)}\right) - 2\gamma. \tag{4.27}$$

This quantity is larger than $\lambda(t^*(A) + \gamma)$ as long as

$$C_1\frac{t^*(A)}{\tau(M)} \leq 1 - \lambda - (2 + \lambda)\frac{\gamma}{t^*(A)}. \tag{4.28}$$

If $\gamma \leq (1 - \lambda)\frac{t^*(A)}{6}$ and $C_1\frac{t^*(A)}{\tau(M)} \leq \frac{1-\lambda}{2}$, then (4.28) is satisfied, giving the desired lower bound on $t_\lambda(B)$ under those two conditions, should $t^*(A) + \gamma$ be smaller than $t_{\max}$. □

As a corollary of this result, we obtain the adaptivity of the t-convex hull estimators of parameter $t_\lambda(\mathcal{X}_n)$.

Corollary 4.3.6. *Let $0 < \lambda < 1$ and $t_{\max} > 0$. Let $0 < d < D$ and $q = (\tau_{\min}, f_{\min}, +\infty, \eta) \in \Theta^d$. Then, if $\tau_{\min} > 2t_{\max}/\lambda$, we have for n large enough*

$$R_n(\mathrm{Conv}(t_\lambda(\mathcal{X}_n), \mathcal{X}_n), \mathcal{Q}^{2,d}_{q,n}, d_H) \leq \left(\frac{\log n}{n}\right)^{2/d}\left(\eta + \frac{130}{\tau_{\min}(\omega_d f_{\min})^{2/d}}\right) \tag{4.29}$$

By letting $t_{\max,n}$ be any sequence converging to 0 and larger that $(c_d \log n/(n f_{\min}))^{1/d}$ (for instance $t_{\max,n} = 1/\log(n)$ or $t_{\max,n} = ((\log n)^2/n)^{1/d}$), we obtain an adaptive estimator on the scale of models $\mathcal{Q}^{2,d}_{q,n}$ for $q \in \Theta^d$, $1 \leq d < D$, i.e. such that

$$\sup_{1\leq d<D}\sup_{q\in\Theta^d}\limsup_n \frac{R_n(\mathrm{Conv}(t_\lambda(\mathcal{X}_n), \mathcal{X}_n), \mathcal{Q}^{2,d}_{q,n}, d_H)}{\mathcal{R}_n(M, \mathcal{Q}^{2,d}_{q,n}, d_H)} \leq C. \tag{4.30}$$

Remark 4.3.7. Note that the previous result is of an asymptotic nature. In particular, should n not be large enough (i.e. if $t^*(\mathcal{X}_n)$ is larger than some fraction of the reach), then the selection procedure is doomed to fail, as the long-scale behavior corresponding to the range $[t^*(\mathcal{X}_n), \tau(M)]$ is too small to be captured by the selection procedure (or even is non-existent). A non-asymptotic choice of the parameter $t_{\max}$ requires to find a lower bound on the reach $\tau(M)$. If estimators of the reach exist [Aam+19; Ber+21] they both require the tuning of some scale parameter h (with respect to $f_{\min}$ for instance), so that it is not clear how we may find such a lower bound in an adaptive manner.

To prove Corollary 4.3.6, we first state an elementary lemma.

Lemma 4.3.8. *Let $A \subset M$ be a finite set of cardinality n. Then,*

$$\varepsilon(A) \geq c_d \tau(M) n^{-1/d}. \tag{4.31}$$

Proof. As $M \subset \bigcup_{x \in A} \mathcal{B}(x, \varepsilon(A))$, one has $|\mathrm{vol}_M| \leq n c_d \varepsilon(A)^d$. As $|\mathrm{vol}_M| \geq \omega_d \tau(M)^d$, we have the conclusion. □

Proof of Corollary 4.3.6. By equation (4.17), if $t_\lambda(\mathcal{X}_n) \geq t^*(\mathcal{Y}_n) - \gamma$, then

$$d_H(\mathrm{Conv}_{t_\lambda(\mathcal{X}_n)}(\mathcal{X}_n), M) \leq \gamma + \frac{(t_\lambda(\mathcal{X}_n) + \gamma)^2}{\tau(M)}. \tag{4.32}$$

This relation holds (we even have $t_\lambda(\mathcal{X}_n) \geq t^*(\mathcal{Y}_n) + \gamma$) as long as Conditions 1, 2 and 3 of Theorem 4.3.5 are satisfied. If $\gamma < \eta (\log n/n)^{2/d}$ and $\tau_{\min} > 2t_{\max}/\lambda$, Conditions 1 and 2 are satisfied as long as $t^*(\mathcal{Y}_n)$ is small enough with respect to λ, $t_{\max}$ and $\tau(M)$ and n is large enough. Also, by Lemma 4.3.8 and Proposition 4.2.3, Condition 3 is satisfied as long as n is large enough. Therefore, Conditions 1, 2 and 3 are satisfied with probability $1 - c_{d,\tau_{\min},f_{\min},\lambda,t_{\max}} \exp(-C_{d,\tau_{\min},f_{\min},\lambda,t_{\max}} n)$, according to Propositions 4.2.3 and 4.2.7. Therefore, (4.32) holds with high probability, and one obtains the conclusion by using the upper bound in Theorem 4.3.5, Proposition 4.2.3 and the fact that $\mathbb{E}[\varepsilon(\mathcal{Y}_n)^2]$ is of order $(\log n/n)^{2/d}$.

To obtain the adaptive behavior (4.30), it suffices to remark that inequality (4.32) holds as long as $\tau_{\min} > 2t_{\max}/\lambda$ and if $t^*(\mathcal{Y}_n)$ is small enough with respect to $t_{\max}$. Using that $t^*(\mathcal{Y}_n)$ is approximately equal to $\varepsilon(\mathcal{Y}_n)$ and using Proposition 4.2.7 yields the conclusion. □

Another possible criterion to ensure the quality of an estimator $\hat{M}$ of a manifold M is to ensure that $\hat{M}$ and M are homotopy equivalent. Although we have no guarantees on the topology of the estimator $\mathrm{Conv}(t_\lambda(\mathcal{X}_n), \mathcal{X}_n)$, our selection procedure also permits to build a simplicial complex homotopy equivalent to M. We write $M \simeq N$ to indicate that the two topological spaces M and N are homotopy equivalent. For $A \subset \mathbb{R}^D$, recall the definition of the Čech simplicial complex of parameter t on A:

$$\mathrm{Cech}(t, A) := \{\sigma \subset A : \ r(\sigma) \leq t\}. \tag{4.33}$$

We will consider that $\mathrm{Cech}(t, A)$ is a topological space by identifying it with its geometric realization.

Corollary 4.3.9. *Let $0 < \lambda < 1$ and $t_{\max} > 0$. Let d be an integer smaller than D and $f_{\min}, \eta > 0$, $\tau_{\min} > 2t_{\max}/\lambda$. Then, for n large enough, and $\gamma_n \leq \eta (\log n/n)^{2/d}$, we have*

$$\sup_{\mu \in \mathcal{Q}^{2,d}_{\tau_{\min},f_{\min},+\infty}(\gamma_n)} \mathbb{P}(M \not\simeq \mathrm{Cech}(5t_\lambda(\mathcal{X}_n), \mathcal{X}_n)) \leq C_0 \exp(-C_1 n), \tag{4.34}$$

where C_0 and C_1 depend on $d, \tau_{\min}, f_{\min}, \eta, \lambda, t_{\max}$.

This rate matches the exponential minimax rate obtained in [Bal+12] for estimating homology groups, i.e. the parameter $t_\lambda(\mathcal{X}_n)$ also allows creating adaptive minimax homology estimators (although in a slightly weaker sense that in Section 4.1).

Proof of Corollary 4.3.9. For the sake of simplicity, we only give a proof for $\eta = 0$ (no noise), the extension to the noise case being made with similar ideas than in the previous proof. According to [CCSL09, Theorem 4.6], if $\varepsilon(\mathcal{X}_n) < \tau(M)/17$ and $4\varepsilon(\mathcal{X}_n) \leq t < \tau(M) - 3\varepsilon(\mathcal{X}_n)$, then $\mathrm{Cech}(t, \mathcal{X}_n) \simeq M$. Also, according to Theorem

4.3.5 and Proposition 4.2.3, if $\varepsilon(\mathcal{X}_n)$ is small enough with respect to λ, $t_{\max}$ and $\tau(M)$, then

$$5t_\lambda(\mathcal{X}_n) \geq 5t^*(\mathcal{X}_n) \geq 5\varepsilon(\mathcal{X}_n)\left(1 - C_0\frac{\varepsilon(\mathcal{X}_n)}{\tau(M)}\right) \geq 4\varepsilon(\mathcal{X}_n) \text{ and} \tag{4.35}$$

$$\begin{aligned} 5t_\lambda(\mathcal{X}_n) &\leq 10\frac{t^*(\mathcal{X}_n)}{\lambda}\left(1 + \frac{t^*(\mathcal{X}_n)}{\tau(M)}\right) \leq 20\frac{t^*(\mathcal{X}_n)}{\lambda} \\ &\leq \tau(M) - 3\varepsilon(\mathcal{X}_n). \end{aligned} \tag{4.36}$$

Therefore, if $\varepsilon(\mathcal{X}_n)$ is small enough, then $M \simeq \mathrm{Cech}(5t_\lambda(\mathcal{X}_n), \mathcal{X}_n)$. We conclude by using Proposition 4.2.7. □

As a last example, we show that the parameter $t_\lambda(\mathcal{X}_n)$ can also be used to estimate tangent spaces in an adaptive way. Let $x \in M$ and $A \subset M$ be a finite set. We denote by $T_x(A,t)$ to be the d-dimensional vector space U which minimizes $d_H(A \cap \mathcal{B}(x,t), x+U)$. This estimator was originally studied in [BSW09]. Recall that the angle between subspaces is denoted by $\angle$.

Corollary 4.3.10. *Let $0 < \lambda < 1$ and $t_{\max} > 0$. Let d be an integer smaller than D and $f_{\min} > 0$, $\tau_{\min} > 2t_{\max}/\lambda$. Then, for n large enough, we have*

$$\sup_{\mu \in \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, +\infty}(\gamma_n)} \mathbb{E}\angle(T_pM, T_p(\mathcal{X}_n, 11t_\lambda(\mathcal{X}_n))) \leq C_0\left(\frac{\log n}{n}\right)^{1/d}, \tag{4.37}$$

where C_0 depends on $d, \tau_{\min}, f_{\min}, \lambda, t_{\max}$.

This rate is the minimax rate (up to logarithmic factors) according to [AL19, Theorem 3]: we obtain an adaptive estimator (once again in a weaker sense that in Section 4.1).

Proof of Corollary 4.3.10. According to [BSW09, Theorem 3.2], for $A \subset M$, if $t < \tau(M)/2$ and $t \geq 10\varepsilon(A)$, then

$$\angle(T_p(A,t), T_pM) \leq C_0\frac{t}{\tau(M)} \tag{4.38}$$

for some absolute constant C_0. According to Theorem 4.3.5 and Proposition 4.2.3, and arguing as in the two previous proofs, $11t_\lambda(\mathcal{X}_n) > 10\varepsilon(\mathcal{X}_n)$ and $11t_\lambda(\mathcal{X}_n) < \tau(M)/2$ as long as $\varepsilon(\mathcal{X}_n) < C_{\tau(M),\lambda,t_{\max}}$. Therefore,

$$\begin{aligned} \mathbb{E}\angle(T_pM, T_p(\mathcal{X}_n, 11t_\lambda(\mathcal{X}_n)) &\leq 11C_0\frac{\mathbb{E}t_\lambda(\mathcal{X}_n)}{\tau(M)} + \mathbb{P}(\varepsilon(\mathcal{X}_n) > C_{\tau(M),\lambda,t_{\max}}) \\ &\leq C_{d,\tau_{\min},f_{\min},\lambda,t_{\max}}\left(\log n/n\right)^{1/d}, \end{aligned}$$

by Theorem 4.3.5 and Proposition 4.2.7. □

4.4 Short-scale behavior of the convexity defect functions

The selection procedure described in Section 4.3 relies on the behavior of the convexity defect function $h(\cdot, \mathcal{X}_n)$ on the range $[t^*(\mathcal{X}_n), \tau(M)]$. However, it appears in numerical experiments (see Figure 4.4) that the convexity defect function also exhibits a behavior worth of interest on the interval $[0, t^*(\mathcal{X}_n)]$: it appears that the convexity defect function $h(t, \mathcal{X}_n)$ stays very close to its maximal value t for t in this range. The next proposition proves that such a behavior indeed appears in a random setting.

Proposition 4.4.1 (Short-scale behavior)**.** *Let d be an integer smaller than D, and let $q = (\tau_{\min}, f_{\min}, f_{\max}, 0) \in \Theta^d$. Let $\mathcal{X}_n$ be a n-sample of law $\mu \in \mathcal{Q}^{2,d}_{q,n}$. Fix $0 < \lambda < 1$. There exist positive constants t_0, C_0, C_1 depending on the parameters of the model and on λ such that the following holds. Let, for $x > 0$, $\phi(x) = \min(1, x)e^{-x}$. Then, for n large enough and $0 < t \leq t_0$, we have*

$$h(t, \mathcal{X}_n) \geq \lambda t \text{ with probabilty larger than } 1 - C_0 \exp(-C_1 n\phi(nm)). \tag{4.39}$$

The probability appearing in (4.39) will be close to 1 as long as t is smaller than a fraction of $(\log n/n)^{1/d}$ and larger than $(1/n)^{(2-\delta)/d}$ for any $0 < \delta < 1$. Therefore, with high probability, the convexity defect function $h(t, \mathcal{X}_n)$ is very close to t for $(1/n)^{(2-\delta)/d} \lesssim t \lesssim (\log n/n)^{1/d}$. On the contrary, standard techniques show that if $t \lesssim (1/n)^{2/d}$, then $h(t, \mathcal{X}_n)$ is null with probability larger than, say, $1/2$, indicating that the lower bound in the previous range is close of being optimal. The arguments to prove Proposition 4.4.1 are of a purely probabilistic nature and do not rely on the geometry of the support of μ. The remainder of the Section is dedicated to proving Proposition 4.4.1.

Let $\mu \in \mathcal{Q}^{2,d}_{\tau_{\min}, f_{\min}, f_{\max}}$ be a probability distribution with support M and let $\mathcal{X}_n$ be a n-sample of law μ. We will use repeatedly in the proof the fact that there exist constants $c_d, C_d > 0$ such that, if $t \leq \tau(M)/4$, then $c_d f_{\min} t^d \leq \mu(B) \leq C_d f_{\max} t^d$ for all balls B of radius t centered at points of M (see Proposition 3.5.7.7).

Lemma 4.4.2. *Assume that $t \leq t_{d,\tau_{\min},f_{\max}}$. There exists a partition $\mathcal{C} = \{U_1, \ldots, U_K\}$ of M into K measurable parts such that:*

1. *for $k = 1, \ldots, K$, U_k contains a ball $V_k = \mathcal{B}_M(x_k, 2t)$,*
2. *for $k = 1, \ldots, K$, $\mu(U_k) = 1/K$,*
3. *we have $c_{d,\tau_{\min},f_{\max}} t^{-d} \leq K \leq C_{d,\tau_{\min},f_{\max}} t^{-d}$.*

Proof. If $t \leq \tau(M)/8$, then $\mu(B) \leq C_d f_{\max} t^d$ for any ball B of radius $2t$. Assume that t is small enough so that $C_d f_{\max} t^d \leq 1/2$ and let K be the largest integer such that $1/K \geq C_d f_{\max} t^d$, so that $1/(2C_d f_{\max} t^d) \leq K \leq 1/(C_d f_{\max} t^d)$. Build $\mathcal{C}$ in the following way. Start with an union of K disjoint balls V_k of radius $2t$, for $k = 1, \ldots, K$, choose W_k any measurable set in $M \setminus \bigcup_{k=1}^K V_k$ with $\mu(W_k) = 1/K - \mu(V_k) \geq 0$ and let $U_k = V_k \cup W_k$. The set $M \setminus \bigcup_{k=1}^K U_k$ is of μ-measure null, so that by adding it to U_1 for instance, we obtain a partition following the required properties. Note that we used the fact that for any $A \subset M$ and $0 \leq p \leq \mu(A)$, there exists a subset $V \subset A$ with $\mu(V) = p$: this holds as μ is absolutely continuous with respect to the volume measure on M. □

We fix such a partition in the following, with balls V_k of radius $(2 - \lambda)t$. Let B_k be the ball sharing its center with V_k, of radius t. For $W \subset M$, let $N(W)$ be the number of points of $\mathcal{X}_n$ in W. We also write N_k for $N(U_k)$. Let x_k be the center of B_k and e be a unit vector in $T_x M$, and denote by A_k^+ (resp. A_k^-) the ball of radius $(1 - \lambda)t/2$ centered at $x^+ = x_k + e(1 + \lambda)t/2$ (resp. $x^- = x_k - e(1 + \lambda)t/2$), see Figure 4.5.

Lemma 4.4.3. *Fix $k = 1, \ldots, K$. If $h(t, \mathcal{X}_n) < \lambda t$ and $N_k = 2$, then we cannot have both $N(A_k^+) = 1$ and $N(A_k^-) = 1$.*

Proof. Let $\sigma = \mathcal{X}_n \cap U_k$. Assume that $N_k = 2$, and that $N(A_k^+) = N(A_k^-) = 1$. Then, σ is made of two points, x_1 and x_2, respectively in A_k^+ and A_k^-. As both points belong to B_k, we have $r(\sigma) \leq t$. Therefore, $d_H(\mathrm{Conv}(\sigma)|\mathcal{X}_n) \leq h(t, \mathcal{X}_n) < \lambda t$. In particular,

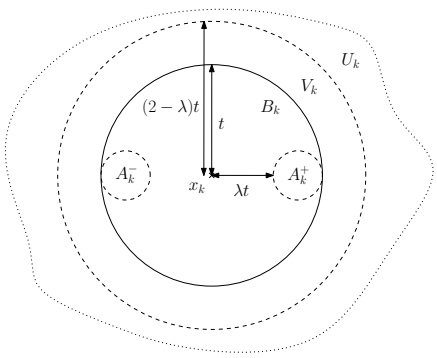


FIGURE 4.5: Any ball with diameter whose one extremity is in A_k^- and the other in A_k^+ is included in U_k.

the middle point x_0 of x_1 and x_2 is at distance less than λt from $\mathcal{X}_n$. Let us show that $\mathcal{B}_M(x_0, |x_1 - x_0|) \subset V_k$. If this is the case, then $d(x_0, \mathcal{X}_n) = |x_1 - x_2|/2 \geq \lambda t$, a contradiction with having $d_H(\mathrm{Conv}(\sigma)|\mathcal{X}_n) < \lambda t$. Let $z \in \mathcal{B}_M(x_0, |x_1 - x_0|)$ and denote by π_e the projection on e. Then,

$$\begin{aligned}|z - x_k| &\leq |z - x_0| + |x_0 - x_k| \leq \frac{|x_1 - x_2|}{2} + |\pi_e(x_0 - x_k)| + |\pi_e^{\perp}(x_0 - x_k)| \\ &\leq t + \frac{(1-\lambda)t}{2} + \frac{(1-\lambda)t}{2} \leq (2-\lambda)t,\end{aligned}$$

concluding the proof. □

Denote by F_k the complementary event of the event $N(A_k^+) = N(A_k^-) = 1$. We obtain the bound

$$\begin{aligned}\mathbb{P}(h(t, \mathcal{X}_n) < \lambda t) &\leq \mathbb{P}(\forall k = 1, \ldots, K,\ N_k \neq 2 \text{ or } (N_k = 2 \text{ and } F_k)) \\ &= \mathbb{E}\left[\mathbb{P}(\forall k = 1, \ldots, K,\ N_k \neq 2 \text{ or } (N_k = 2 \text{ and } F_k)|(N_k)_{k=1,\ldots,K})\right] \\ &\leq \mathbb{E}\left[\prod_{k=1}^{K}(\mathbf{1}\{N_k \neq 2\} + \mathbb{P}(F_k|N_k = 2)\mathbf{1}\{N_k = 2\})\right] \\ &\leq \mathbb{E}\left[\prod_{k=1}^{K}(1 - (1 - \mathbb{P}(F_k|N_k = 2))\mathbf{1}\{N_k = 2\})\right].\end{aligned}$$

Lemma 4.4.4. *There exists a positive constant C_1 such that*

$$\mathbb{P}(F_k|N_k = 2) \leq e^{-C_1} \text{ for } k = 1, \ldots, K.$$

Proof. If $|x_+ - x_k| \leq t \leq 7\tau(M)/24$, then there exists $y_+ \in M$ with $\pi_{x_k}(y_+ - x_k) = x_+ - x_k$ by Proposition 3.5.8. Furthermore, we have $|y_+ - x_k| \leq 8t/7$ and, by Proposition 3.5.7.4, we have $|y_+ - x_+| \leq (8t/7)^2/(2\tau(M)) = 32t^2/(49\tau(M))$. In particular,

$$\mathcal{B}(x_+, (1-\lambda)t/2) \supset \mathcal{B}(y_+, (1-\lambda)t/2 - 32t^2/(49\tau(M))) \supset \mathcal{B}(y_+, (1-\lambda)t/4),$$

if $t \leq 49(1-\lambda)\tau(M)/128$. According to Proposition 3.5.7.2, we therefore have, also assuming that $t \leq \tau(M)/4$,

$$\mu(\mathcal{B}(x_+, (1-\lambda)t/2)) \geq f_{\min}\alpha_d\left(\frac{(1-\lambda)t}{4}\frac{47}{48}\right)^d,$$

and the same inequality holds for x_-.

Let Y_1, Y_2 be two independent random variables sampled according to μ, conditioned on being in U_k. Then, as $\mu(U_k) = m = \alpha_d(1+\delta)f_{\min}(2-\lambda)^d t^d$,

$$\begin{aligned}\mathbb{P}(F_k|N_k = 2) &= 1 - 2\mathbb{P}(Y_1 \in A_k^+)\mathbb{P}(Y_2 \in A_k^-)\\ &= 1 - 2\frac{\mu(\mathcal{B}(x^+, (1-\lambda)t/2))\mu(\mathcal{B}(x^-, (1-\lambda)t/2))}{\mu(U_k)^2}\\ &\le 1 - 2\left(\frac{\left(\frac{47}{48}\frac{1-\lambda}{4}\right)^d}{(1+\delta)(2-\lambda)^d}\right)^2 \le e^{-C_1},\end{aligned}$$

where $C_1 = 2\left(\frac{\left(\frac{47}{48}\frac{1-\lambda}{4}\right)^d}{(1+\delta)(2-\lambda)^d}\right)^2$. □

We finally obtain

$$\mathbb{P}(h(t, \mathcal{X}_n) < \lambda t) \le \mathbb{E}\left[\exp\left(-C_1 \sum_{k=1}^{K} \mathbf{1}\{N_k = 2\}\right)\right]. \tag{4.40}$$

Lemma 4.4.5. *Assume that* $nm \le \max(m^{-1}, (\ln n)^2)$. *Let* $\phi : x \in [0, +\infty) \to \min(1, x)e^{-x}$. *Then,*

$$\mathbb{E}\left[\exp\left(-C_1 \sum_{k=1}^{K} \mathbf{1}\{N_k = 2\}\right)\right] \le C_2 \exp\left(-C_3 n\phi(nm)\right), \tag{4.41}$$

for some positive constants C_2, C_3.

Proof. Let $S = \sum_{k=1}^{K} \mathbf{1}\{N_k = 2\}$. Let $\tilde{n}$ be the number of points of $\mathcal{X}_n$ in $\bigcup_k U_k$, so that $\tilde{n}$ follows a binomial distribution of parameters n and Km. Recall that by construction, $Km \ge c_0$ for some constant c_0 (see Lemma 4.4.2). Conditionally on $\tilde{n}$, the random variable S can be realized as the number of urns containing exactly two balls, in a model where $\tilde{n}$ balls are thrown uniformly in K urns. Let $p_i = \binom{\tilde{n}}{i} K^{-i}(1-K^{-1})^{\tilde{n}-i}$ be the probability that an urn contains exactly i balls. We have $\mathbb{E}[S|\tilde{n}] = Kp_2$, and

$$\begin{aligned}\mathbb{E}[\exp(-C_1 S)|\tilde{n}] &\le \mathbb{E}[\exp(-C_1 Kp_2/2)\mathbf{1}\{S \ge Kp_2/2\}|\tilde{n}] + \mathbb{P}(S < Kp_2/2|\tilde{n})\\ &\le \exp(-C_1 Kp_2/2) + \mathbb{P}(|S - Kp_2| > Kp_2/2|\tilde{n}).\end{aligned} \tag{4.42}$$

Let $v = 2K\max(2p_2, 3p_3)$. According to [BHBO17, Proposition 3.5], if for some $s > 0$,

$$Kp_2/2 \ge \sqrt{4vs} + 2s/3, \tag{4.43}$$

then $\mathbb{P}(|S - Kp_2| > Kp_2/2|\tilde{n}) \le 4e^{-s}$. Recall that $nm^2 \le 1$ by assumption, and that $K \ge c_{\mu,\delta}t^{-d} \ge c_1/m$. We therefore have $n/K^2 \le c_1^{-2}$. Assuming that $\tilde{n} \ge 3$ and using the inequality $\ln(1-K^{-1}) \ge -K^{-1} - K^{-2}$ for $K \ge 2$, we obtain the inequalities

$$p_2 \ge \frac{(\tilde{n}/K)^2}{4e^{c_1^{-2}}}e^{-\tilde{n}/K} \text{ and } p_3 \le \frac{e^3}{6}(\tilde{n}/K)^3 e^{-\tilde{n}/K} \le c_2 p_2(n/K) \tag{4.44}$$

for some positive constant c_2. We consider two different regimes.

• Assume first that $n/K \le 2/(3c_2)$. Then $3p_3 \le 2p_2$ and one can check that $s = Kp_2/100$ satisfies (4.43). Inequality (4.42) then yields that $\mathbb{E}[\exp(-C_1 S)|\tilde{n}] \le 5\exp(-C_1' Kp_2)$ for $C_1' = \min(C_1/2, 1/100)$. To conclude, we remark that for any $\alpha \in (0,1)$, by the Hoeffding inequality, the event $|\tilde{n} - nKm| \le nKm\alpha$ holds with probability at least $1 - \exp(-2n\alpha^2)$. Letting $\alpha = 1/2$, we obtain that, on this event,

$$\frac{1}{2}nm \le \frac{\tilde{n}}{K} \le \frac{3}{2}nm \le \frac{3}{2}\frac{n}{K}mK \le \frac{1}{c_2},$$

where we used that $mK \leq 1$. Therefore, $p_2 \geq c_3(nm)^2 \geq c_4(nm)^2 e^{-nm}$ for some constants c_3 and c_4. The probability of order $\exp(-2n\alpha^2)$ being negligible, we obtain a final bound of order $\exp(-C_1' c_4 K(nm)^2 e^{-nm}) \leq \exp(-C_2 n\phi(nm))$, concluding the proof in the regime $n/K \leq 2/(3c_2)$.

• Otherwise, we have $n/K > 2/(3c_2)$ and we also assume that $|\tilde{n} - nKm| \leq \alpha nKm$ for some $\alpha \in (0,1)$ to fix (this happens with probability $1 - \exp(-2n\alpha^2)$ by Hoeffding's inequality). One can then check using (4.44) that $s = c_5 \tilde{n} e^{-\tilde{n}/K}$ satisfies (4.43) if c_5 is chosen small enough. Furthermore, $s \leq c_6 K p_2$ for some constant c_6 (using (4.44)). The leading term in (4.42) is therefore of the form $\exp(-c_7 \tilde{n} e^{-\tilde{n}/K})$. Let $\alpha = 1/(\ln n)^3$. We have, as $nm \geq c_0 n/K \geq c_8$ and as $nm \leq (\ln n)^2$ (by assumption),

$$c_9 \leq nm(1-\alpha) \leq \frac{\tilde{n}}{K} \leq nm(1+\alpha) \leq nm + \frac{1}{\ln n}.$$

Therefore, $\tilde{n} e^{-\tilde{n}/K} \geq (c_9/2) K e^{-nm}$. The probability of order $\exp(-2n\alpha^2)$ is still negligible, and we obtain a final bound on $\mathbb{E}[\exp(-C_1 S)]$ of order $\exp(-(c_9/2)Ke^{-nm}) \leq \exp(-c_{10} n\phi(nm))$. □

4.5 Numerical considerations

Computing $\mathrm{Conv}(t, \mathcal{X}_n)$ amounts to compute the Čech complex of $\mathcal{X}_n$ of parameter t: we refer to Section 3.6 for a discussion on the computational complexity of this problem. It remains to discuss the cost of computing $t_\lambda(\mathcal{X}_n)$.

The scale $t_\lambda(\mathcal{X}_n)$ is easily obtained once the convexity defect function of the set $\mathcal{X}_n \subset \mathbb{R}^D$ has been computed. By the Carathéodory theorem, one can restrict to simplexes of dimension less than D for the computation of $\mathrm{Conv}(t, \mathcal{X}_n)$. As there are $O(n^{D+1})$ such simplexes, the computation cost of the convexity defect function is prohibitive for large D. We therefore propose to consider only simplexes of dimension 1 in the convexity defect function. Let $\mathrm{Conv}^1(t, \mathcal{X}_n)$ be equal to the union of the edges $e = \{x_1, x_2\} \subset \mathcal{X}_n$ of length smaller than $2t$, and $h^1(t, \mathcal{X}_n) = d_H(\mathcal{X}_n, \mathrm{Conv}^1(t, \mathcal{X}_n))$. We define likewise the parameter $t^1_\lambda(\mathcal{X}_n)$ with the function h being replaced by h^1.

Lemma 4.5.1. *Let $1 \leq d < D$ be an integer and let $c_D = \sqrt{\frac{1}{2} - \frac{1}{2D}}$. Let $B \subset \mathbb{R}^D$ and $t_{\max} > 0$, $0 < \lambda < 1 - c_D$. Then,*

$$t_{\lambda + c_D}(B) \leq t^1_\lambda(B) \leq t_\lambda(B). \tag{4.45}$$

Proof. A direct computation shows that if σ is a D-simplex of radius smaller than t, then the Hausdorff distance between $\mathrm{Conv}(\sigma)$ and the 1-skeleton of σ (the union of its edges) is bounded by $c_D t$. Hence, $h(t, B) \geq h^1(t, B) \geq h(t, B) - c_D t$. The conclusion follows from the definition of $t_\lambda(B)$. □

Hence, if some sets $A, B \subset M$ satisfy the conditions of Theorem 4.3.5 for λ and $\lambda + c_D$, then $t^1_\lambda(B)$ satisfies

$$t^*(A) + \gamma \leq t^1_\lambda(B) \leq \frac{2t^*(A)}{\lambda}\left(1 + \frac{t^*(A)}{\tau(M)}\right) + \frac{6\gamma}{\lambda}.$$

The scale $t^1_\lambda(\mathcal{X}_n)$ can be computed by computing the distance $d_H(e|\mathcal{X}_n)$ for the $n(n-1)$ edges e of $\mathcal{X}_n$. Each distance can be obtained by computing the projections of the set $\mathcal{X}_n$ on the line spanned by e. The time complexity can be further reduced by selecting a random subset of L edges in $\mathcal{X}_n$. If we have no guarantees on the output with such a

strategy, it appears in our experiments that it is similar to $h^1(\cdot, \mathcal{X}_n)$ for L significantly smaller than n^2.

As a numerical illustration of our procedure, we compute the convexity defect function $h^1(\cdot, \mathcal{X}_n)$ of three synthetic datasets: (a) $n_a = 10^3$ points uniformly sampled on the unit circle, (b) $n_b = 10^4$ points sampled on a torus of inner radius 4 and outer radius 1, and (c) $n_c = 10^5$ points sampled on a swiss roll implemented with `scipy` [Vir+20] (which was also used to compute the Hausdorff distance between point clouds). The convexity defect functions (a), (b) and (c) were approximated using the algorithm described in the previous paragraph with parameter $L_a = \infty$ (all pairs computed), $L_b = 10^6$ and $L_c = 10^7$. On each function, displayed in Figure 4.6, the behavior described in Section 4.3 is observed: first a linear growth up to a certain value, then a quadratic growth until the reach of the manifold (equal to 1 in the first two illustrations, and slightly larger than 3 for the swiss roll dataset). We then fix $t_{\max} = 0.5\,\mathrm{diam}(\mathcal{X}_n)/\log(n)$ and compute $t^1_\lambda(\mathcal{X}_n)$ for different values of λ. When λ is very close to 1, $t^1_\lambda(\mathcal{X}_n)$ is always 0, whereas it slowly increases as λ decreases, until reaching $t_{\max}$ at some value $\lambda_{\min}$. As a rule of thumb, we choose $\lambda_* = \frac{1+\lambda_{\min}}{2}$ and select the parameter $t^1_{\lambda_*}(\mathcal{X}_n)$, which is equal to $t_a = 0.049$, $t_b = 0.31$ and $t_c = 0.48$ in the different experiments (a), (b) and (c), while the approximation rates $\varepsilon(\mathcal{X}_n)$ were evaluated (by oversampling) at $\varepsilon_a = 0.021$, $\varepsilon_b = 0.31$ and $\varepsilon_c = 0.33$.

4.6 Discussion and further works

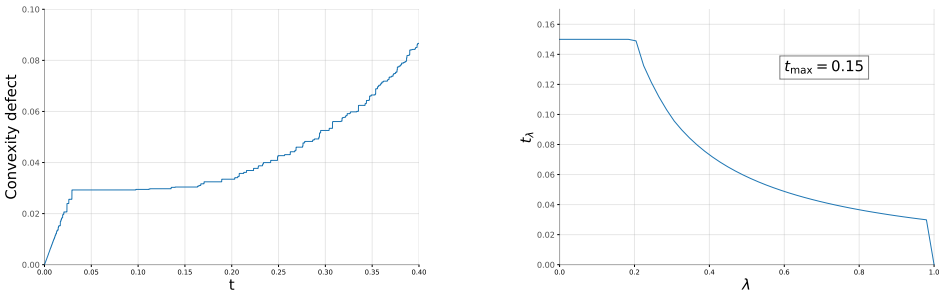
In this article, we introduced a particularly simple manifold estimator, based on a unique rule: add the convex hull of any subset of the set of observations which is of radius smaller than t. After proving that this leads to a minimax estimator for some choice of t, we explained how to select the parameter t by computing the convexity defect function of the set of observations. Our selection procedure actually allows us to find a parameter $t_\lambda(\mathcal{X}_n)$ that is very close to $\varepsilon(\mathcal{X}_n)$ (up to a known multiplicative constant). The selected parameter can therefore be used as a scale parameter in a wide range of procedures in geometric inference. We illustrated this general idea by showing how an adaptive tangent space estimator can be created thanks to $t_\lambda(\mathcal{X}_n)$.

The main limitation to our procedure is its non-robustness to outliers. Indeed, even in the presence of one outlier in $\mathcal{X}_n$, the loss function $t \mapsto d_H(\mathrm{Conv}(t, \mathcal{X}_n), M)$ would be constant, equal to the distance between the outlier and the manifold M: with respect to the Hausdorff distance, all the estimators $\mathrm{Conv}(t, \mathcal{X}_n)$ are then equally bad. Of course, even in that case, we would like to assert that some values of t are "better" than others in some sense. A solution to overcome this issue would be to change the loss function, for instance by using Wasserstein distances on judicious probability measures built on the t-convex hulls $\mathrm{Conv}(t, \mathcal{X}_n)$ instead of the Hausdorff distance.

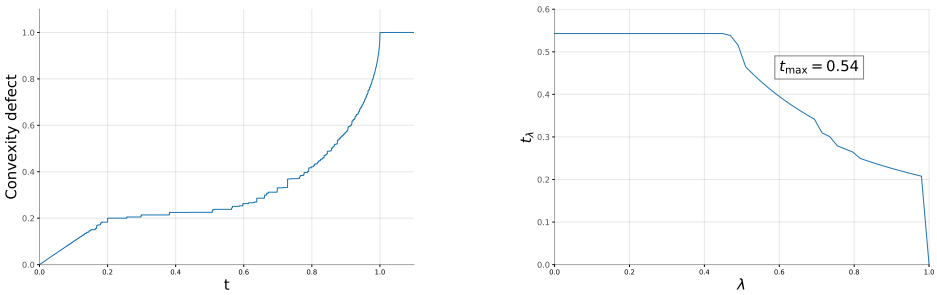
Another way to improve the selection procedure is to exploit the short-scale behavior of the convexity defect function: its linear behavior suggests that selecting the smallest value t such that the convexity defect function is small (whereas we select the largest value $t_\lambda(\mathcal{X}_n)$ such that $h(t, \mathcal{X}_n)$ is large) would also lead to an adaptive estimator. With such a method, the hyperparameter $t_{\max}$ is not needed anymore. We refer to [Div21b] for details on this improved construction.

4.7 Precise lower bound on the minimax risk

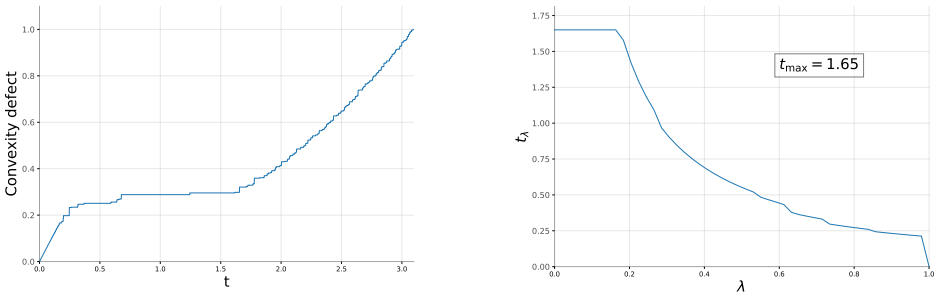
The goal of this section is to show the lower bound in Theorem 4.1.2. To do so, we adapt the construction made in [KZ15] so that the lower bound holds with an explicit



(A) 10^3 points on a circle



(B) 10^4 points on a torus



(C) 10^5 points on a swiss roll

FIGURE 4.6: The convexity defect function of the datasets (a), (b) and (c), and the corresponding choices of $t^1_\lambda(\mathcal{X}_n)$ with respect to λ.

constant. Let $0 < d < D$ and $q = (\tau_{\min}, f_{\min}, f_{\max}, \eta) \in \Theta^d$. We denote by $M(P)$ the underlying manifold of $P \in \mathcal{Q}^{2,d}_{q,n}$. The lower bound is based on Le Cam's lemma:

Lemma 4.7.1. *Let $\mathcal{Q}^{(1)}$, $\mathcal{Q}^{(2)}$ be two subfamilies of $\mathcal{Q}^{2,d}_{q,n}$ which are ε-separated, in the sense that $d_H(M(P^{(1)}), M(P^{(2)})) \geq 2\varepsilon$ for all $P^{(1)} \in \mathcal{Q}^{(1)}$, $P^{(2)} \in \mathcal{Q}^{(2)}$. Then,*

$$\mathcal{R}_n(M, \mathcal{Q}^{2,d}_{q,n}, d_H) \geq \varepsilon \left| \frac{1}{\#\mathcal{Q}^{(1)}} \sum_{P^{(1)} \in \mathcal{Q}^{(1)}} \iota_\# P^{(1)} \wedge \frac{1}{\#\mathcal{Q}^{(2)}} \sum_{P^{(2)} \in \mathcal{Q}^{(2)}} \iota_\# P^{(2)} \right|, \tag{4.46}$$

where $|P \wedge Q|$ is the testing affinity between two distributions P and Q and $\iota : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^D$ is the addition.

To obtain a lower bound on the minimax risk, authors in [KZ15] exhibit two families of manifolds which are ε-separated, and consider the uniform distributions on them. Those manifolds are built by considering a base manifold M_0 which is locally flat, and by adding small bumps on the locally flat part. Such a construction leads to distributions having a density equal roughly to $1/|\mathrm{vol}_{M_0}|$, a constant which might be smaller than $f_{\min}$. If this is the case, then the corresponding submodels are not in $\mathcal{Q}^{2,d}_{q,n}$ and we cannot apply Le Cam's Lemma. Hence, we consider another base manifold, which is a sphere M_0 of radius R slightly larger than $\tau_{\min}$, so that its volume is smaller than $1/f_{\min}$ (this is possible as $f_{\min}\omega_d\tau^d_{\min} \leq \kappa < 1$). The two families are then once again constructed by adding small bumps on M_0. We now detail this construction.

Let $R, \delta > 0$ be two parameters to be fixed later. Let $M_0 \subset \mathbb{R}^{d+1} \subset \mathbb{R}^D$ be the d-sphere of radius R, and let A be a maximal subset of M_0 of even size, which is 4δ-separated. Note that, standard packing arguments (and the formula for the volume of a spherical cap) show that if δ/R is small enough, then the cardinality $2m$ of A satisfies $2m \geq \left(\frac{c_0 R}{\delta}\right)^d$ for some absolute constant c_0. Let $\phi : \mathbb{R} \to \mathbb{R}$ be a smooth function such that $0 \leq \phi \leq 1$, $\phi \equiv 1$ on $[-1, 1]$ and $\phi \equiv 0$ on $\mathbb{R}\backslash[-2, 2]$. For $s \in \{\pm 1\}^A$, we build a diffeomorphism Φ^ε_s by letting for $x \in \mathbb{R}^D$

$$\Phi^\varepsilon_s(x) = x \left(1 + \frac{\varepsilon}{R} \sum_{y \in A} s(y)\phi\left(\frac{|x-y|}{\delta}\right)\right). \tag{4.47}$$

Recall that $\|N\|_{\mathrm{op}}$ denotes the operator norm of a linear application N.

Lemma 4.7.2. *There exists two absolute constants $c_1, c_2 > 0$ such that the following holds. Assume that $\delta \leq R$ and that $c_1\varepsilon/\delta < 1$. Then, the function $\Phi^\varepsilon_s : \mathcal{B}(0, 3R) \to \mathbb{R}^{d+1}$ is a diffeomorphism on its image, with*

$$\sup_{x \in \mathcal{B}(0,3R)} \|\mathrm{id} - d_x\Phi^\varepsilon_s\|_{\mathrm{op}} \leq c_1\varepsilon/\delta \text{ and } \sup_{x \in \mathcal{B}(0,3R)} \left\|d^2_x\Phi^\varepsilon_s\right\|_{\mathrm{op}} \leq c_2\varepsilon/\delta^2. \tag{4.48}$$

Proof. As A is 4δ-separated, at most one term in the sum in (4.47) is non-zero. A computation gives that the derivative of Φ_B is given by, for $x \in \mathcal{B}(0, 3R)$,

$$d_x\Phi^\varepsilon_s(h) = h + h\frac{\varepsilon}{R}\sum_{y \in A} s(y)\phi\left(\frac{|x-y|}{\delta}\right) + x\frac{\varepsilon}{R}\sum_{y \in A}\frac{1}{\delta}s(y)\phi'\left(\frac{|x-y|}{\delta}\right)\frac{\langle x-y, h\rangle}{|x-y|}. \tag{4.49}$$

Hence,

$$\|\mathrm{id} - d_x\Phi^\varepsilon_s\|_{\mathrm{op}} \leq \frac{\varepsilon}{R}\left(\|\phi\|_\infty + |x|\frac{\|\phi'\|_\infty}{\delta}\right) \leq \frac{\varepsilon}{R}\left(\|\phi\|_\infty + 3R\frac{\|\phi'\|_\infty}{\delta}\right) \leq c_1\frac{\varepsilon}{\delta},$$

where $c_1 = c_0\|\phi\|_\infty + 3\|\phi'\|_\infty$. A similar computation gives that $\left\|d_x^2\Phi_s^\varepsilon\right\|_{\mathrm{op}} \le c_2\varepsilon/\delta^2$ for $c_2 = 4\|\phi'\|_\infty + 3\|\phi''\|_\infty$. We eventually show the injectivity: if $\Phi_s^\varepsilon(x) = \Phi_s^\varepsilon(x')$, then x and x' are colinear. Also, if $c_0 = \|\phi\|_\infty + 3\|\phi'\|_\infty$, one can check using (4.49) that the derivative of the function $r \in [0, 3R] \mapsto \langle \Phi_s^\varepsilon(ru), u\rangle$ for u an unit vector is increasing, proving the injectivity. □

Therefore, from [Fed59, Theorem 14.19], we infer that $M_s^\varepsilon := \Phi_s^\varepsilon(M)$ is a manifold with reach larger than

$$\tau(M_s^\varepsilon) \ge R \min\left(1 - c_1\varepsilon/\delta, \frac{(1 - c_1\varepsilon/\delta)^2}{1 + c_1\varepsilon/\delta + Rc_2\varepsilon/\delta^2}\right). \tag{4.50}$$

Also, the volume of M_s^ε is smaller than

$$\begin{aligned}|\mathrm{vol}_{M_s^\varepsilon}| &= \int_{M_0} J\Phi_s^\varepsilon(x)\mathrm{d}x = \omega_d R^d + \sum_{y\in A}\int_{\mathcal{B}_{M_0}(y,2\delta)} (J\Phi_s^\varepsilon(x) - 1)\mathrm{d}x \\ &\le \omega_d R^d + 2mC_d c_1 \frac{\varepsilon}{\delta}|\mathrm{vol}_{M_0}|(\mathcal{B}(y, 2\delta)) \le \omega_d R^d\left(1 + C_d c_1 \frac{\varepsilon}{\delta}\right),\end{aligned} \tag{4.51}$$

where we used that $\det(N) - 1 \le C_d \|N - \mathrm{id}\|_{\mathrm{op}}$ for some constant C_d if N is a matrix of size d with operator norm smaller than 1, the fact that $2m|\mathrm{vol}_{M_0}(\mathcal{B}(y, 2\delta)) \le |\mathrm{vol}_{M_0}|$, and Lemma 4.7.2.

Let $R = \tau_{\min} + \frac{1}{2}\left(\frac{1}{(\omega_d f_{\min})^{1/d}} - \tau_{\min}\right)$ and $\delta = \sqrt{R\varepsilon}\nu$ where $\nu^2 = \frac{2c_2\tau_{\min}}{R-\tau_{\min}}$. With this choice of parameters, one can check that, for ε/δ small enough, $\tau(M_s^\varepsilon) \ge \tau_{\min}$ (by (4.50)) and $|\mathrm{vol}_{M_s^\varepsilon}| \le 1/f_{\min}$ (by (4.51) and using that $\omega_d f_{\min}\tau_{\min}^d \le \kappa < 1$).

We define the family $\mathcal{M}^{(1)}$ of manifolds M_s^ε where s contains exactly m signs $+1$ (and m signs -1). The family $\mathcal{M}^{(2)}$ is defined likewise by considering M_s^ε where s contains exactly $m+1$ or $m-1$ signs $+1$. We then let $\mathcal{Q}^{(1)}$ be the set of distributions $(Q_s^\varepsilon, \delta_0)$ where Q_s^ε is the uniform distribution on a manifold of $M_s^\varepsilon \in \mathcal{M}^{(1)}$, so that $\mathcal{Q}^{(1)}$ is a subset of $\mathcal{Q}_{q,n}^{2,d}$. We then define $\mathcal{Q}^{(2)}$ as follows: let $X \sim Q_s^\varepsilon$ where Q_s^ε is the uniform distribution on a manifold of $M_s^\varepsilon \in \mathcal{M}^{(2)}$. Then, we have $X = \Phi_s^\varepsilon(V)$ for some $V \in M_0$, and we let

$$Y = \Phi_s^{\varepsilon+\gamma}(V), \qquad Z = X - Y.$$

An element of $\mathcal{Q}^{(2)}$ is then given by the law of the couple (Y, Z). Note that for $P^{(2)} \in \mathcal{Q}^{(2)}$, $\iota_\# P^{(2)}$ is the uniform distribution on a manifold of $\mathcal{M}^{(2)}$. Also, $M(P^{(2)})$ is equal to $M_s^{\varepsilon+\gamma} = \Phi_s^{\varepsilon+\gamma} \circ (\Phi_s^\varepsilon)^{-1}(M_s^\varepsilon)$ for some $M_s^\varepsilon \in \mathcal{M}^{(2)}$. By (4.51) and (4.50), its reach is also larger than $\tau_{\min}$, and its volume is smaller than $1/f_{\min}$ if $(\varepsilon+\gamma)/\delta$ is small enough. Note also that $|Z| = |\Phi_s^\varepsilon(V) - \Phi_s^{\varepsilon+\gamma}(V)| \le |V|\gamma/R \le \gamma$. Hence, $\mathcal{Q}^{(2)}$ is indeed a subset of $\mathcal{Q}_{q,n}^d$.

By construction, the two families $\mathcal{Q}^{(1)}$, $\mathcal{Q}^{(2)}$ are $(2\varepsilon+\gamma)$-separated (see Figure 4.7). Hence, we can apply Le Cam's lemma. The exact same computations than in [KZ15, Section 3] show that the testing affinity between $\mathcal{Q}^{(1)}$ and $\mathcal{Q}^{(2)}$ converge to 1 as long as $4m = n/\log n$. Thus, Le Cam's Lemma (4.46) yields

$$\liminf_n \frac{\mathcal{R}_n(M, \mathcal{Q}_{q,n}^{2,d}, d_H)}{\left(\frac{\log n}{n}\right)^{2/d}} \ge \liminf_n \left((m/4)^{2/d}\varepsilon + \frac{\eta}{2}\right). \tag{4.52}$$

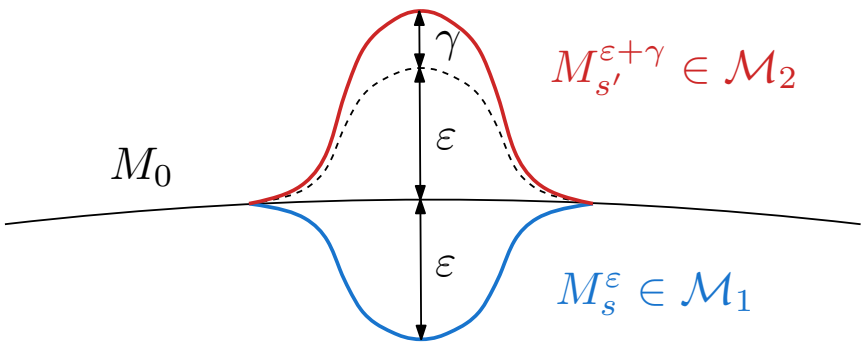


FIGURE 4.7: An element $P^{(1)} \in \mathcal{Q}^{(1)}$ has its first marginal supported on the blue manifold M_s^{ε} (lower bump), whereas an element $P^{(2)} \in \mathcal{Q}^{(2)}$ is such that $P_1^{(2)}$ is supported on the red manifold $M_{s'}^{\varepsilon+\gamma}$ (upper bump), whereas $\iota_{\#}P^{(2)}$ is the uniform distribution on the dotted manifold.

As $2m \geq (c_0 R/\delta)^d$, we therefore have

$$\liminf_n \frac{\mathcal{R}_n(M, \mathcal{Q}_{q,n}^{2,d}, d_H)}{\left(\frac{\log n}{n}\right)^{2/d}} \geq \frac{c_0^2}{8^{2/d}} \frac{R^2}{\delta^2} \varepsilon + \frac{\eta}{2} = \frac{c_0^2}{8^{2/d}} \frac{R}{\nu^2} + \frac{\eta}{2}$$
$$= \frac{c_0^2}{8^{2/d}} \frac{R(R - \tau_{\min})}{2c_2 \tau_{\min}} + \frac{\eta}{2} \geq \frac{c_4}{(\omega_d f_{\min})^{1/d} \tau_{\min}} \left(\frac{1}{(\omega_d f_{\min})^{1/d}} - \tau_{\min} \right) + \frac{\eta}{2},$$

for some absolute constant c_4, where we used that $R - \tau_{\min} = \frac{1}{2}\left(\frac{1}{(\omega_d f_{\min})^{1/d}} - \tau_{\min}\right)$ by definition and that $R \geq \frac{1}{2}(\omega_d f_{\min})^{-1/d}$. As $\tau_{\min} \leq \kappa/(\omega_d f_{\min})^{1/d}$, we obtain the conclusion.

Chapter 5

Reconstruction of measures on manifolds: an optimal transport approach

Density estimation is one of the most fundamental tasks in non-parametric statistics. If efficient methods (from both a theoretical and a practical point of view) exist when the ambient space is of low dimension, minimax rates of estimation become increasingly slow as the dimension increases. To overcome this so-called *curse of dimensionality*, some structural assumptions on the underlying probability are to be made in moderate to high dimensions, which may take different forms, including e.g. the existence of a parametric component [LLW07], the single-index model [Liu+13], sparsity assumptions [Tib96], or constraints on the shape of the support. We focus in this work on the latter, namely on the case where the probability distribution μ generating the observations is assumed to be concentrated on a submanifold M of $\mathbb{R}^D$, of dimension d smaller than D. The topic of density estimation in the manifold setting has been studied for over thirty years, with the emphasis initially being put on reconstructing the density in the case where the manifold M is given—think for instance of datasets lying on the space of orthogonal matrices—notable works including [Hen90; Pel05; Cle+20]. Less attention has been dedicated to the more general setting where the manifold M is unknown and acts as a nuisance parameter. Kernel density estimators on manifolds are designed in [BS17; WW20], where rates are exhibited, respectively in the case where the manifold has a boundary and in the case where the density is Hölder continuous. In [BH19], kernel density estimators are shown to be minimax, and an adaptive procedure is designed, based on Lepski's method, to estimate the unknown density in a point $x \in \mathbb{R}^D$ which is known to belong to the unknown (and possibly nonsmooth) manifold M.

To go beyond the pointwise estimation of μ, even the choice of a relevant loss is nontrivial. Indeed, most standard losses between probability measures (e.g. the L_p distance, the Hellinger distance or the Kullback-Leibler divergence) are degenerate when comparing mutually singular measures, which will typically be the case for measures on two distinct manifolds, even if they are very close to each other with respect to the Hausdorff distance. This implies that the estimation problem is degenerate from a minimax perspective when choosing such losses (see Theorem 5.1.9). On the contrary, the Wasserstein distances W_p, $1 \leq p \leq \infty$ are particularly adapted to this problem, as they are by design robust to small metric perturbations of the support of a measure.

Apart from this first motivation, the use of Wasserstein distances, and more generally of the theory of optimal transport, has shown to be an efficient tool in widely different recent problems of machine learning, with fast implementations and sound theoretical results (see e.g. [PC19] for a survey). From a statistical perspective, most of the attention has been dedicated to studying rates of convergence between a probability

distribution μ and its empirical counterpart μ_n [Dud69; DSS13; FG15; SP18; WB19a; Lei20]. Unsurprisingly, if more regularity is assumed on μ, then it is possible to build estimators with smaller risks than the empirical measure μ_n. Assume for instance that μ is a probability distribution on the cube $[-1,1]^D$, with density f of regularity s (measured through the Besov scale $B^s_{p,q}$). In this setting, it has been shown in [WB19b] that, given n i.i.d. points of law μ, the minimax rate (up to logarithmic factors) for the estimation of μ with respect to the Wasserstein distance W_p is of order

$$\begin{cases} n^{-\frac{s+1}{2s+D}} & \text{if } D \geq 3 \\ n^{-\frac{1}{2}} \log n & \text{if } D = 2 \\ n^{-\frac{1}{2}} & \text{if } D = 1, \end{cases} \tag{5.1}$$

and that this rate is attained by a modified linear wavelet density estimator. Our main contribution consists in extending the results of [WB19b] by allowing the support of the probability to be any d-dimensional compact $\mathcal{C}^k$ submanifold $M \subset \mathbb{R}^D$ for $k \geq 2$. More precisely, assume that some probability μ on M has a lower and upper bounded density f which belongs to the Besov space $B^s_{p,q}(M)$ for some $0 < s \leq k-1$, $1 \leq p < \infty$, $1 \leq q \leq \infty$ (see Section 5.1 for details). We first show (Theorem 5.2.1) that some weighted kernel density estimator that we integrate against the volume measure vol_M on M attains, for the W_p distance, the rate of estimation

$$\begin{cases} n^{-\frac{s+1}{2s+d}} & \text{if } d \geq 3 \\ n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}} & \text{if } d = 2 \\ n^{-\frac{1}{2}} & \text{if } d = 1. \end{cases} \tag{5.2}$$

In the case where the manifold M is unknown, we do not have access to the volume measure vol_M, so that the latter estimator is not computable. We therefore propose to estimate the volume measure vol_M in a preliminary step. Such an estimator $\widehat{\mathrm{vol}}_M$ is defined by using local polynomial estimation techniques from [AL19]. We show that this estimator is a minimax estimator of the volume measure up to logarithmic factors (Theorem 5.2.6), with a risk of order $(\log n/n)^{k/d}$. We then show (Theorem 5.2.7) that a weighted kernel density estimator integrated against $\widehat{\mathrm{vol}}_M$ attains the rate (5.2). Those rates are significantly faster than the rates of (5.1) if $d \ll D$ and are shown to be minimax up to logarithmic factors.

In Section 5.1, we define our statistical model and give some preliminary results on Wasserstein distances. In Section 5.2, we define kernel density estimators on a manifold M, and state our main results. Proofs of the main theorems are then given in Section 5.3.

5.1 Preliminaries

For $1 \leq p \leq \infty$, we let $L_p(M)$ be the set of measurable functions $f : M \to \mathbb{R}$ with finite p-norm $\|f\|_{L_p(M)} := \left(\int f \mathrm{dvol}_M\right)^{1/p}$ (and usual modification if $p = \infty$). We say that a locally integrable function is weakly differentiable if there exists a measurable section ∇f of the tangent bundle TM (uniquely defined almost everywhere) such that for all smooth vector fields w on M with compact support, we have

$$\int f(\nabla \cdot w)\, \mathrm{dvol}_M = -\int (\nabla f) \cdot w\, \mathrm{dvol}_M, \tag{5.3}$$

where $\nabla \cdot w$ denotes the divergence of w (the divergence of w is defined as the real-valued function satisfying (5.3) for every $\mathcal{C}^1$ function f). Furthermore, we will denote by $p^* \in [1, \infty]$ the number satisfying $\frac{1}{p} + \frac{1}{p^*} = 1$.

5.1.1 Besov spaces on manifolds

Let $M \in \mathcal{M}^{k,d}_{\tau_{\min},L}$ for some $k \geq 2$, $\tau_{\min}, L > 0$. We also assume that M is compact. As stated in the introduction, minimax rates for the estimation of a given probability will depend crucially on the regularity of its density f, which is assumed to belong to some Besov space $B^s_{p,q}(M)$. We first introduce Sobolev spaces $H^l_p(M)$ on M for $l \leq k$ an integer, and Besov spaces on M are then defined by real interpolation.

Definition 5.1.1 (Sobolev space on a manifold)**.** *Let $0 \leq l \leq k$, $1 \leq p < \infty$ and let $f \in \mathcal{C}^\infty(M)$. We let*

$$\|f\|_{H^l_p(M)} := \max_{0\leq i\leq l} \left(\int \left\|d^i f(x)\right\|^p_{\mathrm{op}} \mathrm{dvol}_M(x) \right)^{1/p}. \tag{5.4}$$

The space $H^l_p(M)$ is the completion of $\mathcal{C}^\infty(M)$ for the norm $\|\cdot\|_{H^l_p(M)}$.

Remark 5.1.2 (On the case $p = \infty$). The previous definition cannot be extended to the case $p = \infty$. Indeed, the completion of $\mathcal{C}^\infty(M)$ for the norm $\|\cdot\|_{H^l_\infty(M)}$ is equal to $\mathcal{C}^l(M)$, whereas for instance $H^0_\infty(M)$ should be equal to $L_\infty(M)$. For $l = 1$, the space $H^1_p(M)$ can equivalently be defined as the space of weakly differentiable functions f with $\|f\|_{H^1_p(M)} < \infty$, while this definition can be easily extended to the case $p = \infty$. In particular, if $f \in H^1_\infty(M)$, then one can verify that $f \circ \Psi_x \in H^1_\infty(\mathcal{B}_{T_xM}(0, r_0))$ for any $x \in M$. It follows from standard results on Sobolev spaces on domains that $f \circ \Psi_x$ is Lipschitz continuous (see e.g. [Bre10, Proposition 9.3]). Hence, f is also locally Lipschitz continuous. By Rademacher theorem, f is therefore almost everywhere differentiable, and its differential coincides with the weak differential. As a consequence, a function $f \in H^1_\infty(M)$ is Lipschitz continuous, with Lipschitz constant for geodesic distance d_g equal to $\|f\|_{H^1_\infty(M)}$.

For $1 \leq p < \infty$, we introduce the negative homogeneous Sobolev norm $\|\cdot\|_{\dot{H}^{-1}_p(M)}$, defined, for $f \in L_p(M)$ with $\int f \mathrm{dvol}_M = 0$, by

$$\|f\|_{\dot{H}^{-1}_p(M)} := \sup \left\{ \int fg \mathrm{dvol}_M,\ \|\nabla g\|_{L_{p^*}(M)} \leq 1 \right\}, \tag{5.5}$$

where the supremum is taken over all functions $g \in H^1_{p^*}(M)$. For $f \in L_p(M)$, the negative Sobolev norm is defined by

$$\|f\|_{H^{-1}_p(M)} := \sup \left\{ \int fg \mathrm{dvol}_M,\ \|g\|_{H^1_{p^*}(M)} \leq 1 \right\}, \tag{5.6}$$

and the corresponding Banach space is denoted by $H^{-1}_p(M)$.

Proposition 5.1.3. *Let $1 \leq p < \infty$ and $f \in H^{-1}_p(M) \cap L_1(M)$ with $\int f \mathrm{dvol}_M = 0$.*

(i) We have $C_{d,\tau_{\min}} |\mathrm{vol}_M|^{\frac{d-1}{p}-d} \|f\|_{\dot{H}^{-1}_p(M)} \leq \|f\|_{H^{-1}_p(M)} \leq \|f\|_{\dot{H}^{-1}_p(M)}$ for some positive constant $C_{d,\tau_{\min}}$ depending on d and $\tau_{\min}$.

(ii) We have $\|f\|_{\dot{H}^{-1}_p(M)} = \inf\{\|w\|_{L_p(M)},\ \nabla \cdot w = f\}$, where the infimum is taken over all measurable vector fields w on M with finite p-norm, and where $\nabla \cdot w = f$ means that $\int fg \mathrm{dvol}_M = -\int w \cdot \nabla g \mathrm{dvol}_M$ for all $g \in \mathcal{C}^\infty(M)$.

Following [Tri92], Besov spaces on a manifold M are defined as real interpolation of Sobolev spaces.

Definition 5.1.4 (Real interpolation of spaces)**.** *Let A_0, A_1 be two Banach spaces, which continuously embed into some Banach space A. We endow the space $A_0 \cap A_1$ with the norm $\|x\|_{A_0 \cap A_1} = \max\{\|x\|_{A_0}, \|x\|_{A_1}\}$ for $x \in A_0 \cap A_1$ and the space $A_0 + A_1$ with the norm $K(x,1)$ for $x \in A_0 + A_1$, where*

$$K(x,\lambda) := \inf\{\|x_0\|_{A_0} + \lambda\|x_1\|_{A_1},\ x = x_0 + x_1,\ x_0 \in A_0,\ x_1 \in A_1\}, \quad \lambda \geq 0. \tag{5.7}$$

For $\theta \in [0,1]$ and $1 \leq q \leq \infty$, we let

$$\|x\|_{(A_0,A_1)_{\theta,q}} := \left(\int_0^\infty \lambda^{-\theta q} K(x,\lambda)^q \frac{\mathrm{d}\lambda}{\lambda}\right)^{1/q}, \quad x \in A_0 + A_1, \tag{5.8}$$

and $(A_0,A_1)_{\theta,q} := \{x \in A_0 + A_1,\ \|x\|_{(A_0,A_1)_{\theta,q}} < \infty\}$ (with usual modification if $q = \infty$). The pair (A_0,A_1) is called a compatible pair, and $(A_0,A_1)_{\theta,q}$ is the real interpolation between A_0 and A_1 of exponents θ and q.

For A, B two Banach spaces and $F : A \to B$ a bounded operator, we let $\|F\|_{A,B}$ be the operator norm of F. Let (A_0,A_1) and (B_0,B_1) be two compatible pairs. Let $F : A_0 + A_1 \to B_0 + B_1$ be a linear map such that the restriction of F to A_j is a bounded linear map into B_j $(j = 0,1)$. Then, the following interpolation inequality holds [Lun18, Theorem 1.1.6]

$$\|F\|_{(A_0,A_1)_{\theta,q},(B_0,B_1)_{\theta,q}} \leq \|F\|_{A_0,B_0}^{1-\theta}\|F\|_{A_1,B_1}^{\theta}. \tag{5.9}$$

Definition 5.1.5 (Besov space on a manifold)**.** *Let $1 \leq p < \infty$ and $0 < s < k$. The Besov space $B^s_{p,q}(M)$ is defined as $B^s_{p,q}(M) := (L_p(M), H^k_p(M))_{s/k,q}$.*

Basic results from interpolation theory then imply that $\|\cdot\|_{B^s_{p,q}(M)} \leq \|\cdot\|_{B^{s'}_{p,q}(M)}$ if $0 < s \leq s' < k$ (see e.g. [Lun18]).

A crucial point in the study conducted in the next sections is the relation between Wasserstein distances and negative Sobolev norms.

Proposition 5.1.6 (Wasserstein distances and negative Sobolev norms)**.** *Let $1 \leq p < \infty$. Let $M \in \mathcal{M}^{2,d}$ be a manifold with reach $\tau(M) \geq \tau_{\min}$, and let $\mu, \nu \in \mathcal{P}^p_1(\mathbb{R}^D)$ be two probability measures supported on M, absolutely continuous with respect to vol_M. Assume that $\mu, \nu \geq f_{\min} \cdot \mathrm{vol}_M$ for some $f_{\min} > 0$. Then, identifying measures with their densities, we have*

$$\begin{aligned} W_p(\mu,\nu) &\leq p^{-1/p} f_{\min}^{1/p-1}\|\mu - \nu\|_{\dot{H}^{-1}_p(M)} \\ &\leq C_{d,\tau_{\min},f_{\min}}\|\mu - \nu\|_{H^{-1}_p(M)}, \end{aligned} \tag{5.10}$$

for some constant $C_{d,\tau_{\min},f_{\min}}$ depending on d, $\tau_{\min}$ and $f_{\min}$.

In particular, if $p = 1$, then the first inequality in (5.10) is actually an equality by the Kantorovitch-Rubinstein duality formula [Vil08, Particular Case 5.16]. This inequality appears in [Pey18] for $p = 2$ and in [San15, Section 5.5.1] for measures having density with respect to the Lebesgue measure. We carefully adapt their proofs in Section 5.4.2.

5.1.2 Statistical models and the choice of the loss function

Statistical models in interest for this problem are based on the statistical models $\mathcal{P}^{k,d}_{\tau_{\min},L,f_{\min},f_{\max}}$ introduced in Chapter 3, with the additional constraints that conditions on the regularity of the density of the measures are to be made. Furthermore, we require the noise to be orthogonal to the manifold in those models.

Definition 5.1.7 (Noise free model)**.** *Let $d \leq D$ be integers, $k \geq 2$, $0 \leq s < k$ and $1 \leq p < \infty$. Let $M \in \mathcal{M}_d^k$. For $s = 0$, the set $\mathcal{Q}^0(M)$ is the set of probability distributions μ on $\mathbb{R}^D$ absolutely continuous with respect to the volume measure vol_M, with a density f satisfying $f_{\min} \leq f \leq f_{\max}$ almost everywhere. For $s > 0$, the set $\mathcal{Q}^s(M)$ is the set of distributions $\mu \in \mathcal{Q}^0(M)$, with density $f \in B^s_{p,q}(M)$ satisfying $\|f\|_{B^s_{p,q}(M)} \leq L_s$. The model $\mathcal{Q}_d^{s,k}$ is equal to the union of the sets $\mathcal{Q}^s(M)$ for $M \in \mathcal{M}^{k,d}$.*

Definition 5.1.8 (Orthogonal noise model)**.** *Let $d \leq D$ be integers, $k \geq 2$, $0 \leq s < k$, $1 \leq p < \infty$ and $\gamma \geq 0$. The set $\mathcal{Q}_d^{s,k}(\gamma)$ is the set of probability distributions ξ of random variables (Y, Z) where $Y \sim \mu \in \mathcal{Q}_d^{s,k}$ and $Z \in \mathcal{B}(0, \gamma)$ is such that $Z \in T_Y M^\perp$.*

As in the previous chapter, we assume in the orthogonal noise model that we observe a n-sample of law $\iota_\# \xi$ where $\xi \in \mathcal{Q}_d^{s,k}(\gamma)$: concretely, a n-sample is given by $X_1, \ldots, X_n$, where X_i is equal to $Y_i + Z_i$ with Y_i supported on some manifold M and $Z_i \in T_{Y_i} M^\perp$ is of norm smaller than γ. The goal is then to reconstruct the law $\vartheta(\xi) = \mu$ of Y_i. We first show that such a task is impossible if the loss function $\mathcal{L}$ is larger than the total variation distance between measures.

Theorem 5.1.9. *Let $d \leq D$ be integers, $k \geq 2$, $0 \leq s < k$, $1 \leq p < \infty$. Let $\mathcal{L} : \mathcal{P}(\mathbb{R}^D) \times \mathcal{P}(\mathbb{R}^D) \to [0, \infty]$ be a measurable map with respect to the Borel σ-algebra associated to the total variation distance on $\mathcal{P}(\mathbb{R}^D) \times \mathcal{P}(\mathbb{R}^D)$. Assume that $\mathcal{L}(\mu, \nu) \geq g(|\mu - \nu|)$ for a convex nondecreasing function $g : \mathbb{R} \to [0, \infty]$ with $g(0) = 0$. Then, for any $\tau_{\min} > 0$, if $f_{\min}$ is small enough and $L_k, L_s, f_{\max}$ are large enough, we have*

$$\mathcal{R}_n(\mu, \mathcal{Q}_d^{s,k}, \mathcal{L}) \geq g(c_d), \tag{5.11}$$

for some constant $c_d > 0$.

Examples of such losses include the total variation distance, the Hellinger distance (with $g(x) = x$), the Kullback-Leibler divergence (with $g(x) = x^2/2$), and the L_p distance with respect to some dominating measure (with $g(x) = x^p$). We give a proof of Theorem 5.1.9, based on Assouad's lemma, in Section 5.4.7. A simple example of loss $\mathcal{L}$ which is not degenerate for mutually singular measures is given by the W_p distance. As stated in the introduction, we will therefore choose this loss, and study $\mathcal{R}_n(\mu, \mathcal{Q}_d^{s,k}(\gamma), W_p)$, the minimax rate of estimation for μ with respect to W_p, where μ is the first marginal of $\xi \in \mathcal{Q}_d^{s,k}(\gamma)$.

Remark 5.1.10. For $\gamma > 0$, the statistical model $\mathcal{Q}_d^{s,k}(\gamma)$ is not identifiable, in the sense that there exist ξ, ξ' in the model for which $\iota_\# \xi = \iota_\# \xi'$. Having such an equality implies that $W_p(\vartheta(\xi), \vartheta(\xi')) \leq W_p(\vartheta(\xi), \iota_\# \xi) + W_p(\iota_\# \xi', \vartheta(\xi')) \leq 2\gamma$. This inequality is tight up to a constant. Indeed, take Y an uniform random variable on the unit sphere, let ξ be the law of $(Y, 0)$ and ξ' be the law of $((1+\gamma)Y, -\gamma Y)$. Then, ξ and ξ' are in $\mathcal{Q}_d^{s,k}(\gamma)$ and $\iota_\# \xi = \iota_\# \xi'$, whereas, by the Kantorovitch-Rubinstein duality formula,

$$W_p(\vartheta(\xi), \vartheta(\xi')) \geq W_1(\vartheta(\xi), \vartheta(\xi')) \geq \mathbb{E}[\phi((1+\gamma)Y) - \phi(Y)]$$

for any 1-Lipschitz function ϕ. Letting ϕ be the distance to the unit sphere, we obtain that this distance is larger than γ. In that sense, γ represents the maximal precision for the estimation of $\vartheta(\xi)$.

Remark 5.1.11. For ease of notation, we will write in the following $a \lesssim b$ to indicate that there exists a constant C depending on the parameters $p, k, \tau_{\min}, L_s, L_k, f_{\min}, f_{\max}$, **but not on s and D**, such that $a \leq Cb$, and write $a \asymp b$ to indicate that $a \lesssim b$ and $b \lesssim a$. Also, we will write c_α to indicate that a constant c depends on some parameter α.

5.2 Kernel density estimation on an unknown manifold

Before building an estimator in the model $\mathcal{Q}_d^{s,k}(\gamma)$, let us consider the easier problem of the estimation of μ in the case where $\gamma = 0$ (noise free model) and the support M is known. Let $\mu \in \mathcal{Q}^s(M)$ and $Y_1, \dots, Y_n$ be a n-sample of law μ. Let $\mu_n = \frac{1}{n}\sum_{i=1}^n \delta_{Y_i}$ be the empirical measure of the sample. Identify $\mathbb{R}^d$ with $\mathbb{R}^d \times \{0\}^{D-d}$ and consider a kernel $K : \mathbb{R}^D \to \mathbb{R}$ satisfying the following conditions:

- **Condition** A**:** The kernel K is a smooth radial function with support $\mathcal{B}(0,1)$ such that $\int_{\mathbb{R}^d} K = 1$.
- **Condition** $B(m)$**:** The kernel K is of order $m \geq 0$ in the following sense. Let $|\alpha| := \sum_{j=1}^d \alpha_j$ be the length of a multiindex $\alpha = (\alpha_1, \dots, \alpha_d)$. Then, for all multiindexes α^0, α^1 with $0 \leq |\alpha^0| < m$, $0 \leq |\alpha^1| < m + |\alpha_0|$, and with $|\alpha^1| > 0$ if $\alpha^0 = 0$, we have
$$\int_{\mathbb{R}^d} \partial^{\alpha^0} K(v) v^{\alpha^1} \mathrm{d}v = 0, \tag{5.12}$$
where $v^\alpha = \prod_{j=1}^d v_j^{\alpha_j}$ and $\partial^\alpha K$ is the partial derivative of K in the direction α.
- **Condition** $C(\beta)$**:** The negative part K_- of K satisfies $\int_{\mathbb{R}^d} K_- \leq \beta$.

We show in Section 5.4.8 that for every integer $m \geq 0$ and real number $\beta > 0$, there exists a kernel K satisfying conditions A, $B(m)$ and $C(\beta)$. Define the convolution of K with a measure $\nu \in \mathcal{P}(\mathbb{R}^D)$ as
$$K * \nu(x) := \int K(x-y)\mathrm{d}\nu(y), \quad x \in \mathbb{R}^D, \tag{5.13}$$
and, for $h > 0$, let $K_h := h^{-d}K(\cdot/h)$. Let $\rho_h := K_h * \mathrm{vol}_M$ and let $\mu_{n,h}$ be the measure with density $K_h * (\mu_n/\rho_h)$ with respect to vol_M. Dividing by ρ_h ensures that $\mu_{n,h}$ is a measure of mass 1. Remark that the computation of $\mu_{n,h}$ requires to have access to M, that is $\mu_{n,h}$ is an estimator on $\mathcal{Q}^s(M)$ but not on $\mathcal{Q}_d^{s,k}$. By linearity, the expectation of $\mu_{n,h}$ is given by μ_h, the measure having for density $K_h * (\mu/\rho_h)$ on M.

Theorem 5.2.1. *Let $d \leq D$ be integers, $0 < s \leq k-1$ with $k \geq 2$ and $1 \leq p < \infty$. Let $M \in \mathcal{M}^{k,d}$ and $\mu \in \mathcal{Q}^s(M)$ with $Y_1, \dots, Y_n$ a n-sample of law μ. There exists a constant β depending on the parameters of the model such that, if K is a kernel satisfying conditions A, $B(k)$ and $C(\beta)$, then the measure $\mu_{n,h}$ satisfies the following:*

(i) If $(\log n/n)^{1/d} \lesssim h \lesssim 1$, then, with probability larger than $1 - cn^{-k/d}$, the density of $\mu_{n,h}$ is larger than $f_{\min}/2$ and smaller than $2f_{\max}$ everywhere on M.

(ii) We have
$$\mathbb{E}\|\mu - \mu_{n,h}\|_{H_p^{-1}(M)} \leq \|\mu - \mu_h\|_{H_p^{-1}(M)} + \mathbb{E}\|\mu_{n,h} - \mu_h\|_{H_p^{-1}(M)} \tag{5.14}$$
$$\lesssim h^{s+1} + \frac{h^{1-d/2} I_d(h)}{\sqrt{n}}, \tag{5.15}$$
where $I_d(h) = 1$ if $d \geq 3$, $(-\log(h))^{1/2}$ if $d = 2$ and $h^{-1/2}$ if $d = 1$.

(iii) Let $h \asymp n^{-1/(2s+d)}$ if $d \geq 3$, $h \asymp (\log n/n)^{1/d}$ if $d \leq 2$. Define $\mu_{n,h}^0 = \mu_{n,h}$ if $\mu_{n,h}$ is a probability measure and $\mu_{n,h}^0 = \delta_{X_1}$ otherwise. Then,
$$\mathbb{E}W_p(\mu_{n,h}^0, \mu) \lesssim \begin{cases} n^{-\frac{s+1}{2s+d}} & \text{if } d \geq 3, \\ n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}} & \text{if } d = 2, \\ n^{-\frac{1}{2}} & \text{if } d = 1. \end{cases} \tag{5.16}$$

(iv) Furthermore, for any $0 \leq s < k$ and $\tau_{\min} > 0$, if $f_{\min}$ is small enough and if $f_{\max}$ and L_s are large enough, then there exists a manifold $M \in \mathcal{M}_d^k$ such that

$$\mathcal{R}_n(\mu, W_p, \mathcal{Q}^s(M)) \gtrsim \begin{cases} n^{-\frac{s+1}{2s+d}} & \text{if } d \geq 3, \\ n^{-\frac{1}{2}} & \text{if } d \leq 2. \end{cases} \tag{5.17}$$

Remark 5.2.2. The condition $C(\beta)$ on the kernel is only used to ensure that the measure $\mu_{n,h}$ has a lower and upper bounded density on M. An alternative possibility to ensure this property is to assume that the density of μ is Hölder continuous of exponent δ for some $\delta > 0$. Techniques from [BH19] then imply that $\|\mu_{n,h} - \mu\|_{L^\infty(M)} \lesssim h^\delta + n^{-1/2}h^{-d/2} \ll 1$ with high probability, ensuring in particular that the density is lower bounded. If $sp > d$, then every element of $B^s_{p,q}(M)$ is Hölder continuous (by [Tri92, Theorem 7.4.2]), and condition $C(\beta)$ is no longer required. However, Theorem 5.2.1 also holds for non-continuous densities.

Remark 5.2.3. Let K be a nonnegative kernel satisfying conditions A, $B(0)$ and $C(\beta)$. It is straightforward to check that $W_p(\mu_n, \mu_{n,h}) \lesssim h$. Therefore, Theorem 5.2.1(ii) and Proposition 5.1.6 imply in particular that $W_p(\mu_n, \mu) \lesssim h + \frac{h^{1-d/2} I_d(h)}{\sqrt{n}}$. By choosing h of the order $n^{-1/d}$, we obtain that

$$W_p(\mu_n, \mu) \lesssim \begin{cases} n^{-\frac{1}{d}} \text{ if } d \geq 3 \\ n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}} \text{ if } d = 2 \\ n^{-\frac{1}{2}} \text{ if } d = 1. \end{cases} \tag{5.18}$$

Such a result was already shown for $p = \infty$ [Tri+20] with additional logarithmic factors, with a proof very different from ours. See also [Div21a] for a short proof of this result when M is the flat torus.

In (5.15), a classical bias-variance trade-off appears. Namely, the bias of the estimator is of order h^{s+1}, whereas its fluctuations are of order $h^{1-d/2}/\sqrt{n}$ (at least for $d \geq 3$). This decomposition can be compared to the classical bias-variance decomposition for a kernel density estimator of bandwidth h, say for the pointwise estimation of a function of class $\mathcal{C}^s$ on the cube $[0,1]^d$. It is then well-known (see e.g. [Tsy08, Chapter 1]) that the bias of the estimator is of order h^s whereas its variance is of order $h^{-d/2}/\sqrt{n}$. The supplementary factor h appearing both in the bias and fluctuation terms can be explained by the fact that we are using a norm $H_p^{-1}(M)$ instead of a pointwise norm to quantify the risk of the estimator: in some sense, we are estimating the antiderivative of the density rather than the density itself. This is particularly true if $d = 1$ and $p = 1$, where the Wasserstein distance between two measures is given by the L_1 distance between the cumulative distribution functions of the two measures [San15, Proposition 2.17].

