Large Scale computation of Means and Clusters for Persistence Diagrams using Optimal Transport

Théo Lacombe  
Datashape  
Inria Saclay  
théo.lacombe@inria.fr

Marco Cuturi  
Google Brain, and  
CREST, ENSAE  
cuturi@google.com

Steve Oudot  
Datashape  
Inria Saclay  
steve.oudot@inria.fr

Abstract

Persistence diagrams (PDs) are now routinely used to summarize the underlying topology of complex data. Despite several appealing properties, incorporating PDs in learning pipelines can be challenging because their natural geometry is not Hilbertian. Indeed, this was recently exemplified in a string of papers which show that the simple task of averaging a few PDs can be computationally prohibitive. We propose in this article a tractable framework to carry out standard tasks on PDs at scale, notably evaluating distances, estimating barycenters and performing clustering. This framework builds upon a reformulation of PD metrics as optimal transport (OT) problems. Doing so, we can exploit recent computational advances: the OT problem on a planar grid, when regularized with entropy, is convex can be solved in linear time using the Sinkhorn algorithm and convolutions. This results in scalable computations that can stream on GPUs. We demonstrate the efficiency of our approach by carrying out clustering with diagrams metrics on several thousands of PDs, a scale never seen before in the literature.

1 Introduction

Topological data analysis (TDA) has been used successfully in a wide array of applications, for instance in medical (Nicolaou et al., 2011) or material (Hiraoka et al., 2016) sciences, computer vision (Li et al., 2014) or to classify NBA players (Lum et al., 2013). The goal of TDA is to exploit and account for the complex topology (connectivity, loops, holes, etc.) seen in modern data. The tools developed in TDA are built upon persistent homology theory (Edelsbrunner et al., 2000; Zomorodian & Carlsson, 2005; Edelsbrunner & Harer, 2010) whose main output is a descriptor called a persistence diagram (PD) which encodes in a compact form—roughly speaking, a point cloud in the upper triangle of the square $[0,1]^2$—the topology of a given space or object at all scales.

Statistics on PDs. Persistence diagrams have appealing properties: in particular they have been shown to be stable with respect to perturbations of the input data (Cohen-Steiner et al., 2007; Chazal et al., 2009, 2014). This stability is measured either in the so called bottleneck metric or in the $p$-th diagram distance, which are both distances that compute optimal partial matchings. While theoretically motivated and intuitive, these metrics are by definition very costly to compute. Furthermore, these metrics are not Hilbertian, preventing a faithful application of a large class of standard machine learning tools ($k$-means, PCA, SVM) on PDs.

Related work. To circumvent the non-Hilbertian nature of the space of PDs, one can of course map diagrams onto simple feature vectors. Such features can be either finite dimensional (Carrière et al., 2015; Adams et al., 2017), or infinite through kernel functions (Reininghaus et al., 2015; Bubenik, 2015; Carrière et al., 2017). A known drawback of kernel approaches on a rich geometric space such as that formed by PDs is that once PDs are mapped as feature vectors, any ensuing analysis remains in the space of such features (the “inverse image” problem inherent to kernelization). They are therefore...
Histograms, $P_{\text{Images}}$, $\| \cdot \|_2$

Inputs

PDs, $d_2$
Histograms, $L_C^*$
PlImages, $\| \cdot \|_2$

Barycenters

Figure 1: Illustration of differences between Fréchet means with Wasserstein and Euclidean geometry. The top row represents input data, namely persistence diagrams (left), discretization of PDs as histograms (middle), and vectorization of PDs as persistence images in $\mathbb{R}_{100\times100}$ (right) (Adams et al., 2017). The bottom row represents the estimated barycenters (orange scale) with input data (shaded), using the approach of Turner et al. (2014) (left), our optimal transport based approach (middle) and the arithmetic mean of persistence images (right).

not helpful to carry out simple tasks in the space of PDs, such as that of averaging PDs, namely computing the Fréchet mean of a family of PDs. Such problems call for algorithms that are able to optimize directly in the space of PDs, and were first addressed by Mileyko et al. (2011) and Turner (2013). Turner et al. (2014) provides an algorithm that converges to a local minimum of the Fréchet function by successive iterations of the Hungarian algorithm. However, the Hungarian algorithm does not scale well with the size of diagrams, and non-convexity yields potentially convergence to bad local minima.

Contributions. We reformulate the computation of diagram metrics as an optimal transport (OT) problem, opening several perspectives, among them the ability to benefit from entropic regularization (Cuturi, 2013). We provide a new numerical scheme to bound OT metrics, and therefore diagram metrics, with additive guarantees. Unlike previous approximations of diagram metrics, ours can be parallelized and implemented efficiently on GPUs. These approximations are also differentiable, leading to a scalable method to compute barycenters of persistence diagrams. In exchange for a tractable implementation of the $k$-means algorithm in the space of PDs.

Notations for matrix and vector manipulations. When applied to matrices or vectors, operators $\exp$, $\log$, division are always meant element-wise. $u \odot v$ denotes element-wise multiplication (Hadamard product) while $Ku$ denotes the matrix-vector product of $K \in \mathbb{R}^{d \times d}$ and $u \in \mathbb{R}^d$.

2 Background on OT and TDA

OT. Optimal transport is now widely seen as a central tool to compare probability measures (Villani, 2003, 2008; Santambrogio, 2015). Given a space $\mathcal{X}$ endowed with a cost function $c : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$, we consider two discrete measures $\mu$ and $\nu$ on $\mathcal{X}$, namely measures that can be written as positive combinations of diracs, $\mu = \sum_{i=1}^n a_i \delta_{x_i}$, $\nu = \sum_{j=1}^m b_j \delta_{y_j}$ with weight vectors $a \in \mathbb{R}_+^n$, $b \in \mathbb{R}_+^m$ satisfying $\sum_i a_i = \sum_j b_j$ and all $x_i, y_j$ in $\mathcal{X}$. The $n \times m$ cost matrix $C = \langle c(x_i, y_j) \rangle_{ij}$ and the transportation polytope $\Pi(a, b) := \{ P \in \mathbb{R}^{n \times m} \parallel P1_m = a, P^T 1_n = b \}$ define an optimal transport problem whose optimum $L_C$ can be computed using either of two linear programs, dual to each other,

$$L_C(\mu, \nu) := \min_{P \in \Pi(a, b)} \langle P, C \rangle = \max_{(\alpha, \beta) \in \Psi_C} \langle \alpha, a \rangle + \langle \beta, b \rangle \tag{1}$$

where $\langle \cdot, \cdot \rangle$ is the Frobenius dot product and $\Psi_C$ is the set of pairs of vectors $(\alpha, \beta) \in \mathbb{R}^n \times \mathbb{R}^m$ such that their tensor sum $\alpha \oplus \beta$ is smaller than $C$, namely $\forall i, j, \alpha_i + \beta_j \leq C_{ij}$. Note that when $n = m$ and all weights $a$ and $b$ are uniform and equal, the problem above reduces to the computation of an optimal matching, that is a permutation $\sigma \in \mathcal{S}_n$ (with a resulting optimal plan $P$ taking the form $P_{ij} = 1_{\sigma(i)=j}$). That problem has clear connections with diagram distances, as shown in §3.
Input data: point cloud $P$

Persistence diagram

Sublevels sets of $f = \text{dist}_P$

Figure 2: Sketch of persistent homology. $X = \mathbb{R}^3$ and $f(x) = \min_{p \in P} \|x - p\|$ so that sublevel sets of $f$ are unions of balls centered at the points of $P$. First (resp second) coordinate of points in the persistence diagram encodes appearance scale (resp disappearance) of cavities in the sublevel sets of $f$. The isolated red point accounts for the presence of a persistent hole in the sublevel sets, inferring the underlying spherical geometry of the input point cloud.