Before giving a proof of Theorem 5.2.1, let us explain how to extend it to the case where the manifold M is unknown and in the presence of orthogonal noise. The measure $\mu_{n,h}$ is the measure having density $K_h * (\mu_n/\rho_h)$ with respect to vol_M. Of course, if M is unknown, then so is vol_M, and we therefore propose the following estimation procedure of vol_M, using local polynomial estimation techniques from [AL19]. Let $X_1, \ldots, X_n$ be a n-sample in the model with orthogonal noise $\mathcal{Q}_d^{s,k}(\gamma)$, with $X_i = Y_i + Z_i$, Y_i of law μ and $Z_i \in T_{Y_i}M^\perp$ with $|Z_i| \leq \gamma$. Let $\nu_n^{(i)}$ be the empirical measure $\frac{1}{n-1}\sum_{j \neq i} \delta_{X_j - X_i}$. For two positive parameters ℓ, ε, the local polynomial

estimator $(\hat{\pi}_i, \hat{V}_{2,i}, \dots, \hat{V}_{m-1,i})$ of order m at X_j is defined as an element of

$$\underset{\pi, \sup_{2\le j\le m-1}\|V_j\|_{\mathrm{op}}\le \ell}{\arg\min} \nu_n^{(i)} \left(\left| x - \pi(x) - \sum_{j=2}^{m-1} V_j[\pi(x)^{\otimes j}] \right|^2 \mathbf{1}\{x \in \mathcal{B}(0,\varepsilon)\} \right), \tag{5.19}$$

where the argmin is taken over all orthogonal projectors π of rank d and symmetric tensors $V_j : (\mathbb{R}^D)^j \to \mathbb{R}^D$ of order j.[1] Let $\hat{T}_i$ be the image of $\hat{\pi}_i$ and $\hat{\Psi}_i : v \in \mathbb{R}^D \mapsto X_i + v + \sum_{j=2}^{m-1} \hat{V}_{j,i}[v^{\otimes j}]$. We summarize the results of [AL19] in the following proposition (see Section 5.4.1 for details).

Proposition 5.2.4. *With probability at least $1 - cn^{-k/d}$, if $m \le k$, $(\log n/n)^{1/d} \lesssim \varepsilon \lesssim 1$, $\gamma \lesssim \varepsilon$ and $1 \lesssim \ell \lesssim \varepsilon^{-1}$, then,*

$$\max_{1\le i\le n} \angle(T_{Y_i}M, \hat{T}_i) \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1} \tag{5.20}$$

and, for all $1 \le i \le n$, if $v \in \hat{T}_i$ with $|v| \le 3\varepsilon$, we have

$$|\hat{\Psi}_i(v) - \Psi_{Y_i} \circ \pi_{Y_i}(v)| \lesssim \varepsilon^m + \gamma \tag{5.21}$$

$$\left\| d\hat{\Psi}_i(v) - d(\Psi_{Y_i} \circ \pi_{Y_i})(v) \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1}. \tag{5.22}$$

Hence, if γ is of order at most ε^k, by choosing $m = k$, it is possible to approximate the tangent space at Y_i with precision ε^{k-1} and the local parametrization with precision ε^k. In particular, authors in [AL19] show that, with high probability, $\bigcup_{i=1}^n \mathcal{B}_{\hat{\Psi}_i(\hat{T}_i)}(X_i, \varepsilon)$ is at Hausdorff distance less than $\varepsilon^k + \gamma$ from M (up to a constant). We now define an estimator $\widehat{\mathrm{vol}}_M$ of vol_M by using an appropriate partition of unity $(\chi_j)_j$, which is built thanks to the next lemma. We say that a set S is δ-sparse if $|x - y| \ge \delta$ for all distinct points $x, y \in S$. Recall that M^δ denotes the δ-neighborhood of the set M.

Lemma 5.2.5 (Construction of partitions of unity)**.** *Let $\delta \lesssim 1$. Let $S \subset M^\delta$ be a set which is $\frac{7}{3}\delta$-sparse, with $d_H(M^\delta|S) \le 4\delta$. Let $\theta : \mathbb{R}^D \to [0,1]$ be a smooth radial function supported on $\mathcal{B}(0,1)$, which is equal to 1 on $\mathcal{B}(0,1/2)$. Define, for $y \in M^\delta$ and $x \in S$,*

$$\chi_x(y) = \frac{\theta\left(\frac{y-x}{8\delta}\right)}{\sum_{x'\in S} \theta\left(\frac{y-x'}{8\delta}\right)}. \tag{5.23}$$

Then, the sequence of functions $\chi_x : M^\delta \to [0,1]$ for $x \in S$, satisfies (i) $\sum_{x\in S} \chi_x \equiv 1$, with at most c_d non-zero terms in the sum at any given point of M^δ, (ii) $\|\chi_x\|_{\mathcal{C}^l(M^\delta)} \le C_{l,d}\delta^{-l}$ for any $l \ge 0$ and, (iii) χ_x is supported on $\mathcal{B}_{M^\delta}(x, 8\delta)$.

A proof of Lemma 5.2.5 is given in Section 5.4.1. Given a set $S_0 \subset M^\delta$ with $d_H(M^\delta|S_0) \le 5\delta/3$, the farthest sampling algorithm with parameter $7\delta/3$ (see e.g. [AL18, Section 3.3]) outputs a set $S \subset S_0$ which is $7\delta/3$-sparse and $7\delta/3$-close from S: the set S then satisfies the hypothesis of Lemma 5.2.5. The next proposition describes how we may define a minimax estimator $\widehat{\mathrm{vol}}_M$ of the volume measure on M (up to logarithmic factors) using such a partition of unity.

Theorem 5.2.6 (Minimax estimation of the volume measure on M)**.** *Let $d \le D$ be integers and $k \ge 2$. Let $\xi \in \mathcal{Q}_d^{0,k}(\gamma)$ and let $X_1, \dots, X_n$ be a n-sample of law $\iota_\# \xi$. Let $(\log n/n)^{1/d} \lesssim \varepsilon \lesssim 1$, $\gamma \lesssim \varepsilon$, $1 \lesssim \ell \lesssim \varepsilon^{-1}$.*

[1] The existence of such a measurable application follows from the Kuratowski-Ryll-Nardzewski selection theorem [AB06, Theorem 18.13].

(i) *Let $\{X_{i_1}, \dots, X_{i_J}\}$ be the output of the farthest point sampling algorithm with parameter $7\varepsilon/24$ and input $\{X_1, \dots, X_n\}$. With probability larger than $1 - cn^{-k/d}$, there exists a sequence of smooth nonnegative functions $\chi_j : M^{\varepsilon/8} \to [0,1]$ for $1 \le j \le J$, such that χ_j is supported on $\mathcal{B}_{M^{\varepsilon/8}}(X_{i_j}, \varepsilon)$, $\|\chi_j\|_{\mathcal{C}^1(M^{\varepsilon/8})} \lesssim \varepsilon^{-1}$ and $\sum_{j=1}^J \chi_j(z) = 1$ for $z \in M^{\varepsilon/8}$, with at most c_d non-zero terms in the sum.*

(ii) *Let $\hat{\Psi}_i$ be the local polynomial estimator of order $m \le k$ with parameter ε and ℓ, and $\hat{T}_i$ the associated tangent space. Let $\widehat{\mathrm{vol}}_M$ be the measure defined by, for all continuous bounded functions $f : \mathbb{R}^D \to \mathbb{R}$,*

$$\int f(x) \mathrm{d}\widehat{\mathrm{vol}}_M(x) = \sum_{j=1}^J \int_{\hat{\Psi}_{i_j}(\hat{T}_{i_j})} f(x)\chi_j(x)\mathrm{d}x, \tag{5.24}$$

where the integration is taken against the d-dimensional Hausdorff measure on $\hat{\Psi}_{i_j}(\hat{T}_{i_j})$. Then, for $1 \le r \le \infty$, with probability larger than $1 - cn^{-k/d}$, we have, for $\gamma \lesssim \varepsilon^2$,

$$W_r\left(\frac{\widehat{\mathrm{vol}}_M}{|\widehat{\mathrm{vol}}_M|}, \frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}\right) \lesssim \gamma + \varepsilon^m. \tag{5.25}$$

(iii) *In particular, if $m = k$, $\varepsilon \asymp (\log n/n)^{1/d}$ and $\gamma \lesssim \varepsilon^2$, we obtain that*

$$\mathbb{E}W_r\left(\frac{\widehat{\mathrm{vol}}_M}{|\widehat{\mathrm{vol}}_M|}, \frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}\right) \lesssim \gamma + \left(\frac{\log n}{n}\right)^{\frac{k}{d}}. \tag{5.26}$$

Also, for any $\tau_{\min} > 0$ and $0 \le s < k$, if $f_{\min}$ is small enough, and if $f_{\max}, L_k, L_s$ are large enough, then

$$\mathcal{R}_n\left(\frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}, \mathcal{Q}_d^{s,k}(\gamma), W_r\right) \gtrsim \gamma + \left(\frac{1}{n}\right)^{\frac{k}{d}}. \tag{5.27}$$

Let $\hat{\rho}_h := K_h * \widehat{\mathrm{vol}}_M$. We define $\hat{\nu}_{n,h}$ as the measure having density $K_h * (\nu_n/\hat{\rho}_h)$ with respect to the measure $\widehat{\mathrm{vol}}_M$, where $\nu_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ is the empirical measure of the sample $(X_1, \dots, X_n)$.

Theorem 5.2.7. *Let $d \le D$ be integers, $0 < s \le k-1$ with $k \ge 2$ and $1 \le p < \infty$. Let $\xi \in \mathcal{Q}_d^{s,k}(\gamma)$, with μ the first marginal of ξ and let $X_1, \dots, X_n$ be a n-sample of law $\iota_\# \xi$. There exists a constant β depending on the parameters of the model such that the following holds. Assume that K is a kernel satisfying conditions A, $B(k)$ and $C(\beta)$, that $(\log n/n)^{1/d} \lesssim \varepsilon \lesssim h \lesssim 1$, $\gamma \lesssim \varepsilon^2$, $1 \lesssim \ell \lesssim \varepsilon^{-1}$ and consider the estimator $\widehat{\mathrm{vol}}_M$ defined in (5.24) with parameters m, ε and ℓ. Then,*

(i) *The measure $\hat{\nu}_{n,h}$ is a nonnegative measure with probability larger than $1 - cn^{-k/d}$.*

(ii) *Define $\hat{\nu}^0_{n,h} = \hat{\nu}_{n,h}$ if $\hat{\nu}_{n,h}$ is a nonnegative measure and $\hat{\nu}^0_{n,h} = \delta_{X_1}$ otherwise. Then, with probability larger than $1 - cn^{-k/d}$,*

$$W_p(\hat{\nu}^0_{n,h}, \mu^0_{n,h}) \lesssim \gamma + \varepsilon^m. \tag{5.28}$$

(iii) In particular, let $m = \lceil s+1 \rceil$, $\varepsilon \asymp (\ln n/n)^{1/d}$, $\ell \asymp \varepsilon^{-1}$ *and* $h \asymp n^{-1/(2s+d)}$ *if* $d \geq 3$, $h \asymp (\log n/n)^{1/d}$ *if* $d \leq 2$. *Then,*

$$\mathbb{E}W_p(\hat{\nu}^0_{n,h}, \mu) \lesssim \gamma + \begin{cases} n^{-\frac{s+1}{2s+d}} & \text{if } d \geq 3 \\ n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}} & \text{if } d = 2 \\ n^{-\frac{1}{2}} & \text{if } d = 1. \end{cases} \tag{5.29}$$

(iv) Furthermore, if $0 \leq s < k$ *and* $\tau_{\min} > 0$, *for any* $f_{\min}$ *small enough and* $f_{\max}$, L_s, L_k *large enough, we have*

$$\mathcal{R}_n(\mu, \mathcal{Q}^{s,k}_d(\gamma), W_p) \gtrsim \gamma + \begin{cases} n^{-\frac{s+1}{2s+d}} + n^{-\frac{k}{d}} & \text{if } d \geq 3, \\ n^{-\frac{1}{2}} & \text{if } d \leq 2. \end{cases} \tag{5.30}$$

Remark 5.2.8 (Numerical considerations). There are several considerations worth of interest concerning the numerical implementation of the estimators $\widehat{\mathrm{vol}}_M$ and $\hat{\nu}_{n,h}$. In a preprocessing step, one must first solve the optimization problem (5.19) for each element X_{i_j} of the output of the farthest point sampling algorithm. Let N_j be the number of points of the sample at distance less than ε from X_{i_j} (which is with high probability of order $n\varepsilon^d \asymp \log n$). For $k = 2$, minimizing (5.19) is equivalent to performing a PCA on the N_j neighbors of X_{i_j}, with a corresponding time complexity of order $\mathcal{O}(N_j^3)$ with high probability. For $k \geq 3$, as the space of orthogonal projectors of rank d is a non-convex manifold, the minimization of the objective function is more delicate. In [ZJRS16], a Riemannian SVRG procedure is proposed to minimize a functional defined on some Riemannian manifold. Their procedure outputs values whose costs are provably close to the minimal value of the objective function, even for non-convex smooth functions. The implementation of such an algorithm is a promising way to minimize (5.19) in practice.

Then, the uniform measure on M can be approximated by considering the empirical measure $(\hat{U}_M)_N$ of a N-sample of law $\hat{U}_M := \widehat{\mathrm{vol}}_M / |\widehat{\mathrm{vol}}_M|$. To create such a sample, we may use importance sampling techniques to sample according to the measure with density χ_j on $\hat{\Psi}_{i_j}(\hat{T}_{i_j})$. Finally, the measure $\hat{\nu}^{(N)}_{n,h}$ with density $K_h * (\nu_n/\hat{\rho}_h)$ with respect to $(\hat{U}_M)_N$ may be used as a proxy for $\hat{\nu}_{n,h}$.

5.3 Proofs of the main theorems

5.3.1 Bias of the kernel density estimator

The first step to prove Theorem 5.2.1 is to study the bias of the estimator, given by the distance $\|\cdot\|_{H_p^{-1}(M)}$ between μ_h and μ. Write $\tilde{\phi}$ for ϕ/ρ_h. Introduce the operator $A_h : B^s_{p,q}(M) \to H_p^{-1}(M)$ defined for $\phi \in L_1(M)$ and $x \in M$ by

$$A_h\phi(x) := K_h * \left(\frac{\phi(x)}{\rho_h(x)}\right) - \phi(x) = \int_M K_h(x-y)\left(\tilde{\phi}(y) - \tilde{\phi}(x)\right) \mathrm{dvol}_M(x). \tag{5.31}$$

Then,

$$\begin{aligned} \|\mu_h - \mu\|_{H_p^{-1}(M)} = \|A_h f\|_{H_p^{-1}(M)} &\leq \|A_h\|_{B^s_{p,q}(M), H_p^{-1}(M)} \|f\|_{B^s_{p,q}(M)} \\ &\leq \|A_h\|_{B^s_{p,q}(M), H_p^{-1}(M)} L_s. \end{aligned} \tag{5.32}$$

Proposition 5.3.1. *Let* $0 < s \leq k-1$, $1 \leq p < \infty$, *and assume that the kernel* K *is of order* k. *Then, if* $h \lesssim 1$,

$$\|A_h\|_{B^s_{p,q}(M), H_p^{-1}(M)} \lesssim h^{s+1}. \tag{5.33}$$

The proof of Proposition 5.3.1 consists in using the Taylor expansion of a function $\phi \in B^s_{p,q}(M)$, and by using that all polynomial terms of low order in the Taylor expansion disappear when integrated against K, as the kernel K is of sufficiently large order. Namely, we have the following property, whose proof is given in Section 5.4.3.

Lemma 5.3.2. *Assume that the kernel K is of order k and let $B : (\mathbb{R}^D)^j \to \mathbb{R}$ be a tensor of order $1 \le j < k$. Then, for all $x \in M$,*

$$\left| \int_M K_h(x-y) B[(x-y)^{\otimes j}] \mathrm{d}y \right| \lesssim \|B\|_{\mathrm{op}} h^k \tag{5.34}$$

$$|\rho_h(x) - 1| \lesssim h^{k-1} \quad \textit{and} \quad \|\rho_h\|_{\mathcal{C}^j(M)} \lesssim h^{k-1-j} \tag{5.35}$$

Let us now give a sketch of proof of Proposition 5.3.1 in the case $0 < s \le 1$. The $H^{-1}_p(M)$-norm of $A_h\phi$ is by definition equal to

$$\|A_h\phi\|_{H^{-1}_p(M)} = \sup \left\{ \int (A_h\phi) g \mathrm{dvol}_M, \ \|g\|_{H^1_{p^*}(M)} \le 1 \right\}.$$

Let $g \in H^1_{p^*}(M)$ with $\|g\|_{H^1_{p^*}(M)} \le 1$. We use the following symmetrization trick:

$$\begin{aligned}
\int A_h\phi(x) g(x) \mathrm{d}x &= \iint K_h(x-y)(\tilde\phi(y) - \tilde\phi(x)) g(x) \mathrm{d}y \mathrm{d}x \\
&= \iint K_h(y-x)(\tilde\phi(x) - \tilde\phi(y)) g(y) \mathrm{d}y \mathrm{d}x \qquad \text{(by swapping the indexes } x \text{ and } y\text{)} \\
&= \frac{1}{2} \iint K_h(x-y)(\tilde\phi(y) - \tilde\phi(x))(g(x) - g(y)) \mathrm{d}y \mathrm{d}x
\end{aligned} \tag{5.36}$$

where, at the last line, we averaged the two previous lines and used that K is an even function. Informally, as $K_h(x-y) = 0$ if $|x-y| \ge h$, and as ρ_h is roughly constant, we expect $|\tilde\phi(y) - \tilde\phi(x)|$ to be of order h^s and $|g(x) - g(y)|$ to be of order h, leading to a bound of $\int A_h\phi(x)g(x)\mathrm{d}x$ of order h^{s+1}. For $l \ge 1$, the following analog of the symmetrization trick holds.

Lemma 5.3.3 (Symmetrization trick)**.** *There exists $h_0 \lesssim 1$ such that the following holds. Let $0 \le l \le k-1$ be even and let $K^{(l)}(x) = \int_0^1 K_\lambda(x) \frac{(1-\lambda)^{l-1}\lambda^{-l}}{(l-1)!} \mathrm{d}\lambda$ for $x \in \mathbb{R}^D$. Fix $x_0 \in M$ and let $\phi \in \mathcal{C}^\infty(M)$ be a function supported in $\mathcal{B}_M(x_0, h_0)$. Define $\tilde\phi_l := d^l(\tilde\phi \circ \Psi_{x_0}) \circ \tilde\pi_{x_0}$. Let $g \in L_{p^*}(M)$ with $\|g\|_{L_{p^*}(M)} \le 1$. Then, for $h \lesssim 1$, $\int A_h\phi(x)g(x)\mathrm{d}x$ is equal to*

$$\frac{1}{2} \iint_{\mathcal{B}_M(x_0,h_0)^2} K^{(l)}_h(x-y)(\tilde\phi_l(y) - \tilde\phi_l(x)) \left[\pi_{x_0}(x-y)\right]^{\otimes l} (g(x) - g(y)) \, \mathrm{d}y \mathrm{d}x + R, \tag{5.37}$$

where R is a remainder term satisfying $|R| \lesssim \|\tilde\phi\|_{H^l_p(M)} h^{l+1}$. Furthermore, if $l \le k-2$ is even, we have $|R| \lesssim \|\tilde\phi\|_{H^{l+1}_p(M)} h^{l+2}$.

Lemma 5.3.4. *Let $\eta \in \mathcal{C}^\infty(M)$ and let $0 \le l \le k-2$. Assume that either $l = 0$ or that η is supported on $\mathcal{B}_M(x_0, h_0)$. Let $\eta_l = d^l(\eta \circ \Psi_{x_0}) \circ \tilde\pi_{x_0}$. Then, for any $h \lesssim 1$,*

$$\begin{aligned}
&\left(h^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \le h\} \frac{\|\eta_l(x) - \eta_l(y)\|^p_{\mathrm{op}}}{|x-y|^p} \mathrm{d}x \mathrm{d}y \right)^{1/p} \\
&\qquad \lesssim \left(\int_{\mathcal{B}_M(x_0,h_0)} \|\eta_{l+1}(x)\|^p_{\mathrm{op}} \, \mathrm{d}x \right)^{1/p} \lesssim \|\eta\|_{H^{l+1}_p(M)}.
\end{aligned} \tag{5.38}$$

Proofs of Lemma 5.3.3 and Lemma 5.3.4 are found in Section 5.4.3. We may now conclude the proof using those two lemmas. Let $\phi \in \mathcal{C}^\infty(M)$ be a function supported in $\mathcal{B}_M(x_0, h_0)$ and $g \in H^1_{p^*}(M)$ with $\|g\|_{H^1_{p^*}(M)} \leq 1$.

Case 1: s is even Let $l = s$. Assume first that $p > 1$ and that g is smooth. We have

$$\iint_{\mathcal{B}_M(x_0,h_0)^2} |K_{\lambda h}(x-y)| \left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}} |g(x) - g(y)||x-y|^l \mathrm{d}x\mathrm{d}y \tag{5.39}$$

$$\leq \|K\|_\infty (\lambda h)^{l+1-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}} \frac{|g(x)-g(y)|}{|x-y|} \mathrm{d}x\mathrm{d}y$$

$$\leq \|K\|_\infty (\lambda h)^{l+1} \left((\lambda h)^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}}^p \mathrm{d}x\mathrm{d}y \right)^{1/p}$$

$$\times \left((\lambda h)^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \frac{|g(x)-g(y)|^{p^*}}{|x-y|^{p^*}} \mathrm{d}x\mathrm{d}y \right)^{1/p^*}$$

$$\lesssim (\lambda h)^{l+1} \left(2^p (\lambda h)^{-d} \int_{x \in \mathcal{B}_M(x_0,h_0)} \left\|\tilde{\phi}^l(x)\right\|_{\mathrm{op}}^p \mathrm{vol}_M(\mathcal{B}_M(x, \lambda h)) \mathrm{d}x \right)^{1/p} \|g\|_{H^1_{p^*}(M)}$$

$$\lesssim \|\tilde{\phi}\|_{H^l_p(M)} (\lambda h)^{l+1} \lesssim \|\phi\|_{H^l_p(M)} (\lambda h)^{l+1}, \tag{5.40}$$

where at the last line, we used Proposition 3.5.7.7 to control the volume of $\mathcal{B}_M(x, \lambda h)$ and, at the second to last line, we used Lemma 5.3.4. Furthermore, it follows from Leibniz formula for the derivative of a product and Lemma 5.3.2 that $\|\tilde{\phi}\|_{H^l_p(M)} \lesssim \|\phi\|_{H^l_p(M)}$.

As $\mathcal{C}^\infty(M)$ is dense in $H^1_{p^*}(M)$, inequality (5.40) actually holds for every $g \in H^1_{p^*}(M)$. If $p = 1$, then every function $g \in H^1_{p^*}(M)$ with $\|g\|_{H^1_{p^*}(M)} \leq 1$ is Lipschitz continuous for the distance d_g (see Remark 5.1.2). Using that $d_g(x, y) \leq 2|x-y|$ if $|x-y| \leq \tau_{\min}/2$, a similar computation than in the case $p < \infty$ shows that inequality (5.40) also holds if $p = \infty$.

By integrating inequality (5.40) against $\lambda \in (0, 1)$ and by using Lemma 5.3.3, we obtain the inequality $\|A_h \phi\|_{H^{-1}_p(M)} \lesssim h^{s+1} \|\phi\|_{H^s_p(M)}$.

Case 2: s is odd Similarly, we treat the case where $s \leq k-1$ is odd. Let $l = s-1$. Once again, assume first that $p > 1$ and that g is smooth. Then,

$$\iint_{\mathcal{B}_M(x_0,h_0)^2} |K_{\lambda h}(x-y)| \left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}} |g(x) - g(y)||x-y|^l \mathrm{d}x\mathrm{d}y$$

$$\leq \iint_{\mathcal{B}_M(x_0,h_0)^2} |K_{\lambda h}(x-y)| \frac{\left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}}}{|x-y|} \frac{|g(x)-g(y)|}{|x-y|} |x-y|^{l+2} \mathrm{d}x\mathrm{d}y$$

$$\leq \|K\|_\infty (\lambda h)^{l+2-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \frac{\left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}}}{|x-y|} \frac{|g(x)-g(y)|}{|x-y|} \mathrm{d}x\mathrm{d}y$$

$$\leq \|K\|_\infty (\lambda h)^{l+2} \left((\lambda h)^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \frac{\left\|\tilde{\phi}_l(y) - \tilde{\phi}_l(x)\right\|_{\mathrm{op}}^p}{|x-y|^p} \mathrm{d}x\mathrm{d}y \right)^{1/p}$$

$$\times \left((\lambda h)^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq \lambda h\} \frac{|g(x)-g(y)|^{p^*}}{|x-y|^{p^*}} \mathrm{d}x\mathrm{d}y \right)^{1/p^*}$$

$$\lesssim (\lambda h)^{l+2}\|\phi\|_{H^s_p(M)}, \tag{5.41}$$

where at last line we used Lemma 5.3.4 and the inequality $\|\tilde{\phi}\|_{H^l_p(M)} \lesssim \|\phi\|_{H^l_p(M)}$. As in the previous case, the same inequality holds for $g \in H^1_{p^*}(M)$ non necessarily smooth and if $p = 1$. By using Lemma 5.3.3 and by integrating (5.41) against $\lambda \in (0, 1)$, we obtain that $\|A_h\phi\|_{H^{-1}_p(M)} \lesssim h^{s+1}\|\phi\|_{H^s_p(M)}$.

So far, we have proven that

$$\|A_h\phi\|_{H^{-1}_p(M)} \lesssim h^{s+1}\|\phi\|_{H^s_p(M)} \tag{5.42}$$

for all integers $0 \leq s \leq k-1$ and ϕ a smooth function supported on $\mathcal{B}_M(x_0, h_0)$. To obtain the result when ϕ is not supported on some ball $\mathcal{B}_M(x_0, h_0)$, we use an appropriate partition of unity. Indeed, for $\delta = h_0/8$, standard packing arguments show the existence of a set S_0 of cardinality $N \leq c_d|\mathrm{vol}_M|\delta^{-d}$ with $d_H(M^\delta|S_0) \leq 5\delta/3$. By the remark following Lemma 5.2.5, the output S of the farthest point sampling algorithm with parameter $7\delta/3$ satisfies the assumption of Lemma 5.2.5, and is of cardinality smaller than $N \lesssim 1$. We consider such a covering $(\mathcal{B}_M(x, h_0))_{x\in S}$, with associated partition of unity $(\chi_x)_{x\in S}$. Then, $\|A_h\phi\|_{H^{-1}_p(M)}$ is bounded by

$$\begin{aligned}\sum_{x\in S}\|A_h(\chi_x\phi)\|_{H^{-1}_p(M)} &\lesssim h^{s+1}\sum_{x\in S}\|\chi_x\phi\|_{H^s_p(M)}\\ &\lesssim h^{s+1}\sum_{x\in S}\|\chi_x\|_{\mathcal{C}^s(M)}\|\phi\|_{H^s_p(M)} \lesssim h^{l+1}\|\phi\|_{H^s_p(M)},\end{aligned}$$

where the second to last inequality follows from Leibniz rule for the derivative of a product. Also, the last inequality follows from the fact that $(\chi_x)_{|M} = \chi_x \circ i_M$, where $i_M : M \to M^\delta$ is the inclusion, which is a $\mathcal{C}^k$ function with controlled $\mathcal{C}^k$-norm. Hence, $\|\chi_x\|_{\mathcal{C}^s(M)} \lesssim \|\chi_x\|_{\mathcal{C}^s(M^\delta)} \lesssim 1$ by the chain rule.

As $\mathcal{C}^\infty(M)$ is dense in $H^s_p(M)$, this gives the desired bound on the operator norm of $A_h : H^s_p(M) \to H^{-1}_p(M)$ for $0 \leq s \leq k-1$ an integer. To obtain the conclusion for Besov spaces $B^s_{p,q}(M)$, we use the interpolation inequality (5.9). By the reiteration theorem [Lun18, Theorem 1.3.5], for $0 < s < k-1$, $B^s_{p,q}(M) = (L_p(M), H^{k-1}_p(M))_{s/(k-1),q}$, with an equivalent norm. Hence, we have, for $0 < s < k-1$,

$$\begin{aligned}\|A_h\|_{B^s_{p,q}(M),H^{-1}_p(M)} &\lesssim \|A_h\|^{1-\theta}_{L_p(M),H^{-1}_p(M)}\|A_h\|^{\theta}_{H^{k-1}_p(M),H^{-1}_p(M)}\\ &\lesssim h^{1-\frac{s}{k-1}}h^{k\frac{s}{k-1}} \lesssim h^{s+1},\end{aligned}$$

so that Proposition 5.3.1 is proven for $s < k-1$. It remains to prove the inequality in the case $s = k-1$. By Fatou's lemma and the definition of interpolation spaces (5.8), we have, for some constant C not depending on s,

$$\|A_hf\|_{B^{k-1}_{p,q}(M)} \leq \liminf_{\substack{s\to k-1\\ s<k-1}}\|A_hf\|_{B^s_{p,q}(M)} \leq \liminf_{\substack{s\to k-1\\ s<k-1}}\left(Ch^{s+1}\|f\|_{B^s_{p,q}(M)}\right) \leq Ch^k\|f\|_{B^{k-1}_{p,q}(M)},$$

where we used that $\|f\|_{B^s_{p,q}(M)} \leq \|f\|_{B^{k-1}_{p,q}(M)}$. This concludes the proof of Proposition 5.3.1.

5.3.2 Fluctuations of the kernel density estimator

The purpose of this section is to prove the following bound on the fluctuations of the kernel density estimator.

Proposition 5.3.5. *Let $\mu \in \mathcal{Q}^s(M)$ with $Y_1, \dots, Y_n$ a n-sample of law μ. Assume that $h \lesssim 1$ and that $nh^d \gtrsim 1$. Then,*

$$\mathbb{E}\|\mu_{n,h} - \mu_h\|_{H_p^{-1}(M)} \lesssim n^{-1/2} h^{1-d/2} I_d(h), \tag{5.43}$$

where $I_d(h)$ is defined in Theorem 5.2.1.

Let Δ be the Laplace-Beltrami operator on M and $G : U_M \to \mathbb{R}$ be a Green's function, defined on $\{(x,y) \in M \times M,\ x \neq y\}$ (see [Aub82, Chapter 4]). By definition, if $f \in \mathcal{C}^\infty(M)$, then the function $Gf : x \in M \mapsto \int_M G(x,y) f(y) \mathrm{d}y$ is a smooth function satisfying $\Delta G f = f$, with $\nabla G f(x) = \int \nabla_x G(x,y) f(y) \mathrm{d}y$ for $x \in M$. Hence, if $w = \nabla G f$, then $\nabla \cdot w = f$, so that, Proposition 5.1.3 yields

$$\|f\|_{H_p^{-1}(M)} \leq \|f\|_{\dot{H}_p^{-1}(M)} \leq \|\nabla G f\|_{L_p(M)}.$$

By linearity, we have

$$\begin{aligned} \|\mu_{n,h} - \mu_h\|_{H_p^{-1}(M)} &= \|K_h * (\mu_n - \mu)\|_{H_p^{-1}(M)} \\ &\leq \left\| \frac{1}{n} \sum_{i=1}^n \nabla G \left(K_h * \left(\frac{\delta_{Y_i}}{\rho_h(Y_i)} \right) \right) - \mathbb{E}\left[\nabla G \left(K_h * \left(\frac{\delta_{Y_i}}{\rho_h(Y_i)} \right) \right) \right] \right\|_{L_p(M)}. \end{aligned} \tag{5.44}$$

The expectation of the L_p-norm of the sum of i.i.d. centered functions is controlled thanks to the next lemma.

Lemma 5.3.6. *Let $U_1, \dots, U_n$ be i.i.d. functions on $L_p(M)$. Then, the expectation $\mathbb{E}\left\|\frac{1}{n}\sum_{i=1}^n (U_i - \mathbb{E}U_i)\right\|_{L_p(M)}^p$ is smaller than*

$$\begin{cases} n^{-p/2} \int \left(\mathbb{E}\left[|U_1(z)|^2\right]\right)^{p/2} \mathrm{d}z & \text{if } p \leq 2, \\ C_p n^{-p/2} \int \left(\mathbb{E}|U_1(z)|^2\right)^{p/2} \mathrm{d}z + C_p n^{1-p} \int_M \mathbb{E}\left[|U_1(z)|^p\right] \mathrm{d}z & \text{if } p > 2. \end{cases} \tag{5.45}$$

Proof. If $p \leq 2$, one has by Jensen's inequality

$$\mathbb{E}\left|\sum_{i=1}^n (U_i(z) - \mathbb{E}U_i(z))\right|^p \leq \left(\mathbb{E}\left|\sum_{i=1}^n (U_i(z) - \mathbb{E}U_i(z))\right|^2\right)^{p/2} \leq n^{p/2} \left(\mathbb{E}|U_1(z)|^2\right)^{p/2}$$

and (5.45) follows by integrating this inequality against $z \in M$. For $p > 2$, we use Rosenthal inequality [Ros70, Theorem 3] for a fixed $z \in M$, and then integrate the inequality against $z \in M$. □

It remains to bound $\mathbb{E}\left[\left|\nabla G\left(K_h * \left(\frac{\delta_Y}{\rho_h(Y)}\right)\right)(z)\right|^p\right]$ where $Y \sim \mu$, $z \in M$ and $p \geq 2$.

Lemma 5.3.7. *Let $p \geq 2$. Then, for all $z \in M$ and $h \lesssim 1$,*

$$\mathbb{E}\left[\left|\nabla G\left(K_h * \left(\frac{\delta_Y}{\rho_h(Y)}\right)\right)(z)\right|^p\right] \lesssim \begin{cases} 1 & \text{if } d = 1 \\ -\log h & \text{if } p = d = 2 \\ h^{p+d-dp} & \text{else.} \end{cases} \tag{5.46}$$

A proof of Lemma 5.3.7 is found in Section 5.4.4. From (5.44), Lemma 5.3.6 and Lemma 5.3.7, we obtain, in the case $p \geq 2$ and $d \geq 3$

$$\begin{aligned}
\mathbb{E}\|\mu_{n,h} - \mu_h\|_{H_p^{-1}(M)} &\leq \left(\mathbb{E}\|\mu_{n,h} - \mu_h\|^p_{H_p^{-1}(M)}\right)^{1/p} \\
&\leq C_p n^{-1/2} \left(\int \left(\mathbb{E} \left| \nabla G \left(K_h * \left(\frac{\delta_Y}{\rho_h(Y)} \right) \right)(z) \right|^2 \right)^{p/2} \mathrm{d}z \right)^{1/p} \\
&\quad + C_p n^{1/p-1} \left(\int \mathbb{E} \left[\left| \nabla G \left(K_h * \left(\frac{\delta_Y}{\omega_h(Y)} \right) \right)(z) \right|^p \right] \mathrm{d}z \right)^{1/p} \\
&\lesssim n^{-1/2} |\mathrm{vol}_M|^{1/p} h^{1-d/2} + n^{1/p-1} |\mathrm{vol}_M|^{1/p} h^{1+d/p-d}.
\end{aligned}$$

Recalling that $|\mathrm{vol}_M| \leq f_{\min}^{-1} \lesssim 1$ and that $nh^d \gtrsim 1$, one can check that this quantity is smaller up to a constant than $n^{-1/2}h^{1-d/2}$, proving Proposition 5.3.5 in the case $p \geq 2$ and $d \geq 3$. A similar computation shows that Proposition 5.3.5 also holds if $p \leq 2$ or $d \leq 2$.

5.3.3 Proof of Theorem 5.2.1

The proof of (i) is found in Section 5.4.5. Let us now prove (ii). If $0 < s \leq k-1$, by Proposition 5.3.1 and (5.32), we have

$$\|\mu - \mu_h\|_{H_p^{-1}(M)} \leq L_s \|A_h\|_{B^s_{p,q}(M), H_p^{-1}(M)} \lesssim h^{s+1}.$$

Combining this inequality with Proposition 5.3.5 yields (5.15).

Let us prove (iii). Let E be the event described in (i). If E is realized, then $\mu^0_{n,h}$ is equal to $\mu_{n,h}$, and it satisfies $\mu^0_{n,h} \geq \frac{f_{\min}}{2}\mathrm{vol}_M$. Thus, Proposition 5.1.6 yields $W_p(\mu^0_{n,h}, \mu) \lesssim \|\mu_{n,h} - \mu\|_{H_p^{-1}(M)}$. If E is not realized, we bound $W_p(\mu^0_{n,h}, \mu)$ by $\mathrm{diam}(M)$, which is itself bounded by a constant depending only on the parameters of the model (see Proposition 3.5.7.3). Hence,

$$\begin{aligned}
\mathbb{E}W_p(\mu^0_{n,h}, \mu) &\leq \mathbb{E}\left[W_p(\mu^0_{n,h}, \mu)\mathbf{1}\{E\}\right] + \mathrm{diam}(M)\mathbb{P}(E^c) \\
&\lesssim \mathbb{E}\|\mu_{n,h} - \mu\|_{H_p^{-1}(M)} + n^{-k/d},
\end{aligned}$$

and we conclude thanks to (5.15).

Finally, a proof of (iv) is found in Section 5.4.7.

5.3.4 Proofs of Theorem 5.2.6 and Theorem 5.2.7

Proof of Theorem 5.2.6(i).

Assume that $\gamma \leq \varepsilon/24$. Let $\mathcal{X} = \{X_1, \ldots, X_n\}$ and $\mathcal{Y} = \{Y_1, \ldots, Y_n\}$. By the remark following Lemma 5.2.5, the existence of a partition of unity satisfying the requirements of Theorem 5.2.6(i) is ensured as long as $d_H(M^{\varepsilon/8}|\mathcal{X}) \leq 5\varepsilon/24$. We have $d_H(M^{\varepsilon/8}|\mathcal{X}) \leq d_H(M^{\varepsilon/8}|\mathcal{Y}) + \varepsilon/24 \leq d_H(M|\mathcal{Y}) + 4\varepsilon/24$. Hence, the partition of unity exists if $d_H(M|\mathcal{Y}) \leq \varepsilon/24$. This is satisfied with probability larger than $1 - cn^{-k/d}$ if $\varepsilon \gtrsim (\log n/n)^{1/d}$ by [Aam17, Lemma III.23].

Proof of Theorem 5.2.6(ii).

For ease of notation, we will assume that the output $\{X_{i_1}, \ldots, X_{i_J}\}$ of the farthest point sampling algorithm is equal to $\{X_1, \ldots, X_J\}$. Write ν_j for the measure having density χ_j with respect to the d-dimensional Hausdorff measure on $\hat{\Psi}_j(\hat{T}_j)$.

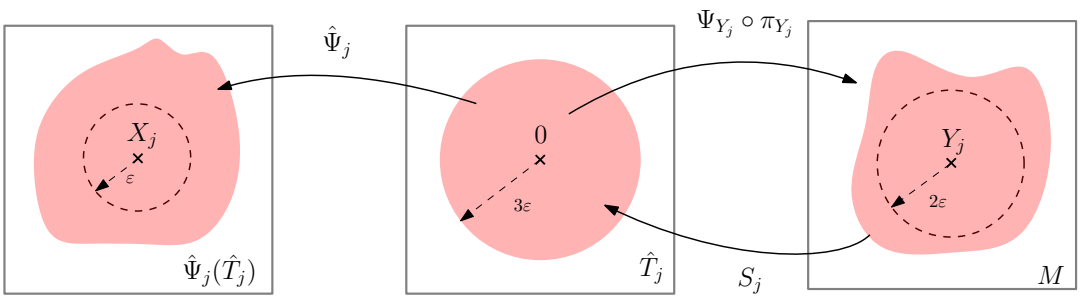


FIGURE 5.1: Illustration of Lemma 5.3.8(a)

Lemma 5.3.8. *If* $(\log n/n)^{1/d} \lesssim \varepsilon \lesssim 1$, *with probability larger than* $1 - cn^{-k/d}$, *for all* $j = 1, \dots, J$:

(a) The map $\Psi_{Y_j} \circ \pi_{Y_j} : \mathcal{B}_{\hat{T}_j}(0, 3\varepsilon) \to M$ *is a diffeomorphism on its image, which contains* $\mathcal{B}_M(Y_j, 2\varepsilon)$. *Let* $S_j : \mathcal{B}_M(Y_j, 2\varepsilon) \to \mathcal{B}_{\hat{T}_j}(0, 3\varepsilon)$ *be the inverse of* $\Psi_{Y_j} \circ \pi_{Y_j}$. *Then,* $\hat{\Psi}_j \circ S_j : \mathcal{B}_M(Y_j, 2\varepsilon) \to \hat{\Psi}_j(\hat{T}_j)$ *is also a diffeomorphism on its image, which contains* $\mathcal{B}_{\hat{\Psi}_j(\hat{T}_j)}(X_j, \varepsilon)$. *Furthermore, for all* $z \in \mathcal{B}_M(Y_j, 2\varepsilon)$, *we have* $|\hat{\Psi}_j \circ S_j(z) - X_j| \geq \frac{7}{8}|z - Y_j|$.

(b) The measure $(\hat{\Psi}_j \circ S_j)^{-1}_{\#}\nu_j$ *has a density* $\tilde{\chi}_j$ *on* M *equal to*

$$\tilde{\chi}_j(z) = \chi_j(\hat{\Psi}_j \circ S_j(z)) J(\hat{\Psi}_j \circ S_j)(z), \text{ for } z \in M, \tag{5.47}$$

where the function is extended by 0 *for* $z \in M \backslash \mathcal{B}_M(Y_j, 2\varepsilon)$.

(c) For $z \in \mathcal{B}_M(Y_j, 2\varepsilon)$, *we have*

$$|\hat{\Psi}_j \circ S_j(z) - z| \lesssim \varepsilon^m + \gamma, \tag{5.48}$$
$$|\tilde{\chi}_j(z) - \chi_j(z)| \lesssim \varepsilon^m + \gamma. \tag{5.49}$$

A proof of Lemma 5.3.8 is found in Section 5.4.6. Let $\hat{M}_\varepsilon = \bigcup_{j=1}^J \mathcal{B}_{\hat{\Psi}_j(\hat{T}_j)}(X_j, \varepsilon)$ be the support of $\widehat{\mathrm{vol}}_M$.

Lemma 5.3.9. *Let* $1 \leq r \leq \infty$. *Let* $\phi : M \to \mathbb{R}$, $\tilde{\phi} : \hat{M}_\varepsilon \to \mathbb{R}$ *be functions satisfying* $\phi_{\min} \leq \phi, \tilde{\phi} \leq \phi_{\max}$ *for some positive constants* $\phi_{\min}, \phi_{\max} > 0$. *Assume further that for all* $j = 1, \dots, J$ *and for all* $z \in M$ *we have,* $|\tilde{\phi}(\hat{\Psi}_j \circ S_j(z)) - \phi(z)| \leq T$. *Then, with probability larger than* $1 - cn^{-k/d}$, *we have*

$$W_r\left(\frac{\tilde{\phi} \cdot \widehat{\mathrm{vol}}_M}{|\tilde{\phi} \cdot \widehat{\mathrm{vol}}_M|}, \frac{\phi \cdot \mathrm{vol}_M}{|\phi \cdot \mathrm{vol}_M|}\right) \lesssim C_0(T + \varepsilon^m + \gamma), \tag{5.50}$$

where C_0 *depends on* $\phi_{\min}$ *and* $\phi_{\max}$.

In particular, inequality (5.25) is a consequence of Lemma 5.3.9 with $\phi \equiv \tilde{\phi} \equiv 1$.

Proof. Assume first that $r < \infty$. If $(\varepsilon^m + \gamma) \gtrsim 1$, there is nothing to prove, so we may assume that $(\varepsilon^m + \gamma) \leq 1/(2Cc_d)$, where c_d is the constant of Lemma 5.2.5 and $C := \sup_{z \in M} |\tilde{\chi}_j(z) - \chi_j(z)|/(\varepsilon^m + \gamma)$. We have the bound

$$
\begin{aligned}
W_r\left(\frac{\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M}{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|},\frac{\phi\cdot\mathrm{vol}_M}{|\phi\cdot\mathrm{vol}_M|}\right) &= \frac{1}{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|^{1/r}}W_r\left(\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M,\phi\cdot\mathrm{vol}_M\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right)\\
&\leq \frac{1}{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|^{1/r}}\left(W_r\left(\sum_{j=1}^J\tilde{\phi}\cdot\nu_j,\sum_{j=1}^J(\hat{\Psi}_j\circ S_j)_\#^{-1}(\tilde{\phi}\cdot\nu_j)\right)\right.\\
&\left.+W_r\left(\sum_{j=1}^J(\hat{\Psi}_j\circ S_j)_\#^{-1}(\tilde{\phi}\cdot\nu_j),\phi\cdot\mathrm{vol}_M\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right)\right)
\end{aligned}
\tag{5.51}
$$

We use Proposition 5.1.6 to bound the second term in (5.51). By a change of variables, the density of $(\hat{\Psi}_j\circ S_j)_\#^{-1}(\tilde{\phi}\cdot\nu_j)$ is given by $\tilde{\phi}_j : z\mapsto\tilde{\phi}(\hat{\Psi}_j\circ S_j(z))\tilde{\chi}_j(z)$. With probability larger than $1-cn^{-k/d}$, we have for $z\in M$,

$$
\sum_{j=1}^J\tilde{\chi}_j(z)\geq\sum_{j=1}^J\chi_j(z)-Cc_d(\varepsilon^m+\gamma)\geq 1-\frac{1}{2}=\frac{1}{2}.
$$

Hence, by Proposition 5.1.6,

$$
\begin{aligned}
&W_r\left(\sum_{j=1}^J(\hat{\Psi}_j\circ S_j)_\#^{-1}(\tilde{\phi}\cdot\nu_j),\phi\cdot\mathrm{vol}_M\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right)\\
&\leq r^{-1/r}\left(\frac{2}{\phi_{\min}}\right)^{1-1/r}\left\|\sum_{j=1}^J\tilde{\phi}_j-\phi\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right\|_{H_r^{-1}(M)}\\
&\leq\left(\frac{2}{\phi_{\min}}\vee 1\right)\left\|\sum_{j=1}^n\tilde{\phi}_j-\phi\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right\|_{L_r(M)}\\
&\leq\left(\frac{2}{\phi_{\min}}\vee 1\right)\left(\left\|\sum_{j=1}^J\tilde{\phi}_j-\phi\right\|_{L_r(M)}+\frac{||\phi\cdot\mathrm{vol}_M|-|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M||}{|\phi\cdot\mathrm{vol}_M|}\|\phi\|_{L_r(M)}\right).
\end{aligned}
$$

Remark that $\tilde{\chi}_j(z)\leq 2$ for any $z\in M$. Therefore, we have according to Lemma 5.3.8, $|\tilde{\phi}_j(z)-\phi(z)\chi_j(z)|\leq 2T+\phi_{\max}|\chi_j(z)-\tilde{\chi}_j(z)|\lesssim T+\phi_{\max}(\varepsilon^m+\gamma)$. Hence, we have the bound,

$$
\begin{aligned}
||\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|-|\phi\cdot\mathrm{vol}_M||\leq\left\|\sum_{j=1}^J\tilde{\phi}_j-\phi\right\|_{L_1(M)}&\leq\left\|\sum_{j=1}^J\tilde{\phi}_j-\phi\right\|_{L_r(M)}|\mathrm{vol}_M|^{1-1/r}\\
&\leq\left\|\sum_{j=1}^J\tilde{\phi}_j-\phi\right\|_{L_\infty(M)}|\mathrm{vol}_M|\lesssim T+\phi_{\max}(\varepsilon^m+\gamma).
\end{aligned}
\tag{5.52}
$$

As $\|\phi\|_{L_r(M)}\leq|\mathrm{vol}_M|^{1/r}\phi_{\max}$ and $|\phi\cdot\mathrm{vol}_M|\geq\phi_{\min}|\mathrm{vol}_M|$, we finally obtain that

$$
W_r\left(\sum_{j=1}^J(\hat{\Psi}_j\circ S_j)_\#^{-1}(\tilde{\phi}\cdot\nu_j),\phi\cdot\mathrm{vol}_M\frac{|\tilde{\phi}\cdot\widehat{\mathrm{vol}}_M|}{|\phi\cdot\mathrm{vol}_M|}\right)\lesssim C_{\phi_{\min},\phi_{\max}}\left(T+\varepsilon^m+\gamma\right),
$$

with the constant $C_{\phi_{\min},\phi_{\max}}$ in the upper bound depending on $\phi_{\min}$ and $\phi_{\max}$, but not on r.

To bound the first term in (5.51), consider the transport plan $\sum_{j=1}^{J}(\mathrm{id}, (\hat{\Psi}_j \circ S_j)^{-1})_{\#}(\tilde{\phi} \cdot \nu_j)$, which has, according to Lemma 5.3.8, a cost bounded by

$$\sum_{j=1}^{J} \int |y - (\hat{\Psi}_j \circ S_j)^{-1}(y)|^r \mathrm{d}(\tilde{\phi} \cdot \nu_j)(y) \lesssim \phi_{\max} \left(\varepsilon^m + \gamma\right)^r |\widehat{\mathrm{vol}}_M|.$$

As $|\widehat{\mathrm{vol}}_M| \lesssim |\mathrm{vol}_M| + T + \phi_{\max}(\varepsilon^m + \gamma)$, we obtain the desired bound. By letting $r \to \infty$, and remarking that the different constants involved are independent of r, we observe that the same bound holds for $r = \infty$. □

Remark 5.3.10. Inequality (5.52) with $\phi \equiv \phi' \equiv 1$ gives a bound on the distance between the total mass of $\widehat{\mathrm{vol}}_M$ and the volume $|\mathrm{vol}_M|$ of M: choosing $k = m$, it is of order $\varepsilon^k + \gamma$ with probability larger than $1 - cn^{-k/d}$.

Proof of Theorem 5.2.6(iii).

Inequality (5.26) is a consequence of Theorem 5.2.6(ii), whereas the lower bound on the minimax risk (5.27) is proven in Section 5.4.7.

Proof of Theorem 5.2.7.

Note first that $\hat{\nu}_{n,h}$ is indeed a measure of mass 1. We show in Lemma 5.4.6 that

$$T := \max_{j=1\dots J} \sup_{z \in \mathcal{B}(Y_j,\varepsilon)} \left| K_h * \left(\frac{\nu_n}{\hat{\rho}_h}\right)(\hat{\Psi}_j \circ S_j(z)) - K_h * \left(\frac{\mu_n}{\rho_h}\right)(z) \right|$$

satisfies $T \lesssim \varepsilon^m + \gamma$ with probability larger than $1 - cn^{-k/d}$. As $f_{\min}/2 \leq K_h * (\mu_n/\rho_h) \leq 2f_{\max}$ on M by Theorem 5.2.1(i), and as every $y \in \hat{M}_\varepsilon$ is in the image of $\hat{\Psi}_j \circ S_j$ for some $j = 1 \dots J$, we have $f_{\min}/3 \leq K_h * (\nu_n/\hat{\rho}_h) \leq 3f_{\max}$ on $\hat{M}_\varepsilon$ should $\varepsilon^k + \gamma$ be small enough. This proves Theorem 5.2.1(i) and, together with Lemma 5.3.9, this also proves Theorem 5.2.7(ii). Theorem 5.2.7(iii) is a consequence of Theorem 5.2.7(ii) and Theorem 5.2.7(iv) is proven in Section 5.4.7.

5.4 Appendix to Chapter 5

5.4.1 Geometric properties of $\mathcal{C}^k$ manifolds with positive reach and their estimators

Let $M \in \mathcal{M}^{k,d}_{\tau_{\min},L}$ for some $k \geq 2$ and $\tau_{\min}, L > 0$. We first give elementary properties of $\mathcal{C}^k$ manifolds.

Lemma 5.4.1. *Let $x \in M$. The following properties hold:*

(i) There exists a map $N_x : \mathcal{B}_{T_xM}(0, r_0) \to T_xM^\perp$ satisfying $dN_x(0) = 0$, and such that, for $u \in \mathcal{B}_{T_xM}(0, r_0)$, we have $\Psi_x(u) = x + u + N_x(u)$ with $|N_x(u)| \leq L|u|^2$.

(ii) There exist tensors $B^1_x, \dots, B^{k-1}_x$ of operator norm controlled by a constant depending on L, d, k and $\tau_{\min}$, such that, if $u \in T_xM$ satisfies $|u| \leq C_{k,d,L}$, then $J\Psi_x(u) = 1 + \sum_{i=2}^{k-1} B^i_x[u^{\otimes i}] + R_x(u)$, with $|R_x(u)| \leq C'_{k,d,L}|u|^k$.

Proof. By a Taylor expansion of Ψ_x at $u=0$, we have $\Psi_x(u) = x + u + N_x(u)$, with $N_x(u) = \int_0^1 d^2\Psi_x(tu)[u^{\otimes 2}]\mathrm{d}t$. Hence, $|N_x(u)| \le L|u|^2$. Furthermore, as $\tilde{\pi}_x \circ \Psi_x(u) = u$, we have $\pi_x(N_x(u)) = 0$, i.e. N_x takes its values in $T_xM^\perp$. This proves (i).

Let us prove (ii). We have $d\Psi_x(u) = \mathrm{id}_{T_xM} + dN_x(u)$, and $d\Psi_x(u)^* d\Psi_x(u) = \mathrm{id}_{T_xM} + (dN_x(u))^* dN_x(u)$. Therefore,

$$J\Psi_x(u) = \sqrt{\det(d\Psi_x(u)^* d\Psi_x(u))} = \sqrt{\det(\mathrm{id}_{T_xM} + (dN_x(u))^* dN_x(u))}.$$

One has $dN_x(u) = dN_x(0) + \sum_{j=2}^{k-1} \frac{d^j N_x(0)}{(j-1)!}[u^{\otimes(j-1)}] + R_x(u)$, with $|R_x(u)| \le C_{k,L}|u|^{k-1}$ and $dN_x(0) = 0$. Hence, $(dN_x(u))^* dN_x(u)$ is written as $\sum_{j=2}^{k-1} B_j[u^{\otimes j}] + R'_x(u)$, with $|R'_x(u)| \le C'_{k,l}|u|^k$. The operator norm of this operator is smaller than, say, $1/2$ for $|u|$ sufficiently small, and we conclude the proof by writing a Taylor expansion at 0 of the function $F \mapsto \sqrt{\det(\mathrm{id} + F)}$. □

We now prove Lemma 5.2.5, on the construction of smooth partitions of unity based on some set S which is sufficiently sparse and dense over a tubular neighborhood of M.

Proof of Lemma 5.2.5. Consider the functions θ and $(\chi_x)_{x\in S}$ as in the statement of the lemma, and, for $y \in M^\delta$, let $Z(y) = \sum_{x'\in S} \theta\left(\frac{y-x'}{8\delta}\right)$. As $d_H(M^\delta|S) \le 4\delta$, we have $Z(y) \ge 1$ and the quantity $\chi_x(y)$ is well-defined. The function χ_x is smooth, and we have $\sum_{x\in S}\chi_x \equiv 1$ on M^δ. One has $d^l\chi_x(y)$ which is written as a sum of terms of the form $d^{l-j}\theta\left(\frac{y-x}{8\delta}\right) d^j(Z^{-1})(y)$, and $d^j(Z^{-1})(y)$ is equal to a sum of terms of the form $Z^{j'-j-2}(y)d^{j'}Z(y)$ for $1 \le j' \le j$. Also, $\left\|d^j\theta\left(\frac{y-x'}{8\delta}\right)\right\|_{\mathrm{op}} \le C_j\delta^{-j}$ and $\left\|d^jZ(y)\right\|_{\mathrm{op}} \le C_j\delta^{-j}\sum_{x\in S}\mathbf{1}\{|x-y| \le 8\delta\}$. Hence, as $Z \ge 1$, we have for any $l \ge 0$

$$\left\|d^l\chi_x(y)\right\|_{\mathrm{op}} \le C'_l\delta^{-l}\sum_{x\in S}\mathbf{1}\{|x-y| \le 8\delta\}.$$

It remains to bound this sum. If $x \in \mathcal{B}(y, 8\delta)$, then $\pi_M(x) \in \mathcal{B}(\pi_M(y), 10\delta)$. Also, for $x \ne x' \in S$, we have $|\pi_M(x) - \pi_M(x')| \ge |x - x'| - 2\delta \ge 2\delta$. In particular, the balls $\mathcal{B}_M(\pi_M(x), \delta)$ for $x \in S$ are pairwise disjoint, and are all included in $\mathcal{B}_M(\pi_M(y), 11\delta)$. Therefore, if $11\delta \le \tau(M)/4$, using Proposition 3.5.8.7 twice, we obtain that $\mathrm{vol}_M(\mathcal{B}_M(\pi_M(x), \delta)) \ge c_d\delta^d$, and that

$$\begin{aligned}\sum_{x\in S}\mathbf{1}\{|x-y| \le 8\delta\} &\le \sum_{x\in S}\mathbf{1}\{|x-y| \le 8\delta\}\frac{\mathrm{vol}_M(\mathcal{B}_M(\pi_M(x), \delta))}{c_d\delta^d} \\ &\le \frac{\mathrm{vol}_M(\mathcal{B}_M(\pi_M(y), 11\delta))}{c_d\delta^d} \le c'_d.\end{aligned}$$

This concludes the proof. □

We end this section by detailing the properties of the local polynomial estimators $\hat{\Psi}_i$ and $\hat{T}_i$ defined in [AL19]. In particular, we prove Proposition 5.2.4. Recall that $X_i = Y_i + Z_i$ with $Y_i \in M$ and $|Z_i| \le \gamma$. Aamari and Levrard introduce tensors $V^*_{j,i}$ which are defined as $d^j\Psi_{X_i}(0)/j!$, where $d^j\Psi_{X_i}(0)$ is the jth differential of Ψ_{X_i} at 0 (see the proof of Lemma 2 in [AL19] for details). In particular, we have $V^*_{1,i} = \pi_{Y_i}$. Furthermore, as $\tilde{\pi}_{Y_j} \circ \Psi_{Y_j} = \mathrm{id}$, we have $\pi_{Y_j} \circ V^*_{j,i} = 0$ for $j \ge 2$.

Lemma 5.4.2. *With probability larger than $1 - cn^{-k/d}$, for any $1 \le i \le n$,*

(i) We have $\angle(T_{Y_i}M, \hat{T}_i) \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1}$.

(ii) *For* $v \in \hat{T}_i$*, we have* $\hat{\Psi}_i(v) = X_i + v + \hat{N}_i(v)$*, where* $\hat{N}_i : \hat{T}_i \to \hat{T}_i^{\perp}$ *is defined by* $\hat{N}_i(v) = \sum_{j=2}^{m-1} \hat{V}_{j,i}[v^{\otimes j}]$.

(iii) *For any* $2 \leq j < m$, $\left\| \hat{V}_{j,i} \circ \hat{\pi}_i - V_{j,i}^* \circ \pi_{Y_i} \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-j} + \gamma\varepsilon^{-j}$.

(iv) *For* $v \in \mathcal{B}_{\hat{T}_i}(0, 3\varepsilon)$*, we have*

$$|\hat{\Psi}_i(v) - \Psi_{Y_i}(\pi_{Y_i}(v))| \lesssim \varepsilon^m + \gamma, \tag{5.53}$$

$$|\hat{N}_i(v) - N_{Y_i}(\pi_{Y_i}(v))| \lesssim \varepsilon^m + \gamma, \tag{5.54}$$

$$\left\| d\hat{\Psi}_i(v) - d(\Psi_{Y_i} \circ \pi_{Y_i})(v) \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1} \tag{5.55}$$

$$\left\| d\hat{N}_i(v) - d(N_{Y_i} \circ \pi_{Y_i})(v) \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1}. \tag{5.56}$$

Proof of Proposition 5.2.4. Lemma 5.4.2(i) is stated in Theorem 2 in [AL19]. Remark that for $x \in \mathcal{B}(X_i, \varepsilon)$, with $\tilde{x} = x - X_i$, and any orthogonal projection π,

$$\begin{aligned} &\left| \tilde{x} - \pi(\tilde{x}) - \sum_{j=2}^{m-1} V_j[\pi(\tilde{x})^{\otimes j}] \right|^2 \\ &\quad = \left| \tilde{x} - \pi(\tilde{x}) - \sum_{j=2}^{m-1} \pi^{\perp} \circ V_j[\pi(\tilde{x})^{\otimes j}] \right|^2 + \left| \sum_{j=2}^{m-1} \pi \circ V_j[\pi(\tilde{x})^{\otimes j}] \right|^2 \end{aligned}$$

so that we may always assume that the tensors $\hat{V}_{j,i}$ minimizing the criterion (5.19) satisfy $\hat{\pi}_i \circ \hat{V}_{j,i} = 0$ for $j \geq 2$. This proves Lemma 5.4.2(ii).

We prove Lemma 5.4.2(iii) by induction on $2 \leq j < m$. The result for $j = 2$ is stated in [AL19, Theorem 2]. It is shown in [AL19] (see Equation (3)) that there exist tensors $V'_{j,i}$ for $1 \leq j < m$ satisfying with probability larger than $1 - cn^{-k/d}$,

$$\left\| V'_{j,i} \circ \pi_{Y_i} \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-j} + \gamma\varepsilon^{-j}. \tag{5.57}$$

The tensors $V'_{j,i}$ are defined by the relations, for $y \in M$ close enough to Y_i,

$$\begin{aligned} y - Y_i &= \pi_{Y_i}(y - Y_i) + \sum_{j=2}^{m-1} V_{j,i}^*[\pi_{Y_i}(y - Y_i)^{\otimes j}] + R(y - Y_i) \\ y - Y_i - \hat{\pi}_i(y - Y_i) - \sum_{j=2}^{m-1} \hat{V}_{j,i}[\hat{\pi}_i(y - Y_i)^{\otimes j}] &= \sum_{j=1}^{m-1} V'_{j,i}[\pi_{Y_i}(y - Y_i)^{\otimes j}] + R'(y - Y_i), \end{aligned}$$

with $|R(y - Y_i)|, |R'(y - Y_i)| \lesssim \varepsilon^m$, see the proof of Lemma 3 in [AL19]. In particular, for $j \geq 2$, noting that $\pi_{Y_i} \circ V_{j,i}^* = 0$, we see that $V'_{j,i} \circ \pi_{Y_i}$ is written as the sum of $(\pi_{Y_i} - \hat{\pi}_i) \circ V_{j,i}^* + (V_{j,i}^* \circ \pi_{Y_i} - \hat{V}_{j,i} \circ \hat{\pi}_i)$ and of a sum of terms proportional to

$$\hat{V}_{j',i}[\hat{\pi}_i \circ V_{a_1,i}^* \circ \pi_{Y_i}, \ldots, \hat{\pi}_i \circ V_{a_{j'},i}^* \circ \pi_{Y_i}], \tag{5.58}$$

where $2 \leq j' < j$ and $a_1 + \cdots + a_{j'} = j$, $1 \leq a_1, \ldots, a_{j'} < j$. There exists in particular an index in the sum which is larger than 2. Assume without loss of generality that

$a_1, \dots, a_l > 1$ and $a_{l+1}, \dots, a_{j'} = 1$, so that $\hat{\pi}_i \circ \hat{V}_{a_u,i} = 0$ for $1 \le u \le l$. Then,

$$\begin{aligned}
&\left\| \hat{V}_{j',i}[\hat{\pi}_i \circ V^*_{a_1,i} \circ \pi_{Y_i}, \dots, \hat{\pi}_i \circ V^*_{a_l,i} \circ \pi_{Y_i}, \dots, \hat{\pi}_i \circ V^*_{a_{j'},i} \circ \pi_{Y_i}] \right\|_{\mathrm{op}} \\
&= \left\| \hat{V}_{j',i}[\hat{\pi}_i \circ (V^*_{a_1,i} - \hat{V}_{a_1,i}) \circ \pi_{Y_i}, \dots, \hat{\pi}_i \circ (V^*_{a_l,i} - \hat{V}_{a_l,i}) \circ \pi_{Y_i}, \dots, \hat{\pi}_i \circ V^*_{a_{j'},i} \circ \pi_{Y_i}] \right\|_{\mathrm{op}} \\
&\lesssim \ell \prod_{u=1}^{l} \left\| V^*_{a_u,i} \circ \pi_{Y_i} - \hat{V}_{a_u,i} \circ \pi_{Y_i} \right\|_{\mathrm{op}} \\
&\lesssim \ell \prod_{u=1}^{l} \left(\left\| V^*_{a_u,i} \circ \pi_{Y_i} - \hat{V}_{a_u,i} \circ \hat{\pi}_i \right\|_{\mathrm{op}} + \ell \left\| \pi_{Y_i} - \hat{\pi}_i \right\|_{\mathrm{op}} \right) \\
&\lesssim \varepsilon^{-1} \prod_{u=1}^{l} \left(\varepsilon^{m-a_u} + \gamma \varepsilon^{-a_u} + \varepsilon^{m-2} + \gamma \varepsilon^{-2} \right) \\
&\lesssim \varepsilon^{-1} (\varepsilon^{lm-(j-l)} + \gamma^l \varepsilon^{-(j-l)}) \lesssim \varepsilon^{m-j} + \gamma \varepsilon^{-j},
\end{aligned}$$

where at the last line we use the induction hypothesis as well as Lemma 5.4.2(i), the fact that $\sum_{u=1}^{l} a_u = j - l$ and that $\ell \lesssim \varepsilon^{-1}$. As $\left\| (\pi_{Y_i} - \hat{\pi}_i) \circ V^*_{j,i} \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-1} + \gamma \varepsilon^{-1}$, we obtain that

$$\left\| (V^*_{j,i} \circ \pi_{Y_i} - \hat{V}_{j,i} \circ \hat{\pi}_i) - V'_{j,i} \circ \pi_{Y_i} \right\|_{\mathrm{op}} \lesssim \varepsilon^{m-j} + \gamma \varepsilon^{-j}.$$

Hence, using (5.57),

$$\begin{aligned}
\left\| V^*_{j,i} \circ \pi_{Y_i} - \hat{V}_{j,i} \circ \hat{\pi}_i \right\|_{\mathrm{op}} &\le \left\| (V^*_{j,i} \circ \pi_{Y_i} - \hat{V}_{j,i} \circ \hat{\pi}_i) - V'_{j,i} \circ \pi_{Y_i} \right\|_{\mathrm{op}} + \left\| V'_{j,i} \circ \pi_{Y_i} \right\|_{\mathrm{op}} \\
&\lesssim \varepsilon^{m-j} + \gamma \varepsilon^{-j}.
\end{aligned}$$

We now may prove (5.53). Indeed, for $v \in \mathcal{B}_{\hat{T}_i}(0, 3\varepsilon)$, we have $\hat{\Psi}_i(v) = X_i + v + \sum_{j=2}^{m-1} \hat{V}_{j,i}[v^{\otimes j}]$, whereas by a Taylor expansion, $\Psi_{Y_i} \circ \pi_{Y_i}(v) = Y_i + \pi_{Y_i}(v) + \sum_{j=2}^{m-1} V_{j,i}[\pi_{Y_i}(v)^{\otimes j}] + R(v)$, with $|R(v)| \lesssim \varepsilon^m$. By Lemma 5.4.2(iii), the difference between the two quantities is bounded with high probability by a sum of terms of order $(\varepsilon^{m-j} + \gamma \varepsilon^{-j})|v|^j \lesssim \varepsilon^m + \gamma$. Inequality (5.54) is directly implied by (5.53) and Lemma 5.4.2(i). Inequality (5.55) is proven as (5.53), by noting that, for $h \in \hat{T}_i$,

$$\begin{cases}
d(\Psi_{Y_j} \circ \pi_{Y_j})(v)[h] = \pi_{Y_j}(h) + \sum_{j=2}^{m-1} j V^*_{j,i}[\pi_{Y_j}(v), \pi_{Y_j}(h)^{\otimes (j-1)}] + R'(v)h \\
d\hat{\Psi}_j(v)[h] = h + \sum_{j=2}^{m-1} j \hat{V}_{j,i}[v, h^{\otimes (j-1)}],
\end{cases}$$

with $\|R'(v)\|_{\mathrm{op}} \lesssim \varepsilon^{m-1}$. Equation (5.56) is shown in a similar way. □

5.4.2 Properties of negative Sobolev norms

Proof of Proposition 5.1.3. The second inequality in (i) is trivial. The assertion (ii) is stated in [BCS10, Theorem 2.1] for an open set $\Omega \subset \mathbb{R}^d$, and their proof can be straightforwardly adapted to the manifold setting. It remains to prove the first inequality in (i). Note that for any g with $\|\nabla g\|_{L_{p^*}(M)} \le 1$, one has $\int f g \mathrm{dvol}_M = \int f (g - \int g \mathrm{dvol}_M) \mathrm{dvol}_M$ as $\int f \mathrm{dvol}_M = 0$. Also, by Poincaré inequality (see [BCH18, Theorem 0.6]),

$$\left\| g - \int_M g \right\|_{L_{p^*}(M)} \le C^{\frac{1}{p}} R^{\frac{d}{p^*} + \frac{1}{p}} \|\nabla g\|_{L_{p^*}(M)} \le C^{\frac{1}{p}} R^{\frac{d}{p^*} + \frac{1}{p}},$$

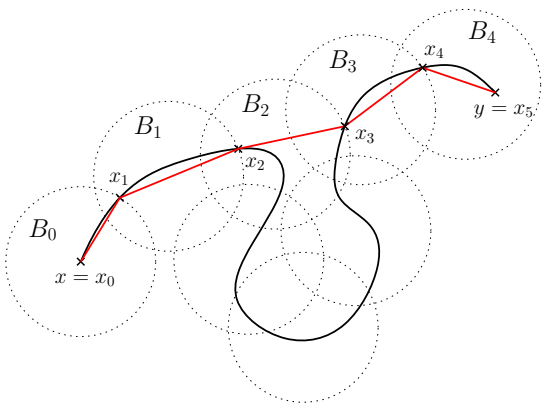


FIGURE 5.2: Illustration of the construction in the proof of Lemma 5.4.3

where $R = \max\{d_g(x,y),\ x,y \in M\}$ and C depends on d and on a lower bound κ on the Ricci curvature of M. Therefore, $\left\|g - \int_M g\right\|_{H^1_{p^*}(M)} \leq C^{\frac{1}{p}} R^{\frac{d}{p^*}+\frac{1}{p}}$. The quantity κ can be further lower bounded by a constant depending on $\tau_{\min}$ and d. Indeed, a bound on the second fundamental form of M entails a bound on the Ricci curvature according to Gauss equation (see e.g. [Car92, Chapter 6]), and the second fundamental form is controlled by the reach of M, see Proposition 3.5.6. As $C^{\frac{1}{p}} \leq C \vee 1$, to conclude, it suffices to bound the geodesic diameter of M. This is done in the following lemma. □

Lemma 5.4.3. *The geodesic diameter of M satisfies* $\sup_{x,y\in M} d_g(x,y) \leq c_d|\mathrm{vol}_M|\tau_{\min}^{1-d}$.

Proof. Consider a covering of M by N open balls of radius $r_1 = \tau(M)/4$ (for the Euclidean distance) and let $x, y \in M$. Such a covering exists with $N \leq c_d|\mathrm{vol}_M|r_1^{-d}$ by standard packing arguments. Let $\gamma : [0,\ell] \to M$ be a unit speed curve between x and y. Let B_0 be the ball of the covering such that $x \in B_0$. If $y \in B_0$, then $|x-y| \leq 2r_1$, and by [NSW08, Proposition 6.3], we have $d_g(x,y) \leq 4r_1$. Otherwise, let $t_0 = \inf\{t \in [0,\ell],\ \forall t' \geq t,\ \gamma(t') \notin B_0\}$. Then $x_1 := \gamma(t_0)$ belong to the boundary of B_0, and is also in some other ball B_1. By the previous argument, we have $d_g(x,x_1) \leq 4r_1$. If $y \in B_1$, then $d_g(x_1,y) \leq 4r_1$ and $d_g(x,y) \leq 8r_1$. Otherwise, we define $t_1 = \inf\{t \in [t_0,\ell],\ \forall t' \geq t,\ \gamma(t') \notin B_1\}$ and we iterate the same argument. At the end, we obtain a sequence $x = x_0, x_1, \ldots, x_I$ of points in M with associated balls B_i which contain x_i, such that $y \in B_I$ and $d_g(x_i, x_{i+1}) \leq 4r_1$. Furthermore, all the balls B_i are pairwise distinct. As $d_g(x_I, y) \leq 4r_1$, we have $\ell \leq (I+1)4r_1 \leq (N+1)4r_1 \leq 8Nr_1$. By letting γ be a geodesic, we obtain in particular $\ell = d_g(x,y) \leq 8Nr_1 \leq 8c_d|\mathrm{vol}_M|r_1^{1-d}$. □

Proof of Proposition 5.1.6. Given a measurable map $\rho : [0,1] \to \mathcal{P}^p$, E_t a vectorial measure absolutely continuous with respect to ρ_t (see [San15, Box 4.2]) and $v(x,t)$ a time-depending vector field, defined as the density of E_t with respect to ρ_t, we define the Benamou-Brenier functional

$$\mathcal{B}_p(\rho, E) := \int |v(x,t)|^p \mathrm{d}\rho_t(x)\mathrm{d}t. \tag{5.59}$$

The Benamou-Brenier formula [BB00; Bre03] asserts that for $\mu, \nu \in \mathcal{P}_1^p$ supported on some ball of radius R,

$$W_p^p(\mu,\nu) = \min\left\{\mathcal{B}_p(\rho,E),\ \partial_t\rho_t + \nabla\cdot E_t = 0, \rho_0 = \mu, \rho_1 = \nu\right\}, \tag{5.60}$$

where ρ_t is supported on the ball of radius R, and the continuity equation $\partial_t\rho+\nabla\cdot E=\mu-\nu$ has to be understood in the distributional sense, i.e.

$$\int_{[0,1]\times\mathbb{R}^D}\partial_t\phi(t,x)\mathrm{d}\rho(t,x)+\int_{[0,1]\times\mathbb{R}^D}\nabla\phi(t,x)\cdot\mathrm{d}E(t,x)=0, \tag{5.61}$$

for all $\phi\in\mathcal{C}^1((0,1)\times\mathcal{B}(0,R))$ with compact support.

Assume that μ has a density f_0 and ν has a density f_1 on M. As $\tau(M)>0$, the existence of a probability measure of mass 1, supported on M, with density larger than $f_{\min}$ implies that $|\mathrm{vol}_M|$ is finite, so that M is compact, see Proposition 3.5.7.3. It is in particular included in a ball $\mathcal{B}(0,R)$ for some R large enough. Let w be a vector field on M with $\nabla\cdot w=\mu-\nu$ in a distributional sense, i.e. $\int\nabla g\cdot w=-\int g(\mu-\nu)$ for all $g\in\mathcal{C}^1(M)$. Let $\rho_t=(1-t)\mu+t\nu$ and define E the vector measure having density w with respect to $\mathrm{Leb}_1\times\mathrm{vol}_M$, where Leb_1 is the Lebesgue measure on $[0,1]$. Then (ρ,E) satisfies the continuity equation and $E=v\cdot\rho$ where $v(t,x)=\frac{w(x)}{(1-t)f_0(x)+tf_1(x)}$ for $t\in[0,1]$, $x\in M$. Hence,

$$\begin{aligned}W_p^p(\mu,\nu)&\le\int_0^1\int\frac{1}{p}|v|^p\mathrm{d}\rho\\&=\frac{1}{p}\int_0^1\int\frac{|w(x)|^p}{|(1-t)f_0(x)+tf_1(x)|^p}((1-t)f_0(x)+tf_1(x))\mathrm{d}x\mathrm{d}t\\&\le\frac{1}{p}\int|w(x)|^p\mathrm{d}x\frac{1}{f_{\min}^{p-1}}.\end{aligned}$$

By taking the infimum on vector fields w on M satisfying $\nabla\cdot w=\mu-\nu$ and using Proposition 5.1.3, we obtain the conclusion. The second inequality in (5.10) follows from Proposition 5.1.3. □

5.4.3 Proofs of Section 5.3.1

Proof of Lemma 5.3.2. We first prove (5.34). Note that if $|x-y|\ge h$ for $x,y\in M$, then $K_h(x-y)=0$. Hence, by a change of variable, using that $\mathcal{B}_M(x,h)\subset\Psi_x(\mathcal{B}_{T_xM}(0,h))$ as π_x is 1-Lipschitz continuous,

$$\begin{aligned}\int_M K_h(x-y)B[(x-y)^{\otimes j}]\mathrm{d}y&=\int_{\mathcal{B}_{T_xM}(0,h)}K_h(x-\Psi_x(v))B[(x-\Psi_x(v))^{\otimes j}]J\Psi_x(v)\mathrm{d}v\\&=\int_{\mathcal{B}_{T_xM}(0,1)}K\left(\frac{x-\Psi_x(hv)}{h}\right)B[(x-\Psi_x(hv))^{\otimes j}]J\Psi_x(hv)\mathrm{d}v.\end{aligned}$$

As the functions Ψ_x and K are $\mathcal{C}^k$, according to Lemma 5.4.1(i) and Lemma 5.4.1(ii), we can write by a Taylor expansion, for $v,u\in\mathcal{B}_{T_xM}(0,r_0)$,

$$\begin{cases}\Psi_x(v)=x+v+\sum_{i=2}^{k-1}\frac{d^i\Psi_x(0)}{i!}[v^{\otimes i}]+R_1(x,v)\\J\Psi_x(v)=1+\sum_{i=2}^{k-1}B_x^i[v^{\otimes i}]+R_2(x,v)\\K(v+u)=K(v)+\sum_{i=1}^{k-1}\frac{d^iK(v)}{i!}[u^{\otimes i}]+R_3(v,u)\\B[(v+u)^{\otimes j}]=B[v^{\otimes j}]+\sum_{\emptyset\neq\sigma\subset\{1,\dots,j\}}B[v^\sigma,u^{\sigma^c}],\end{cases} \tag{5.62}$$

where $|R_j(x,v)|\le C_j|v|^k$ for $j=1,2$, $|R_3(v,u)|\le C_3|u|^k$ and (v^σ,u^{σ^c}) is the j-tuple whose lth entry is equal to v if $l\in\sigma$, u otherwise. We obtain that

$$\frac{x-\Psi_x(hv)}{h}=-v-\sum_{i=2}^{k-1}\frac{d^i\Psi_x(0)}{i!}[(hv)^{\otimes i}]h^{-1}-R_1(x,hv)h^{-1},$$

and that the expression $K\left(\frac{x-\Psi_x(hv)}{h}\right)B[(x-\Psi_x(hv))^{\otimes j}]J\Psi_x(hv)$ is written as a sum of terms of the form

$$C_{i_0,i_1,i_2}h^{-i_0}d^{i_0}K(v)[(d^{i_1}\Psi_x(0)[(hv)^{\otimes i_1}])^{\otimes i_0}]F_{i_2}[(hv)^{\otimes i_2}] \tag{5.63}$$

for $0 \le i_0 \le k-1$, $2 \le i_1 \le k-1$ and $j \le i_2 \le k'$, where F_{i_2} is some tensor of order i_2 and k' is some integer depending on k and j, plus a remainder term smaller than $\|B\|_{\mathrm{op}}|hv|^{k-1+j}$ up to a constant depending on k, j, L_k and K. The terms for which $i_0i_1+i_2-i_0 \ge k$ are smaller than $\|B\|_{\mathrm{op}}h^k$ up to a constant, whereas the integrals of the other the terms are null as the kernel is of order k. The first inequality in (5.35) is proven in a similar manner. Let us now bound $\|\rho_h\|_{\mathcal{C}^j(M)}$. Given $x \in M$, we have to bound $\left\|d^j(\rho_h \circ \Psi_x)(0)\right\|_{\mathrm{op}}$. We have

$$d^j(\rho_h \circ \Psi_x)(0) = h^{-j}\int_{\mathcal{B}_{T_xM}(0,h)}(d^jK)_h(x-\Psi_x(v))J\Psi_x(v)\mathrm{d}v.$$

Therefore, using the same argument as before, we obtain that $\left\|d^j(\rho_h \circ \Psi_x)(0)\right\|_{\mathrm{op}} \lesssim h^{k-1-j}$. □

Proof of Lemma 5.3.3. Let $0 \le l \le k-1$ be even, $\phi \in \mathcal{C}^\infty(M)$ be supported in $\mathcal{B}_M(x_0,h_0)$ for some h_0 small enough and $g \in L_{p^*}(M)$ with $\|g\|_{L_{p^*}(M)} \le 1$. Let $x = \Psi_{x_0}(u) \in \mathcal{B}_M(x_0,h_0)$ and let $\tilde{\phi}_{x_0} = \tilde{\phi} \circ \Psi_{x_0}$. Recall that $\tilde{\phi}_l = d^l\tilde{\phi}_{x_0} \circ \tilde{\pi}_{x_0}$. We have $K_h(x-\Psi_{x_0}(v)) \neq 0$ only if $|x-\Psi_{x_0}(v)| \le h$. Hence, as $|x-\Psi_{x_0}(v)| \ge |u-v|$ (recall that Ψ_{x_0} is the inverse of the projection $\tilde{\pi}_{x_0}$), the function $K_h(x-\Psi_{x_0}(\cdot))$ is supported on $\mathcal{B}_{T_{x_0}M}(u,h) \subset \mathcal{B}_{T_{x_0}M}(0,r_0) =: B_0$ for h, h_0 small enough. Thus,

$$\begin{aligned} A_h\phi(x) &= \int_{\mathcal{B}_M(x,h)} K_h(x-y)(\tilde{\phi}(y)-\tilde{\phi}(x))\mathrm{d}y \\ &= \int_{B_0} K_h(x-\Psi_{x_0}(v))(\tilde{\phi}_{x_0}(v)-\tilde{\phi}_{x_0}(u))J\Psi_{x_0}(v)\mathrm{d}v. \end{aligned}$$

We may write

$$\tilde{\phi}_{x_0}(v)-\tilde{\phi}_{x_0}(u) = \sum_{i=1}^{l-1}\frac{d^i\tilde{\phi}_{x_0}(u)}{i!}[(v-u)^{\otimes i}] + \int_0^1 d^l\tilde{\phi}_{x_0}(u+\lambda(v-u))[(v-u)^{\otimes l}]\frac{(1-\lambda)^{l-1}}{(l-1)!}\mathrm{d}\lambda.$$

Each term $\int_{B_0}K_h(x-\Psi_{x_0}(v))\frac{d^i\tilde{\phi}_{x_0}(u)}{i!}[(v-u)^{\otimes i}]J\Psi_{x_0}(v)\mathrm{d}v$ is equal to

$$\int_M K_h(x-y)\frac{d^i\tilde{\phi}_{x_0}(\tilde{\pi}_{x_0}(x))}{i!}[(\pi_{x_0}(y-x))^{\otimes i}]\mathrm{d}y,$$

and is therefore of order smaller than $h^k\max_{1\le i\le l}\left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}}$ by Lemma 5.3.2. Hence, $A_h\phi(x)$ is equal to the sum of a remainder term of order $h^k\max_{1\le i\le l}\left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}}$ and of

$$\begin{aligned} &\int_0^1\int_{B_0}K_h(x-\Psi_{x_0}(v))d^l\tilde{\phi}_{x_0}(u+\lambda(v-u))[(v-u)^{\otimes l}]\frac{(1-\lambda)^{l-1}}{(l-1)!}J\Psi_{x_0}(v)\mathrm{d}v\mathrm{d}\lambda \\ &= \int_0^1\int_{B_0}K_h(x-\Psi_{x_0}(v))\left(d^l\tilde{\phi}_{x_0}(u+\lambda(v-u))-d^l\tilde{\phi}_{x_0}(u)\right)[(v-u)^{\otimes l}]\frac{(1-\lambda)^{l-1}}{(l-1)!} \\ &\qquad J\Psi_{x_0}(v)\mathrm{d}v\mathrm{d}\lambda \\ &\quad + R_1(x), \end{aligned}$$

where $|R_1(x)| \lesssim h^k \max_{1\le i\le l} \left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}}$ by Lemma 5.3.2. We now fix $\lambda \in (0,1)$ and write, by a change of variables, and as $\mathcal{B}_{T_{x_0}M}(u,h) \subset B_0$ for h_0, h small enough,

$$U(x) := \int_{B_0} K_h(x-\Psi_{x_0}(v)) \left(d^l\tilde{\phi}_{x_0}(u+\lambda(v-u)) - d^l\tilde{\phi}_{x_0}(u)\right)[(v-u)^{\otimes l}]J\Psi_{x_0}(v)\mathrm{d}v$$
$$= \int_{B_0} K_h\left(x-\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right)\right)\left(d^l\tilde{\phi}_{x_0}(w) - d^l\tilde{\phi}_{x_0}(u)\right)\left[\frac{(w-u)^{\otimes l}}{\lambda^l}\right]$$
$$J\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right)\frac{\mathrm{d}w}{\lambda^d}$$

Note that $|K_h(u)-K_h(v)| \lesssim h^{-d-1}|u-v|\mathbf{1}\{|u|\le h \text{ or } |v|\le h\}$, and that, as Ψ_{x_0} is $\mathcal{C}^2$,

$$\left|x-\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right) - \frac{x-\Psi_{x_0}(w)}{\lambda}\right|$$
$$\le \left|\frac{d\Psi_{x_0}(u)[w-u]-(x-\Psi_{x_0}(w))}{\lambda}\right| + \frac{L_k|w-u|^2}{2\lambda^2}$$
$$\le \frac{L_k|w-u|^2}{\lambda} \lesssim \frac{|w-u|^2}{\lambda},$$

whereas, as $J\Psi_{x_0}$ is Lipschitz continuous,

$$\left|J\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right) - J\Psi_{x_0}(w)\right| \lesssim \left|u+\frac{w-u}{\lambda}-w\right| \lesssim \frac{|w-u|}{\lambda}.$$

Hence, $U(x)$ is equal to the sum of

$$\lambda^{-l}\int_{B_0} K_{h\lambda}\left(x-\Psi_{x_0}(w)\right)\left(d^l\tilde{\phi}_{x_0}(w) - d^l\tilde{\phi}_{x_0}(u)\right)[(w-u)^{\otimes l}]J\Psi_{x_0}(w)\,\mathrm{d}w$$
$$= \lambda^{-l}\int_M K_{h\lambda}(x-y)\left(\tilde{\phi}_l(y)-\tilde{\phi}_l(x)\right)[(\pi_{x_0}(y-x))^{\otimes l}]\mathrm{d}y,$$

and of a remainder term smaller than

$$\lambda^{-l}\int_{B_0}\left|\lambda^{-d}K_h\left(x-\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right)\right)J\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right)\right.$$
$$\left. - K_{h\lambda}\left(x-\Psi_{x_0}(w)\right)J\Psi_{x_0}(w)\right| \times \left\|d^l\tilde{\phi}_{x_0}(w)-d^l\tilde{\phi}_{x_0}(u)\right\|_{\mathrm{op}}|w-u|^l\mathrm{d}w$$
$$\lesssim \lambda^{-l}\int_{|w-u|\lesssim\lambda h}\left(\frac{|w-u|^2}{(\lambda h)^{d+1}}J\Psi_{x_0}\left(u+\frac{w-u}{\lambda}\right) + |K_{h\lambda}(x-\Psi_{x_0}(w))|\frac{|w-u|}{\lambda}\right)$$
$$\times \left\|d^l\tilde{\phi}_{x_0}(w)-d^l\tilde{\phi}_{x_0}(u)\right\|_{\mathrm{op}}|w-u|^l\mathrm{d}w$$
$$\lesssim h^{l+1}(\lambda h)^{-d}\int_{|w-u|\lesssim\lambda h}\left\|d^l\tilde{\phi}_{x_0}(w)-d^l\tilde{\phi}_{x_0}(u)\right\|_{\mathrm{op}}\mathrm{d}w.$$

Putting all the estimates together, we may now write $\int_M A_h\phi(x)g(x)\mathrm{d}x$ as $S+R_2$, where, by the symmetrization trick (using that l is even)

$$S = \iint_{M\times M} K_h^{(l)}(x-y)\left(\tilde{\phi}_l(y)-\tilde{\phi}_l(x)\right)[(\pi_{x_0}(y-x))^{\otimes l}]g(x)\mathrm{d}y\mathrm{d}x$$
$$= \iint_{M\times M} K_h^{(l)}(x-y)\left(\tilde{\phi}_l(x)-\tilde{\phi}_l(y)\right)[(\pi_{x_0}(x-y))^{\otimes l}]g(y)\mathrm{d}y\mathrm{d}x$$
$$= \frac{1}{2}\iint_{M\times M} K_h^{(l)}(x-y)\left(\tilde{\phi}_l(y)-\tilde{\phi}_l(x)\right)[(\pi_{x_0}(x-y))^{\otimes l}](g(x)-g(y))\mathrm{d}y\mathrm{d}x,$$

and, as $A_h\phi$ is supported on $\mathcal{B}_M(x_0, h_0+h) \subset \mathcal{B}_M(x, 2h_0)$ if h is small enough, R_2 is smaller than,

$$h^{l+1}(\lambda h)^{-d} \int_{x\in\mathcal{B}_M(x,2h_0)} \int_{|w-\tilde{\pi}_{x_0}(x)|\lesssim\lambda h} \left\| d^l\tilde{\phi}_{x_0}(w) - d^l\tilde{\phi}_{x_0}(\tilde{\pi}_{x_0}(x)) \right\|_{\mathrm{op}} |g(x)|\mathrm{d}w\mathrm{d}x \tag{5.64}$$

$$+ \int_M h^k \max_{1\le i\le l} \left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}} |g(x)|\mathrm{d}x$$

$$\lesssim h^{l+1}(\lambda h)^{-d} \int_{w\in\mathcal{B}_M(x,3h_0)} \left\| d^l\tilde{\phi}_{x_0}(w)\right\|_{\mathrm{op}} \int_{|w-\tilde{\pi}_{x_0}(x)|\lesssim\lambda h} |g(x)|\mathrm{d}x\mathrm{d}w \tag{5.65}$$

$$+ h^{l+1} \int_{x\in\mathcal{B}_M(x,2h_0)} \left\|\tilde{\phi}_l(x)\right\|_{\mathrm{op}} |g(x)|\mathrm{d}x + \int_M h^k \max_{1\le i\le l} \left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}} |g(x)|\mathrm{d}x,$$

where we also used Lemma 3.5.87. By the chain rule,

$$\max_{1\le i\le l} \left\|\tilde{\phi}_i(x)\right\|_{\mathrm{op}} \lesssim \max_{1\le i\le l} \left\| d^i\tilde{\phi}(x)\right\|_{\mathrm{op}} \lesssim \sum_{i=1}^{l} \left\| d^i\tilde{\phi}(x)\right\|_{\mathrm{op}}.$$

Hence, applying Hölder's inequality and using that $\|g\|_{L_{p^*}(M)} \le 1$ show that the two last terms in (5.65) are of order $h^{l+1}\|\tilde{\phi}\|_{H_p^l(M)}$. To bound the first term in (5.65), remark that by Young's inequality for integral operators [Sog17, Theorem 0.3.1], if $\mathcal{T}_{\lambda h}(g)(y) = (\lambda h)^{-d}\int_{|x-y|\lesssim\lambda h} |g(x)|\mathrm{d}x$, then $\|\mathcal{T}_{\lambda h}g\|_{L_{p^*}(M)} \lesssim \|g\|_{L_{p^*}(M)}$. This yields, by Hölder's inequality,

$$h^{l+1} \int_{w\in\mathcal{B}_M(x,3h_0)} \left\| d^l\tilde{\phi}_{x_0}(w)\right\|_{\mathrm{op}} \mathcal{T}_{h\lambda}(g)(\Psi_{x_0}(w))\mathrm{d}w \lesssim h^{l+1}\|\tilde{\phi}\|_{H_p^l(M)},$$

which concludes the proof of the first statement of Lemma 5.3.3. To bound the remainder term in terms of $\|\tilde{\phi}\|_{H_p^{l+1}(M)}$, we bound the second term in (5.64) in the same fashion, while, to bound the first term, we write, by a change of variables,

$$\int_{\mathcal{B}_M(x_0,2h_0)} \int_{|w-\tilde{\pi}_{x_0}(x)|\lesssim\lambda h} \left\| d^l\tilde{\phi}_{x_0}(w) - d^l\tilde{\phi}_{x_0}(\tilde{\pi}_{x_0}(x))\right\|_{\mathrm{op}} |g(x)|\mathrm{d}x\mathrm{d}w$$

$$\le \int_0^1 \int_{\mathcal{B}_M(x_0,2h_0)} \int_{|w-\tilde{\pi}_{x_0}(x)|\lesssim\lambda h} \left\| d^{l+1}\tilde{\phi}_{x_0}(\tilde{\pi}_{x_0}(x) + \lambda'(w-\tilde{\pi}_{x_0}(x)))\right\|_{\mathrm{op}}$$

$$\times |\tilde{\pi}_{x_0}(x) - w||g(x)|\mathrm{d}x\mathrm{d}w\mathrm{d}\lambda'$$

$$\lesssim h\int_0^1 \int_{\mathcal{B}_M(x_0,2h_0)} \int_{|u-\tilde{\pi}_{x_0}(x)|\lesssim\lambda'\lambda h} \left\| d^{l+1}\tilde{\phi}_{x_0}(u)\right\|_{\mathrm{op}} |g(x)|\mathrm{d}x\frac{\mathrm{d}u}{\lambda'^d}\mathrm{d}\lambda',$$

and this term is bounded as the first term in (5.65) by $h(h\lambda)^d\|\tilde{\phi}\|_{H_p^{l+1}(M)}$, concluding the proof of Lemma 5.3.3. □

Proof of Lemma 5.3.4. By the chain rule, we have that, for any $u \in \mathcal{B}_{T_{x_0}M}(0, h_0)$, $\left\| d^{l+1}(\eta\circ\Psi_{x_0})(u)\right\|_{\mathrm{op}} \lesssim \max_{1\le i\le l+1} \left\| d^i\eta(\Psi_{x_0}(u))\right\|_{\mathrm{op}}$. Hence, by a change of variables,

$$\int_{\mathcal{B}_M(x_0,h_0)} \|\eta_{l+1}(x)\|_{\mathrm{op}}^p \mathrm{d}x \lesssim \int_{\mathcal{B}_{T_{x_0}M}(0,h_0)} \max_{1\le i\le l+1} \left\| d^i\eta(\Psi_{x_0}(u))\right\|_{\mathrm{op}}^p \mathrm{d}u$$

$$\lesssim \sum_{i=1}^{l+1} \int_{\mathcal{B}_{T_{x_0}M}(0,h_0)} \left\| d^i\eta(\Psi_{x_0}(u))\right\|_{\mathrm{op}}^p \mathrm{d}u$$

$$\lesssim \sum_{i=1}^{l+1} \int_{\mathcal{B}_{T_{x_0}M}(0,h_0)} \left\| d^i\eta(\Psi_{x_0}(u))\right\|_{\mathrm{op}}^p J\Psi_{x_0}(u)\mathrm{d}u \lesssim \|\eta\|_{H_p^{l+1}(M)}^p,$$

where we used at last line that, by Lemma 3.5.8(ii), $J\Psi_{x_0}(u) \geq 1/2$ for $|u| \leq h_0$ if h_0 is small enough. To prove the first inequality, write

$$\begin{aligned}
&h^{-d} \iint_{\mathcal{B}_M(x_0,h_0)^2} \mathbf{1}\{|x-y| \leq h\} \frac{\|\eta_l(x) - \eta_l(y)\|_{\mathrm{op}}^p}{|x-y|^p} \mathrm{d}x\mathrm{d}y \\
&\lesssim h^{-d} \iint_{\mathcal{B}_{T_{x_0}M}(0,h_0)^2} \mathbf{1}\{|\Psi_{x_0}(u) - \Psi_{x_0}(v)| \leq h\} \frac{\left\|d^l(\eta \circ \Psi_{x_0})(u) - d^l(\eta \circ \Psi_{x_0})(v)\right\|_{\mathrm{op}}^p}{|\Psi_{x_0}(u) - \Psi_{x_0}(v)|^p} \mathrm{d}u\mathrm{d}v \\
&\lesssim h^{-d} \int_0^1 \iint_{\mathcal{B}_{T_{x_0}M}(0,h_0)^2} \mathbf{1}\{|u-v| \leq h\} \left\|d^{l+1}(\eta \circ \Psi_{x_0})(u + \lambda(v-u))\right\|_{\mathrm{op}}^p \mathrm{d}u\mathrm{d}v\mathrm{d}\lambda \\
&\lesssim h^{-d} \int_0^1 \iint_{\mathcal{B}_{T_{x_0}M}(0,2h_0)^2} \mathbf{1}\{|w-u| \leq \lambda h\} \left\|d^{l+1}(\eta \circ \Psi_{x_0})(w)\right\|_{\mathrm{op}}^p \mathrm{d}u\mathrm{d}w\lambda^{-d}\mathrm{d}\lambda \\
&\lesssim \int_0^1 \int_{\mathcal{B}_{T_{x_0}M}(0,2h_0)} \left\|d^{l+1}(\eta \circ \Psi_{x_0})(w)\right\|_{\mathrm{op}}^p \mathrm{d}w \lesssim \int_{\mathcal{B}_M(x_0,h_0)} \|\eta_{l+1}(x)\|_{\mathrm{op}}^p \,\mathrm{d}x,
\end{aligned}$$

where at the second to last line, we used that $w = u + \lambda(v-u)$ is of norm smaller than $2h_0$ if $|u| \leq h_0$ and $|v-u| \leq h \leq h_0$, and, at the last line, we used that $J\Psi_{x_0}(w) \geq 1/2$ for $|w|$ small enough. □

5.4.4 Proof of Lemma 5.3.7

Lemma 5.3.7 is heavily based on the following classical control on the gradient of the Green function.

Lemma 5.4.4. *Let $x, y \in M$, then*

$$|\nabla_x G(x,y)| \lesssim \frac{1}{d_g(x,y)^{d-1}} \leq \frac{1}{|x-y|^{d-1}}. \tag{5.66}$$

Proof. For $d \geq 2$, a proof of Lemma 5.4.4 is found in [Aub82, Theorem 4.13]. See also [Hir96, Theorem 5.2] for a proof with more explicit constants in the case $d \geq 3$. Constants in their proofs depend on d, bounds on the curvature of M, $|\mathrm{vol}_M|$ and the geodesic diameter of M. As, those three last quantities can be further bounded by constants depending on $\tau_{\min}$, $f_{\min}$ and d, see Lemma 5.4.3 and [NSW08, Proposition 6.1], this concludes the proof. For $d = 1$, M is isometric to a circle, for which a closed formula for G exists [Bur94], and satisfies $|\nabla_x G(x,y)| \leq 1$. □

Recall that, by Lemma 5.3.2, $|\rho_h(x)| \geq 1/2$ for all $x \in M$. Therefore, Lemma 5.4.4 yields

$$\left|\nabla G\left(K_h * \left(\frac{\delta_x}{\rho_h}\right)\right)(z)\right| = \left|\int_M \nabla_z G(z,y) \frac{K_h(x-y)}{\rho_h(x)} \mathrm{d}y\right| \lesssim \int_{\mathcal{B}_M(x,h)} \frac{\|K\|_\infty h^{-d}}{|z-y|^{d-1}} \mathrm{d}y.$$

If $d = 1$, this quantity is smaller than a constant as $\mathrm{vol}_M(\mathcal{B}_M(x,h)) \lesssim h^d$ by Lemma 3.5.87. We then obtain directly the result in this case by integrating this inequality against $f(x)\mathrm{d}x$. If $d \geq 2$, we use the following argument.

- If $|x-z| \geq 2h$ and $y \in \mathcal{B}_M(x,h)$, then $|z-y| \geq |x-z| - h \geq |x-z|/2$. Therefore, by Proposition 3.5.7.7,

$$\int_{\mathcal{B}_M(x,h)} \frac{\|K\|_\infty h^{-d}}{|z-y|^{d-1}} \mathrm{d}y \leq \frac{2^{1-d}\|K\|_\infty h^{-d}}{|x-z|^{d-1}} \mathrm{vol}_M(\mathcal{B}_M(x,h)) \lesssim \frac{1}{|x-z|^{d-1}}.$$

- If $|x-z| \leq 2h$, then

$$\int_{\mathcal{B}_M(x,h)} \frac{\|K\|_\infty h^{-d}}{|z-y|^{d-1}} \mathrm{d}y \leq \int_{\mathcal{B}_M(z,3h)} \frac{\|K\|_\infty h^{-d}}{|z-y|^{d-1}} \mathrm{d}y$$
$$\leq \int_{\mathcal{B}_{T_zM}(0,3h)} \frac{\|K\|_\infty h^{-d} J\Psi_z(u)}{|z-\Psi_z(u)|^{d-1}} \mathrm{d}u \lesssim h^{-d} \int_{\mathcal{B}_{T_zM}(0,3h)} \frac{\mathrm{d}u}{|u|^{d-1}} \lesssim h^{1-d},$$

  where at the last line we used that $|z-\Psi_z(u)| \geq |u|$ and that $J\Psi_z(u) \lesssim 1$ by Lemma 5.4.1.

Hence,

$$\mathbb{E}\left[|\nabla(G(K_h * \delta_X))(z)|^p\right] = \int_M f(x)|\nabla(G(K_h * \delta_x))(z)|^p \mathrm{d}x$$
$$\leq f_{\max}\left(\int_{\mathcal{B}_M(z,2h)} |\nabla(G(K_h * \delta_x))(z)|^p \mathrm{d}x + \int_{M\setminus\mathcal{B}_M(z,2h)} |\nabla(G(K_h * \delta_x))(z)|^p \mathrm{d}x\right)$$
$$\lesssim \int_{\mathcal{B}_M(z,2h)} h^{(1-d)p} \mathrm{d}x + \int_{M\setminus\mathcal{B}_M(z,2h)} |z-x|^{(1-d)p} \mathrm{d}x$$
$$\lesssim h^{(1-d)p+d} + \int_{M\setminus\mathcal{B}_M(z,2h)} |z-x|^{(1-d)p} \mathrm{d}x.$$

The latter integral is bounded by

$$\int_{2h\leq|x-z|\leq r_0} |z-x|^{(1-d)p} \mathrm{d}x + \int_{|x-z|\geq r_0} |z-x|^{(1-d)p} \mathrm{d}x$$
$$\leq \int_{2h\leq|\Psi_z(u)-z|\leq r_0} |z-\Psi_z(u)|^{(1-d)p} J\Psi_z(u)\mathrm{d}u + |\mathrm{vol}_M| r_0^{(1-d)p}$$
$$\lesssim \int_{14h/8\leq|u|\leq r_0} |u|^{(1-d)p}\mathrm{d}u + 1 \lesssim h^{(1-d)p+d} \text{ if } (1-d)p+d<0,$$

where at the last line we use that $|u| \leq |z-\Psi_z(u)| \leq 8|u|/7$ by Proposition 3.5.8. If $d>2$ or if $d=2$ and $p>2$, the condition $(1-d)p+d<0$ is always satisfied. If $d=2$ and $p=2$, then $\int_{14h/8\leq|u|\leq h_0} |u|^{(1-d)p}\mathrm{d}u$ is of order $-\log h$, concluding the proof.

5.4.5 Proof of Theorem 5.2.1(i)

Let f be the density of μ and $\tilde{f} = f/\rho_h$. By Lemma 5.3.2, $f_{\min}(1-c_0h^{k-1}) \leq \tilde{f} \leq f_{\max}(1+c_0h^{k-1})$ for h small enough. We have

$$K_h * f(x) = \int_M K_h(x-y)\tilde{f}(y)\mathrm{d}y = \int_{\mathcal{B}_{T_xM}(0,h)} K_h(x-\Psi_x(v))\tilde{f}\circ\Psi_x(v)J\Psi_x(v)\mathrm{d}v$$
$$\geq \int_{\mathcal{B}_{T_xM}(0,h)} K_h(v)\tilde{f}\circ\Psi_x(v)J\Psi_x(v)\mathrm{d}v \tag{5.67}$$
$$-\int_{\mathcal{B}_{T_xM}(0,h)} |K_h(x-\Psi_x(v)) - K_h(v)|\tilde{f}\circ\Psi_x(v)J\Psi_x(v)\mathrm{d}v. \tag{5.68}$$

By Lemma 3.5.8(i), the quantity $|K_h(x-\Psi_x(v)) - K_h(v)|$ is bounded by $\frac{\|K\|_{\mathcal{C}^1(\mathbb{R}^d)}}{h^{d+1}}|x-v-\Psi_x(v)| \lesssim \frac{|v|^2}{h^{d+1}}$, so that the second term in the right-hand side of (5.68) is bounded by $Cf_{\max}\int_{\mathcal{B}_{T_xM}(0,h)} \frac{|v|^2}{h^{d+1}}\mathrm{d}v \lesssim h$. Also, using that $|J\Psi_x(v)-1| \leq c_1|v|$ by Lemma

3.5.8, the first term is larger than

$$\begin{aligned}
&f_{\min}(1-c_0h^{k-1})(1-c_1h)\int_{\mathbb{R}^d}K_+(v)\mathrm{d}v - f_{\max}(1+c_1h)(1+c_0h^{k-1})\int_{\mathbb{R}^d}K_-(v)\mathrm{d}v\\
&= f_{\min}(1-c_2h)\left(1+\int_{\mathbb{R}^d}K_-(v)\mathrm{d}v\right) - f_{\max}(1+c_2h)\int_{\mathbb{R}^d}K_-(v)\mathrm{d}v\\
&= f_{\min}(1-c_2h) - (f_{\max}(1+c_2h)-f_{\min}(1-c_2h))\int_{\mathbb{R}^d}K_-(v)\mathrm{d}v\\
&\geq f_{\min}(1-c_2h) - (f_{\max}(1+c_2h)-f_{\min}(1-c_2h))\beta\\
&\geq 3f_{\min}/4,
\end{aligned}$$

if $\beta < f_{\min}/(4(f_{\max}-f_{\min}))$ and h is small enough. Likewise, we show that $K_h * \tilde{f}(x) \leq 3f_{\max}/2$. It remains to show that $|K_h * \tilde{f}(x) - K_h * (\mu_n/\rho_h)(x)|$ is small enough for all $x \in M$ with high probability. Note that $K_h * \tilde{f} - K_h * (\mu_n/\rho_h)$ is L-Lipschitz with $L \lesssim h^{-d-1}$. Let $t = f_{\min}/4$ and consider a covering of M by N balls $\mathcal{B}_M(x_j, t/(2L))$. By standard packing arguments, such a covering exists with $N \lesssim (L/t)^d$. If $|K_h * \tilde{f}(x_j) - K_h * \mu_n(x_j)| \leq t/2$ for all $j = 1,\dots,N$, then $\|K_h * \tilde{f} - K_h * \mu_n\|_{L_\infty(M)} \leq t/2 + Lt/(2L) \leq t$. Hence, using Bernstein inequality [GN15, Theorem 3.1.7], as $|K_h(x_j - Y_i)| \leq \|K\|_{\mathcal{C}^0(\mathbb{R}^D)}h^{-d}$ and $\mathrm{Var}(K_h(x_j - Y_i)) \leq \|K^2\|_{\mathcal{C}^0(\mathbb{R}^D)}h^{-d}$, we obtain

$$\begin{aligned}
\mathbb{P}(\|K_h * \tilde{f} - K_h * \mu_n\|_{L_\infty(M)} \geq t) &\leq \mathbb{P}(\exists j,\ |K_h * \tilde{f}(x_j) - K_h * \mu_n(x_j)| \geq t/2)\\
&\lesssim (L/t)^d\mathbb{P}(|K_h * \tilde{f}(x_j) - K_h * \mu_n(x_j)| \geq t/2) \lesssim h^{-d(d+1)}\exp(-Cnh^d).
\end{aligned}$$

Choosing $nh^d = C'\log n$ for C' large enough yields the conclusion.

5.4.6 Proofs of Section 5.3.4

We first prove Lemma 5.3.8.

Proof of (a). The application $\Psi_{Y_j} \circ \pi_{Y_j} : \mathcal{B}_{\hat{T}_j}(0, 3\varepsilon) \to M$ is a diffeomorphism on $\mathcal{B}_{\hat{T}_j}(0, 3\varepsilon)$, as the composition of the diffeomorphisms Ψ_{Y_j} and $(\pi_{Y_j})_{|\hat{T}_j}$ (recall that $\angle(\hat{T}_j, T_{Y_j}M) \lesssim \varepsilon^{m-1} + \gamma\varepsilon^{-1} \lesssim 1$ by Proposition 5.2.4). Furthermore, as $\tilde{\pi}_{Y_j}$ is 1-Lipschitz continuous and using the bound on the angle,

$$\mathcal{B}_M(Y_j, 2\varepsilon) \subset \Psi_{Y_j}(\mathcal{B}_{T_{Y_j}M}(0, 2\varepsilon)) \subset (\Psi_{Y_j} \circ \pi_{Y_j})(\mathcal{B}_{\hat{T}_j}(0, 3\varepsilon)).$$

This proves the first part of Lemma 5.3.8(a). Let $S_j : \mathcal{B}_M(Y_j, 2\varepsilon) \to \mathcal{B}_{\hat{T}_j}(0, 3\varepsilon)$ be the inverse of $\Psi_{Y_j} \circ \pi_{Y_j}$. By Lemma 5.4.2(ii), $\hat{\Psi}_j$ is injective on $\hat{T}_j$, while, for $v \in \hat{T}_j$ with $|v| \leq 3\varepsilon$,

$$\left\|\mathrm{id} - d\hat{\Psi}_j(v)\right\|_{\mathrm{op}} \leq \left\|\sum_{a=2}^{m-1} a\hat{V}_{a,j}[\cdot, v^{\otimes(a-1)}]\right\| \lesssim \ell\varepsilon \leq 1/2 \tag{5.69}$$

if $\ell \lesssim \varepsilon^{-1}$ is small enough. Hence, $\hat{\Psi}_j : \mathcal{B}_{\hat{T}_j}(0, 3\varepsilon) \to \hat{\Psi}_j(\hat{T}_j)$ is a diffeomorphism on its image, and $\hat{\Psi}_j \circ S_j$ is a diffeomorphism as a composition of diffeomorphisms. Note that the inverse of $\hat{\Psi}_j$ is given by $\hat{\pi}_j(\cdot - X_j)$, so that $\mathcal{B}_{\hat{\Psi}_j(\hat{T}_j)}(X_j, \varepsilon) \subset \hat{\Psi}_j(\mathcal{B}_{\hat{T}_j}(0, \varepsilon))$. Furthermore, by Proposition 3.5.8,

$$(\Psi_{Y_j} \circ \pi_{Y_j})(\mathcal{B}_{\hat{T}_j}(0, \varepsilon)) \subset \Psi_{Y_j}(\mathcal{B}_{T_{Y_j}}(0, \varepsilon)) \subset \mathcal{B}_M(Y_j, 8\varepsilon/7),$$

so that $(\hat{\Psi}_j \circ S_j)(\mathcal{B}_M(Y_j, 2\varepsilon))$ contains $\mathcal{B}_{\hat{\Psi}_j(\hat{T}_j)}(X_j, \varepsilon)$. Furthermore, these inclusions of balls also hold for any $\varepsilon' \leq \varepsilon$, proving that $|\hat{\Psi}_j \circ S_j(z) - X_j| \geq (7/8)|z - Y_j|$ for any $z \in \mathcal{B}_M(Y_j, 2\varepsilon)$.

Proof of (b). The formula for the density $\tilde{\chi}_j$ follows from a change of variables.

Proof of (c). The inequality (5.48) follows from Proposition 5.2.4. We now prove that

$$|\pi_{Y_i}(z - \hat{\Psi}_j \circ S_j(z))| \lesssim \varepsilon(\varepsilon^m + \gamma). \tag{5.70}$$

Let $u \in \hat{T}_j$ be such that $z = \Psi_{Y_j} \circ \pi_{Y_j}(u)$ and $y = \hat{\Psi}_j(u)$. Recall that $X_j \in T_{Y_j}M^\perp$ by assumption, so that $\pi_{Y_j}(X_j - Y_j) = 0$. Also, by Lemma 3.5.8(i), we have $\Psi_{Y_j}(\pi_{Y_j}(u)) = Y_j + \pi_{Y_j}(u) + N_{Y_j}(\pi_{Y_j}(u))$ with $N_{Y_j}(\pi_{Y_j}(u)) \in T_{Y_j}M^\perp$, while by Lemma 5.4.2(ii), we have $\hat{\Psi}_j(u) = X_j + u + \hat{N}_j(u)$ with $\hat{N}_j(u) \in \hat{T}_j^\perp$. Hence,

$$\begin{aligned}
|\pi_{Y_j}(z - y)| &= |\pi_{Y_j}(Y_j + \pi_{Y_j}(u) + N_{Y_j}(\pi_{Y_j}(u)) - (X_j + u + \hat{N}_j(u)))| \\
&= |\pi_{Y_j}(N_{Y_j}(\pi_{Y_j}(u)) - \hat{N}_j(u))| \\
&\leq \angle(T_{Y_j}M, \hat{T}_j)|N_{Y_j}(\pi_{Y_j}(u)) - \hat{N}_j(u)| + |\hat{\pi}_j(N_{Y_j}(\pi_{Y_j}(u)) - \hat{N}_j(u))| \\
&\lesssim (\varepsilon^{m-1} + \gamma\varepsilon^{-1})(\varepsilon^m + \gamma) + |\hat{\pi}_j(\pi_{Y_j}^\perp(N_{Y_j}(\pi_{Y_j}(u))))| \\
&\lesssim (\varepsilon^{m-1} + \gamma\varepsilon^{-1})(\varepsilon^m + \gamma) + \angle(T_{Y_j}M, \hat{T}_j)|N_{Y_j}(\pi_{Y_j}(u))| \\
&\lesssim (\varepsilon^{m-1} + \gamma\varepsilon^{-1})(\varepsilon^m + \gamma + \varepsilon^2) \lesssim (\varepsilon^{m-1} + \gamma\varepsilon^{-1})(\varepsilon^2 + \gamma),
\end{aligned}$$

where we used Proposition 5.2.4 to bound $\angle(T_{Y_j}M, \hat{T}_j)$, Lemma 5.4.2 to bound $|N_{Y_j}(\pi_{Y_j}(u)) - \hat{N}_j(u)|$ and Lemma 3.5.8 to bound $|N_{Y_j}(\pi_{Y_j}(u))|$. Recalling that $\gamma \lesssim \varepsilon^2$ by assumption, we obtain (5.70).

To prove inequality (5.49), we first bound $|\chi_j(\hat{\Psi}_j \circ S_j(z)) - \chi_j(z)|$ and then bound $|J(\hat{\Psi}_j \circ S_j)(z) - 1|$. The first bound is based on the following elementary lemma.

Lemma 5.4.5. *Let $\theta : \mathbb{R}^D \to \mathbb{R}$ be a smooth radial function. Then, $|\theta(x) - \theta(y)| \leq \frac{\|\theta\|_{\mathcal{C}_2(\mathbb{R}^D)}}{2}||x|^2 - |y|^2|$.*

Proof. As $d\theta(0) = 0$, one can write $\theta(x) = \tilde{\theta}(|x|^2)$ for some function $\tilde{\theta}$ which is Lipschitz continuous with Lipschitz constant $\frac{\|d^2\theta\|_\infty}{2}$. This implies the conclusion. □

Recall from the proof of Lemma 5.2.5 that we have $\chi_j(z) = \zeta_j(z)/\sum_{i=1}^J \zeta_i(z)$ where $\zeta_i = \theta\left(\frac{z - X_i}{\varepsilon}\right)$ for some smooth radial function θ, and that furthermore, there is at most c_d non-zero terms in the sum in the denominator, which is always larger than 1. Hence, if we control for every $i = 1, \ldots, J$ the difference $||z - X_i|^2 - |\hat{\Psi}_j \circ S_j(z) - X_i|^2|$, then we obtain a control on $|\chi_j(z) - \chi_j(\hat{\Psi}_j \circ S_j(z))|$. We have by (5.48) and (5.70),

$$\begin{aligned}
&||\hat{\Psi}_j \circ S_j(z) - X_i|^2 - |z - X_i|^2| = ||\hat{\Psi}_j \circ S_j(z) - z|^2 + 2(\hat{\Psi}_j \circ S_j(z) - z) \cdot (z - X_i)| \\
&\lesssim (\varepsilon^m + \gamma)^2 + |(\hat{\Psi}_j \circ S_j(z) - z) \cdot (z - Y_i)| + |(\hat{\Psi}_j \circ S_j(z) - z) \cdot (X_i - Y_i)| \\
&\lesssim (\varepsilon^m + \gamma)^2 + |\pi_{Y_j}(\hat{\Psi}_j \circ S_j(z) - z) \cdot \pi_{Y_j}(z - Y_i)| \\
&\qquad + |\pi_{Y_j}^\perp(\hat{\Psi}_j \circ S_j(z) - z) \cdot \pi_{Y_j}^\perp(z - Y_i)| + (\varepsilon^m + \gamma)\gamma \\
&\lesssim (\varepsilon^m + \gamma)^2 + \varepsilon(\varepsilon^m + \gamma)|z - Y_i| + (\varepsilon^k + \gamma)|\pi_{Y_j}^\perp(z - Y_i)| + (\varepsilon^m + \gamma)\gamma.
\end{aligned}$$

By Proposition 3.5.7.4, $|\pi_{Y_j}^\perp(z - Y_i)| \leq |\tilde{\pi}_{Y_j}^\perp(z)| + |\tilde{\pi}_{Y_j}^\perp(Y_i)| \lesssim \varepsilon^2 + |Y_i - Y_j|^2$ and $\gamma, \varepsilon^m \lesssim \varepsilon^2$. Hence, we obtain that

$$||\hat{\Psi}_j \circ S_j(z) - X_i|^2 - |z - X_i|^2| \lesssim (\varepsilon^m + \gamma)(\varepsilon^2 + |Y_i - Y_j|^2). \tag{5.71}$$

Therefore,

$$\left|\theta\left(\frac{z-X_i}{\varepsilon}\right)-\theta\left(\frac{\hat{\Psi}_j\circ S_j(z)-X_i}{\varepsilon}\right)\right| \lesssim \frac{(\varepsilon^m+\gamma)(\varepsilon^2+|Y_i-Y_j|^2)}{\varepsilon^2} = (\varepsilon^m+\gamma)\left(1+\frac{|Y_i-Y_j|^2}{\varepsilon^2}\right). \tag{5.72}$$

Note also that if $|Y_i-Y_j|\geq 3\varepsilon$, then $|z-X_i|\geq |X_i-X_j|-|z-X_j|\geq 3\varepsilon-\varepsilon-3\gamma\geq\varepsilon$, while by the same argument $|\hat{\Psi}_j\circ S_j(z)-X_i|\geq\varepsilon$. Hence, both terms in the left-hand side of (5.72) are null in that case. Thus, we may assume that $|Y_i-Y_j|\leq 3\varepsilon$, so that $\left|\theta\left(\frac{z-X_i}{\varepsilon}\right)-\theta\left(\frac{\hat{\Psi}_j\circ S_j(z)-X_i}{\varepsilon}\right)\right|\lesssim\varepsilon^m+\gamma$. From the definition of $\chi_j(z)$, and as the function $t\mapsto 1/t$ is Lipschitz on $[1,\infty[$, we obtain that $|\chi_j(z)-\chi_j(\hat{\Psi}_j\circ S_j(z))|\lesssim\varepsilon^m+\gamma$.

We now prove a bound on $|J(\hat{\Psi}_j\circ S_j)(z)-1|$. One has, for $u=S_j(z)\in\hat{T}_j$,

$$|J(\hat{\Psi}_j\circ S_j)(z)-1| = \frac{|J\hat{\Psi}_j(u)-J(\Psi_{Y_j}\circ\pi_{Y_j})(u)|}{J(\Psi_{Y_j}\circ\pi_{Y_j})(u)}.$$

By Lemma 3.5.8(i) and Lemma 5.4.2(ii), we have $\left\|\mathrm{id}_{\hat{T}_j}-d(\Psi_{Y_j}\circ\pi_{Y_j})(u)\right\|_{\mathrm{op}}\lesssim|u|$ and $\left\|\mathrm{id}_{\hat{T}_j}-d\hat{\Psi}_j(u)\right\|_{\mathrm{op}}\lesssim|u|$. As a consequence, both Jacobians are larger than, say $1/2$ for u small enough, and, as the function $A\in\mathbb{R}^{d\times d}\mapsto\sqrt{\det(A)}$ is c_d Lipschitz on the set of matrices with $\det(A)\geq 1/2$ and $\|A\|_{\mathrm{op}}\leq 2$, we have

$$|J(\hat{\Psi}_j\circ S_j)(z)-1|\leq 2c_d\left\|d\hat{\Psi}_j(u)^*d\hat{\Psi}_j(u)-d(\Psi_{Y_j}\circ\pi_{Y_j})(u)^*d(\Psi_{Y_j}\circ\pi_{Y_j})(u)\right\|_{\mathrm{op}}. \tag{5.73}$$

Recall that $\hat{\Psi}_j(u)=X_j+u+\hat{N}_j(u)$ and $\Psi_{Y_j}\circ\pi_{Y_j}(u)=Y_j+\pi_{Y_j}(u)+N_{Y_j}\circ\pi_{Y_j}(u)$. We may write

$$d\hat{\Psi}_j(u)^*d\hat{\Psi}_j(u)=\mathrm{id}_{\hat{T}_j}+(d\hat{N}_j(u))^*d\hat{N}_j(u)\quad\text{and}$$
$$d(\Psi_{Y_j}\circ\pi_{Y_j})(u)^*d(\Psi_{Y_j}\circ\pi_{Y_j})(u)=\hat{\pi}_j\pi_{Y_j}\hat{\pi}_j+(d(N_{Y_j}\circ\pi_{Y_j})(u))^*d(N_{Y_j}\circ\pi_{Y_j})(u).$$

One has $\left\|\mathrm{id}_{\hat{T}_j}-\hat{\pi}_j\pi_{Y_j}\hat{\pi}_j\right\|_{\mathrm{op}}=\left\|\hat{\pi}_j\pi_{Y_j}^{\perp}\pi_{Y_j}^{\perp}\hat{\pi}_j\right\|_{\mathrm{op}}\leq\angle(T_{Y_j}M,\hat{T}_j)^2\lesssim(\varepsilon^{m-1}+\gamma\varepsilon^{-1})^2\lesssim\varepsilon^m+\gamma$ (recall that $\gamma\lesssim\varepsilon^2$). Furthermore, by Lemma 5.4.2(iv),

$$\begin{aligned}&\left\|(d\hat{N}_j(u))^*d\hat{N}_j(u)-(d(N_{Y_j}\circ\pi_{Y_j})(u))^*d(N_{Y_j}\circ\pi_{Y_j})(u)\right\|_{\mathrm{op}}\\&\quad\leq\left(\left\|d\hat{N}_j(u)\right\|_{\mathrm{op}}+\left\|d(N_{Y_j}\circ\pi_{Y_j})(u)\right\|_{\mathrm{op}}\right)\left\|d\hat{N}_j(u)-d(N_{Y_j}\circ\pi_{Y_j})(u)\right\|_{\mathrm{op}}\\&\quad\lesssim\varepsilon(\varepsilon^{m-1}+\gamma\varepsilon^{-1})\lesssim\varepsilon^m+\gamma.\end{aligned}$$

Putting together (5.73) with those two inequalities, we obtain that $|J(\hat{\Psi}_j\circ S_j)(z)-1|\lesssim\varepsilon^m+\gamma$, concluding the proof of Lemma 5.3.8.

To conclude the section, we state and prove Lemma 5.4.6, which gives an upper bound on the quantity T appearing in Lemma 5.3.9 for $\phi=K_h*(\nu_n/\hat{\rho}_h)$ and $\phi'=K_h*(\mu_n/\rho_h)$.

Lemma 5.4.6. *The quantity* $T=\max_{j=1\ldots J}\sup_{z\in\mathcal{B}(Y_j,\varepsilon)}|\phi(\hat{\Psi}_j\circ S_j(z))-\phi'(z)|$ *satisfies* $T\lesssim\varepsilon^m+\gamma$ *with probability larger than* $1-cn^{-k/d}$.

Proof. For $z \in \mathcal{B}(Y_j, \varepsilon)$, we have

$$|\phi(\hat{\Psi}_j \circ S_j(z)) - \phi'(z)| \leq \frac{1}{n} \sum_{i=1}^{n} \left| \frac{K_h * \delta_{X_i}(\hat{\Psi}_j \circ S_j(z))}{\hat{\rho}_h(X_i)} - \frac{K_h * \delta_{Y_i}(z)}{\rho_h(Y_i)} \right|.$$

Fix an index $i \in \{1, \dots, n\}$. By Proposition 3.5.7.4, as $X_i - Y_i \in T_{Y_i} M^{\perp}$, we have for $z \in M$,

$$||z - Y_i|^2 - |z - X_i|^2| = ||X_i - Y_i|^2 - 2(z - Y_i) \cdot (X_i - Y_i)| \leq \gamma^2 + |z - Y_i|^2 \frac{\gamma}{\tau_{\min}}.$$

This inequality together with (5.71) and Lemma 5.4.5 yield

$$\begin{aligned}
&|K_h(X_i - \hat{\Psi}_j \circ S_j(z)) - K_h(Y_i - z)| \\
&\quad \leq |K_h(X_i - \hat{\Psi}_j \circ S_j(z)) - K_h(X_i - z)| + |K_h(X_i - z) - K_h(Y_i - z)| \\
&\quad \lesssim h^{-d-2} \left((\varepsilon^m + \gamma)(\varepsilon^2 + |Y_i - Y_j|^2) + \gamma^2 + \gamma |z - Y_i|^2 \right).
\end{aligned}$$

We may assume that $|Y_i - Y_j| \leq 3h$ and $|z - Y_i| \leq 2h$, for otherwise both quantities in the left-hand site of the above equation are zero. Hence, as $\gamma \lesssim \varepsilon \lesssim h$ by assumption, we have

$$|K_h(X_i - \hat{\Psi}_j \circ S_j(z)) - K_h(Y_i - z)| \lesssim h^{-d}(\varepsilon^m + \gamma) \mathbf{1}\{Y_i \in \mathcal{B}_M(z, 2h)\}. \tag{5.74}$$

Let us now bound $|\hat{\rho}_h(\hat{\Psi}_j \circ S_j(X_i)) - \rho_h(Y_i)|$. By the triangle inequality, and using (5.49) and (5.74), we obtain that this quantity is smaller than

$$\begin{aligned}
&\sum_{j=1}^{J} \int_M |\tilde{\chi}_j(z) K_h(X_i - \hat{\Psi}_j \circ S_j(z)) - \chi_j(z) K_h(Y_i - z)| \mathrm{d}z \\
&\lesssim \sum_{j=1}^{J} \int_M \Bigg(\mathbf{1}\{z \in \mathcal{B}_M(Y_j, 2\varepsilon)\}(\varepsilon^m + \gamma)|K_h(Y_i - z)| \\
&\qquad\qquad + \tilde{\chi}_j(z) h^{-d}(\varepsilon^m + \gamma) \mathbf{1}\{z \in \mathcal{B}_M(Y_i, 2h)\} \Bigg) \mathrm{d}z \\
&\lesssim h^{-d}(\varepsilon^m + \gamma) \sum_{j=1}^{J} \int_M \mathbf{1}\{z \in \mathcal{B}_M(Y_j, 2\varepsilon)\} \mathbf{1}\{z \in \mathcal{B}_M(Y_i, 2h)\} \mathrm{d}z \\
&\lesssim \varepsilon^d h^{-d}(\varepsilon^m + \gamma) \sum_{j=1}^{J} \mathbf{1}\{|Y_j - Y_i| \leq 4h\} \\
&\lesssim h^{-d}(\varepsilon^m + \gamma) \sum_{j=1}^{J} \mathbf{1}\{|Y_j - Y_i| \leq 4h\} \mathrm{vol}_M(\mathcal{B}_M(Y_j, \varepsilon/8)) \\
&\lesssim h^{-d}(\varepsilon^m + \gamma) \mathrm{vol}_M(\mathcal{B}_M(Y_i, 5h)) \lesssim \varepsilon^m + \gamma,
\end{aligned}$$

where we use that $\{X_1, \dots, X_J\}$ is $7\varepsilon/24$-sparse, so that $\{Y_1, \dots, Y_J\}$ is $\varepsilon/4$-sparse. Therefore, the balls $\mathcal{B}_M(Y_j, \varepsilon/8)$ for $|Y_j - Y_i| \leq 4h$ are pairwise distinct, and are all included in $\mathcal{B}_M(Y_i, 4h + \varepsilon/8) \subset \mathcal{B}_M(Y_i, 5h)$. We conclude by Proposition 3.5.7.7.

Letting $N(z, 2h)$ be the number of points Y_i belonging to $\mathcal{B}_M(z, 2h)$, we obtain

$$|\phi(\hat{\Psi}_j \circ S_j(z)) - \phi'(z)| \lesssim \frac{1}{n}\sum_{i=1}^{n}\Bigg(|K_h(Y_i - z)|(\varepsilon^m + \gamma) + h^{-d}(\varepsilon^m + \gamma)\mathbf{1}\{Y_i \in \mathcal{B}_M(z, 2h)\}\Bigg)$$
$$\lesssim \frac{N(z, 2h)}{nh^d}(\varepsilon^m + \gamma).$$

If, for every $z \in M$ and some $\lambda > 0$, $N(z, 2h) \leq \lambda nh^d$, then we have the conclusion. Let us bound

$$P_0 = \mathbb{P}(\exists z \in M,\ N(z, 2h) > \lambda nh^d).$$

If $N(z, 2h) > \lambda nh^d$, then there exists a point Y_i with $N(Y_i, 4h) \geq N(z, 2h) > \lambda nh^d$. Hence, $P_0 \leq n\mathbb{P}(N(Y_1, 4h) > \lambda nh^d)$. Conditionally on Y_1, $N(Y_1, 4h) = 1 + U$ with U a binomial random variable of parameters $n - 1$ and $\mu(\mathcal{B}_M(Y_1, 4h)) \leq f_{\max}\mathrm{vol}_M(\mathcal{B}_M(Y_1, 4h)) \lesssim h^d$ (see Proposition 3.5.7.7). In particular, for λ large enough, the probability P_0 is smaller than $n^{-k/d}$ by Hoeffding's inequality. □

5.4.7 Lower bounds on minimax risks

In this section, we prove the different lower bounds on minimax risks stated in the article. The main tool used will be Assouad's lemma. Fix as in Chapter 3 a statistical model $(\mathcal{Y}, \mathcal{H}, \mathcal{Q})$ with $\mathcal{Q} \subset \mathcal{P}_1(\mathcal{Y})$ and $\vartheta : \mathcal{Y} \to (E, \mathcal{L})$ a measurable function taking its values in some semi-metric space $(E, \mathcal{L})$. We further assume that we observe n i.i.d. observations from law $\iota_\# \xi$ for some $\xi \in \mathcal{Q}$, with ι being the addition in our case.

Lemma 5.4.7 (Assouad's lemma [Yu97]). *Let $m \geq 1$ be an integer and $\mathcal{Q}_m = \{\xi_\sigma,\ \sigma \in \{-1, 1\}^m\} \subset \mathcal{Q}$ be a set of probability measures. Assume that for all $\sigma, \sigma' \in \{-1, 1\}^m$,*

$$\mathcal{L}(\vartheta(\xi_\sigma), \vartheta(\xi_{\sigma'})) \geq |\sigma - \sigma'|\delta, \tag{5.75}$$

where $|\sigma - \sigma'| = \sum_{i=1}^m \mathbf{1}\{\sigma(i) \neq \sigma'(i)\}$ is the Hamming distance between σ and σ'. Then,

$$\mathcal{R}_n(\vartheta, \mathcal{Q}, \mathcal{L}) \geq m\frac{\delta}{16}\left(1 - \max\left\{TV(\iota_\#\xi_\sigma, \iota_\#\xi_{\sigma'}),\ |\sigma - \sigma'| = 1\right\}\right)^{2n}. \tag{5.76}$$

The lower bound on the minimax rates we prove are actually going to hold on the smaller model of uniform distributions on manifolds.

Definition 5.4.8. *Let $k \geq 2$ and $\gamma \geq 0$. The set $\mathcal{Q}_d^k(\gamma)$ is the set of probability distributions ξ of random variables (Y, Z), where Y follows the uniform distribution on some manifold $M \in \mathcal{M}_d^k$ with $f_{\max}^{-1} \leq |\mathrm{vol}_M| \leq f_{\min}^{-1}$, and $Z \in \mathcal{B}(0, \gamma)$ is such that $Z \in T_Y M^\perp$. The statistical model is completed by letting $(\mathcal{Y}, \mathcal{H})$ be $\mathbb{R}^D \times \mathbb{R}^D$ endowed with its Borel σ-algebra, ι be the addition $\mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^D$ and $\vartheta(\xi)$ be the first marginal μ of ξ.*

We write $\mathcal{Q}_d^k$ for $\mathcal{Q}_d^k(0)$. One can check that $\mathcal{Q}_d^k(\gamma) \subset \mathcal{Q}_d^{k,s}(\gamma)$, with parameter $L_s = f_{\min}^{-1/p} \vee f_{\max}^{1-1/p}$. Therefore, a lower bound on the minimax risk on the model $\mathcal{Q}_d^k(\gamma)$ yields a lower bound on the minimax risk on the model $\mathcal{Q}_d^{k,s}(\gamma)$ should the parameter L_s be large enough.

We build a subfamily of manifolds indexed by $\sigma \in \{-1, 1\}^m$ following [AL19]. By [AL19, Section C.2], there exists a manifold $M \subset \mathbb{R}^{d+1}$ of reach $2\tau_{\min}$, of volume

$C_d\tau_{\min}^d$ which contains $\mathcal{B}_{\mathbb{R}^d}(0,\tau_{\min})$. Let $\delta > 0$ and consider a family of m points $x_1,\dots,x_m \in \mathcal{B}_{\mathbb{R}^d}(0,\tau_{\min}/2)$, with $|x_i - x_{i'}| \geq 4\delta$ for $i \neq i'$ and $c_d(\tau_{\min}/\delta)^d \leq m \leq C_d(\tau_{\min}/\delta)^d$. Let $0 < \Lambda < \delta$ and let $\phi : \mathbb{R}^{d+1} \to [0,1]$ be a smooth radial function supported on $\mathcal{B}(0,1)$, with $\phi \equiv 1$ on $\mathcal{B}(0,1/2)$. Let e be the unit vector in the $(d+1)$th direction. We then let, for $\sigma \in \{-1,1\}^m$,

$$\Phi_\sigma^\Lambda(x) = x + \sum_{i=1}^m \frac{\sigma_i + 1}{2}\Lambda\phi\left(\frac{x - x_i}{\delta}\right)e. \tag{5.77}$$

Let $M_\sigma^\Lambda = \Phi_\sigma^\Lambda(M)$ and μ_σ^Λ be the the uniform measure on M_σ^Λ. If $\Lambda \leq c_{k,d,\tau_{\min}}\delta^k$, then $\mu_\sigma^\Lambda \in \mathcal{Q}_d^k$, provided that L_k is large enough [AL19, Lemma C.13]. If $\sigma_i = 1$, the volume of $\Phi_\sigma^\Lambda(\mathcal{B}_{\mathbb{R}^d}(x_i,\delta))$ satisfies, with ω_d the volume of the d-dimensional unit ball,

$$\begin{aligned}\left|\mathrm{vol}_{M_\sigma^\Lambda}(\Phi_\sigma^\Lambda(\mathcal{B}_{\mathbb{R}^d}(x_i,\delta)) - \omega_d\delta^d\right| &\leq \int_{\mathcal{B}_{\mathbb{R}^d}(x_i,\delta)} |J\Phi_\sigma^\Lambda(x) - 1|\mathrm{d}x \\ &\leq \int_{\mathcal{B}_{\mathbb{R}^d}(x_i,\delta)} \left|\sqrt{1 + \Lambda^2\delta^{-2}\left|\nabla\phi\left(\frac{x-x_i}{\delta}\right)\right|^2} - 1\right|\mathrm{d}x \leq C_d\delta^d\Lambda^2\delta^{-2}.\end{aligned}$$

Hence, for δ small enough, we have $||\mathrm{vol}_{M_\sigma^\Lambda}| - C_d\tau_{\min}^d| \leq mC_d\delta^d\Lambda^2\delta^{-2} \leq C_d\tau_{\min}^d/3$, as $m \leq C_d(\tau_{\min}/\delta)^d$ and $\Lambda \leq c_{k,d,\tau_{\min}}\delta^k$. As a consequence, if $|\sigma - \sigma'| = 1$, with for instance $\sigma_i = 1$ and $\sigma_i' = -1$, then

$$\mathrm{TV}(\mu_\sigma^\Lambda, \mu_\sigma'^\Lambda) \leq \max(\mu_\sigma^\Lambda(\Phi_\sigma^\Lambda(\mathcal{B}_{\mathbb{R}^d}(x_i,\delta))), \mu_{\sigma'}^\Lambda(\mathcal{B}_{\mathbb{R}^d}(x_i,\delta)) \leq C_{d,\tau_{\min}}\delta^d. \tag{5.78}$$

We may now prove the different minimax lower bounds using Assouad's Lemma on the family $\{\mu_\sigma^\Lambda,\ \sigma \in \{-1,1\}^m\}$.

Proof of Theorem 5.1.9. As g is nondecreasing and convex, by Jensen's inequality, we may assume without loss of generality that $\mathcal{L} = \mathrm{TV}$. Let $\Gamma = |(\mu_\sigma^\Lambda - \mu_{\sigma'}^\Lambda)(B_i)|$, where $B_i = \mathcal{B}_{\mathbb{R}^d}(x_i,\delta)$ and $\sigma(i) \neq \sigma'(i)$. Then, $\mathrm{TV}(\mu_\sigma^\Lambda, \mu_{\sigma'}^\Lambda) \geq |\sigma - \sigma'|\Gamma$. Furthermore, if for instance $\sigma'(i) = 1$, $\Gamma \geq \mu_{\sigma'}^\Lambda(B_i) = (\omega_d\delta^d)/|\mathrm{vol}_{M_{\sigma'}^\Lambda}| \geq c_d\delta^d/\tau_{\min}^d$. By Assouad's Lemma,

$$\begin{aligned}\mathcal{R}_n(\mu;\mathcal{Q}_d^{s,k};\mathrm{TV}) \geq \mathcal{R}_n(\mu;\mathcal{Q}_d^k;\mathrm{TV}) &\geq \frac{m}{16}c_d\frac{\delta^d}{\tau_{\min}^d}\left(1 - C_{d,\tau_{\min}}\delta^d\right)^{2n} \\ &\geq C_d\left(1 - C_{d,\tau_{\min}}\delta^d\right)^{2n}.\end{aligned}$$

We obtain the conclusion by letting δ go to 0. □

Lemma 5.4.9. *For any $\tau_{\min} > 0$ and $1 \leq r \leq \infty$, for $f_{\min}$ small enough and $f_{\max}$, L_k large enough, one has*

$$\mathcal{R}_n\left(\frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}, \mathcal{Q}_d^k(\gamma), W_r\right) \gtrsim \gamma + n^{-k/d}. \tag{5.79}$$

Proof. As, $W_r \geq W_1$, we may assume that $r = 1$. Let $\sigma, \sigma' \in \{-1,1\}^m$ with $\sigma(i) \neq \sigma'(i)$. Let $p_{\sigma(i)} = \mathrm{vol}_{M_\sigma^\Lambda}(\mathcal{B}(x_i,\delta))$ and $U_{\sigma,i}^\Lambda = p_{\sigma(i)}^{-1}(\mathrm{vol}_{M_\sigma^\Lambda})_{|\mathcal{B}(x_i,\delta)}$. By the Kantorovitch-Rubinstein duality formula, $W_1(\mu,\nu) = \max\int f\mathrm{d}(\mu - \nu)$, where the maximum is taken over all 1-Lipschitz continuous functions $f : \mathbb{R}^D \to \mathbb{R}$. Let $f : x \mapsto x \cdot e$. Assume for instance that $\sigma(i) = -1$ and $\sigma'(i) = 1$. We have $f(x) = 0$ for $x \in \mathcal{B}_{M_\sigma^\Lambda}(x_i,\delta)$ and $f(x) = \Lambda$ for $x \in \mathcal{B}_{M_{\sigma'}^\Lambda}(x_i,\delta/2)$. Therefore, we have, as $p_{\sigma'(i)} \leq c\delta^{-d}$,

$$W_1(U_{\sigma,i}^\Lambda, U_{\sigma',i}^\Lambda) \geq p_{\sigma'(i)}^{-1}\Lambda\omega_d(\delta/2)^d \geq c_1\Lambda.$$

Note also that $|p_{\sigma(i)} - p_{\sigma'(i)}| \leq \left|\mathrm{vol}_{M_\sigma^\Lambda}(\Phi_\sigma^\Lambda(\mathcal{B}_{\mathbb{R}^d}(x_i,\delta)) - \omega_d\delta^d\right| \leq C_d\delta^d\Lambda^2\delta^{-2}$. Furthermore, $||\mathrm{vol}_{M_\sigma^\Lambda}| - |\mathrm{vol}_{M_{\sigma'}^\Lambda}|| \leq \sum_{i=1}^m |p_{\sigma(i)} - p_{\sigma'(i)}| \leq |\sigma - \sigma'|C_d\delta^d\Lambda^2\delta^{-2}$. Let f_i be a function such that $W_1(U_{\sigma,i}^\Lambda, U_{\sigma',i}^\Lambda) = \int f d(U_{\sigma,i}^\Lambda - U_{\sigma',i}^\Lambda)$. One can choose f_i such that $f_i(x_i) = 0$, so that the maximum of $|f_i|$ on $\mathcal{B}(x_i,\delta)$ is at most δ. One can then change the value of f_i outside the ball without changing the value of the integral, so that f_i is supported on $\mathcal{B}(x_i, 2\delta)$ and 1-Lipschitz continuous. Consider the function f obtained by gluing together the different functions f_i. The function f is 1-Lipschitz continuous, so that

$$\begin{aligned}
W_1\left(\mu_\sigma^\Lambda, \mu_{\sigma'}^\Lambda\right) &\geq \sum_{i=1}^m \left(\frac{p_{\sigma(i)}}{|\mathrm{vol}_{M_\sigma^\Lambda}|}U_{\sigma,i}^\Lambda - \frac{p_{\sigma'(i)}}{|\mathrm{vol}_{M_{\sigma'}^\Lambda}|}U_{\sigma',i}^\Lambda\right)(f) \\
&\geq \sum_{i=1}^m \frac{p_{\sigma(i)}}{|\mathrm{vol}_{M_\sigma^\Lambda}|}(U_{\sigma,i}^\Lambda - U_{\sigma',i}^\Lambda)(f) - |p_{\sigma(i)} - p_{\sigma'(i)}|\frac{|U_{\sigma',i}^\Lambda(f)|}{|\mathrm{vol}_{M_\sigma^\Lambda}|} \\
&\qquad - p_{\sigma'(i)}|U_{\sigma',i}^\Lambda(f)|\left|\frac{1}{|\mathrm{vol}_{M_\sigma^\Lambda}|} - \frac{1}{|\mathrm{vol}_{M_{\sigma'}^\Lambda}|}\right| \\
&\geq \sum_{i=1}^m \frac{p_{\sigma(i)}}{|\mathrm{vol}_{M_\sigma^\Lambda}|}W_1(U_{\sigma,i}^\Lambda, U_{\sigma',i}^\Lambda) - \sum_{i=1}^m c_4|p_{\sigma(i)} - p_{\sigma'(i)}|\delta\mathbf{1}\{\sigma(i) \neq \sigma'(i)\} \\
&\qquad - c_5\delta|\sigma - \sigma'|\delta^d\Lambda^2\delta^{-2} \\
&\geq \sum_{i=1}^m \mathbf{1}\{\sigma(i) \neq \sigma'(i)\}(c_6\delta^d\Lambda - c_4\delta^d\Lambda^2\delta^{-1}) - c_5\delta|\sigma - \sigma'|\delta^d\Lambda^2\delta^{-2} \\
&\geq c_7\delta^d\Lambda|\sigma - \sigma'|.
\end{aligned}$$

Hence, letting $\Lambda = c_{k,d,\tau_{\min},L_k}\delta^k$ and $\delta = n^{-1}$, we have, by Assouad's Lemma,

$$\mathcal{R}_n\left(\frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}, \mathcal{Q}_d^k(\gamma), W_r\right) \gtrsim n^{-k/d}.$$

Consider now the case $\gamma > 0$. Let M_0 be the d-dimensional sphere of radius $\tau_{\min}$ and M_1 be the d-dimensional sphere of radius $\tau_{\min} + \delta$. Let Y be uniform on M_1, and let ξ be the law of $(Y, 0)$. Also, let ξ' be the law of $((1+\gamma/\tau_{\min})Y, -\gamma/\tau_{\min}Y)$. Then, $\iota_\#\xi = \iota_\#\xi'$, whereas $W_1\left(\frac{\mathrm{vol}_{M_0}}{|\mathrm{vol}_{M_0}|}, \frac{\mathrm{vol}_{M_1}}{|\mathrm{vol}_{M_1}|}\right) \geq \gamma$. We conclude by Le Cam lemma [Yu97] that $\mathcal{R}_n\left(\frac{\mathrm{vol}_M}{|\mathrm{vol}_M|}, \mathcal{Q}_d^k(\gamma), W_r\right) \gtrsim \gamma$. □

Proof of Theorem 5.2.1(iv). Let $a_n = n^{-\frac{s+1}{2s+d}}$ if $d \geq 3$ and $a_n = n^{-1/2}$ if $d \leq 2$. As $W_p \geq W_1$, we may assume without loss of generality that $r = 1$, and up to rescaling, we assume that $\tau_{\min} = \sqrt{d}$. Consider the manifold $M \subset \mathbb{R}^{d+1}$ containing $\mathcal{B}_{\mathbb{R}^d}(0, \sqrt{d})$ of the previous proof. In particular, M contains the cube $[-1,1]^d$. We adapt the proof of Theorem 3 in [WB19b], where authors consider a family of functions $f_\sigma : [-1,1]^d \to M$ indexed by $\sigma \in \{-1,1\}^m$, with $f_\sigma = 1 + n^{-1/2}\sum_{j=1}^m \sigma_j\psi_j$, where $(\psi_j)_{j=1,\dots,m}$ are elements of a wavelet basis of $[-1,1]^d$ (see [WB19b, Appendix E] for details on the construction of the wavelet basis). If $m \lesssim n^{d/(2s+d)}$, then $t_0 \leq f_\sigma \leq t_1$ for some positive constants $t_0 < 1 < t_1$, and $\|f_\sigma\|_{B_{p,q}^s([-1,1]^d)} \lesssim 1$. Define a function g_σ by $g_\sigma(x) = f_\sigma(x)$ if $x \in [-1,1]^d$ and $g_\sigma(x) = 1$ otherwise. The function g_σ satisfies $t_0 \leq g_\sigma \leq t_1$, as well as $\|g_\sigma\|_{B_{p,q}^s(M)} \lesssim \|f_\sigma\|_{B_{p,q}^s} + |\mathrm{vol}_M|^{1/p} \lesssim 1$. Such an inequality is clear for the $\|\cdot\|_{H_p^l(M)}$ norm for l an integer, as $\|g_\sigma\|_{H_p^l(M)}^p = \|g_\sigma\|_{H_p^l([-1,1]^d)}^p + \|g_\sigma\|_{H_p^l(M\setminus[-1,1]^d)}^p$, while the result follows from interpolation for Besov spaces [Lun18, Corollary 1.1.7]. Also, as

$\int_{[-1,1]^d} f_\sigma = 1$, we have $\int g_\sigma = |\mathrm{vol}_M|$, and $g_\sigma/|\mathrm{vol}_M|$ is larger than $f_{\min} = t_0/|\mathrm{vol}_M|$ and smaller than $f_{\max} = t_1/|\mathrm{vol}_M|$. Hence, identifying measures with their densities, the set

$$\mathcal{Q}_m = \{\mu_\sigma = g_\sigma/|\mathrm{vol}_M|,\ \sigma \in \{-1,1\}^m\}$$

is a subset of $\mathcal{Q}_d^{s,k}$ for $f_{\min}$ small enough and L_k, L_s, $f_{\max}$ large enough. Furthermore, for $\sigma, \sigma' \in \{-1,1\}^m$, $\mathrm{TV}(\mu_\sigma, \mu_{\sigma'}) = \mathrm{TV}(f_\sigma, f'_\sigma)$, while $W_1(\mu_\sigma, \mu_{\sigma'}) = W_1(f_\sigma, f_{\sigma'})$ by the Kantorovitch-Rubinstein duality formula. Hence, applying Assouad's inequality in the same fashion than in [WB19b, Theorem 3] yields that $\mathcal{R}_n(\mu, \mathcal{Q}_d^{s,k}, W_1) \gtrsim a_n$. □

Proof of Theorem 5.2.7(iv). According to Lemma 5.4.9,

$$\mathcal{R}_n(\mu, \mathcal{Q}_d^{s,k}, W_p) \geq \mathcal{R}_n(\mu, \mathcal{Q}_d^{k}, W_p) \gtrsim \gamma + n^{-k/d},$$

and according to Theorem 5.2.1(iv), $\mathcal{R}_n(\mu, \mathcal{Q}_d^{s,k}, W_p) \gtrsim a_n$. □

5.4.8 Existence of kernels satisfying conditions A, $B(m)$ and $C(\beta)$

The goal of the section is to prove the existence of a kernel K satisfying the conditions A, $B(m)$ and $C(\beta)$ stated at the beginning of Section 5.2.

If K is a radial kernel, we have by integration by parts, as K is smooth with compact support,

$$\int_{\mathbb{R}^d} \partial^{\alpha_0} K(v) v^{\alpha_1} \mathrm{d}v = C_{\alpha_0,\alpha_1} \int_{\mathbb{R}^d} K(v) v^{\alpha_1+\alpha_0} \mathrm{d}v = C'_{\alpha_0,\alpha_1} \int_{\mathbb{R}} K(r) r^{d+|\alpha_0|+|\alpha_1|-1} \mathrm{d}r.$$

Hence, to show the existence of such a kernel, it suffices to find for every $m \geq 0$ a smooth even function $K : \mathbb{R} \to \mathbb{R}$ supported on $[-1,1]$ satisfying

- **Condition A':** $\int_{\mathbb{R}} K(r) r^{d-1} \mathrm{d}r = (C'_{0,0})^{-1}$,
- **Condition $B'(m)$:** $\int_{\mathbb{R}} K(r) r^{d+i-1} \mathrm{d}r = 0$ for $i = 1, \dots, m$,
- **Condition $C'(\beta)$:** $\int_{\mathbb{R}} K(r)^- r^{d-1} \mathrm{d}r \leq \beta$.

We show by recursion on m that for any $\beta > 0$, there exists a such a kernel. For $m = 0$, let K_0 be any smooth even nonnegative function supported on $[-1,1]$. Then, letting $K = (C'_{0,0})^{-1} K_0 / \int_{\mathbb{R}} K_0$, we obtain a kernel K satisfying the desired conditions for any $\beta > 0$. Consider now the case $m > 0$. Let $\beta > 0$.

- If $m + d$ is even, then any K satisfying conditions A', $B'(m-1)$ and $C'(\beta)$ will also satisfy $B'(m)$. Indeed, as K is even, we have $\int_{\mathbb{R}} K(r) r^{m+d-1} \mathrm{d}r = 0$, so that the induction step is proven.
- If $m+d$ is odd, let K be a kernel satisfying conditions A', $B'(m-1)$ and $C'(\beta/2)$. We use the following lemma.

Lemma 5.4.10. *For $i \geq 0$, let $e_i : x \in \mathbb{R} \mapsto x^{i+d-1}$ and fix an integer $m > 0$. Then, for any $a \in \mathbb{R}$, let F_a be the set of smooth functions $f : (1,\infty) \to \mathbb{R}$ with compact support satisfying $\int f e_i = 0$ for $0 \leq i < m$ and $\int f e_m = a$. Then,*

$$\inf \left\{ \int |f(r)| r^{d-1} \mathrm{d}r,\ f \in F_a \right\} = 0. \tag{5.80}$$

Assume first the lemma. Let $a = -\frac{1}{2}\int_{\mathbb{R}} K(r)r^{m+d-1}$ and $f \in F_a$. Then,

$$\begin{cases} \int (K(r)+f(|r|))r^{d-1}\mathrm{d}r = (C'_{0,0})^{-1} + \int f(|r|)r^{d-1}\mathrm{d}r = (C'_{0,0})^{-1} \\ \int (K(r)+f(|r|))r^{i+d-1}\mathrm{d}r = \int f(|r|)r^{i+d-1}\mathrm{d}r = 0 \text{ for } 0 < i < m \\ \int (K(r)+f(|r|))r^{m+d-1}\mathrm{d}r = \int K(r)r^{m+d-1}\mathrm{d}r + 2\int_1^\infty f(r)r^{m+d-1}\mathrm{d}r = 0. \end{cases}$$

Hence, the kernel $K + f(|\cdot|)$ satisfies the condition $B'(m)$. Also, we have, as $K(r) = 0$ if $|r| \geq 1$,

$$\begin{aligned} \int_{\mathbb{R}} (K(r)+f(|r|))_- r^{d-1}\mathrm{d}r &= \int_{\mathbb{R}} K(r)_-\mathrm{d}r + 2\int_1^\infty f(r)_- r^{d-1}\mathrm{d}r \\ &\leq \beta/2 + \int_1^\infty |f(r)|r^{d-1}\mathrm{d}r, \end{aligned}$$

where we used at the last line that

$$\int_1^\infty f(r)_- r^{d-1}\mathrm{d}r = \int_1^\infty f(r)_+ r^{d-1}\mathrm{d}r = \frac{1}{2}\int_1^\infty |f(r)|r^{d-1}\mathrm{d}r.$$

Lemma 5.4.10 asserts the existence of $f \in F_a$ with $\int |f(r)|r^{d-1}\mathrm{d}r \leq \beta/2$. For such a choice of f, the kernel $\tilde{K} = K + f(|\cdot|)$ satisfies also $C'(\beta)$. Finally, f has a compact support, included in $[0, R]$ for some $R > 0$. The kernel $\tilde{K}_{1/R}$ is supported on $\mathcal{B}(0,1)$, and satisfies conditions A', $B'(m)$ and $C'(\beta)$. This concludes the induction step, and the proof of the existence of kernels satisfying conditions A, $B(m)$ and $C(\beta)$.

Proof of Lemma 5.4.10. Consider functions f supported on $[r_0, r_1]$ for some $1 < r_0 \leq r_1$ to fix. Let G_{r_0,r_1} be the subspace of $L_2([r_0,r_1])$ spanned by the functions e_i for $0 \leq i \leq m-1$ and let g_m be the projection of e_m on $G^\perp_{r_0,r_1}$ the orthogonal space of G_{r_0,r_1}, with L_2 norm ℓ. The function $f = \frac{ag_m}{\ell^2}$ is a polynomial of degree m restricted to $[r_0, r_1]$ and satisfies $\int fe_i = 0$ for $0 \leq i \leq m-1$ by construction, with $\int fe_m = \frac{a}{\ell^2}\int e_m g_m = a$. Also, we have for any polynomial $P \in G_{r_0,r_1}$,

$$\begin{aligned} \|e_m - P\|^2_{L_2([r_0,r_1])} &= \int_{r_0}^{r_1} |r^{m+d-1} - P(r)|^2\mathrm{d}r = \int_1^{\frac{r_1}{r_0}} r_0|(r_0 r)^{d+m-1} - P(rr_0)|^2\mathrm{d}r \\ &= r_0^{2(d+m)-1}\int_1^{\frac{r_1}{r_0}} |r^{d+m-1} - r_0^{-(d+m-1)}P(rr_0)|^2\mathrm{d}r. \end{aligned}$$

As $r \mapsto r_0^{-(d+m-1)}P(rr_0)$ is an element of $G_{1,r_1/r_0}$, letting $r_1 = 2r_0$, we obtain

$$\begin{aligned} \ell^2 = \|g_m\|^2_{L_2([r_0,r_1])} &= \min_{P\in G_{r_0,r_1}} \|e_m - P\|^2_{L_2([r_0,r_1])} \\ &= r_0^{2(d+m)-1}\min_{P\in G_{1,2}} \|e_m - P\|^2_{L_2([1,2])} = Cr_0^{2(d+m)-1}, \end{aligned}$$

where $C = C_m > 0$ is the distance between e_m restricted to $[1,2]$ and $G_{1,2}$. The function f is not smooth so that it does not belong to F_a. To overcome this issue, we consider a smooth kernel ρ on $\mathbb{R}$ satisfying $\int \rho = 1$ and $\int \rho(r)r^i\mathrm{d}r = 0$ for $i = 1, \ldots, m+d-1$, with support included in $\mathcal{B}_{\mathbb{R}}(0, r_0/2)$. See e.g. [BH19, Section 3.2] for the construction of such a kernel ρ. The map $\rho * f$ is supported on $(1,\infty)$ and it is straightforward to check that $\rho * f \in F_a$ for $r_0 > 2$. By Young's inequality, $\|\rho * f\|_{L_2(\mathbb{R})} \leq \|\rho\|_\infty \|f\|_{L_2(\mathbb{R})}$, so that

$$\begin{aligned} \int |\rho * f(r)|r^{d-1}\mathrm{d}r &\leq \left(\int_{r_0/2}^{5r_0/2} r^{2d-2}\mathrm{d}r\right)^{1/2} \|\rho * f\|_{L_2(\mathbb{R})} \leq \left(c_d r_0^{2d-1}\right)^{1/2} \|\rho\|_\infty \|f\|_{L_2(\mathbb{R})} \\ &\leq C_{d,m} a r_0^{-m} \end{aligned}$$

By letting r_0 goes to ∞, we see that $\inf\left\{\int |f(r)|r^{d-1}\mathrm{d}r,\ f \in F_a\right\} = 0$. □

Part II

Statistical descriptors in the space of persistence diagrams

Chapter 6

Structure of the space of persistence diagrams

In this chapter, we make the connection between the p-bottleneck metrics between persistence diagrams introduced in Chapter 3 and optimal partial transport metrics introduced by Figalli and Gigli [FG10]. Making this link explicit allows us to introduce distances FG_p between non-discrete measures on $\Omega := \{u = (u_1, u_2) \in \mathbb{R}^2 : \ u_1 < u_2\}$, while we call the corresponding metric space $(\mathcal{M}^p, \mathrm{FG}_p)$ the space of *persistence measures*. In particular, in Section 6.5, we leverage the study of the metric and topological properties of this space to show the existence of p-Fréchet means of distributions on $\mathcal{D}^p$.

6.1 Elements of optimal partial transport

Let $\mathcal{X}$ be some Polish locally compact metric space. In Chapter 3, we introduced the theory of optimal transport, which allowed us to compare two measures μ and ν on $\mathcal{P}(\mathcal{X})$ having the same mass by considering the different ways of transporting the distribution μ towards the distribution ν. In certain situations, measures having different masses may naturally appear, while the total mass of a measure may carry a physical meaning worth of interest. In that case, it is therefore not satisfactory to normalize the measures, and extending optimal transport to measures of different masses is needed. This more general problem is referred to as optimal *partial* transport. Two main approaches have been proposed in the literature.

A first class of methods consists in relaxing the marginal constraints on the transport plans $\pi \in \Pi(\mu, \nu)$, while penalizing the difference between the marginals of π and μ and ν (for instance by the Kullback-Leibler divergence). Such approaches were first introduced for computational purposes, as computing this relaxed distance, called the Sinkhorn distance, turns out to be a strictly convex problem with fast minimization procedures available [CD14]. This class of distances was then studied theoretically, and both the geometry of the corresponding spaces and the statistical properties of such objects are bustling research topics [Chi+15; KMV16].

Another possibility consists in using a waste function $\omega : \mathcal{X} \to (0, +\infty)$ to throw away the excess mass between μ and ν. Informally, we can now either match an element of mass $\mu(\mathrm{d}x)$ to another element $\nu(\mathrm{d}y)$ with cost $d(x, y)^p$, or throw it away with cost $\omega(x)$. The most investigated case in the literature is the case $\omega \equiv \mathrm{cst}$ [HR95; Han94; PR14], although the general case was considered for $p = 1$ in [Gui02]. In [FG10], Figalli and Gigli consider measures supported on some *bounded* open set $\Omega \subset \mathbb{R}^d$ and consider the waste function $\omega = d(\cdot, \partial\Omega)^p$, while this problem was then further generalized to asymmetric settings [MJT14]. The p-bottleneck distances introduced in Chapter 3 share key ideas with the distance introduced by Figalli and Gigli, with the caveat that the space Ω is not bounded, causing some technical difficulties.

We introduce the more general problem where some locally compact Polish space $\mathcal{X}$ is partitioned into an open set Ω_0 and a closed reservoir of mass $\mathcal{R}$, i.e. $\mathcal{X} = \Omega_0 \sqcup \mathcal{R}$. An element of mass $\mu(\mathrm{d}x)$ can either be mapped to some $\nu(\mathrm{d}y)$, with cost $d(x,y)^p$, or to the reservoir $\mathcal{R}$, with cost $d(x,\mathcal{R})^p$ (and similarly for ν). Formally, we introduce the following generalization of [FG10, Problem 1.1].

Definition 6.1.1. *Let $p \in [1,+\infty)$. Let $\mathcal{M}^p(\Omega_0,\mathcal{R})$ be the set of Radon measures μ supported on Ω_0 satisfying*

$$\int_{\Omega_0} d(x,\mathcal{R})^p \mathrm{d}\mu(x) < +\infty.$$

Given $\mu,\nu \in \mathcal{M}^p(\Omega_0,\mathcal{R})$, the set of admissible transport plans (or couplings) $\mathrm{Adm}(\mu,\nu)$ *is defined as the set of Radon measures π on $\mathcal{X}\times\mathcal{X}$ satisfying for all Borel sets $A,B \subset \Omega_0$,*

$$\pi(A\times\mathcal{X}) = \mu(A) \quad \text{and} \quad \pi(\mathcal{X}\times B) = \nu(B).$$

The cost of $\pi \in \mathrm{Adm}(\mu,\nu)$ is defined as

$$C_p(\pi) := \iint_{\mathcal{X}\times\mathcal{X}} d(x,y)^p \mathrm{d}\pi(x,y). \tag{6.1}$$

The Figalli-Gigli distance $\mathrm{FG}_p(\mu,\nu)$ *is then defined as*

$$\mathrm{FG}_p(\mu,\nu) := \inf\{C_p(\pi)^{1/p} : \ \pi \in \mathrm{Adm}(\mu,\nu)\}. \tag{6.2}$$

Plans $\pi \in \mathrm{Adm}(\mu,\nu)$ realizing the infimum in (6.2) are called optimal. *The set of optimal transport plans between μ and ν for the cost $(x,y)\mapsto d(x,y)^p$ is denoted by* $\mathrm{Opt}_p(\mu,\nu)$.

We introduce the following definition, which shows how to build an element of $\mathrm{Adm}(\mu,\nu)$ given a map $f:\mathcal{X}\to\mathcal{X}$ satisfying some balance condition (see Figure 6.1).

Definition 6.1.2. *Let $\mu,\nu \in \mathcal{M}(\Omega_0)$. Consider $f:\mathcal{X}\to\mathcal{X}$ a measurable function satisfying for all Borel set $B\subset\Omega_0$*

$$\mu(f^{-1}(B)\cap\Omega_0) + \nu(B\cap f(\mathcal{R})) = \nu(B). \tag{6.3}$$

Define for all Borel sets $A,B\subset\mathcal{X}$,

$$\pi(A\times B) = \mu(f^{-1}(B)\cap\Omega_0\cap A) + \nu(\Omega_0\cap B\cap f(A\cap\mathcal{R})). \tag{6.4}$$

π is called the transport plan induced *by the* transport map *f.*

One can easily check that we have indeed $\pi(A\times\mathcal{X}) = \mu(A)$ and $\pi(\mathcal{X}\times B) = \nu(B)$ for any Borel sets $A,B\subset\Omega_0$, so that $\pi\in\mathrm{Adm}(\mu,\nu)$ (see Figure 6.1).