**Entropic Regularization.** Solving the optimal transport problem is intractable for large data. Cuturi proposes to consider a regularized formulation of that problem using entropy, namely:

$$\mathcal{L}^\gamma_C(a, b) := \min_{P \in \Pi(a, b)} \langle P, C \rangle - \gamma h(P)$$

$$= \max_{\alpha \in \mathbb{R}^n, \beta \in \mathbb{R}^m} \langle \alpha, a \rangle + \langle \beta, b \rangle - \gamma \sum_{i,j} e^{\frac{\alpha_i + \beta_j - C_{i,j}}{\gamma}},$$

where $\gamma > 0$ and $h(P) := -\sum_{i,j} P_{ij} \log P_{ij} - 1$. Because the negentropy is 1-strongly convex, that problem has a unique solution $P^\gamma$ which takes the form, using first order conditions,

$$P^\gamma = \text{diag}(u^\gamma) K \text{diag}(v^\gamma) \in \mathbb{R}^{n \times m},$$

where $K = e^{-C}$ (term-wise exponentiation), and $(u^\gamma, v^\gamma) \in \mathbb{R}^n \times \mathbb{R}^m$ is a fixed point of the Sinkhorn map (term-wise divisions):

$$S : (u, v) \mapsto \left(\frac{a}{K v}, \frac{b}{K^T u}\right).$$

Note that this fixed point is the limit of any sequence $(u_{t+1}, v_{t+1}) = S(u_t, v_t)$, yielding a straightforward algorithm to estimate $P^\gamma$. Cuturi considers the transport cost of the optimal regularized plan, $S_C^\gamma(a, b) := \langle P^\gamma, C \rangle = \langle u^\gamma \rangle^T K \text{diag}(v^\gamma)$, to define a Sinkhorn divergence between $a, b$ (here $\circ$ is the term-wise multiplication). One has that $S_C^\gamma(a, b) \rightarrow \mathcal{L}_C(a, b)$ as $\gamma \rightarrow 0$, and more precisely $P^\gamma$ converges to the optimal transport plan solution of (1) with maximal entropy. That approximation can be readily applied to any problem that involves terms in $L_C$, notably barycenters (Cuturi & Doucet, 2014; Solomon et al., 2015; Benamou et al., 2015).

**Eulerian setting.** When the set $\mathcal{X}$ is finite with cardinality $d$, $\mu$ and $\nu$ are entirely characterized by their probability weights $a, b \in \mathbb{R}_d^\mu$ and are often called histograms in an Eulerian setting. When $\mathcal{X}$ is not discrete, as when considering the plane $[0, 1]^2$, we therefore have a choice of representing measures as sums of diracs, encoding their information through locations, or as discretized histograms on a planar grid of arbitrary granularity. Because the latter setting is more effective for entropic regularization (Solomon et al., 2015), this is the approach we will favor in our computations.

**Persistent homology and Persistence Diagrams.** Given a topological space $\mathcal{X}$ and a real-valued function $f : \mathcal{X} \rightarrow \mathbb{R}$, persistent homology provides—under mild assumptions on $f$, taken for granted in the remaining of this article—a topological signature of $f$ built on its sublevel sets $(f^{-1}((-\infty, t]))_{t \in \mathbb{R}}$, and called a persistence diagram (PD), denoted as $\text{Dgm}(f)$. In practice, it is of the form $\text{Dgm}(f) = \sum_{i=1}^n \delta_{x_i}$, namely a point measure with finite support included in $\mathbb{R}_2 := \{(s, t) \in \mathbb{R}^2 | s < t\}$. Each point $(s, t)$ in $\text{Dgm}(f)$ can be understood as a topological feature (connected component, loop, hole...) which appears at scale $s$ and disappears at scale $t$ in the sublevel sets of $f$. Comparing the persistence diagrams of two functions $f, g$ measures their difference from a topological perspective: presence of some topological features, difference in appearance scales, etc. The space of PDs is naturally endowed with a partial matching metric defined as ($p \geq 1$):

$$d_p(D_1, D_2) := \left(\min_{\zeta \in \Pi(D_1, D_2)} \sum_{(x,y) \in \zeta} \|x - y\|^p_p + \sum_{s \in D_1 \cup D_2 \setminus \zeta} \|s - \pi_D(s)\|^p_p\right)^{\frac{1}{p}},$$

(6)
where $\Gamma(D_1, D_2)$ is the set of all partial matchings between points in $D_1$ and points in $D_2$ and $\pi_\Delta(s)$ denotes the orthogonal projection of an (unmatched) point $s$ to the diagonal $\{(x, x) \in \mathbb{R}^2, x \in \mathbb{R}\}$. The mathematics of OT and diagram distances share a key idea, that of matching, but differ on an important aspect: diagram metrics can cope, using the diagonal as a sink, with measures that have a varying total number of points. We solve this gap by leveraging an unbalanced formulation for OT.

### 3 Fast estimation of diagram metrics using Optimal Transport

In the following, we start by explicitly formulating (6) as an optimal transport problem. Entropic smoothing provides us a way to approximate (6) with controllable error. In order to benefit mostly from that regularization (matrix parallel execution, convolution, GPU—as showcased in (Solomon et al., 2015)), implementation requires specific attention, as described in propositions 2, 3, 4.

**PD metrics as Optimal Transport.** The main differences between (6) and (1) are that PDs do not generally have the same mass, i.e. number of points (counted with multiplicity), and that the diagonal plays a special role by allowing to match any point $x$ in a given diagram with its orthogonal projection $\pi_\Delta(x)$ onto the diagonal. Guittet’s formulation for partial transport (2002) can be used to account for this by creating a “sink” bin corresponding to that diagonal and allowing for different total masses.

The idea of representing the diagonal as a single point already appears in the bipartite graph problem of Edelsbrunner & Harer (2010) (Ch.VIII). The important aspect of the following proposition is the clarification of the partial matching problem (6) as a standard OT problem (1).

Let $\mathbb{R}^2_+ \cup \{\Delta\}$ be $\mathbb{R}^2_+$ extended with a unique virtual point $\{\Delta\}$ encoding the diagonal. We introduce the linear operator $R$ which, to a finite non-negative measure $\mu$ supported on $\mathbb{R}^2_+$, associates a dirac on $\Delta$ with total mass equal to $\mu$, namely $R: \mu \mapsto |\mu|\delta_\Delta$.

**Proposition 1.** Let $D_1 = \sum_{i=1}^{n_1} \delta_{x_i}$ and $D_2 = \sum_{j=1}^{n_2} \delta_{y_j}$ be two persistence diagrams with respectively $n_1$ points $x_1 \ldots x_{n_1}$ and $n_2$ points $y_1 \ldots y_{n_2}$. Let $p \geq 1$. Then:

$$d_p(D_1, D_2)^p = L_C(D_1 + RD_2, D_2 + RD_1),$$

where $C$ is the cost matrix with block structure

$$C = \begin{pmatrix} \tilde{C} \\ v^T \\ 0 \end{pmatrix} \in \mathbb{R}^{(n_1+1) \times (n_2+1)}$$

where $u_i = \|x_i - \pi_\Delta(x_i)\|_p$, $v_j = \|y_j - \pi_\Delta(y_j)\|_p$, $\tilde{C}_{ij} = \|x_i - y_j\|_p$, for $i \leq n_1$, $j \leq n_2$.

The proof seamlessly relies on the fact that, when transporting point measures with the same mass (number of points counted with multiplicity), the optimal transport problem is equivalent to an optimal matching problem (see §2). Details are left to the supplementary material.

**Entropic approximation of diagram distances.** Following the correspondence established in Proposition 1, entropic regularization can be used to approximate the diagram distance $d_p(D_1, D_2)$. Given two persistence diagrams $D_1, D_2$ with respective masses $n_1$ and $n_2$, let $n := n_1 + n_2$, $a = (1_{n_1}, n_2) \in \mathbb{R}^{n_1+1}$, $b = (1_{n_2}, n_1) \in \mathbb{R}^{n_2+1}$, and $P_t^\gamma = \text{diag}(u_t^\gamma)K\text{diag}(v_t^\gamma)$ where $(u_t^\gamma, v_t^\gamma)$ is the output after $t$ iterations of the Sinkhorn map (5). Adapting the bounds provided by Altschuler et al. (2017), we can bound the error of approximating $d_p(D_1, D_2)^p$ by $(P_t^\gamma, C)$:

$$|d_p(D_1, D_2)^p - \langle P_t^\gamma, C \rangle| \leq 2\gamma n \log(n) + \text{dist}(\bar{P}_t^\gamma, \Pi(a, b))\|C\|_\infty$$

where $\text{dist}(P, \Pi(a, b)) := \|P1 - a\|_1 + \|P^T1 - b\|_1$ (that is, error on marginals).

Dvurechensky et al. (2018) prove that iterating the Sinkhorn map (5) gives a plan $P_t^\gamma$ satisfying $\text{dist}(\bar{P}_t^\gamma, \Pi(a, b)) < \varepsilon$ in $\mathcal{O}\left(\frac{\|C\|^2}{\varepsilon^2} \ln(n)\right)$ iterations. Given (9), a natural choice is thus to take $\gamma = \frac{\varepsilon}{n \ln(n)}$ for a desired precision $\varepsilon$, which lead to a total of $\mathcal{O}\left(\frac{n \ln(n)\|C\|^2}{\varepsilon^2}\right)$ iterations in the Sinkhorn loop. These results can be used to pre-tune parameters $t$ and $\gamma$ to control the approximation error due to smoothing. However, these are worst-case bounds, controlled by max-norms, and are often too pessimistic in practice. To overcome this phenomenon, we propose on-the-fly error control, using approximate solutions to the smoothed primal (2) and dual (3) optimal transport problems, which provide upper and lower bounds on the optimal transport cost.

**Upper and Lower Bounds.** The Sinkhorn algorithm, after at least one iteration ($t \geq 1$), produces feasible dual variables $(\alpha_t^\gamma, \beta_t^\gamma) = (\gamma \log(u_t^\gamma), \gamma \log(v_t^\gamma)) \in \Psi_C$ (see below (1) for a definition).
Their objective value, as measured by $\langle \alpha^*_t, a \rangle + \langle \beta^*_t, b \rangle$, performs poorly as a lower bound of the true optimal transport cost (see Fig. 3 and §5 below) in most of our experiments. To improve on this, we compute the so-called $\mathcal{C}$-transform (Santambrogio, 2015, §1.6), defined as:

$$\forall j, (\alpha^*_t)^c_j = \max_i \{C_{ij} - \alpha_i\}, j \leq n_2 + 1.$$ 

Applying a $C^T$-transform on $\langle \alpha^*_t \rangle^c$, we recover two vectors $\langle \alpha^*_t \rangle^c \in \mathbb{R}^{n_1+1}$, $\langle \beta^*_t \rangle^c \in \mathbb{R}^{n_2+1}$. One can show that for any feasible $\alpha, \beta$, we have that (Peyré & Cuturi, 2018, Prop 3.1)

$$\langle \alpha, a \rangle + \langle \beta, b \rangle \leq \langle \alpha^c, a \rangle + \langle \alpha^c, b \rangle.$$

When $C$’s top-left block is the squared Euclidean metric, this problem can be cast as that of computing the Moreau envelope of $\alpha$. In a Eulerian setting and when $\mathcal{X}$ is a finite regular grid which we will consider, we can use either the linear-time Legendre transform or the Parabolic Envelope algorithm (Lacut, 2010, §2.2.1, §2.2.2) to compute the $C$-transform in linear time with respect to the grid resolution $d$.

Unlike dual iterations, the primal iterate $P^*_t$ does not belong to the transport polytope $\Pi(a, b)$ after a finite number $t$ of iterations. We use the rounding_to_feasible algorithm provided by Altschuler et al. (2017) to compute efficiently a feasible approximation $\tilde{R}^*_t$ of $P^*_t$ that does belong to $\Pi(a, b)$. Putting these two elements together, we obtain

$$\langle (\alpha^*_t)^c, a \rangle + \langle (\beta^*_t)^c, b \rangle \leq L_C(a, b) \leq \langle \tilde{R}^*_t, C \rangle.$$  

(10)

Therefore, after iterating the Sinkhorn map (5) $t$ times, we have that if $M^*_t - m^*_t$ is below a certain criterion $\epsilon$, then we can guarantee that $(R^*_t, C)$ is a fortiori an $\epsilon$-approximation of $L_C(a, b)$. Observe that one can also have a relative error control: if one has $M^*_t - m^*_t \leq \epsilon M^*_t$, then $(1 - \epsilon)M^*_t \leq L_C(a, b) \leq M^*_t$. Note that $m^*_t$ might be negative but can always be replaced by $\max(m^*_t, 0)$ since we know $C$ has non-negative entries (and therefore $L_C(a, b) \geq 0$), while $M^*_t$ is always non-negative.

**Discretization.** For simplicity, we assume in the remaining that our diagrams have their support in $[0, 1]^2 \cap \mathbb{R}^2$. From a numerical perspective, encoding persistence diagrams as histograms on the square offers numerous advantages. Given a uniform grid of size $d \times d$ on $[0, 1]^2$, we associate to a given diagram $D$ a matrix-shaped histogram $a \in \mathbb{R}^{d \times d}$ such that $a_{ij}$ is the number of points in $D$ belonging to the cell located at position $(i, j)$ in the grid (we transition to bold-faced small letters to insist on the fact that these histograms must be stored as square matrices). To account for the total mass, we add an extra encoding mass on $\Delta$. We extend the operator $\mathbf{R}$ to histograms, associating to a histogram $a \in \mathbb{R}^{d \times d}$ its total mass on the $(d^2 + 1)$-th coordinate. One can show that the approximation error resulting from that discretization is bounded above by $\frac{1}{2}(|D_1|^2 + |D_2|^2)$ (see the supplementary material).

**Convolutions.** In the Eulerian setting, where diagrams are matrix-shaped histograms of size $d \times d = d^2$, the cost matrix $C$ has size $d^2 \times d^2$. Since we will use large values of $d$ to have low discretization error (typically $d = 100$), instantiating $C$ is usually intractable. However, Solomon et al. (2015)
showed that for regular grids endowed with a separable cost, each Sinkhorn iteration (as well as other key operations such as evaluating Sinkhorn’s divergence $S^2_\gamma$) can be performed using Gaussian convolutions, which amounts to performing matrix multiplications of size $d \times d$, without having to manipulate $d^2 \times d^2$ matrices. Our framework is slightly different due to the extra dimension $\{\Delta\}$, but we show that equivalent computational properties hold. This observation is crucial from a numerical perspective. Our ultimate goal being to efficiently evaluate (11), (12) and (14), we provide implementation details.

Let $(u, u_\Delta)$ be a pair where $u \in \mathbb{R}^{d \times d}$ is a matrix-shaped histogram and $u_\Delta \in \mathbb{R}_+$ is a real number accounting for the mass located on the virtual point $\{\Delta\}$. We denote by $\overrightarrow{u}$ the $d^2 \times 1$ column vector obtained when reshaping $u$. The $(d^2 + 1) \times (d^2 + 1)$ cost matrix $C$ and corresponding kernel $K$ are given by

$$C = \begin{pmatrix} \overrightarrow{C} & \overrightarrow{\Delta} \\ \overrightarrow{\Delta}^T & 0 \end{pmatrix}, \quad K = \begin{pmatrix} \overrightarrow{K} & \overrightarrow{\Delta} \\ \overrightarrow{\Delta}^T & 0 \end{pmatrix},$$

where $\overrightarrow{C} = ((i, i') - (j, j'))^T_{(j') = \pi_\Delta((i, i')))}$. $C$ and $K$ as defined above will never be instantiated, because we can rely instead on $c \in \mathbb{R}^{d \times d}$ defined as $c_{ij} = |i - j|^p$ and $k = e^{-\frac{c}{\gamma}}$.

**Proposition 2** (Iteration of Sinkhorn map). The application of $K$ to $(u, u_\Delta)$ can be performed as:

$$(u, u_\Delta) \mapsto (k(u\Delta)^T) + u_\Delta k, (u, u_\Delta) + u_\Delta$$

(11)

where $\langle \cdot, \cdot \rangle$ denotes the Frobenius dot-product in $\mathbb{R}^{d \times d}$.

We now introduce $m := k \circ c$ and $m_\Delta := k_\Delta \circ c_\Delta$ ($\circ$ denotes term-wise multiplication).

**Proposition 3** (Computation of $S^2_\gamma$). Let $(u, u_\Delta), (v, v_\Delta) \in \mathbb{R}^{d \times d+1}$. The transport cost of $P := \text{diag}(\overrightarrow{u}, u_\Delta)K\text{diag}(\overrightarrow{v}, v_\Delta)$ can be computed as:

$$\langle \text{diag}(\overrightarrow{u}, u_\Delta)K\text{diag}(\overrightarrow{v}, v_\Delta), C \rangle = \langle \text{diag}(\overrightarrow{u}, u_\Delta)K\text{diag}(\overrightarrow{v}, v_\Delta), C \rangle + u_\Delta \langle v, m_\Delta \rangle + v_\Delta \langle u, m_\Delta \rangle,$$

(12)

where the first term can be computed as:

$$\langle \text{diag}(\overrightarrow{u}, u_\Delta)K\text{diag}(\overrightarrow{v}, v_\Delta), C \rangle = \|u \otimes (m(ku^T)^T + k(mv^T)^T)\|_1.$$

(13)

Finally, consider two histograms $(a, a_\Delta), (b, b_\Delta) \in \mathbb{R}^{d \times d} \times \mathbb{R}$, let $R \in \Pi((a, a_\Delta), (b, b_\Delta))$ be the rounded matrix of $P$ (see the supplementary material or (Altschuler et al., 2017)). Let $r(P), c(P) \in \mathbb{R}^{d \times d} \times \mathbb{R}$ denote the first and second marginal of $P$ respectively. We introduce (using term-wise min and divisions):

$$X = \min \left( \frac{(a, a_\Delta)}{r(P)}, 1 \right), \quad Y = \min \left( \frac{(b, b_\Delta)}{c(\text{diag}(X)(P))}, 1 \right),$$

along with $P' = \text{diag}(X)P\text{diag}(Y)$ and the marginal errors:

$$\langle e_r, (r_\Delta) \rangle = (a, a_\Delta) - r(P'), \quad \langle e_c, (c_\Delta) \rangle = (b, b_\Delta) - c(P'),$$