Remark 6.1.3. Since we have no constraints on $\pi(\mathcal{R}\times\mathcal{R})$, one may always assume that a plan π satisfies $\pi(\mathcal{R}\times\mathcal{R}) = 0$, so that measures $\pi\in\mathrm{Adm}(\mu,\nu)$ are supported on

$$E_{\Omega_0} := (\mathcal{X}\times\mathcal{X})\backslash(\mathcal{R}\times\mathcal{R}). \tag{6.5}$$

The case $\Omega_0 = \Omega$ and $\mathcal{R} = \partial\Omega$ will be particularly relevant to the setting of Topological Data Analysis. In particular, we will show that the Figalli-Gigli distance coincides with the p-bottleneck distance between persistence diagrams. If all the results appearing in the remaining of the chapter hold in the general case, we will settle with the choice $(\Omega_0,\mathcal{R}) = (\Omega,\partial\Omega)$ to keep the connection with persistence diagrams explicit. We will write $\mathcal{M}^p$ instead of $\mathcal{M}^p(\Omega,\partial\Omega)$ and call this space the *space of persistence measures*, while the quantity $\mathrm{Pers}_p(\mu) := \int_\Omega d(x,\partial\Omega)^p \mathrm{d}\mu(x)$ is the *total persistence* of $\mu\in\mathcal{M}^p$.

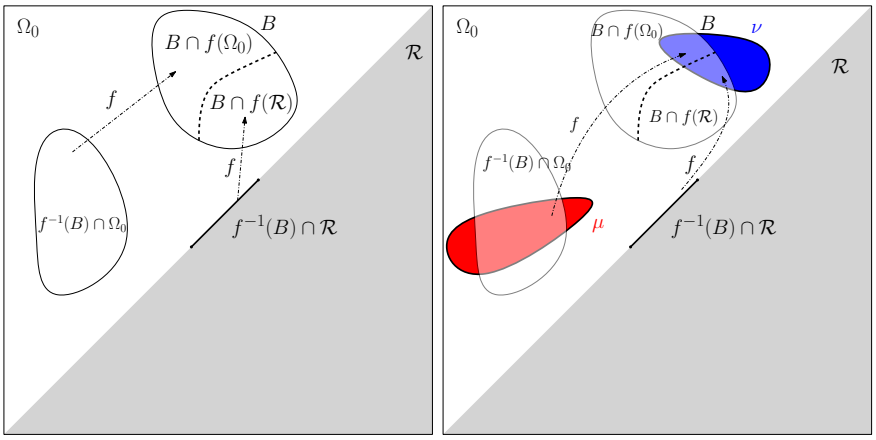


FIGURE 6.1: A transport map f must satisfy that the mass $\nu(B)$ (light blue) is the sum of the mass $\mu(f^{-1}(B) \cap \Omega_0)$ given by μ that is transported by f onto B (light red) and the mass $\nu(B \cap f(\mathcal{R}))$ coming from $\mathcal{R}$ and transported by f onto B. The case $(\Omega_0, \mathcal{R}) = (\Omega, \partial\Omega)$ is displayed.

Remark 6.1.4. The choices of reservoir $\mathcal{R}$ and groundspace Ω_0 are actually very flexible. In particular, one can recover the optimal transport problem with waste function w on Ω_0 by letting $\mathcal{R}$ be the graph of Ω_0 (in $\Omega_0 \times \mathbb{R}$), while Ω_0 is identified with $\Omega_0 \times \{0\}$. As such, the following propositions also hold in this framework.

6.2 General properties of $\mathcal{M}^p$

This section is dedicated to general properties of the metric space $(\mathcal{M}^p, \mathrm{FG}_p)$. In particular, we show that FG_p coincides with d_p when comparing persistence diagrams, so that $\mathcal{M}^p$ is a metric extension of $\mathcal{D}^p$.

Remark 6.2.1. If a (Borel) measure μ satisfies $\mathrm{Pers}_p(\mu) < \infty$, then for any Borel set $A \subset \Omega$ satisfying $d(A, \partial\Omega) := \inf_{x \in A} d(x, \partial\Omega) > 0$, we have:

$$\mu(A) d(A, \partial\Omega)^p \leq \int_A d(x, \partial\Omega)^p \mathrm{d}\mu(x) \leq \int_\Omega d(x, \partial\Omega)^p \mathrm{d}\mu(x) = \mathrm{Pers}_p(\mu) < \infty, \quad (6.6)$$

so that $\mu(A) < \infty$. In particular, μ is automatically a Radon measure.

Proposition 6.2.2. *Let $\mu, \nu \in \mathcal{M}$. The set of transport plans $\mathrm{Adm}(\mu, \nu)$ is sequentially compact for the vague topology on E_Ω. Moreover, if $\mu, \nu \in \mathcal{M}^p$, for this topology,*

- *$\pi \in \mathrm{Adm}(\mu, \nu) \mapsto C_p(\pi)$ is lower semi-continuous.*
- *$\mathrm{Opt}_p(\mu, \nu)$ is a non-empty sequentially compact set.*
- *FG_p is lower semi-continuous, in the sense that for sequences $(\mu_n)_n, (\nu_n)_n$ in $\mathcal{M}^p$ satisfying $\mu_n \xrightarrow{v} \mu$ and $\nu_n \xrightarrow{v} \nu$, we have*

$$\mathrm{FG}_p(\mu, \nu) \leq \liminf_{n \to \infty} \mathrm{FG}_p(\mu_n, \nu_n).$$

Moreover, FG_p is a metric on $\mathcal{M}^p$.

These properties are mentioned in [FG10, pages 4-5] in the bounded case, and corresponding proofs adapt straightforwardly to the general case. For the sake of completeness, we provide a detailed proof in Section 6.6.

For $r > 0$, let $\Omega_r := \{u \in \Omega : \ d(u, \partial\Omega) > r\}$.

Lemma 6.2.3. *Let $\mu \in \mathcal{M}^p$. For $r > 0$, let μ_r be the restriction of μ to Ω_r. Then $\mathrm{FG}_p(\mu_r, \mu) \to 0$ when $r \to 0$. Similarly, if $a \in \mathcal{D}^p$, we have $d_p(a_r, a) \to 0$.*

Proof. Let $\pi \in \mathrm{Adm}(\mu, \mu_r)$ be the transport plan induced by the identity map on Ω_r, and the projection onto $\partial\Omega$ on $\overline{\Omega}\backslash\Omega_r$. As π is sub-optimal, one has:

$$\mathrm{FG}_p^p(\mu, \mu_r) \leq C_p(\pi) = \int_{\Omega\backslash\Omega_r} d(x, \partial\Omega)^p \mathrm{d}\mu(x) = \mathrm{Pers}_p(\mu) - \mathrm{Pers}_p(\mu_r).$$

Thus, by the monotone convergence theorem applied to μ with the functions $f_r : x \mapsto d(x, \partial\Omega)^p \cdot \mathbf{1}\{x \in \Omega\backslash\Omega_r\}$, $\mathrm{FG}_p(\mu, \mu_r) \to 0$ as $r \to 0$. Similar arguments show that $d_p(a_r, a) \to 0$ as $r \to 0$. □

Proposition 6.2.4. *For $a, b \in \mathcal{D}^p$, $\mathrm{FG}_p(a, b) = d_p(a, b)$.*

Proof. Let $a, b \in \mathcal{D}^p$ be two persistence diagrams. If a and b are finite, than the equality is shown in [LCO18, Proposition 1].

In the general case, let $r > 0$. Due to (6.6), the diagrams a_r and b_r defined in Lemma 6.2.3 have a finite mass (thus finite number of points). Therefore, $d_p(a_r, b_r) = \mathrm{FG}_p(a_r, b_r)$. By Lemma 6.2.3, the former converges to $d_p(a, b)$ while the latter converges to $\mathrm{FG}_p(a, b)$, giving the conclusion. □

Proposition 6.2.5. *The space $(\mathcal{M}^p, \mathrm{FG}_p)$ is a Polish metric space.*

As for Proposition 6.2.2, this proposition appears in [FG10, Proposition 2.7] in the bounded case, while a proof is found in Section 6.6.

We now state one of our main result: a characterization of convergence in $(\mathcal{M}^p, \mathrm{FG}_p)$.

Theorem 6.2.6. *Let $\mu, \mu_1, \mu_2, \ldots$ be measures in $\mathcal{M}^p$. Then,*

$$\mathrm{FG}_p(\mu_n, \mu) \to 0 \Leftrightarrow \begin{cases} \mu_n \xrightarrow{v} \mu, \\ \mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu). \end{cases} \tag{6.7}$$

This result is analog to the characterization of convergence of probability measures in the Wasserstein space (see Chapter 3) and can be found in [FG10, Proposition 2.7] in the case where the ground space is bounded. While the proof of the direct implication can be easily adapted from [FG10] (it can be found in Section 6.6), a new proof is needed for the converse implication.

Proof of the converse implication. For a given compact set $K \subset \Omega$, we denote its complementary set in Ω by K^c, its interior set by $\mathring{K}$, and its boundary by ∂K. Let $\mu, \mu_1, \mu_2 \ldots$ be elements of $\mathcal{M}^p$ and assume that $\mu_n \xrightarrow{v} \mu$ and $\mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu)$. Since

$$\mathrm{FG}_p(\mu_n, \mu) \leq \mathrm{FG}_p(\mu_n, 0) + \mathrm{FG}_p(\mu, 0) = \mathrm{Pers}_p(\mu_n)^{1/p} + \mathrm{Pers}_p(\mu)^{1/p},$$

the sequence $(\mathrm{FG}_p(\mu_n, \mu))_n$ is bounded. Thus, if we show that $(\mathrm{FG}_p(\mu_n, \mu))_n$ admits 0 as an unique accumulation point, then the convergence holds. Up to extracting a subsequence, we may assume that $(\mathrm{FG}_p(\mu_n, \mu))_n$ converges to some limit. For $n \geq 0$, let $\pi_n \in \mathrm{Opt}(\mu_n, \mu)$ be a corresponding optimal transport plan. Let K be a compact subset of Ω. Recall from Chapter 3 (Proposition 3.1.8) that relative compactness for the vague convergence of a sequence $(\mu_n)_n$ is equivalent to $\sup_n\{\mu_n(K)\} < \infty$ for every compact $K \subset \Omega$. Therefore, for any compact $K \subset \Omega$, and $n \in \mathbb{N}$,

$$\pi_n((K \times \Omega) \cup (\Omega \times K)) \leq \mu_n(K) + \mu(K) \leq \sup_k \mu_k(K) + \mu(K) < \infty.$$

As any compact of $E_{\overline{\Omega}}$ is included is some set of the form $(K \times \Omega) \cup (\Omega \times K)$, for $K \subset \Omega$ any compact subset, using Proposition 3.1.8 again, it follows that $(\pi_n)_n$ is also relatively compact for the vague convergence.

Let thus π be the limit of any converging subsequence of $(\pi_n)_n$, whose indexes are still denoted by n. As $\mu_n \xrightarrow{v} \mu$, π is necessarily in $\mathrm{Opt}_p(\mu, \mu)$ (see [FG10, Proposition 2.3]), i.e. π is supported on $\{(x, x) : \ x \in \Omega\}$. The vague convergence of $(\mu_n)_n$ and the convergence of $(\mathrm{Pers}_p(\mu_n))_n$ to $\mathrm{Pers}_p(\mu)$ imply that for a given compact set $K \subset \Omega$, we have

$$\begin{aligned}
&\limsup_{n\to\infty} \int_{K^c} d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) \\
&= \limsup_{n\to\infty} \left(\mathrm{Pers}_p(\mu_n) - \int_K d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) \right) \\
&= \mathrm{Pers}_p(\mu) - \liminf_n \int_{\mathring{K}} d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) - \liminf_n \int_{\partial K} d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) \\
&\leq \mathrm{Pers}_p(\mu) - \int_{\mathring{K}} d(x, \partial\Omega)^p \mathrm{d}\mu(x) \text{ by the Portmanteau theorem} \\
&= \int_{\overline{K^c}} d(x, \partial\Omega)^p \mathrm{d}\mu(x),
\end{aligned}$$

where the Portmanteau theorem is recalled in Chapter 3. As $\mathrm{Pers}_p(\mu)$ is finite, for $\varepsilon > 0$, there exists some compact set $K \subset \Omega$ with

$$\limsup_n \int_{K^c} d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) < \varepsilon \quad \text{and} \quad \int_{K^c} d(x, \partial\Omega)^p \mathrm{d}\mu(x) < \varepsilon. \tag{6.8}$$

Let $s : \Omega \to \partial\Omega$ be the projection on $\partial\Omega$ for the metric d. Such a projection is not unique for $q = 1$ or for the more general reservoir $\mathcal{R}$, but we can always select a measurable projection s [CR03]. We consider the following transport plan $\tilde{\pi}_n$ (consider informally that what went from K to K^c and from K^c to K is now transported onto the diagonal, while everything else is unchanged):

$$\begin{cases}
\tilde{\pi}_n = \pi_n & \text{on } K^2 \sqcup (K^c)^2, \\
\tilde{\pi}_n = 0 & \text{on } K \times K^c \sqcup K^c \times K, \\
\tilde{\pi}_n(A \times B) = \pi_n(A \times B) + \pi_n(A \times (s^{-1}(B) \cap K^c)) & \text{for } A \subset K,\ B \subset \partial\Omega, \\
\tilde{\pi}_n(A \times B) = \pi_n(A \times B) + \pi_n(A \times (s^{-1}(B) \cap K)) & \text{for } A \subset K^c,\ B \subset \partial\Omega, \\
\tilde{\pi}_n(A \times B) = \pi_n(A \times B) + \pi_n((s^{-1}(A) \cap K^c) \times B) & \text{for } A \subset \partial\Omega,\ B \subset K, \\
\tilde{\pi}_n(A \times B) = \pi_n(A \times B) + \pi_n((s^{-1}(A) \cap K) \times B) & \text{for } A \subset \partial\Omega,\ B \subset K^c.
\end{cases} \tag{6.9}$$

Note that $\tilde{\pi}_n \in \mathrm{Adm}(\mu_n, \mu)$: for instance, for $A \subset K$ a Borel set,

$$\begin{aligned}
\tilde{\pi}_n(A \times \overline{\Omega}) &= \tilde{\pi}_n(A \times K) + \tilde{\pi}_n(A \times K^c) + \tilde{\pi}_n(A \times \partial\Omega) \\
&= \pi_n(A \times K) + 0 + \pi_n(A \times \partial\Omega) + \pi_n(A \times (s^{-1}(\partial\Omega) \cap K^c)) \\
&= \pi_n(A \times \overline{\Omega}) = \mu_n(A),
\end{aligned}$$

and it is shown likewise that the other constraints are satisfied. As $\tilde{\pi}_n$ is suboptimal, $\mathrm{FG}_p^p(\mu_n, \mu) \leq \int_{\overline{\Omega}^2} d(x, y)^p \mathrm{d}\tilde{\pi}_n(x, y)$. The latter integral is equal to a sum of different terms, and we will show that each of them converges to 0. Assume without loss of generality that the compact set K belongs to an increasing sequence of compact sets whose union is Ω, with $\pi(\partial(K \times K)) = 0$ for all compacts of the sequence.

- We have $\iint_{K^2} d(x,y)^p \mathrm{d}\tilde{\pi}_n(x,y) = \iint_{K^2} d(x,y)^p \mathrm{d}\pi_n(x,y)$. The lim sup of the integral is less than or equal to $\iint_{K^2} d(x,y)^p \mathrm{d}\pi(x,y)$ by the Portmanteau theorem (applied to the sequence $(d(x,y)^p \mathrm{d}\pi_n(x,y))_n$), and, recalling that π is supported on the diagonal of $E_{\overline{\Omega}}$, this integral is equal to 0.

- For optimality reasons, any optimal transport plan must be supported on the set $\{d(x,y)^p \leq d(x,\partial\Omega)^p + d(y,\partial\Omega)^p\}$ (this fact is detailed in [FG10, Proposition 2.3]). It follows that

$$\begin{aligned}\iint_{(K^c)^2} d(x,y)^p \mathrm{d}\tilde{\pi}_n(x,y) &= \iint_{(K^c)^2} d(x,y)^p \mathrm{d}\pi_n(x,y) \\ &\leq \int_{K^c} d(x,\partial\Omega)^p \mathrm{d}\mu_n(x) + \int_{K^c} d(y,\partial\Omega)^p \mathrm{d}\mu(y).\end{aligned}$$

  Taking the lim sup in n, and then letting K goes to Ω, this quantity converges to 0 by (6.8).

- We have

$$\begin{aligned}&\iint_{K\times\partial\Omega} d(x,\partial\Omega)^p \mathrm{d}\tilde{\pi}_n(x,y) \\ &= \iint_{K\times\partial\Omega} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) + \iint_{K\times K^c} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) \\ &= \iint_{K\times\overline{\Omega}} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) - \iint_{K^2} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) \\ &= \int_K d(x,\partial\Omega)^p \mathrm{d}\mu_n(x) - \iint_{K^2} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y)\end{aligned}$$

  By the Portmanteau theorem applied to the sequence $(d(x,\partial\Omega)^p \mathrm{d}\mu_n(x))_n$, the lim sup of the first term is less than or equal to $\int_K d(x,\partial\Omega)^p \mathrm{d}\mu(x)$. Recall that we assume that $\pi(\partial(K\times K)) = 0$. By applying the second characterization of Portmanteau theorem (see Proposition 3.1.11) on the second term to the sequence $(d(x,y)^p \mathrm{d}\pi_n(x,y))_n$, and using that π is supported on the diagonal of $E_{\overline{\Omega}}$, we obtain that the limsup of the second term is less than or equal to $-\iint_{K^2} d(x,\partial\Omega)^p \mathrm{d}\pi(x,y) = -\int_K d(x,\partial\Omega)^p \mathrm{d}\mu(x)$. Therefore, the lim sup of the integral is equal to 0.

- The three remaining terms (corresponding to the three last lines of the definition (6.9)) are treated likewise this last case.

Finally, we have proven that $(\mathrm{FG}_p(\mu_n,\mu))_n$ is bounded and that for any converging subsequence $(\mu_{n_k})_k$, $\mathrm{FG}_p(\mu_{n_k},\mu)$ converges to 0. It follows that $\mathrm{FG}_p(\mu_n,\mu) \to 0$. □

Remark 6.2.7. The assumption $\mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu)$ is crucial to obtain convergence with respect to FG_p assuming vague convergence. For example, the sequence defined by $\mu_n := \delta_{(n,n+1)}$ converges vaguely to $\mu = 0$ and $(\mathrm{Pers}_p(\mu_n))_n$ does converge (it is constant), while $\mathrm{FG}_p(\mu_n, 0) \nrightarrow 0$. This does not contradict Theorem 6.2.6 since $\mathrm{Pers}_p(\mu) = 0 \neq \lim_n \mathrm{Pers}_p(\mu_n)$.

Theorem 6.2.6 implies some useful results. First, it entails that the topology of the metric FG_p is stronger than the vague topology. As a consequence, the following corollary holds, using Proposition 3.1.12 ($\mathcal{D}^p$ is closed in $\mathcal{M}^p$ for the vague topology).

Corollary 6.2.8. *$\mathcal{D}^p$ is closed in $\mathcal{M}^p$ for the metric FG_p.*

We recover in particular that the space $(\mathcal{D}^p, \mathrm{FG}_p)$ is a Polish space (Proposition 6.2.5), a result already proved in [MMH11, Theorems 7 and 12] with a different approach.

Secondly, we show that the vague convergence of μ_n to μ along with the convergence of $\mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu)$ is equivalent to the weak convergence of a weighted measure. For $\mu \in \mathcal{M}^p$, let us introduce the Borel measure with finite mass $\mu^{(p)}$ defined, for a Borel subset $A \subset \Omega$, as:

$$\mu^{(p)}(A) = \int_A d(x, \partial\Omega)^p \mathrm{d}\mu(x). \tag{6.10}$$

Corollary 6.2.9. *The space $(\mathcal{M}^p, \mathrm{FG}_p)$ is homeomorphic to $\mathcal{P}(\Omega)$ endowed with the weak topology, through the map $\mu \in \mathcal{M}^p \mapsto \mu^{(p)} \in \mathcal{P}(\Omega)$. In particular, for a sequence $(\mu_n)_n$ and a persistence measure $\mu \in \mathcal{M}^p$, we have*

$$\mathrm{FG}_p(\mu_n, \mu) \to 0 \text{ if and only if } \mu_n^{(p)} \xrightarrow{w} \mu^{(p)}.$$

Proof. We first show the equivalence of the two convergences. Consider $\mu, \mu_1, \mu_2, \dots \in \mathcal{M}^p$ and assume that $\mathrm{FG}_p(\mu_n, \mu) \to 0$. By Theorem 6.2.6, this is equivalent to $\mu_n \xrightarrow{v} \mu$ and $\mu_n^{(p)}(\Omega) = \mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu) = \mu^{(p)}(\Omega)$. Since for any continuous function f compactly supported, the map $x \mapsto d(x, \partial\Omega)^p f(x)$ is also continuous and compactly supported, $\mu_n \xrightarrow{v} \mu$ implies $\mu_n^{(p)} \xrightarrow{v} \mu^{(p)}$. Likewise, the map $x \mapsto d(x, \partial\Omega)^{-p} f(x)$ is continuous and compactly supported, so that $\mu_n^{(p)} \xrightarrow{v} \mu^{(p)}$ also implies $\mu_n \xrightarrow{v} \mu$. Hence, $\mu_n \xrightarrow{v} \mu$ is equivalent to $\mu_n^{(p)} \xrightarrow{v} \mu^{(p)}$. By Proposition 3.1.10, the vague convergence $\mu_n^{(p)} \xrightarrow{v} \mu^{(p)}$ along with the convergence of the masses is equivalent to $\mu_n^{(p)} \xrightarrow{w} \mu^{(p)}$.

So far, we have proved that both the application $G : \mu \in \mathcal{M}^p \to \mu^{(p)} \in \mathcal{P}(\Omega)$ and its inverse are sequentially continuous. As the space $\mathcal{M}^p$ is a metric space and the space $\mathcal{P}(\Omega)$ is metrizable [Var58], sequential continuity is equivalent to continuity, so that we have the conclusion. □

We end this section with a characterization of relatively compact sets in $(\mathcal{M}^p, \mathrm{FG}_p)$.

Proposition 6.2.10. *A set F is relatively compact in $(\mathcal{M}^p, \mathrm{FG}_p)$ if and only if the set $\{\mu^{(p)} : \mu \in F\}$ is tight and $\sup_{\mu \in F} \mathrm{Pers}_p(\mu) < \infty$.*

Proof. From Corollary 6.2.9, the relative compactness of a set $F \subset \mathcal{M}^p$ for the metric FG_p is equivalent to the relative compactness of the set $\{\mu^{(p)} : \mu \in F\}$ for the weak convergence. Recall that all $\mu^{(p)}$ have a finite mass, as $\mu^{(p)}(\Omega) = \mathrm{Pers}_p(\mu) < \infty$. Therefore, one can use Prokhorov's theorem (Proposition 3.1.9) to conclude. □

Remark 6.2.11. This characterization is equivalent to the one described in [MMH11, Theorem 21] for persistence diagrams. The notions introduced by the authors of off-diagonally birth-death boundedness, and uniformness are rephrased using the notion of tightness, standard in measure theory.

We end this section with a remark on the existence of transport maps, assuming that one of the two measures has a density with respect to the Lebesgue measure on Ω. We denote by $f_\# \mu$ the pushforward of a measure μ by a map f, defined by $f_\# \mu(A) = \mu(f^{-1}(A))$ for A a Borel set.

Remark 6.2.12. Following [FG10, Corollary 2.5], one can prove that if $\mu \in \mathcal{M}^2$ has a density with respect to the Lebesgue measure on Ω, then for any measure $\nu \in \mathcal{M}^2$, there exists an unique optimal transport plan π between μ and ν for the OT_2 metric. The restriction of this transport plan to $\Omega \times \overline{\Omega}$ is equal to $(\mathrm{id}, T)_\# \mu$ where $T : \Omega \to \overline{\Omega}$

is the gradient of some convex function, whereas the transport plan restricted to $\partial\Omega \times \Omega$ is given by $(s, \mathrm{id})_\#(\nu - T_\#\mu)$, where $s : \Omega \to \partial\Omega$ is the projection on the diagonal. A proof of this fact in the context of persistence measures would require to introduce various notions that are out of the scope covered by this chapter. We refer the interested reader to [FG10, Proposition 2.3] and [AGS08, Theorem 6.2.4] for details.

6.3 Persistence measures in the finite setting

In practice, many statistical results regarding persistence diagrams are stated for sets of diagrams with uniformly bounded number of points [Kwi+15; CCO17], and the specific properties of FG_p in this setting are therefore of interest. Introduce for $m \geq 0$ the subset $\mathcal{M}^p_{\leq m}$ of $\mathcal{M}^p$ defined as $\mathcal{M}^p_{\leq m} := \{\mu \in \mathcal{M}^p : \ \mu(\Omega) \leq m\}$, and the set $\mathcal{M}^p_f$ of finite persistence measures, $\mathcal{M}^p_f := \bigcup_{m\geq 0} \mathcal{M}^p_{\leq m}$. Define similarly the set $\mathcal{D}_{\leq m}$ (resp. $\mathcal{D}_f$). Note that the assumption $\mathrm{Pers}_p(a) < \infty$ is always satisfied for a finite diagram a (which is not true for general Radon measures), so that the exponent p is not needed when defining $\mathcal{D}_{\leq m}$ and $\mathcal{D}_f$.

Proposition 6.3.1. *$\mathcal{M}^p_f$ (resp. $\mathcal{D}_f$) is dense in $\mathcal{M}^p$ (resp. $\mathcal{D}^p$) for the metric FG_p.*

Proof. This is a straightforward consequence of Lemma 6.2.3. Indeed, if $\mu \in \mathcal{M}^p$ and $r > 0$, then (6.6) implies that μ_r is of finite mass. □

Let $\tilde{\Omega} = \Omega \sqcup \{\partial\Omega\}$ be the quotient of $\overline{\Omega}$ by the closed subset $\partial\Omega$—i.e. we encode the diagonal by just one point (still denoted by $\partial\Omega$). The distance d on $\overline{\Omega}^2$ induces naturally a function $\tilde{d}$ on $\tilde{\Omega}^2$, defined for $x, y \in \Omega$ by $\tilde{d}(x, y) = d(x, y)$, $\tilde{d}(x, \partial\Omega) = \tilde{d}(\partial\Omega, x) = d(x, s(x))$ and $\tilde{d}(\partial\Omega, \partial\Omega) = 0$. However, $\tilde{d}$ is not a distance since one can have $\tilde{d}(x, y) > \tilde{d}(x, \partial\Omega) + \tilde{d}(y, \partial\Omega)$. Define

$$\rho(x, y) := \min\{\tilde{d}(x, y), \tilde{d}(x, \partial\Omega) + \tilde{d}(y, \partial\Omega)\}. \tag{6.11}$$

It is straightforward to check that ρ is a distance on $\tilde{\Omega}$ and that $(\tilde{\Omega}, \rho)$ is a Polish space. One can then define the Wasserstein distance $W_{p,\rho}$ with respect to ρ for finite measures on $\tilde{\Omega}$ which have the same masses, that is the infimum of $\tilde{C}_p(\tilde{\pi}) := \iint_{\tilde{\Omega}^2} \rho(x, y)^p \mathrm{d}\tilde{\pi}(x, y)$, for $\tilde{\pi}$ a transport plan with corresponding marginals. The following theorem states that the problem of computing the FG_p metric between two persistence measures with finite masses can be turn into the one of computing the Wasserstein distances between two measures supported on $\tilde{\Omega}$ with the same mass. Recall that $s : \Omega \to \partial\Omega$ is the orthogonal projection (or a measurable projection in the general case).

Proposition 6.3.2. *Let $\mu, \nu \in \mathcal{M}^p_f$ and $r \geq \mu(\Omega)+\nu(\Omega)$. Define $\tilde{\mu} = \mu+(r-\mu(\Omega))\delta_{\partial\Omega}$ and $\tilde{\nu} = \nu + (r - \nu(\Omega))\delta_{\partial\Omega}$. Then $\mathrm{FG}_p(\mu, \nu) = W_{p,\rho}(\tilde{\mu}, \tilde{\nu})$.*

Before proving Proposition 6.3.2, we need the two following lemmas:

Lemma 6.3.3. *Let $\mu, \nu \in \mathcal{M}^p_f$ and $r \geq \max(\mu(\Omega), \nu(\Omega))$. Let $\tilde{\mu} := \mu + (r - \mu(\Omega))\delta_{\partial\Omega}$, $\tilde{\nu} := \nu + (r - \nu(\Omega))\delta_{\partial\Omega}$ and $s : \Omega \to \partial\Omega$ be the orthogonal projection on the diagonal.*

1. *Define $T(\mu, \nu)$ the set of plans $\pi \in \mathrm{Adm}(\mu, \nu)$ satisfying $\pi(\{(x, y) \in \Omega \times \partial\Omega : y \neq s(x)\}) = \pi(\{(x, y) \in \partial\Omega \times \Omega : \ x \neq s(y)\}) = 0$ along with $\pi(\partial\Omega \times \partial\Omega) = 0$. Then, $\mathrm{Opt}_p(\mu, \nu) \subset T(\mu, \nu)$.*

2. *Let $\pi \in T(\mu,\nu)$ be such that $\mu(\Omega) + \pi(\partial\Omega \times \Omega) \leq r$. Define $\iota(\pi) \in \Pi(\tilde{\mu},\tilde{\nu})$ by, for Borel sets $A, B \subset \Omega$,*

$$\begin{cases} \iota(\pi)(A \times B) = \pi(A \times B), \\ \iota(\pi)(A \times \{\partial\Omega\}) = \pi(A \times \partial\Omega), \\ \iota(\pi)(\{\partial\Omega\} \times B) = \pi(\partial\Omega \times B), \\ \iota(\pi)(\{\partial\Omega\} \times \{\partial\Omega\}) = r - \mu(\Omega) - \pi(\partial\Omega \times \Omega) \geq 0. \end{cases} \tag{6.12}$$

Then, $C_p(\pi) = \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\iota(\pi)(x,y)$.

3. *Let $\tilde{\pi} \in \Pi(\tilde{\mu},\tilde{\nu})$. Define $\kappa(\tilde{\pi}) \in T(\mu,\nu)$ by,*

$$\begin{cases} \kappa(\tilde{\pi})(A \times B) = \tilde{\pi}(A \times B) & \text{for } A, B \subset \Omega, \\ \kappa(\tilde{\pi})(A \times B) = \tilde{\pi}((A \cap s^{-1}(B)) \times \{\partial\Omega\}) & \text{for } A \subset \Omega, B \subset \partial\Omega, \\ \kappa(\tilde{\pi})(A \times B) = \tilde{\pi}(\{\partial\Omega\} \times (B \cap s^{-1}(A))) & \text{for } A \subset \partial\Omega, B \subset \Omega, \\ \kappa(\tilde{\pi})(\partial\Omega, \partial\Omega) = 0. \end{cases}$$

Then, $\iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y) = C_p(\kappa(\tilde{\pi}))$.

Proof.

1. Consider $\pi \in \mathrm{Adm}(\mu,\nu)$, and define π' that coincides with π on $\Omega \times \Omega$, and is such that we enforce mass transported on the diagonal to be transported on its orthogonal projection: more precisely, for all Borel set $A \subset \Omega$, $B \subset \partial\Omega$, $\pi'(A \times B) = \pi((s^{-1}(B) \cap A) \times B)$ and $\pi'(B \times A) = \pi(B \times (s^{-1}(B) \cap A))$. Note that $\pi' \in T(\mu,\nu)$. Since $s(x)$ is the unique minimizer of $y \mapsto d(x,y)^p$, it follows that $C_p(\pi') \leq C_p(\pi)$, with equality if and only if $\pi \in T(\mu,\nu)$, and thus $\mathrm{Opt}_p(\mu,\nu) \subset T(\mu,\nu)$.

2. Write $\tilde{\pi} = \iota(\pi)$. The mass $\tilde{\pi}(\{\partial\Omega\} \times \{\partial\Omega\})$ is nonnegative by definition. One has for all Borel sets $A \subset \Omega$,

$$\begin{aligned} \tilde{\pi}(A \times \tilde{\Omega}) &= \tilde{\pi}(A \times \Omega) + \tilde{\pi}(A \times \{\partial\Omega\}) \\ &= \pi(A \times \Omega) + \pi(A \times \partial\Omega) = \pi(A \times \overline{\Omega}) = \mu(A) = \tilde{\mu}(A). \end{aligned}$$

Similarly, $\tilde{\pi}(\tilde{\Omega} \times B) = \tilde{\nu}(B)$ for all $B \subset \Omega$. Observe also that

$$\tilde{\pi}(\{\partial\Omega\} \times \tilde{\Omega}) = \tilde{\pi}(\{\partial\Omega\} \times \{\partial\Omega\}) + \tilde{\pi}(\{\partial\Omega\} \times \Omega) = r - \mu(\Omega) = \tilde{\mu}(\{\partial\Omega\}).$$

Similarly, $\tilde{\pi}(\tilde{\Omega} \times \{\partial\Omega\}) = \tilde{\nu}(\{\partial\Omega\})$. It gives that $\iota(\pi) \in \Pi(\tilde{\mu},\tilde{\nu})$, so that ι is well defined. Observe that

$$\begin{aligned} \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y) &= \iint_{\Omega\times\Omega} d(x,y)^p \mathrm{d}\pi(x,y) \\ &\quad + \int_\Omega d(x,\partial\Omega)^p \mathrm{d}\pi(x,\partial\Omega) \\ &\quad + \int_\Omega d(\partial\Omega,y)^p \mathrm{d}\pi(\partial\Omega,y) + 0 \\ &= C_p(\pi) \text{ as } \pi \in T(\mu,\nu). \end{aligned}$$

3. Write $\pi = \kappa(\tilde{\pi})$. For $A \subset \Omega$ a Borel set,

$$\begin{aligned} \pi(A \times \overline{\Omega}) &= \pi(A \times \Omega) + \pi(A \times \partial\Omega) \\ &= \tilde{\pi}(A \times \Omega) + \tilde{\pi}(A \times \{\partial\Omega\}) = \tilde{\pi}(A \times \tilde{\Omega}) = \mu(A). \end{aligned}$$

Similarly, $\pi(\overline{\Omega} \times B) = \nu(B)$ for all $B \subset \Omega$. Therefore, $\pi \in \mathrm{Adm}(\mu, \nu)$, and by construction, if a point $x \in \Omega$ is transported on $\partial\Omega$, it is transported on $s(x)$, so that $\pi \in T(\mu, \nu)$. Observe that $\mu(\Omega) + \pi(\partial\Omega \times \Omega) \leq \tilde{\pi}(\tilde{\Omega} \times \tilde{\Omega}) = r$, so that $\iota(\pi)$ is well defined. Also, $\iota(\pi) = \tilde{\pi}$, so that, according to point 2, $C_p(\pi) = \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y)$. □

We show that the inequality $\mathrm{FG}_p(\mu, \nu) \leq W_{p,\rho}(\tilde{\mu}, \tilde{\nu})$ holds as long as the condition $r \geq \max(\mu(\Omega), \nu(\Omega))$ holds.

Lemma 6.3.4. *Let $\mu, \nu \in \mathcal{M}_f^p$ and $r \geq \max(\mu(\Omega), \nu(\Omega))$. Let $\tilde{\mu} := \mu + (r - \mu(\Omega))\delta_{\partial\Omega}$, $\tilde{\nu} := \nu + (r - \nu(\Omega))\delta_{\partial\Omega}$. Then, $\mathrm{FG}_p(\mu, \nu) \leq W_{p,\rho}(\tilde{\mu}, \tilde{\nu})$.*

Proof. Let $\tilde{\pi} \in \Pi(\tilde{\mu}, \tilde{\nu})$. Define the set $H := \{(x,y) \in \tilde{\Omega}^2 : \ \rho(x,y) = d(x,y)\}$, and let H^c be its complementary set in $\tilde{\Omega}^2$, i.e. the set where $\rho(x,y) = d(x,\partial\Omega) + d(\partial\Omega, y)$. Define $\tilde{\pi}' \in \mathcal{M}(\tilde{\Omega}^2)$ by, for Borel sets $A, B \subset \Omega$:

$$\begin{cases} \tilde{\pi}'(A \times B) = \tilde{\pi}((A \times B) \cap H) \\ \tilde{\pi}'(A \times \{\partial\Omega\}) = \tilde{\pi}((A \times \tilde{\Omega}) \cap H^c) + \tilde{\pi}(A \times \{\partial\Omega\}) \\ \tilde{\pi}'(\{\partial\Omega\} \times B) = \tilde{\pi}((\tilde{\Omega} \times B) \cap H^c) + \tilde{\pi}(\{\partial\Omega\} \times B). \end{cases}$$

We easily check that $\tilde{\pi}' \in \Pi(\tilde{\mu}, \tilde{\nu})$. Also, using $(a+b)^p \geq a^p + b^p$ for positive a, b, we have

$$\begin{aligned} \iint_{\tilde{\Omega}\times\tilde{\Omega}} \rho(x,y)^p \mathrm{d}\tilde{\pi}(x,y) &= \iint_H \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y) \\ &\quad + \iint_{H^c} (\tilde{d}(x,\partial\Omega) + \tilde{d}(\partial\Omega, y))^p \mathrm{d}\tilde{\pi}(x,y) \\ &\geq \iint_H \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}'(x,y) \\ &\quad + \iint_{H^c} \left(\tilde{d}(x,\partial\Omega)^p + \tilde{d}(y,\partial\Omega)^p\right) \mathrm{d}\tilde{\pi}(x,y) \\ &= \iint_{\tilde{\Omega}\times\tilde{\Omega}} d(x,y)^p \mathrm{d}\tilde{\pi}'(x,y) \\ &\geq \inf_{\tilde{\pi}' \in \Pi(\tilde{\mu},\tilde{\nu})} \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}'(x,y). \end{aligned}$$

We conclude by taking the infimum on $\tilde{\pi}$ that

$$W_{p,\rho}(\tilde{\mu}, \tilde{\nu}) \geq \inf_{\tilde{\pi}' \in \Pi(\tilde{\mu},\tilde{\nu})} \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}'(x,y).$$

Since $\rho(x,y) \leq \tilde{d}(x,y)$, it follows that

$$W_{p,\rho}^p(\tilde{\mu}, \tilde{\nu}) = \inf_{\tilde{\pi} \in \Pi(\tilde{\mu},\tilde{\nu})} \iint_{\tilde{\Omega}^2} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y). \tag{6.13}$$

Since $\tilde{d}$ is continuous, the infimum in the right hand side of (6.13) is reached [Vil08, Theorem 4.1]. Consider thus $\tilde{\pi} \in \Pi(\tilde{\mu}, \tilde{\nu})$ which realizes the infimum. We can write, using Lemma 6.3.3,

$$\begin{aligned} W_{p,\rho}^p(\tilde{\mu}, \tilde{\nu}) &= \iint_{\tilde{\Omega}^2} \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y) = \iint_{\overline{\Omega}\times\overline{\Omega}} d(x,y)^p \mathrm{d}\kappa(\tilde{\pi})(x,y) \\ &\geq \inf_{\pi \in T(\mu,\nu)} \iint_{\overline{\Omega}\times\overline{\Omega}} d(x,y)^p \mathrm{d}\pi(x,y) = \mathrm{FG}_p^p(\mu, \nu), \end{aligned}$$

which concludes the proof. □

Proof of Proposition 6.3.2. Let $\pi \in T(\mu,\nu)$. As $\mu(\Omega)+\pi(\partial\Omega\times\Omega) \leq \mu(\Omega)+\nu(\Omega) \leq r$, one can define $\tilde{\pi} = \iota(\pi)$. Since $\rho(x,y) \leq \tilde{d}(x,y)$, we have $\tilde{C}_p(\tilde{\pi}) \leq \iint \tilde{d}(x,y)^p \mathrm{d}\tilde{\pi}(x,y) = C_p(\pi)$ (Lemma 6.3.3). Taking infimum gives $W_{p,\rho}(\tilde{\mu},\tilde{\nu}) \leq \mathrm{FG}_p(\mu,\nu)$. The other inequality holds according to Lemma 6.3.4. □

Remark 6.3.5. The starting idea of this theorem—informally, "adding the mass of one diagram to the other and vice-versa"—is known in TDA as a *bipartite graph matching* [EH10, Ch. VIII.4] and used in practical computations [KMN17]. Here, Proposition 6.3.2 states that solving this bipartite graph matching problem can be formalized as computing a Wasserstein distance on the metric space $(\tilde{\Omega},\rho)$ and as such, makes sense (and remains true) for more general measures.

Remark 6.3.6. Proposition 6.3.2 is useful for numerical purposes since it allows us in applications, when dealing with a finite set of finite measures (in particular diagrams), to directly use the various tools developed in computational optimal transport [PC19] to compute Wasserstein distances. This alternative to the combinatorial algorithms considered in the literature [KMN17; Tur+14] is studied in detail in [LCO18]. This result is also helpful to prove the existence of p-Fréchet means of sets of persistence measures, Section 6.5 below.

6.4 The FG_∞ distance

In classical optimal transport, the ∞-Wasserstein distance is known to have a much more erratic behavior than its $p<\infty$ counterparts [San15, Section 5.5.1]. However, in the context of persistence diagrams, the bottleneck distance defined in Chapter 3 appears naturally as an interleaving distance between persistence modules and satisfies strong stability results: it is thus worthy of interest. It also happens that, when restricted to diagrams having some specific finiteness properties, most irregular behaviors are suppressed and a convenient characterization of convergence exists.

Definition 6.4.1. *Recall that* $\mathrm{spt}(\mu)$ *denote the support of a measure* μ *and define* $\mathrm{Pers}_\infty(\mu) := \sup\{d(x,\partial\Omega),\ x\in\mathrm{spt}(\mu)\}$. *Let*

$$\mathcal{M}^\infty := \{\mu\in\mathcal{M}:\ \mathrm{Pers}_\infty(\mu)<\infty\} \quad \textit{and} \quad \mathcal{D}^\infty := \mathcal{D}\cap\mathcal{M}^\infty. \tag{6.14}$$

For $\mu,\nu\in\mathcal{M}^\infty$ *and* $\pi\in\mathrm{Adm}(\mu,\nu)$, *let* $C_\infty(\pi) := \sup\{d(x,y):\ (x,y)\in\mathrm{spt}(\pi)\}$ *and let*

$$\mathrm{FG}_\infty(\mu,\nu) := \inf\{C_\infty(\pi):\ \pi\in\mathrm{Adm}(\mu,\nu)\}. \tag{6.15}$$

The set of transport plans minimizing (6.15) *is denoted by* $\mathrm{Opt}_\infty(\mu,\nu)$.

Recall that $E_{\overline{\Omega}} = (\overline{\Omega}\times\overline{\Omega})\backslash(\partial\Omega\times\partial\Omega)$.

Proposition 6.4.2. *Let* $\mu,\nu\in\mathcal{M}^\infty$. *For the vague topology on* $E_{\overline{\Omega}}$,

- *the map* $\pi\in\mathrm{Adm}(\mu,\nu)\mapsto C_\infty(\pi)$ *is lower semi-continuous.*
- *The set* $\mathrm{Opt}_\infty(\mu,\nu)$ *is a non-empty sequentially compact set.*
- FG_∞ *is lower semi-continuous.*

Moreover, FG_∞ *is a metric on* $\mathcal{M}^\infty$.

The proofs of these results are found in Section 6.6. As in the case $p<\infty$, FG_∞ and d_∞ coincide on $\mathcal{D}^\infty$.

Proposition 6.4.3. *For $a, b \in \mathcal{D}^\infty$, $\mathrm{FG}_\infty(a,b) = d_\infty(a,b)$.*

Proof. Consider two diagrams $a, b \in \mathcal{D}^\infty$, written as $a = \sum_{i\in I} \delta_{x_i}$ and $b = \sum_{j\in J} \delta_{y_j}$, where $I, J \subset \mathbb{N}$ are (possibly infinite) sets of indices. The marginals constraints imply that a plan $\pi \in \mathrm{Adm}(\mu,\nu)$ is supported on $(\{x_i\}_i \cup \partial\Omega) \times (\{y_j\}_j \cup \partial\Omega)$. If some of the mass $\pi(\{x_i\}, \partial\Omega)$ (resp. $\pi(\partial\Omega, \{y_j\})$) is sent on a point other than the projection of x_i (resp. y_j) on the diagonal $\partial\Omega$, then the cost of such a plan can always be (strictly if $q > 1$) reduced. Introduce the matrix C indexed on $(-J \cup I) \times (-I \cup J)$ defined by

$$\begin{cases} C_{i,j} = d(x_i, y_j) & \text{for } i,j > 0, \\ C_{i,j} = d(\partial\Omega, y_j) & \text{for } i < 0, j > 0, \\ C_{i,j} = d(x_i, \partial\Omega) & \text{for } i > 0, j < 0, \\ C_{i,j} = 0 & \text{for } i,j < 0. \end{cases} \tag{6.16}$$

In this context, an element of $\mathrm{Opt}(a,b)$ can be written a matrix P indexed on $(-J \cup I) \times (-I \cup J)$, and marginal constraints state that P must belong to the set of doubly stochastic matrices $\mathcal{S}$. Therefore, $\mathrm{FG}_\infty(a,b) = \inf_{P\in\mathcal{S}} \sup\{C_{i,j} : (i,j) \in \mathrm{spt}(P)\}$, where $\mathcal{S}$ is the set of doubly stochastic matrices indexed on $(-J \cup I) \times (-I \cup J)$, and $\mathrm{spt}(P)$ denotes the support of P, that is the set $\{(i,j),\ P_{i,j} > 0\}$.

Let $P \in \mathcal{S}$. For any $k \in \mathbb{N}$, and any set of distinct indices $\{i_1, \dots, i_k\} \subset -J \cup I$, we have

$$k = \sum_{k'=1}^{k} \underbrace{\sum_{j\in -I\cup J} P_{i_{k'},j}}_{=1} = \sum_{j\in -I\cup J} \underbrace{\sum_{k'=1}^{k} P_{i_{k'},j}}_{\leq 1}.$$

Thus, the cardinality of $\{j : \exists k' \text{ such that } (i_{k'}, j) \in \mathrm{spt}(P)\}$ must be larger than k. Said differently, the marginals constraints impose that any set of k points in a must be matched to *at least* k points in b (points are counted with eventual repetitions here). Under such conditions, the Hall's marriage theorem (see [Hal86, p. 51]) guarantees the existence of a permutation matrix P' with $\mathrm{spt}(P') \subset \mathrm{spt}(P)$. As a consequence,

$$\begin{aligned} \sup\{C_{i,j} : (i,j) \in \mathrm{spt}(P)\} &\geq \sup\{C_{i,j} : (i,j) \in \mathrm{spt}(P')\} \\ &\geq \inf_{P'\in\mathcal{S}'} \sup\{C_{i,j} : (i,j) \in \mathrm{spt}(P')\} = d_\infty(a,b), \end{aligned}$$

where $\mathcal{S}'$ denotes the set of permutations matrix indexed on $(-J \cup I) \times (-I \cup J)$. Taking the infimum on $P \in \mathcal{S}$ on the left-hand side and using that $\mathcal{S}' \subset \mathcal{S}$ finally gives that $\mathrm{FG}_\infty(a,b) = d_\infty(a,b)$. □

Proposition 6.4.4. *The space $(\mathcal{M}^\infty, \mathrm{FG}_\infty)$ is complete.*

Proof. Let $(\mu_n)_n$ be a Cauchy sequence for FG_∞. Fix a compact $K \subset \Omega$, and pick $\varepsilon = d(K, \partial\Omega)/2$. There exists n_0 such that for $n > n_0$, $\mathrm{FG}_\infty(\mu_n, \mu_{n_0}) < \varepsilon$. Let $K_\varepsilon := \{x \in \Omega : d(x,K) \leq \varepsilon\}$. By considering $\pi_n \in \mathrm{Opt}_\infty(\mu_n, \mu_{n_0})$, and since $\mathrm{FG}_\infty(\mu_n, \mu_{n_0}) < \varepsilon$, we have that

$$\mu_n(K) = \pi_n(K \times \overline{\Omega}) = \pi_n(K \times K_\varepsilon) \leq \mu_{n_0}(K_\varepsilon). \tag{6.17}$$

Therefore, $(\mu_n(K))_n$ is uniformly bounded, and Proposition 3.1.8 implies that $(\mu_n)_n$ is relatively compact. Finally, the exact same computations as in the proof of the completeness for $p < \infty$ (see Section 6.6) show that $(\mu_n)_n$ converges for the FG_∞ metric. □

Remark 6.4.5. Contrary to the case $p < \infty$, the space $\mathcal{D}^\infty$ (and therefore $\mathcal{M}^\infty$) is not separable. Indeed, for $I \subset \mathbb{N}$, define the diagram $a_I := \sum_{i\in I} \delta_{(i,i+1)} \in \mathcal{D}^\infty$. The family $\{a_I : I \subset \mathbb{N}\}$ is uncountable, and for two distinct I, I', $\mathrm{FG}_\infty(a_I, a_{I'}) = \frac{\sqrt{2}}{2}$. This result is similar to [BV18, Theorem 4.20].

We now show that the direct implication in Theorem 6.2.6 still holds in the case $p = \infty$.

Proposition 6.4.6. *Let $\mu, \mu_1, \mu_2, \dots$ be measures in $\mathcal{M}^\infty$. If $\mathrm{FG}_\infty(\mu_n, \mu) \to 0$, then $(\mu_n)_n$ converges vaguely to μ and $\mathrm{Pers}_\infty(\mu_n)$ converges to $\mathrm{Pers}_\infty(\mu)$.*

Proof. First, the convergence of $\mathrm{Pers}_\infty(\mu_n)$ towards $\mathrm{Pers}_\infty(\mu)$ is a consequence of the reverse triangle inequality:

$$|\mathrm{Pers}_\infty(\mu_n) - \mathrm{Pers}_\infty(\mu)| = |\mathrm{FG}_\infty(\mu_n, 0) - \mathrm{FG}_\infty(\mu, 0)| \leq \mathrm{FG}_\infty(\mu_n, \mu),$$

which converges to 0 as n goes to ∞.

We now prove the vague convergence. Let $f \in C_c(\Omega)$, whose support is included in some compact set K. For any $\varepsilon > 0$, there exists a L-Lipschitz function f_ε, whose support is included in K, with $\|f - f_\varepsilon\|_\infty \leq \varepsilon$. Observe that $\sup_k \mu_k(K) < \infty$ using the same arguments than for (6.17). Let $\pi_n \in \mathrm{Opt}_\infty(\mu_n, \mu)$. We have

$$\begin{aligned}
|\mu_n(f) - \mu(f)| &\leq |\mu_n(f - f_\varepsilon)| + |\mu(f - f_\varepsilon)| + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)| \\
&\leq (\mu_n(K) + \mu(K))\varepsilon + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)| \\
&\leq (\sup_k \mu_k(K) + \mu(K))\varepsilon + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)|.
\end{aligned}$$

Also,

$$\begin{aligned}
|\mu_n(f_\varepsilon) - \mu(f_\varepsilon)| &= \left| \iint_{\overline{\Omega}^2} (f_\varepsilon(x) - f_\varepsilon(y)) \mathrm{d}\pi_n(x, y) \right| \\
&\leq \iint_{\overline{\Omega}^2} |f_\varepsilon(x) - f_\varepsilon(y)| \mathrm{d}\pi_n(x, y) \\
&\leq L \iint_{(K\times\overline{\Omega})\cup(\overline{\Omega}\times K)} d(x, y) \mathrm{d}\pi_n(x, y) \text{ as } f_\varepsilon \text{ is } L\text{-Lipschitz continuous} \\
&\leq L C_\infty(\pi_n)(\pi_n(K \times \overline{\Omega}) + \pi_n(\overline{\Omega} \times K)) \\
&\leq L \mathrm{FG}_\infty(\mu_n, \mu) \left(\sup_k \mu_k(K) + \mu(K) \right).
\end{aligned}$$

This last quantity converge to 0 as n goes to ∞ for fixed ε. Therefore, taking the $\limsup$ in n and then letting ε go to 0, we obtain that $\mu_n(f) \to \mu(f)$. □

Remark 6.4.7. As for the case $1 \leq p < \infty$, Proposition 6.4.6 implies that FG_∞ metricizes the vague convergence, and thus using Propositions 6.4.3 and 3.1.12, we have that $(\mathcal{D}^\infty, d_\infty)$ is closed in $(\mathcal{M}^\infty, \mathrm{FG}_\infty)$ and is—in particular—complete.

Contrary to the $p < \infty$ case, a converse of Proposition 6.4.6 does not hold, even on the subspace of persistence diagrams (see Figure 6.2). To recover a space with a structure more similar to $\mathcal{D}^p$, it is useful to look at a smaller set. Introduce $\mathcal{D}_0^\infty$ the set of persistence diagrams such that for all $r > 0$, there is a finite number of points of the diagram of persistence larger than r and recall that $\mathcal{D}_f$ denotes the set of persistence diagrams with finite number of points.

Proposition 6.4.8. *The closure of $\mathcal{D}_f$ for the distance FG_∞ is $\mathcal{D}_0^\infty$.*

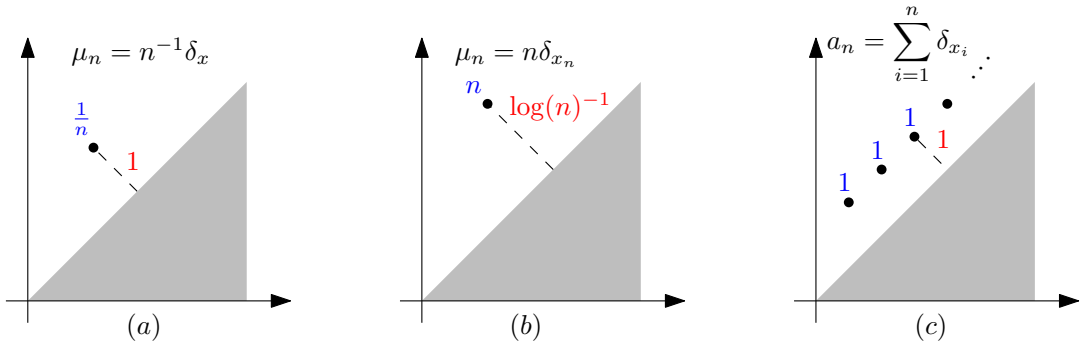


FIGURE 6.2: Illustration of differences between FG_p, FG_∞, and vague convergences. Blue color represents the mass on a point while red color designates distances. (a) A case where $\mathrm{FG}_p(\mu_n, 0) \to 0$ for any $p < \infty$ while $\mathrm{FG}_\infty(\mu_n, 0) = 1$. (b) A case where $\mathrm{FG}_\infty(\mu_n, 0) \to 0$ while for all $p < \infty$, $\mathrm{FG}_p(\mu_n, \mu) \to \infty$. (c) A sequence of persistence diagrams $a_n \in \mathcal{D}^\infty$, where $(a_n)_n$ converges vaguely to $a = \sum_i \delta_{x_i}$ and $\mathrm{Pers}_\infty(a_n) = \mathrm{Pers}_\infty(a)$, but (a_n) does not converge to a for FG_∞.

Proof. Consider $a \in \mathcal{D}_0^\infty$. By definition, for all $n \in \mathbb{N}$, a has a finite number of points with persistence larger than $\frac{1}{n}$, so that the restriction a_n of a to points with persistence larger than $\frac{1}{n}$ belongs to $\mathcal{D}_f$. As $\mathrm{FG}_\infty(a, a_n) \leq \frac{1}{n} \to 0$, $\mathcal{D}_0^\infty$ is contained in the closure of $\mathcal{D}_f$.

Conversely, consider a diagram $a \in \mathcal{D}^\infty \backslash \mathcal{D}_0^\infty$. There is a constant $r > 0$ such that a has infinitely many points with persistence larger than r. For any finite diagram $a' \in \mathcal{D}_f$, we have $\mathrm{FG}_\infty(a', a) \geq r$, so that a is not the limit for the FG_∞ metric of any sequence in $\mathcal{D}_f$. □

Remark 6.4.9. The space $\mathcal{D}_0^\infty$ is exactly the set introduced in [Blu+14, Theorem 3.5] as the completion of $\mathcal{D}_f$ for the bottleneck metric d_∞. Here, we recover that $\mathcal{D}_0^\infty$ is complete as a closed subset of the complete space $\mathcal{D}^\infty$.

Define for $r > 0$ and $a \in \mathcal{D}$, $a^{(r)}$ the persistence diagram restricted to Ω_r (as in Lemma 6.2.3). The following characterization of convergence holds in $\mathcal{D}_0^\infty$.

Proposition 6.4.10. *Let $a, a_1, a_2, \ldots$ be persistence diagrams in $\mathcal{D}_0^\infty$. Then,*

$$\mathrm{FG}_\infty(a_n, a) \to 0 \Leftrightarrow \begin{cases} a_n \xrightarrow{v} a, \\ (a_n^{(r)})_n \text{ is tight for all positive } r. \end{cases}$$

Proof. Let us prove first the direct implication. Proposition 6.4.6 states that the convergence with respect to FG_∞ implies the vague convergence. Fix $r > 0$. By definition, $a^{(r)}$ is made of a finite number of points, all included in some open bounded set $U \subset \Omega$. As $a_n^{(r)}(U^c)$ is a sequence of integers, the bottleneck convergence implies that for n large enough, $a_n^{(r)}(U^c)$ is equal to 0. Thus, $(a_n^{(r)})_n$ is tight.

Let us prove the converse. Consider $a \in \mathcal{D}_0^\infty$ and a sequence $(a_n)_n$ that converges vaguely to a, with $(a_n^{(r)})$ tight for all $r > 0$. Fix $r > 0$ and let $x_1, \ldots, x_K$ be an enumeration of the points in $a^{(r)}$, the point x_k being present with multiplicity $m_k \in \mathbb{N}$. Denote by $\mathcal{B}(x, \varepsilon)$ (resp. $\overline{\mathcal{B}}(x, \varepsilon)$) the open (resp. closed) ball of radius ε centered at x. By the Portmanteau theorem, for ε small enough,

$$\begin{cases} \liminf_{n\to\infty} a_n(\mathcal{B}(x_k, \varepsilon)) \geq a(\mathcal{B}(x_k, \varepsilon)) = m_k \\ \limsup_{n\to\infty} a_n(\overline{\mathcal{B}}(x_k, \varepsilon)) \leq a(\overline{\mathcal{B}}(x_k, \varepsilon)) = m_k, \end{cases}$$

so that, for n large enough, there are exactly m_k points of a_n in $\mathcal{B}(x_k, \varepsilon)$ (since $(a_n(\mathbb{B}"B(x_k, \varepsilon)))_n$ is a converging sequence of integers). The tightness of $(a_n^{(r)})_n$ implies the existence of some compact $K \subset \Omega$ such that for n large enough, $a_n^{(r)}(K^c) = 0$ (as the measures take their values in $\mathbb{N}$). Applying Portmanteau's theorem to the closed set $K' := K \setminus \bigcup_{i=1}^{K} B(x_i, \varepsilon)$ gives

$$\limsup_{n\to\infty} a_n^{(r)}(K') \leq a^{(r)}(K') = 0.$$

This implies that for n large enough, there are no other points in a_n with persistence larger than r and thus $\mathrm{FG}_\infty(a^{(r)}, a_n)$ is less than or equal to $r + \varepsilon$. Finally,

$$\limsup_{n\to\infty} \mathrm{FG}_\infty(a_n, a) \leq \limsup_{n\to\infty} \mathrm{FG}_\infty(a_n, a^{(r)}) + r \leq 2r + \varepsilon.$$

Letting $\varepsilon \to 0$ then $r \to 0$, the bottleneck convergence holds. □

Remark 6.4.11 (Related work with $p = +\infty$ in standard optimal transport.). Although it has been less studied than the W_p distances for finite p, there exist some stimulating works on the W_∞ distance. In particular, [CDPJ08] introduces the notion of restrictable transport plans: these are the transport plans π_∞ which appear as the limit as $p \to \infty$ of optimal plans π_p for W_p. Such optimal plans appear to have nice restriction properties and satisfy a form of cyclical monotonicity—an important notion in optimal transport theory that is not introduced in this work for the sake of concision. We conjecture that the existence and main properties of restrictable transport plans also hold in the framework of persistence measures with the FG_∞ distance.

6.5 Fréchet means of persistence measures

In this section, we state the existence of p-Fréchet means for probability distributions supported on $\mathcal{M}^p$. We start with the finite case (i.e. averaging finitely many persistence measures) and then extend the result to any probability distribution with finite p-th moment. We then study the specific case of distributions supported on $\mathcal{D}^p$ (i.e. averaging persistence diagrams), and show that in the finite setting, the set of p-Fréchet means is a convex set whose extreme points are in $\mathcal{D}^d$ (i.e. are actual persistence diagrams). We assume that $1 < p < \infty$ throughout this section.

Remark 6.5.1. Once again, the content of this section also holds in the more general setting where a general ground space Ω_0 and reservoir $\mathcal{R}$ are considered. Besides being a locally compact Polish space, one needs to assume that $\mathcal{X} = \Omega_0 \sqcup \mathcal{R}$ is a *geodesic* space for Fréchet means to exist. This property ensures that a Fréchet mean of two Diracs δ_x and δ_y) exists (and is given by the "middle" of a geodesic joining x to y if both points are sufficiently far away from the reservoir $\mathcal{R}$).

Recall that $(\mathcal{M}^p, \mathrm{FG}_p)$ is a Polish space. The space $(\mathcal{P}_1^p(\mathcal{M}^p), W_{p,\mathrm{FG}_p})$ is the space of probability measures P supported on $\mathcal{M}^p$, equipped with the W_{p,FG_p} metric, which are at a finite distance from δ_0—the Dirac mass supported on the empty diagram—i.e.

$$W^p_{p,\mathrm{FG}_p}(P, \delta_0) = \int_{\nu\in\mathcal{M}^p} \mathrm{FG}_p^p(\nu, 0)\mathrm{d}P(\nu) = \int_{\nu\in\mathcal{M}^p} \mathrm{Pers}_p(\nu)\mathrm{d}P(\nu) < \infty.$$

We recall the definition of p-Fréchet mean from Chapter 3.

Definition 6.5.2. *Let $P \in \mathcal{P}_1^p(\mathcal{M}^p)$. A measure $\mu^* \in \mathcal{M}^p$ is a p-*Fréchet mean *of P if it minimizes $\mathcal{E} : \mu \in \mathcal{M}^p \mapsto \int_{\nu\in\mathcal{M}^p} \mathrm{FG}_p^p(\mu, \nu)\mathrm{d}P(\nu)$.*

6.5.1 p-Fréchet means in the finite case

Let P be of the form $\sum_{i=1}^N \lambda_i \delta_{\mu_i}$ with $N \in \mathbb{N}$, μ_i a persistence measure of finite mass m_i, and $(\lambda_i)_i$ non-negative weights that sum to 1. Define $m_{\text{tot}} := \sum_{i=1}^N m_i$. To prove the existence of p-Fréchet means for such a P, we show that, in this case, p-Fréchet means correspond to p-Fréchet means for the Wasserstein distance of some distribution on $\mathcal{M}^p_{m_{\text{tot}}}(\tilde{\Omega})$, the sets of measures on $\tilde{\Omega}$ that all have the same mass m_{tot} (see Section 6.3), a problem well studied in the literature [AC11; CE10; COO15a].

We start with a lemma which affirms that if a measure μ has too much mass (larger than m_{tot}), then it cannot be a p-Fréchet mean of $\mu_1 \dots \mu_N$.

Lemma 6.5.3. *We have* $\inf\{\mathcal{E}(\mu) : \ \mu \in \mathcal{M}^p\} = \inf\{\mathcal{E}(\mu) : \ \mu \in \mathcal{M}^p_{\leq m_{\text{tot}}}\}$.

Proof. The idea of the proof is to show that if a measure μ has some mass that is mapped to the diagonal in each transport plan between μ and μ_i, then we can build a measure μ' by "removing" this mass, and then observe that such a measure μ' has a smaller energy.

Let thus $\mu \in \mathcal{M}^p$. Let $\pi_i \in \text{Opt}_p(\mu_i, \mu)$ for $i = 1, \dots, N$. The measure $A \subset \Omega \mapsto \pi_i(\partial\Omega \times A)$ is absolutely continuous with respect to μ. Therefore, it has a density f_i with respect to μ. Define for $A \subset \Omega_0$ a Borel set,

$$\mu'(A) := \mu(A) - \int_A \min_j f_j(x) \mathrm{d}\mu(x),$$

and, for $i = 1, \dots, N$, a measure π'_i, equal to π_i on $\Omega \times \overline{\Omega}$ and which satisfies for $A \subset \Omega_0$ a Borel set,

$$\pi'_i(\partial\Omega \times A) = \pi'_i(s(A) \times A) := \pi_i(\partial\Omega \times A) - \int_A \min_j f_j(x) \mathrm{d}\mu(x),$$

where s is the orthogonal projection on $\partial\Omega$. As $\pi_i(\partial\Omega \times A) = \int_A f_i(x)\mathrm{d}\mu(x)$, $\pi'_i(A)$ is nonnegative, and as $\pi_i(\partial\Omega \times A) \leq \mu(A)$, it follows that $\mu'(A)$ is nonnegative. To prove that $\pi'_i \in \text{Adm}(\mu_i, \mu')$, it is enough to check that for $A \subset \Omega_0$, $\pi'_i(\overline{\Omega} \times A) = \mu'(A)$:

$$\begin{aligned}\pi'_i(\overline{\Omega} \times A) &= \pi_i(\Omega_0 \times A) + \pi_i(\partial\Omega \times A) - \int_A \min_j f_j(x)\mathrm{d}\mu(x) \\ &= \mu(A) - \int_A \min_j f_j(x)\mathrm{d}\mu(x) = \mu'(A).\end{aligned}$$

Also,

$$\begin{aligned}\mu'(\Omega) &= \int_\Omega (1 - \min_j f_j)\mathrm{d}\mu(x) \leq \sum_{j=1}^N \int_\Omega (1 - f_j)\mathrm{d}\mu(x) \\ &= \sum_{j=1}^N (\mu(\Omega) - \pi_j(\partial\Omega \times \Omega)) = \sum_{j=1}^N (\pi_j(\overline{\Omega} \times \Omega) - \pi_j(\partial\Omega \times \Omega)) \\ &= \sum_{j=1}^N \pi_j(\Omega \times \Omega) \leq \sum_{j=1}^N \pi_j(\Omega \times \overline{\Omega}) = \sum_{j=1}^N m_j = m_{\text{tot}}.\end{aligned}$$

and thus $\mu'(\Omega) \leq m_{\text{tot}}$. To conclude, observe that

$$\begin{aligned}\mathcal{E}(\mu') &\leq \sum_{i=1}^{N} \lambda_i C_p(\pi_i') = \sum_{i=1}^{N} \lambda_i \left(\iint_{\Omega\times\overline{\Omega}} d(x,y)^p \mathrm{d}\pi_i(x,y) \right. \\ &\qquad \left. + \iint_{\partial\Omega\times\Omega} d(x,y)^p \mathrm{d}\pi_i(x,y) - \int_{\Omega} d(x,\partial\Omega)^p \min_j f_j(x) \mathrm{d}\mu(x) \right) \\ &\leq \sum_{i=1}^{N} \lambda_i C_p(\pi) = \mathcal{E}(\mu).\end{aligned}$$

□

Recall that $W_{p,\rho}$ denote the Wasserstein distance between measures with same mass supported on the metric space $(\tilde{\Omega}, \rho)$ (see Chapter 3 and Section 6.3).

Proposition 6.5.4. *Let* $\Psi : \mu \in \mathcal{M}^p_{\leq m_{\text{tot}}} \mapsto \tilde{\mu} \in \mathcal{M}^p_{m_{\text{tot}}}(\tilde{\Omega})$, *where* $\tilde{\mu} := \mu + (m_{\text{tot}} - \mu(\Omega))\delta_{\partial\Omega}$. *The functionals*

$$\mathcal{E} : \mu \in \mathcal{M}^p_{\leq m_{\text{tot}}} \mapsto \sum_{i=1}^{N} \lambda_i \mathrm{FG}^p_p(\mu, \mu_i) \text{ and}$$
$$\mathcal{F} : \tilde{\mu} \in \mathcal{M}^p_{m_{\text{tot}}}(\tilde{\Omega}) \mapsto \sum_{i=1}^{N} \lambda_i W^p_{p,\rho}(\tilde{\mu}, \Psi(\mu_i)),$$

have the same infimum values and $\arg\min \mathcal{E} = \Psi^{-1}(\arg\min \mathcal{F})$.

Proof. Let G be the set of $\mu \in \mathcal{M}^p$ such that, for all i, there exists $\pi_i \in \mathrm{Opt}_p(\mu_i, \mu)$ with $\pi_i(\Omega, \partial\Omega) = 0$. By point 2 of Lemma 6.3.3, for $\mu \in G$ and $\pi_i \in \mathrm{Opt}_p(\mu_i, \mu)$ with $\pi_i(\Omega, \partial\Omega) = 0$, $\iota(\pi_i)$ is well defined and satisfies

$$\mathrm{FG}^p_p(\mu_i, \mu) = C_p(\pi_i) = \iint_{\tilde{\Omega}\times\tilde{\Omega}} \tilde{d}(x,y)^p \mathrm{d}\iota(\pi_i)(x,y) \geq \tilde{C}_p(\iota(\pi_i)) \geq W^p_{p,\rho}(\tilde{\mu}_i, \tilde{\mu}),$$

so that $\mathcal{F}(\Psi(\mu)) \leq \mathcal{E}(\mu)$. As, by Lemma 6.3.4, $\mathcal{E} \leq \mathcal{F} \circ \Psi$, we therefore have $\mathcal{E}(\mu) = \mathcal{F}(\Psi(\mu))$ for $\mu \in G$.

We now show that if $\mu \notin G$, then there exists $\mu' \in \mathcal{M}^p$ with $\mathcal{E}(\mu') < \mathcal{E}(\mu)$. Let $\mu \notin G$ and $\pi_i \in \mathrm{Opt}_p(\mu_i, \mu)$. Assume that for some i, we have $\pi_i(\Omega, \partial\Omega) > 0$, and introduce $\nu \in \mathcal{M}^p$ defined as $\nu(A) = \pi_i(A, \partial\Omega)$ for $A \subset \Omega$. Define

$$T : x \in \Omega \mapsto \arg\min_{y\in\Omega} \left\{ \lambda_i d(x,y)^p + \sum_{j\neq i} \lambda_j d(y, \partial\Omega)^p \right\} \in \Omega. \tag{6.18}$$

Note that this function is well defined, with the value of the objective function in $T(x)$ being strictly smaller than the value in $s(x)$, where $s(x)$ is the projection of x on $\partial\Omega$ (in the general case $(\Omega_0, \mathcal{R})$, a minimizer $T(x)$ is found on the geodesic between x and some projection $s(x)$).

Consider the measure $\mu' = \mu + (T_\# \nu)$, where $T_\# \nu$ is the push-forward of ν by the application T. Consider the transport plan π_i' deduced from π_i where ν is transported onto $T_\# \nu$ instead of being transported to $\partial\Omega$ (see Figure 6.3). More precisely, π_i' is the measure on $\overline{\Omega} \times \overline{\Omega}$ defined by, for Borel sets $A, B \subset \Omega$:

$$\pi_i'(A \times B) = \pi_i(A \times B) + \nu(A \cap T^{-1}(B)),$$
$$\pi_i'(A \times \partial\Omega) = 0, \quad \pi_i'(\partial\Omega \times B) = \pi_i(\partial\Omega \times B).$$

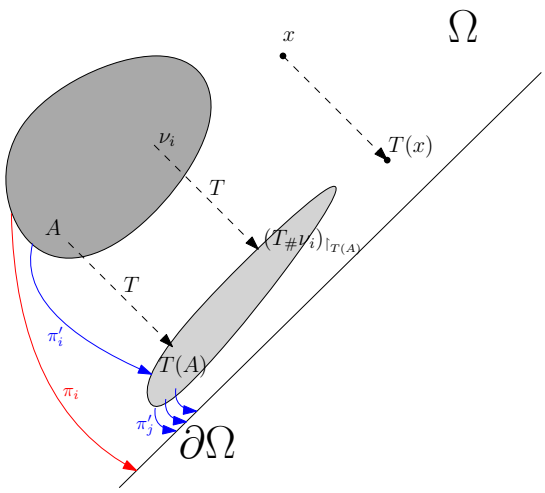


FIGURE 6.3: Global picture of the proof. The main idea is to observe that the cost induced by π_i (red) is strictly greater than the sum of costs induces by the π'_is (blue), which leads to a strictly better energy.

We have $\pi'_i \in \mathrm{Adm}(\mu_i, \mu')$. Indeed, for Borel sets $A, B \subset \Omega$:

$$\pi'_i(A \times \overline{\Omega}) = \pi'_i(A \times \Omega) = \pi_i(A \times \Omega) + \nu(A) = \pi_i(A \times \overline{\Omega}) = \mu_i(A),$$

and

$$\begin{aligned}\pi'_i(\overline{\Omega} \times B) &= \pi'_i(\Omega \times B) + \pi'_i(\partial\Omega \times B) \\ &= \pi_i(\Omega \times B) + \nu(T^{-1}(B)) + \pi_i(\partial\Omega \times B) \\ &= \mu(B) + T_\#\nu(B) = \mu'(B).\end{aligned}$$

Using π'_i instead of π_i changes the transport cost by the quantity

$$\int_\Omega [d(x, T(x))^p - d(x, \partial\Omega)^p] \mathrm{d}\nu(x) \leq 0.$$

In a similar way, we define for $j \neq i$ the plan $\pi'_j \in \mathrm{Adm}(\mu_j, \mu')$ by transporting the mass induced by the newly added $(T_\#\nu)$ to the diagonal $\partial\Omega$. Using these modified transport plans increases the total cost by

$$\sum_{j \neq i} \lambda_j \int_\Omega d(T(x), \partial\Omega)^p \mathrm{d}\nu(x).$$

One can observe that, as the value of the objective function at $T(x)$ in (6.18) is smaller than the value at $s(x)$,

$$\int_\Omega \left[\lambda_i \left(d(x, T(x))^p - d(x, \partial\Omega)^p \right) + \sum_{j \neq i} \lambda_j d(T(x), \partial\Omega)^p \right] \mathrm{d}\nu(x) < 0$$

due to the fact that $\nu(\Omega) > 0$.

Therefore, the total transport cost induced by the $(\pi'_i)_{i=1\ldots N}$ is strictly less or equal to $\mathcal{E}(\mu)$, and thus $\mathcal{E}(\mu') < \mathcal{E}(\mu)$. Finally, we have

$$\inf_{\mu \in \mathcal{M}^p_{\leq m_{tot}}} \mathcal{E}(\mu) = \inf_{\mu \in G} \mathcal{E}(\mu) = \inf_{\mu \in G} \mathcal{F}(\Psi(\mu)) \geq \inf_{\mu \in \mathcal{M}^p_{\leq m_{tot}}} \mathcal{F}(\Psi(\mu)) \geq \inf_{\mu \in \mathcal{M}^p_{\leq m_{tot}}} \mathcal{E}(\mu),$$

where the last inequality comes from $\mathcal{F} \circ \Psi \geq \mathcal{E}$ (Lemma 6.3.4). Therefore, $\inf \mathcal{E} = \inf \mathcal{F} \circ \Psi$, which is equal to $\inf \mathcal{F}$, as Ψ is a bijection. Also, if μ is a minimizer of $\mathcal{E}$ (should it exist), then $\mu \in G$ and $\mathcal{E}(\mu) = \mathcal{F}(\Psi(\mu))$. Therefore, as the infimum are equal, $\Psi(\mu)$ is a minimizer of $\mathcal{F}$. Reciprocally, if $\tilde{\mu}$ is a minimizer of $\mathcal{F}$, then, by Lemma 6.3.4, $\mathcal{F}(\tilde{\mu}) \geq \mathcal{E}(\Psi^{-1}(\tilde{\mu}))$, and, as the infimum are equal, $\Psi^{-1}(\tilde{\mu})$ is a minimizer of $\mathcal{E}$. □

The existence of minimizers $\tilde{\mu}$ of $\mathcal{F}$, that is "Wasserstein barycenter" (i.e. p-Fréchet means for the Wasserstein distance) of $\tilde{P} := \sum_{i=1}^{N} \lambda_i \delta_{\tilde{\mu}_i}$, is well-known (see [LGL16, Proposition 1]). Proposition 6.5.4 asserts that $\Psi^{-1}(\tilde{\mu})$ is a minimizer of $\mathcal{E}$ on $\mathcal{M}^p_{\leq m_{\text{tot}}}$, and thus a p-Fréchet mean of P according to Lemma 6.5.3. We therefore have proved the existence of p-Fréchet means in the finite case.

6.5.2 Existence and consistency of p-Fréchet means

We now extend the results of the previous section to the p-Fréchet means of general probability measures supported on $\mathcal{M}^p$. First, we show a *consistency* result, in the vein of [LGL16, Theorem 3].

Proposition 6.5.5. *Let P_n, P be probability measures in $\mathcal{P}^p_1(\mathcal{M}^p)$. Assume that each P_n has a p-Fréchet mean μ_n and that $W_{p,\mathrm{FG}_p}(P_n, P) \to 0$. Then, the sequence $(\mu_n)_n$ is relatively compact in $(\mathcal{M}^p, \mathrm{FG}_p)$, and any limit of a converging subsequence is a p-Fréchet mean of P.*

Proof. In order to prove relative compactness of $(\mu_n)_n$, we use the characterization stated in Proposition 3.1.8. Consider a compact set $K \subset \Omega$. We have, because of (6.6),

$$\begin{aligned}\mu_n(K)^{\frac{1}{p}} &\leq \frac{1}{d(K, \partial\Omega)} \mathrm{FG}_p(\mu_n, 0) = \frac{1}{d(K, \partial\Omega)} W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, \delta_0) \\ &\leq \frac{1}{d(K, \partial\Omega)} \left(W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P_n) + W_{p,\mathrm{FG}_p}(P_n, \delta_0) \right)\end{aligned}$$

Since μ_n is a p-Fréchet mean of P_n, it minimizes $\{W_{p,\mathrm{FG}_p}(\delta_\nu, P_n) : \nu \in \mathcal{M}^p\}$, and in particular $W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P_n) \leq W_{p,\mathrm{FG}_p}(\delta_0, P_n)$. Furthermore, as by assumption $W_{p,\mathrm{FG}_p}(P_n, P) \to 0$, we have that $\sup_n W_{p,\mathrm{FG}_p}(P_n, \delta_0) < \infty$. As a consequence $\sup_n \mu_n(K) < \infty$, and Proposition 3.1.8 allows us to conclude that the sequence $(\mu_n)_n$ is relatively compact for the vague convergence.

To conclude the proof, we use the following two lemmas, whose proofs are found in Section 6.6.

Lemma 6.5.6. *Under the same hypothesis than Proposition 6.5.5, there exists a subsequence $(\mu_{n_k})_k$ of $(\mu_n)_n$ which vaguely converges towards μ a p-Fréchet mean of P and there exists $\nu \in \mathcal{M}^p$ such that $\mathrm{FG}_p(\mu_{n_k}, \nu) \to \mathrm{FG}_p(\mu, \nu)$ as $k \to \infty$.*

Lemma 6.5.7. *Let $\mu, \mu_1, \mu_2, \dots \in \mathcal{M}^p$. Then, $\mathrm{FG}_p(\mu_n, \mu) \to 0$ if and only if (i) $\mu_n \xrightarrow{v} \mu$ and (ii) there exists a persistence measure $\nu \in \mathcal{M}^p$ such that $\mathrm{FG}_p(\mu_n, \nu) \to \mathrm{FG}_p(\mu, \nu)$.*

Let $\mu'_k = \mu_{n_k}$ be any subsequence of μ_n. We want to show that there exists a subsequence of μ'_k which converges with respect to the FG_p metric towards some p-Fréchet mean of P. By Lemma 6.5.6 applied to the sequence $(\mu'_k)_k$, there exists a subsequence μ'_{k_l} which converges vaguely to some p-Fréchet mean μ of P, and some ν with $\mathrm{FG}_p(\mu'_{k_l}, \nu) \to \mathrm{FG}_p(\mu, \nu)$ as $l \to \infty$. By Lemma 6.5.7, this implies that μ'_{k_l} converges to μ with respect to the FG_p metric, showing the conclusion. □

As the finite case is solved, generalization follows easily using Proposition 6.5.5.

Theorem 6.5.8. *For any probability distribution P supported on $\mathcal{M}^p$ with finite p-th moment, the set of p-Fréchet means of P is a non-empty compact convex set of $\mathcal{M}^p$.*

Proof. We first prove the non-emptiness. Let $P = \sum_{i=1}^N \lambda_i \mu_i$ be a probability measure on $\mathcal{M}^p$ with finite support $\mu_1, \dots, \mu_N$. According to Proposition 6.3.1, there exists sequences $(\mu_i^{(n)})_n$ in $\mathcal{M}_f^p$ with $\mathrm{FG}_p(\mu_i^{(n)}, \mu_i) \to 0$. As a consequence of the result of Section 6.5.1, the probability measures $P^{(n)} := \sum_i \lambda_i \delta_{\mu_i^{(n)}}$ admit p-Fréchet means. Furthermore, $W^p_{p,\mathrm{FG}_p}(P^{(n)}, P) \leq \sum_i \lambda_i \mathrm{FG}_p^p(\mu_i^{(n)}, \mu_i)$ so that this quantity converges to 0 as $n \to \infty$. It follows from Proposition 6.5.5 that P admits a p-Fréchet mean.