**Proposition 4** (Computation of upper bound $\langle R, C \rangle$). The transport cost induced by $R$ can be computed as:

$$\langle R, C \rangle = \langle \text{diag}(X \otimes (u, u_\Delta))K\text{diag}(Y \otimes (v, v_\Delta)), C \rangle$$

$$+ \frac{1}{\|e_c\|_1 + (e_c_\Delta)}(\|e_c^Tc_\Delta\|_1 + \|e_c^Tc_\Delta\|_1 + (e_c_\Delta) \langle e_r, c_\Delta \rangle + (e_r_\Delta) \langle e_c, c_\Delta \rangle).$$

(14)

Note that the first term can be computed using (12)

**Parallelization and GPU.** Using a Eulerian representation is particularly beneficial when applying Sinkhorn’s algorithm, as shown by Cuturi (2013). Indeed, the Sinkhorn map (5) only involves matrix-vector operations. When dealing with a large number of histograms, concatenating these histograms and running Sinkhorn’s iterations in parallel as matrix-matrix product results in significant speedup that can exploit GPGPU to compare a large number of pairs simultaneously. This makes our approach especially well-suited for large sets of persistence diagrams.
We can now estimate distances between persistence diagrams with Alg. 1 in parallel by performing only \((d \times d)\)-sized matrix multiplications, leading to a computational scaling in \(d^3\) where \(d\) is the grid resolution parameter. Note that a standard stopping threshold in Sinkhorn iteration process is to check the error to marginals \(\text{dist}(P, \Pi(a, b))\), as motivated by (9).

### 4 Smoothed barycenters for persistence diagrams

**OT formulation for barycenters.** We show in this section that the benefits of entropic regularization also apply to the computation of barycenters of PDs. As the space of PD is not Hilbertian but only a metric space, the natural definition of barycenters is to formulate them as Fréchet means for the \(d_p\) metric, as first introduced (for PDs) in (Mileyko et al., 2011).

**Definition.** Given a set of persistence diagrams \(D_1, \ldots, D_N\), a barycenter of \(D_1 \ldots D_N\) is any solution of the following minimization problem:

\[
\min_{\mu \in \mathcal{M}_+(\mathbb{R}^{2d})} \mathcal{E}(\mu) := \sum_{i=1}^{N} L_C(\mu + RD_i, D_i + R\mu)
\]  

where \(C\) is defined as in (8) with \(p = 2\) (but our approach adapts easily to any finite \(p \geq 1\)), and \(\mathcal{M}_+(\mathbb{R}^{2d})\) denotes the set of non-negative finite measures supported on \(\mathbb{R}^{2d}\). \(\mathcal{E}(\mu)\) is the energy of \(\mu\).

Let \(\hat{\mathcal{E}}\) denotes the restriction of \(\mathcal{E}\) to the space of persistence diagrams (finite point measures). Turner et al. (2014) proved the existence of minimizers of \(\hat{\mathcal{E}}\) and proposed an algorithm that converges to a local minimum of the functional, using the Hungarian algorithm as a subroutine. Their algorithm will be referred to as the \(B\)-Munkres Algorithm. The non-convexity of \(\hat{\mathcal{E}}\) can be a real limitation in practice since \(\hat{\mathcal{E}}\) can have arbitrarily bad local minima (see Lemma 1 in the supplementary material). Note that minimizing \(\mathcal{E}\) instead of \(\hat{\mathcal{E}}\) will not give strictly better minimizers (see Proposition 6 in the supplementary material). We then apply entropic smoothing to this problem. This relaxation offers differentiability and circumvents both non-convexity and numerical scalability.

**Entropic smoothing for PD barycenters.** In addition to numerical efficiency, an advantage of smoothed optimal transport is that \(a \mapsto L_C^{\gamma}(a, b)\) is differentiable. In the Eulerian setting, its gradient is given by centering the vector \(\gamma \log(u^{\gamma})\) where \(u^{\gamma}\) is a fixed point of the Sinkhorn map (5), see (Cuturi & Doucet, 2014). This result can be adapted to our framework, namely:

**Proposition 5.** Let \(D_1 \ldots D_N\) be PDs, and \((a_i)_i\), the corresponding histograms on a \(d \times d\) grid. The gradient of the functional \(\mathcal{E}^{\gamma} : z \mapsto \sum_{i=1}^{N} L_C^{\gamma}(z + Ra_i, a_i + Rz)\) is given by

\[
\nabla_z \mathcal{E}^{\gamma} = \gamma \left( \sum_{i=1}^{N} \log(u_i^{\gamma}) + R^T \log(v_i^{\gamma}) \right)
\]
where \( R^T \) denotes the adjoint operator \( R \) and \((u_i^n, v_i^n)\) is a fixed point of the Sinkhorn map obtained while transporting \( z + Ra_i \) onto \( a_i + Rz \).

As in (Cuturi & Doucet, 2014), this result follows from the envelope theorem, with the added subtlety that \( z \) appears in both terms depending on \( u \) and \( v \). This formula can be exploited to compute barycenters via gradient descent, yielding Algorithm 2. Following (Cuturi & Doucet, 2014, §4.2), we used a multiplicative update. This is a particular case of mirror descent (Beck & Teboulle, 2003) and is equivalent to a (Bregman) projected gradient descent on the positive orthant, retaining positive coefficients throughout iterations.

As it can be seen in Fig. 4, the barycentric persistence diagrams are smeared. If one wishes to recover more spiked diagrams, quantization and/or entropic sharpening (Solomon et al., 2015, §6.1) can be applied, as well as smaller values for \( \gamma \) that impact computational speed or numerical stability. We will consider these extensions in future work.

**A comparison with linear representations.** When doing statistical analysis with PDs, a standard approach is to transform a diagram into a finite dimensional vector—in a stable way—and then perform statistical analysis with an Euclidean structure. This approach does not preserve the Wasserstein-like geometry of the diagram space and thus loses the algebraic interpretability of PDs. Fig. 1 gives a qualitative illustration of the difference between Wasserstein barycenters (Fréchet mean) of PDs and Euclidean barycenters (linear means) of persistence images (Adams et al., 2017), a commonly used vectorization for PDs (Makarenko et al., 2016; Zeppelzauer et al., 2016; Obayashi et al., 2018).

## 5 Experiments

All experiments are run with \( p = 2 \), but would work with any finite \( p \geq 1 \). This choice is consistent with the work of Turner et al. (2014) for barycenter estimation.

**A large scale approximation.** Iterations of Sinkhorn map (5) yield a transport cost whose value converges to the true transport cost as \( \gamma \to 0 \) and the number of iterations \( t \to \infty \) (Cuturi, 2013). We quantify in Fig. 3 this convergence experimentally using the upper and lower bounds provided in (10) through \( t \) and for decreasing \( \gamma \). We consider a set of \( N = 100 \) pairs of diagrams randomly generated with 100 to 150 points in each diagram, and discretized on a \( 100 \times 100 \) grid. We run Alg. 1 for different \( \gamma \) ranging from \( 10^{-1} \) to \( 5 \times 10^{-4} \) along with corresponding upper and lower bounds described in (10). For each pair of diagrams, we center our estimates by removing the true distance, so that the target cost is 0 across all pairs. We plot median, top 90\% and bottom 10\% percentiles for both bounds. Using the \( C \)-transform provides a much better lower bound in our experiments. This is however inefficient in practice: despite a theoretical complexity linear in the grid size, the sequential structure of the algorithms described in (Lucet, 2010) makes them unsuited for GPGPU to our knowledge.

We then compare the scalability of Alg. 1 with respect to the number of points in diagrams with that of Kerber et al. (2017) which provides a state-of-the-art algorithm with publicly available code—referred to as \textit{Hera}—to estimate distances between diagrams. For both algorithms, we compute the average time \( t_n \) to estimate a distance between two random diagrams having from \( n \) to \( 2n \) points where \( n \) ranges from 10 to 5000. In order to compare their scalability, we plot in Fig. 5 the ratio \( t_n/t_{10} \) of both algorithms, with \( \gamma_n = 10^{-1}/n \) in Alg. 1.

### Algorithm 2 Smoothed approximation of PD barycenter

**Input:** PDs \( D_1, \ldots, D_N \), learning rate \( \lambda \), smoothing parameter \( \gamma > 0 \), grid step \( d \in \mathbb{N} \).