If P has infinite support, following [LGL16], it can be approximated (in W_{p,FG_p}) by a empirical probability measure $P_n = \frac{1}{n}\sum_{i=1}^n \delta_{\mu_i}$ where the μ_i are i.i.d. from P. We know that P_n admits a p-Fréchet mean since its support is finite, and thus, applying Proposition 6.5.5 once again, we obtain that P admits a p-Fréchet mean.

Finally, the compactness of the set of p-Fréchet means follows from Proposition 6.5.5 applied with $P_n = P$: if $(\mu_n)_n$ is a sequence of p-Fréchet means, then the sequence is relatively compact in $(\mathcal{M}^p, \mathrm{FG}_p)$, and any converging subsequence is also a p-Fréchet mean of P. Also, the convexity of the set of p-Fréchet means follows from the convexity of FG_p^p (see Lemma 8.1.3 in Chapter 8): if μ_1, μ_2 are two p-Fréchet means with energy $\mathcal{E}(\mu_1) = \mathcal{E}(\mu_2) = E_0$ and $0 \leq \lambda \leq 1$, then

$$\begin{aligned}
\mathcal{E}(\lambda\mu_1 + (1-\lambda)\mu_2) &= \int_{\nu \in \mathcal{M}^p} \mathrm{FG}_p^p(\lambda\mu_1 + (1-\lambda)\mu_2, \nu)\mathrm{d}P(\nu) \\
&\leq \int_{\nu \in \mathcal{M}^p} (\lambda \mathrm{FG}_p^p(\mu_1, \nu) + (1-\lambda)\mathrm{FG}_p^p(\mu_2, \nu))\mathrm{d}P(\nu) \\
&= \lambda\mathcal{E}(\mu_1) + (1-\lambda)\mathcal{E}(\mu_2) = E_0,
\end{aligned}$$

so that $\lambda\mu_1 + (1-\lambda)\mu_2$ is also a p-Fréchet mean.

□

6.5.3 p-Fréchet means in $\mathcal{D}^p$

We now prove the existence of p-Fréchet means for distributions of persistence diagrams (i.e. probability distributions supported on $\mathcal{D}^p$), extending the results of [MMH11], in which authors prove their existence for specific probability distributions (namely distributions with compact support or specific rates of decay). Theorem 6.5.10 below asserts two different things: that $\arg\min\{\mathcal{E}(a) : a \in \mathcal{D}^p\}$ is non empty, and that $\min\{\mathcal{E}(a) : a \in \mathcal{D}^p\} = \min\{\mathcal{E}(\mu) : \mu \in \mathcal{M}^p\}$, i.e a persistence measure cannot perform strictly better than an optimal persistence diagram when averaging diagrams. As for p-Fréchet means in $\mathcal{M}^p$, we start with the finite case. The following lemma actually gives a geometric description of the set of p-Fréchet means obtained when averaging a finite number of finite diagrams.

Lemma 6.5.9. *Consider $a_1, \dots, a_N \in \mathcal{D}_f$, weights $(\lambda_i)_i$ that sum to 1, and let $P := \sum_{i=1}^N \lambda_i \delta_{a_i}$. Then, the set of minimizers of $\mu \mapsto \sum_{i=1}^N \lambda_i \mathrm{FG}_p^p(\mu, a_i)$ is a non empty convex subset of $\mathcal{M}_f^p$ whose extreme points belong to $\mathcal{D}_f$. In particular, P admits a p-Fréchet mean in $\mathcal{D}_f$.*

The proof of this lemma is delayed to Section 6.6. Note that, as a straightforward consequence, if P has a unique minimizer in $\mathcal{D}_f$ (which is generically true [Tur13]), then so it does in $\mathcal{M}_f^p$.

Theorem 6.5.10. *For any probability distribution P supported on $\mathcal{D}^p$ with finite p-th moment, the set of p-Fréchet means of P contains an element of $\mathcal{D}^p$.*

Proof. To prove the existence of a p-Fréchet mean which is a persistence diagram, we argue as in the proof of Theorem 6.5.8, using additionally the fact that $\mathcal{D}^p$ is closed in $\mathcal{M}^p$ (Proposition 3.1.12). □

6.6 Additional proofs

For the sake of completeness, we first present proofs which either require very few adaptations from corresponding proofs in [FG10] or which are close to standard proofs in optimal transport theory.

Proofs of Proposition 6.2.2 and Proposition 6.4.2.

- For $\pi \in \mathrm{Adm}(\mu,\nu)$ supported on $E_{\overline{\Omega}}$, and for any compact sets $K,\ K' \subset \Omega$, one has $\pi((K\times\overline{\Omega})\cup(\overline{\Omega}\times K')) \leq \mu(K)+\nu(K') < \infty$. As any compact subset of $E_{\overline{\Omega}}$ is included in a set of the form $(K\times\overline{\Omega})\cup(\overline{\Omega}\times K')$, Proposition 3.1.8 implies that $\mathrm{Adm}(\mu,\nu)$ is relatively compact for the vague convergence on $E_{\overline{\Omega}}$. Also, if a sequence $(\pi_n)_n$ in $\mathrm{Adm}(\mu,\nu)$ converges vaguely to some $\pi \in \mathcal{M}(E_{\overline{\Omega}})$, then the marginals of π are still μ and ν. Indeed, if f is a continuous function with compact support on Ω, then
$$\begin{aligned}\int_{E_\Omega} f(x)\mathrm{d}\pi(x,y) &= \lim_n \int_{E_\Omega} f(x)\mathrm{d}\pi_n(x,y) = \lim_n \int_\Omega f(x)\mathrm{d}\mu_n(x)\\ &= \int_\Omega f(x)\mathrm{d}\mu(x),\end{aligned}$$
and we show likewise that the second marginal of π is ν. Hence, $\mathrm{Adm}(\mu,\nu)$ is closed and relatively compact in $\mathcal{M}(E_{\overline{\Omega}})$: it is therefore sequentially compact.

- To prove the second point of Proposition 6.2.2, consider $\pi,\pi_1,\pi_2,\dots$ such that $\pi_n \xrightarrow{v} \pi$, and introduce $\pi'_n : A \mapsto \iint_A d(x,y)^p \mathrm{d}\pi_n$. The sequence $(\pi'_n)_n$ still converges vaguely to $\pi' : A \mapsto \iint_A d(x,y)^p\mathrm{d}\pi$. the Portmanteau theorem (Proposition 3.1.11) applied with the open set $E_{\overline{\Omega}}$ to the measures $\pi'_n \xrightarrow{v} \pi'$ implies that
$$C_p(\pi) = \pi'(E_{\overline{\Omega}}) \leq \liminf_n \pi'_n(E_{\overline{\Omega}}) = \liminf_n C_p(\pi_n),$$
i.e. C_p is lower semi-continuous.

- We now prove the lower semi-continuity of C_∞. Let $(\pi_n)_n$ be a sequence converging vaguely to π on $E_{\overline{\Omega}}$ and let $r > \liminf_{n\to\infty} C_\infty(\pi_n)$. The set $U_r = \{(x,y)\in E_{\overline{\Omega}} :\ d(x,y) > r\}$ is open. By the Portmanteau theorem (Proposition 3.1.11), we have
$$0 = \liminf_{n\to\infty} \pi_n(U_r) \geq \pi(U_r).$$
Therefore, $\mathrm{spt}(\pi) \subset U_r^c$ and $C_\infty(\pi) \leq r$. As this holds for any $r > \liminf_{n\to\infty} C_\infty(\pi_n)$, we have $\liminf_{n\to\infty} C_\infty(\pi_n) \geq C_\infty(\pi)$.

- We show that for any $1 \leq p \leq \infty$, the lower semi-continuity of C_p and the sequential compactness of $\mathrm{Adm}(\mu,\nu)$ imply that 1. $\mathrm{Opt}_p(\mu,\nu)$ is a non-empty compact set for the vague topology on $E_{\overline{\Omega}}$ and that 2. FG_p is lower semi-continuous.

1. Let $(\pi_n)_n$ be a minimizing sequence of (6.2) or (6.15) in $\mathrm{Adm}(\mu,\nu)$. As $\mathrm{Adm}(\mu,\nu)$ is sequentially compact, it has an adherence value π, and the lower semi-continuity implies that $C_p(\pi) \leq \liminf_{n\to\infty} C_p(\pi_n) = \mathrm{FG}_p^p(\mu,\nu)$, so that $\mathrm{Opt}_p(\mu,\nu)$ is non-empty. Using once again the lower semi-continuity of C_p, if a sequence in $\mathrm{Opt}_p(\mu,\nu)$ converges to some limit, then the cost of the limit is less than or equal to (and thus equal to) $\mathrm{FG}_p^p(\mu,\nu)$, i.e. the limit is in $\mathrm{Opt}_p(\mu,\nu)$. The set $\mathrm{Opt}_p(\mu,\nu)$ being closed in the sequentially compact set $\mathrm{Adm}(\mu,\nu)$, it is also sequentially compact.
2. Let $\mu_n \xrightarrow{v} \mu$ and $\nu_n \xrightarrow{v} \nu$. One has

$$\liminf_n \mathrm{FG}_p(\mu_n,\nu_n) = \lim_k \mathrm{FG}_p(\mu_{n_k},\nu_{n_k})$$

for some subsequence $(n_k)_k$. For ease of notation, we will still use the index n to denote this subsequence. If the limit is infinite, there is nothing to prove. Otherwise, consider $\pi_n \in \mathrm{Opt}_p(\mu_n,\nu_n)$. For any compact sets $K,\ K' \subset \Omega$, one has $\pi_n((K\times\overline{\Omega})\cup(\overline{\Omega}\times K')) \leq \sup_n \mu_n(K)+\sup_n \nu_n(K') < \infty$. Therefore, by Proposition 3.1.8, there exists a subsequence $(\pi_{n_k})_k$ which converges vaguely to some measure $\pi \in \mathrm{Adm}(\mu,\nu)$. Note that the first (resp. second) marginal of π is equal to the limit μ (resp. ν) of the first (resp. second) marginal of (π_{n_k}), so that π is in $\mathrm{Adm}(\mu,\nu)$. Therefore,

$$\mathrm{FG}_p^p(\mu,\nu) \leq C_p(\pi) \leq \liminf_{n\to\infty} C_p(\pi_n) = \liminf_{n\to\infty} \mathrm{FG}_p^p(\mu_n,\nu_n).$$

- Finally, we prove that FG_p is a metric on $\mathcal{M}^p$. Let $\mu,\nu,\lambda \in \mathcal{M}^p$. The symmetry of FG_p is clear. If $\mathrm{FG}_p(\mu,\nu) = 0$, then there exists $\pi \in \mathrm{Adm}(\mu,\nu)$ supported on $\{(x,x),\ x \in \Omega\}$. Therefore, for a Borel set $A \subset \Omega$, $\mu(A) = \pi(A\times\overline{\Omega}) = \pi(A\times A) = \pi(\overline{\Omega}\times A) = \nu(A)$, and $\mu = \nu$. To prove the triangle inequality, we need a variant on the gluing lemma, stated in [FG10, Lemma 2.1]: for $\pi_{12} \in \mathrm{Opt}(\mu,\nu)$ and $\pi_{23} \in \mathrm{Opt}(\nu,\lambda)$ there exists a measure $\gamma \in \mathcal{M}(\overline{\Omega}^3)$ such that the marginal corresponding to the first two entries (resp. two last entries), when restricted to $E_{\overline{\Omega}}$, is equal to π_{12} (resp. π_{23}), and induces a zero cost on $\partial\Omega\times\partial\Omega$. Therefore, by the triangle inequality and the Minkowski inequality,

$$\begin{aligned}
\mathrm{FG}_p(\mu,\lambda) &\leq \left(\int_{\overline{\Omega}^2} d(x,z)^p \mathrm{d}\gamma(x,y,z)\right)^{1/p} \\
&\leq \left(\int_{\overline{\Omega}^2} d(x,y)^p \mathrm{d}\gamma(x,y,z)\right)^{1/p} + \left(\int_{\overline{\Omega}^2} d(y,z)^p \mathrm{d}\gamma(x,y,z)\right)^{1/p} \\
&= \left(\int_{\overline{\Omega}^2} d(x,y)^p \mathrm{d}\pi_{12}(x,y)\right)^{1/p} + \left(\int_{\overline{\Omega}^2} d(y,z)^p \mathrm{d}\pi_{23}(y,z)\right)^{1/p} \\
&= \mathrm{FG}_p(\mu,\nu) + \mathrm{FG}_p(\nu,\lambda).
\end{aligned}$$

The proof is similar for $p = \infty$.

□

Proof of Proposition 6.2.5. We first show the separability. Consider for $k > 0$ a partition of Ω into squares (C_i^k) of side length 2^{-k}, centered at points x_i^k. Let F be the set of all measures of the form $\sum_{i\in I} q_i \delta_{x_i^k}$ for q_i positive rationals, $k > 0$ and I a finite subset of $\mathbb{N}$. Our goal is to show that the countable set F is dense in $\mathcal{M}^p$. Fix $\varepsilon > 0$, and $\mu \in \mathcal{M}^p$. The proof is in three steps.

1. Since $\mathrm{Pers}_p(\mu) < \infty$, there exists a compact $K \subset \Omega$ such that $\mathrm{Pers}_p(\mu) - \mathrm{Pers}_p(\mu_0) < \varepsilon^p$, where μ_0 is the restriction of μ to K. By considering the transport plan between μ and μ_0 induced by the identity map on K and the projection onto the diagonal on $\overline{\Omega}\backslash K$, it follows that $\mathrm{FG}_p^p(\mu, \mu_0) \leq \mathrm{Pers}_p(\mu) - \mathrm{Pers}_p(\mu_0) \leq \varepsilon^p$.

2. Consider k such that $2^{-k} \leq \varepsilon/(\sqrt{2}\mu(K)^{1/p})$ and denote by I the indices corresponding to squares C_i^k intersecting K. Let $\mu_1 = \sum_{i\in I}^{\infty} \mu_0(C_i^k)\delta_{x_i^k}$. One can create a transport map between μ_0 and μ_1 by mapping each square C_i^k to its center x_i^k, so that

$$\mathrm{FG}_p(\mu_0, \mu_1) \leq \left(\sum_i \mu_0(C_i^k)(\sqrt{2}\cdot 2^{-k})^p\right)^{1/p} \leq \mu(K)^{1/p}\sqrt{2}\cdot 2^{-k} \leq \varepsilon.$$

3. Consider, for $i \in I$, q_i a rational number satisfying $q_i \leq \mu_0(C_i^k)$ and $|\mu_0(C_i^k) - q_i| \leq \varepsilon^p / \left(\sum_{i\in I} d(x_i^k, \partial\Omega)^p\right)$. Let $\mu_2 = \sum_{i\in I} q_i\delta_{x_i^k}$. Consider the transport plan between μ_2 and μ_1 that fully transports μ_2 onto μ_1, and transport the remaining mass in μ_1 onto the diagonal. Then,

$$\mathrm{FG}_p(\mu_1, \mu_2) \leq \left(\sum_{i\in I} |\mu_0(C_i^k) - q_i| d(x_i^k, \partial\Omega)^p\right)^{1/p} \leq \varepsilon.$$

As $\mu_2 \in F$ and $\mathrm{FG}_p(\mu, \mu_2) \leq 3\varepsilon$, the separability is proven.

To prove that the space is complete, consider a Cauchy sequence $(\mu_n)_n$. As the sequence $(\mathrm{Pers}_p(\mu_n))_n = (\mathrm{FG}_p^p(\mu_n, 0))_n$ is a Cauchy sequence, it is bounded. Therefore, for $K \subset \Omega$ a compact set, (6.6) implies that $\sup_n \mu_n(K) < \infty$. Proposition 3.1.8 implies that $(\mu_n)_n$ is relatively compact for the vague topology on Ω. Consider $(\mu_{n_k})_k$ a subsequence converging vaguely on Ω to some measure μ. By the lower semi-continuity of FG_p,

$$\mathrm{Pers}_p(\mu) = \mathrm{FG}_p^p(\mu, 0) \leq \liminf_{k\to\infty} \mathrm{FG}_p^p(\mu_{n_k}, 0) < \infty,$$

so that $\mu \in \mathcal{M}^p$. Using once again the lower semi-continuity of FG_p,

$$\begin{aligned}\mathrm{FG}_p(\mu_n, \mu) &\leq \liminf_{k\to\infty} \mathrm{FG}_p(\mu_n, \mu_{n_k})\\ \lim_{n\to\infty} \mathrm{FG}_p(\mu_n, \mu) &\leq \lim_{n\to\infty} \liminf_{k\to\infty} \mathrm{FG}_p(\mu_n, \mu_{n_k}) = 0,\end{aligned}$$

ensuring that $\mathrm{FG}_p(\mu_n, \mu) \to 0$, that is the space is complete. □

Proof of the direct implication of Theorem 6.2.6. Let $\mu, \mu_1, \mu_2, \ldots$ be elements of $\mathcal{M}^p$ and assume that the sequence $(\mathrm{FG}_p(\mu_n, \mu))_n$ converges to 0. The triangle inequality implies that $\mathrm{Pers}_p(\mu_n) = \mathrm{FG}_p^p(\mu_n, 0)$ converges to $\mathrm{Pers}_p(\mu) = \mathrm{FG}_p^p(\mu, 0)$. Let $f \in C_c(\Omega)$, whose support is included in some compact set K. For any $\varepsilon > 0$, there exists a Lipschitz function f_ε, with Lipschitz constant L and whose support is included in K, with the ∞-norm $\|f - f_\varepsilon\|_\infty$ less than or equal to ε. The convergence of $\mathrm{Pers}_p(\mu_n)$ and (6.6) imply that $\sup_k \mu_k(K) < \infty$. Let $\pi_n \in \mathrm{Opt}_p(\mu_n, \mu)$, we have

$$\begin{aligned}|\mu_n(f) - \mu(f)| &\leq |\mu_n(f - f_\varepsilon)| + |\mu(f - f_\varepsilon)| + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)|\\ &\leq (\mu_n(K) + \mu(K))\varepsilon + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)|\\ &\leq (\sup_k \mu_k(K) + \mu(K))\varepsilon + |\mu_n(f_\varepsilon) - \mu(f_\varepsilon)|.\end{aligned}$$

Also,

$$
\begin{aligned}
|\mu_n(f_\varepsilon) - \mu(f_\varepsilon)| &\leq \iint_{\overline{\Omega}^2} |f_\varepsilon(x) - f_\varepsilon(y)| \mathrm{d}\pi_n(x,y) \quad \text{where } \pi_n \in \mathrm{Opt}(\mu_n, \mu) \\
&\leq L \iint_{(K\times\overline{\Omega})\cup(\overline{\Omega}\times K)} d(x,y)\mathrm{d}\pi_n(x,y) \\
&\leq L\pi_n((K\times\overline{\Omega})\cup(\overline{\Omega}\times K))^{1-\frac{1}{p}} \left(\iint_{(K\times\overline{\Omega})\cup(\overline{\Omega}\times K)} d(x,y)^p \mathrm{d}\pi_n(x,y) \right)^{\frac{1}{p}} \\
&\qquad \text{by Hölder's inequality.} \\
&\leq L \left(\sup_k \mu_k(K) + \mu(K) \right)^{1-\frac{1}{p}} \mathrm{FG}_p(\mu_n, \mu) \xrightarrow[n\to\infty]{} 0.
\end{aligned}
$$

Therefore, taking the limsup in n and then letting ε goes to 0, we obtain that $\mu_n(f) \to \mu(f)$. □

The following proof is already found in [LGL16]. We reproduce it here for the sake of completeness.

Proof of Lemma 6.5.6. Recall that P_n is a sequence in $\mathcal{P}_1^p(\mathcal{M}^p)$ such that each P_n has a p-Fréchet mean μ_n and that $W_{p,\mathrm{FG}_p}(P_n, P) \to 0$ for some $P \in \mathcal{P}_1^p(\mathcal{M}^p)$. According to the beginning of the proof of Proposition 6.5.5, the sequence $(\mu_n)_n$ is relatively compact for the vague convergence. Let $\nu \in \mathcal{M}^p$ and let μ be the vague limit of some subsequence, which, for ease of notations, will be denoted as the initial sequence. By Skorokhod's representation theorem [Bil13, Theorem 6.7], as P_n converges weakly to P, there exists a probabilistic space on which are defined random variables $\boldsymbol{\mu} \sim P$ and $\boldsymbol{\mu_n} \sim P_n$ for $n \geq 0$, such that $\boldsymbol{\mu_n}$ converges almost surely with respect to the FG_p metric towards $\boldsymbol{\mu}$. Using those random variables, we have

$$
\begin{aligned}
\mathcal{E}(\nu) &= \mathbb{E}\mathrm{FG}_p^p(\nu, \boldsymbol{\mu}) = W_{p,\mathrm{FG}_p}^p(\delta_\nu, P) \\
&= \lim_n W_{p,\mathrm{FG}_p}^p(\delta_\nu, P_n) \text{ since } W_{p,\mathrm{FG}_p}(P_n, P) \to 0 \\
&= \lim_n \mathbb{E}\mathrm{FG}_p^p(\nu, \boldsymbol{\mu_n}) \\
&\geq \lim_n \mathbb{E}\mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu_n}) \text{ since } \mu_n \text{ is a barycenter of } P_n \\
&\geq \mathbb{E} \liminf_n \mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu_n}) \text{ by Fatou's lemma} \\
&\geq \mathbb{E}\mathrm{FG}_p^p(\mu, \boldsymbol{\mu}) = \mathcal{E}(\mu) \text{ by lower semi-continuity of } \mathrm{FG}_p \text{ (Proposition 6.2.2).}
\end{aligned} \tag{6.19}
$$

This implies that μ is a barycenter of P. We are now going to show that, almost surely, $\liminf_n \mathrm{FG}_p(\mu_n, \boldsymbol{\mu}) = \mathrm{FG}_p(\mu, \boldsymbol{\mu})$. This concludes the proof by letting n_k be the subsequence attaining the liminf for some fixed realization of $\boldsymbol{\mu}$. By plugging in $\nu = \mu$ in (6.19), all the inequalities become equalities, and in particular,

$$
\lim_n W_{p,\mathrm{FG}_p}^p(\delta_{\mu_n}, P_n) = \lim_n \mathbb{E}\mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu_n}) = \mathbb{E}\mathrm{FG}_p^p(\mu, \boldsymbol{\mu}) = W_{p,\mathrm{FG}_p}^p(\delta_\mu, P).
$$

This yields

$$
\begin{aligned}
0 &\leq W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P) - W_{p,\mathrm{FG}_p}(\delta_\mu, P) \\
&\leq W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P_n) + W_{p,\mathrm{FG}_p}(P_n, P) - W_{p,\mathrm{FG}_p}(\delta_\mu, P) \to 0
\end{aligned}
$$

as n goes to $+\infty$, i.e. $\lim_n W_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P) = W_{p,\mathrm{FG}_p}(\delta_\mu, P)$. Therefore,

$$\begin{aligned}\mathbb{E}\mathrm{FG}_p^p(\mu, \boldsymbol{\mu}) &= W^p_{p,\mathrm{FG}_p}(\delta_\mu, P) = \lim_n W^p_{p,\mathrm{FG}_p}(\delta_{\mu_n}, P) = \lim_n \mathbb{E}\mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu}) \\ &\geq \mathbb{E}\liminf_n \mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu}) \text{ by Fatou's lemma} \\ &\geq \mathbb{E}\mathrm{FG}_p^p(\mu, \boldsymbol{\mu}) \text{ by lower semi-continuity of } \mathrm{FG}_p.\end{aligned}$$

As $\liminf_n \mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu}) \geq \mathrm{FG}_p^p(\mu, \boldsymbol{\mu})$ and $\mathbb{E}\liminf_n \mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu}) = \mathbb{E}\mathrm{FG}_p^p(\mu, \boldsymbol{\mu})$, we actually have $\liminf_n \mathrm{FG}_p^p(\mu_n, \boldsymbol{\mu}) = \mathrm{FG}_p^p(\mu, \boldsymbol{\mu})$ almost surely, concluding the proof. □

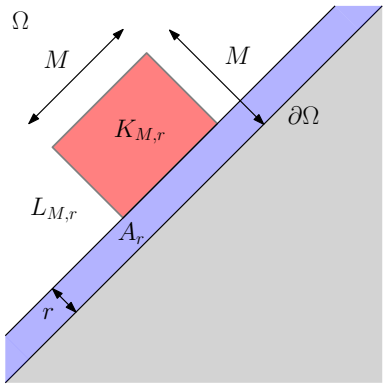


FIGURE 6.4: Partition of Ω used in the proof of Lemma 6.5.7.

We end this section by giving the proof of two technical lemmas of Section 6.5.

Proof of Lemma 6.5.7. For the direct implication, take $\nu = 0$ and apply Theorem 6.2.6.

Let us prove the converse implication. Assume that $\mu_n \xrightarrow{v} \mu$ and $\mathrm{FG}_p(\mu_n, \nu) \to \mathrm{FG}_p(\mu, \nu)$ for some $\nu \in \mathcal{D}^p$. The vague convergence of $(\mu_n)_n$ implies that $\mu^{(p)}$ is the only possible accumulation point for weak convergence of the sequence $(\mu_n^{(p)})_n$. Therefore, it is sufficient to show that the sequence $(\mu_n^{(p)})_n$ is relatively compact for weak convergence (i.e. tight and bounded in total variation, see Proposition 3.1.9). Indeed, this would mean that $(\mu_n^{(p)})$ converges weakly to $\mu^{(p)}$, or equivalently by Proposition 3.1.10 that $\mu_n \xrightarrow{v} \mu$ and $\mathrm{Pers}_p(\mu_n) \to \mathrm{Pers}_p(\mu)$. The conclusion is then obtained thanks to Theorem 6.2.6.

Thus, let $(\mu_n)_n$ be any subsequence and $(\pi_n)_n$ be corresponding optimal transport plans between μ_n and ν. The vague convergence of $(\mu_n)_n$ implies that $(\pi_n)_n$ is relatively compact with respect to the vague convergence on E_Ω. Let π be a limit of any converging subsequence of $(\pi_n)_n$, which indexes are still denoted by n. One can prove that $\pi \in \mathrm{Opt}(\mu, \nu)$ (see [FG10, Proposition 2.3]). For $r > 0$, recall that $\Omega_r = \{x \in \Omega : \ d(x, \partial\Omega) > r\}$ and define $A_r := \{x \in \Omega : \ d(x, \partial\Omega) \leq r\}$, so that $\Omega = \Omega_r \sqcup A_r$. Write also $\overline{A}_r$ for $A_r \cup \partial\Omega$. Consider $\eta > 1$. We can write

$$\begin{aligned}&\int_{A_r} d(x, \partial\Omega)^p \mathrm{d}\mu_n(x) = \iint_{A_r \times \overline{\Omega}} d(x, \partial\Omega)^p \mathrm{d}\pi_n(x, y) \\ &= \iint_{A_r \times \Omega_{\eta r}} d(x, \partial\Omega)^p \mathrm{d}\pi_n(x, y) + \iint_{\overline{A}_r \times \overline{A}_{\eta r}} d(x, \partial\Omega)^p \mathrm{d}\pi_n(x, y) \\ &\overset{(*)}{\leq} \frac{1}{(\eta - 1)^p} \iint_{A_r \times (\Omega_{\eta r})} d(x, y)^p \mathrm{d}\pi_n(x, y) + \iint_{\overline{A}_r \times \overline{A}_{\eta r}} d(x, \partial\Omega)^p \mathrm{d}\pi_n(x, y)\end{aligned}$$

$$\leq \frac{1}{(\eta-1)^p}\mathrm{FG}_p^p(\mu_n,\nu) + 2^{p-1}\left(\iint\limits_{\overline{A}_r\times\overline{A}_{\eta r}} d(x,y)^p \mathrm{d}\pi_n(x,y) + \iint\limits_{\overline{A}_r\times\overline{A}_{\eta r}} d(y,\partial\Omega)^p \mathrm{d}\pi_n(x,y)\right)$$

$$\leq \frac{1}{(\eta-1)^p}\mathrm{FG}_p^p(\mu_n,\nu) + 2^{p-1}\left(\mathrm{FG}_p^p(\mu_n,\nu) - \iint\limits_{E_\Omega\backslash(\overline{A}_r\times\overline{A}_{\eta r})} d(x,y)^p \mathrm{d}\pi_n(x,y) + \int_{A_{\eta r}} d(y,\partial\Omega)^p \mathrm{d}\nu(y)\right)$$

where $(*)$ holds because $d(x,y) \geq (\eta-1)r \geq (\eta-1)d(x,\partial\Omega)$ for $(x,y) \in A_r \times A_{\eta r}^c$. Therefore,

$$\limsup_{n\to\infty} \int_{A_r} d(x,\partial\Omega)^p \mathrm{d}\mu_n(x) \leq \frac{1}{(\eta-1)^p}\mathrm{FG}_p^p(\mu,\nu) + 2^{p-1}\Bigg(\mathrm{FG}_p^p(\mu,\nu) - \iint\limits_{E_\Omega\backslash(\overline{A}_r\times\overline{A}_{\eta r})} d(x,y)^p \mathrm{d}\pi(x,y) + \int_{A_{\eta r}} d(y,\partial\Omega)^p \mathrm{d}\nu(y)\Bigg)$$

Note that at the last line, we used the Portmanteau theorem (see Proposition 3.1.11) on the sequence of measures $(d(x,y)^p \mathrm{d}\pi_n(x,y))_n$ for the open set $E_\Omega\backslash(\overline{A}_r \times \overline{A}_{\eta r})$. Letting r goes to 0, then η goes to infinity, one obtains

$$\lim_{r\to 0}\limsup_{n\to\infty} \int_{A_r} d(x,\partial\Omega)^p \mathrm{d}\mu_n(x) = 0.$$

The second part consists in showing that there can not be mass escaping "at infinity" in the subsequence $(\mu_n^{(p)})_n$. Fix $r, M > 0$. For $x \in \Omega$, denote $s(x)$ the projection of x on $\partial\Omega$. Pose

$$K_{M,r} := \{x \in \Omega_r : \ d(x,\partial\Omega) < M, d(s(x),0) < M\}$$

and $L_{M,r}$ the closure of $\Omega\backslash(A_r \cup K_{M,r})$ (see Figure 6.4). For $r' > 0$,

$$\begin{aligned}
\int_{L_{M,r}} d(x,\partial\Omega)^p \mathrm{d}\mu_n(x) &= \iint\limits_{L_{M,r}\times\overline{\Omega}} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) \\
&= \iint\limits_{L_{M,r}\times(L_{M/2,r'}\cup\overline{A}_{r'})} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) + \iint\limits_{L_{M,r}\times K_{M/2,r'}} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) \\
&\leq 2^{p-1} \iint\limits_{L_{M,r}\times(L_{M/2,r'}\cup\overline{A}_{r'})} d(x,y)^p \mathrm{d}\pi_n(x,y) \\
&\quad + 2^{p-1} \iint\limits_{L_{M,r}\times(L_{M/2,r'}\cup\overline{A}_{r'})} d(\partial\Omega,y)^p \mathrm{d}\pi_n(x,y) \\
&\quad + \iint\limits_{L_{M,r}\times K_{M/2,r'}} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y).
\end{aligned}$$

We treat the three parts of the sum separately. As before, taking the lim sup in n and letting M goes to ∞, the first part of the sum converges to 0 (apply the Portmanteau theorem on the open set $E_\Omega\backslash(L_{M,r} \times (L_{M/2,r'} \cup \overline{A}_{r'}))$. The second part is less than or equal to

$$2^{p-1}\int_{L_{M/2,r'}\cup A_{r'}} d(y,\partial\Omega)^p \mathrm{d}\nu(y),$$

which converges to 0 as $M \to \infty$ and $r' \to 0$. For the third part, notice that if $(x,y) \in L_{M,r} \times K_{M/2,r'}$, then

$$d(x,\partial\Omega) \le d(x,s(y)) \le d(x,y) + d(y,s(y)) \le d(x,y) + \frac{M}{2} \le 2d(x,y).$$

Therefore,

$$\begin{aligned}\iint\limits_{L_{M,r}\times K_{M/2,r'}} d(x,\partial\Omega)^p \mathrm{d}\pi_n(x,y) &\le 2^p \iint\limits_{L_{M,r}\times K_{M/2,r'}} d(x,y)^p \mathrm{d}\pi_n(x,y)\\ &\le 2^p \iint\limits_{L_{M,r}\times \overline{\Omega}} d(x,y)^p \mathrm{d}\pi_n(x,y).\end{aligned}$$

As before, it is shown that $\limsup_n \iint_{L_{M,r}\times\overline{\Omega}} d(x,y)^p \mathrm{d}\pi_n(x,y)$ converges to 0 when M goes to infinity by applying the Portmanteau theorem on the open set $E_\Omega \backslash (L_{M,r} \times \overline{\Omega})$.

Finally, we have shown, that by taking r small enough and M large enough, one can find a compact set $\overline{K_{M,r}}$ such that $\int_{\Omega\backslash\overline{K_{M,r}}} d(x,\partial\Omega)^p \mathrm{d}\mu_n = \mu_n^{(p)}(\Omega\backslash\overline{K_{M,r}})$ is uniformly small: $(\mu_n^{(p)})_n$ is tight. As we have

$$\begin{aligned}\mu_n^{(p)}(\Omega) &= \mathrm{Pers}_p(\mu_n) = \mathrm{FG}_p^p(\mu_n, 0)\\ &\le (\mathrm{FG}_p(\mu_n,\nu) + \mathrm{FG}_p(\nu,0))^p \to (\mathrm{FG}_p(\mu,\nu) + \mathrm{FG}_p(\nu,0))^p,\end{aligned}$$

it is also bounded in total variation. Hence, $(\mu_n^{(p)})_n$ is relatively compact for the weak convergence: this concludes the proof. □

Proof of Lemma 6.5.9. Let $P = \sum_{i=1}^N \lambda_i \delta_{a_i}$ a probability distribution with $a_i \in \mathcal{D}_f$ of mass $m_i \in \mathbb{N}$, and define $m_{\mathrm{tot}} = \sum_{i=1}^N m_i$. By Proposition 6.5.4, every p-Fréchet mean a of P is in correspondence with a p-Fréchet mean for the Wasserstein distance $\tilde{a}$ of $\tilde{P} = \sum_{i=1}^N \lambda_i \delta_{\tilde{a}_i}$, where $\tilde{a}_i = a_i + (m_{\mathrm{tot}} - m_i)\delta_{\partial\Omega}$, with a being the restriction of $\tilde{a}$ to Ω.

Let thus fix $m \in \mathbb{N}$, and let $\tilde{a}_1, \dots, \tilde{a}_N$ be point measures of mass m in $\tilde{\Omega}$. Write $\tilde{a}_i = \sum_{j=1}^m \delta_{x_{i,j}}$, so that $x_{i,j} \in \tilde{\Omega}$ for $1 \le i \le N$, $1 \le j \le m$, with the $x_{i,j}$s non-necessarily distinct. Define

$$T : (x_1, \dots, x_N) \in \tilde{\Omega}^N \mapsto \arg\min \left\{ \sum_{i=1}^N \lambda_i \rho(x_i, y)^p : \ y \in \tilde{\Omega} \right\} \in \tilde{\Omega}. \tag{6.20}$$

Since we assume $p > 1$, T is well-defined and is continuous, while in the general case the existence of a measurable minimizer follows from standard arguments [CR03]. Using the localization property stated in [COO15a, Section 2.2], we know that the support of a p-Fréchet mean of $\tilde{P}$ is included in the finite set

$$S := \{T(x_{1,j_1}, \dots, x_{N,j_N}) : \ 1 \le j_1, \dots, j_N \le m\}.$$

Let $K = m^N$ and let $z_1, \dots, z_K$ be an enumeration of the points of S (with potential repetitions). Denote by $\mathrm{Gr}(z_k)$ the N elements $x_1, \dots, x_N$, with $x_i \in \mathrm{spt}(\tilde{a}_i)$, such that $z_k = T(x_1, \dots, x_N)$. It is explained in [COO15a, Section 2.3], that finding a p-Fréchet mean of $\tilde{P}$ is equivalent to finding a minimizer of the problem

$$\inf_{(\gamma_1,\dots,\gamma_N)\in\Pi} \sum_{i=1}^N \lambda_i \iint_{\tilde{\Omega}^2} \rho(x_i, y)^p \mathrm{d}\gamma_i(x_i, y), \tag{6.21}$$

where Π is the set of plans $(\gamma_i)_{i=1,\dots,N}$, with γ_i having for first marginal $\tilde{a}_i$, and such that all γ_is share the same (non-fixed) second marginal. Furthermore, we can assume without loss of generality that $(\gamma_1 \dots \gamma_N)$ is supported on $(\mathrm{Gr}(z_k), z_k)_k$, i.e. a point z_k in the p-Fréchet mean is necessary transported to its corresponding grouping $\mathrm{Gr}(z_k)$ by (optimal) $\gamma_1, \dots \gamma_N$ [COO15a, Section 2.3]. For such a minimizer, the common second marginal is a p-Fréchet mean of $\tilde{P}$.

A potential minimizer of (6.21) is described by a vector $\gamma = (\gamma_{i,j,k}) \in \mathbb{R}_+^{NmK}$ such that:

$$\begin{cases} \text{for } 1 \le i \le N,\ 1 \le j \le m, & \sum_{k=1}^{K} \gamma_{i,j,k} = 1 \text{ and} \\ \text{for } 2 \le i \le N,\ 1 \le k \le K, & \sum_{j=1}^{m} \gamma_{1,j,k} = \sum_{j=1}^{m} \gamma_{i,j,k}. \end{cases} \tag{6.22}$$

Let $c \in \mathbb{R}^{NmK}$ be the vector defined by $c_{i,j,k} = \mathbf{1}\{x_{i,j} \in \mathrm{Gr}(z_k)\}\lambda_i \rho(x_{i,j}, z_k)^p$. Then, the problem (6.21) is equivalent to

$$\underset{\gamma \in \mathbb{R}_+^{NmK}}{\text{minimize}}\, \gamma^T c \quad \text{under the constraints (6.22).} \tag{6.23}$$

The set of p-Fréchet means of P are in bijection with the set of minimizers of this Linear Programming problem (see [Sch03, Section 5.15]), which is given by a face of the polyhedron described by the equations (6.22). Hence, if we show that this polyhedron is integer (i.e. its vertices have integer values), then it would imply that the extreme points of the set of p-Fréchet means of P are point measures, concluding the proof. The constraints (6.22) are described by a matrix A of size $(Nm + (N-1)K) \times NmK$ and a vector $b = [\mathbf{1}_{Nm}, \mathbf{0}_{(N-1)K}]$, such that $\gamma \in \mathbb{R}^{NmK}$ satisfies (6.22) if and only if $A\gamma = b$. A sufficient condition for the polyhedron $\{Ax \le b\}$ to be integer is to satisfy the following property (see [Sch03, Section 5.17]): for all $u \in \mathbb{Z}^{NmK}$, the dual problem

$$\max\{y^T b,\ y \ge 0 \text{ and } y^T A = u\} \tag{6.24}$$

has either no solution (i.e. there is no $y \ge 0$ satisfying $y^T A = u$), or it has an integer optimal solution y.

For y satisfying $y^T A = u$, write $y = [y^0, y^1]$ with $y^0 \in \mathbb{R}^{Nm}$ and $y^1 \in \mathbb{R}^{(N-1)K}$, so that y^0 is indexed on $1 \le i \le N,\ 1 \le j \le m$ and y^1 is indexed on $2 \le i \le N,\ 1 \le k \le K$. One can check that, for $2 \le i \le N,\ 1 \le j \le m,\ 1 \le k \le K$:

$$u_{1,j,k} = y^0_{1,j} + \sum_{i'=2}^{N} y^1_{i',k} \quad \text{and} \quad u_{i,j,k} = y^0_{i,j} - y^1_{i,k}, \tag{6.25}$$

so that,

$$\begin{aligned} y^T b &= \sum_{i=1}^{N}\sum_{j=1}^{m} y^0_{i,j} = \sum_{j=1}^{m} y^0_{1,j} + \sum_{i=2}^{N}\sum_{j=1}^{m} y^0_{i,j} \\ &= \sum_{j=1}^{m}(u_{1,j,k} - \sum_{i=2}^{N} y^1_{i,k}) + \sum_{i=2}^{N}\sum_{j=1}^{m}(u_{i,j,k} + y^1_{i,k}) \\ &= \sum_{i=1}^{N}\sum_{j=1}^{m} u_{i,j,k}. \end{aligned}$$

Therefore, the function $y^T b$ is constant on the set $P := \{y \ge 0,\ y^T A = u\}$, and any point of the set is an argmax. We need to check that if the set P is non-empty, then it contains a vector with integer coordinates: this would conclude the proof. A solution of the homogeneous equation $y^T A = 0$ satisfies $y^0_{i,j} = y^1_{i,k} = \lambda_i$ for $i \ge 2$ and

$y^0_{1,j} = -\sum_{i=2}^N y^1_{i,k} = -\sum_{i=2}^N \lambda_i$ and reciprocally, any choice of $\lambda_i \in \mathbb{R}$ gives rise to a solution of the homogeneous equation. For a given u, one can verify that the set of solutions of $y^T A = u$ is given, for $\lambda_i \in \mathbb{R}$, by

$$\begin{cases} y^0_{1,j} = \sum_{i=1}^N u_{i,j,k} - \sum_{i=2}^N \lambda_i \\ y^0_{i,j} = \lambda_i \text{ for } i \geq 2, \\ y^1_{i,k} = -u_{i,j,k} + \lambda_i \text{ for } i \geq 2. \end{cases}$$

Such a solution exists if and only if for all j, $U_j := \sum_{i=1}^N u_{i,j,k}$ does not depend on k and for $i \geq 2$, $U_{i,k} := u_{i,j,k}$ does not depend on j. For such a vector u, P corresponds to the $\lambda_i \geq 0$ with $\lambda_i \geq \max_k U_{i,k}$ and $U_j \geq \sum_{i=1}^N \lambda_i$. If this set is non empty, it contains as least the point corresponding to $\lambda_i = \max\{0, \max_k U_{i,k}\}$, which is an integer: this point is integer valued, concluding the proof. $\square$

Chapter 7

On the choice of weight functions for linear representations of persistence diagrams

A wide class of representations of persistence diagrams, including the persistence surface [Ada+17] (variants of this object have been also introduced [Che+15; KHF16; Rei+15]), the accumulated persistence function [BM19] or the persistence silhouette [Cha+15a] are conveniently expressed as a linear expression of the points of the diagram.

Definition 7.0.1 (Linear representations)**.** *Let $f : \Omega \to B$ be a map, where B is some Banach space. The map $\Psi_f : \mathcal{D}^p \to B$ defined by $\Psi_f(a) = a(f) = \sum_{u \in a} f(u)$ is called the* linear representation *associated with f.*

In this chapter, we explore the behavior of linear representations in two different ways. First, in Section 7.1, using the characterization of convergence with respect to the Figalli-Gigli metric FG_p given in Chapter 6, we give a description of all continuous linear representations. In particular, we highlight the importance of weighting the representation by the distance to the diagonal to the power p: the representations of the form $\Psi_{d(\cdot,\partial\Omega)^p \cdot f}$ with f continuous bounded are the only continuous ones with respect to FG_p. In applications, Lipschitz continuity is often more desirable than continuity. For $p = 1$, we therefore show a general stability result for linear representations, which is based on a version of the Kantorovitch-Rubinstein duality formula for persistence diagrams. Although obtaining a stability result for $p > 1$ is somewhat less straightforward, we also give an inequality for bounding the distance between linear representations by the FG_p distance for general p. In this case, the importance of weighting the underlying map f by the distance to the diagonal is once again shown.

Our second approach consists in taking an asymptotic point of view, by studying the behavior of Čech and Rips persistence diagrams built on top of large random point clouds. Assume for instance that a point cloud $\mathcal{X}$ is located on some Riemannian manifold M. Under this assumption, the Čech persistence diagram $a = \mathrm{dgm}_q^C(\mathcal{X})$ of the data set is made of two different types of points: points a_{true} far away from the diagonal, which estimate the diagram of the manifold M, and points a_{noise} close to the diagonal, which are generally considered to be "topological noise" (see Figure 7.1). This interpretation is a consequence of the stability theorem for persistence diagrams; see Chapter 3. If the relevant information lies in the structure of the manifold, then the topological noise indeed represents true noise, and linear representations of the form $\Psi_f(a)$ are bound to fail if $\Psi_f(a_{\text{noise}})$ is dominating $\Psi_f(a_{\text{true}})$. Once again, we showcase the advantage of using a weight function $w : \Omega \to \mathbb{R}$. If w is chosen properly, i.e. small enough when close to the diagonal, then one can hope that $\Psi_{wf}(a_{\text{true}})$ can be

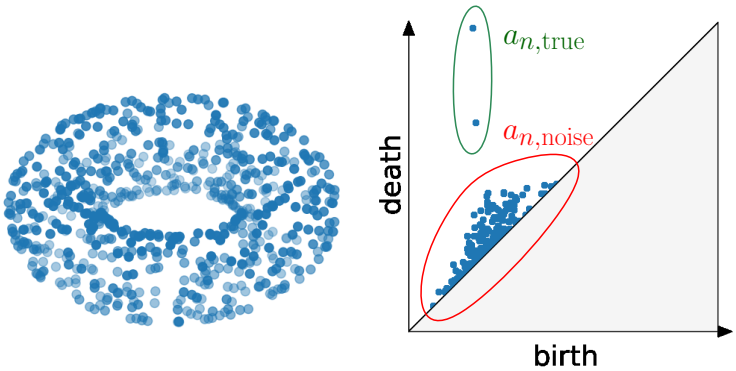


FIGURE 7.1: The persistence diagram for homology of degree 1 of the Rips filtration of $n = 700$ i.i.d. points uniformly sampled on a torus.

separated from $\Psi_{wf}(a_{\text{noise}})$. We address this question from an asymptotic perspective: for which weight functions does $\Psi_{wf}(a_{\text{noise}})$ converge to 0?

Of course, for this question to make sense, a model for the dataset has to be specified. A simple model is given by a Poisson (or binomial) process $\mathcal{X}_n$ of intensity n in a cube of dimension d. We then denote by $\text{dgm}_q^K(\mathcal{X}_n)$ the persistence diagram of $\mathcal{X}_n$ built with either the Čech ($K = C$) or the Rips ($K = R$) filtration for q-dimensional homology. In this setting, there are no "true" topological features (other than the trivial topological feature of $[0,1]^d$ being connected), and thus the diagram based on the sampled data is uniquely made of topological noise. A first promising result is the vague convergence of the persistence measure $\mu_q^n := n^{-1}\text{dgm}_q^K(n^{1/d}\mathcal{X}_n)$, which was proven in [HST18] for homogeneous Poisson processes in the cube and in [GTT19] for binomial processes on manifolds. However, vague convergence is not enough for our purpose, as neither f nor w have good reasons to have compact support. Our main result, Theorem 7.2.4 extends results of [GTT19], for processes on the cube, to a stronger convergence, allowing test functions to have both non-compact support (but to converge to 0 near the diagonal) and to have polynomial growth. As a corollary of this general result, the convergence of the p-th total persistence is shown, as well as convergence of μ_q^n for the Figalli-Gigli metric.

Theorem 7.0.2. *Let $p \geq 0$ and let κ be a density on $[0,1]^d$ such that $0 < \inf \kappa \leq \sup \kappa < \infty$. Let $\mathcal{X}_n$ be either a binomial process with parameters n and κ or a Poisson process of intensity $n\kappa$ in the cube $[0,1]^d$. Then, with probability one, as $n \to \infty$*

$$n^{\frac{\alpha}{d}-1}\text{Pers}_p(\text{dgm}_q^K(\mathcal{X}_n)) \to \mu_q^\kappa(\text{pers}^p) < \infty \tag{7.1}$$

for some non-zero persistence measure μ_q^κ.

Furthermore, if $\mu_q^n := n^{-1}\text{dgm}_K(n^{1/d}\mathcal{X}_n)$ and $p \geq 1$, we have

$$\text{FG}_p(\mu_q^n, \mu_q^\kappa) \to 0. \tag{7.2}$$

Remark that (7.2) is a consequence of (7.1) and of the vague convergence of μ_q^n proven in [HST18], by using the characterization of convergence for the Figalli-Gigli metric (Theorem 6.2.6). If $a_n := \text{dgm}_q^K(\mathcal{X}_n')$ is built on a point cloud $\mathcal{X}_n'$ of size n on a d-dimensional manifold, one can expect $a_{n,\text{noise}}$ to behave similarly to that of $\text{dgm}_q^K(\mathcal{X}_n)$ for $\mathcal{X}_n$ a n-sample on a d-dimensional cube (a manifold looking locally like a cube). Therefore, for $p > 0$, the quantity $\text{Pers}_p(a_{n,\text{noise}})$ should be close to $\text{Pers}_p(\text{dgm}_q^K(\mathcal{X}_n))$, and it can be expected to converge to 0 if and only if the weight function pers^p is such that $p > d$. As such, we obtain the following heuristic: *a weight*

function of the form pers^p *with* $p > d$ *is sensible if the data lies near a* d*-dimensional object.*

Further properties of the process $(\mathrm{dgm}_q^K(\mathcal{X}_n))_n$ are also shown, namely non-asymptotic rates of decays for the number of points in said diagrams, and the absolute continuity of the marginals of μ_q^κ with respect to the Lebesgue measure on $\mathbb{R}$.

Related work Techniques used to derive the large sample results indicated above are closely related to the field of geometric probability, which is the study of geometric quantities arising naturally from point processes in $\mathbb{R}^d$. A classical result in this field, see [Ste88], proves the convergence of the total length of the minimum spanning tree built on n i.i.d. points in the cube. This pioneering work can be seen as a 0-dimensional special case of our general results about persistence diagrams built for homology of dimension q. This type of result has been extended to a large class of functionals in the works of J. E. Yukich and M. Penrose (see for instance [MY99; Yuk00; PY03] and [Pen03] or [Yuk06] for monographs on the subject).

The study of higher dimensional properties of such processes is much more recent. Known results include convergence of Betti numbers for various models and under various asymptotics (see [Kah11; KM13; YSA17; BO17]). The paper [BKS17] finds bounds on the persistence of cycles in random complexes, and [HST18] proves limit theorems for persistence diagrams built on homogeneous point processes. The latter is extended to non-homogeneous processes in [Tri17], and to processes on manifolds in [GTT19]. Note that our results constitute a natural extension of [Tri17]. In [STY17], higher dimensional analogs of minimum spanning trees, called minimal spanning acycles, were introduced. Minimal spanning acycles exhibits strong links with persistence diagrams and our main theorem can be seen as a convergence result for weighted minimal spanning acycle on geometric random complexes. [STY17] also proves the convergence of the total 1-persistence for Linial-Meshulam random complexes, which are models of random simplicial complexes of a combinatorial nature rather than a geometric nature.

7.1 Continuity and stability of linear representations

As mentioned in the introduction, a *linear representation* of persistence measures (in particular persistence diagrams) is a mapping $\Phi_f : \mathcal{M}^p \to B$ for some Banach space B of the form $\mu \mapsto \mu(f)$, where $f : \Omega \to B$ is some chosen function. Using such a representation, one can turn a sample of diagrams into a sample of vectors, making the use of machine learning tools easier. Of course, a minimal expectation is that Φ_f should be continuous. In practice, building a linear representation generally follows the same pattern: first consider a "nice" function g, e.g. a gaussian distribution, then introduce a weight with respect to the distance to the diagonal $d(\cdot, \partial\Omega)^p$, and prove that $\mu \mapsto \mu(g(\cdot)d(\cdot, \partial\Omega)^p)$ has some regularity properties (continuity, stability, etc.). Applying Theorem 6.2.6, we show that this approach always gives a continuous linear representation, and that it is the only way to do so.

For B a Banach space (typically $\mathbb{R}^d$), define the class of functions:

$$\mathcal{C}^0_{b,p} = \left\{ f : \Omega \to B : \ f \text{ is continuous and } x \mapsto \frac{f(x)}{d(x, \partial\Omega)^p} \text{ is bounded} \right\}. \tag{7.3}$$

Proposition 7.1.1. *Let* B *be a Banach space and* $f : \Omega \to B$ *a function. The linear representation* $\Psi_f : \mathcal{M}^p \to B$ *is continuous with respect to* FG_p *if and only if* $f \in \mathcal{C}^0_{b,p}$.

Proof. Consider first the case $B = \mathbb{R}$. Let $f \in \mathcal{C}^0_{b,p}$ and $\mu, \mu_1, \mu_2 \cdots \in \mathcal{M}^p$ be such that $\mathrm{FG}_p(\mu_n, \mu) \to 0$. Recall the definition (6.10) of $\mu^{(p)}$. Using Corollary 6.2.9, having $\mathrm{FG}_p(\mu_n, \mu) \to 0$ means that $\mu_n^{(p)} \xrightarrow{w} \mu^{(p)}$, and thus that

$$\int_\Omega \frac{f(x)}{d(x, \partial\Omega)^p} \mathrm{d}\mu_n^{(p)}(x) \to \int_\Omega \frac{f(x)}{d(x, \partial\Omega)^p} \mathrm{d}\mu^{(p)}(x),$$

that is

$$\Psi_f(\mu_n) = \int_\Omega f(x) \mathrm{d}\mu_n(x) \to \int_\Omega f(x) \mathrm{d}\mu(x) = \Psi_f(\mu),$$

i.e. Ψ_f is continuous with respect to FG_p.

Now, let B be any Banach space. [Nie11, Theorem 2] states that if a sequence of measures $(\mu_n)_n$ weakly converges to μ, then $\mu_n(f) \to \mu(f)$ for any continuous bounded function $g : \Omega \to B$. Applying this result to the sequence $(\mu_n^{(p)}$ with $g = f/d(\cdot, \partial\Omega)^p$ yields the desired result.

Conversely, let $f : \Omega \to B$. Assume first that f is not continuous in some $x \in \Omega$. There exist a sequence $(x_n)_n \in \Omega^{\mathbb{N}}$ such that $x_n \to x$ but $f(x_n) \nrightarrow f(x)$. Let $\mu_n = \delta_{x_n}$ and $\mu = \delta_x$. We have $\mathrm{FG}_p(\mu_n, \mu) \to 0$, but $\mu_n(f) = f(x_n) \nrightarrow f(x_0) = \mu(f)$, so that the linear representation $\mu \mapsto \mu(f)$ cannot be continuous.
Then, assume that f is continuous but that $x \mapsto \frac{f(x)}{d(x,\partial\Omega)^p}$ is not bounded. Let thus $(x_n)_n \in \Omega^{\mathbb{N}}$ be a sequence such that $\left\| \frac{f(x_n)}{d(x_n,\partial\Omega)^p} \right\| \to +\infty$. Define the measure $\mu_n := \frac{1}{\|f(x_n)\|} \delta_{x_n}$. Observe that $\mathrm{FG}_p(\mu_n, 0) = \frac{d(x_n,\partial\Omega)^p}{\|f(x_n)\|} \to 0$ by hypothesis. However, $\|\mu_n(f)\| = 1$ for all n, allowing us to conclude once again that $\mu \mapsto \mu(f)$ cannot be continuous. □

Examples of such linear representations commonly used in applications of TDA include for instance the persistence surface, persistence silhouettes and (weighted) Betti curves, all introduced in Section 3.9.

Stability in the case $p = 1$. Continuity is a basic expectation when embedding a set of diagrams in some Banach space B. One could however ask for more, e.g. some Lipschitz regularity: given a representation $\Psi : \mathcal{M}^p \to B$, one may want to have $\|\Psi(\mu) - \Psi(\nu)\| \leq C \cdot \mathrm{FG}_p(\mu, \nu)$ for some constant C. This property is generally referred to as "stability" in the TDA community and is generally obtained with $p = 1$, see for example [Ada+17, Theorem 5], [CCO17, Theorem 3.3 & 3.4], [Som+18, Section4], [Rei+15, Theorem 2], etc.

Here, we still consider the case of linear representations, and show that stability always holds with respect to the distance FG_1. Informally, this is explained by the fact that when $p = 1$, the cost function $(x, y) \mapsto d(x, y)^p$ is actually a distance.

Proposition 7.1.2. *Define $\mathcal{L}$ the set of Lipschitz continuous functions $f : \overline{\Omega} \to \mathbb{R}$ with Lipschitz constant less than or equal to 1 and that satisfy $f(\partial\Omega) = 0$. Let T be any set, and consider a family $(f_t)_{t\in T}$ with $f_t \in \mathcal{L}$. Then the linear representation $\Psi : \mu \mapsto (\mu(f_t))_{t\in T}$ is 1-Lipschitz continuous in the following sense:*

$$\|\Psi(\mu) - \Psi(\nu)\|_\infty := \sup_{t\in T} |(\mu - \nu)(f_t)| \leq \mathrm{FG}_1(\mu, \nu), \tag{7.4}$$

for any measures $\mu, \nu \in \mathcal{M}^1$.

Proof. Consider $\mu, \nu \in \mathcal{M}^1$, and $\pi \in \mathrm{Opt}(\mu, \nu)$ an optimal transport plan. Let $t \in T$. We have:

$$\begin{aligned}(\mu - \nu)(f_t) &= \int_\Omega f_t(x)\mathrm{d}\mu(x) - \int_\Omega f_t(y)\mathrm{d}\nu(y) = \iint_{\overline{\Omega}\times\overline{\Omega}} (f_t(x) - f_t(y))\mathrm{d}\pi(x,y) \\ &\leq \iint_{\overline{\Omega}\times\overline{\Omega}} d(x,y)\mathrm{d}\pi(x,y) = \mathrm{FG}_1(\mu,\nu),\end{aligned}$$

and thus, $\|\Psi(\mu) - \Psi(\nu)\|_\infty \leq \mathrm{FG}_1(\mu,\nu)$. □

In particular, if $f : \overline{\Omega} \to B$, where B is some Banach space, is 1-Lipschitz with $f(\partial\Omega) = 0$, then one can let $T = B_1^*$ (the unit ball of the dual of B) and $f_t(x) := t(f(x))$ for $t \in T$. We then obtain that $\|\Psi_f(\mu) - \Psi_f(\nu)\| \leq \mathrm{FG}_1(\mu,\nu)$, i.e. that $\Psi_f : (\mathcal{M}^1, \mathrm{FG}_1) \to (B, \|\cdot\|)$ is 1-Lipschitz.

Remark 7.1.3. One actually has a converse of such an inequality, i.e. it can be shown that

$$\mathrm{FG}_1(\mu,\nu) = \max\{(\mu-\nu)(f) : \ f \in \mathcal{L}\}. \tag{7.5}$$

This equation is an adapted version of the well-known Kantorovich-Rubinstein formula, which is itself a particular version in the case $p = 1$ of the duality formula in optimal transport, see for example [Vil08, Theorem 5.10] and [San15, Theorem 1.39]. A proof of (7.5) would require to introduce several optimal transport notions. The interested reader can consult Proposition 2.3 in [FG10] for details.

Stability for general weight functions Instead of weighting a representation by the distance to the diagonal $d(\cdot, \partial\Omega)^p$ for some $p \geq 1$, one could use other schemes. For instance, in [KFH17, Corollary 12], representations of diagrams are shown to be Lipschitz with respect to the FG_1 distance for weight functions of the form $w : u \in \Omega = \arctan(B \cdot \mathrm{pers}(u)^\alpha)$ with $\alpha > m+1, B > 0$, provided the diagrams are built with the sublevels of functions defined on a space $\mathcal{X}$ having bounded m-th total persistence. The stability result is proved for a particular function $f : \Omega \to B$ defined by $u \in \Omega \mapsto f(u) = K(u, \cdot)$, with K a bounded Lipschitz kernel and B the associated RKHS (short for Reproducing Kernel Hilbert Space, see [Aro50] for a monograph on the subject). We present a generalization of the stability result to (i) general weight functions w, (ii) any bounded Lipschitz function f, and (iii) we only require $\alpha > m$.

Consider weight functions $w : \Omega \to \mathbb{R}_+$ of the form $w(u) = \tilde{w}(\mathrm{pers}(u))$ for $u \in \Omega$, for a differentiable function $\tilde{w} : \mathbb{R}_+ \to \mathbb{R}_+$ satisfying $\tilde{w}(0) = 0$, and, for some $A > 0$, $\alpha \geq 1$,

$$\forall r \geq 0, \ |\tilde{w}'(r)| \leq A r^{\alpha-1}. \tag{7.6}$$

Examples of such functions include $w : u \mapsto \arctan(B \cdot \mathrm{pers}(u)^\alpha)$ for $B > 0$ and $w : u \mapsto \mathrm{pers}(u)^\alpha$. We denote the class of such weight functions by $\mathbb{W}(\alpha, A)$. In contrast to [KFH17], the function f does not necessarily take its values in a RKHS, but simply in a Banach space. Given $R > 0$, we let $\mathcal{D}_R^p$ be the set of persistence diagrams a with $\mathrm{Pers}_p(a) \leq R$ (i.e. $\mathcal{D}_R^p$ is the ball of radius R^p centered at 0 in $\mathcal{D}^p$).

Theorem 7.1.4. *Let $(B, \|\cdot\|)$ be a Banach space, let $f : \Omega \to B$ be a Lipschitz continuous function and let $w \in \mathbb{W}(\alpha, A)$ with $A > 0$, $\alpha \geq 1$. Fix $t \in [0,1]$ and let $p_1 = p\frac{\alpha}{p-1}$ and $p_2 = p\frac{\alpha-t}{p-t}$. Given $R_1, R_2 > 0$ and two diagrams a and b in $\mathcal{D}^p \cap \mathcal{D}_{R_1}^{p_1} \cap \mathcal{D}_{R_2}^{p_2}$, we have*

$$\|\Psi_{wf}(a) - \Psi_{wf}(b)\| \leq \mathrm{Lip}(f)\frac{A}{\alpha}R_1^{1-\frac{1}{p}}\mathrm{FG}_p(a,b) + \|f\|_\infty A\,(2R_2)^{1-\frac{t}{p}}\,\mathrm{FG}_p(a,b)^t. \tag{7.7}$$

Proof. We only treat the case $p < \infty$, the proof being easily adapted to the case $p = \infty$.

Fix two persistence diagrams a and b. Denote $\mu = w \cdot a$ (resp. $\nu = w \cdot b$) the measure having density w with respect to a (resp. b). Fix $\varepsilon > 0$ and let γ be a matching between a and b such that the cost of the matching is smaller than $\mathrm{FG}_p(a, b) + \varepsilon$. Define

$$\tilde{\mu} = \sum_{u \in a \cup \partial\Omega} w(\gamma(u))\delta_u.$$

Note that as the cost of γ is finite, there is a finite numbers on points $u \in \partial\Omega$ with $\gamma(u) \neq u$, so that $w(\gamma(u)) \neq 0$ only for a finite number of elements in the definition of $\tilde{\mu}$. Remark also that $\tilde{\mu}$ is of finite mass, with $|\tilde{\mu}| = |\nu|$. We have

$$\begin{aligned} \|\Psi_{wf}(a) - \Psi_{wf}(b)\| = \|\mu(f) - \nu(f)\| &\leq \|\mu(f) - \tilde{\mu}(f)\| + \|\tilde{\mu}(f) - \nu(f)\| \\ &\leq \|f\|_\infty |\mu - \tilde{\mu}| + \mathrm{Lip}(f) W_1(\tilde{\mu}, \nu). \end{aligned} \tag{7.8}$$

We bound the two terms in the sum separately. Let us first bound $W_1(\tilde{\mu}, \nu)$. Consider an optimal transport plan between $\tilde{\mu}$ and ν, which is built by mapping every point $u \in a \cup \partial\Omega$ towards $\gamma(u) \in b \cup \partial\Omega$. We have

$$W_1(\tilde{\mu}, \nu) \leq \sum_{u \in a \cup \partial\Omega} w(\gamma(u))|u - \gamma(u)|.$$

Let p' be the conjugate exponent of p, defined by $\frac{1}{p} + \frac{1}{p'} = 1$. As condition (7.6) implies that $|w(u)| \leq \frac{A}{\alpha}\mathrm{pers}(u)^\alpha$, the distance $W_1(\tilde{\mu}, \nu)$ is bounded by

$$\begin{aligned} \sum_{u \in a \cup \partial\Omega} w(\gamma(u))|u - \gamma(u)| &\leq \left(\sum_{u \in a \cup \partial\Omega} w(\gamma(u))^{p'} \right)^{1/p'} \left(\sum_{u \in a \cup \partial\Omega} |u - \gamma(u)|^p \right)^{1/p} \\ &\leq \frac{A}{\alpha} \left(\sum_{u \in a \cup \partial\Omega} \mathrm{pers}(\gamma(r))^{p'\alpha} \right)^{1/p'} \mathrm{FG}_p(a, b) \\ &\leq \frac{A}{\alpha} R_1^{1/p'} \mathrm{FG}_p(a, b), \end{aligned} \tag{7.9}$$

where R_1 is a bound on $\mathrm{Pers}_{\alpha p'}(b)$. We now treat the first part of the sum in (7.8). For u_1, u_2, in Ω with $\mathrm{pers}(u_1) \leq \mathrm{pers}(u_2)$, define the path with unit speed $h : [\mathrm{pers}(u_1), \mathrm{pers}(u_2)] \to \Omega$ by

$$h(t) = u_2 \frac{t - \mathrm{pers}(u_1)}{\mathrm{pers}(u_2) - \mathrm{pers}(u_1)} + u_1 \frac{\mathrm{pers}(u_2) - t}{\mathrm{pers}(u_2) - \mathrm{pers}(u_1)},$$

so that it satisfies $\mathrm{pers}(h(t)) = t$. The quantity $|w(u_1) - w(u_2)|$ is bounded by

$$\begin{aligned} \int_{\mathrm{pers}(u_1)}^{\mathrm{pers}(u_2)} |\nabla w(h(t)).h'(t)| dt &\leq \int_{\mathrm{pers}(u_1)}^{\mathrm{pers}(u_2)} A \ \mathrm{pers}(h(t))^{\alpha - 1} dt \\ &\leq \int_{\mathrm{pers}(u_1)}^{\mathrm{pers}(u_2)} A \ t^{\alpha - 1} dt \\ &= \frac{A}{\alpha} (\mathrm{pers}(u_2)^\alpha - \mathrm{pers}(u_1)^\alpha). \end{aligned}$$

For $0 < y < x$ and $0 \leq a \leq 1$, using the convexity of $t \mapsto t^\alpha$, it is easy to see that $x^\alpha - y^\alpha \leq \alpha(x - y)^a x^{\alpha - a}$. Define $q = \frac{p}{a}$, $q' = \frac{q'}{q' - 1}$ and $M(u) := \max(\mathrm{pers}(u), \mathrm{pers}(\gamma(u)))$.

We have,

$$\begin{aligned}
|\mu - \tilde{\mu}| &= \sum_{u \in a \cup \partial\Omega} |w(u) - w(\gamma(u))| \\
&\leq A \sum_{u \in a \cup \partial\Omega} |\mathrm{pers}(u) - \mathrm{pers}(\gamma(u))|^t M(u)^{\alpha - t} \\
&\leq A \left(\sum_{u \in a \cup \partial\Omega} |\mathrm{pers}(u) - \mathrm{pers}(\gamma(u))|^{tq} \right)^{1/q} \left(\sum_{u \in a \cup \partial\Omega} M(u)^{q'(\alpha - t)} \right)^{1/q'} \\
&\leq A \mathrm{FG}_{tq}(a,b)^a \left(\sum_{u \in a \cup \partial\Omega} \left(\mathrm{pers}(u)^{q'(\alpha-t)} + \mathrm{pers}(\gamma(u))^{q'(\alpha-t)} \right) \right)^{1/q'} \\
&\leq A \mathrm{FG}_{tq}(a,b)^t 2^{1/q'} R_2^{1/q'}, \qquad (7.10)
\end{aligned}$$

where R_2 is a bound on $\mathrm{Pers}_{q'(\alpha-t)}(a)$ and $\mathrm{Pers}_{q'(\alpha-t)}(b)$. Combining equations (7.8), (7.9) and (7.10) concludes the proof. □

The total persistence $\mathrm{Pers}_q(a)$ of a diagram a can often be controlled. This is for instance the case if the diagrams are built with Lipschitz continuous functions $\phi : \mathcal{X} \to \mathbb{R}$, and $\mathcal{X}$ is a space having bounded m-th total persistence (see Chapter 3). In that case, we are able to give a simpler stability result than Theorem 7.1.4.

Corollary 7.1.5. *Let $q \geq 0$ an integer, $A > 0$, $\alpha \geq 1$ and consider a space $\mathcal{X}$ having bounded m-th total persistence for some $m \geq 1$ and constant $C_{\mathcal{X},m}$. Suppose that $\phi_1, \phi_2 : \mathcal{X} \to \mathbb{R}$ are two tame Lipschitz continuous functions, $w \in \mathbb{W}(\alpha, A)$, and $t \in [0,1]$. Let $m \leq p \leq \infty$ be such that $\alpha \geq m + t\left(1 - \frac{m}{p}\right) \geq 0$. Let $C_0 = C_{\mathcal{X},m} \max\{\mathrm{Lip}(\phi_1)^m, \mathrm{Lip}(\phi_2)^m\}$ and ℓ be the maximum persistence in the two diagrams $\mathrm{dgm}_q(\phi_1), \mathrm{dgm}_q(\phi_2)$. Then, we have*

$$\begin{aligned}
\|\Psi_{wf}(\mathrm{dgm}_q(\phi_1)) - \Psi_{wf}(\mathrm{dgm}_q(\phi_2))\| \leq C_1 \mathrm{FG}_p(\mathrm{dgm}_q(\phi_1), \mathrm{dgm}_q(\phi_2)) \\
+ C_2 \mathrm{FG}_p(\mathrm{dgm}_q(\phi_1), \mathrm{dgm}_q(\phi_2))^t, \qquad (7.11)
\end{aligned}$$

where $C_1 = \mathrm{Lip}(f)\frac{A}{\alpha}\ell^{\alpha - m\left(1-\frac{1}{p}\right)} C_0^{1-\frac{1}{p}}$ and $C_2 = \|f\|_\infty A \ell^{\alpha - m - t\left(1-\frac{m}{p}\right)} (2C_0)^{1-\frac{t}{p}}$.

Proof. Corollary 7.1.5 follows by using the definition of a space implying bounded m-th total persistence along with the inequality $\mathrm{Pers}_{t_1+t_2}(a) \leq \mathrm{Pers}_\infty(a)^{t_1} \mathrm{Pers}_{t_2}(a)$ for any persistence diagram a. □

If $\alpha > m + 1$ and $p = \infty$, then the result is similar to Theorem 3.3 in [KFH17]. However, Corollary 7.1.5 implies that the representations are still continuous (actually Hölder continuous) when $\alpha \in (m, m+1]$, and this is the novelty of the result. Indeed, for such an α, one can always choose t small enough so that the stability result (7.11) holds. The proofs of Theorem 7.1.4 and Corollary 7.1.5 consist of adaptations of similar proofs in [KFH17].

Remark 7.1.6. *(a)* One cannot expect to obtain an inequality of the form (7.7) without quantities R_1 and R_2 related to the total persistence of the diagrams appearing on the right-hand side. For instance, in the case $p = \infty$, it is clear that adding an arbitrary number of points near the diagonal will not change the bottleneck distance between the diagrams, whereas the distance between representations can become arbitrarily large.

(b) Laws of large numbers stated in the next section (see Theorem 8.2.5), show that

Corollary 7.1.5 is optimal. Indeed, take $w = \mathrm{pers}^\alpha$ and $f \equiv 1$. Let $\mathcal{X} = [0,1]^d$ be the d-dimensional cube, which has bounded m-th total persistence for $m > d$. Let $\mathcal{X}_n$ be a sample of n i.i.d. points on $\mathcal{X}$. Letting ϕ_1 be the distance function to $\mathcal{X}_n$, we obtain that $\mathrm{dgm}_q(\phi_1) = \mathrm{dgm}_q^C(\mathcal{X}_n)$, the Čech persistence diagram of the set $\mathcal{X}_n$. We let $\phi_2 = 0$, so that $\mathrm{dgm}_q(\phi_2) = 0$. Therefore,

$$\|\Psi_{wf}(\mathrm{dgm}_q(\phi_1)) - \Psi_{wf}(\mathrm{dgm}_q(\phi_2))\| = \mathrm{Pers}_\alpha(\mathrm{dgm}_q^C(\mathcal{X}_n)).$$

We will see in the next section that this quantity does not converge to 0 for $\alpha \leq d$ (it even diverges if $\alpha < d$), whereas the bottleneck distance between $\mathrm{dgm}_q^C(\mathcal{X}_n)$ and the empty diagram does converge to 0. As such, it is impossible to obtain an inequality of the form (7.11) for $\alpha \leq m$.

We end this section by giving a foretaste of the asymptotic study of persistence diagrams developed in the next section. The following corollary presents rates of convergence of representations in a random setting. Let $\mathcal{X}_n = \{X_1, \dots, X_n\}$ be a n-sample of i.i.d. points from a distribution on some manifold M. We are interested in the convergence of the representation $\Psi_{wf}(\mathrm{dgm}_q^C(\mathcal{X}_n))$ to the representation $\Psi_{wf}(\mathrm{dgm}_q^C(M))$. We obtain the following corollary.

Corollary 7.1.7. *Consider a d-dimensional compact Riemannian manifold M, and let $\mathcal{X}_n = \{X_1, \dots, X_n\}$ be a n-sample of i.i.d. points from a distribution having a density κ with respect to the volume measure on M. Assume that $0 < \inf \kappa \leq \sup \kappa < \infty$. Let $w \in \mathbb{W}(\alpha, A)$ for some $A > 0, \alpha > d$, and let $f : \Omega \to B$ be a Lipschitz continuous function. Then, for n large enough,*

$$\mathbb{E}\left[\|\Psi_{wf}(\mathrm{dgm}_q^C(\mathcal{X}_n)) - \Psi_{wf}(\mathrm{dgm}_q^C(M))\|\right] \leq C\|f\|_\infty \frac{\alpha}{\alpha - d}\left(\frac{\ln n}{n}\right)^{\frac{\alpha}{d}-1}, \tag{7.12}$$

where C is a constant depending on M, A and the density κ.

The study of the next section will show that this rate of convergence is tight up to logarithmic factors. Once again, this indicates that Corollary 7.1.5 is close to being tight.

Proof. As already discussed, Theorem 7.1.4 can be applied with $\phi_n = d(\cdot, \mathcal{X}_n)$ and ϕ the null function on the manifold M. Take $p = \infty$, $d < \alpha$ and $0 < t < \min(1, \alpha - d)$:

$$\begin{aligned}
&\|\Psi_{wf}(\mathrm{dgm}_q(\phi_n)) - \Psi_{wf}(\mathrm{dgm}_q(\phi))\| \\
&\quad \leq \mathrm{Lip}(f)\frac{A}{\alpha}\mathrm{Pers}_\alpha(\mathrm{dgm}_q(\phi_n))) \cdot d_\infty(\mathrm{dgm}_q(\phi_n), \mathrm{dgm}_q(\phi)) \\
&\qquad + 2\|f\|_\infty A\mathrm{Pers}_{\alpha-t}(\mathrm{dgm}_q(\phi_n))d_\infty(\mathrm{dgm}_q(\phi_n), \mathrm{dgm}_q(\phi))^t.
\end{aligned} \tag{7.13}$$

We mentioned in Chapter 3 that, for $m > d$, we have the inequality $\mathrm{Pers}_m(\mathrm{dgm}_q(\phi_n)) \leq mC_M\|\phi_n\|^{m-d}/(m-d)$ for some constant C_M depending only on M. Moreover, the stability theorem for the bottleneck distance ensures that $d_\infty(\mathrm{dgm}_q(\phi_n), \mathrm{dgm}_q(\phi)) \leq \|\phi_n\|_\infty$. Therefore,

$$\begin{aligned}
&\|\Psi_{wf}(\mathrm{dgm}_q(\phi_n)) - \Psi_{wf}(\mathrm{dgm}_q(\phi))\| \\
&\quad \leq \mathrm{Lip}(f)\frac{\alpha A C_{\mathcal{X}}}{\alpha - d}\|\phi_n\|_\infty^{\alpha-d+1} + \|f\|_\infty \frac{2AC_M(\alpha - t)}{\alpha - t - d}\|\phi_n\|_\infty^{\alpha-t-d+t} \\
&\quad \leq \mathrm{Lip}(f)\frac{\alpha A C_M}{\alpha - d}\|\phi_n\|_\infty^{\alpha-d+1} + \|f\|_\infty \frac{2AC_M\alpha}{\alpha - d}\|\phi_n\|_\infty^{\alpha-d},
\end{aligned} \tag{7.14}$$

where, in the last line, the second term was minimized over $t \in [0,1]$. The quantity $\|\phi_n\|_\infty$ is the Hausdorff distance between $\mathcal{X}_n$ and M. Elementary techniques of geometric probability (see for instance [Cue09]) show that if M is a compact d-dimensional manifold, then $\mathbb{E}[\|\phi_n\|_\infty^\beta] \leq c\left(\frac{\ln n}{n}\right)^{\beta/d}$ for $\beta \geq 0$, where c is some constant depending on $\beta, M, \inf\kappa$ and $\sup\kappa$. Therefore, the first term of the sum (7.14) being negligible,

$$\mathbb{E}\left[\|\Psi_{wf}(\mathrm{dgm}_q(\phi_n)) - \Psi_{wf}(\mathrm{dgm}_q(\phi))\|\right] \leq \\ \|f\|_\infty \frac{2AC_M\alpha}{\alpha - d} c\left(\frac{\ln n}{n}\right)^{(\alpha-d)/d} + o\left(\left(\frac{\ln n}{n}\right)^{(\alpha-d)/d}\right).$$

In particular, the conclusion holds for any $C > 2AC_M c$, for n large enough. □

7.2 Limit laws on large persistence diagrams

As a gentle introduction to the formalism used later, we first recall some known results from geometric probability on the study of Betti numbers, and we also detail relevant results of [HST18; Tri17; GTT19].

7.2.1 Prior work

In the following, K refers to either the Čech or the Rips filtration. Let κ be a density on $[0,1]^d$ such that:

$$0 < \inf\kappa \leq \sup\kappa < \infty. \tag{7.15}$$

Note that the cube $[0,1]^d$ could be replaced by any compact convex body (i.e. the boundary of an open bounded convex set). However, the proofs (especially geometric arguments of Section 7.4.1) become much more involved in this greater generality. To keep the main ideas clear, we therefore restrict ourselves to the case of the cube. We indicate, however, when challenges arise in the more general setting.

Let $(X_i)_{i\geq 1}$ be a sequence of i.i.d. random variables sampled from density κ and let $(N_i)_{i\geq 1}$ be an independent sequence of Poisson variables with parameter i. In the following $\mathcal{X}_n$ denotes either $\{X_1, \ldots, X_n\}$, a binomial process of intensity κ and of size n, or $\{X_1, \ldots, X_{N_n}\}$, a Poisson process of intensity $n\kappa$. The fact that the binomial and Poisson processes are built in this fashion is not important for weak laws of large numbers (only the law of the variables is of interest), but it is crucial for strong laws of large numbers to make sense.

Recall the definition of the persistent Betti numbers

$$\beta_{r,s}(\mathrm{dgm}_q^K(\mathcal{X}_n)) := \mathrm{dgm}_q^K(\mathcal{X}_n)(\lrcorner_{r,s}), \tag{7.16}$$

where $\lrcorner_{r,s} = \{u = (u_1, u_2) \in \Omega : \ u_1 \leq r \leq s \leq u_2\}$ for $0 \leq r \leq s$.

Theorem 7.2.1 (Theorem 1.4 in [Tri17]). *Let $r > 0$ and $q \geq 0$. Then, with probability one, $n^{-1}\beta_{r,r}(\mathrm{dgm}_q^K(n^{1/d}\mathcal{X}_n))$ converges to some constant. The convergence also holds in expectation.*

The theorem is originally stated with the Čech filtration but its generalization to the Rips filtration (or even to more general filtrations considered in [HST18]) is straightforward. The proof of this theorem is based on a simple, yet useful geometric lemma, which still holds for the persistent Betti numbers, as proven in [HST18]. Recall that for $j \geq 0$, $\mathcal{S}_j(K)$ denote the j-skeleton of the simplicial complex K.

Lemma 7.2.2 (Lemma 2.11 in [HST18]). *Let $\mathcal{X} \subset \mathcal{Y}$ be two subsets of $\mathbb{R}^d$. Then*

$$|\beta_{r,s}(\mathrm{dgm}_q^K(\mathcal{X})) - \beta_{r,s}(\mathrm{dgm}_q^K(\mathcal{Y}))| \leq \sum_{j=q}^{q+1} |\mathcal{S}_j(K^s(\mathcal{Y}))\backslash\mathcal{S}_j(K^s(\mathcal{X}))|. \tag{7.17}$$

In [HST18], this lemma was used to prove the convergence of expectations of diagrams of stationary point processes. As indicated in [GTT19, Remark 2.4], this lemma can also be used to prove the convergence of the expectations of diagrams for non-homogeneous binomial processes on manifold. Set $\mu_q^n = n^{-1}\mathrm{dgm}_q^K(n^{1/d}\mathcal{X}_n)$. Remark 2.4 in [GTT19] implies the following theorem.

Theorem 7.2.3 (Remark 2.4 in [GTT19] and Theorem 1.5 in [HST18]). *Let κ be a probability density function on a d-dimensional compact $\mathcal{C}^1$ manifold M (or the cube), with $\int_M \kappa^j(z)dz < \infty$ for $j \in \mathbb{N}$. Then, for $q \geq 0$, there exists a unique Radon measure μ_q^κ on Ω such that*

$$\mathbb{E}[\mu_q^n] \xrightarrow[n\to\infty]{v} \mu_q^\kappa \tag{7.18}$$

and

$$\mu_n \xrightarrow[n\to\infty]{v} \mu_q^\kappa \ a.s.. \tag{7.19}$$

The measure μ_q^κ is called the persistence diagram of intensity κ for the filtration K.

The measure $\mathbb{E}[\mu_q^n]$ is by definition the unique measure defined by $\mathbb{E}[\mu_q^n](A) := \mathbb{E}[\mu_q^n(A)]$ for every Borel set A. We will investigate in detail the behavior or such measures, that we call expected persistence diagrams, in Chapter 8.

7.2.2 Main results

A function $\phi : \Omega \to \mathbb{R}$ is said to vanish on the diagonal if

$$\lim_{\varepsilon\to 0} \sup_{\mathrm{pers}(r)\leq\varepsilon} |\phi(r)| = 0. \tag{7.20}$$

Denote by $\mathcal{C}_0(\Omega)$ the set of all such functions. The weight functions of Section 7.1 all lie in $\mathcal{C}_0(\Omega)$. We say that a function $\phi : \Omega \to \mathbb{R}$ has polynomial growth if there exist two constants $A, \alpha > 0$, such that

$$|\phi(r)| \leq A\left(1 + \mathrm{pers}(r)^\alpha\right). \tag{7.21}$$

The class $\mathcal{C}_{\mathrm{poly}}(\Omega)$ of functions in $\mathcal{C}_0(\Omega)$ with polynomial growth constitutes a reasonable class of functions $w \cdot \phi$ one may want to build a representation with. Our goal is to extend the convergence of Theorem 7.2.3 to this larger class of functions. Convergence of measures μ_n to μ with respect to $\mathcal{C}_{\mathrm{poly}}(\Omega)$, i.e. $\forall\phi \in \mathcal{C}_{\mathrm{poly}}(\Omega)$, $\mu_n(\phi) \xrightarrow[n\to\infty]{} \mu(\phi)$, is denoted by $\xrightarrow{v_p}$. Note that this class of functions is standard: it is for instance known to characterize p-th Wasserstein convergence in optimal transport (see Chapter 3).

Theorem 7.2.4. *(i) For $q \geq 0$, there exists a unique Radon measure μ_q^κ such that $\mathbb{E}[\mu_q^n] \xrightarrow[n\to\infty]{v_p} \mu_q^\kappa$ and, with probability one, $\mu_q^n \xrightarrow[n\to\infty]{v_p} \mu_q^\kappa$. The measure μ_q^κ is called the q-th persistence diagram of intensity κ for either the Čech or Rips filtration. It does not depend on whether $\mathcal{X}_n$ is a Poisson or a binomial process, and is of positive finite mass.*

(ii) The convergence also holds pointwise for the L_p distance: for all $\phi \in \mathcal{C}_{\mathrm{poly}}(\Omega)$, and for all $p \geq 1$, $\mu_q^n(\phi) \xrightarrow[n\to\infty]{L_p} \mu_q^\kappa(\phi)$. In particular, $|\mu_q^\kappa(\phi)| < \infty$.

Remark 7.2.5. *(a)* Remark 2.4 together with Theorem 1.1 in [GTT19] imply that the measure μ_q^κ has the following expression:

$$\mu_q^\kappa(\phi) = \mathbb{E}\left[\int_\Omega \phi(r\kappa(X)^{-1/d})d\mu_q(r)\right] \ \forall \phi \in \mathcal{C}_c(\Omega), \tag{7.22}$$

where $\mu_q = \mu_q^{\mathbf{1}}$ is the q-th persistence diagram of uniform density on $[0,1]^d$, appearing in Theorem 7.2.3, and the expectation is taken with respect to a random variable X having a density κ.

(b) Assume $q = 0$ and $d = 1$. Then, the persistence diagram $\mathrm{dgm}_0^K(\mathcal{X}_n)$ is simply the collection of the intervals $(X_{(i+1)} - X_{(i)})$ where $X_{(1)} < \cdots < X_n$ is the order statistics of $\mathcal{X}_n$. The measure $\mathbb{E}[\mu_0^n]$ can be explicitly computed: it converges to a measure having density $u \mapsto \mathbb{E}[\exp(-u\kappa(X))\kappa(X)]$ with respect to the Lebesgue measure on $\mathbb{R}_+$, where X has density κ. Take κ the uniform density on $[0,1]$: one sees that this is coherent with the basic fact that the spacings of a homogeneous Poisson process on $\mathbb{R}$ are distributed according to an exponential distribution. Moreover, the expression (7.22) is found again in this special case.

(c) Theorem 1.9 in [HST18] states that the support of $\mu_q^{\mathbf{1}}$ is Ω. Using Equation (7.22), the same holds for μ_q^κ.

(d) Theorem 7.0.2 is a direct corollary of Theorem 7.2.4. Indeed, we have

$$\begin{aligned} n^{\frac{\alpha}{d}-1}\mathrm{Pers}_\alpha(\mathrm{dgm}_q^K(\mathcal{X}_n)) &:= n^{\frac{\alpha}{d}-1} \sum_{r\in \mathrm{dgm}_q^K(\mathcal{X}_n)} \mathrm{pers}^\alpha(r) \\ &= n^{-1} \sum_{r\in \mathrm{dgm}_q^K(\mathcal{X}_n)} \mathrm{pers}^\alpha(n^{-\frac{1}{d}}r) \\ &= \mu_q^n(\mathrm{pers}^\alpha), \end{aligned}$$

a quantity which converges to $\mu_q^\kappa(\mathrm{pers}^\alpha)$. The relevance of Theorem 7.0.2 is illustrated in Figure 7.2, where Čech complexes are computed on random samples on the torus.

The core of the proof of Theorem 7.2.4 consists in a control of the number of points appearing in diagrams. This bound is obtained thanks to geometric properties satisfied by the Čech and Rips filtrations. Finding good requirements to impose on a filtration K for this control to hold is an interesting question. The following states some non-asymptotic controls of the number of points in diagrams which are interesting by themselves.

Proposition 7.2.6. *Let $M \geq 0$ and define $U_M = \mathbb{R} \times [M, \infty)$. Then, there exist constants $c_1, c_2 > 0$ (which can be made explicit) depending on κ and q, such that, for any $t > 0$,*

$$\mathbb{P}(\mu_q^n(U_M) > t) \leq c_1 \exp(-c_2(M^d + t^{1/(q+1)})). \tag{7.23}$$

As an immediate corollary, the moments of the total mass $|\mu_q^n|$ are uniformly bounded. However, the proof of the almost sure finiteness of $\sup_n |\mu_q^n|$ is much more intricate. Indeed, we are unable to control directly this quantity, and we prove that a majorant of $|\mu_q^n|$ satisfies concentration inequalities. The majorant arises as the number of simplicial complexes of a simpler process, whose expectation is also controlled.

It is natural to wonder whether μ_q^κ has some density with respect to the Lebesgue measure on Ω: it is the case for the for $d = 1$, and it is shown in Chapter 8 that $\mathbb{E}[\mu_q^n]$ also has a density. Even if those elements are promising, it is not clear whether the limit μ_q^κ has a density in a general setting. However, we are able to prove that the marginals of μ_q^κ have densities.

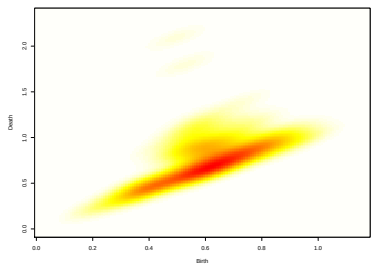
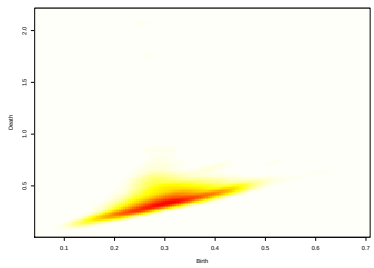
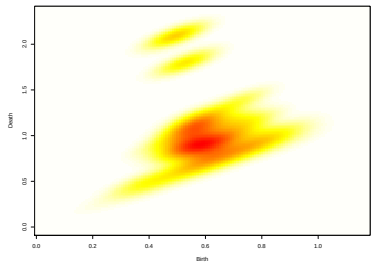
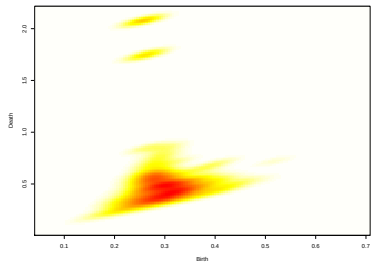
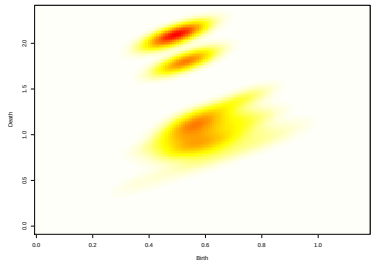
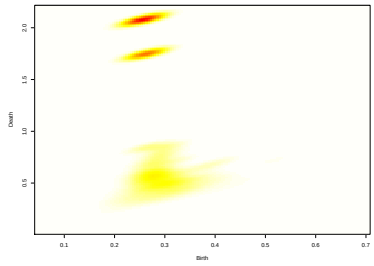
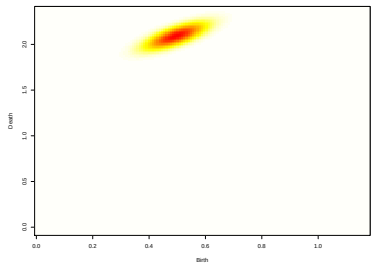
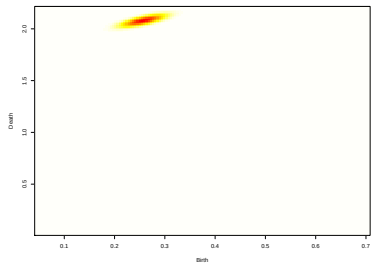
Weight function	$n = 500$	$n = 2000$
pers^0		
pers^1		
pers^2		
pers^{100}		

FIGURE 7.2: For $n = 500$ or 2000 points uniformly sampled on the torus, persistence surfaces [Ada+17] for different weight functions are displayed. For $\alpha < 2$, the mass of the topological noise is far larger than the mass of the true signal, the latter being comprised by the two points with high-persistence. For $\alpha = 2$, the two points with high-persistence are clearly distinguishable. For $\alpha = 100$, the noise has also disappeared, but so has one of the point with high-persistence.

Proposition 7.2.7. *Let π_1 (resp. π_2) be the projection on the x-axis (resp. y-axis). Then, for $q > 0$, the pushforwards $(\pi_1)_\#(\mu_q^\kappa)$ and $(\pi_2)_\#(\mu_q^\kappa)$ have densities with respect to the Lebesgue measure on $\mathbb{R}$. For $q = 0$, $(\pi_2)_\#(\mu_q^\kappa)$ has a density.*

7.3 Discussion

The tuning of the weight functions in representations of persistence diagrams is a critical issue in practice. When the statistician has good reasons to believe that the data lies near a d-dimensional structure, we give, through two different approaches (stability and limit theorems), a heuristic to tune this weight function: a weight of the form pers^α with $\alpha \geq d$ is sensible. The study carried out in this paper allowed us to show new results on the asymptotic structure of random persistence diagrams. While the existence of a limiting measure in a weak sense was already known, we strengthen the convergence, by showing that the convergence holds for the Figalli-Gigli metrics FG_p. Some results about the properties of the limit are also shown, namely that it has a finite mass, finite moments, and that its marginals have densities with respect to the Lebesgue measure. The fact that the limit behavior of the random persistence diagram is sensitive to the dimension d can also be used to define a notion of fractal dimension for measures via persistent homology, see [Ada+20].

Challenging open questions on this asymptotic behavior include:

- Existence of a density for the limiting measure: An approach for obtaining such results would be to control the numbers of points of a diagram in some square $[r_1, r_2] \times [s_1, s_2]$.
- Convergence of the number of points in the diagrams: The number of points in the diagrams is a quantity known to be not stable (motivating the use of bottleneck distances, which is blind to them). However, experiments show that this number, conveniently rescaled, converges in this setting. An analog of Lemma 7.2.2 for the number of points in the diagrams with small persistence would be crucial to attack this problem.
- Generalization to manifolds: While the vague convergence of the rescaled diagrams is already proven in [GTT19], allowing test functions without compact support appears to be a challenge. Once again, the crucial issue consists in controlling the total number of points in the diagrams.

7.4 Proofs of Section 7.2

7.4.1 Proof of Proposition 7.2.6

First, as the right hand side of the inequality (7.23) does not depend on n, one may safely assume that μ_q^n is built with the binomial process. The proof is based on two observations.

(i) Denote by $\phi(\sigma)$ the *filtration time* of some simplex σ, given by $r(\sigma)$ for the Čech filtration and $\text{diam}(\sigma)$ for the Rips filtration. Recall the definition of a *negative* and *positive* simplexes from Chapter 3. A simplex σ is said to be *negative* in the filtration $K(\mathcal{X}_n)$ if σ is not included in any cycle of $K(\phi(\sigma), \mathcal{X}_n)$. A basic result of persistent homology states that points in $\text{dgm}_q^K(\mathcal{X}_n)$ are in bijection with pair of simplexes, one negative and one positive (i.e. non-negative). Moreover, the death time r_2 of a point $r = (r_1, r_2)$ of the diagram is exactly $\phi(\sigma)$ for some negative $(q+1)$-simplex σ.

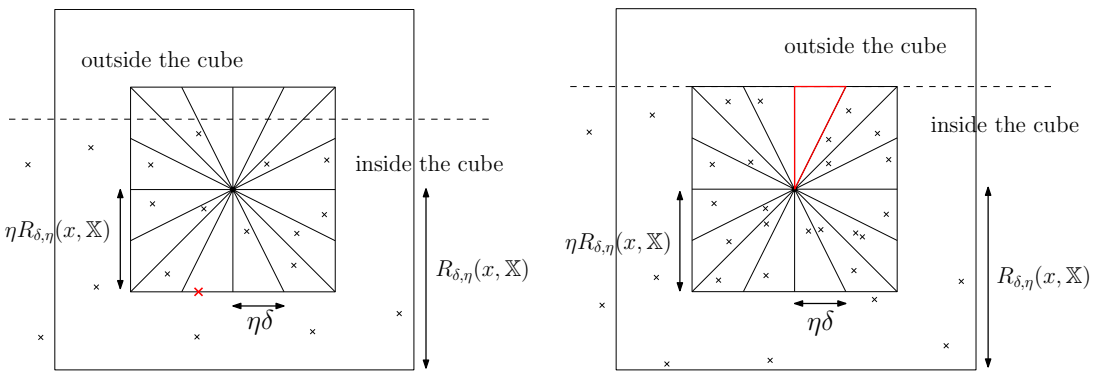


FIGURE 7.3: *Illustration of the definition of $R := R_{\delta,\eta}(x,\mathcal{X})$ for some two point clouds $\mathcal{X}$. The dashed line indicates the boundary of $[0,1]^d$. On the left display, the radius R is such that there is a point (indicated in red) on $C_j^\delta(x,R)$. On the right display, there is a cone $A_j^\delta(x,R)$, indicated in red, for which $C_j^\delta(x,R)$ is on some face of the cube $[0,1]^d$.*

Therefore, $n\mu_q^n(U_M)$ is equal to $N_q(\mathcal{X}_n, M)$, the number of negative $(q+1)$-simplexes in the filtration $K(\mathcal{X}_n)$ appearing after $M_n := n^{-1/d}M$.

(ii) The number of negative simplexes in the Čech and Rips filtration can be efficiently bounded thanks to elementary geometric arguments.

Geometric arguments for the Rips filtration

We have

$$N_q(\mathcal{X}_n, M) = \frac{1}{q+2}\sum_{i=1}^{n} \#\Xi(X_i, \mathcal{X}_n), \tag{7.24}$$

where, for $x \in \mathcal{X}$, with $\mathcal{X}$ a finite set, $\Xi(x,\mathcal{X})$ is the set of negative $(q+1)$-simplexes (and therefore of size $q+2$) in $\mathrm{Rips}(\mathcal{X})$ that are containing x, and have a filtration time larger than M_n. The following construction is inspired by the proof of Lemma 2.4 in [MY99].

The angle (with respect to 0) of two vectors $x, y \in \mathbb{R}^d$ is defined as

$$\angle xy := \arccos\left(\frac{\langle x, y\rangle}{|x||y|}\right).$$

The angular section of a cone A is defined as $\sup_{x,y\in A}\angle xy$. Denote by $C(x,r)$ the cube centered at x of side length $2r$. For $0<\delta<1$, and for each face of the cube $C(x,r)$, consider a regular grid with spacing δr, so that the center of each face is one of the grid points. This results in a partition of the boundary of the cube $C(x,r)$ into $(d-1)$-dimensional cubes $\left(C_j^\delta(x,r)\right)_{j=1\dots Q}$ of side length δr. Using this partition of the boundary of $C(x,r)$, we construct a partition of $C(x,r)$ into closed convex cones $(A_j^\delta(x,r))_{j=1\dots Q}$, where each cone $A_j^\delta(x,r)$ is defined as a d-simplex spanned by x and one of the $(d-1)$-dimensional cubes $C_j^\delta(x,r)$ of side length δr on a face of $C(x,r)$. In other words, the point x is the apex of each $A_j^\delta(x,r)$, and $C_j^\delta(x,r)$ is its base. We call two such cones $A_j^\delta(x,r)$ and $A_{j'}^\delta(x,r)$ *adjacent*, if $A_j^\delta(x,r)\cap A_{j'}^\delta(x,r) \neq \{x\}$.

Fix $0<\eta<1$, and define $R_{\delta,\eta}(x,\mathcal{X}_n)$ to be the smallest radius r so that each cone $A_j^\delta(x,\eta r)$ in $C(x,\eta r)$ either contains a point of $\mathcal{X}_n$ other than x, or is not a subset of $(0,1)^d$ (see Figure 7.3 for an illustration).

Lemma 7.4.1. *Let $x \in [0,1]^d$. Fix $\delta > 0$, and $0 < r \leq \frac{1}{2}$, and let $A_j^\delta(x,r)$ be a cone of $C(x,r)$ whose base $C_j^\delta(x,r)$ intersects $[0,1]^d$. Then, either $A_j^\delta(x,r)$ is a subset of $[0,1]^d$, or there exists a cone $A_{j'}^\delta(x,r)$ of $C(x,r)$ adjacent to $A_j^\delta(x,r)$ that is a subset of $[0,1]^d$.*

Proof. A necessary and sufficient condition for a cone $A_j^\delta(x,r)$ to be a subset of $[0,1]^d$ is that $C_j^\delta(x,r) \subset [0,1]^d$. Suppose that this is not the case, i.e. we have $C_j^\delta(x,r) \setminus [0,1]^d \neq \emptyset$. For each coordinate $i = 1, \ldots, d$ for which $C_j^\delta(x,r)$ extends beyond a face of $[0,1]^d$, move one step in the 'opposite' direction, and find the corresponding adjacent cone. The fact that $r \leq 1/2$ ensures that these (at most d) steps, each of size $r\delta$, do not make the exterior boundary of the corresponding adjacent cone extend beyond any of the opposite faces of the cube corresponding to the directions of the steps. □

Note that the angular section (with respect to x) of the union of a cone $A_j^\delta(x,r)$ and its adjacent cones is bounded by $c\delta$ for some constant c.

Lemma 7.4.2. *Let $\eta = \min\{1/\sqrt{d}, 1/2\}$. There exists a $\delta = \delta(d) > 0$, such that each simplex σ of $\Xi(x, \mathcal{X}_n)$ is included in $C(x, R_{\delta,\eta}(x, \mathcal{X}_n))$. Furthermore, $\Xi(x, \mathcal{X}_n)$ is empty if $R_{\delta,\eta}(x, \mathcal{X}_n) > M_n$.*

Proof. To ease notation, denote $R_{\delta,\eta}(x, \mathcal{X}_n)$ by R. We are going to prove that all negative simplexes containing x are included in $C(x,R)$, a fact that proves the two assertions of the lemma. First, if $\eta R \geq 1/2$, then $C(x,R)$ contains $[0,1]^d$ and the result is trivial. So, assume that $\eta R < 1/2$, and consider a $(q+1)$-simplex $\sigma = \{x, x_1, \ldots, x_{q+1}\}$ that is not contained in $C(x,R)$. Assume without loss of generality that x_1 is the point in σ maximizing the distance to x, which in particular means that x_1 is not in $C(x,R)$. The line $[x, x_1]$ hits $C(x, \eta R)$ at some cone $A_j^\delta(x, \eta R)$. By Lemma 7.4.1 and the definition of R, if A^δ denotes the union of $A_j^\delta(x, \eta R)$ and its adjacent cones in $C(x, \eta R)$, then there exists a point z of $\mathcal{X}_n$ in $A^\delta \subset C(x, \eta R)$ and the angle $\angle xzx_1$ formed by $[z,x]$ and $[z,x_1]$ is in smaller than $c\delta$. Let us prove that all the $(q+1)$-simplexes σ_t of the form $(\sigma \setminus \{t\}) \cup \{z\}$, for $t \in \sigma$, have a filtration time smaller than $r(\sigma)$. If this is the case, then the cycle formed by the σ_t's and σ is contained in the complex at time $r(\sigma)$, meaning that σ is not negative, concluding the proof. Therefore, it suffices to prove that $|z - x| \leq r(\sigma)$ and that $|z - x_i| \leq r(\sigma)$ for all i:

- $|z - x| \leq \sqrt{d}\eta R \leq |x - x_1|$.
- If $\angle xzx_1 < c\delta \leq \pi/3$,

$$\begin{aligned} |z - x_1|^2 &= |z - x|^2 + |x_1 - x|^2 - 2\langle z - x, x_1 - x\rangle \\ &\leq |z - x|^2 + |x_1 - x|^2 - |z - x||x_1 - x| \leq |x_1 - x|^2 \leq r(\sigma)^2. \end{aligned}$$

For $i \geq 2$, we have $|x - x_i| \leq |x - x_1|$ by assumption. Let $I(z)$ denote the set of all $t \in \mathbb{R}^d$ with $|z - t| \geq |x - t|$ and $|z - t| \geq |x_1 - t|$, i.e. $I(z)$ is the intersection of two half spaces (see Figure 7.4). Let $F_x(z) = d(I(z), x)$. If we find a δ with $F_x(z) > |x - x_1|$ for all $z \in A^\delta$, then no x_i is in $I(z)$, whatever the position of $z \in A^\delta$ is, meaning that all x_i's satisfy $|z - x_i| \leq \max\{|x - x_i|, |x_1 - x_i|\} \leq r(\sigma)$, concluding the proof. The method of Lagrange multipliers shows that $F_x(z)^2$ is a continuous function of z, with a known (but complicated) expression. A straightforward study of this expression shows that for δ small enough, the minimum of F_x on A^δ can be made arbitrarily large: therefore, there exists δ such that $F_x(z) > \sqrt{d} \geq |x - x_1|$, for all $z \in A^\delta$. □

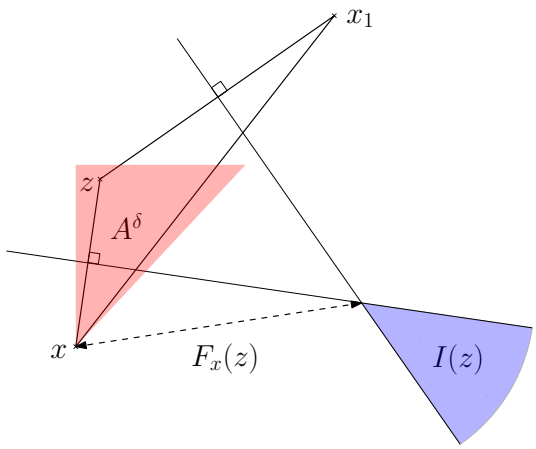


FIGURE 7.4: *The geometric construction used in the proof of Lemma 7.4.2. The red region represents A^δ whereas the blue region represents $I(z)$ for some point z in A^δ. If δ is made sufficiently small, the distance $F_x(z)$ between x and $I(z)$ can be made arbitrarily large.*

Construction for the Čech filtration

A similar construction works for the Čech filtration, but the arguments are slightly different. First, note that each negative simplex σ in the Čech filtration is such that there exists a subsimplex σ' of σ that enters in the filtration at the same time $r(\sigma)$ as σ, and so that $r(\sigma)$ is the circumradius of σ'. Then

$$\begin{aligned} N_q(\mathcal{X}_n, M) &= \sum_{\sigma \in \mathrm{Cech}_{q+1}(\mathcal{X}_n)} \mathbf{1}\{\sigma \text{ negative},\ r(\sigma) \geq M\} \\ &= \sum_{\sigma \in \mathrm{Cech}_{q+1}(\mathcal{X}_n)} \frac{1}{\#\sigma'} \sum_{i=1}^{n} \mathbf{1}\{\sigma \text{ negative},\ r(\sigma) \geq M,\ X_i \in \sigma'\} \\ &\leq \sum_{i=1}^{n} \#\Xi'(X_i, \mathcal{X}_n), \end{aligned}$$

where $\Xi'(x, \mathcal{X}_n)$ the set of negative $(q+1)$-simplexes σ in the Čech filtration $\mathrm{Cech}(\mathcal{X}_n)$ with $r(\sigma) \geq M$ and $x \in \sigma'$.

Lemma 7.4.3. *For $\eta = \min\{1/\sqrt{d}, 1/2\}$ and some $\delta = \delta(d) > 0$, each simplex σ of $\Xi'(x, \mathcal{X}_n)$ is included in $C(x, R_{\delta,\eta}(x, \mathcal{X}_n))$. Furthermore, $\Xi'(x, \mathcal{X}_n)$ is empty if $R_{\delta,\eta}(x, \mathcal{X}_n) > M_n$.*

Proof. Recall the definition of $C(x, r)$ and the partition of $C(x, r)$ into the cones $(A_j^\delta(x, r))_{j=1\ldots Q}$ with corresponding bases $(C_j^\delta(x, r))_{j=1\ldots Q}$. As above, denote $R_{\delta,\eta}(x, \mathcal{X}_n)$ by R. Let $\sigma = \{x, x_1, \ldots, x_{q+1}\}$ denote a $(q+1)$-simplex not included in $C(x, R)$, with $r(\sigma) \geq M$. As in the Rips case, the result is trivial if $\eta R \geq 1/2$. By definition of the Čech filtration, the intersection $\bigcap_{i=0}^{q+1} B(x_i, r(\sigma))$ consists of a singleton $\{y\}$. If there is a point z of $\mathcal{X}_n$ in $B(y, r(\sigma))$, then, by the nerve theorem applied to $\sigma \cup \{z\}$, we can conclude with similar arguments as in Lemma 7.4.2 that σ is positive in the filtration, meaning that every negative $\sigma \in \Xi(x, \mathcal{X}_n)$ has to be included in $C(x, R)$.

Let us prove the existence of such a z. As $x \in \sigma'$, the distance between x and y is equal to $r(\sigma) \geq R$. Therefore, the line $[x, y]$ hits $C(x, \eta R)$ in some cone $A_j^\delta(x, \eta R)$, whose base $C_j^\delta(x, r)$ intersects $[0, 1]^d$, as it intersects $[x_0, y]$. As in the Rips case, there exists a point z of $\mathcal{X}_n$ in $C(x, \eta R)$ such that the angle made by z, x and y is smaller than $c\delta$. As before, it can then be argued that $|y - z| \leq r(\sigma)$, concluding the proof. $\square$

Remark 7.4.4. Note that the fact that the support of κ is the cube only enters the picture through the geometric arguments used here and in the above proof. Some more refined work is needed to show that a similar construction holds when the cube is replaced by a convex body.

In the following, fix $\eta = \min\{1/\sqrt{d}, 1/2\}$, choose δ sufficiently small, and let $R_{\delta,\eta}(x, \mathcal{X}_n), A_j^\delta(x, r)$ and $C_j^\delta(x, r)$ be denoted by $R(x, \mathcal{X}_n), A_j(x, r)$ and $C_j(x, r)$ respectively. Both $\Xi(x, \mathcal{X}_n)$ and $\Xi'(x, \mathcal{X}_n)$ are included in the set of $(q+1)$-tuples of $\mathcal{X}_n \cap C(x, R(x, \mathcal{X}_n))$, so that the following inequality holds for either the Rips or the Čech filtration:

$$N_q(\mathcal{X}_n, M) \leq \sum_{i=1}^{n} \mathbf{1}\{R(X_i, \mathcal{X}_n) > M_n\} \left(\#(\mathcal{X}_n \cap C(X_i, R(X_i, \mathcal{X}_n)))\right)^{q+1}. \tag{7.25}$$

Denote $R(X_1, \mathcal{X}_n)$ by R_n. As we will see, an estimate of the tail of R_n is sufficient to get a control of $N_q(\mathcal{X}_n, M)$. The probability $\mathbb{P}(R_n > t)$ is bounded by the probability that one of the cones pointing at X_1, of radius $t/2$, wholly included in the cube $[0,1]^d$, is empty. Conditionally on X_1, this probability is exactly the probability that a binomial process with parameters $n-1$ and κ does not intersect this cone. Therefore,

$$\mathbb{P}(R_n > t) \leq c \exp(-cnt^d), \tag{7.26}$$

and we obtain, for $\lambda > 0$,

$$\begin{aligned} \mathbb{E}\left[e^{\lambda n R_n^d}\right] &= \int_1^\infty \mathbb{P}(\lambda n R_n^d > \ln(t)) dt \\ &\leq \int_1^\infty c \exp\left(-c\frac{\ln(t)}{\lambda}\right) dt < \infty \text{ if } \lambda < c/2. \end{aligned} \tag{7.27}$$

Lemma 7.4.5. *The random variable $\#(\mathcal{X}_n \cap C(X_1, R_n))$ has exponential tail bounds: for $t > 0$,*

$$\mathbb{P}(\#(\mathcal{X}_n \cap C(X_1, R_n)) > t) \leq c \exp(-ct).$$

Proof. Conditionally on X_1 and R_n, two possibilities may occur. In the first one, the cube centered at X_1 of radius ηR_n contains a point on its boundary, in the cone $A_{j_0}(X_1, \eta R_n)$. Denote this event E and let Q_0 be the number of cones wholly included in the support. The configuration of $\mathcal{X}_n$ is a binomial process conditioned to have at least one point in the cones $A_j(X_1, \eta R_n)$ wholly included in the cube, except for $j = j_0$, and a point on $C_{j_0}(X_1, \eta R_n)$. In this case, $\#(\mathcal{X}_n \cap C(X_1, R_n))$ is equal to $Q_0 + Z$, where Z is a binomial variable of parameters $n - Q_0$ and

$$\int_{C(X_1,R_n)\setminus A_{j_0}(X_1,\eta R_n)} \kappa(x) dx \leq c R_n^d.$$

Therefore, for $\beta > 0$, using a Chernoff bound and a classical bound on the moment generating function of a binomial variable:

$$\begin{aligned} \mathbb{P}(\#(\mathcal{X}_n \cap C(X_1, R_n)) > t | R_n, Q_0, E) &\leq \mathbb{P}(Q_0 + Z > t | R_n, Q_0) \\ &\leq \frac{e^{\beta Q_0} \mathbb{E}[e^{\beta Z} | R_n]}{e^{\beta t}} \\ &\leq \frac{e^{\beta Q} e^{cnR_n^d(e^\beta - 1)}}{e^{\beta t}}, \end{aligned}$$

where Q is the number of elements in the partition of $C(x,R)$. Take β sufficiently small so that $\mathbb{E}[e^{cnR_n^d(e^\beta-1)}]<\infty$ (such a β exists by equation (7.27)). We have the conclusion in this first case.

The other possibility is that there exists a cone not wholly included in the cube containing no point of $\mathcal{X}_n$. In this case, the configuration of $\mathcal{X}_n$ is a binomial process conditioned on having at least one point in the cones $A_j(X_1,R_n)$ wholly included in cube and no point in a certain cone not wholly included in the cube. Likewise, a similar bound is shown. □

We are now able to finish the proof of Proposition 7.2.6: for $p\geq 1$,

$$\begin{aligned}
&\mathbb{E}[\mu_q^n(U_M)^p]=\mathbb{E}\left[\left(\frac{N_q(\mathcal{X}_n,M)}{n}\right)^p\right]\\
&\leq\frac{1}{(q+2)^p}\mathbb{E}\left[\left(\frac{\sum_{i=1}^n\mathbf{1}\{R(X_i,\mathcal{X}_n)>M_n\}\left(\#(\mathcal{X}_n\cap C(X_i,R(X_i,\mathcal{X}_n)))\right)^{q+1}}{n}\right)^p\right]\\
&\leq\frac{1}{(q+2)^p}\mathbb{E}\left[\mathbf{1}\{R_n>M_n\}\#(\mathcal{X}_n\cap C(X_1,R_n))^{p(q+1)}\right]\text{ by Jensen's inequality}\\
&\leq\frac{1}{(q+2)^p}\left(P(R_n>M_n)\mathbb{E}[\#(\mathcal{X}_n\cap C(X_1,R_n))^{2p(q+1)}]\right)^{1/2}.
\end{aligned}$$

Lemma 7.4.5 implies that, for $p'>0$,

$$\mathbb{E}\left[\#(\mathcal{X}_n\cap C(X_1,R_n))^{p'}\right]\leq\int_1^\infty ce^{-Ct^{1/p'}}dt=\frac{p'c}{C^{p'}}\int_1^\infty u^{p'-1}e^{-u}du=\frac{c}{C^{p'}}(p')!.$$

Therefore, for $q\geq 1$,

$$\mathbb{E}[\mu_q^n(U_M)^{p/(q+1)}]\leq c\frac{1}{(q+2)^{p/(q+1)}}\exp(-cM^d)\left((2p)!C^{-2p}\right)^{1/2}\leq\exp(-cM^d)c^pp!.$$

To finish the proof, we use a simple lemma relating the moments of a random variable to its tail.

Lemma 7.4.6. *Let X be a positive random variable such that there exists constants $A,C>0$ with*

$$\mathbb{E}[X^k]\leq AC^kk!. \tag{7.28}$$

Then, there exists a constant $c>0$ such that $\forall x>0,\mathbb{P}(X>x)\leq A\exp(-cx)$.

Proof. Fix $\lambda=\frac{1}{2C}$. The moment generating function of X in λ is bounded by:

$$\mathbb{E}\left[e^{\lambda X}\right]=\sum_{k\geq 0}\frac{\lambda^k\mathbb{E}[X^k]}{k!}\leq A\sum_{k\geq 0}\lambda^kC^k=A.$$

Therefore, using a Chernoff bound, $\mathbb{P}(X>x)\leq A\exp(-\lambda x)$. □

Apply Lemma 7.4.6 to $X=\mu_q^n(U_M)^{1/(q+1)}$ to obtain the assertion of Proposition 7.2.6.

7.4.2 Proof of Theorem 7.2.4

Step 1: Convergence for functions vanishing on the diagonal

The first step of the proof is to show that the convergence holds $C_0(\Omega)$, the set of continuous bounded functions vanishing of the diagonal. The crucial part of the proof consists in using Proposition 7.2.6, which bounds the total number of points in the diagrams. An elementary lemma from measure theory is then used to show that it implies the a.s. convergence for vanishing functions. We say that a sequence of measures $(\mu_q^n)_{n\geq 0}$ converges C_0-vaguely to μ if $\mu_q^n(\phi) \to \mu(\phi)$ for all functions ϕ in $C_0(\Omega)$.

Lemma 7.4.7. *Let E be a locally compact Hausdorff space. Let $(\mu_n)_{n\geq 0}$ be a sequence of Radon measure on E which converges vaguely to some measure μ. If $\sup_n |\mu_n| < \infty$, then $(\mu_n)_{n\geq 0}$ converges C_0-vaguely to μ.*

Proof. Let (h_q) be a sequence of functions with compact support converging to 1 and let $\phi \in C_0(E)$. Fix $\varepsilon > 0$. By definition of $C_0(E)$, there exists a compact set K_ε such that f is smaller than ε outside of K_ε. For q large enough, the support of h_q includes K_ε. Let $\phi_q = \phi \cdot h_q$. Then,

$$\begin{aligned}|\mu_n(\phi) - \mu(\phi)| &\leq |\mu_n(\phi) - \mu_n(\phi_q)| + |\mu_n(\phi_q) - \mu(\phi_q)| + |\mu(\phi_q) - \mu(\phi)| \\ &\leq (\sup_n |\mu_n| + |\mu|)\varepsilon + |\mu_n(\phi_q) - \mu(\phi_q)|.\end{aligned}$$

As $(\mu_n)_n$ converges vaguely to μ, the last term of the sum converges to 0 when ε is fixed. Hence, we have $\limsup_{n\to\infty} |\mu_n(\phi) - \mu(\phi)| \leq (\sup_n |\mu_n| + |\mu|)\,\varepsilon$. As this holds for all $\varepsilon > 0$, $\mu_n(\phi)$ converges to $\mu(\phi)$. □

Taking $M = 0$ in Proposition 7.2.6, we see that $\sup_n \mathbb{E}[|\mu_q^n|] < \infty$. Therefore, the C_0-vague convergence of $\mathbb{E}[\mu_q^n]$ is shown in the binomial setting. To show that the convergence also holds almost surely for $|\mu_q^n|$, we need to show that $\sup_n |\mu_q^n| < \infty$. For this, we use concentration inequalities. We do not show concentration inequalities for $|\mu_q^n|$ directly. Instead, we derive concentration inequalities for $\sum_{i=1}^n \#(\mathcal{X}_n \cap C(X_i, R(X_i, \mathcal{X}_n)))^{q+1}$, which is a majorant of $|\mu_q^n|$. Recall that $R(X_i, \mathcal{X}_n)$ is defined as the smallest radius R such that, for some fixed parameter $\eta > 0$, and for each $j = 1 \dots Q$, $A_j(X_i, \eta R)$, either contains a point of $\mathcal{X}_n$ different than X_i, or is not contained in the cube. To ease the notations, we denote $R(X_i, \mathcal{X}_n)$ by $R_{i,n}$.

Lemma 7.4.8. *Fix $M \geq 0$ and define $Z_n^M = \sum_{i=1}^n \#(\mathcal{X}_n \cap C(X_i, R_{i,n}))^q \mathbf{1}\{R_{i,n} \geq M\}$. Then, for every $\varepsilon > 0$, there exists a constant $c_\varepsilon > 0$ such that*

$$\mathbb{P}(|Z_n^M - \mathbb{E}[Z_n^M]| > t) \leq \frac{n^{\frac{3}{2}+\varepsilon}}{t^3} \exp(-c_\varepsilon n^{-1} M^d). \tag{7.29}$$

The constant c_ε depends on ε, d, q and κ.

As a consequence of the concentration inequality, $n^{-1} Z_n^0$ is almost surely bounded. Indeed, choose $\varepsilon < 1/2$:

$$\mathbb{P}(n^{-1}|Z_n^0 - \mathbb{E}[Z_n^0]| > t) \leq \frac{n^{\frac{3}{2}+\varepsilon}}{(nt)^3} = \frac{n^{-\frac{3}{2}+\varepsilon}}{t^3}.$$

By Borel-Cantelli lemma, almost surely, for n large enough, we have $n^{-1}|Z_n^0 - \mathbb{E}[Z_n^0]| \leq 1$. Moreover, $\sup_n n^{-1}\mathbb{E}[Z_n^0]$ is finite. As a consequence, $\sup_n n^{-1} Z_n^0$ is almost surely finite. As this is an upper bound of $\sup_n |\mu_q^n|$, we have proven that $\sup_n |\mu_q^n| < \infty$

almost surely. By Lemma 7.4.7, the sequence μ_q^n converges C_0-vaguely to μ. The proof of Lemma 7.4.8 is based on an inequality of the Efron-Stein type and is rather long and technical. It can be found in Section 7.4.4.

We now briefly consider the Poisson setting. Define $\tilde{\mu}_q^n = \mu_q^{N_n} \times (N_n/n)$, where $(N_i)_{i\geq 1}$ is some sequence of independent Poisson variables of parameter n, independent of $(X_i)_{i\geq 1}$.

- $\mathbb{E}[|\tilde{\mu}_q^n|] = \mathbb{E}\left[\frac{N_n}{n}\mathbb{E}[|\mu_q^{N_n}||N_n]\right] \leq \sup_n \mathbb{E}[|\mu_q^n|] < \infty$. Therefore, C_0-convergence of the expected diagram holds in the Poisson setting.
- Likewise, it is sufficient to show that $\sup_n \frac{N_n}{n} < \infty$ to conclude to the C_0-convergence of the diagram in the Poisson setting. Fix $t > 1$. It is shown in the chapter 1 of the monograph [Pen03] that $\mathbb{P}(N_n > nt) \leq \exp(-nH(t))$, where $H(t) = 1 - t + t\ln t$. This gives us

$$\begin{aligned}\mathbb{P}\left(\sup_n \frac{N_n}{n} \leq t\right) &= \prod_{n\geq 0}(1 - \mathbb{P}(N_n > nt)) \\ &\geq \prod_{n\geq 0}(1 - \exp(-nH(t))) = \exp\left(\sum_{n\geq 0}\ln(1 - \exp(-nH(t)))\right)\end{aligned} \tag{7.30}$$

The series $\sum_n \ln(1 - x^n)$ is equal to $-\sum_n \sigma(n)/nx^n$ when $|x| < 1$, and where $\sigma(n)$ is the sum of the proper divisors of n. Therefore it is a power series, and is continuous on $]-1, 1[$. Since t tends to infinity, $\exp(-H(t))$ converges to 0, and thus the quantity appearing in the right hand side of (7.30) converges to 1 as t tends to infinity.

Step 2: Convergence for functions with polynomial growth

The second step consists in extending the convergence to functions $\phi \in C_{\text{poly}}(\Omega)$. We only show the result for binomial processes. The proof can be adapted to the Poisson case using similar techniques as at the end of Step 1. The core of the proof is a bound on the number of points in a diagram with high persistence. For $M > 0$, define $T_M = \{r = (r_1, r_2) \in \Omega \text{ s.t. } \text{pers}(r) \geq M\}$. Let $P_n(M) = n\mu_q^n(T_M)$ denote the number of points in the diagram with persistence larger than M. We also introduce the quantity $\text{Pers}_\alpha(M; a) := \sum_{u\in a} \text{pers}(u)^\alpha \mathbf{1}\{\text{pers}(u) \geq M\}$ for a a persistence diagram.

First, we show that the expectation of $P_n(M)$ converges to 0 at an exponential rate when M tends to ∞. The random variable $P_n(M)$ is bounded by $n\mu_q^n(U_M)$. By Proposition 7.2.6, recalling that q is the degree of homology,

$$\begin{aligned}\mathbb{E}\big[P_n(M)\big] &\leq \int_0^\infty \mathbb{P}\big(n\mu_q^n(U_M) \geq t\big)dt \\ &\leq \int_0^\infty c\exp\big(-c(M^d + (t/n)^{1/(q+1)}\big)dt \\ &\leq cn\exp(-cM^d)\int_0^\infty \exp(-u)qu^q du = cn\exp\big(-cM^d\big)\end{aligned} \tag{7.31}$$

Fix a sequence (g_M) of continuous functions with support inside the complement of T_M taking their values in $[0, 1]$, equal to 1 on T_{M-1}^c. Let ϕ be a function with polynomial growth, i.e. satisfying (7.21) for some $A, \alpha > 0$. Define $\phi_M = \phi \cdot g_M$. We have the decomposition:

$$\mathbb{E}[\mu_q^n(\phi)] = (\mathbb{E}[\mu_q^n(\phi)] - \mathbb{E}[\mu_q^n(\phi_M)]) + \mathbb{E}[\mu_q^n(\phi_M)]. \tag{7.32}$$

As $\phi_M \in C_0(\Omega)$, the second term on the right converges to $\mu(\phi_M)$. The first term on the right is bounded by

$$\begin{aligned}\mathbb{E}[\mu_q^n(\phi)] - \mathbb{E}[\mu_q^n(\phi_M)] &\leq \mathbb{E}[\mu_q^n(A(1+\mathrm{pers}^\alpha)(1-g_M))] \\ &\leq A\mathbb{E}[P_n(M)]/n + A\mathbb{E}[\mathrm{Pers}_\alpha(M;\mathrm{dgm}_q^K(\mathcal{X}_n))]/n \\ &\leq cA\exp\left(-cM^d\right) + A\mathbb{E}[\mathrm{Pers}_\alpha(M;\mathrm{dgm}_q^K(\mathcal{X}_n))]/n, \end{aligned} \tag{7.33}$$

using inequality (7.31). It is shown in [CS+10] that

$$\mathrm{Pers}_\alpha(M;\mathrm{dgm}_q^K(\mathcal{X}_n)) \leq M^\alpha P_n(M) + \alpha\int_M^\infty P_n(\varepsilon)\varepsilon^{\alpha-1}d\varepsilon.$$

Hence, by Fubini's theorem and inequality (7.31):

$$\mathbb{E}[\mathrm{Pers}_\alpha(M;\mathrm{dgm}_q^K(\mathcal{X}_n))]/n \leq cM^\alpha\exp\left(-cM^d\right) + c\alpha\int_M^\infty \exp\left(-c\varepsilon^d\right)\varepsilon^{\alpha-1}d\varepsilon. \tag{7.34}$$

and this quantity goes to 0 as M goes to infinity. Moreover, applying this inequality to $M=0$, we get that $C_0 = \sup_n \mathbb{E}[\mu_q^n(\phi)] < \infty$. Therefore, $\lim_{n\to\infty}\mathbb{E}[\mu_q^n(\phi_M)] = \mu(\phi_M) \leq C_0$. By the monotone convergence theorem, $\mu(\phi_M)$ converges to $\mu(\phi)$ when ϕ is non negative, with $\mu(\phi)$ finite by the latter inequality. If ϕ is not always non negative, we conclude by separating its positive and negative parts. Finally, looking at the bounds (7.33) and (7.34),

$$\limsup_{n\to\infty}|\mathbb{E}[\mu_q^n(\phi)] - \mu(\phi)| \leq \limsup_{n\to\infty}(\mathbb{E}[\mu_q^n(\phi)] - \mathbb{E}[\mu_q^n(\phi_M)]) + |\mu(\phi_M) - \mu(\phi)| \xrightarrow[M\to\infty]{} 0.$$

We now prove that $\mu_q^n(\phi) - \mathbb{E}[\mu_q^n(\phi)]$ converges a.s. to 0. Similar to the above, it is enough to show that $P_n(M)$ is almost surely bounded by a quantity independent of n, which converges to 0 at an exponential rate when M goes to ∞. The random variable $(q+2)P_n(M)$ is bounded by Z_n^M, which is defined in Lemma 7.4.8, and whose expectation is controlled. Therefore, it remains to show that Z_n^M is close to its expectation. We have

$$\begin{aligned}&\limsup_{n\to\infty}|\mu_q^n(\phi) - \mathbb{E}[\mu_q^n(\phi)]| \\ &\leq \limsup_{n\to\infty}\left(|\mu_q^n(\phi-\phi_M)| + |(\mu_q^n - \mathbb{E}[\mu_q^n])(\phi_M)| + |\mathbb{E}[\mu_q^n](\phi-\phi_M)|\right) \\ &\leq \limsup_{n\to\infty}|\mu_q^n(\phi-\phi_M)| + 0 + cA\exp\left(-cM^d\right) + cM^\alpha\exp\left(-cM^d\right) \\ &\quad + c\alpha\int_M^\infty \exp\left(-c\varepsilon^d\right)\varepsilon^{\alpha-1}d\varepsilon \end{aligned} \tag{7.35}$$

by inequalities (7.33) and (7.34). The random variable $|\mu_q^n(\phi-\phi_M)|$ is bounded by

$$\begin{aligned}&An^{-1}\left(P_n(M) + M^\alpha P_n(M) + \alpha\int_M^\infty P_n(\varepsilon)\varepsilon^{\alpha-1}d\varepsilon.\right) \\ &\leq An^{-1}\left(Z_n^{M_n} + M^\alpha Z_n^{M_n} + \alpha\int_M^\infty Z_n^{\varepsilon_n}\varepsilon^{\alpha-1}d\varepsilon,\right) \end{aligned} \tag{7.36}$$

where $M_n = n^{-1/d}M$ and $\varepsilon_n = n^{-1/d}\varepsilon$. As a consequence of Lemma 7.4.8, by choosing ε so that $-3/2+\varepsilon < -1$,

$$\mathbb{P}\left(\sup_n n^{-1}|Z_n^{M_n} - \mathbb{E}[Z_n^{M_n}]| > t\right) \leq c\frac{\exp(-cM^d)}{t^3}.$$

Fixing $t = \exp(-(c/6)M^d)$ and using Borel-Cantelli lemma, for $M \in \mathbb{N}$ large enough, $\sup_n n^{-1}|Z_n^{M_n} - \mathbb{E}[Z_n^{M_n}]| < \exp(-(c/6)M^d)$. Also, $\mathbb{E}[Z_n^{M_n}] \leq nc\exp(-cM^d)$. Therefore, for $\alpha \geq 0$,

$$\lim_{M\to\infty} \limsup_{n\to\infty} n^{-1} M^\alpha Z_n^{M_n} = 0 \text{ a.s.}$$

The third term in the sum (7.36) is less straightforward to treat. As Z_n^M is a decreasing function of M, for $M \in \mathbb{N}$ large enough and with $k_n = n^{-1/d}k$:

$$\begin{aligned}
\int_M^\infty n^{-1} Z_n^{\varepsilon_n} \varepsilon^{\alpha-1} d\varepsilon &\leq \sum_{k\geq M} n^{-1} Z_n^{k_n} \int_k^{k+1} \varepsilon^{\alpha-1} d\varepsilon \\
&\leq \sum_{k\geq M} c\exp(-ck^d)\frac{1}{\alpha}\left((k+1)^\alpha - k^\alpha\right) \\
&\leq \sum_{k\geq M} c\exp(-ck^d)\frac{k^\alpha 2^\alpha}{\alpha} = o(1).
\end{aligned}$$

As a consequence, $\lim_{M\to\infty}\limsup_n |\mu_q^n(\phi - \phi_M)| = 0$. As the three last terms appearing in inequality (7.35) also converges to 0 when M goes to infinity, we have proven that $\mu_q^n(\phi) - \mathbb{E}[\mu_q^n(\phi)]$ converges a.s. to 0. Therefore, $\mu_q^n(\phi)$ converges a.s. to $\mu(\phi)$.

Finally, we have to prove assertion (ii) in Theorem 7.2.4, i.e. that the convergence holds in L_p. As the convergence holds in probability, it is sufficient to show that $(\mu_q^n(\phi)^p)_n$ is uniformly integrable. Observing that $\mathbb{E}[\mu_q^n(\phi)^p \mathbf{1}\{\mu_q^n(\phi)^p > M\}] \leq \left(\mathbb{E}[\mu_q^n(\phi)^{2p}]\mathbb{P}(\mu_q^n(\phi)^p > M)\right)^{1/2}$, uniform integrability follows from $\sup_n \mathbb{E}[\mu_q^n(\phi)^p] < \infty$ for any $p > 1$. We have

$$\mu_q^n(\phi)^p \leq \mu_q^n(A(1+\text{pers}^\alpha))^p \leq 2^{p-1}(A^p|\mu_q^n|^p + \mu_q^n(\text{pers}^\alpha)^p),$$

and from Proposition 7.2.6 we easily obtain that $\mathbb{E}[|\mu_q^n|^p]$ is uniformly bounded. We treat the other part by assuming without loss of generality that p is an integer:

$$\begin{aligned}
\mathbb{E}[\mu_q^n(\text{pers}^\alpha)^p] &\leq \frac{1}{n^p}\mathbb{E}\left[\left(\int_0^\infty P_n(\varepsilon)\varepsilon^{\alpha-1}d\varepsilon\right)^p\right] \\
&= \frac{1}{n^p}\mathbb{E}\left[\int_{[0,\infty[^p} P_n(\varepsilon_1)\cdots P_n(\varepsilon_p)(\varepsilon_1\cdots\varepsilon_p)^{\alpha-1}d\varepsilon_1\cdots\varepsilon_p\right] \\
&= \frac{1}{n^p}\int_{[0,\infty[^p} \mathbb{E}[P_n(\varepsilon_1)\cdots P_n(\varepsilon_p)](\varepsilon_1\cdots\varepsilon_p)^{\alpha-1}d\varepsilon_1\cdots\varepsilon_p \\
&\leq \frac{1}{n^p}\int_{[0,\infty[^p} \left(\mathbb{E}[P_n(\varepsilon_1)^p]\cdots\mathbb{E}[P_n(\varepsilon_p)^p]\right)^{1/p}(\varepsilon_1\cdots\varepsilon_p)^{\alpha-1}d\varepsilon_1\cdots\varepsilon_p \\
&\leq \frac{1}{n^p}\int_{[0,\infty[^p} \left(n^{p^2}c\exp(-c(\varepsilon_1^d+\cdots+\varepsilon_p^d))\right)^{1/p}(\varepsilon_1\cdots\varepsilon_p)^{\alpha-1}d\varepsilon_1\cdots\varepsilon_p \\
&= c\int_{[0,\infty[^p} \exp\left(-\frac{c}{p}(\varepsilon_1^d+\cdots+\varepsilon_p^d)\right)(\varepsilon_1\cdots\varepsilon_p)^{\alpha-1}d\varepsilon_1\cdots\varepsilon_p \\
&= c\left(\int_0^\infty \exp\left(-\frac{c}{p}\varepsilon^d\right)\varepsilon^{\alpha-1}d\varepsilon\right)^p < \infty.
\end{aligned}$$

7.4.3 Proof of Proposition 7.2.7

The proof relies on the regularity of the number of simplexes appearing at certain scales.

Lemma 7.4.9. *Let $q \geq 0$. For $r_1 < r_2$, let $F_q(\mathcal{X}_n, r_1, r_2)$ be the number of q-simplexes σ in the filtration $K(\mathcal{X}_n)$ with $\phi(\sigma) \in [r_1, r_2]$. Assume that $\mathcal{X}_n$ is a binomial n-sample of density κ. Then,*

$$n^{-1} F_q(n^{1/d}\mathcal{X}_n, r_1, r_2) \xrightarrow[n\to\infty]{L_2} F_q(r_1, r_2), \tag{7.37}$$

where $F_q(r_1, r_2) \leq c r_2^{2dq-1}|r_2 - r_1|$.

Proof. For a finite set $\mathcal{X} \subset \mathbb{R}^d$, define

$$\xi^{r_1,r_2}(x, \mathcal{X}) = \frac{1}{q+1} \sum_{\sigma \in \mathcal{K}_q(\mathcal{X})} \mathbf{1}\{\phi(\sigma) \in [r_1, r_2] \text{ and } x \in \sigma\}.$$

Then, $F_q(\mathcal{X}_n, r_1, r_2) = \sum_{x\in\mathcal{X}} \xi^{r_1,r_2}(x, \mathcal{X}_n)$. In [PY03], the convergence in L_2 of such functionals $\xi(x, \mathcal{X})$ is shown under two conditions. The first one of them is called stabilization. Let $\mathcal{P}$ be a homogeneous Poisson process in $\mathbb{R}^d$. A quantity $\xi(x, \mathcal{X})$ is stabilizing if, with probability one, there exists some random radius $R < \infty$ such that, for all finite sets A which are equal to $\mathcal{P}$ on $\mathcal{B}(0, R)$,

$$\xi(0, \mathcal{P} \cap \mathcal{B}(0, R)) = \xi(0, A),$$

Denote this quantity by $\xi_\infty(\mathcal{P})$. In our case, ξ^{r_1,r_2} is stabilizing with $R = 2r_2$. The second condition is a moment condition: there exists some number $\beta > 2$ such that

$$\sup_n \mathbb{E}[\xi(n^{1/d}X_1, n^{1/d}\mathcal{X}_n)^\beta] < \infty.$$

Once again, ξ^{r_1,r_2} possesses this property: the random variable $\xi^{r_1,r_2}(n^{1/d}X_1, n^{1/d}\mathcal{X}_n)$ is bounded by the number of q-simplexes of $K(\mathcal{X}_n)$ containing X_1 and being included in $\mathcal{B}(X_1, 2n^{-1/d}r_2)$. This number of q-simplexes is bounded by $\#(\mathcal{X}_n \cap \mathcal{B}(X_1, 2n^{-1/d}r_2))^q$, which, in turn, is stochastically dominated by a binomial random variable with parameters n and $cn^{-1}r_2^d$. In particular, its moment of order $3q$ is smaller than a constant independent of n. This means that the moment condition is satisfied. Applying the main theorem of [PY03], convergence (7.37) is obtained, with $F_q(r_1, r_2) = \mathbb{E}[\xi_\infty^{r_1,r_2}(\mathcal{P})]$, where $\xi_\infty^{r_1,r_2}(\mathcal{P}) = \xi^{r_1,r_2}(0, \mathcal{P} \cap \mathcal{B}(0, 2r_2))$. The set $\mathcal{P} \cap \mathcal{B}(0, 2r_2)$ can be expressed as $\{X_1, \ldots, X_N\}$, where $(X_i)_{i\geq 0}$ is a sequence of i.i.d. uniform random variables on $\mathcal{B}(0, 2r_2)$, and N is an independent Poisson variable with parameter cr_2^d. Therefore,

$$\begin{aligned}
\mathbb{E}[\xi_\infty^{r_1,r_2}(\mathcal{P})] &= \mathbb{E}\left[\sum_{i_1,\ldots,i_q} \mathbf{1}\{\phi(\{0, X_{i_1}, \ldots, X_{i_q}\}) \in [r_1, r_2]\}\right] \\
&= \mathbb{E}\left[\frac{N!}{(N-q)!}\right] \mathbb{P}(\phi(\{0, X_1, \ldots, X_q\}) \in [r_1, r_2]) \\
&\leq c r_2^{2dq-1}|r_2 - r_1|.
\end{aligned}$$

The last inequality is a consequence of (i) the fact that the q-th factorial moment of N equals cr_2^{dq}, and (ii) of the following lemma. □

Lemma 7.4.10. *If $X_1, \ldots, X_q$ is a q-sample of the uniform distribution on $\mathcal{B}(0, 2) \subset \mathbb{R}^d$, and r is either the filtration time of the Čech or Rips filtration, then, for any $0 < a < b \leq 2$,*

$$\mathbb{P}(\phi(0, X_1, \ldots, X_q) \in [a, b]) \leq C_{q,d}|a - b|, \tag{7.38}$$

for some constant depending on d and q.

Proof. Such an inequality holds if the filtration time $\phi(0, X_1, \ldots, X_q)$ has a bounded density on $[0, 2]$. We treat separately the case of the Rips and of the Čech filtration.

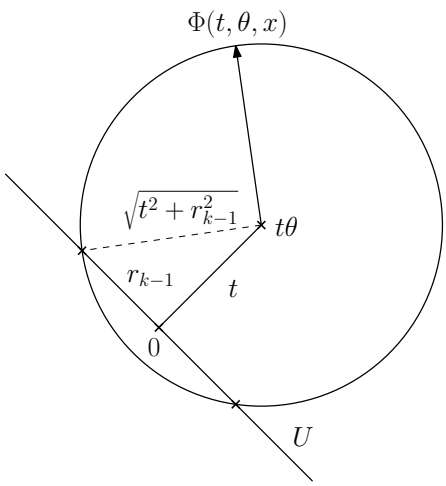


FIGURE 7.5: Definition of Φ. We display the plane $V(\theta)$.

Rips filtration The quantity $\phi(\{0, X_1, \ldots, X_q\}) = \mathrm{diam}(\{0, X_1, \ldots, X_q\})$ is equal to $|X_i|$ or $|X_i - X_j|$ for some indexes i, j. Hence, one has $\mathbb{P}(\phi(0, X_1, \ldots, X_q) \in [a, b]) \leq q\mathbb{P}(|X_1| \in [a, b]) + \frac{q(q-1)}{2}\mathbb{P}(|X_1 - X_2| \in [a, b])$. The random variables $|X_1|$ and $|X_1 - X_2|$ have bounded densities on $[0, 2]$, so that the result follows.

Čech filtration Let $r'(\{x_1, \ldots, x_k\})$ be the radius of the circumsphere of $x_1, \ldots, x_k$. Then, $\phi(x_1, \ldots, x_q) = r'(x_{i_1}, \ldots, x_{i_k})$ for a certain subset of $\{1, \ldots, q\}$. Hence,

$$\mathbb{P}(\phi(0, X_1, \ldots, X_q) \in [a, b]) \leq \sum_{\sigma \subset \{1,\ldots,q\}} (\mathbb{P}(r'(0, X_\sigma) \in [a, b]) + \mathbb{P}(r'(X_\sigma) \in [a, b])). \tag{7.39}$$

We are going to show that $r'(X_\sigma)$ has a bounded density on $[0, 2]$ by induction on k, and it is then shown likewise that $r'(0, X_\sigma)$ has a bounded density. For $k = 2$, $r'(X_\sigma)$ is the distance between X_1 and X_2, which has a bounded density. If $k > 2$, we let r_k be the circumradius of $\{X_1, \ldots, X_k\}$, r_{k-1} the circumradius of $\{X_2, \ldots, X_k\}$, with associated circumcenters z_k, z_{k-1}, respectively, and U be the affine $(k-2)$-dimensional space spanned by $\{X_2, \ldots, X_k\}$. The vector $z_k - z_{k-1}$ is orthogonal to U and therefore $r_k^2 = |z_k - z_{k-1}|^2 + r_{k-1}^2$. For any subspace E, we let π_E be the orthogonal projection onto E, $E^\perp$ be the orthogonal space from E and S_E be the unit sphere in E. Without loss of generality we assume that $z_{k-1} = 0$, so that U is a subspace of $\mathbb{R}^d$. For any $\theta \in S_{U^\perp}$, we let $V(\theta) = U + \mathbb{R}\theta$. Let θ_0 be any vector in $S_{U^\perp}$, with $V_0 = V(\theta_0)$ and introduce the function $\Phi : \mathbb{R}^+ \times S_{U^\perp} \times S_{V_0} \to \mathbb{R}^d$ defined by

$$\Phi(t, \theta, x) = t\theta + \sqrt{t^2 + r_{k-1}^2} R(\theta)x,$$

where $R(\theta)$ is an isometry from V_0 to $V(\theta)$ defined by $R(\theta)x = \pi_U(x) + (x \cdot \theta_0)\theta$ for $x \in V_0$. Notice that, for each $\theta \in S_{U^\top}$, we have $\Phi(t, \theta, x) \in V(\theta)$. See also Figure 7.5.

Fact. *The function Φ is injective and we have $\{r_k \in [a, b]\} \subset \{X_1 \in \Phi(A_{r_{k-1}})\}$, where $A_{r_{k-1}} = M_{a,b} \times S_{U^\perp} \times S_{V_0}$ and $M_{a,b} = \{t \geq 0,\ a^2 \leq t^2 + r_{k-1}^2 \leq b^2\}$.*

The proof of this fact is given below. We continue the proof of the lemma by assuming that the fact holds. Letting λ_d denote the Lebesgue measure on $\mathbb{R}^d$, and c_d^{-1}

the d-dimensional volume of $\mathcal{B}(0,2)$, we have

$$\begin{aligned}\mathbb{P}(r'(X_\sigma)\in[a,b]) &= \mathbb{E}[\mathbb{P}(r_k\in[a,b]|r_{k-1})] \le \mathbb{E}\left[\mathbb{P}(X_1\in\Phi(A_{r_{k-1}})|r_{k-1})\right]\\ &\le c_d\mathbb{E}\left[\lambda_d(\Phi(A_{r_{k-1}}))\right] = c_d\mathbb{E}\left[\int_{A_{r_{k-1}}} J\Phi(t,\theta_1,\theta_2)\mathrm{d}t\mathrm{d}\theta_1\mathrm{d}\theta_2\right] \end{aligned} \tag{7.40}$$

Let us compute the Jacobian $J\Phi(y)$ of Φ at some point $y=(t,\theta,x)\in A_{r_{k-1}}$. The tangent space of $S_{U^\perp}$ at θ is equal to $U^\perp\cap(\mathbb{R}\theta)^\perp = V(\theta)^\perp$ and the tangent space of S_{V_0} at x is equal to $V_0\cap(\mathbb{R}x)^\perp$. We compute the partial derivatives:

$$\begin{aligned}
\partial_t\Phi(y)[h_0] &= \theta h_0 + \frac{th_0}{\sqrt{t^2+r_{k-1}^2}}R(\theta)x, && h_0\in\mathbb{R}\\
\partial_\theta\Phi(y)[h_1] &= h_1 t + \sqrt{t^2+r_{k-1}^2}(x\cdot\theta_0)h_1 && h_1\in V(\theta)^\perp\\
\partial_x\Phi(y)[h_2] &= \sqrt{t^2+r_{k-1}^2}R(\theta)h_2 && h_2\in V_0\cap(\mathbb{R}x)^\perp.
\end{aligned}$$

We decompose the space $\mathbb{R}^d$ as follows. Let $g=R(\theta)x\in V(\theta)$, $G=(\mathbb{R}g)^\perp\cap V(\theta)$, and $H=V(\theta)^\perp$. Then, $\pi_{\mathbb{R}g}+\pi_G+\pi_H=\mathrm{id}$ (recall that π_E denotes the orthogonal projection onto E). Also, note that, as $h_2\in V_0\cap(\mathbb{R}x)^\perp$ is orthogonal to x, and $R(\theta)$ is an isometry, the vector $R(\theta)h_2$ is orthogonal to $g=R(\theta)x$. We have with $s_{k-1}=\sqrt{t^2+r_{k-1}^2}$ that

$$\begin{cases}\pi_{\mathbb{R}g}\partial_t\Phi(y)[h_0] = \left((\theta\cdot g)h_0+\frac{th_0}{s_{k-1}}\right)g\\ \pi_{\mathbb{R}g}\partial_\theta\Phi(y)[h_1]=0\\ \pi_{\mathbb{R}g}\partial_x\Phi(y)[h_2]=0\end{cases}$$

$$\begin{cases}\pi_G\partial_t\Phi(y)[h_0] = \pi_G\theta h_0\\ \pi_G\partial_\theta\Phi(y)[h_1]=0\\ \pi_G\partial_x\Phi(y)[h_2] = s_{k-1}\pi_G R(\theta)h_2\end{cases}$$

$$\begin{cases}\pi_H\partial_t\Phi(y)[h_0]=0\\ \pi_H\partial_\theta\Phi(y)[h_1] = h_1t+s_{k-1}(x\cdot\theta_0)h_1\\ \pi_H\partial_x\Phi(y)[h_2]=0.\end{cases}$$

Hence, remarking that $\pi_G R(\theta)$ is an isometry from $V_0\cap(\mathbb{R}x)^\perp$ to $G=V(\theta)\cap(\mathbb{R}g)^\perp$,

$$\begin{aligned}J\Phi(y) &= \left|\theta\cdot g+\frac{t}{s_{k-1}}\right|\times\left|\det\left(s_{k-1}\pi_G R(\theta)_{|V_0\cap(\mathbb{R}x)^\perp}\right)\right|\times\left|\det\left((t+s_{k-1}x\cdot\theta_0)\,\mathrm{id}_H\right)\right|\\ &\le 2\times s_{k-1}^{k-2}\times(t+s_{k-1}x\cdot\theta_0)^{d-k+1}\\ &\le 2^{d-k+2}s_{k-1}^{d-1}.\end{aligned}$$

Therefore, letting $t_0=\sqrt{a^2-r_{k-1}^2}$ and $t_1=\sqrt{b^2-r_{k-1}^2}$, we may bound (7.40) as follows

$$\begin{aligned}\mathbb{P}(r'(X_\sigma)\in[a,b]) &\le c_d\mathbb{E}\left[\int_{A_{r_{k-1}}} 2^{d-k+2}\left(t^2+r_{k-1}^2\right)^{(d-1)/2}\mathrm{d}t\mathrm{d}\theta_1\mathrm{d}\theta_2\right]\\ &\le c_{d,k}\mathbb{E}\left[\int_{t_0}^{t_1}(t^2+r_{k-1}^2)^{(d-1)/2}\mathrm{d}t\right]\end{aligned}$$

Introduce $F : x \mapsto \int_0^{\sqrt{x^2-r_{k-1}^2}} (t^2 + r_{k-1}^2)^{(d-1)/2} \mathrm{d}t$. Then,

$$F'(x) = x^{d-1} \times \frac{x}{\sqrt{x^2 - r_{k-1}^2}} = \frac{x^d}{\sqrt{x^2 - r_{k-1}^2}}$$

and, letting f_{k-1} be the density of r_{k-1} on $[0, 2]$,

$$\begin{aligned}
\mathbb{P}(r'(X_\sigma) \in [a, b]) &\leq c_{d,k} \mathbb{E}\left[\int_a^b F'(x) \mathrm{d}x\right] \\
&\leq c_{d,k} \int_a^b \int_0^b \mathbf{1}\{x \geq r_{k-1}\} f_{k-1}(r_{k-1}) \frac{x^d}{\sqrt{x^2 - r_{k-1}^2}} \mathrm{d}x \mathrm{d}r_{k-1} \\
&\leq c'_{d,k} \int_a^b x^d \int_0^x \frac{1}{\sqrt{x^2 - r_{k-1}^2}} \mathrm{d}r_{k-1} \mathrm{d}x \\
&\leq c'_{d,k,} \int_a^b x^d \int_0^1 \frac{1}{\sqrt{1 - u^2}} \mathrm{d}u \mathrm{d}x \leq c''_{d,k} |b - a|,
\end{aligned}$$

where at the last line we used that the function $x \mapsto x^d$ is bounded on $[0, 2]$. Hence, $r'(X_\sigma)$ has a bounded density on $[0, 2]$, and the induction step is proven. It remains to verify the Fact.

Proof of Fact. We first prove the injectivity. Let $v = \Phi(t, \theta, x)$ for some $y = (t, \theta, x) \in \mathbb{R}^+ \times S_{U^\perp} \times S_{V_0}$. Then, $\pi_{U^\perp}(y)$ is colinear with θ, so that θ is determined up to a sign by y. Let S_1 be the sphere in U, centered at 0, of radius r_{k-1}, and let S_2 be the unique sphere in $V(\theta)$ containing both y and S_1. Then $y \in S_2$, while the center of S_2 is $t\theta$, so that t and θ are uniquely determined by y. It follows that $R(\theta)x = \frac{y - t\theta}{\sqrt{t^2 + r_{k-1}^2}}$ is also uniquely determined by y, and so is x, showing the injectivity of Φ.

Let $t = |z_k - z_{k-1}|$ and $\theta = (z_k - z_{k-1})/t$. As $z_k - z_{k-1}$ is orthogonal to U, we have $\theta \in S_{U^\perp}$. The point X_1 lies inside the sphere of the space spanned by U and $z_k - z_{k-1}$, centered at z_k, of radius $r_k = \sqrt{t^2 + r_{k-1}^2} \in [a, b]$. Therefore, $X_1 = t\theta + \sqrt{t^2 + r_{k-1}^2} y$, where y is some unit vector in $V(\theta)$, which can be written as $R(\theta)x$ for some $x \in V_0$. Hence, $X_1 \in \Phi(A_{r_{k-1}})$. This completes the proof of the Fact and of the lemma. □

We may now prove Proposition 7.2.7. Fix $0 < r_1 < r_2$. We wish to show that, as r_1 and r_2 get closer, $(\pi_1)_\# \mu_q^\kappa(]r_1, r_2[)$ goes to 0. By the Portemanteau Theorem, $(\pi_1)_\# \mu_q^\kappa([r_1, r_2]) \leq \liminf_n (\pi_1)_\# \mu_q^n(]r_1, r_2[)$. It is shown in Lemma 7.4.9 that this quantity is smaller than $c r_2^{2dq-1} |r_2 - r_1|$, a quantity which converges to 0 when r_2 goes to r_1. A similar proof holds for $(\pi_2)_\# \mu_q^\kappa$.

7.4.4 Proof of Lemma 7.4.8

The lemma is based on an inequality of the Efron-Stein type, combined with Markov's inequality.

Theorem 7.4.11 (Theorem 2 in [Bou+05]). *Let $\mathcal{X}$ be a measurable set and $F : \mathcal{X}^n \to \mathbb{R}$ a measurable function. Define a n-sample $\mathcal{X}_n = \{X_1, \ldots, X_n\}$ and let $Z = F(\mathcal{X}_n)$. If $\mathcal{X}'_n$ is an independent copy of $\mathcal{X}_n$, denote $Z'_i = F(X_1, \ldots, X_{i-1}, X'_i, X_{i+1}, \ldots, X_n)$. Define*

$$V = \sum_{i=1}^n \mathbb{E}[(Z - Z'_i)^2 | \mathcal{X}_n].$$

Then, for $p \geq 2$, there exists a constant C_p depending only on p such that

$$\mathbb{E}[|Z - \mathbb{E}[Z]|^p] \leq C_p \mathbb{E}[V^{p/2}].$$

Denote $\mathcal{X}_n^i = \mathcal{X}_n \backslash \{X_i\}$ and $S(X_i, \mathcal{X}_n) = \#(\mathcal{X}_n \cap C(X_i, R_{i,n}))^q \mathbf{1}\{R_{i,n} \geq M\}$. We will apply Theorem 7.4.11 to $F(\mathcal{X}_n) = \sum_{i=1}^n S(X_i, \mathcal{X}_n)$. The quantity $(Z - Z_i')^2$ is bounded by $2(Z - Z_i)^2 + 2(Z_i' - Z_i)^2$, where $Z_i = F(\mathcal{X}_n^i)$. For most X_j's, $S(X_j, \mathcal{X}_n) = S(X_j, \mathcal{X}_n^i)$, and therefore V can be efficiently bounded. More precisely,

$$\begin{aligned}
\mathbb{E}[V^{p/2}] &= \mathbb{E}\left[\left(\sum_{i=1}^n \mathbb{E}[(Z - Z_i')^2 | \mathcal{X}_n]\right)^{p/2}\right] \\
&\leq n^{p/2} \mathbb{E}[(Z - Z_n')^p] && \text{(by Jensen's inequality)} \\
&\leq n^{p/2} 2^{p-1} \mathbb{E}[(Z - Z_n)^p + (Z_n' - Z_n)^p] \\
&= n^{p/2} 2^p \mathbb{E}[(Z - Z_n)^p] \text{ as } (Z, Z_n) \sim (Z_n', Z_n) \\
&= 2^p n^{p/2} \mathbb{E}\left[\left(S(X_n, \mathcal{X}_n) + \sum_{j=1}^{n-1} (S(X_j, \mathcal{X}_n) - S(X_j, \mathcal{X}_{n-1}))\right)^p\right] \\
&\leq 2^p n^{p/2} 2^{p-1} \left(\mathbb{E}[S(X_n, \mathcal{X}_n)^p] + \mathbb{E}\left[\left(\sum_{j=1}^{n-1} (S(X_j, \mathcal{X}_n) - S(X_j, \mathcal{X}_{n-1}))\right)^p\right]\right).
\end{aligned} \tag{7.41}$$

Fix $p = 3$. Lemma 7.4.5 shows that for $p \geq 1$, $B_p = \sup_n \mathbb{E}[S(X_n, \mathcal{X}_n)^p] < \infty$. Define $Y_j = (S(X_j, \mathcal{X}_n) - S(X_j, \mathcal{X}_{n-1}))$. Denote G_j the event that $X_n \in C(X_j, R_{j,n-1})$. If G_j is not realized, then $Y_j = 0$. Expanding the product,

$$\begin{aligned}
\mathbb{E}\left[\left(\sum_{j=1}^{n-1} (S(X_j, \mathcal{X}_n) - S(X_j, \mathcal{X}_{n-1}))\right)^3\right] &\leq \sum_{j_1, j_2, j_3} \mathbb{E}\left[\mathbf{1}\{G_{j_1} \cap G_{j_2} \cap G_{j_3}\} Y_{j_1} Y_{j_2} Y_{j_3}\right] \\
&\leq \sum_{j_1, j_2, j_3} \mathbb{P}\left(G_{j_1} \cap G_{j_2} \cap G_{j_3}\right)^{1/q'} \mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{p'}\right]^{1/p'},
\end{aligned} \tag{7.42}$$

where $\frac{1}{p'} + \frac{1}{q'} = 1$ and $p' \geq 1$ is some quantity to be fixed later.

- We first bound $\mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{p'}\right]$. If $Y_{j_1} \neq 0$, then $R_{j_1,n-1} > M$. Therefore,

$$\mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{p'}\right] \leq \sqrt{\mathbb{P}(R_{j_1,n-1} > M) \mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{2p'}\right]}.$$

Also, $\mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{2p'}\right] \leq \mathbb{E}\left[Y_{j_1}^{6p'}\right] \leq B_{6p'}$, as $0 \leq Y_{j_1} \leq S(X_{j_1}, \mathcal{X}_n)$. Therefore, using inequality (7.26):

$$\mathbb{E}\left[(Y_{j_1} Y_{j_2} Y_{j_3})^{p'}\right] \leq c \exp(-cM^d).$$

- We now bound the probability $\mathbb{P}(G_{j_1} \cap G_{j_2} \cap G_{j_3})$.

If $j_1 = j_2 = j_3$, then it is clear that $\mathbb{P}(G_{j_1} \cap G_{j_2} \cap G_{j_3}) \leq c/n$. However, in the general case, the joint law of the different $R_{j_i,n-1}$s becomes of interest. To ease the notation, assume that $j_i = i$ and denote $R_{i,n-1}$ simply by R_i. Also, define D_{ij} the distance between X_i and X_j. The fact that inequality (7.26) still holds conditionally on X_1, X_2 and X_3, and with the joint laws of R_1, R_2 and R_3, will be repeatedly used.

Lemma 7.4.12. *The following bound holds:*

$$\mathbb{P}(R_1 \geq t_1, R_2 \geq t_2, R_3 \geq t_3 | X_1, X_2, X_3) \leq c \exp\big(- cn(t_1^d + t_2^d + t_3^d)\big) \tag{7.43}$$

Proof. Suppose that $\max t_i = t_1$. Inequality (7.26) states that $\mathbb{P}(R_1 \geq t_1) \leq c\exp(-cnt_1^d)$. Likewise, it is straightforward to show that a similar bound holds conditionally on X_1, X_2 and X_3. As $t_1^d \geq \frac{t_1^d+t_2^d+t_3^d}{3}$, the result follows. □

Let us prove that $\mathbb{P}(G_1 \cap G_2) \leq c/n^2$. If the event is realized, then X_n is in the intersection of $C(X_1, R_1)$ and $C(X_2, R_2)$. Therefore, this intersection is non empty and $D_{12} \leq \sqrt{d}(R_1 + R_2)$. Hence,

$$\begin{aligned}
\mathbb{P}(G_1 \cap G_2) &\leq \mathbb{P}(D_{12} \leq \sqrt{d}(R_1 + R_2) \text{ and } X_n \in C(X_1, R_1) \cap C(X_2, R_2)) \\
&\leq 2\mathbb{P}(D_{12} \leq 2\sqrt{d}R_1 \text{ and } X_n \in C(X_1, R_1)) \\
&= 2\mathbb{E}\left[\mathbf{1}\{D_{12} \leq 2\sqrt{d}R_1\} P(X_n \in C(X_1, R_1) | \mathcal{X}_{n-1})\right] \\
&\leq 2c\mathbb{E}\left[\mathbf{1}\{D_{12} \leq 2\sqrt{d}R_1\} R_1^d\right] \\
&\leq 2c\mathbb{E}\left[\int_{(D_{12}/(2\sqrt{d}))^d} P(R_{1,n-1}^d \geq t | X_1, X_2) dt\right] \\
&\leq 2c\mathbb{E}\left[\int_{(D_{12}/(2\sqrt{d}))^d} \exp(-cnt) dt\right] \\
&\leq \frac{c}{n}\mathbb{E}\left[\exp(-cnD_{12}^d)\right] \\
&= \frac{c}{n}\int_0^1 \mathbb{P}(cnD_{12}^d \leq -\ln(t)) dt \\
&\leq \frac{c}{n}\int_0^1 \frac{-\ln(t)}{cn} dt = \frac{c}{n^2}.
\end{aligned}$$

Finally, we bound $\mathbb{P}(G_1 \cap G_2 \cap G_3)$. If the event is realized, then

$$\begin{cases} D_{12} \leq \sqrt{d}(R_1 + R_2) \\ D_{23} \leq \sqrt{d}(R_2 + R_3) \\ D_{13} \leq \sqrt{d}(R_1 + R_3) \end{cases} \implies \begin{cases} D_{12} \leq 2\sqrt{d}R_1 \text{ or } D_{12} \leq 2\sqrt{d}R_2 \\ D_{23} \leq 2\sqrt{d}R_2 \text{ or } D_{23} \leq 2\sqrt{d}R_3 \\ D_{13} \leq 2\sqrt{d}R_1 \text{ or } D_{13} \leq 2\sqrt{d}R_3 \end{cases}$$

This last event is an union of eight events. Each of these event is either bounded by an event of the form $(D_{12} \leq 2\sqrt{d}R_1$ and $D_{13} \leq 2\sqrt{d}R_1)$ (six events), or by an event of the form $(D_{12} \leq 2\sqrt{d}R_1$ and $D_{23} \leq 2\sqrt{d}R_2$ and $D_{13} \leq 2\sqrt{d}R_3)$ (two events). Using this, we obtain

$$\begin{aligned}
&\mathbb{P}(G_1 \cap G_2 \cap G_3) \\
&\quad \leq 6\mathbb{P}(X_n \in C(X_1, R_1) \text{ and } D_{12} \leq 2\sqrt{d}R_1 \text{ and } D_{13} \leq 2\sqrt{d}R_1) \\
&\quad + 2\mathbb{P}(X_n \in C(X_1, R_1) \text{ and } D_{12} \leq 2\sqrt{d}R_1 \text{ and } D_{23} \leq 2\sqrt{d}R_2 \text{ and } D_{13} \leq 2\sqrt{d}R_3) \\
&\quad \leq c\mathbb{E}[R_1^d \mathbf{1}\{D_{12} \leq 2\sqrt{d}R_1 \text{ and } D_{13} \leq 2\sqrt{d}R_1\}] \\
&\quad + c\mathbb{E}[R_1^d \mathbf{1}\{D_{12} \leq 2\sqrt{d}R_1 \text{ and } D_{23} \leq 2\sqrt{d}R_2 \text{ and } D_{13} \leq 2\sqrt{d}R_3\}] \\
&\quad = c\mathbb{E}\left[\int_{\left(\frac{\max(D_{12}, D_{13})}{2\sqrt{d}}\right)^d}^{\infty} \mathbb{P}(R_1^d \geq u | X_1, X_2, X_3) du\right] \\
&\quad + c\mathbb{E}\left[\int_{\left(\frac{D_{12}}{2\sqrt{d}}\right)^d}^{\infty} \mathbb{P}\left(R_1^d \geq u \text{ and } R_2 \geq \frac{D_{23}}{2\sqrt{d}} \text{ and } R_3 \geq \frac{D_{13}}{2\sqrt{d}} \middle| X_1, X_2, X_3\right) du\right]
\end{aligned}$$

$$
\begin{aligned}
&\leq c\mathbb{E}\left[\int_{\left(\frac{\max(D_{12},D_{13})}{2\sqrt{d}}\right)^d}^{\infty} e^{-cnu}du\right] + c\mathbb{E}\left[\int_{\left(\frac{D_{12}}{2\sqrt{d}}\right)^d}^{\infty} e^{\left(-cn(u+D_{23}^d+D_{13}^d)\right)}du\right] \\
&= \frac{c}{n}\mathbb{E}\left[e^{-cn\max(D_{12},D_{13})^d}\right] + \frac{c}{n}\mathbb{E}\left[e^{-cn(D_{12}^d+D_{23}^d+D_{13}^d)}\right] \\
&\leq 2\frac{c}{n}\mathbb{E}\left[e^{-cn\max(D_{12},D_{13})^d}\right] = \frac{c}{n}\int_0^1 \mathbb{P}\left(\max(D_{12},D_{13})^d \leq \frac{-\ln(t)}{cn}\right)dt \\
&\leq \frac{c}{n}\int_0^1 \left(\frac{-\ln(t)}{cn}\right)^2 dt = \frac{c}{n^3}.
\end{aligned}
$$

Finally, inequality (7.42) becomes

$$
\begin{aligned}
\mathbb{E}[V^{3/2}] &\leq cn^{3/2}(\exp(-cM^d) + \exp(-cM^d)(n^{1-1/q'} + n^{2-2/q'} + n^{3-3/q'}) \\
&\leq cn^{3/2+3(1-1/q')}\exp(-cM^d).
\end{aligned}
$$

Choose $p' = 3/\varepsilon$ and apply Markov inequality to conclude.