**Output:** Estimated barycenter \( z \)

**Init:** \( z \) uniform measure above the diagonal.

Cast each \( D_i \) as an histogram \( a_i \) on a \( d \times d \) grid

**while** \( z \) changes **do**

Iterate \( S \) defined in (5) in parallel between all the pairs \((z + Ra_i), (a_i + Rz)\), using (11).

\[
\nabla := \gamma (\sum_i \log(u_i^n) + R^T \log(v_i^n))
\]

\[
z := z \odot \exp(-\lambda \nabla)
\]

**end while**

If Want energy **then**

Compute \( \frac{1}{N} \sum_i S^\gamma_c(z + Ra_i, a_i + Rz) \) using (12)

**end if**

Return \( z \)
We compare our Alg. 2 (referred to as Sinkhorn) to the combinatorial algorithm of Turner et al. (2014) (referred to as B-Munkres). We use the script munkres.py provided on the website of K.Turner for their implementation. We record in Fig. 6 running times of both algorithms on a set of 10 diagrams having from $n$ to $2n$ points, $n$ ranging from 1 to 500, on Intel Xeon 2.3 GHz (CPU) and P100 (GPU, Sinkhorn only). When running Alg. 2, the gradient descent is performed until $|\mathcal{E}(\mathbf{z}_{t+1})/\mathcal{E}(\mathbf{z}_t) - 1| < 0.01$, with $\gamma = 10^{-1}/n$ and $d = 50$. Our experiment shows that Alg. 2 drastically outperforms B-Munkres as the number of points $n$ increases. We interrupt B-Munkres at $n = 30$, after which computational time becomes an issue.

Aside from computational efficiency, we highlight the benefits of operating with a convex formulation in Fig. 7. Due to non-convexity, the B-Munkres algorithm is only guaranteed to converge to a local minima, and its output depends on initialization. We illustrate on a toy set of $N = 3$ diagrams how our algorithm avoids local minima thanks to the Eulerian approach we take.

We now merge Alg. 1 and Alg. 2 in order to perform unsupervised clustering via $k$-means on PDs. We work with the 3D-shape database provided by Sumner & Popović and generate diagrams in the same way as in (Carrière et al., 2015), working in practice with 5000 diagrams with 50 to 100 points each. The database contains 6 classes: camel, cat, elephant, horse, head, and face. In practice, this unsupervised clustering algorithm detects two main clusters: faces and heads on one hand, camels and horses on the other hand are systematically grouped together. Fig. 8 illustrates the convergence of our algorithm and the computed centroids for the aforementioned clusters.

### 6 Conclusion

In this work, we took advantage of a link between PD metrics and optimal transport to leverage and adapt entropic regularization for persistence diagrams. Our approach relies on matrix manipulations rather than combinatorial computations, providing parallelization and efficient use of GPUs. We provide bounds to control approximation errors. We use these differentiable approximations to estimate barycenters of PDs significantly faster than existing algorithm, and showcase their application by clustering thousand diagrams built from real data. We believe this first step will open the way for new statistical tools for TDA and ambitious data analysis applications of persistence diagrams.
Acknowledgments. We thank the anonymous reviewers for the fruitful discussion. TL was supported by the AMX, École polytechnique. MC acknowledges the support of a Chaire d’Excellence de l’Idex Paris-Saclay.

References

Adams, H., Emerson, T., Kirby, M., Neville, R., Peterson, C., Shipman, P., Chepushtanova, S., Hanson, E., Motta, F., and Ziegelmeier, L. Persistence images: a stable vector representation of persistent homology. *Journal of Machine Learning Research*, 18(8):1–35, 2017.

Agueh, M. and Carlier, G. Barycenters in the wasserstein space. *SIAM Journal on Mathematical Analysis*, 43(2):904–924, 2011.

Altschuler, J., Weed, J., and Rigollet, P. Near-linear time approximation algorithms for optimal transport via sinkhorn iteration. In *Advances in Neural Information Processing Systems*, pp. 1961–1971, 2017.

Anderes, E., Borgwardt, S., and Miller, J. Discrete wasserstein barycenters: optimal transport for discrete data. *Mathematical Methods of Operations Research*, 84(2):389–409, 2016.

Beck, A. and Teboulle, M. Mirror descent and nonlinear projected subgradient methods for convex optimization. *Operations Research Letters*, 31(3):167–175, 2003.

Benamou, J.-D., Carlier, G., Cuturi, M., Nenna, L., and Peyré, G. Iterative bregman projections for regularized transportation problems. *SIAM Journal on Scientific Computing*, 37(2):A1111–A1138, 2015.

Bubenik, P. Statistical topological data analysis using persistence landscapes. *The Journal of Machine Learning Research*, 16(1):77–102, 2015.

Carlier, G., Oberman, A., and Oudet, E. Numerical methods for matching for teams and wasserstein barycenters. *ESAIM: Mathematical Modelling and Numerical Analysis*, 49(6):1621–1642, 2015.

Carrière, M., Oudot, S. Y., and Ovsjanikov, M. Stable topological signatures for points on 3d shapes. In *Computer Graphics Forum*, volume 34, pp. 1–12. Wiley Online Library, 2015.

Carrière, M., Cuturi, M., and Oudot, S. Sliced wasserstein kernel for persistence diagrams. In *34th International Conference on Machine Learning*, 2017.

Chazal, F., Cohen-Steiner, D., Glisse, M., Guibas, L. J., and Oudot, S. Y. Proximity of persistence modules and their diagrams. In *Proceedings of the twenty-fifth annual symposium on Computational geometry*, pp. 237–246. ACM, 2009.

Chazal, F., De Silva, V., and Oudot, S. Persistence stability for geometric complexes. *Geometriae Dedicata*, 173(1):193–214, 2014.

Cohen-Steiner, D., Edelsbrunner, H., and Harer, J. Stability of persistence diagrams. *Discrete & Computational Geometry*, 37(1):103–120, 2007.

Cuturi, M. Sinkhorn distances: Lightspeed computation of optimal transport. In *Advances in Neural Information Processing Systems*, pp. 2292–2300, 2013.

Cuturi, M. and Doucet, A. Fast computation of wasserstein barycenters. In *International Conference on Machine Learning*, pp. 685–693, 2014.

Dvurechensky, P., Gasnikov, A., and Kroshnin, A. Computational optimal transport: Complexity by accelerated gradient descent is better than by sinkhorn’s algorithm. In Dy, J. and Krause, A. (eds.), *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pp. 1367–1376, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR. URL http://proceedings.mlr.press/v80/dvurechensky18a.html.

Edelsbrunner, H. and Harer, J. *Computational topology: an introduction*. American Mathematical Soc., 2010.

Edelsbrunner, H., Letscher, D., and Zomorodian, A. Topological persistence and simplification. In *Foundations of Computer Science, 2000. Proceedings. 41st Annual Symposium on*, pp. 454–463. IEEE, 2000.

Fréchet, M. Les éléments aléatoires de nature quelconque dans un espace distancié. In *Annales de l’institut Henri Poincaré*, volume 10, pp. 215–310. Presses universitaires de France, 1948.
Guittet, K. *Extended Kantorovich norms: a tool for optimization*. PhD thesis, INRIA, 2002.

Hiraoka, Y., Nakamura, T., Hirata, A., Escolar, E. G., Matsue, K., and Nishiura, Y. Hierarchical structures of amorphous solids characterized by persistent homology. *Proceedings of the National Academy of Sciences*, 113(26):7035–7040, 2016.

Kerber, M., Morozov, D., and Nigmetov, A. Geometry helps to compare persistence diagrams. *Journal of Experimental Algorithmics (JEA)*, 22(1):1–4, 2017.

Li, C., Ovsjanikov, M., and Chazal, F. Persistence-based structural recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp. 1995–2002, 2014.

Lucet, Y. What shape is your conjugate? a survey of computational convex analysis and its applications. *SIAM review*, 52(3):505–542, 2010.

Lum, P., Singh, G., Lehman, A., Ishkanov, T., Vejdemo-Johansson, M., Alagappan, M., Carlsson, J., and Carlsson, G. Extracting insights from the shape of complex data using topology. *Scientific reports*, 3:1236, 2013.

Makarenko, N., Kalimoldayev, M., Pak, I., and Yessenaliyeva, A. Texture recognition by the methods of topological data analysis. *Open Engineering*, 6(1), 2016.

Mileyko, Y., Mukherjee, S., and Harer, J. Probability measures on the space of persistence diagrams. *Inverse Problems*, 27(12):124007, 2011.

Moreau, J.-J. Proximité et dualité dans un espace hilbertien. *Bull. Soc. Math. France*, 93(2):273–299, 1965.

Nicolaou, M., Levine, A. J., and Carlsson, G. Topology based data analysis identifies a subgroup of breast cancers with a unique mutational profile and excellent survival. *Proceedings of the National Academy of Sciences*, 108(17):7265–7270, 2011.

Obayashi, I., Hiraoka, Y., and Kimura, M. Persistence diagrams with linear machine learning models. *Journal of Applied and Computational Topology*, 1(3-4):421–449, 2018.

Peyré, G. and Cuturi, M. Computational Optimal Transport, 2018. URL http://arxiv.org/abs/1803.00567.

Reininghaus, J., Huber, S., Bauer, U., and Kwitt, R. A stable multi-scale kernel for topological machine learning. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 4741–4748, 2015.

Santambrogio, F. Optimal transport for applied mathematicians. *Birkäuser, NY*, 2015.

Schrijver, A. *Theory of linear and integer programming*. John Wiley & Sons, 1998.

Solomon, J., De Goes, F., Peyré, G., Cuturi, M., Butscher, A., Nguyen, A., Du, T., and Guibas, L. Convolutional wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Transactions on Graphics (TOG)*, 34(4):66, 2015.

Sumner, R. W. and Popović, J. Deformation transfer for triangle meshes. In *ACM Transactions on Graphics (TOG)*, volume 23, pp. 399–405. ACM, 2004.

Turner, K. Means and medians of sets of persistence diagrams. *arXiv preprint arXiv:1307.8300*, 2013.

Turner, K., Mileyko, Y., Mukherjee, S., and Harer, J. Fréchet means for distributions of persistence diagrams. *Discrete & Computational Geometry*, 52(1):44–70, 2014.

Villani, C. *Topics in optimal transportation*. Number 58. American Mathematical Soc., 2003.

Villani, C. *Optimal transport: old and new*, volume 338. Springer Science & Business Media, 2008.

Zeppelzauer, M., Zieliński, B., Juda, M., and Seidl, M. Topological descriptors for 3d surface analysis. In *International Workshop on Computational Topology in Image Context*, pp. 77–87. Springer, 2016.

Zomorodian, A. and Carlsson, G. Computing persistent homology. *Discrete & Computational Geometry*, 33(2):249–274, 2005.
7 Supplementary material

7.1 Omitted proofs from Section 3

Diagram metrics as optimal transport: We recall that we consider \( D_1 = \sum_{i=1}^{n_1} \delta_{x_i} \) and \( D_2 = \sum_{j=1}^{n_2} \delta_{y_j} \) two persistence diagrams with respectively \( n_1 \) points \( x_1 \ldots x_{n_1} \) and \( n_2 \) points \( y_1 \ldots y_{n_2} \), \( p \geq 1 \), and \( C \) is the cost matrix with block structure

\[
C = \begin{pmatrix} \hat{C} & u \\ v^T & 0 \end{pmatrix} \in \mathbb{R}^{(n_1+1) \times (n_2+1)},
\]

Proof of Prop 1. Let \( n = n_1 + n_2 \) and \( \mu = D_1 + RD_2, \nu = D_2 + RD_1 \). Since \( \mu, \nu \) are point measures, that is discrete measures of same mass \( n \) with integer weights at each point of their support, finding \( \inf_{P \in \Pi(\mu,\nu)} \langle P, C \rangle \) is an assignment problem of size \( n \) as introduced in §2. It is equivalent to finding an optimal matching \( P \in \Sigma_n \), representing some permutation \( \sigma \in \mathfrak{S}_n \) for the cost matrix \( \hat{C} \in \mathbb{R}^{n \times n} \) built from \( C \) by repeating the last line \( u \) in total \( n_1 \) times, the last column \( v \) in total \( n_2 \) times, and replacing the lower right corner \( 0 \) by a \( n_1 \times n_2 \) matrix of zeros. The optimal \( \sigma \) defines a partial matching \( \zeta \) between \( D_1 \) and \( D_2 \), defined by \( (x_i, y_j) \in \zeta \) iff \( j = \sigma(i) \), \( 1 \leq i \leq n_1, 1 \leq j \leq n_2 \). Such pairs of points induce a cost \( \|x_i - y_j\|^p \), while other points \( s \in D_1 \cup D_2 \) (referred to as unmatched) induce a cost \( \|s - \pi_\Delta(s)\|^p \). Then:

\[
L_C(\mu, \nu) = \min_{P \in \Sigma_n} \langle \hat{C}, P \rangle
= \min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} \hat{C}_{\sigma(i)}
= \min_{\zeta \in \Gamma(D_1, D_2)} \sum_{(x_i, y_j) \in \zeta} \|x_i - y_j\|^p + \sum_{s \in D_1 \cup D_2} \|s - \pi_\Delta(s)\|^p
= d_p(D_1, D_2)^p.
\]

Error control due to discretization: Let \( D_1, D_2 \) be two diagrams and \( a, b \) their respective representations as \( d \times d \) histograms. For two histograms, \( L_C(a + Rb, b + Ra) = d_p(D_1' + RD_2', D_2' + RD_1') \) where \( D_1', D_2' \) are diagrams deduced from \( D_1, D_2 \) respectively by moving any mass located at \( (x, y) \in \mathbb{R}^2 \) to \( \left( \frac{\lfloor x d \rfloor}{d}, \frac{\lfloor y d \rfloor}{d} \right) \), inducing at most an error of \( \frac{1}{d^2} \) for each point. We identify \( a, b \) and \( D_1', D_2' \) in the following. We recall that \( d_p(\cdot, \cdot) \) is a distance over persistence diagrams and thus satisfy triangle inequity, leading to:

\[
|d_p(D_1, D_2) - L_C(a + Rb, b + Ra)^{\frac{p}{2}}| \leq d_p(D_1, D_1') + d_p(D_2, D_2').
\]

Thus, the error made is upper bounded by \( \frac{1}{d}(|D_1|^\frac{1}{2} + |D_2|^\frac{1}{2}) \).

Propositions 2, 3, 4: We keep the same notations as in the core of the article and give details regarding the iteration schemes provided in the paper.

Proof of prop 2. Given an histogram \( u \in \mathbb{R}^{d \times d} \) and a mass \( u_\Delta \in \mathbb{R}_+ \), one can observe that (see below):

\[
\hat{K}u = k(ku^T)^T.
\]

In particular, the operation \( u \mapsto \hat{K}u \) can be perform by only manipulating matrices in \( \mathbb{R}^{d \times d} \). Indeed, observe that:

\[
\hat{K}_{ij,kl} = e^{-(i-k)^2/\gamma} e^{-(j-l)^2/\gamma} = k_{ik}k_{jl}.
\]
so we have:
\[
(\hat{K}u)_{i,j} = \sum_{k,l} K_{ij,kl} u_{k,l}
\]
\[
= \sum_{k,l} k_{ik} k_{jl} u_{k,l} = \sum_{k} k_{ik} \sum_{l} k_{jl} u_{kl}
\]
\[
= \sum_{k} k_{ik} (ku^T)_{j,k} = (k(u^T)^T)_{i,j}.
\]
Thus we have in our case:
\[
K(u, u_\Delta) = (\hat{K}u + u_\Delta k_\Delta, \langle u, k_\Delta \rangle + u_\Delta)
\]
where \(\langle a, b \rangle\) designs the Frobenius dot product between two histograms \(a, b \in \mathbb{R}^{d \times d}\). Note that these computations only involves manipulation of matrices with size \(d \times d\). \(\square\)

**Proof of prop 3.**
\[
\langle \text{diag}(\mathbf{u}) \hat{K} \text{diag}(\mathbf{v}), \hat{C} \rangle = \sum_{ijkl} u_{ij} k_{ij} k_{kl} [c_{ik} + c_{jl}] v_{kl}
\]
\[
= \sum_{ijkl} u_{ij} (|k_{ik} c_{ik}| k_{jl} v_{kl} + k_{ik} k_{jl} c_{jl} v_{kl})
\]
\[
= \sum_{ij} u_{ij} \sum_{kl} (m_{ik} k_{ij} v_{kl} + k_{ik} m_{jl} v_{kl})
\]
Thus, we finally have:
\[
\langle \text{diag}(\mathbf{u}) \hat{K} \text{diag}(\mathbf{v}), \hat{C} \rangle = \| u \otimes (m(kv^T)^T + kmv^T)^T \|_1
\]
And finally, taking the \(\{\Delta\}\) bin into considerations,
\[
\langle \text{diag}(\mathbf{u}, u_\Delta) \hat{K} \text{diag}(\mathbf{v}, v_\Delta), C \rangle = \langle \text{diag}(\mathbf{u}) \hat{K} \text{diag}(\mathbf{v}, v_\Delta) U_{\Delta} (\mathbf{u} \Delta \otimes \hat{K} \Delta), \langle \hat{C}, \hat{C}_\Delta \rangle \rangle = \langle \text{diag}(\mathbf{u}) \hat{K} \text{diag}(\mathbf{v}), \hat{C} \rangle + u_\Delta \langle v, k_\Delta \otimes c_\Delta \rangle + v_\Delta \langle u, k_\Delta \otimes c_\Delta \rangle
\]
Remark: First term correspond to the cost of effective mapping (point to point) and the two others to the mass mapped to the diagonal. \(\square\)

To address the last proof, we recall below the rounding_to_feasible algorithm introduced by Altschuler et al.; \(r(P)\) and \(c(P)\) denotes respectively the first and second marginal of a matrix \(P\).