Chapter 8

The expected persistence diagram

We have established in the previous chapter various properties of the behavior of linear representations of persistence diagrams by taking two approaches: studying their stability, and their asymptotic behavior under certain generative models. In this chapter, we focus on the behavior of linear representations in a random non-asymptotic setting. Assume that $a_1, \ldots, a_n \sim P$ is a n-sample of persistence diagrams. To analyze this sample, one can choose a linear representation Ψ_f, and consider the vectors $\Psi_f(a_1), \ldots, \Psi_f(a_n)$. If one wants to understand the behavior of this random sample, it is probably best to start by considering simple quantities such as the sample mean

$$\frac{\Psi_f(a_1) + \cdots + \Psi_f(a_n)}{n}, \tag{8.1}$$

which approximates the expectation $\mathbb{E}_{a\sim P}[\Psi_f(a)]$. As $\Psi_f(a) = a(f)$, the integration of f against a seen as a measure, this is in turn equal to $\int_\Omega f(u)\mathrm{d}\mathbb{E}[a](u)$, where $\mathbb{E}[a]$ is the expected value of the random measures $a \sim P$. We call this object, which is central to understand the average behavior of linear representations of persistence diagrams, the *expected persistence diagram of* P, that we denote either by $\mathbb{E}_{a\sim P}[a]$ or $E(P)$.

We show in the following various properties of expected persistence diagrams. First, we show that expected persistence diagrams possess a (smooth) density in a wide variety of settings (i.e. for filtrations built on top of random point clouds, but also for the sublevel sets of random functions such as the Brownian motion, see Section 8.2).

Second, we inquire about stability properties of the expected persistence diagram: if P_1 and P_2 are close, then so should be $E(P_1)$ and $E(P_2)$. Stability is treated in two different ways. When no assumptions are made on the underlying laws P_1 and P_2, we prove a general 1-Lipschitz inequality with respect to the Wasserstein distance between P_1 and P_2. When the persistence diagrams are built on top of random point clouds, Section 8.2 ensures that the corresponding expected persistence diagrams possess densities on Ω. In that case, we are then able to give stronger stability results relating the densities of the expected persistence diagrams and the densities of the underlying processes, see Section 8.2.4.

We then focus on the estimation of the expected persistence diagram in a statistical setting. Given a n-sample $a_1, \ldots, a_n$ of law $P \in \mathcal{P}_1(\mathcal{D})$, we study in Section 8.3 a very natural estimator, the *empirical expected persistence diagram*, defined by

$$\overline{a}_n := \frac{a_1 + \cdots + a_n}{n}. \tag{8.2}$$

We show that this estimator is a minimax estimator of the expected persistence diagram $E(P)$ with respect to the FG_p-distance on a large class of models, with a minimax rate of order $n^{-1/(2p)}$. More surprisingly, we show that this estimator is minimax even on models where $E(P)$ is assumed to have a smooth density, with the same rate of

convergence. The empirical expected persistence diagram has the advantage of being very simple (it consists in "superposing" the different persistence diagrams $a_1, \dots, a_n$), but has the drawback of being possibly very large, its number of points being equal to the total number of points in all the persistence diagrams of the sample. To overcome this issue, we consider in Section 8.5 the quantization of the expected persistence diagram: given a fixed number of points k, this is the best approximation of the expected persistence diagram supported on k points. We propose an online algorithm to compute a quantization of the empirical expected persistence diagram and show that—provided a good initialization—the output of our algorithm approximates a quantization of the expected persistence diagram at an appropriate rate. Both the performance of the empirical expected persistence diagram and of its quantization are then illustrated on synthetic examples.

Finally, we investigate in Section 8.4 the estimation of $E(P)$ with respect to the L_2-norm on Ω in the case where $E(P)$ possesses a density. In that case, we show that smoothing the empirical persistence diagram $\overline{a}_n$ is a good idea, and that such an object is related to the persistence surface of a diagram introduced by [Ada+17]. We then propose a selection procedure for the smoothing parameter and showcase our procedure on simple numerical experiments.

Throughout this chapter, persistence diagrams in numerical experiments are computed using the `Gudhi` library [Mar+14] and FG_p distances are computed building on tools available from the `POT` library [FC17].

8.1 The expected persistence diagram

Given a probability distribution $P \in \mathcal{P}_1(\mathcal{M}(\Omega))$, the expected persistence diagram $E(P)$ associated to P is given by the relation $E(P)(A) := \mathbb{E}[\mu(A)]$ if $\mu \sim P$ and $A \subset \Omega$ a Borel set. Note that by Fubini's theorem, this assignment indeed defines a Radon measure on Ω as long as the minimal requirement $\mathbb{E}[\mu(K)] < \infty$ for every compact set $K \subset \Omega$ is satisfied (we then say that P is integrable). Of particular interest for us is the case where P is supported on $\mathcal{D} \subset \mathcal{M}(\Omega)$, that is $\mu \sim P$ is always a persistence diagram, although all the results of this section hold without this assumption. It is useful to know when the expected persistence diagram $E(P)$ actually belongs to $\mathcal{M}^p$ (and can therefore be compared using the Figalli-Gigli metrics FG_p). We show that this condition is equivalent to having $P \in \mathcal{P}_1^p(\mathcal{M}^p)$. Furthermore, in that case, an alternative way of defining the expected persistence diagram is possible. Let $I_p : \mathcal{M}^p \to \mathcal{P}(\Omega)$ be the function defined by $I_p(\mu) = \mu^{(p)}$, the measure with density $d(\cdot, \partial\Omega)^p$ with respect to $\mu \in \mathcal{M}^p$ introduced in Chapter 6. The space $\mathcal{P}(\Omega)$ endowed with the total variation is a Banach space, so that the Bochner integral is well-defined in this space, see e.g. [Die84, Chapter 4]. Therefore, an alternative possibility to define $E(P)$ is to pushforward P to $\mathcal{P}(\Omega)$ with I^p, define the expected value in the Banach space using the Bochner integral, and then go back to $\mathcal{M}^p$ with I_p^{-1}. We show that this definition is equivalent to the first one, and it will sometimes be useful to use this alternative definition to exploit properties of the Bochner integral.

Lemma 8.1.1. *Let P be an integrable probability distribution on $\mathcal{P}_1(\mathcal{M}(\Omega))$ and let $1 \le p \le \infty$. Let $\mu \sim P$. Then, we have the equivalence*

1. $E(P) \in \mathcal{M}^p$,
2. $P \in \mathcal{P}_1^p(\mathcal{M}^p)$,
3. $\mathbb{E}[\mathrm{Pers}_p(\mu)] < \infty$.

Furthermore, in that case, for $p < \infty$, we have $E(P) = I_p^{-1}(\mathbb{E}[I^p(\mu)])$, where $\mathbb{E}[I^p(\mu)]$ is the Bochner integral of $I^p(\mu)$ in the Banach space $(\mathcal{P}(\Omega), |\cdot|)$.

Proof. The equivalence between the two last items follows from the definition of $\mathcal{P}_1^p(\mathcal{M}^p)$, as $\mathrm{Pers}_p(\mu) = \mathrm{FG}_p^p(\mu, 0)$. To prove the equivalence between the first and the last item, it suffices to show that $\mathrm{Pers}_p(E(P)) = \mathbb{E}[\mathrm{Pers}_p(\mu)]$. This is implied by writing $d(\cdot, \partial\Omega)^p$ as a simple function $\sum_i a_i \mathbf{1}\{A_i\}$ for some positive numbers a_i and Borel sets A_i, and then using the definition of $E(P)$ as well as Fubini's theorem.

Also, the random variable $I^p(\mu)$ is Bochner integrable if $\mathbb{E}[|I^p(\mu)|] < \infty$, with $|I^p(\mu)| = \mathrm{Pers}_p(\mu)$. Therefore, we indeed have the Bochner integrability of $I^p(\mu)$, with, for $K \subset \Omega$ a compact set,

$$\begin{aligned} I_p^{-1}(\mathbb{E}[I^p(\mu)])(K) &= \int_K \frac{1}{d(u, \partial\Omega)^p} \mathrm{d}\mathbb{E}[I^p(\mu)](u) = \mathbb{E}\left[\int_K \frac{1}{d(u, \partial\Omega)^p} \mathrm{d}I^p(\mu)(u)\right] \\ &= \mathbb{E}\left[\int_K \mathrm{d}\mu(u)\right] = \mathbb{E}[\mu](K), \end{aligned}$$

with the second equality following from properties of the Bochner integral (namely, that the expectation commutes with continuous linear forms). □

We now address the question of the stability of the expected persistence diagram with respect to the underlying phenomenon generating them. As a first result, we exploit the convexity of the function FG_p^p and use Jensen's inequality to give a simple inequality relating the distance between two expected persistence diagrams $E(P_1)$ and $E(P_2)$ and the Wasserstein distance $W_{p,\mathrm{FG}_p}(P_1, P_2)$ between the associated probability measures.

Proposition 8.1.2. *Let $P_1, P_2 \in \mathcal{P}_1^p(\mathcal{D}^p)$. Then,*

$$\mathrm{FG}_p(E(P_1), E(P_2)) \leq W_{p,\mathrm{FG}_p}(P_1, P_2). \tag{8.3}$$

To prove Proposition 8.1.2, we first show that the function FG_p^p is convex.

Lemma 8.1.3. *For $1 \leq p < \infty$, the function $\mathrm{FG}_p^p : \mathcal{M}^p \times \mathcal{M}^p \to \mathbb{R}$ is convex.*

Proof. Fix $\mu_1, \mu_2, \nu_1, \nu_2 \in \mathcal{M}^p$ and $t \in [0, 1]$. Our goal is to show that

$$\mathrm{FG}_p^p(t\mu_1 + (1-t)\mu_2, t\nu_1 + (1-t)\nu_2) \leq t\mathrm{FG}_p^p(\mu_1, \nu_1) + (1-t)\mathrm{FG}_p^p(\mu_2, \nu_2).$$

Let $\pi_{11} \in \mathrm{Opt}_p(\mu_1, \nu_1)$ and $\pi_{22} \in \mathrm{Opt}_p(\mu_2, \nu_2)$. It is straightforward to check that $\pi := t\pi_{11} + (1-t)\pi_{22}$ is an admissible plan between $t\mu_1 + (1-t)\mu_2$ and $t\nu_1 + (1-t)\nu_2$. The cost of this admissible plan is $t\mathrm{FG}_p^p(\mu_1, \nu_1) + (1-t)\mathrm{FG}_p^p(\mu_2, \nu_2)$, which is therefore larger than $\mathrm{FG}_p^p(t\mu_1 + (1-t)\mu_2, t\nu_1 + (1-t)\nu_2)$. □

We then use the following result, which is a particular case of [Per74, Theorem 3.10].

Proposition 8.1.4. *Let $(V, \|\cdot\|)$ be a Banach space and $C \subset \mathcal{X}$ a closed convex set. Let Q be a probability measure on $\mathcal{X}$ endowed with its Borelian σ-algebra, which is supported on C. Assume that $\int \|x\| \mathrm{d}Q(x) < \infty$. Let $f : C \to [0, \infty)$ be a continuous convex function with $\int f(x)\mathrm{d}Q(x) < \infty$. Then*

$$f\left(\int x \mathrm{d}Q(x)\right) \leq \int f(x)\mathrm{d}Q(x),$$

where $\int x\mathrm{d}Q(x)$ denotes the Bochner integral of x with respect to Q.

Proof of Proposition 8.1.2. Let $V = \mathcal{C}_b(\Omega)^* \times \mathcal{C}_b(\Omega)^*$ which is a Banach space (endowed with the product total variation norm). Let $C = \mathcal{P}(\Omega) \times \mathcal{P}(\Omega)$, which is convex and closed (closedness follows immediately from the definition of the total variation $|\cdot|$) and let $f = \mathrm{FG}_p^p \circ (I_p^{-1}, I_p^{-1}) : C \to \mathbb{R}$. The continuity of I_p^{-1} implies that f is continuous and Lemma 8.1.3 implies the convexity of f. Let P_1, P_2 be two probability measures in $\mathcal{P}_1^p(\mathcal{M}^p)$ and γ be an optimal coupling between P_1 and P_2. We let Q be the image measure of γ by (I_p, I_p), so that

$$\begin{aligned}\int_{x\in V} \|x\| \mathrm{d}Q(x) &= \int_{\mu_1,\mu_2\in\mathcal{M}^p} \max(|\mu_1^{(p)}|, |\mu_2^{(p)}|)\mathrm{d}\gamma(\mu_1,\mu_2) \\ &\leq \int_{\mu_1} \mathrm{Pers}_p(\mu_1)\mathrm{d}P_1(\mu_1) + \int_{\mu_2} \mathrm{Pers}_p(\mu_2)\mathrm{d}P_2(\mu_2) < \infty\end{aligned}$$

and that

$$\int_{x\in V} f(x)\mathrm{d}Q(x) = \int_{\mu_1,\mu_2\in\mathcal{M}^p} \mathrm{FG}_p^p(\mu_1,\mu_2)\mathrm{d}\gamma(\mu_1,\mu_2) = W^p_{p,\mathrm{FG}_p}(P_1,P_2) < \infty.$$

Also, we have

$$\begin{aligned}\int_{x\in V} x\mathrm{d}Q(x) &= \int_{\nu_1,\nu_2\in\mathcal{M}^p} (\nu_1,\nu_2)\mathrm{d}(I_p,I_p)_\#\gamma(\nu_1,\nu_2) \\ &= \left(\int_{\nu_1\in\mathcal{M}^p} \nu_1 \mathrm{d}(I_p)_\# P_1(\nu_1), \int_{\nu_2\in\mathcal{M}^p} \nu_2 \mathrm{d}(I_p)_\# P_2(\nu_2)\right),\end{aligned}$$

so that by Lemma 8.1.1, $f\left(\int x\mathrm{d}Q(x)\right) = \mathrm{FG}_p^p(\mathbb{E}[\mu_1], \mathbb{E}[\mu_2])$, where $\mu_1 \sim P_1$ and $\mu_2 \sim P_2$. Proposition 8.1.2 yields the conclusion. □

Using stability results on the distances d_p $(= \mathrm{FG}_p)$ between persistence diagrams (see Section 3.8.4), one is able to obtain a more precise control between the expectations in some situations.

Proposition 8.1.5. *Let ξ_1, ξ_2 be two probability distributions on some metric space $(\mathcal{X}, d)$ which implies bounded p'-total persistence and let $p \leq p'+1$. Fix an integer $q \geq 0$. For $i = 1, 2$, let $\mathcal{X}_n^{(i)}$ be a set of n random i.i.d. points sampled according to ξ_i. Then,*

$$\mathrm{FG}_p(\mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)})], \mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})]) \leq C_{p,p'} n^{1/p} W_{p-p'}(\xi_1,\xi_2)^{1-\frac{p'}{p}}. \tag{8.4}$$

Letting $p \to \infty$, we obtain the following simple bottleneck stability result

$$\mathrm{FG}_\infty(\mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)})], \mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})]) \leq W_\infty(\xi_1,\xi_2). \tag{8.5}$$

Spaces implying bounded total persistence include for instance compact Riemannian manifolds, graphs, or simplicial complexes. For $p < \infty$, the bound in (8.4) is of order $n^{1/p}$. This constant is however not tight, see Chapter 7 for asymptotic results on $\mathrm{dgm}_q^C \mathcal{X}_n^{(i)})$ for n-samples on the cube.

Proof. Let P_1 be the law of $\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)})$, P_2 be the law of $\mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})$ and let γ be any coupling between $\mathcal{X}_n^{(1)}$ a n-sample of law ξ_1, and $\mathcal{X}_n^{(2)}$ a n-sample of law ξ_2. Then, the law of $(\mathrm{dgm}(\mathcal{X}_n^{(1)}), \mathrm{dgm}(\mathcal{X}_n^{(2)}))$ is a coupling between P_1 and P_2. Thus, Proposition 8.1.2 yields

$$\mathrm{FG}_p^p(\mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)})], \mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})]) \leq \mathbb{E}_\gamma[\mathrm{FG}_p^p(\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)}), \mathrm{dgm}_q^C(\mathcal{X}_n^{(2)}))].$$

It is stated in [CS+10, Wasserstein Stability Theorem] that

$$\mathrm{FG}_p^p(\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)}), \mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})) \leq C_{p,p'} d_H(\mathcal{X}_n^{(1)}, \mathcal{X}_n^{(2)})^{p-p'},$$

where $C_{p,p'}$ depends on p, p' and $\mathcal{X}$, and d_H is the Hausdorff distance between sets. By taking the infimum on transport plans γ, we obtain

$$\mathrm{FG}_p^p(\mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(1)})], \mathbb{E}[\mathrm{dgm}_q^C(\mathcal{X}_n^{(2)})]) \leq C_{p,p'} W_{p-p',d_H}^{p-p'}(\xi_1^{\otimes n}, \xi_2^{\otimes n}),$$

where W_{p,d_H} is the p-Wasserstein distance between probability distributions on compact sets of the space $\mathcal{X}$, endowed with the Hausdorff distance. Lemma 15 of [Cha+15b] states that

$$W_{p-p',d_H}^{p-p'}(\xi_1^{\otimes n}, \xi_2^{\otimes n}) \leq n \cdot W_{p-p'}^{p-p'}(\xi_1, \xi_2),$$

concluding the proof. □

Note that this proposition illustrates the usefulness of introducing new distances FG_p: considering the proximity between linear expectations requires to extend the metrics d_p to Radon measures.

8.2 Regularity of the expected persistence diagram

Our next contribution to the study of the expected persistence diagram consists in showing that in two different kinds of situations (e.g. filtrations built on point clouds in Theorem 8.2.5 or filtration built with the sublevel sets of a Brownian motion in Theorem 8.2.17), the expected persistence diagram $\mathbb{E}[a]$, which is a measure on Ω, has a density λ with respect to the Lebesgue measure on Ω. Therefore, $\mathbb{E}[\Psi_f(a)]$ is equal to $\int_\Omega f(u)\lambda(u)\mathrm{d}u$, and if properties of the density λ are shown (such as smoothness), those properties will also apply to the expectation of the representation Ψ_f. Note that Theorem 8.2.17 is, to our knowledge, one of the first result about the *persistent* homology of Gaussian random fields.

More precisely, in Theorem 8.2.5, we consider filtrations $K(\mathcal{X})$ built on top of a random point cloud X (e.g. K is the Čech filtration or the Rips filtration). The main argument to prove the existence of a density for the expected persistence diagram then relies on the basic observation that for a random point cloud $\mathcal{X}$ of given size n, the filtration $K(\mathcal{X})$ can induce a finite number of ordering configurations of the simplices. The core of the proof consists in showing that, under suitable assumptions, this ordering is locally constant for almost all $\mathcal{X}$. As one needs to use geometric arguments, having properties only satisfied almost everywhere is not sufficient for our purpose. One needs to show that properties hold in a stronger sense, namely that the set on which it is satisfied is a dense open set. Hence, a convenient framework to obtain such properties is given by subanalytic geometry (see [Shi97] for a monograph on the subject). Subanalytic sets are a class of subsets of $\mathbb{R}^d$ that are locally defined as linear projections of sets defined by analytic equations and inequations. As most considered filtrations in Topological Data Analysis result from real algebraic constructions, such sets naturally appear in practice. On open sets where the combinatorial structure of the filtration is constant, the way the points in the diagrams are matched to pairs of simplices is fixed: only the times/scales at which those simplices appear change, see Section 3.8.3. Under an assumption of smoothness of those times, and using the coarea formula, one then deduces the existence of a density for $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$.

Background on subanalytic sets We now give basic results on subanalytic geometry, whose proofs are given in Section 8.6. See [Shi97] for a thorough review of the subject. Let $M \subset \mathbb{R}^D$ be a connected real analytic submanifold, possibly with boundary, whose dimension is denoted by d.

Definition 8.2.1. *A subset X of M is* semianalytic *if each point of M has a neighborhood $U \subset M$ such that $X \cap U$ is of the form*

$$\bigcup_{i=1}^{p} \bigcap_{j=1}^{q} X_{ij}, \tag{8.6}$$

where X_{ij} is either $f_{ij}^{-1}(\{0\})$ or $f_{ij}^{-1}((0,\infty))$ for some analytic functions $f_{ij} : U \to \mathbb{R}$.

Definition 8.2.2. *A subset X of M is* subanalytic *if for each point of M, there exists a neighborhood U of this point, a real analytic manifold N and A, a relatively compact semianalytic set of $N \times M$, such that $X \cap U$ is the projection of A on M. A function $f : X \to \mathbb{R}$ is subanalytic if its graph is subanalytic in $M \times \mathbb{R}$. The set of real-valued subanalytic functions on X is denoted by $\mathcal{S}(X)$.*

A point x in a subanalytic subset X of M is smooth (of dimension k) if, in some neighborhood of x in M, X is an analytic submanifold (of dimension k). The maximal dimension of a smooth point of X is called the dimension of X. The smooth points of X of dimension d are called regular, and the other points are called singular. The set $\mathrm{Reg}(X)$ of regular points of X is an open subset of M, possibly empty; the set of singular points is denoted by $\mathrm{Sing}(X)$.

Lemma 8.2.3. *(i) For $f \in \mathcal{S}(M)$, the set $A(f)$ on which f is analytic is an open subanalytic set of M. Its complement is a subanalytic set of dimension smaller than d.*

Fix X a subanalytic subset of M. Assume that $f, g : X \to \mathbb{R}$ are subanalytic functions such that the image of a bounded set is bounded. Then,

(ii) The functions fg and $f + g$ are subanalytic.

(iii) The sets $f^{-1}(\{0\})$ and $f^{-1}((0,\infty))$ are subanalytic in M.

As a consequence of point (i), for $f \in \mathcal{S}(M)$, one can define its gradient ∇f everywhere but on some subanalytic set of dimension smaller than d.

Lemma 8.2.4. *Let X be a subanalytic subset of M. If the dimension of X is smaller than d, then $\mathcal{H}_d(X) = 0$.*

As a direct corollary, we always have

$$\mathcal{H}_d(X) = \mathcal{H}_d(\mathrm{Reg}(X)). \tag{8.7}$$

Write $\mathcal{N}(M)$ for the class of subanalytic subsets X of M with $\mathrm{Reg}(X) = \emptyset$. We have just shown that $\mathcal{H}_d \equiv 0$ on $\mathcal{N}(M)$. They form a special class of negligeable sets. We say that a property is verified *almost subanalytically everywhere* (a.s.e.) if the set on which it is not verified is included in a set of $\mathcal{N}(M)$. For example, Lemma 8.2.3 implies that ∇f is defined a.s.e..

Statements of the main results Let $n > 0$ be an integer and M a real analytic compact d-dimensional connected submanifold possibly with boundary. Let Δ_n be the standard n-dimensional simplicial complex, given by all the non-empty subsets of $\{1, \dots, n\}$. Let $\varphi = (\varphi[\sigma])_{\sigma \in \Delta_n} : M^n \to \mathbb{R}^{\Delta_n}$ be a continuous function. The function φ will be used to construct the persistence diagram and is called a *filtering function*: a simplex σ is added in the filtration at the time $\varphi[\sigma]$. For $x = (x_1, \dots, x_n) \in M^n$ and for σ a simplex, define $x(\sigma) := (x_j)_{j \in \sigma}$. We make the following assumptions on φ:

(K1) *Absence of interaction:* For $\sigma \in \Delta_n$, $\varphi[\sigma](x)$ only depends on $x(\sigma)$.

(K2) *Invariance by permutation:* For $\sigma \in \Delta_n$ and for $(x_1, \dots, x_n) \in M^n$, if τ is a permutation of $\{1, \dots, n\}$ whose support is included in σ, then $\varphi[\sigma](x_{\tau(1)}, \dots, x_{\tau(n)}) = \varphi[\sigma](x_1, \dots, x_n)$.

(K3) *Monotony:* For $\sigma \subset \sigma' \in \Delta_n$, $\varphi[\sigma] \leq \varphi[\sigma']$.

(K4) *Compatibility:* For a simplex $\sigma \in \Delta_n$ and for $j \in \sigma$, if $\varphi[\sigma](x_1, \dots, x_n)$ is not a function of x_j on some open set U of M^n, then $\varphi[\sigma] \equiv \varphi[\sigma \backslash \{j\}]$ on U.

(K5) *Smoothness:* The function φ is subanalytic and the gradient of each of its entries (which is defined a.s.e.) is non vanishing a.s.e..

Assumptions (K2) and (K3) ensure that a filtration $K(x)$ can be defined thanks to φ by:

$$\forall \sigma \in \Delta_n,\ \sigma \in K(t, x) \Longleftrightarrow \varphi[\sigma](x) \leq t. \tag{8.8}$$

Assumption (K1) means that the moment a simplex is added in the filtration only depends on the position of its vertices, but not on their relative position in the point cloud. For $\sigma \in \Delta_n$, the gradient of $\varphi[\sigma]$ is a vector field in TM^n. Its projection on the jth coordinate is denoted by $\nabla^j \varphi[\sigma]$: it is a vector field in TM defined a.s.e.. The persistence diagram of the filtration $K(x)$ for q-dimensional homology is denoted by $\mathrm{dgm}_q(K(x))$.

Theorem 8.2.5. *Fix $n \geq 1$. Assume that M is a real analytic compact d-dimensional connected submanifold possibly with boundary and that X is a random variable on M^n having a density with respect to the Hausdorff measure $\mathcal{H}_{dn}$. Assume that K satisfies the assumptions (K1)-(K5). Then, for $q \geq 0$, the expected persistence diagram $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ has a density with respect to the Lebesgue measure on Ω.*

Remark 8.2.6. The condition that M is compact can be relaxed in most cases: it is only used to ensure that the subanalytic functions appearing in the proof satisfy the boundedness condition of Lemma 8.2.3. For the Čech and Vietoris-Rips filtrations, one can directly verify that the function φ (and therefore the functions appearing in the proofs) satisfies it when $M = \mathbb{R}^d$. Indeed, in this case, the filtering functions are semi-algebraic.

Classical filtrations such as the Vietoris-Rips and Čech filtrations do not satisfy the full set of assumptions (K1)-(K5). Specifically, they do not satisfy the second part of assumption (K5): all singletons $\{j\}$ are included at time 0 in those filtrations so that $\varphi[\{j\}] \equiv 0$, and the gradient $\nabla \varphi[\{j\}]$ is therefore null everywhere. This leads to a well-known phenomenon on Vietoris-Rips and Čech diagrams: all the non-infinite points of the diagram for 0-dimensional homology are included in the vertical line $\{0\} \times [0, \infty)$. A theorem similar to Theorem 8.2.5 still holds in this case:

Theorem 8.2.7. *Fix $n \geq 1$. Assume that M is a real analytic compact d-dimensional connected submanifold and that $\mathcal{X}$ is a random variable on M^n having a density with respect to the Hausdorff measure $\mathcal{H}_{dn}$. Define assumption (K5'):*

(K5') The function φ is subanalytic and the gradient of its entries σ of size larger than 1 is non vanishing a.s.e.. Moreover, for $\{j\}$ a singleton, $\varphi[\{j\}] \equiv 0$.

Assume that $\mathcal{K}$ satisfies the assumptions (K1)-(K4) and (K5'). Then, for $q \geq 1$, $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ has a density with respect to the Lebesgue measure on Ω. Moreover, $\mathbb{E}[\mathrm{dgm}_0(K(\mathcal{X}))]$ has a density with respect to the Lebesgue measure on the vertical line $\{0\} \times [0, \infty)$.

The proof of Theorem 8.2.7 is very similar to the proof of Theorem 8.2.5. It is therefore relegated with other additional proofs in Section 8.6.

One can easily generalize Theorem 8.2.5 and assume that the size of the point process X is itself random. For $n \in \mathbb{N}$, define a function $\varphi^{(n)} : M^n \to \mathbb{R}^{\Delta_n}$ satisfying the assumption (K1)-(K5). If x is a finite subset of M, define $K(x)$ by the filtration associated to $\varphi^{(\#x)}$ where $\#x$ is the size of x. We obtain the following corollary, proven in Section 8.6.

Corollary 8.2.8. *Assume that X has some density with respect to the law of a Poisson process on M of intensity $\mathcal{H}_d$, such that $\mathbb{E}\left[2^{\#X}\right] < \infty$. Assume that K satisfies the assumptions (K1)-(K5). Then, for $q \geq 0$, $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ has a density with respect to the Lebesgue measure on Ω.*

The condition $\mathbb{E}\left[2^{\#X}\right] < \infty$ ensures the existence of the expected persistence diagram and is for example satisfied when X is a Poisson process with finite intensity.

As the way the filtration is created is smooth, one may actually wonder whether the density of $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ is smooth as well: it is the case as long as the way the points are sampled is smooth.

Theorem 8.2.9. *Fix $0 \leq k \leq \infty$ and assume that $X \in M^n$ has some density of class $\mathcal{C}^k$ with respect to $\mathcal{H}_{nd}$. Then, for $q \geq 0$, the density of $\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ is of class $\mathcal{C}^k$.*

The proof is based on classical results of continuity under the integral sign as well as an use of the implicit function theorem: it can be found in Section 8.6.

As a corollary of Theorem 8.2.9, we obtain the smoothness of various expected descriptors computed on persistence diagrams. For instance, the expected birth distribution and the expected death distribution have smooth densities under the same hypothesis, as they are obtained by projection of the expected diagram on some axis. Another example is the smoothness of the expected Betti curves. We recall the definition of the Betti curve introduced in Section 3.9: the Betti number at scale t of a persistence diagram a is defined as $\beta_t(a) := a(\lrcorner_{t,t})$, where $\lrcorner_{t,t} = \{u = (u_1, u_2) \in \Omega : u_1 \leq t \leq u_2\}$. The Betti curve is then the function $\beta(a) : t \in \mathbb{R} \mapsto \beta_t(a)$. The Betti curves are step functions which can be used as statistics, as in [Ume17] where they are used for a classification task on time series. With few additional work (see proof in Section 8.6), the expected Betti curves are shown to be smooth.

Corollary 8.2.10. *Under the same hypothesis than Theorem 8.2.9, for $q \geq 0$, the expected Betti curve $\mathbb{E}[\beta(\mathrm{dgm}_q(K(\mathcal{X}))]$ is a $\mathcal{C}^k$ function.*

8.2.1 Proof of Theorem 8.2.5

First, one can always replace M^n by $A(\varphi) = \bigcap_{\sigma \in \Delta_n} A(\varphi[\sigma])$, as Lemma 8.2.3 implies that it is an open set whose complement is in $\mathcal{N}(M^n)$. We will therefore assume that φ is analytic on M^n.

Given $x \in M^n$, the different values taken by $\varphi(x)$ on the filtration can be written $t_1 < \cdots < t_L$. Define $E_l(x)$ the set of simplices σ such that $\varphi[\sigma](x) = t_l$. The sets $E_1(x), \ldots, E_L(x)$ form a partition of Δ_n denoted by $\mathcal{A}(x)$.

Lemma 8.2.11. *For a.s.e. $x \in M^n$, for $l \geq 1$, $E_l(x)$ has a unique minimal element σ_l (for the partial order induced by inclusion).*

Proof. Fix $\sigma, \sigma' \subset \{1, \dots, n\}$ with $\sigma \neq \sigma'$ and $\sigma \cap \sigma' \neq \emptyset$. consider the subanalytic functions $f : x \in M^n \mapsto \varphi[\sigma](x) - \varphi[\sigma'](x)$ and $g : x \in M^n \mapsto \varphi[\sigma](x) - \varphi[\sigma \cap \sigma'](x)$. The set

$$C(\sigma, \sigma') := \{f = 0\} \cap \{g > 0\}. \tag{8.9}$$

is a subanalytic subset of M^n. Assume that it contains some open set U. On U, $\varphi[\sigma](x)$ is equal to $\varphi[\sigma'](x)$. Therefore, it does not depend on the entries x_j for $j \in \sigma \backslash \sigma'$. Hence, by assumption (K4), $\varphi[\sigma](x)$ is actually equal to $\varphi[\sigma \cap \sigma'](x)$ on U. This is a contradiction with having $g > 0$ on U. Therefore, $C(\sigma, \sigma')$ does not contain any open set, and all its points are singular: $C(\sigma, \sigma')$ is in $\mathcal{N}(M^n)$. If $\sigma \cap \sigma' = \emptyset$, similar arguments show that $C(\sigma, \sigma') = \{f = 0\}$ cannot contain any open set: it would contradict assumption (K5). On the complement of

$$C := \bigcup_{\sigma \neq \sigma' \subset \{1, \dots, n\}} C(\sigma, \sigma'), \tag{8.10}$$

having $\varphi[\sigma](x) = \varphi[\sigma'](x)$ implies that $\sigma \cap \sigma' \neq \emptyset$ and that $\varphi[\sigma](x) = \varphi[\sigma \cap \sigma'](x)$. This show the existence of a unique minimal element σ_l to $E_l(x)$ on the complement of C. This property is therefore a.s.e. satisfied. □

Lemma 8.2.12. *A.s.e., $x \mapsto \mathcal{A}(x)$ is locally constant.*

Proof. Fix $\mathcal{A}_0 = \{E_1, \dots, E_l\}$ a partition of Δ_n induced by some filtration, with minimal elements $\sigma_1, \dots, \sigma_l$. Consider the subanalytic functions F, G defined, for $x \in M^n$, by

$$F(x) = \sum_{l=1}^{L} \sum_{\sigma \in E_l} (\varphi[\sigma](x) - \varphi[\sigma_l](x)) \text{ and } G(x) = \sum_{l \neq l'} (\varphi[\sigma_l](x)) - \varphi[\sigma_{l'}](x))^2 .$$

The set $\{x \in M^n, \mathcal{A}(x) = \mathcal{A}_0\}$ is exactly the set $C(\mathcal{A}_0) = \{F = 0\} \cap \{G > 0\}$, which is subanalytic. The sets $C(\mathcal{A}_0)$ for all partitions $\mathcal{A}_0$ of Δ_n define a finite partition of the space M^n. On each open set $\mathrm{Reg}(C(\mathcal{A}_0)))$, the application $x \mapsto \mathcal{A}(x)$ is constant. Therefore, $x \mapsto \mathcal{A}(x)$ is locally constant everywhere but on $\bigcup_{\mathcal{A}_0} \mathrm{Sing}(C(\mathcal{A}_0)) \in \mathcal{N}(M^n)$. □

Therefore, the space M^n is partitioned into a negligeable set of $\mathcal{N}(M^n)$ and some open subanalytic sets $U_1, \dots, U_R$ on which $\mathcal{A}$ is constant.

Lemma 8.2.13. *Fix $1 \leq r \leq R$ and assume that $\sigma_1, \dots, \sigma_L$ are the minimal elements of $\mathcal{A}$ on U_r. Then, for $1 \leq l \leq L$ and $j \in \sigma_l$, $\nabla^j \varphi[\sigma_l] \neq 0$ a.s.e. on U_r.*

Proof. By minimality of σ_l, for $j \in \sigma_l$, the subanalytic set $\{\nabla^j \varphi[\sigma_l] = 0\} \cap U_r$ cannot contain an open set. It is therefore in $\mathcal{N}(M^n)$. □

Fix $1 \leq r \leq R$ and write

$$V_r = U_r \bigg\backslash \left(\bigcup_{l=1}^{L} \bigcup_{j=1}^{|\sigma_l|} \{\nabla^j \varphi[\sigma_l] = 0\} \right).$$

The complement of V_r in U_r is still in $\mathcal{N}(M^n)$. For $x \in V_r$, $\mathrm{dgm}_q[K(x)]$ is written $\sum_{i=1}^{N} \delta_{u_i}$, where

$$u_i = (\varphi[\sigma_{l_1}](x), \varphi[\sigma_{l_2}](x)) =: (b_i, d_i).$$

The integer N and the simplices σ_{l_1}, σ_{l_2} depend only on V_r. Note that d_i is always larger than b_i, so that σ_{l_2} cannot be included in σ_{l_1}. The map $x \mapsto u_i$ has its differential of rank 2. Indeed, take $j \in \sigma_{l_2} \backslash \sigma_{l_1}$. By Lemma 8.2.13, $\nabla^j \varphi[\sigma_{l_2}](x) \neq 0$. Also, as $\varphi[\sigma_{l_1}]$ only depends on the entries of x indexed by σ_{l_1} (assumption (K1)), $\nabla^j \varphi[\sigma_{l_1}](x) = 0$. Furthermore, take j' in σ_{l_1}. By Lemma 8.2.13, $\nabla^{j'} \varphi[\sigma_{l_1}](x) \neq 0$. This implies that the differential is of rank 2.

We now compute the qth persistence diagram for $q \geq 0$. Let κ be the density of $\mathcal{X}$ with respect to the measure $\mathcal{H}_{nd}$ on M^n. Then,

$$\begin{aligned}
\mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))] &= \sum_{r=1}^{R} \mathbb{E}\left[\mathbf{1}\{\mathcal{X} \in V_r\} \mathrm{dgm}_q(K(X))\right] \\
&= \sum_{r=1}^{R} \mathbb{E}\left[\mathbf{1}\{\mathcal{X} \in V_r\} \sum_{i=1}^{N_r} \delta_{u_i}\right] \\
&= \sum_{r=1}^{R} \sum_{i=1}^{N_r} \mathbb{E}\left[\mathbf{1}\{\mathcal{X} \in V_r\} \delta_{u_i}\right]
\end{aligned}$$

Let μ_{ir} be the measure $\mathbb{E}[\mathbf{1}\{\mathcal{X} \in V_r\}\delta_{u_i}]$. To conclude, it suffices to show that this measure has a density with respect to the Lebesgue measure on Ω. This is a consequence of the coarea formula. Define the function $\Phi_{ir} : x \in V_r \mapsto u_i = (\varphi[\sigma_{l_1}](x), \varphi[\sigma_{l_2}](x))$. We have already seen that Φ_{ir} is of rank 2 on V_r, so that $J\Phi_{ir} > 0$. By the coarea formula (see Theorem 3.5.13), for a Borel set B in Ω,

$$\begin{aligned}
\mu_{ir}(B) &= \mathbb{P}(\Phi_{ir}(\mathcal{X}) \in B, \mathcal{X} \in V_r) \\
&= \int_{V_r} \mathbf{1}\{\Phi_{ir}(x) \in B\} \kappa(x) d\mathcal{H}_{nd}(x) \\
&= \int_{u \in B} \int_{x \in \Phi_{ir}^{-1}(\{u\})} (J\Phi_{ir}(x))^{-1} \kappa(x) d\mathcal{H}_{nd-2}(x) du.
\end{aligned}$$

Therefore, μ_{ir} has a density with respect to the Lebesgue measure on Ω equal to, for $u \in \Omega$,

$$\lambda_{ir}(u) = \int_{x \in \Phi_{ir}^{-1}(\{u\})} (J\Phi_{ir}(x))^{-1} \kappa(x) d\mathcal{H}_{nd-2}(x). \tag{8.11}$$

Finally, $\mathbb{E}[\mathrm{dgm}_q(K(X))]$ has a density equal to

$$\lambda(u) = \sum_{r=1}^{R} \sum_{i=1}^{N_r} \int_{x \in \Phi_{ir}^{-1}(\{u\})} (J\Phi_{ir}(x))^{-1} \kappa(x) d\mathcal{H}_{nd-2}(x). \tag{8.12}$$

8.2.2 Examples

We now note that the Vietoris-Rips and the Čech filtrations satisfy the assumptions (K1)-(K4) and (K5') when $M = \mathbb{R}^d$ is an Euclidean space. Note that similar arguments show that weighted versions of those filtrations (see [Buc+16]) satisfy assumptions (K1)-(K5).

Vietoris-Rips filtration Let $x \in M^n$ and $\sigma \in \Delta_n$ be a simplex. For the Vietoris-Rips filtration, $\varphi[\sigma](x) = \max_{i,j \in \sigma} |x_i - x_j|$. The function φ clearly satisfies (K1), (K2) and (K3). It is also subanalytic, as it is the maximum of semi-algebraic functions.

Also, we have $\varphi[\sigma](x) = |x_i - x_j|$ for some indices i, j. Those indices are locally stable, and $\varphi[\sigma](x) = \varphi[\{i,j\}](x)$: hypothesis (K4) is satisfied. Furthermore, on this set,

$$\nabla\varphi[\{i,j\}](x) = \left(\frac{x_i - x_j}{|x_i - x_j|}, \frac{x_j - x_i}{|x_i - x_j|}\right) \neq 0. \tag{8.13}$$

Hence, (K5') is also satisfied: both Theorem 8.2.7 and Theorem 8.2.9 are satisfied for the Vietoris-Rips filtration.

Čech filtration Recall that the ball centered at x of radius r is denoted by $\mathcal{B}(x,r)$. For the Čech filtration,

$$\varphi[\sigma](x) = \inf_{r>0}\left\{\bigcap_{j\in\sigma}\mathcal{B}(x_j,r) \neq \emptyset\right\}. \tag{8.14}$$

First, it is clear that (K1), (K2) and (K3) are satisfied by φ.

We give without proof a characterization of the Čech complex.

Proposition 8.2.14. *Let x be in M^n and fix $\sigma \in \Delta_n$. If the circumcenter of $x(\sigma)$ is in the convex hull of $x(\sigma)$, then $\varphi[\sigma](x)$ is the radius of the circumsphere of $x(\sigma)$. Otherwise, its projection on the convex hull belongs to the convex hull of some subsimplex $x(\sigma')$ of $x(\sigma)$ and $\varphi[\sigma](x) = \varphi[\sigma'](x)$.*

Definition 8.2.15. *The Cayley-Menger matrix of a k-simplex $x = (x_1, \dots, x_k) \in M^k$ is the symmetric matrix $(\mathrm{CM}(x)_{i,j})_{i,j}$ of size $k+1$, with zeros on the diagonal, such that $\mathrm{CM}(x)_{1,j} = 1$ for $j > 1$ and $\mathrm{CM}(x)_{i+1,j+1} = |x_i - x_j|^2$ for $i, j \leq k$.*

Proposition 8.2.16 (see [Cox30])**.** *Let $x \in M^k$ be a point in general position. Then, the Cayley-Menger matrix $\mathrm{CM}(x)$ is invertible with $(\mathrm{CM}(x))^{-1}_{1,1} = -2r^2$, where r is the radius of the circumsphere of x. The kth other entries of the first line of $\mathrm{CM}(x)^{-1}$ are the barycentric coordinates of the circumcenter.*

Therefore, the application which maps a simplex to its circumcenter is analytic, and the set on which the circumcenter of a simplex belongs in the interior of its convex hull is a subanalytic set. On such a set, the function φ is also analytic, as it is the square root of the inverse a matrix which is polynomial in x. Furthermore, on the open set on which the circumcenter is outside the convex hull, we have shown that $\varphi[\sigma](x) = \varphi[\sigma'](x)$ for some subsimplex J': assumption (K4) is satisfied.

Finally, let us show that assumption (K5') is satisfied. The previous paragraph shows the subanalyticity of φ. For $\sigma \in \Delta_n$ a simplex, there exists some subsimplex σ' such that $\varphi[\sigma](x)$ is the radius of the circumsphere of $x(\sigma')$. It is clear that there cannot be an open set on which this radius is constant. Thus, $\nabla\varphi[\sigma]$ is a.s.e. non null.

8.2.3 The expected persistence diagram of a Brownian motion

Another instance of random objects one can build filtrations on are random functions. The most fundamental instance of such functions is the Brownian motion $B : t \in [0,1] \mapsto B_t \in \mathbb{R}$, defined as the continuous Gaussian random field on $\mathbb{R}$ having covariance function $C(t_1, t_2) = t_1 \wedge t_2$ (see [LG16, Chapter 2] for a concise and rigorous introduction). The continuity of B ensures that the persistence module induced by the 0-level homology of its sublevel sets is q-tame (see Section 3.8). In particular, the persistence diagram $\mathrm{dgm}(B)$ of this persistence module is well-defined, but may contain accumulation points close to the diagonal. To put it another way, $\mathrm{dgm}(B)$ belongs to $\mathcal{D}$ but not to $\mathcal{D}^f$, the space of finite persistence diagrams.

Theorem 8.2.17. *The random persistence diagram* $\mathrm{dgm}(B)$ *is integrable and its expectation* $\mathbb{E}[\mathrm{dgm}(B)]$ *has a density with respect to the Lebesgue measure.*

The result holds as the persistent Betti numbers, defined by

$$\beta_{r,s} := \beta_{r,s}(\mathrm{dgm}(B)) = \mathrm{dgm}(B)(]-\infty, r] \times [s, \infty[),$$

have a particularly convenient expression in this setting. Indeed, $\beta^{r,s}$ is exactly the number of upward crossings of the band $[r, s]$ by the Brownian motion. The law of this quantity is explicitly known, and happens to be continuous with respect to r and s. Standard measure theoretic arguments are then enough to conclude.

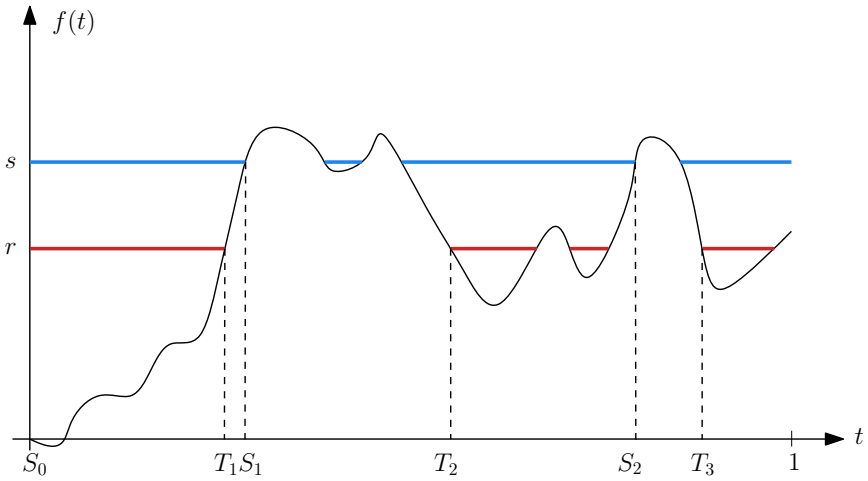


FIGURE 8.1: Example of a function $f : [0, 1] \to \mathbb{R}$ with $\beta^{r,s} = 3$. The red region corresponds to $f^{-1}((-\infty, r])$ and the blue region to $f^{-1}((-\infty, s])$.

More precisely, for $a \in \mathbb{R}$, define $T(a) := \inf\{t > 0,\ B_t = a\}$. Then, $T(a)$ has a density with respect to the Lebesgue measure equal to

$$f_a(t) = \frac{a}{\sqrt{2\pi t^3}} \exp\left(-\frac{a^2}{2t}\right).$$

Assume that $0 < r < s$ (similar arguments hold when both numbers are negative or if $r < 0 < s$). Define $T_0 = S_0 = 0$ and for $i \geq 0$

$$T_{i+1} := \inf\{t \geq S_i,\ B_t = r\},$$
$$S_{i+1} := \inf\{t \geq T_{i+1},\ B_t = s\}.$$

Then $\beta^{r,s}$ is equal to $\max\{k \geq 0,\ T_k \leq 1\}$ (see Figure 8.1) and $\mathbb{P}(\beta^{r,s} \geq k) = \mathbb{P}(T_k \leq 1)$. First, note that T_1 is equal to $T(r)$. Also, by Markov property, for $i \geq 1$, conditionally on S_i, $T_{i+1} - S_i$ has the same law than $T(s-r)$, and so does $S_{i+1} - T_{i+1}$ conditionally on T_{i+1}. Therefore for $k \geq 2$,

$$\begin{aligned}\mathbb{P}(\beta^{r,s} \geq k) &= \mathbb{P}(T_k \leq 1)\\ &= \int_{\Sigma_{2k-2}} f_r(t_1) f_{s-r}(s_1) f_{s-r}(t_2) \cdots f_{s-r}(s_{k-1}) f_{s-r}(t_k) \mathrm{d}s\mathrm{d}t,\end{aligned}$$

where $\Sigma_{2k-2} := \{u = (t_1, \dots, t_k, s_1, \dots, s_{k-1}) \in \mathbb{R}^{2k-1},\ t_i \geq 0,\ s_i \geq 0 \text{ and } \sum_{i=1}^{k} t_i + \sum_{i=1}^{k-1} s_i \leq 1\}$. Therefore,

$$\begin{aligned}
\mathbb{E}[\beta^{r,s}] &= \sum_{k\geq 1} \mathbb{P}(\beta^{r,s} \geq k) \\
&= \sum_{k\geq 1} \int_{\Sigma_{2k-2}} f_r(t_1) f_{s-r}(s_1) f_{s-r}(t_2) \cdots f_{s-r}(s_{k-1}) f_{s-r}(t_k) \mathrm{d}s\mathrm{d}t \\
&= \sum_{k\geq 1} \int_{\Sigma_{2k-2}} \frac{r(s-r)^{2k-2}}{\prod_{i=1}^{2k-1} \sqrt{2\pi u_i^3}} \exp\left(-\frac{r^2}{2u_1} - \frac{(s-r)^2}{2} \sum_{i=2}^{2k-1} u_i^{-1} \right) \mathrm{d}u \\
&:= \sum_{k\geq 1} \int_{\Sigma_k} G_k(u; r, s) \mathrm{d}u := \sum_{k\geq 1} I_k(r, s).
\end{aligned}$$

Note first that this sum is finite. Indeed, for $b \geq 0$, the function $x \in [0,1] \mapsto x^{-1} + \frac{\ln(x)}{b}$ is bounded from below by $b^{-1}(1 + \ln(b))$. Therefore,

$$\begin{aligned}
G_k(u; r, s) &\leq \frac{r(s-r)^{2k-2}}{(2\pi)^{k-1/2}} \exp\Bigg(-\frac{r^2}{2}\frac{3}{r^2}\left(1 + \ln\left(\frac{r^2}{3}\right)\right) \\
&\qquad - (2k-2)\frac{(s-r)^2}{2}\frac{3}{(s-r)^2}\left(1 + \ln\left(\frac{(s-r)^2}{3}\right)\right)\Bigg) \\
&= \frac{r(s-r)^{2k-2}}{(2\pi)^{k-1/2}} \exp\left(-(2k-1)\frac{3}{2}(1 - \ln 3) - \ln(r^3) - (2k-2)\ln((s-r)^3) \right) \\
&= \frac{r^{-2}(s-r)^{-4(k-1)}}{(2\pi)^{k-1/2}} BC^k
\end{aligned}$$

for some constants B, C. As the volume of Σ_k is $\frac{\sqrt{k+1}}{k!}$, $\sum_{k\geq 0} I_k(r,s)$ is finite. This implies that $\mathrm{dgm}(B)$ is indeed integrable. Moreover, it is possible to find a local bound of $I_k(r,s)$ independent of r and s: using classical results on the continuity of parametric integrals, one has that $\mathbb{E}[\beta^{r,s}] = \mu(A_{r,s})$ is continuous in r and s. Using the similar bounds on the derivatives of $I_k(r,s)$, one can show that $(r,s) \mapsto \mu(A_{r,s})$ is a $\mathcal{C}^1$ function. This implies that μ is absolutely continuous with respect to the Lebesgue measure on Ω.

We end this section by mentioning that the behavior of persistence diagrams of one-dimensional stochastic processes has been further investigated by Daniel Perez [Per20].

8.2.4 Stability of expected persistence diagrams: the smooth case

We end this section by mentioning a stronger stability result between expected persistence diagrams in the case where they have densities. Indeed, if, in Section 8.1, we provided a general stability result for expected persistence diagrams with respect to the Figalli-Gigli metrics, in the case where the expected persistence diagrams possess densities, there exist other, stronger metrics of interest to compare expected persistence diagrams. We address stability in this particular setting by using the L_1 and L_∞ distances.

Theorem 8.2.18. *Let $n \geq 1$ and M be a real analytic compact d-dimensional connected submanifold possibly with boundary. Let $\mathcal{X}_1$ (resp. $\mathcal{X}_2$) be a random variable on M^n having a density κ_1 (resp. κ_2) with respect to the Hausdorff measure $\mathcal{H}_{dn}$. Assume that K satisfies the assumptions (K1)-(K5) (or (K5')). Let $\overline{\lambda}_1$ be the density of the*

normalized *measure* $\mathbb{E}\left[\frac{\mathrm{dgm}_q(K(\mathcal{X}_1))}{|\mathrm{dgm}_q(K(\mathcal{X}_1))|}\right]$ *and* $\overline{\lambda}_2$ *be the density of* $\mathbb{E}\left[\frac{\mathrm{dgm}_q(K(\mathcal{X}_2))}{|\mathrm{dgm}_q(K(\mathcal{X}_2))|}\right]$. *Also, let* λ_1 *and* λ_2 *be the non-normalized densities. Then,*

$$\|\overline{\lambda}_1 - \overline{\lambda}_2\|_{L_1(\Omega)} \leq \|\kappa_1 - \kappa_2\|_{L_1(M^n)}, \text{ and} \tag{8.15}$$

$$\|\lambda_1 - \lambda_2\|_{L_1(\Omega)} \leq C_n |\mathrm{vol}_M|^n \|\kappa_1 - \kappa_2\|_\infty, \tag{8.16}$$

where C_n *is the expected number of points in the persistence diagram built with the filtration* K *on* n *i.i.d. uniform points on* M.

It is conjectured (and even proved for $M = [0,1]^d$ in Chapter 7) that C_n is of order n when K is either the Rips or the Čech filtration.

Proof. Consider first the non-normalized case. Given the expression (8.11), one can write for $u \in \Omega$:

$$\lambda_1(u) - \lambda_2(u) = \sum_{r=1}^{R} \sum_{i=1}^{N_r} \int_{x \in \Phi_{ir}^{-1}(\{u\})} (J\Phi_{ir}(x))^{-1} (\kappa_1(x) - \kappa_2(x)) d\mathcal{H}_{nd-2}(x),$$

so that

$$\begin{aligned}
&\int_\Omega |\lambda_1(u) - \lambda_2(u)| du \\
&\leq \sum_{r=1}^{R} \sum_{i=1}^{N_r} \int_\Omega \int_{x \in \Phi_{ir}^{-1}(\{u\})} (J\Phi_{ir}(x))^{-1} |\kappa_1(x) - \kappa_2(x)| d\mathcal{H}_{nd-2}(x) \\
&= \sum_{r=1}^{R} \sum_{i=1}^{N_r} \int_{V_r} \mathbb{1}\{\Phi_{ir}(x) \in \Omega\} |\kappa_1(x) - \kappa_2(x)| d\mathcal{H}_{nd}(x) \text{ by the coarea formula} \\
&= \sum_{r=1}^{R} N_r \int_{V_r} |\kappa_1(x) - \kappa_2(x)| d\mathcal{H}_{nd}(x) \\
&\leq \sum_{r=1}^{R} N_r \mathcal{H}_{nd}(V_r) \|\kappa_1 - \kappa_2\|_\infty \\
&= \mathcal{H}_{nd}(M^n) \sum_{r=1}^{R} N_r \frac{\mathcal{H}_{nd}(V_r)}{\mathcal{H}_{nd}(M^n)} \|\kappa_1 - \kappa_2\|_\infty = \mathcal{H}_d(M)^n C_n \|\kappa_1 - \kappa_2\|_\infty.
\end{aligned}$$

Inequality (8.15) is likewise obtained. □

8.3 Minimax estimation of the expected persistence diagram

A natural way to estimate the expected persistence diagram of P is to consider its empirical counterpart, which simply reads $\overline{a}_n := \frac{1}{n}(a_1 + \cdots + a_n)$. By leveraging techniques from optimal transport theory, we show that $\overline{a}_n$ approximates $E(P)$ at the parametric rate $n^{-1/2}$ with respect to the loss FG_p^p under non-restrictive assumptions, and that it is optimal from a minimax perspective. We actually consider the more general case where $\mu \sim P$ is a general persistence measure, with $\overline{\mu}_n = \frac{\mu_1 + \cdots + \mu_n}{n}$ the empirical expected persistence diagram.

Before exhibiting rates of convergence, we show that the consistency of the empirical expected persistence diagram can be directly obtained from the convergence results of Chapter 6.

Lemma 8.3.1. *Let $P \in \mathcal{P}_1^p(\mathcal{M}^p)$. Let $(\mu_n)_{n\geq 1}$ be a sequence of i.i.d. variables of law P and let $\overline{\mu}_n = \frac{1}{n}(\mu_1 + \cdots + \mu_n)$. Then,*

$$\mathrm{FG}_p(\overline{\mu}_n, E(P)) \xrightarrow[n\to\infty]{} 0 \text{ almost surely.} \tag{8.17}$$

Proof. By the strong law of large numbers applied to the function $d(\cdot, \partial\Omega)^p$, we have $\mathrm{Pers}_p(\overline{\mu}_n) \to \mathrm{Pers}_p(E(P))$ almost surely. Also, for any continuous function $f : \Omega \to \mathbb{R}$ with compact support, we have $\overline{\mu}_n(f) \to E(P)(f)$ almost surely. This convergence also holds almost surely for any countable family $(f_i)_i$ of functions. Applying this result to a countable convergence-determining class for the vague convergence, we obtain that $(\overline{\mu}_n)_n$ converges vaguely towards $E(P)$ almost surely. We conclude thanks to Theorem 6.2.6. □

Rates of convergence are obtained by making stronger assumptions on the distribution P. Let A_L be the ℓ_1-ball in $\mathbb{R}^2$ centered at $(-L/\sqrt{8}, L/\sqrt{8})$ of radius $L/\sqrt{2}$ (see Figure 8.2). For $0 \leq q \leq \infty$ and $L, M > 0$, we let $\mathcal{M}^q_{L,M}$ be the set of measures $\mu \in \mathcal{M}^q$ which are supported on A_L, with $\mathrm{Pers}_q(\mu) \leq M$. Let $\mathcal{P}^q_{L,M}$ be the set of probability distributions which are supported on $\mathcal{M}^q_{L,M}$. It is known that persistence diagrams belong to the set $\mathcal{M}^q_{L,M}$ as long as they are built as the sublevel sets of Lipschitz continuous functions $f : \mathcal{X} \to \mathbb{R}$ for some metric space $\mathcal{X}$ implying bounded q total persistence.

In particular, for $q > 0$, no constraints on the total number of points of the persistence diagram are imposed. This is particularly interesting in applications, where the number of points in persistence diagrams is likely to be large, while their total persistence Pers_q may be moderate, see e.g. Chapter 7 for asymptotics in the case of the Čech and Rips persistence diagrams of large samples on the cube.

Theorem 8.3.2. *Let $1 \leq p < \infty$ and $0 \leq q < p$. Let $P \in \mathcal{P}^q_{L,M}$ and let $\mu_1, \ldots, \mu_n$ be a n-sample from law P. If $\overline{\mu}_n$ is the associated empirical expected persistence diagram, then,*

$$\mathbb{E}[\mathrm{FG}_p^p(\overline{\mu}_n, E(P))] \leq cML^{p-q}\left(\frac{1}{n^{1/2}} + \frac{a_p(n)}{n^{p-q}}\right), \tag{8.18}$$

where c depends on p and q, and $a_p(n) = 1$ if $p > 1$, $\log(n)$ if $p = 1$.

In particular, if $p \geq q + 1/2$, we obtain a parametric rate of convergence of $n^{-1/2}$. This is always the case if $q = 0$, i.e. if we assume that all the diagrams sampled according to P have less than M points. According to Theorem 3.8.11, it is also the case if $\mu_i = \mathrm{dgm}(f_i)$ for some random 1-Lipschitz functions $f_i : \mathcal{X} \to \mathbb{R}$, where $\mathcal{X}$ is a metric space implying bounded q total persistence. $p \geq q + 1/2$.

Before proving Theorem 8.3.2, we give a general upper bound on the distance FG_p between two measures in $\mathcal{M}^p$. The bound is based on a classical multiscale approach to control a transportation distance between two measures, appearing for instance in [SP18]. Let $J \in \mathbb{N}$. For $k \geq 0$, let $B_k = \{x \in A_L : \ d(x, \partial\Omega) \in (L2^{-(k+1)}, L2^{-k}]\}$. The sets $\{B_k\}_{k\geq 0}$ form a partition of A_L. We then consider a sequence of nested partitions $\{\mathcal{S}_{k,j}\}_{j=1}^J$ of B_k, where $\mathcal{S}_{k,j}$ is made of $N_{k,j}$ squares of sidelength $\varepsilon_{k,j} = L2^{-(k+1)}2^{-j}$. See also Figure 8.2. Let $\mu_{|B_k}$ be the measure μ restricted to B_k and $\mu_k = \frac{\mu_{|B_k}}{\mu(B_k)}$ be the conditional probability on B_k. If $\mu(B_k) = 0$, we let μ_k be any fixed measure, for instance the uniform distribution on B_k.

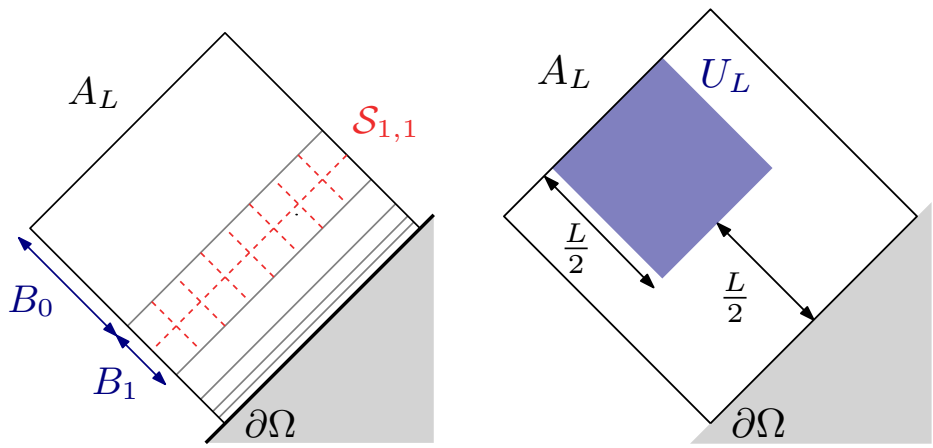


FIGURE 8.2: Partition of A_L used in the proof of Theorem 8.3.2

Lemma 8.3.3. *Let μ, ν be two measures in $\mathcal{M}^p$, supported on A_L. Then, for any $J \geq 0$, with $c_p = 2^{-p/2}(1 + 1/(2^p - 1))$,*

$$\mathrm{FG}_p^p(\mu,\nu) \leq 2^{p/2} L^p \sum_{k\geq 0} 2^{-kp} \Big(2^{-Jp}(\mu(B_k) \wedge \nu(B_k)) + c_p|\mu(B_k) - \nu(B_k)| + \sum_{\substack{1\leq j\leq J \\ S\in\mathcal{S}_{k,j-1}}} 2^{-jp}|\mu(S) - \nu(S)| \Big).$$

Proof. Denote by m_k the quantity $\mu(B_k) \wedge \nu(B_k)$. We build a transport plan as follows: let $\pi_k \in \Pi(\mu_k, \nu_k)$ be an optimal plan (in the sense of W_p). If $\mu(B_k) \leq \nu(B_k)$, then $\mu(B_k)\pi_k$ is a transport plan between $\mu_{|B_k}$ and $\frac{\mu(B_k)}{\nu(B_k)}\nu_{|B_k}$. We then build an admissible plan between the $\frac{\mu(B_k)}{\nu(B_k)}\nu_{|B_k}$ and $\nu_{|B_k}$ by making move $\left(1 - \frac{\mu(B_k)}{\nu(B_k)}\right)\nu_{|B_k}$ to the diagonal, with cost bounded by $\left(1 - \frac{\mu(B_k)}{\nu(B_k)}\right)\nu(B_k)(L2^{-k})^p$. Acting in a similar way if $\nu(B_k) \leq \mu(B_k)$, we obtain a total cost of

$$\sum_{k\geq 0} \Big(m_k W_p^p(\mu_k, \nu_k) + L^p 2^{-kp}|\mu(B_k) - \nu(B_k)| \Big), \tag{8.19}$$

which is therefore an upper bound on $\mathrm{FG}_p^p(\mu,\nu)$. Lemma 6 in [SP18] shows that

$$W_p^p(\mu_k, \nu_k) \leq 2^{p/2} L^p 2^{-(k+1)p} \Big(2^{-Jp} + \sum_{\substack{1\leq j\leq J \\ S\in\mathcal{S}_{k,j-1}}} 2^{-jp}|\mu_k(S) - \nu_k(S)| \Big). \tag{8.20}$$

Furthermore, one can check that

$$m_k|\mu_k(S) - \nu_k(S)| \leq |\mu(S) - \nu(S)| + \frac{\nu(S) \wedge \mu(S)}{\mu(B_k) \vee \nu(B_k)}|\mu(B_k) - \nu(B_k)|.$$

By summing over $S \in \mathcal{S}_{k,j+1}$, we obtain that

$$m_k \sum_{S\in\mathcal{S}_{k,j-1}} |\mu_k(S) - \nu_k(S)| \leq \sum_{S\in\mathcal{S}_{k,j-1}} |\mu(S) - \nu(S)| + |\mu(B_k) - \nu(B_k)|. \tag{8.21}$$

By using that $\sum_{j=1}^J 2^{-pj} \leq 2^{-p}/(1 - 2^{-p})$, and by putting together inequalities (8.19), (8.20) and (8.21), one obtains the inequality of Lemma 8.3.3. □

Before proving Theorem 8.3.2, we state a useful inequality. Let $\mu \in \mathcal{M}^q_{M,L}$ and let $B \subset \Omega$ be at distance ℓ from the diagonal $\partial\Omega$. Then,

$$\mu(B) = \int_B \frac{d(x,\partial\Omega)^q}{d(x,\partial\Omega)^q} \mathrm{d}\mu(x) \leq M\ell^{-q}. \tag{8.22}$$

Proof of Theorem 8.3.2. Consider a distribution $P \in \mathcal{P}^q_{M,L}$. Remark first that for any measure $\mu \in \mathcal{M}^q_{M,L}$, we have $\mu(B_k) \leq ML^{-q}2^{kq}$ one by (8.22). Let μ be a random persistence diagram of law P and $\overline{\mu}_n$ be the empirical expected persistence diagram associated to a n-sample of law P. By the Cauchy-Schwartz inequality, given a Borel set $A \subset \Omega$, we have

$$\mathbb{E}|\overline{\mu}_n(A) - E(P)(A)| \leq \sqrt{\frac{\mathbb{E}[\mu(A)^2]}{n}}. \tag{8.23}$$

The Cauchy-Schwartz inequality also yields, as $|\mathcal{S}_{k,j-1}| = 2^{k+1}4^{j-1}$,

$$\begin{aligned}\sum_{S\in\mathcal{S}_{k,j-1}} \mathbb{E}|\hat{\mu}_n(S) - E(P)(S)| &\leq \sum_{S\in\mathcal{S}_{k,j-1}} \sqrt{\frac{\mathbb{E}[\mu(S)^2]}{n}} \leq \sqrt{\frac{\mathbb{E}\left[\sum_{S\in\mathcal{S}_{k,j-1}} \mu(S)^2\right]}{n}|\mathcal{S}_{k,j-1}|} \\ &\leq \sqrt{\frac{\mathbb{E}\left[\mu(B_k)^2\right]}{n}|\mathcal{S}_{k,j-1}|} \leq \frac{ML^{-q}2^{kq}}{\sqrt{n}} 2^{\frac{k+1}{2}} 2^{j-1}.\end{aligned}$$

Note also that $\sum_{S\in\mathcal{S}_{k,j-1}} \mathbb{E}|\hat{\mu}_n(S) - E(P)(S)| \leq 2E(P)(B_k) \leq 2ML^{-q}2^{kq}$ and that $\overline{\mu}_n(B_k) \wedge E(P)(B_k) \leq ML^{-q}2^{kq}$. By using those three previous inequalities, Lemma 8.3.3 and inequality (8.23), we obtain that

$$\begin{aligned}&\mathbb{E}[\mathrm{FG}^p_p(\overline{\mu}_n, E(P))] \\ &\leq 2^{p/2}ML^{p-q}\sum_{k\geq 0} 2^{-kp}\left((2^{-Jp}2^{kq} + \frac{c_p}{\sqrt{n}}2^{kq} + \sum_{j=1}^{J} 2^{-jp}2^{kq}\left(2 \wedge \frac{2^{\frac{k+1}{2}}2^{j-1}}{\sqrt{n}}\right)\right) \\ &\leq c_{p,q}ML^{p-q}\Big(2^{-Jp} + \frac{1}{\sqrt{n}} + S\Big),\end{aligned}$$

where $S = \sum_{k\geq 0}\sum_{j=1}^{J} 2^{k(q-p)}2^{-jp}\left(1 \wedge \frac{2^{\frac{k}{2}}2^j}{\sqrt{n}}\right)$. To bound S, we remark that if $k \geq \log_2(n)$, then the minimum in the definition of S is equal to 1. Therefore, letting $b_J = 1$ if $p > 1$ and $b_J = J$ if $p = 1$, we find that S is smaller than

$$\begin{aligned}&\sum_{k=0}^{\log_2(n)}\sum_{j=1}^{J}\frac{2^{k(q-p+1/2)}2^{(1-p)j}}{\sqrt{n}} + \sum_{k\geq\log_2(n)}\sum_{j=1}^{J} 2^{-kp}2^{-jp} \\ &\leq c_p b_J \sum_{k=0}^{\log_2(n)}\frac{2^{k(q+1/2-p)}}{\sqrt{n}} + c_p n^{-p} \\ &\leq c_{p,q} b_J (n^{-1/2} \vee n^{q-p}).\end{aligned}$$

Finally, if $p > 1$, we may set $J = +\infty$ and obtain a bound of order $ML^{p-q}(n^{-1/2} + n^{q-p})$. If $p = 1$, we choose $J = (q-p)(\log n)/(2p)$ to obtain a rate of order $n^{-1/2} + n^{q-p}\log n$. □

From a statistical perspective, it is natural to wonder if better estimates of $E(P)$ exist. A possible way to answer this question is given by the minimax framework. Let

$\mathcal{Q}$ be a set of probability distributions on $\mathcal{M}^p$. We recall that the minimax rate for the estimation of $E(P)$ on $\mathcal{Q}$ is given by

$$\mathcal{R}_n(E(P), \mathcal{Q}, \mathrm{FG}_p^p) := \inf_{\hat{\mu}_n} \sup_{P \in \mathcal{Q}} \mathbb{E}[\mathrm{FG}_p^p(\hat{\mu}_n, E(P))], \tag{8.24}$$

where the infimum is taken over all possible estimators of $E(P)$. An estimator attaining the rate $\mathcal{R}_n(E(P), \mathcal{Q}, \mathrm{FG}_p^p)$ (up to a constant) is called minimax, i.e. an estimator is minimax on the class $\mathcal{Q}$ if it has the best possible risk uniformly on this class. We show that the empirical expected persistence diagram $\overline{\mu}_n$ is a minimax estimator on $\mathcal{P}_{L,M}^q$ as long as $p \geq q + 1/2$.

Theorem 8.3.4. *Let $1 \leq p < \infty$ and $q \geq 0$, $L, M > 0$. One has, for some c depending on p and q,*

$$\mathcal{R}_n(E(P), \mathcal{P}_{L,M}^q, \mathrm{FG}_p^p) \geq cML^{p-q}n^{-1/2}. \tag{8.25}$$

As the expected persistence diagram $E(P)$ is known to have a smooth density in a wide variety of settings, it could be expected (likewise it is the case in density estimation [Tsy08] or for measure reconstruction on manifolds in Chapter 5), that one could make use of this regularity to obtain substantially faster minimax rates on appropriate models. Surprisingly enough, using results from statistical optimal transport theory, we show that whatever regularity is assumed on the expected persistence diagram, no estimators can perform better than the empirical expected persistence diagram $\overline{\mu}_n$ for the FG_p loss (from a minimax perspective). Let $B_{p',q'}^s$ be the set of functions $\Omega \to \mathbb{R}$ in the Besov space of parameters $s \geq 0$ and $1 \leq p', q' \leq \infty$, see e.g. [Här+12] for an introduction to Besov spaces. Consider the model $\mathcal{P}_{L,M,T}^{q,s}$ of probability distributions $P \in \mathcal{P}_{L,M}^q$ whose expected persistence diagram $E(P)$ belongs to $B_{p',q'}^s$ with associated norm smaller than T/M.

Theorem 8.3.5. *Let $1 \leq p < \infty$, $q, s \geq 0$, $L, M, T > 0$ and $1 \leq p', q' \leq \infty$. One has*

$$\mathcal{R}_n(E(P), \mathcal{P}_{L,M,T}^{q,s}, \mathrm{FG}_p^p) \geq cML^{p-q}n^{-1/2}, \tag{8.26}$$

where c depends on s, p', q', p, q and T.

The proof of Theorem 8.3.5 is based on a similar result appearing in [WB19b], where minimax rates of estimation with respect to the Wasserstein distance W_p are exhibited for smooth densities on the cube.

Proof of Theorem 8.3.4. As $\mathcal{P}_{L,M,T}^{q,s} \subset \mathcal{P}_{L,M}^q$, we have $\mathcal{R}_n(\mathcal{P}_{L,M}^q) \geq \mathcal{R}_n(\mathcal{P}_{L,M,T}^{q,s})$. Therefore, Theorem 8.3.5, whose proof is found below, directly implies Theorem 8.3.4. □

Proof of Theorem 8.3.5. We first consider the case $q = 0$. If μ, ν are two measures on Ω of mass smaller than M, then $\mathrm{FG}_p(\mu, \nu) = W_{p,\rho}(\Phi(\mu), \Phi(\nu))$, where ρ is the distance on $\tilde{\Omega} := \Omega \cup \{\partial\Omega\}$ defined by $\forall x, y \in \tilde{\Omega}$,

$$\rho(x, y) = \min(|x - y|, d(x, \partial\Omega) + d(y, \partial\Omega))$$

and $\Phi(\mu) = \mu + (2M - |\mu|)\delta_{\partial\Omega}$ (see Proposition 6.3.2). Remark that $\rho(x, y) = |x - y|$ if $x, y \in U_L$, where $U_L \subset A_L$ is any ℓ_1-ball of radius $L/\sqrt{8}$ at distance $L/2$ from the diagonal, see Figure 8.2. As Φ is a bijection, the minimax rates for the estimation of $E(P)$ is therefore equal to

$$\inf_{\Phi(\hat{\mu}_n)} \sup_{P \in \mathcal{P}_{L,M,T}^{0,s}} \mathbb{E}[W_{p,\rho}^p(\Phi(\hat{\mu}_n), \Phi(E(P)))].$$

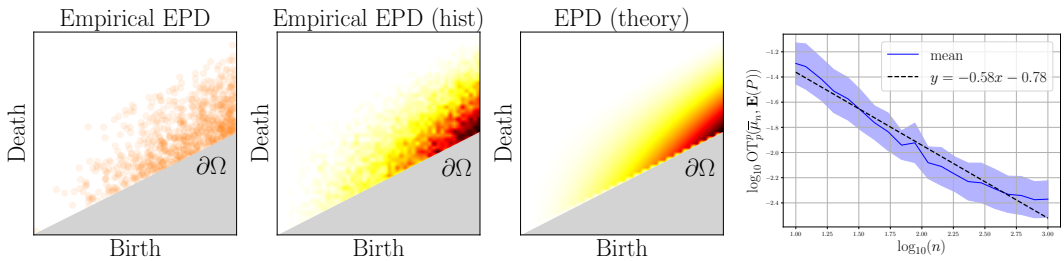


FIGURE 8.3: From left to right. (a) Empirical expected persistence diagram $\overline{\mu}_n$ with $n = 10^3$. (b) Histogram of the empirical expected persistence diagram on a 50×50 grid. (c) expected persistence diagram $E(P)$ of P, displayed on the same grid. (d) Distance $\mathrm{FG}_p^p(\overline{\mu}_n, E(P))$ for $p = 2$ for different values of n in log-log scale (mean and standard deviation over 100 runs). A linear regression shows a convergence rate of order $n^{-0.58}$, close to the theoretical rate of $n^{-1/2}$ indicated by Theorem 8.3.2.

Let $\mathcal{Q}$ be the set of probability measures on U_L whose densities belong to $B^s_{p',q'}$ with associated norm smaller than T/M. Then, $\mathcal{P}^{0,s}_{M,L,T}$ contains in particular the set of all distributions P for which $\mu \sim P$ satisfies $\Phi(\mu) = M\delta_x$ and x is sampled according to some law $\tau \in \mathcal{Q}$. For such a distribution P, one has $\Phi(E(P)) = M\tau$, so that the minimax rate is larger than

$$\inf_{\hat{a}_n} \sup_{\tau \in \mathcal{Q}} \mathbb{E}[W_p^p(\hat{a}_n, M\tau)],$$

where the infimum is taken on all measurable functions based on K observations of the form $M\delta_{x_i}$ with $x_1, \ldots, x_n$ a n-sample of law $\tau \in \mathcal{Q}$. Hence, we have shown that the minimax rate for the estimation of $E(P)$ with respect to FG_p is larger up to a factor M than the minimax rate for the estimation of $\tau \in \mathcal{Q}$ given n i.i.d. observations of law τ. As the minimax rate for this problem is known to be larger than $L^p/\sqrt{n}$ [WB19b, Theorem 5], we obtain the conclusion in the case $q = 0$.

For the general case $q > 0$, we remark that if $M' = ML^{-q}$ then $\mathcal{P}^{0,s}_{M',L}$ is included in $\mathcal{P}^{q,s}_{M,L,T}$. In particular, the minimax rate on $\mathcal{P}^{q,s}_{M,L,T}$ is larger than the minimax rate on $\mathcal{P}^{0,s}_{M',L,T}$, which is larger than $c\frac{M'L^p}{\sqrt{n}} = c\frac{ML^{p-q}}{\sqrt{n}}$ for some constant $c > 0$. □

Remark 8.3.6. In the classical setting of the estimation of a measure thanks to a n-sample with respect to the Wasserstein distance, it has been noted several times [TS15; WB19b; Div21a] that the problem of estimating the underlying measure is significantly easier if the measure has a lower bounded density on its domain. In particular, it is known that the risk for the W_p^p loss of the empirical measure attains the faster rate $n^{-p/2}$ (instead of $n^{-1/2}$) under this hypothesis. If such a result is likely to hold for the FG_p^p loss under similar hypothesis, assuming that the expected persistence diagram has a lower bounded density on some bounded domain U in Ω appears to be unreasonable. Indeed, this would imply that the density exhibits a sharp change of behavior at the boundary of U, whereas the density of the expected persistence diagram is known to be typically smooth on Ω according to Section 8.2. Whether there exists a more realistic assumption on the expected persistence diagram for which the rate of convergence of the empirical expected persistence diagram is $n^{-p/2}$ remains an open question.

Numerical illustration We showcase the rate of convergence of Theorem 8.3.2. There are only few cases where explicit expressions for the expected persistence diagram

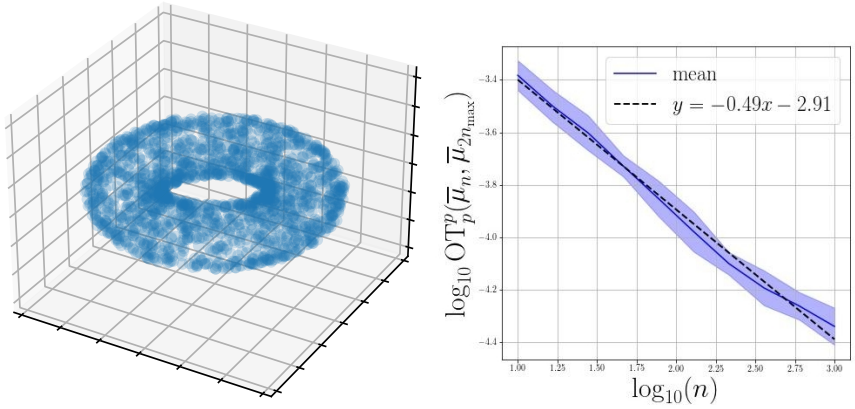


FIGURE 8.4: The convergence rate for a point cloud sampled on the surface of a torus, exhibiting a rate of $n^{-1/2}$.

of a process are known. For instance, for Čech persistence diagrams based on a random sample of points, the corresponding expected persistence diagram is known in closed-form only if the sample is supported on $\mathbb{R}$, see Chapter 7. We therefore first consider a simple setting where an explicit expression can be derived. Let X be a set of N triangles $T_1, \ldots, T_N$, where N is uniform on $\{1, \ldots, 20\}$. We let $f : X \to \mathbb{R}$ be a random piecewise constant function, which is equal to $U_{i,j}$ on the jth edge of the triangle T_i, where the variables $(U_{i,j})$ are i.i.d. uniform variables on $[0, 1]$. Furthermore, the function f is equal to $\max_{j=1,2,3} U_{i,j} + V_i$ on the inside of the triangle T_i, where the V_is are independent, independent from the $U_{i,j}$s, and follow a Beta distribution $\beta(1, 3)$. Let P be the distribution of the associated random persistence diagram. Let **rec** be the rectangle $[r_1, r_2] \times [s_1, s_2]$ for $r_1 \leq r_2 \leq s_1 \leq s_2$. Then,

$$E(P)(\mathbf{rec}) = 30 \int_{r_1}^{r_2} t^2 \mathbb{P}(s_1 - t \leq V \leq s_2 - t) \mathrm{d}t, \tag{8.27}$$

where $V \sim \beta(1, 3)$. In practice, we compute $E(P)$ on a discretization of $[0, 1] \times [0, 2]$ through a grid of size 50×50. Meanwhile, we sample empirical expected persistence diagrams $\overline{\mu}_n$ for $10 \leq n \leq 10^3$. In order to estimate $\mathrm{FG}_p^p(\overline{\mu}_n, E(P))$, we also turn these expected persistence diagrams into histograms on the same grid, and then compute the FG_p distance between two histograms. See Figure 8.3 for an illustration which showcases in particular the expected rate $n^{-1/2}$.

We also exhibit the convergence of the empirical expected persistence diagram in a more usual setting for the TDA practitioner. Namely, we build a random point cloud $\mathcal{X}$ with 10^3 points sampled on the surface of a torus with outer radius $r_1 = 5$ and inner radius $r_2 = 2$, and then consider the corresponding random Čech diagram for the 1-dimensional homology. Given n realizations of $\mathcal{X}$, we compute the empirical expected persistence diagram $\overline{\mu}_n$, where n ranges from 10 to $n_{max} = 1000$. As no closed-form for the corresponding expected persistence diagram is known, we use as a proxy the empirical expected persistence diagram based on a sample of size $2n_{max}$, and then showcase in Figure 8.4 the convergence of $\mathrm{FG}_p^p(\overline{\mu}_n, \overline{\mu}_{2n_{max}})$ at rate $n^{-1/2}$.

8.4 Persistence surface as a kernel density estimator

Among the different linear representations, the persistence surface is of particular interest. It is defined as the convolution of a diagram with a gaussian kernel. Hence, the mean persistence surface can be seen as a kernel density estimator of the density λ

of Theorem 8.2.5. As a consequence, the general theory of kernel density estimation applies and gives theoretical guarantees about various statistical procedures. As an illustration, we consider the bandwidth selection problem for persistence surfaces. Whereas authors in [Ada+17] state that any reasonable bandwidth is sufficient for a classification task, we give arguments for the opposite when no "obvious" shapes appear in the diagrams. We then propose a cross-validation scheme to select the bandwidth matrix. The consistency of the procedure is shown using Stone's theorem [Sto84]. This procedure is implemented on a set of toy examples illustrating its relevance.

Persistence surface is a representation of persistence diagrams introduced by Adams *et al.* [Ada+17]. It consists in a convolution of a diagram with a kernel, a general idea that has been repeatedly and fruitfully exploited, with slight variations, for instance in [Che+15; KHF16; Rei+15]. For $K : \mathbb{R}^2 \to \mathbb{R}$ a kernel and $h \geq 0$, we let for $u \in \mathbb{R}^2$,

$$K_h(u) = h^{-2} K(u/h). \tag{8.28}$$

For a a diagram, $K : \mathbb{R}^2 \to \mathbb{R}$ a kernel, $h \geq 0$ and $w : \mathbb{R}^2 \to \mathbb{R}_+$ a weight function, one defines the persistence surface of a with kernel K and weight function w by:

$$\forall u \in \mathbb{R}^2,\ \mathrm{Surf}_{w,h}(a)(u) := \Phi_{wK_h}(a)(u) = \sum_{v \in a} w(v) K_h(u - v). \tag{8.29}$$

Assume that $\mathcal{X}$ is some point process satisfying the assumptions of Theorem 8.2.5. Then, for $q \geq 1$, $\mu := \mathbb{E}[\mathrm{dgm}_q(K(\mathcal{X}))]$ has some density λ with respect to the Lebesgue measure on Ω. Therefore, $w \cdot \mu$, the measure having density w with respect to μ, has a density equal to $w \cdot \lambda$ with respect to the Lebesgue measure. The mean persistence surface $\mathbb{E}[\mathrm{Surf}_{w,h}(\mathrm{dgm}_q(K(\mathcal{X})))]$ is exactly the convolution of $w \cdot \mu$ by the kernel function K_h. As such, the persistence surface $\mathrm{Surf}_{w,h}(\mathrm{dgm}_q(K(\mathcal{X})))$ is actually a kernel density estimator of $w \cdot \lambda$.

If a point cloud approximates a shape, then its persistence diagram (for the Čech filtration for instance) is made of numerous points with small persistences and a few meaningful points of high persistences which correspond to the persistence diagram of the "true" shape. As one is interested in the latter points, a weight function w, which is typically an increasing function of the persistence, is used to suppress the importance of the topological noise in the persistence surface, see Chapter 7. Authors in [Ada+17] argue that in this setting, the choice of the bandwidth h has few effects for statistical purposes (e.g. classification), a claim supported by numerical experiments on simple sets of synthetic data, e.g. torus, sphere, three clusters, etc.

However, in the setting where the datasets are more complicated and contain no obvious "real" shapes, one may expect the choice of the bandwidth parameter h to become more critical: there are no highly persistent, easily distinguishable points in the diagrams anymore and the precise structure of the density functions of the processes becomes of interest. We show that a cross validation approach allows the bandwidth selection task to be done in an asymptotically consistent way. This is a consequence of a generalization of Stone's theorem [Sto84] when observations are not random vectors but random measures.

Let $P \in \mathcal{P}^0_{L,M}$ for certain parameters $L, M > 0$: if $\mu \sim P$, then $|\mu| \leq M$ and μ is supported on A_L. We further assume that the expected persistence diagram $E(P)$ has a bounded density λ. Given a kernel $K : \mathbb{R}^2 \to \mathbb{R}$ and a bandwidth h, we define the kernel density estimator

$$\forall u \in \Omega,\ \lambda_{n,h}(u) := K_h * \overline{\mu}_n(u) = \frac{1}{n} \sum_{i=1}^{n} \int K_h(u - v) \mathrm{d}\mu_i(v). \tag{8.30}$$

The optimal bandwidth h_{opt} minimizes the Mean Integrated Square Error (MISE)

$$\text{MISE}(h) := \mathbb{E}\left[\|\lambda - \lambda_{n,h}\|^2_{L_2(\Omega)}\right] = \mathbb{E}\left[\int (\lambda(u) - \lambda_{n,h}(u))^2 du\right]. \tag{8.31}$$

Of course, as λ is unknown, MISE(h) cannot be computed. Minimizing MISE(h) is equivalent to minimizing $J(h) := \text{MISE}(h) - \|\lambda\|^2_{L_2(\Omega)}$. Define

$$\lambda^{(i)}_{n,h}(u) := \frac{1}{n-1}\sum_{j\neq i}\int K_h(u-v)\mathrm{d}\mu_j(v) \tag{8.32}$$

and

$$\hat{J}(h) := \frac{1}{n^2}\sum_{i,j}\iint K^{(2)}_h(u-v)\mathrm{d}\mu_i(u)\mathrm{d}\mu_j(v) - \frac{2}{n}\sum_i\int \lambda^{(i)}_{n,h}(u)\mathrm{d}\mu_i(u), \tag{8.33}$$

where $K^{(2)} : u \mapsto \int K(u-v)K(v)\mathrm{d}v$ denotes the convolution of K with itself. The quantity $\hat{J}(h)$ is an unbiased estimator of $J(h)$. The selected bandwidth $\hat{h}$ is then chosen to be equal to $\arg\min_h \hat{J}(h)$.

The following theorem is a straightforward generalization of Stone's theorem (see [Sto84]) in the case where observations are random measures.

Theorem 8.4.1. *Assume that the kernel K is nonnegative, Hölder continuous and has a maximum attained in 0. Then, under the previous assumptions, $\hat{h}$ is asymptotically optimal in the sense that*

$$\frac{\|\lambda - \lambda_{n,\hat{h}}\|_{L_2(\Omega)}}{\|\lambda - \lambda_{n,h_{\text{opt}}}\|_{L_2(\Omega)}} \xrightarrow[N\to\infty]{} 1 \text{ a.s..} \tag{8.34}$$

Note that the gaussian kernel $K(x) = \exp(-|x|^2/2)$ satisfies the assumptions of Theorem 8.4.1.

The quality of the optimal estimator can also be studied. Indeed, a straightforward adaptation of the classical study of kernel density estimator (as presented for example in [Tsy08]) to the case of a sample of i.i.d. random measures shows that there exists a choice h_n of bandwidth depending on n and on the (unknown) regularity of λ such that the estimator λ_{n,h_n} is a consistent estimator of λ in the sense that $\mathbb{E}[\|\lambda - \lambda_{n,h_n}\|^2_{L_2(\Omega)}] \to 0$. Therefore, Theorem 8.4.1 asserts that the cross-validation procedure is consistent. We may furthermore inquire about the rate of convergence of the estimator λ_{n,h_n}. Once again, adapting classical results from [Tsy08] to the case of random measures, one can see that the optimal rate will be of order $n^{-s/(2s+2)}$ if λ is of regularity s. As such, contrary to the Figalli-Gigli loss (in Section 8.3), the rates of convergence are impacted by the underlying smoothness when using a more classical L_2 to estimate the density of the expected persistence diagram.

Let $\mathcal{X}_1, \dots, \mathcal{X}_n$ be i.i.d. processes on M having a density with respect to the law of a Poisson process of intensity $\mathcal{H}_d$ (with no bounds on the potential size of the diagrams). As M implies bounded p-total persistence for $p > d$, we know that the Čech persistence diagrams $\text{dgm}^{\text{C}}(\mathcal{X}_i)$ will satisfy $\text{Pers}_p(\text{dgm}^C_q(\mathcal{X}_i)) < C$ for $p > d$ and some deterministic constant C. Let λ be the density of the expected persistence diagram $\mathbb{E}[\text{dgm}^C_q(\mathcal{X}_1)]$. Assume that λ is bounded and has compact support, and let $\mu_i = d(\cdot, \partial\Omega)^p \cdot \text{dgm}^{\text{C}}(\mathcal{X}_i)$, the measure with density $d(\cdot, \partial\Omega)^p$ with respect to the ith diagram. Then, Theorem 8.4.1 can be applied to the sample $\mu_1, \dots, \mu_n$, and we have the equality

$$\lambda_{n,h} = \frac{1}{n}\sum_{i=1}^n \text{Surf}_{w,h}(\text{dgm}^{\text{C}}(\mathcal{X}_i)),$$

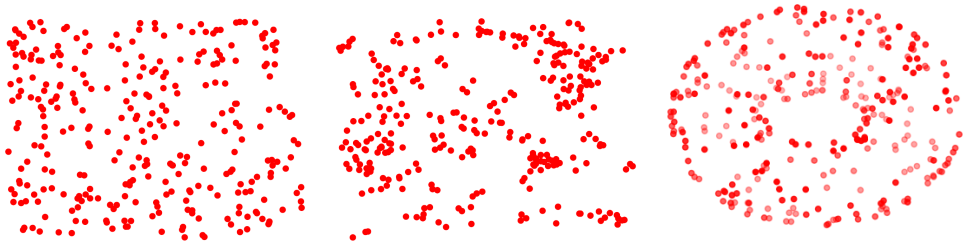


FIGURE 8.5: Realization of the processes (a), (b) and (c).

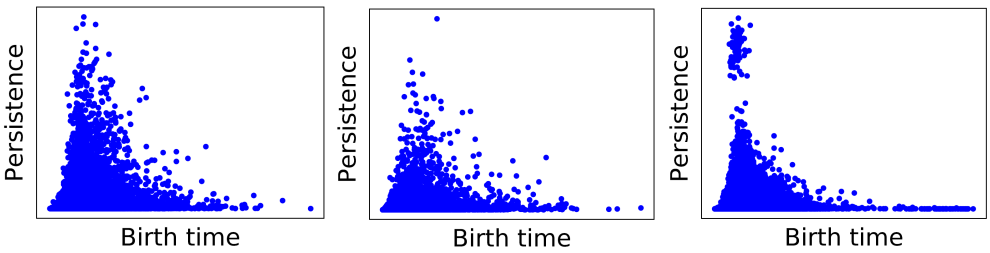


FIGURE 8.6: Superposition of the $N = 40$ diagrams of class (a), (b) and (c), transformed under the map $u \to (r_1, r_2 - r_1)$.

with $w = d(\cdot, \partial\Omega)^p$. Therefore, *the cross validation procedure* (8.33) *to select the bandwidth h in the persistence surface ensures that the mean persistence surface is a consistent estimator of $w \cdot \lambda$.*

Numerical illustration We showcase the bandwidth selection procedure for the persistent surface on simple experiments. Three sets of synthetic data are considered (see Figure 8.5). The first one (a) is made of $N = 40$ sets of $n = 300$ i.i.d. points uniformly sampled in the square $[0, 1]^2$. The second one (b) is made of N samples of a clustered process: $n/3$ cluster's centers are uniformly sampled in the square. Each center is then replaced with 3 i.i.d. points following a normal distribution of standard deviation $0.01 \times n^{-1/2}$. The third dataset (c) is made of N samples of n uniform points on a torus of inner radius 1 and outer radius 2. For each set, a Čech persistence diagram for 1-dimensional homology is computed. Persistence diagrams are then transformed under the map $(r_1, r_2) \mapsto (r_1, r_2 - r_1)$, so that they now live in the upper-left quadrant of the plane. Figure 8.6 shows the superposition of the diagrams in each class. One may observe the slight differences in the structure of the topological noise over the classes (a) and (b). The cluster of most persistent points in the diagrams of class (c) correspond to the two holes of a torus and are distinguishable from the rest of the points in the diagrams of the class, which form topological noise. The persistence diagrams are weighted by the weight function $w(u) = (r_2 - r_1)^3$, as advised in [KFH17] for two-dimensional point clouds. The bandwidth selection procedure will be applied to the measures having density w with respect to the diagrams, e.g. a measure is a sum of weighted Dirac measures.

For each class of dataset, the score $\hat{J}(h)$ is computed for 50 values h evenly spaced on a log-scale between 10^{-5} and 1. Note that the computation of $\hat{J}(h)$ only involves the computations of $K_h(u_1 - u_2)$ for points u_1, u_2 in different diagrams. Hence, the complexity of the computation of $\hat{J}(h)$ is in $O(T^2)$, where T is the sum of the number of points in the diagrams of a given class. If this is too costly, one may use a subsampling approach to estimate the integrals. The selected bandwidth were respectively $h = 0.22, 0.60, 0.17$. Persistence surfaces for the selected bandwidth are

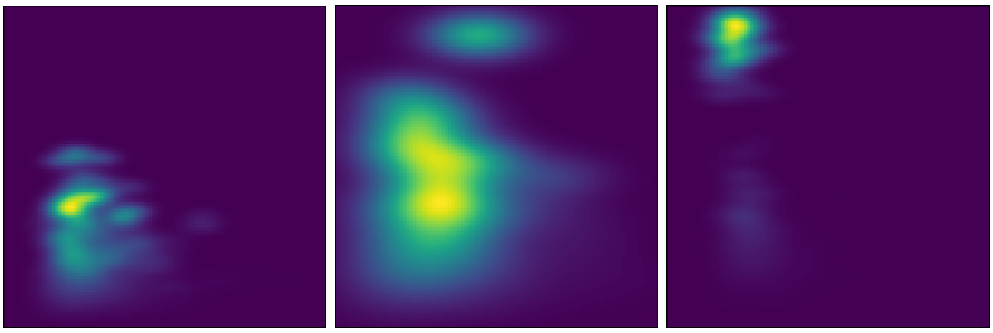


FIGURE 8.7: Persistence surfaces for each class (a), (b) and (c), computed with the weight function $w(u) = (r_2 - r_1)^3$ and with the bandwidth matrix selected by the cross-validation procedure.

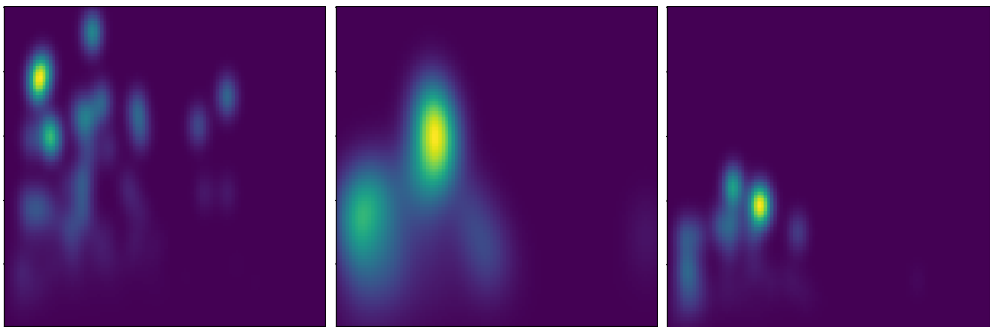


FIGURE 8.8: Persistence surfaces for each person A,B and C, computed with the weight function $w(u) = (r_2 - r_1)^3$ and with the bandwidth matrix selected by the cross-validation procedure.

displayed in Figure 8.7. The persistence of the "true" points of the torus are sufficient to suppress the topological noise: only two yellow areas are seen in the persistence surface of the torus. Note that the two areas can be separated, whereas it is not obvious when looking at the superposition of the diagrams, and would not have been obvious with an arbitrary choice of bandwidth. The bandwidth for class (b) may look to have been chosen too large. However, there is much more variability in class (b) than in the other classes: this phenomenon explains that the density is less peaked around a few selected areas than in class (a).

The cross-validation scheme has also been applied to non-synthetic data: the walk of 3 persons A, B and C, has been recorded using the accelerometer sensor of a smartphone in their pocket, giving rise to 3 multivariate time series in $\mathbb{R}^3$. Using a sliding window, each series has been split in a list of 10 times series made of 200 consecutive points. Using a time-delay embedding technique, those new time series are embedded into $\mathbb{R}^9$: these are the point clouds on which we build the Rips filtration. For each person, the set of 10 persistence diagrams is transformed under the map $(r_1, r_2) \mapsto (r_1, r_2 - r_1)$. The persistence diagrams are weighted by the weight function $w(u) = (r_2 - r_1)^3$. For each person, the scores $\hat{J}(h)$ are computed for 20 values h evenly spaced on a log-scale between 10^{-3} and 10^{-1}. The selected bandwidths are $0.0089, 0.01833$ and 0.0089 and the corresponding persistence surfaces are displayed in Figure 8.8. The three images show very distinct patterns: a reasonable machine learning algorithm will easily make the distinction between the three classes using the images as input.

8.5 Quantization of the expected persistence diagram

The problem of the quantization of a measure, namely approximating a given measure with another measure with support of fixed size, has been studied in depth when those measures are supported on $\mathbb{R}^d$ equipped with its natural Euclidean geometry, see for instance [GL07; Fis10; Lev15; BSW18]. In the context of persistence diagrams, where the quantization problem is generally referred to as computing *codebooks* or *bag-of-words* [Zie+19; Zie+20], existing methods propose to quantize persistence diagrams running a k-mean algorithm on the diagram points. The intuition that points in a diagram that are close to the boundary $\partial\Omega$ of the half-plane Ω represent less important topological features is taken into account through the introduction of weight functions, requiring to introduce an important hyper-parameter whose choice is unclear in general (although we proposed heuristics in Chapter 7).

We propose an alternative approach to quantize persistence diagrams. It differs from the latter on two aspects: first, we do not quantize a single diagram but work in an *online* fashion with a sequence of observed diagrams. Second, we work with the Figalli-Gigli metric FG_p. In doing so, we directly take the boundary $\partial\Omega$ into account in the formulation of our problem without needing to introduce a weight function. Our quantization algorithm significantly builds on [CLR20, Alg. 2]. The main difference is that Chazal, Levrard, and Royer intend to quantize a measure with respect to the 2-Wasserstein distance on $\mathbb{R}^d$, while we work with the metric FG_p on $\Omega \subset \mathbb{R}^2$. This change of perspective introduces some specificities in our problem and allows us to derive results more suited to the context of persistence diagrams. Furthermore, while standard algorithms work with $p = 2$, we propose a simple variation to encompass the case $p = +\infty$, central in TDA as one retrieves the so-called *bottleneck* distance.

This section consists of three steps. In Section 8.5.1, we introduce and study the problem of quantizing persistence measures with respect to the metric FG_p, proving in particular the existence of optimal quantizers in general. Section 8.5.2 provides an online algorithm specifically designed to quantize expected persistence diagrams based on a sequence of observed diagrams $\mu_1, \ldots, \mu_n$ and provide theoretical guarantees of convergence. Finally, we provide numerical experiments in Section 8.5.3.

8.5.1 Quantization for persistence measures.

Let $\mu \in \mathcal{M}^p$ be a persistence measure and k be a fixed integer. The goal of the quantization problem is to build a measure $\nu = \sum_{j=1}^k m_j \delta_{c_j}$ supported on a set of k points $\mathbf{c} = (c_1, \ldots, c_k)$ called a *codebook* (while the $(c_j)_j$s are called *centroids*) that approximates μ in an optimal way. Existing works (including previous works in the TDA literature) treat this problem over the space of probability measures equipped with the Wasserstein metric W_p over $\mathbb{R}^d$. Here, we use the metric FG_p instead, more suited to persistence diagrams, leading to benefits discussed in Remark 8.5.2 below. Our problem consists in minimizing the quantity $((m_1, c_1), \ldots, (m_k, c_k)) \mapsto \mathrm{FG}_p\left(\sum_j m_j \delta_{c_j}, \mu\right)$ where $m_j \in \mathbb{R}_+$ and $c_j \in \Omega$. However, we show in Lemma 8.5.3 below that—as in the standard problem using the metric W_p—this problem can be reduced to an optimization problem on the codebook $\mathbf{c} \in \Omega^k$ only. To that aim, we introduce a notion of *Voronoï tesselation* relative to a codebook $\mathbf{c}$, with the subtlety that points closer to the diagonal $\partial\Omega$ define a specific cell, see Figure 8.9 for an illustration.

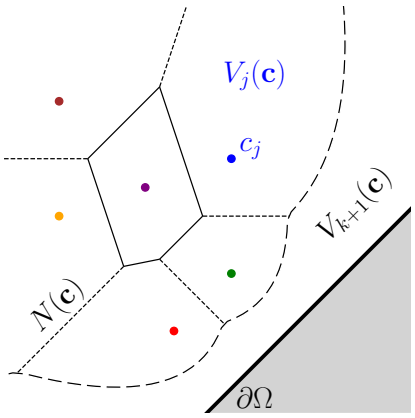


FIGURE 8.9: Example of partition $V_1(\mathbf{c}), \dots, V_{k+1}(\mathbf{c})$ for a given codebook $\mathbf{c}$.

Definition 8.5.1. *Let $\mathbf{c} = (c_1 \dots c_k) \in \Omega^k$ and denote by convention $c_{k+1} := \partial\Omega$, so that in particular $|x - c_{k+1}| := d(x, \partial\Omega)$. Define for $1 \le j \le k+1$,*

$$\begin{aligned} V_j(\mathbf{c}) :=& \{x \in \Omega,\ \forall j' < j, |x - c_j| \le |x - c_{j'}| \text{ and } \forall j' > j, |x - c_j| < |x - c_{j'}|\}, \\ N(\mathbf{c}) :=& \{x \in \Omega,\ \exists j < j' \text{ such that } x \in V_j(\mathbf{c}) \text{ and } |x - c_j| = |x - c_{j'}|\}. \end{aligned} \tag{8.35}$$

Observe that $V_1(\mathbf{c}), \dots, V_{k+1}(\mathbf{c})$ form a partition of Ω.

Remark 8.5.2. The difference between our approach and previous ones (in particular [CLR20]) lies in the presence of the "diagonal cell" $V_{k+1}(\mathbf{c})$. This cell introduces parabolic-shaped boundaries which slightly change the geometry of our problem. However, it has two major benefits. First, we do not "waste" centroids $(c_j)_{j=1}^k$ to encode points close to the diagonal (which are generally accounting for topological noise). Second, our approach does not require the introduction of a weight function (that artificially lowers the mass of points close to the diagonal), as typically done; removing the dependency on an important hyper-parameter.

The following lemma states that given a persistence measure μ and a codebook $\mathbf{c} = (c_1, \dots, c_k)$, it is always optimal to set $m_j = \mu(V_j(\mathbf{c}))$.

Lemma 8.5.3. *Let $\mathbf{c} = (c_1, \dots, c_k)$. Let $\hat{\mu}(\mathbf{c}) := \sum_{j=1}^k \mu(V_j(\mathbf{c}))\delta_{c_j}$ and let $\nu = \sum_{j=1}^k m_j \delta_{c_j}$ for some $m_1, \dots, m_k \ge 0$. Then $\mathrm{FG}_p(\hat{\mu}(\mathbf{c}), \mu) \le \mathrm{FG}_p(\nu, \mu)$.*

Proof of Lemma 8.5.3. Fix a codebook $\mathbf{c} = (c_1 \dots c_k)$. Let $T_{\mathbf{c}} : x \mapsto c_j$ if $x \in V_j(\mathbf{c})$ $(1 \le j \le k)$ and $\pi_{\partial\Omega}(x)$ if $x \in V_{k+1}(\mathbf{c})$. Let π be the pushforward of μ by the map $x \mapsto (x, T_{\mathbf{c}}(x))$, extended on $\overline{\Omega} \times \overline{\Omega}$ by $\pi(U, \overline{\Omega}) = 0$ for $U \subset \partial\Omega$ (intuitively, π pushes the mass of μ on their nearest neighbor in $\{c_1 \dots c_{k+1}\}$). One has, for $A, B \subset \Omega$, $\pi(A, \overline{\Omega}) = \mu((\mathrm{id}, T_c)^{-1}(A, \overline{\Omega})) = \mu(A)$, and $\pi(\overline{\Omega}, B) = \mu(T_c^{-1}(B)) = \sum_j \mu(V_j(\mathbf{c}))\mathbf{1}\{c_j \in B\}$, that is π is an admissible between the measures μ and $\sum_j \mu(V_j(\mathbf{c}))\delta_{c_j}$. Hence,

$$\mathrm{FG}_p^p\left(\mu, \sum_j \mu(V_j(\mathbf{c}))\delta_{c_j}\right) \le \int_{\overline{\Omega}} \min_{1 \le j \le k+1} |x - c_j|^p \mathrm{d}\mu(x).$$

Let $(m_1 \dots m_k)$ be a vector of non-negative weights, let $\nu = \sum_{j=1}^k m_j \delta_{c_j}$, and π be an admissible transport plan between μ and ν. One has

$$\begin{aligned}\int_{\overline{\Omega}\times\overline{\Omega}} |x-y|^p \mathrm{d}\pi(x,y) &= \sum_{j=1}^{k+1} \int_{\overline{\Omega}} |x-c_j|^p \mathrm{d}\pi(x,c_j) \\ &\geq \sum_{j=1}^{k+1} \int_{\overline{\Omega}} \min_{j'} |x-c_{j'}|^p \mathrm{d}\pi(x,c_j) \\ &\geq \int_{\overline{\Omega}} \min_{j'} |x-c_{j'}|^p \mathrm{d}\mu(x) \\ &\geq \mathrm{FG}_p^p\left(\mu, \sum_{j=1}^k \mu(V_j(\mathbf{c}))\delta_{c_j}\right).\end{aligned}$$

Taking the infimum over π gives the conclusion. □

Therefore, quantizing μ boils down to the choice of the codebook $\mathbf{c}$. Formally, given a persistence measure μ to be quantized, a parameter $1 \leq p < \infty$ and an integer k, the quantization problem in the space of persistence measures consists in minimizing $R_{k,p} : \Omega^k \to \mathbb{R}$ defined for $\mathbf{c} \in \Omega^k$ by

$$R_{k,p}(\mathbf{c}) := \mathrm{FG}_p(\hat{\mu}(\mathbf{c}), \mu) = \left(\sum_{j=1}^{k+1} \int_{V_j(\mathbf{c})} |x-c_j|^p \mathrm{d}\mu(x)\right)^{\frac{1}{p}}, \tag{8.36}$$

To alleviate notations, we write R_k instead of $R_{k,p}$ when the parameter p does not play a significant role. The value $R_k(\mathbf{c})$ is called the *distortion* achieved by $\mathbf{c}$. Let $R_k^* := \inf_{\mathbf{c}\in\Omega^k} R_k(\mathbf{c})$ and let $\mathbf{C}_k := \arg\min_{\mathbf{c}\in\Omega^k} R_k(\mathbf{c})$ be the set of optimal codebooks. Note that $R_k^* = 0$ if (and only if) $|\operatorname{spt}(\mu)| \leq k$. From now on, *we assume that μ has at least k points in its support.*

We can now state the main result of this subsection: the existence of an optimal codebook $\mathbf{c}^*$ for any persistence measure in $\mathcal{M}^p$. This result shares key ideas with [GL07, Theorem 4.12], although we replace the assumption of finite p-th moment of the measure to be quantized by the assumption of finite total persistence $\mathrm{Pers}_p(\mu) < \infty$.

Proposition 8.5.4 (Existence of minimizers)**.** *The set of optimal codebooks $\mathbf{C}_k$ is a non-empty compact set. Furthermore, if $\mathbf{c}^* \in \mathbf{C}_k$, then, for all $1 \leq j \neq j' \leq k$, $\mu(V_j(\mathbf{c}^*)) > 0$ and $c_j^* \neq c_{j'}^*$.*

To prove Proposition 8.5.4, we first introduce the following lemma, which states elementary properties of optimal codebooks. For technical reasons, we extend the function R_k to $\overline{\Omega}^k$, by noting that if $c_j \in \partial\Omega$, then the Voronoï cell $V_j(\mathbf{c})$ is empty by definition, see (8.35).

Lemma 8.5.5. *Let $\mathbf{c} \in \overline{\Omega}^k$ be such that there exists $1 \leq j \leq k$ with $\mu(V_j(\mathbf{c}^*)) = 0$. Then, $R_k(\mathbf{c}) > R_k^*$.*

In particular, if two centroids of a codebook $\mathbf{c}$ are equal or if a centroid c_j of $\mathbf{c}$ belongs to $\partial\Omega$, then the condition of the above lemma is satisfied, so that the $\mathbf{c}$ cannot be optimal. This proves the second part of Proposition 8.5.4.

Proof. Let $\mathbf{c} = (c_1, \dots, c_k) \in \overline{\Omega}^k$. Assume that without loss of generality that $\mu(V_1(\mathbf{c})) = 0$. Let $\mathbf{c}_0 = (c_2, \dots, c_k) \in \overline{\Omega}^{k-1}$ (that is, $\mathbf{c}$ where we removed the first

centroid). Assume first that $\mu(V_{k+1}(\mathbf{c})) > 0$, that is there is some mass transported onto the diagonal. Consider a compact subset $A \subset V_{k+1}(\mathbf{c})$ such that $\mu(A) > 0$ and the diameter $\mathrm{diam}(A)$ of A is smaller than the distance $d(A, \partial\Omega)$ between A and $\partial\Omega$. Let $c' \in A$ and observe that, for $x \in A$, $|x - c'| < d(x, \partial\Omega)$. Therefore,

$$\int_A |x - c'|^p \mathrm{d}\mu(x) < \int_A d(x, \partial\Omega)^p \mathrm{d}\mu(x).$$

Consider the measure $\nu = \hat{\mu}(\mathbf{c}_0) + \mu(A)\delta_{c'}$. Then

$$\begin{aligned}
&\mathrm{FG}_p^p(\nu, \mu) \\
&\leq \sum_{j=1}^{k} \int_{V_j(\mathbf{c})} |x - c_j|^p \mathrm{d}\mu(x) + \int_{V_{k+1}(\mathbf{c})\setminus A} d(x, \partial\Omega)^p \mathrm{d}\mu(x) + \int_A |x - c'|^p \mathrm{d}\mu(A) \\
&< R_k(\mathbf{c}),
\end{aligned}$$

thus $\mathbf{c}$ cannot be optimal. We can thus assume that $\mu(V_{k+1}(\mathbf{c})) = 0$, in which case we can reproduce the proof of [GL07, Theorem 4.1], which gives that $\mathbf{c}$ cannot be optimal either in that case, yielding the conclusion. □

Lemma 8.5.6. *R_k is continuous.*

Proof. For a given $x \in \overline{\Omega}$, the map $\mathbf{c} \mapsto \min_i |x - c_i|^p$ is continuous and upper bounded by $d(x, \partial\Omega)^p$. Thus, R_k is continuous by dominated convergence as we have finite p-total persistence. □

Lemma 8.5.7. *Let $0 \leq \lambda < R^*_{k-1}$. Then, the set $\{\mathbf{c} \in \overline{\Omega}^k : R_k(\mathbf{c}) \leq \lambda\}$ is compact.*

Proof. Fix $\lambda < R^*_{k-1}$. The set is closed by continuity of R_k, so that it suffices to show that it is bounded. Let $\mathbf{c}$ be such that $R_k(\mathbf{c}) \leq \lambda$. Pick L such that $\int_{A_L} d(x, \partial\Omega)^p \mathrm{d}\mu(x) \geq \lambda$ and $\int_{A_L^c} d(x, \partial\Omega)^p \mathrm{d}\mu(x) < R^*_{k-1} - \lambda$. Such a L exists since $\int_\Omega d(x, \partial\Omega)^p \mathrm{d}\mu(x) = \mathrm{Pers}_p(\mu) = R^*_0 \geq R^*_{k-1}$. Then, all the c_js must be in A_{2L}. Indeed, assume without loss of generality that $c_1 \in A^c_{2L}$. Then $V_1(\mathbf{c}) \subset A^c_L$, as any point in A_L is closer to the diagonal than to c_1. Therefore,

$$\begin{aligned}
R^*_{k-1} \leq& \sum_{j=2}^{k+1} \int_{V_j(\mathbf{c})} |x - c_j|^p \mathrm{d}\mu(x) + \int_{V_1(\mathbf{c})} \min_{j \in \{2 \ldots k+1\}} |x - c_j|^p \mathrm{d}\mu(x) \\
\leq& R_k(\mathbf{c}) + \int_{V_1(\mathbf{c})} d(x, \partial\Omega)^p \mathrm{d}\mu(x) \\
\leq& R_k(\mathbf{c}) + \int_{A^c_L} d(x, \partial\Omega)^p \mathrm{d}\mu(x) \\
<& \lambda + R^*_{k-1} - \lambda = R^*_{k-1},
\end{aligned}$$

leading to a contradiction. □

Finally, we are ready to prove Proposition 8.5.4.

Proof of Proposition 8.5.4. We show by recursion on $0 \leq m \leq k$ that $R^*_m < R^*_{m-1}$ and that $\mathbf{C}_m$ is a non-empty compact set (with the convention $R^*_{-1} = +\infty$). The initialization holds as $R^*_0 = \mathrm{Pers}_p(\mu) < +\infty$ with the empty codebook being optimal. We now prove the induction step. Let $\mathbf{c} = (c_1, \ldots, c_{m-1}) \in \mathbf{C}_{m-1}$. Consider $\mathbf{c}' = (c_1, c_1, c_2, \ldots, c_{m-1})$. Then, $\mu(V_1(\mathbf{c}')) = 0$, so that $R^*_{m-1} = R_{m-1}(\mathbf{c}) = R_m(\mathbf{c}') > R^*_m$ by Lemma 8.5.5. Furthermore, pick $\lambda \in (R^*_m, R^*_{m-1})$. Then, R^*_m is equal to the

infimum of R_m on the set $\{\mathbf{c} \in \overline{\Omega}^k : R_m(\mathbf{c}) \leq \lambda\}$, which is compact according to Lemma 8.5.7. As the function R_k is continuous, the set of minimizers $\mathbf{C}_m$ is a non-empty compact set, concluding the induction step. □

Corollary 8.5.8. *The following quantities are positive:*

$$\begin{aligned} D_{\min} &:= \inf_{\mathbf{c}^* \in \mathbf{C}_k, 1 \leq j \neq j' \leq k+1} |c_j^* - c_{j'}^*|, \\ m_{\min} &:= \inf_{\mathbf{c}^* \in \mathbf{C}_k, 1 \leq j \leq k} \mu(V_j(\mathbf{c}^*)). \end{aligned} \tag{8.37}$$

Proof of Corollary 8.5.8. The quantities being minimized in the definitions of $D_{\min}$ and $m_{\min}$ are both continuous functions of $\mathbf{c}^*$. As the set $\mathbf{C}_k$ is compact, the minima are attained, and cannot be equal to 0 according to Proposition 8.5.4. □

Computational aspects. One could consider to numerically solve the quantization problem (8.36) deriving optimization algorithms based on their counterpart in the optimal transport literature [CD14], see [Lac20, Section 7.2] for instance. However, using such techniques to quantize empirical expected persistence diagrams would not be satisfactory for two reasons. First, the empirical expected persistence diagram has in general a large number of points, hindering computational efficiency. Second, we want to leverage the fact that we observe a sequence of diagrams $\mu_1, \ldots, \mu_n$, and not only their sum, to design an online algorithm that remains tractable with large sequences of large diagrams.

8.5.2 Quantization of an empirical expected persistence diagram

In Algorithm 1, we propose an online algorithm—adapted from [CLR20, Alg. 2] to the context of persistence diagrams and with arbitrary $p > 1$ instead of $p = 2$—that takes a sequence of observed persistence diagrams $\mu_1, \ldots, \mu_n$ (a n-sample of law P) and outputs a codebook $(c_1, \ldots, c_k)$ aiming at approximating $E(P)$. The algorithm relies on an update function U_p for $p > 1$ defined as

$$U_p(t, \mathbf{c}, \mu, \mu') := \mathbf{c} - \frac{\left(\frac{\mu(V_j(\mathbf{c}))}{\mu'(V_j(\mathbf{c}))}\left(c_j - v_p(\mathbf{c}, \mu)_j\right)\right)_j}{t+1}, \tag{8.38}$$

where $v_p(\mathbf{c}, \mu)_j$ is the *p-center* of mass of μ over the cell $V_j(\mathbf{c})$:

$$v_p(\mathbf{c}, \mu)_j := \arg\min_y \left(\int_{V_j(\mathbf{c})} |y - x|^p \mathrm{d}\mu(x)\right)^{\frac{1}{p}}. \tag{8.39}$$

When $p = 2$, one simply has $v_2(\mathbf{c}, \mu)_j = \int_{V_j(\mathbf{c})} x \frac{\mathrm{d}\mu(x)}{\mu(V_j(\mathbf{c}))}$ and if in addition $\mu = \mu'$, the update (8.38) simplifies to

$$c_j \mapsto \frac{t}{t+1} c_j + \frac{1}{t+1} \int_{V_j(\mathbf{c})} x \frac{\mathrm{d}\mu(x)}{\mu(V_j(\mathbf{c}))},$$

so that roughly speaking, we are pushing c_j toward the usual center of mass of μ over the cell $V_j(\mathbf{c})$, similar to what is done when using the Lloyd algorithm to solve the k-means problem [Llo82]. More generally, (8.38) can be understood as pushing c_j toward the point that would decrease the distortion $R_{k,p}$ over the cell $V_j(\mathbf{c})$ the most, using a step-size (or learning rate) $\frac{1}{t+1}$. There is no closed-form for v_p for $p \neq 2$, though standard convex solvers may be used [Gon89]. When $p = +\infty$, a central situation

Algorithm 1: Online quantization of EPDs

Input: A sequence $\mu_1, \dots, \mu_n$, integer k, parameter p.
Preprocess: Divide indices $\{1, \dots, n\}$ into batches $(B_1, \dots, B_T)$ of size $(n_1, \dots, n_T)$. Furthermore, divide $(B_t)_t$ into two halves $B_t^{(1)}$ and $B_t^{(2)}$.
Set $\overline{\mu}_t^{(\alpha)} := \frac{2}{n_t} \sum_{i \in B_t^{(\alpha)}} \mu_i$ for $1 \leq t \leq T, \alpha \in \{1, 2\}$.
Init: Sample $c_1^{(0)} \dots c_k^{(0)}$ from the diagrams.
for $t = 0, \dots, T-1$ **do**
  $c^{(t+1)} = U_p(\mathbf{c}^{(t)}, \overline{\mu}_{t+1}^{(1)}, \overline{\mu}_{t+1}^{(2)})$ using (8.38)
end for
Output: The final codebook $\mathbf{c}^{(T)}$.

in TDA as it means working with the bottleneck distance FG_∞, computing v_∞ boils down to get the center of the *smallest enclosing circle* of $V_j(\mathbf{c}) \cap \mathrm{spt}(\mu)$. When μ is a discrete measure (e.g. an empirical expected persistence diagram), this problem can be solved in linear time with respect to the number of points of μ that belong to $V_j(\mathbf{c})$ [Meg83].

Note that in Algorithm 1, the split of batches $B_t = (B_t^{(1)}, B_t^{(2)})$ is only required for technical considerations (see the proof of Theorem 8.5.10 and [CLR20]). In practice, this algorithm can be used without further assumptions and empirically, using $B_t = B_t^{(1)} = B_t^{(2)}$ yields substantially similar results. We provide a theoretical analysis of Algorithm 1 in the case $p = 2$, in particular through Theorem 8.5.10 which states that this algorithm is nearly optimal as a way to quantize $E(P)$, provided the initialization is good enough. As in Section 8.3, we consider a probability distribution $P \in \mathcal{P}_{L,M}^p$. For $t > 0$ and $A \subset \Omega$, recall that $A^t := \{x \in \Omega : \exists a \in A, |x - a| \leq t\}$ is the t-neighborhood of A.

Definition 8.5.9 (Margin condition)**.** *Let $\mathbf{c}^*$ be an optimal quantizer of $E(P)$. We say that P satisfies a* margin condition *of parameter $\lambda > 0$ and radius r_0 at $\mathbf{c}^*$ if, for all $t \in [0, r_0]$, one has $E(P)(N(\mathbf{c}^*)^t) \leq \lambda t$.*

Margin-like conditions on optimal codebook are standard in quantization literature [TM16; Lev18]. Informally, it indicates that the expected persistence diagram concentrates around k poles, aside from the mass that is distributed close to the diagonal $\partial\Omega$; the smaller the λ, the more concentrated the measure. Note that this condition holds as long as the $E(P)$ has a bounded density (although with possibly large λ), so that it is satisfied in the framework of Section 8.2

The following theorem states that given a n-sample of law P, Algorithm 1 outputs in $T = \frac{n}{\log(n)}$ steps a codebook $\mathbf{c}^{(T)}$ that approximates (in expectation) an optimal codebook $\mathbf{c}^*$ for $E(P)$ at rate $\frac{\log(n)}{n}$, to be compared with the optimal rate of $\frac{1}{n}$ [Lev18, Proposition 7]. It echoes [CLR20, Theorem 5] with the difference that, thanks to the diagonal cell V_{k+1}, we require a uniform bound on the total persistence of the measures rather than a uniform bound on their total mass, a more natural assumption in TDA.

Theorem 8.5.10. *Let $p = 2$. Let $P \in \mathcal{P}_{L,M}^2$ and let $\mathbf{c}^*$ be an optimal codebook for $E(P)$. Assume that P satisfies a margin condition at $\mathbf{c}^*$ with parameters r_0 large enough and λ small enough (with respect to $D_{\min}, m_{\min}, L$ and M). Let $\mu_1, \dots, \mu_n$ be a n-sample of law P and $B_1, \dots, B_T$ be equally sized batches of length $C_1 \log(n)$. Finally, let $\mathbf{c}^{(T)}$ denote the output of Algorithm 1. There exists $R_0 > 0$ such that if $|\mathbf{c}^{(0)} - \mathbf{c}^*| \leq R_0$, then*

$$\mathbb{E}|\mathbf{c}^{(T)} - \mathbf{c}^*|^2 \leq C_2(\log n)/n,$$

where C_1, C_2 and R_0 are constants depending on $p, L, M, k, D_{\min}$ and $m_{\min}$.

The remainder of this section is dedicated to proving Theorem 8.5.10. In the following, we fix a distribution P supported on $\mathcal{M}^p_{L,M}$ and we consider $\mathbf{c}^*$ be an optimal codebook of $E(P)$. The different constants encountered in this section all depend on the parameters $p, L, M, k, D_{\min}$ and $m_{\min}$. In particular, we introduce the quantity

$$m_{\max} := \sup_{\mu \in \mathcal{M}^p_{L,M}} \sup_{1 \le j \le k} \mu(V_j(\mathbf{c}^*)).$$

Note that $m_{\max} \le \frac{2^p M}{D^p_{\min}}$ as $\int_{V_j(\mathbf{c}^*)} \mathrm{d}\mu(x) \le \frac{2^p}{D^p_{\min}} \int_{V_j(\mathbf{c}^*)} d(x, \partial\Omega)^p \mathrm{d}\mu(x)$.

The proof of Theorem 8.5.10 follows the proof of [CLR20, Theorem 5]. As a first step, we show that it is enough to prove the following lemma, which relates the loss of $\mathbf{c}^{(t)}$ and the loss of $\mathbf{c}^{(t+1)}$.

Lemma 8.5.11. *There exists $R_0 > 0$ such that, if $|c_j^{(0)} - c_j^*| \le R_0$ for $1 \le j \le k$, then*

$$\mathbb{E}|\mathbf{c}^{(t+1)} - \mathbf{c}^*|^2 \le \left(1 - \frac{C_0}{t+1}\right) \mathbb{E}|\mathbf{c}^{(t)} - \mathbf{c}^*|^2 + \frac{C_1}{(t+1)^2},$$

for some constants $C_0 > 1$, $C_1 > 0$.

Proof of Theorem 8.5.10. From Lemma 8.5.11, we show by induction that $u_t := \mathbb{E}|\mathbf{c}^{(t)} - \mathbf{c}^*|^2$ satisfies $u_t \le \frac{\alpha}{t+1}$ for $\alpha = C_1/(C_0 - 1)$. This concludes the proof as T is of order $n/\log(n)$. The initialization holds by assumption as long as $R_0 \le \alpha$, whereas we have by induction

$$\begin{aligned} u_{t+1} &\le \left(1 - \frac{C_0}{t+1}\right) \frac{\alpha}{t+1} + \frac{C_1}{(t+1)^2} \\ &\le \frac{\alpha}{(t+1)^2} (t + 1 - C_0 + C_1/\alpha) = \frac{\alpha t}{(t+1)^2}, \end{aligned}$$

which is smaller than $\alpha/(t+2)$. □

The proof of Lemma 8.5.11 is a close adaptation of [CLR20, Lemma 21]. The proof of the latter contains tedious computations (that we do not reproduce here) which can be adapted *mutatis mutandis* to our setting once the two following key results are shown. Given a codebook $\mathbf{c}$, we let $p_j(\mathbf{c}) = E(P)(V_j(\mathbf{c}))$ and similarly, given a n-sample $\mu_1, \dots, \mu_n$ of law P, we let $\hat{p}_j(\mathbf{c}) = \overline{\mu}_n(V_j(\mathbf{c}))$. Note that if $|\mathbf{c} - \mathbf{c}^*|$ is small enough, one has $p_j(\mathbf{c}) \le 2m_{\max}$. Also, we let $w_p(\mathbf{c}, \mu)_j := \mu(V_j(\mathbf{c}))v_p(\mathbf{c}, \mu)_j$ for $\mu \in \mathcal{M}^p$ and $1 \le j \le k$. Recall that we assume that the expected persistence diagram $E(P)$ satisfies the margin condition (Definition 8.5.9) with parameters λ and r_0 around the optimal codebook $\mathbf{c}^*$.

Lemma 8.5.12 (Lemma 22 in [CLR20])**.** *Let R_0 be small enough respect to $r_0 D^2_{\min}/L^2$ and let $\mathbf{c}$ be such that $|\mathbf{c} - \mathbf{c}^*| \le R_0$. Then, we have*

$$\sum_{j=1}^k |p_j(\mathbf{c}) - p_j(\mathbf{c}^*)| \le 2\lambda r_0,$$

and

$$|w_2(\mathbf{c}, E(P)) - (p_j(\mathbf{c}^*)\mathbf{c}^*_j)_j| \le 7\sqrt{2}\lambda \frac{L^3}{D^2_{\min}} |\mathbf{c} - \mathbf{c}^*|.$$

As $w_2(\mathbf{c}^*, E(P))_j = p_j(\mathbf{c}^*)\mathbf{c}^*_j$, Lemma 8.5.12 indicates that the application $\mathbf{c} \mapsto w_2(\mathbf{c}, E(P))$ is Lipschitz continuous around an optimal codebook $\mathbf{c}^*$, a key property to show the convergence of the sequence $(\mathbf{c}^{(t)})_t$.

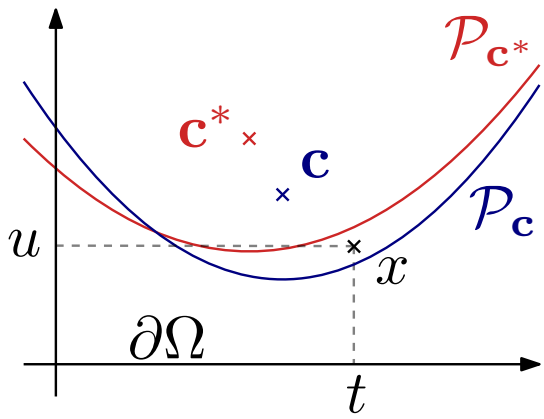


FIGURE 8.10: Illustration of the proof of Lemma 8.5.12

Lemma 8.5.13 (Lemma 24 in [CLR20]). *Let $\mathbf{c}$ be a codebook such that $\hat{p}_j(\mathbf{c}) \leq 2m_{\max}$ (which is always possible if $|\mathbf{c} - \mathbf{c}^*|$ is small enough). Then, with probability larger than $1 - 2ke^{-x}$, we have, for all $1 \leq j \leq k$,*

$$|\hat{p}_j(\mathbf{c}) - p_j(\mathbf{c})| \leq \sqrt{\frac{4m_{\max}p_j(\mathbf{c})x}{n}} + \frac{2m_{\max}x}{3n}. \tag{8.40}$$

Moreover, with probability larger than $1 - e^{-x}$, we have

$$|w_2(\mathbf{c}, \overline{\mu}_n) - w_2(\mathbf{c}, E(P))| \leq 2m_{\max}L\sqrt{\frac{2k}{n}}\left(1 + \sqrt{\frac{x}{2}}\right). \tag{8.41}$$

The proof of this lemma follows from standard concentration inequalities.

Proof of Lemma 8.5.13. Equation (8.40) follows from Bernstein inequality applied to the real-valued random variable $0 \leq \hat{p}_j(\mathbf{c}) \leq 2m_{\max}$, with variance bounded by $\mathbb{E}[\mu(V_j(\mathbf{c}))^2]/n \leq m_{\max}p_j(\mathbf{c})/n$.

For equation (8.41), we introduce the function $f_j : x \mapsto x\mathbf{1}\{x \in V_j(\mathbf{c})\}$, so that $w_2(\mathbf{c}, \mu)_j = \mu(f_j)$, the integral of f_j against μ. We have $w_2(\mathbf{c}, \mu_n)_j - w_2(\mathbf{c}, E(P))_j = n^{-1}\sum_{i=1}^n(\mu_i(f_j) - E(P)(f_j))$. Note that $|\mu_i(f_j)| \leq \sqrt{2}L \cdot 2m_{\max}$. We write

$$\begin{aligned}
&\mathbb{E}\left|\frac{1}{n}\sum_{i=1}^n(\mu_i(f_j) - E(P)(f_j))_j\right| \\
&\leq \sqrt{\mathbb{E}\left|\frac{1}{n}\sum_{i=1}^n(\mu_i(f_j) - E(P)(f_j))_j\right|^2} \\
&\leq \sqrt{\frac{1}{n}\mathbb{E}\left|(\mu_1(f_j))_j\right|^2} \leq 2\sqrt{\frac{k}{n}}\sqrt{2}Lm_{\max}.
\end{aligned}$$

Also, note that $F(\mu_1, \ldots, \mu_n) = |w_2(\mathbf{c}, \mu_n) - w_2(\mathbf{c}, E(P))|$ satisfies a bounded difference condition of parameter $4\sqrt{2}Lm_{\max}$ [BLM13, Section 6.1]. A bounded difference inequality [BLM13, Theorem 6.2] yields the result. □

The proof of Lemma 8.5.12 relies on the following lemma, that essentially tells that the area of misclassified points when using a codebook $\mathbf{c}$ instead of an optimal one $\mathbf{c}^*$ can be controlled linearly in terms of $|\mathbf{c}^* - \mathbf{c}|$. Note that this result is well-known when boundaries between the cells are hyperplanes (as it is the case in standard quantization), it remains to treat the case when the boundary is a parabola. Let $d(x, A)$ be the distance from a point $x \in \Omega$ to $A \subset \Omega$.

Lemma 8.5.14. *Let $\mathbf{c}^*$ be an optimal codebook, and $\mathbf{c} \in A_L^k$. Let $x \in A_L$ and $1 \le j \le k$. Assume that $x \in V_j(\mathbf{c}^*) \cap V_{k+1}(\mathbf{c})$. Then, $d(x, \partial V_j(\mathbf{c}^*)) \le \frac{7L^2}{2D_{\min}^2}|\mathbf{c}^* - \mathbf{c}|$. Symmetrically, if $x \in V_{k+1}(\mathbf{c}^*) \cap V_j(\mathbf{c})$, one has $d(x, \partial V_{k+1}(\mathbf{c}^*)) \le \frac{7L^2}{2D_{\min}^2}|\mathbf{c}^* - \mathbf{c}|$.*

Proof of Lemma 8.5.14. For convenience, we write in this proof the coordinates of points in the basis $(\partial\Omega, \partial\Omega^\perp)$, that $x \in \Omega$ will have coordinates (a, b) where a is the projection of x on $\partial\Omega$ and $b = d(x, \partial\Omega)$. Also, given $y = (a, b) \in \Omega$, we let $\mathcal{P}_y$ be the parabola with focus y and directrix $\partial\Omega$. To put it another way, if $y = (a, b)$, then $\mathcal{P}_y$ is the image of $\partial\Omega$ by the map

$$f(a, b, \cdot) : t \mapsto \frac{(t-a)^2}{2b} + \frac{b}{2}.$$

One can check that for all $t \in [-L/2, L/2]$, if $b = d(y, \partial\Omega) \ge D_{\min}$, we have $\left|\frac{\partial f}{\partial a}\right| \le \frac{L}{D_{\min}}$ and $\left|\frac{\partial f}{\partial b}\right| \le \frac{1}{2} + \frac{(t-a)^2}{b}\frac{1}{b} \le \frac{1}{2} + \frac{2L^2}{D_{\min}^2}$.

Let $c_j^* = (a^*, b^*)$ and $c_j = (a, b)$. Let $x = (t, u) \in V_j(\mathbf{c}^*) \cap V_{k+1}(\mathbf{c})$. Then, $u \ge f(a^*, b^*, t)$, whereas $u \le f(a, b, t)$. The distance $d(x, \partial V_j(\mathbf{c}^*))$ is smaller than $u - f(a^*, b^*, t)$

$$\begin{aligned}
&u - f(a^*, b^*, t) \le f(a, b, t) - f(a^*, b^*, t) \\
&\le |f(a^*, b^*, t) - f(a, b^*, t)| + |f(a, b^*, t) - f(a, b, t)| \\
&\le \int_{a\wedge a^*}^{a\vee a^*} \left|\frac{\partial f}{\partial a}(\alpha, b^*, t)\right| \mathrm{d}\alpha + \int_{b\wedge b^*}^{b\vee b^*} \left|\frac{\partial f}{\partial b}(a, \beta, t)\right| \mathrm{d}\beta \\
&\le \frac{L}{D_{\min}}|a - a^*| + \left(\frac{1}{2} + \frac{2L^2}{D_{\min}^2}\right)|b - b^*| \\
&\le \left(\frac{1}{2} + \frac{L}{D_{\min}} + \frac{2L^2}{D_{\min}^2}\right)|\mathbf{c} - \mathbf{c}^*| \le \frac{7}{2}\frac{L^2}{D_{\min}^2}|\mathbf{c} - \mathbf{c}^*|,
\end{aligned}$$

which proves the claim. □

Proof of Lemma 8.5.12. This proof is inspired from [Lev15, Appendix A.3]. Let us prove the first point. One has, with $t = \frac{7L^2}{2D_{\min}^2}|\mathbf{c} - \mathbf{c}^*| \le r_0$,

$$\begin{aligned}
&\sum_{j=1}^k |p_j(\mathbf{c}) - p_j(\mathbf{c}^*)| = \sum_{j=1}^k |E(P)(V_j(\mathbf{c})) - E(P)(V_j(\mathbf{c}^*)| \\
&\le 2\sum_j \sum_{j'\neq j} E(P)(V_j(\mathbf{c}) \cap V_{j'}(\mathbf{c}^*)) \le 2E(P)[N(\mathbf{c}^*)^t] \le 2\lambda t \le 2\lambda r_0.
\end{aligned}$$

where we applied Lemma 8.5.14 and the margin condition. To prove the second inequality, remark that $w_2(\mathbf{c}, E(P))_j = \int_{V_j(\mathbf{c})} x \mathrm{d}E(P)(x)$. Therefore,

$$\begin{aligned}
|w_2(\mathbf{c}, E(P)) - w_2(\mathbf{c}^*, E(P))| &\le \sum_{j=1}^k |w_2(\mathbf{c}, E(P))_j - w_2(\mathbf{c}^*, E(P))_j| \\
&\le \sum_{j=1}^k \left|\int_{V_j(\mathbf{c})} x \mathrm{d}E(P)(x) - \int_{V_j(\mathbf{c}^*)} x \mathrm{d}E(P)(x)\right| \\
&\le 2\sum_j \sum_{j'\neq j} \int_{V_j(\mathbf{c})\cap V_{j'}(\mathbf{c}^*)} |x| \mathrm{d}E(P)(x) \\
&\le 2\sqrt{2}L\lambda t \le 7\sqrt{2}\lambda \frac{L^3}{D_{\min}^2}|\mathbf{c} - \mathbf{c}^*|.
\end{aligned}$$

□

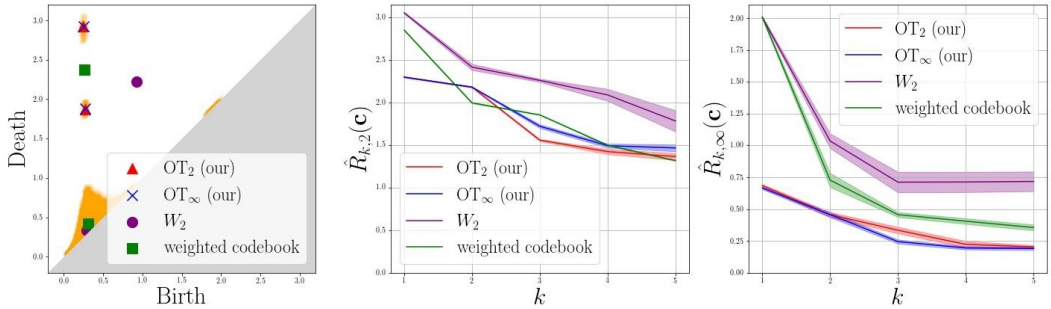


FIGURE 8.11: From left to right: (a) The quantization output for the different approaches considered with $k = 2$. As our approach accounts for the diagonal through the cell V_{k+1}, our codebooks retrieve the two clusters present in the expected persistence diagram, while other approaches have one centroid used to account for the mass close to the diagonal. (b,c) The average distortion $R_{k,p}$ over 10 runs for the different methods, with $p = 2$ and $p = +\infty$.

8.5.3 Numerical illustrations

We now illustrate the behavior of Algorithm 1 using $p = 2$ and $p = \infty$ (referred to as "FG$_2$" and "FG$_\infty$", respectively) and compare it to two natural alternatives. [CLR20, Alg. 2] is essentially the same algorithm without the "diagonal cell" $V_{k+1}(\mathbf{c})$; as such, centroids are dramatically influenced by points close to the diagonal which are likely to be abundant in standard applications of TDA. It is referred to as "W_2" in our illustrations, as it relies on quantization with respect to the Wasserstein distance with $p = 2$. The second alternative, referred to as "weighted codebook", is the one proposed in [Zie+20], which can be summarized in the following way: consider the empirical expected persistence diagram $\overline{a}_n$ built on top of observations $a_1, \ldots, a_n$ (that is, concatenate the diagrams), and then subsample N points in the support of the empirical expected persistence diagram, with the subtlety that the probability of choosing a point $x \in \mathrm{spt}(\overline{\mu}_n)$ depends on a weight function $w : \Omega \to \mathbb{R}_+$. Typical choices for w are of the form $w(x) = \min\left(\max\left(0, \frac{(d(x,\partial\Omega)^q - \lambda)}{\theta - \lambda}\right), 1\right)$ for some parameters (λ, q, θ); the goal being to favor sampling points far from the diagonal. Zieliński et al. propose, in practice, to sample $N = 10^4$ points and to set $q = 1$, while λ and θ are the 0.05 and 0.95 quantiles of the distribution of $\{d(x, \partial\Omega)^q,\ x \in \mathrm{spt}(\overline{\mu}_n)\}$, respectively. We use these parameters in our experiments. One then runs the Lloyd algorithm (k-means) on the set of N points that have been sampled to obtain a quantization of the empirical expected persistence diagram.

We compare the different approaches in the following experiment. We randomly sample a point cloud $\mathcal{X}$ of size m on the surface of a torus with radii (r_1, r_2), where m, r_1, r_2 are random variables that respectively follow a Poisson distribution of parameter $\lambda \in \mathbb{N}$, a uniform distribution over $[R_1 - \varepsilon, R_1 + \varepsilon]$ and a uniform distribution over $[R_2 - \varepsilon, R_2 + \varepsilon]$. We use $\lambda = 2,000, \varepsilon = 0.1, R_1 = 5$ and $R_2 = 2$ in our experiments. Given such a random point cloud $\mathcal{X}$, we build the Čech persistence diagram of its 1-dimensional features, denoted by a, leading to a distribution P of persistence diagrams. We then build a n-sample $a_1, \ldots, a_n$ with $n = 100$ and, for $k \in \{1, \ldots, 5\}$, compute the different codebooks returned by the aforementioned methods, using batches of size 10 for FG$_2$, FG$_\infty$ and W_2. All algorithms are initialized in the same way: we select the k points of highest persistence in the first diagram a_1. To compare the quality of these codebooks, we evaluate their distortion (8.36) with $p = 2$ and $p = \infty$. As we do not

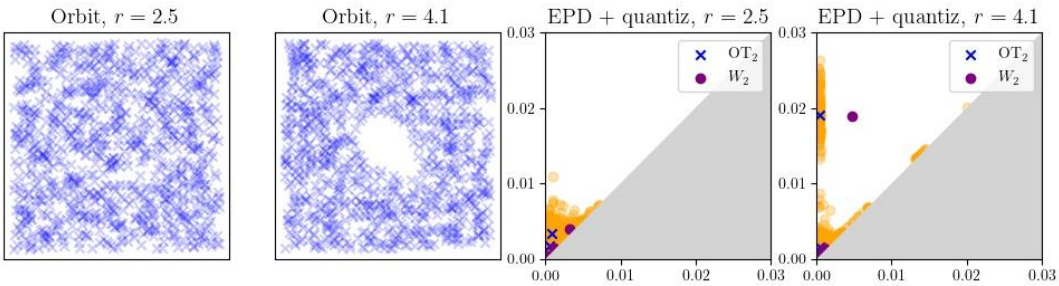


FIGURE 8.12: Orbits, expected persistence diagrams and quantizations for two classes. In the rightmost image, the top centroid using the "W_2" algorithm is shifted to the right with respect to the "FG_2" algorithm, as it takes into account points with small persistence but with large coordinates. The latter corresponds to the diagonal centroid in the "FG_2" approach.

have access to the true expected persistence diagram $E(P)$, we approximate this quantity through its empirical counterpart $\hat{R}_{k,p}(\mathbf{c}) := \left(\int_\Omega \min_{1\le j\le c_{k+1}} |x - c_j|^p \mathrm{d}\overline{a}_n(x)\right)^{\frac{1}{p}}$, while $\hat{R}_{k,\infty}(\mathbf{c}) = \max_{x\in \mathrm{spt}(\overline{a}_n)} \min_j |x - c_j|$. Results are given in Figure 8.11. Interestingly, when $p = 2$ our approach is on a par with the weighted codebook approach, but becomes substantially better when evaluated with $p = \infty$, that is using the bottleneck distance which is the most natural metric to handle persistence diagrams.

We perform another experiment on the `ORBIT5K` dataset [Ada+17, Section 6.4.1], a benchmark dataset in TDA made of 5 classes with 1000 observations each (split into 70%/30% training/test) representing different dynamical systems, turned into persistence diagrams through Čech filtrations. For each class $i \in \{1, \dots, 5\}$, we compute a 2-quantization $\nu^{(i)}$ using our FG_2 algorithm and a 3-quantization $\zeta^{(i)}$ using the standard W_2 approach [CLR20], i.e. without the diagonal cell V_{k+1} (but with an additional centroid). We then build two simple classifiers: the predicted class assigned to a test diagram μ is $\mathrm{argmin}_i\{\mathrm{FG}_2(\mu, \nu^{(i)})\}$ (resp. $(\mu, \zeta^{(i)})$). Our FG_2 classifier achieves a decent test accuracy of 61%. Advanced (kernels,DL) methods in TDA reach between 72% and 87% of accuracy [Car+20, Table 1]; but we stress that our classifier is extremely simple (we summarize a whole training class by a measure with only $k = 2$ points!), showcasing that our quantizations summarize the training persistence diagrams in an informative way. More importantly, the W_2 classifier (with $k = 3$) only achieves 50% of test accuracy even though benefiting from an additional centroid, illustrating the importance of properly accounting for the diagonal as done in our approach.

8.6 Additional proofs

Proof of Lemma 8.2.3. (i) Section I.2.1 in [Shi97] states that $A(f)$ is subanalytic. Therefore, its complement E is also subanalytic: it is enough to show that E is of empty interior to conclude.

Lemma 8.6.1. *The set F of points x where f is not analytic but G_f is locally a real analytic manifold in $(x, f(x))$ is a subanalytic set of empty interior.*

We prove Lemma 8.6.1 below. The set E is the union of F and of $E \cap G$ where G is the projection on M of $\mathrm{Sing}(G_f)$. As, by definition, $\mathrm{Sing}(G_f)$ is of empty interior, G is also of empty interior. Therefore, E is of empty interior, which is equivalent to say that its dimension is smaller than d.

(i) See [Shi97, Section II.1.1].

(ii) See [Shi97, Section II.1.6].

□

Proof of Lemma 8.6.1. Assume F contains an open set U. Replacing U by a smaller open set if necessary, there exists some local parametrization of $U_f = \{(x, f(x)),\ x \in U\}$ by some analytic function $\Phi : V \to \mathbb{R}$, V being a neighborhood of U_f in $M \times \mathbb{R}$. Denote by $\nabla^u \Phi \in \mathbb{R}$ the gradient of Φ with respect to the real variable $u \in \mathbb{R}$. The set Z on which $\nabla^u \Phi = 0$ is an analytic subset of V. As G_f is the graph of a function, $Z \cap G_f$ is made of isolated points: one can always assume that those points are not in U_f. Therefore, there exists some neighborhood V' of U_f which does not intersect Z. One can now apply the analytic implicit function theorem (see for instance [KK83, Section 8]) anywhere on U_f: for $(x_0, u_0) \in U_f$, there exists some neighborhood $W \subset V'$ and an analytic function $g : Z \to \mathbb{R}$, Z being a neighborhood of x_0, such that, on W

$$\Phi(x, u) = 0 \Longleftrightarrow u = g(x).$$

As we also have $\Phi(x, u) = 0$ if and only if $u = f(x)$, $f \equiv g$ on Z and f is analytic on Z. This is a contradiction with having f not analytic in every point of U. □

Proof of Lemma 8.2.4. Let k be the dimension of X. First, one can always assume that X is closed, as $\mathcal{H}_d(\overline{X}) \geq \mathcal{H}_d(X)$. Therefore, there exists some real analytic manifold N of dimension k and a proper real analytic mapping $\Psi : N \to M$ such that $\Psi(N) = X$ (see [Shi97, Section I.2.1]). The set X can be written as the union of some compact sets X_K for $K \geq 0$. It is enough to show that $\mathcal{H}_d(X_K) = 0$. The set X_K can be written $\Psi(\Psi^{-1}(X_K))$, where $\Psi^{-1}(X_K)$ is some compact subset of N. We have $\mathcal{H}_d(\Psi^{-1}(X_K)) = 0$ because N is of dimension $k < d$. Furthermore, as Ψ is analytic on Y, it is Lipschitz on $\Psi^{-1}(X_K)$. Therefore, $\mathcal{H}_d(\Psi(\Psi^{-1}(X_K))) = \mathcal{H}_d(X_K)$ is also null. □

Proof of Theorem 8.2.7. Let us indicate how to change the proof of Theorem 8.2.5 when assumption (K5') is satisfied instead of assumption (K5). In the partition $E_1(x), \ldots, E_L(x)$ of Δ_n, the set $E_1(x)$ plays a special role: it corresponds to the value $r_1 = 0$ and contains all the singletons, which satisfy $\varphi[\{j\}] \equiv 0$ by assumption. Lemma 8.2.11 holds for $l > 1$ and one can always define $\sigma_1 = \{1\}$ to be a minimal element of $E_1(x)$. With this convention in mind, it is straightforward to check that Lemma 8.2.12 still holds and that Lemma 8.2.13 is satisfied as well for $l > 1$. Now, one can define in a likewise manner the sets V_r. For $x \in V_r$, the diagram $\mathrm{dgm}_q(K(x))$ is still decomposed $\sum_{i=1}^N \delta_{u_i}$, with $u_i = (\varphi[\sigma_{l_1}](x), \varphi[\sigma_{l_2}](x))$. If $q > 0$, the end of the proof is similar. However, for $q = 0$, the pairs of simplices $(\sigma_{l_1}, \sigma_{l_2})$ are made of one singleton J_{l_1} and of one 2-simplex σ_{l_2}. As φ is null on singletons, the points in this diagram are all included in the vertical line $L_0 := \{0\} \times [0, \infty)$. The map $\Phi_{ir} : x \in V_r \mapsto u_i \in L_0$ has a differential of rank 1, as Lemma 8.2.13 ensures that $\nabla^j \varphi[\sigma_{l_2}](x) \neq 0$ for $j \in \sigma_{l_2}$. One can apply the coarea formula to Φ_{ir} to conclude to the existence of a density with respect to the Lebesgue measure on L_0. □

Proof of Corollary 8.2.8. The diagram $\mathrm{dgm}_q(K(X))$ can be written

$$\mathrm{dgm}_q(K(X)) = \sum_{n \geq 0} \mathbf{1}\{|X| = n\} \mathrm{dgm}_q(K(X)), \tag{8.42}$$

and Theorem 8.2.5 states that $\mathbf{1}\{|X| = n\}\mathrm{dgm}_q(K(X))$ has a density λ_n with respect to the Lebesgue measure on Ω. Take B a Borel set in Ω:

$$\begin{aligned}\mathbb{E}[\mathrm{dgm}_q(K(X))](B) &= \sum_{n\geq 0} \mathbb{E}[\mathbf{1}\{|X| = n\}\mathrm{dgm}_q(K(X))](B) \\ &= \sum_{n\geq 0} \int_B \lambda_n = \int_B \sum_{n\geq 0} \lambda_n \text{ by Fubini-Torelli's theorem.}\end{aligned}$$

It is possible to use Fubini-Torelli's theorem because $\mathbb{E}[\mathrm{dgm}_q(K(X))](B)$ is finite. Indeed, as $\mathrm{dgm}_q(K(X))$ is always made of less than $2^{\#X}$ points, and as we have supposed that $\mathbb{E}\left[2^{\#X}\right] < \infty$, the measure $\mathbb{E}[\mathrm{dgm}_q(K(X))]$ is finite as well. □

Proof of Theorem 8.2.9. Given the expression (8.11), it is sufficient to show that integrating a function along the fibers is a smooth operation in the fibers. We only show that the density is continuous. Continuity of the higher orders derivatives is obtained in a similar fashion. The proof is a standard application of the implicit function theorem.

Using the same notations than in the proof of Theorem 8.2.5, fix $1 \leq r \leq R$ and $1 \leq i \leq N_r$. We will show that λ_{ir} is continuous. As the indices r and i are now fixed, we drop the dependency in the notation: $V := V_r$ and $\Phi := \Phi_{ir}$. By using a partition of unity and taking local diffeomorphisms, one can always assume that $V \subset \mathbb{R}^{nd}$. Define the function $f : (x, u) \in V \times \Omega \mapsto \Phi(x) - u \in \mathbb{R}^2$. We have already shown in the proof of Theorem 8.2.5 that for $x_0 \in V$, there exists two indices a_1 and a_2 (depending on x_0) such that the minor $M(x_0) = (D\Phi(x_0))_{a_{1,2}}$ is invertible. Rewrite $x \in V$ in (y, z) where $z = (x_{a_1}, x_{a_2}) \in \mathbb{R}^2$. By the implicit function theorem, for (x_0, u_0) such that $f(x_0, u_0) = 0$, there exists a neighborhood $\mathcal{O}_{x_0} \subset V \times \Omega$ of (x_0, u_0) and an analytic function $g_{x_0} : W_{y_0} \times Y_{u_0} \to \mathbb{R}^2$ defined on a neighborhood of (y_0, u_0) such that for $(x, u) \in \mathcal{O}_{x_0}$

$$f(x, u) = 0 \iff z = g_{x_0}(y, u).$$

The sets $(\mathcal{O}_{x_0})_{x_0\in V}$ constitutes an open cover of the fiber $f^{-1}(0)$. Consider a smooth partition of unity $(\rho_{x_0})_{x_0\in V}$ subordinate to this cover. Then, for all $(x, u) \in f^{-1}(0)$

$$(J\Phi(x))^{-1}\kappa(x) = \sum_{x_0\in V} \rho_{x_0}(y, u, g_{x_0}(y, u))(J\Phi(y, g_{x_0}(y, u)))^{-1}\kappa(y, g_{x_0}(y, u))$$

Therefore,

$$\begin{aligned}\lambda_{ir}(u) &= \int_{x\in\Phi^{-1}(u)} (J\Phi(x))^{-1}\kappa(x)\mathrm{d}\mathcal{H}_{nd-2}(x) \\ &= \sum_{x_0\in V} \int_{y\in W_{y_0}} \rho_{x_0}(y, u, g_{x_0}(y, u))(J\Phi(y, g_{x_0}(y, u)))^{-1}\kappa(y, g_{x_0}(y, u))\mathrm{d}y. \quad (8.43)\end{aligned}$$

We are now faced with a classical continuity under the integral sign problem. First, the Cauchy-Binet formula (see [KH04, Example 2.15]) states that $J\Phi$ is equal to the square root of the sum of the squares of the determinants of all 2×2 minors of $D\Phi$. Therefore, $J\Phi(x)$ is larger than the determinant of $M(x)$, the minor of f of indices a_1 and a_2. The implicit function theorem gives the exact value of $M(x)$. Indeed, for $X = (x, u) \in \mathcal{O}_{x_0}$, and for any index k,

$$\frac{\partial g}{\partial X_k}(y, u) = -\left(M^{-1} \cdot \frac{\partial f}{\partial X_k}\right)(y, u, g(y, u)) \quad (8.44)$$

Take $X_k = u_{1,2}$. Then, $\partial f / \partial X_k = (-1, 0)$, resp. $(0, -1)$. Therefore,

$$M^{-1}(y, u, g(y, u)) = \frac{\partial g}{\partial u}(y, u, g(y, u)) \tag{8.45}$$

As ρ_{x_0} has a compact support, it suffices to show that the integrand is bounded by a constant independent of u. The only issue is that $(J\Phi)^{-1}$ may diverge. Equation (8.45) shows that it is bounded by $\det \partial g / \partial u$. This is bounded, as g is analytic on the compact support of ρ_{x_0}: each term in the sum (8.43) is continuous. By the compactness of M and $f^{-1}(0)$, all the partitions of unity can be taken finite, and a finite sum of continuous functions is continuous. This proves the continuity of λ. □

Proof of Corollary 8.2.10. Define $f(t, u)$ to be equal to 1 if $u_1 \leq t \leq u_2$ and 0 otherwise. Then, $\beta_t(\mathrm{dgm}_q(K(X))))$ is equal to $\mathrm{dgm}_q(K(X))(f(t, \cdot))$. Therefore, the expectation $\mathbb{E}[\beta_t(\mathrm{dgm}_q(K(X)))]$ is equal to

$$\int \lambda(u) f(r, u) du. \tag{8.46}$$

As we assumed that the hypothesis of Theorem 8.2.9 were satisfied, the density λ is smooth. Moreover, $\lambda(u) f(r, u)$ is smaller than $\lambda(u)$. The function λ being integrable, one can apply the continuity under the integral sign theorem to conclude that $t \mapsto \mathbb{E}[\beta_t(\mathrm{dgm}_q(K(X)))]$ is continuous. Higher-order derivatives are obtained in a similar fashion. □

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Titre : Quelques contributions à l'inférence géométrique pour les variétés et à l'étude statistique des diagrammes de persistance

Mots clés : inférence géométrique, analyse topologique des données, transport optimal, diagramme de persistance

Résumé : L'analyse topologique des données consiste en un ensemble de méthodes permettant d'extraire des informations topologiques et géométriques de jeux de données. Nous abordons ici ce domaine sous deux angles différents.

Dans un premier temps, nous considérons des techniques d'inférence géométrique, qui visent à reconstruire des invariants géométriques d'une variété à partir d'un nuage de points proche de celle-ci. Nous étudions d'une part le problème de construire des estimateurs adaptatifs de cette variété, et d'autre part la question de la reconstruction de la probabilité générant les données.

Dans un second temps, nous nous intéressons à la théorie de l'homologie persistante pour l'analyse de données. Un objet central dans cette théorie, le diagramme de persistance, permet de résumer de manière multi-échelle un jeu de données. Nous participons à l'étude statistique des diagrammes de persistance de plusieurs façons : tout d'abord en étudiant la structure métrique de l'espace des diagrammes de persistance, ensuite en définissant une notion de moyenne linéaire dans cet espace. Diverses propriétés de cet objet moyen sont alors exhibées (comportement asymptotique, régularité, etc.).

Title: Contributions to geometric inference on manifolds and to the statistical study of the space of persistence diagrams

Keywords: geometric inference, topological data analysis, optimal transport, persistence diagram

Abstract: Topological data analysis (or TDA for short) consists in a set of methods aiming to extract topological and geometric information from complex nonlinear datasets. This field is here tackled from two different perspectives.

First, we consider techniques from geometric inference, whose goal is to reconstruct geometric invariants of a manifold thanks to a random sample. We study from one hand the question of building an adaptive manifold estimator, and on the other hand the question of reconstructing the probability generating the observations.

Second, we study persistent homology theory in TDA. A central tool in this theory, the persistence diagram, allows one to summarize in a multiscale fashion a dataset. We participate to the statistical study of persistence diagrams in several ways: first, by studying the metric structure of the space of persistence diagrams, and second, by defining a notion of linear expectation in this space. Diverse properties of this average object are then exhibited (asymptotic behavior, regularity, etc.)