**Algorithm 3** Rounding algorithm of Altschuler et al. (2017)

1: **Input:** \(P \in \mathbb{R}^{d \times d}\), desired marginals \(r, c\).  
2: **Output:** \(F(P) \in \Pi(r, c)\) close to \(P\).  
3: \(X = \min \left( \frac{r}{\pi^r}, 1 \right) \in \mathbb{R}^d\)  
4: \(P' = \text{diag}(X) P\)  
5: \(Y = \min \left( \frac{c}{\pi^c}, 1 \right) \in \mathbb{R}^d\)  
6: \(P'' = P' \text{diag}(Y)\)  
7: \(e_r = r - r(P''), e_c = c - c(P'')\)  
8: **return** \(F(P) := P'' + e_r e_c^T / \| e_c \|_1\)

**Proof of prop 4.** By straightforward computations, the first and second marginals of \(P'_t = \text{diag}(\mathbf{u}) \hat{K} \text{diag}(\mathbf{v})\) are given by:
\[
\left( \sum_{kl} u_{ij} K_{ij,kl} v_{kl} \right)_{ij} = u \otimes (Kv), \quad \left( \sum_{ij} u_{ij} K_{ij,kl} v_{kl} \right)_{kl} = (uK) \otimes v.
\]
Observe that $Kv$ and $uK$ can be computed using Proposition 2.

Now, the transport cost computation is:
\[
\langle F(P^T_t), C \rangle = \langle \text{diag}(X) P^T_t \text{diag}(Y), C \rangle + \langle e_r e^T_c / \|e_c\|_1, C \rangle \\
= \langle \text{diag}(X \odot u) K \text{diag}(Y \odot v), C \rangle + \frac{1}{\|e_c\|_1} \sum_{ijkl} (e_r)_{ij} (e_c)_{kl} [c_{ik} + c_{jl}] 
\]
The first term is the transport cost induced by a rescaling of $u$ and $v$. The barycenters). We refer the reader to (Santambrogio, 2015; Villani, 2008) for more details.

Consider now the second term. Without considering the additional bin $\{\Delta\}$, we have:
\[
\sum_{ijkl} (e_r)_{ij} (e_c)_{kl} [c_{ik} + c_{jl}] = \sum_{ijkl} (e_r)_{ij} \sum_k c_{ik} (e_c)_{kl} + \sum_{ijkl} (e_r)_{ij} \sum_l c_{jl} (e_c)_{kl} \\
= \sum_{ijkl} (e_r)_{ij} (ce_{c}d)_{il} + \sum_{ijkl} (e_r)_{ij} (ce^T_c)_{jk} \\
= \|e^T_c c_e\|_1 + \|e_r c^T_c\|_1,
\]
so when we consider our framework (with $\{\Delta\}$), it comes:
\[
\langle \left( e_r, (e_r)_{\Delta} \right), \left( e_c, (e_c)_{\Delta} \right), C \rangle = \langle \left( e_r e^T_c (e_c)_{\Delta} e_r, (e_c)_{\Delta} e_r \right), \left( \hat{C} e^T_c \hat{C} \Delta, 0 \right) \rangle \\
= \langle e_r e^T_c, \hat{C} \rangle + (e_c)_{\Delta} \langle e_r, c_e \rangle + (e_r)_{\Delta} \langle e_c, c_e \rangle.
\]
Putting things together finally proves the claim. \hfill \square

## 7.2 Omitted proofs from Section 4

We first observe that $\mathcal{E}$ does not have local minimum (while $\hat{E}$ does). For $x \in \mathbb{R}^2 \cup \{\Delta\}$, we extend the Euclidean norm by $\|x - \Delta\|$ the distance from $x$ to its orthogonal projection onto the diagonal $\pi_\Delta(x)$. In particular, $\|\Delta - \Delta\| = 0$. We denote by $c$ the corresponding cost function (continuous analogue of the matrix $C$ defined in (8)).

**Proposition (Convexity of $\mathcal{E}$).** For any two measures $\mu, \mu' \in \mathcal{M}_+(\mathbb{R}^2)$ and $t \in (0, 1)$, we have:
\[
\mathcal{E}((1-t)\mu + t\mu') \leq (1-t)\mathcal{E}(\mu) + t\mathcal{E}(\mu') \tag{18}
\]

**Proof.** We denote by $\alpha_i, \beta_i$ the dual variables involved when computing the optimal transport plan between $(1-t)\mu + t\mu' + RD_i$ and $D_i + R((1-t)\mu + t\mu')$. Note that maximum are taken over the set $\alpha_i, \beta_i | \alpha_i + \beta_i \leq c$ (with $\alpha \oplus \beta : (x, y) \mapsto \alpha(x) + \beta(y)$):
\[
\mathcal{E}((1-t)\mu + t\mu') = \frac{1}{n} \sum_{i=1}^n L_c((1-t)\mu + t\mu' + RD_i, D_i + (1-t)R\mu + tR\mu') \\
= \frac{1}{n} \sum_{i=1}^n \max \{ \langle \alpha_i, (1-t)\mu + t\mu' + RD_i \rangle + \langle \beta_i, D_i + (1-t)R\mu + tR\mu' \rangle \} \\
= \frac{1}{n} \sum_{i=1}^n \max \{ (1-t) \left( \langle \alpha_i, \mu + RD_i \rangle + \langle \beta_i, D_i + R\mu \rangle \right) + \\
+ t \max \{ \langle \alpha_i, \mu' + RD_i \rangle + \langle \beta_i, D_i + R\mu' \rangle \} \} \\
\leq \frac{1}{n} \sum_{i=1}^n (1-t) \max \{ \langle \alpha_i, \mu + RD_i \rangle + \langle \beta_i, D_i + R\mu \rangle \} \\
+ t \max \{ \langle \alpha_i, \mu' + RD_i \rangle + \langle \beta_i, D_i + R\mu' \rangle \} \\
= (1-t) \frac{1}{n} \sum_{i=1}^n L_c(\mu + RD_i, D_i + R\mu) + t \frac{1}{n} \sum_{i=1}^n L_c(\mu' + RD_i, D_i + R\mu') \\
= (1-t)\mathcal{E}(\mu) + t\mathcal{E}(\mu')
\]

---

1Optimal transport between non-discrete measures was not introduced in the core of this article for the sake of concision. It is a natural extension of notions introduced in §2 (distances, primal and dual problems, barycenters). We refer the reader to (Santambrogio, 2015; Villani, 2008) for more details.
Tightness of the relaxation. The following result states that the minimization problem (15) is a tight relaxation of the problem considered by Turner et al. in sense that global minimizers of $\mathcal{E}$ (which are, by definition, persistence diagrams) are (global) minimizers of $\mathcal{G}$.

**Proposition 6.** Let $D_1, \ldots, D_N$ be a set of persistence diagrams. Diagram $D_i$ has mass $m_i \in \mathbb{N}$ while $m_{\text{tot}} = \sum m_i$ denotes the total mass of the dataset. Consider the normalized dataset $\tilde{D}_1, \ldots, \tilde{D}_N$ defined by $\tilde{D}_i := D_i + (m_{\text{tot}} - m_i)\delta_{\Delta}$. Then the functional

$$
\mathcal{G} : \mu \mapsto \frac{1}{N} \sum_{i=1}^N \mathcal{L}_c(\mu + (m_{\text{tot}} - |\mu|)\delta_{\Delta}, \tilde{D}_i)
$$

(19)

where $\mu \in \{\mathcal{M}_+(\mathbb{R}^2_+) : \max_i m_i \leq |\mu| \leq m_{\text{tot}}\}$ has the same minimizers as (15).

This allows to apply known results from OT theory, linear programming, and integrality of solutions of LPs with totally unimodular constraint matrices and integral constraint vectors (Schrijver, 1998), which provides results on the tightness of our relaxation.

**Corollary (Properties of barycenters for PDs).** Let $\mu^\ast$ be a minimizer of (15). Then $\mu^\ast$ satisfies:

(i) (Carlier et al., 2015) Localization: $x \in \text{supp}(\mu^\ast) \Rightarrow x$ minimizes $z \mapsto \sum_{i=1}^n \|x_i - z\|^2_2$

for some $x_i \in \text{supp}(\tilde{D}_i)$. This function admit a unique minimizer in $\mathbb{R}^2_+ \cup \{\Delta\}$, thus the support of $\mu^\ast$ is discrete.

(ii) $\mathcal{G}$ admits persistence diagrams (that is point measures) as minimizers (so does $\mathcal{E}$).

We introduce an intermediate function $\mathcal{F}$, which appears to have same minimizers as $\mathcal{E}$ and $\mathcal{G}$, which will allow us to conclude that $\mathcal{E}$ and $\mathcal{G}$ have same minimizers.

**Proposition.** Let $\mu^\ast \in \mathcal{M}_+(\mathbb{R}^2_+)$ be a minimizer of $\mathcal{E}$ and $(P_i)$ the corresponding optimal transport plans. Then for all $i$, $P_i$ fully transports $D_i$ onto $\mu^\ast$ (i.e. $P_i(x, \Delta) = 0$ for any $x \in \text{supp}(D_i)$). In particular, $|\mu^\ast| \geq \max m_i$ and $\mathcal{E}$ has the same minimizers as:

$$
\mathcal{F}(\mu) := \frac{1}{N} \sum_{i=1}^N \mathcal{L}_c(\mu, D_i + (|\mu| - m_i)\delta_{\Delta})
$$

(20)

where $\mu \in \mathcal{M}_+(\mathbb{R}^2_+)$ and satisfies $|\mu| \geq \max m_i$

**Proof.** Fix $i \in \{1, \ldots, N\}$. Let $P_i$ be an optimal transport plan between $\mu^\ast + m_i\delta_{\Delta}$ and $D_i + |\mu^\ast|\delta_{\Delta}$. Let $x \in \text{supp}(D_i)$. Assume that there is a fraction of mass $t > 0$ located at $x$ that is transported to the diagonal $\Delta$.

Consider the measure $\mu^\prime := \mu^\ast + t\delta_{x^\prime}$, where $x^\prime = \frac{x + (N-1)x_{\Delta}}{N}$. We now define the transport plan $P_{i,1}^\prime$ which is adapted from $P_i$ by transporting the previous mass to $x^\prime$ instead of $\Delta$ (inducing a cost $t\|x - x^\prime\|^2$ instead of $t\|x - \Delta\|^2$). Extend all other optimal transport plans $(P_{i,j})_{j \neq i}$ to $P_{i,1}^\prime$ by transporting the mass $t$ located at $x^\prime$ in $\mu^\ast$ to the diagonal $\Delta$ (inducing a total cost $(N-1)t\|x^\prime - \Delta\|^2$), and everything else remains unchanged. One can observe that the new $(P_{i,j}^\prime)$ are admissible transport plans from $\mu^\prime + m_j\delta_{\Delta}$ to $D_j + |\mu^\prime|\delta_{\Delta}$ (respectively) inducing an energy $\mathcal{E}(\mu^\prime)$ strictly smaller than $\mathcal{E}(\mu^\ast)$, leading to a contradiction since $\mathcal{E}(\mu^\ast)$ is supposed to be optimal.

To prove equivalence between the two problems considered (in the sense that they have the same minimizers), we introduce $\mu^\ast_{\mathcal{F}}$ and $\mu^\ast_{\mathcal{G}}$ which are minimizers of $\mathcal{E}$ and $\mathcal{F}$ respectively. Note that the existence of minimizers is given by standard arguments in optimal transport theory (lower semi-continuity of $\mathcal{E}, \mathcal{F}, \mathcal{G}$ and relative compactness of minimizing sequences, see for example (Agueh & Carlier, 2011, Prop. 2.3)). We first observe that $\mathcal{E}(\mu) \leq \mathcal{F}(\mu)$ for all $\mu$ (adding the same amount of mass on the diagonal can only decrease the optimal transport cost).

This allows us to write:

$$
\mathcal{F}(\mu^\ast_{\mathcal{F}}) = \mathcal{E}(\mu^\ast_{\mathcal{F}}) = \mathcal{E}(\mu^\ast_{\mathcal{G}}) \leq \mathcal{G}(\mu^\ast_{\mathcal{F}}) \leq \mathcal{G}(\mu^\ast_{\mathcal{G}}) \leq \mathcal{F}(\mu^\ast_{\mathcal{G}})
$$

We can remove $m_i\delta_{\Delta}$ from both sides since $\mu^\ast_{\mathcal{F}}$ is a minimizer of $\mathcal{E}$ since $\mathcal{E}(\mu) \leq \mathcal{F}(\mu)$ since $\mu^\ast_{\mathcal{G}}$ is a minimizer of $\mathcal{F}$
Hence, all these inequalities are actually equalities, thus minimizers of $\mathcal{E}$ are minimizers of $\mathcal{F}$ and vice-versa.

We can now prove that $\mathcal{F}$ as the same minimizers as $\mathcal{G}$ which will finally prove Proposition 6.

**Proof of Proposition 6.** Let $\mu^*_G$ be a minimizer of $\mathcal{G}$. Consider $\mu_\Delta := (m_{tot} - |(G_\hat{\mu})|)\delta_\Delta$. We observe that $\mu_\Delta$ is always transported on $\{\Delta\}$ (inducing a cost of 0) for each of the transport plan $P_1 \in \Pi(\mu^*_G + \mu_\Delta, \hat{D}_i)$ for minimality considerations (as in previous proof). Observe also (as in previous proof) that $\mathcal{G}(\mu) \leq \mathcal{F}(\mu)$ for any measure $\mu$, yielding:

\[
\begin{align*}
\mathcal{G}(\mu^*_G) &= \mathcal{F}(\mu^*_G) \\
&\geq \mathcal{F}(\mu^*_\mathcal{F}) \\
&\geq \mathcal{G}(\mu^*_\mathcal{F}) \\
&\geq \mathcal{G}(\mu^*_G)
\end{align*}
\]

This implies that minimizers of $\mathcal{G}$ are minimizers of $\mathcal{F}$ (and thus of $\mathcal{E}$) and conversely.

**Details for Corollary of Proposition 6**

(i) Given $N$ diagrams $D_1 \ldots D_N$ and $(x_1 \ldots x_N) \in \text{supp}(\hat{D}_1) \times \cdots \times \text{supp}(\hat{D}_N)$, among which $k$ of them are equals to $\Delta$, on can easily observe (this is mentioned in Turner et al. (2014)) that $z \mapsto \sum_{i=1}^{N-k}\|z - x_i\|^2$ admits a unique minimizer $x^* = \frac{(N-k)\pi + k \Delta(z)}{N\pi + k \Delta}$, where $\pi$ is the arithmetic mean of the $(N - k)$ non-diagonal points in $x_1 \ldots x_N$.

The localization property (see §2.2 of Carlier et al. (2015)) states that the support of any barycenter is included in the set $S$ of such $x^*$'s which is finite, proving in particular that barycenters of $\hat{D}_1 \ldots \hat{D}_N$ have a discrete support included in some known set. Note that a similar result is also mentioned in Anderes et al. (2016).

(ii) As a consequence of previous point, one can describe a barycenter of $\hat{D}_1 \ldots \hat{D}_N$ as a vector of weight $w \in \mathbb{R}^s_+$, where $s$ is the cardinality of $S$ and cast the barycenter problem as a Linear Programming (LP) one (see for example §3.2 in Anderes et al. (2016) or §3.2 and 2.4 in Carlier et al. (2015)). More precisely, the problem is equivalent to:

\[
\begin{align*}
\text{minimize } & w^T c \\
\text{s.t.} & \forall i = 1 \ldots N, A_iw = b_i
\end{align*}
\]

Here, $c \in \mathbb{R}^s$ is defined as $c_j = \sum_{k=1}^{N} \|x^*_j - x_{k,j}\|^2$, where $x^*_j$ is the mean (as defined above) associated to $(x_{k,j})$ for each point of its support. Note that each $b_i$ has integer coordinates and that $A_i$ is totally unimodular (see Schrijver, 1998), and thus among optimal $w$, some of them have integer coordinates.

**Bad local minima of $\hat{\mathcal{E}}$.** The following lemma illustrate specific situation which lead algorithms proposed by Turner et al. to get stuck in bad local minima.

**Lemma 1.** For any $\kappa \geq 1$, there exists a set of diagrams such that $\hat{\mathcal{E}}$ admits a local minimizer $D_{\text{loc}}$ satisfying:

\[
\hat{\mathcal{E}}(D_{\text{loc}}) \geq \kappa \hat{\mathcal{E}}(D_{\text{opt}})
\]

where $D_{\text{opt}}$ is a global minimizer. Furthermore, there exist sets of diagrams so that the B-Munkres algorithm always converges to such a local minimum when initialized with one of the input diagram.

**Proof.** We consider the configuration of Fig. 9a where we consider two diagrams with 1 point (blue and green diagram) and their correct barycenter (red diagram) along with the orange diagram (2 points). It is easy to observe that when restricted to the space of persistence diagram, the orange diagram is a minimizer of the function $\hat{\mathcal{E}}$ (in which the algorithm could get stuck if initialized poorly). It achieves an energy of $\frac{1}{2}(\frac{1}{2} + \frac{1}{2})^2 + (\frac{1}{2} + \frac{1}{2})^2 = 1$ while the red diagram achieves an energy of...
\( \frac{1}{2}(\sqrt{\epsilon^2} + \sqrt{\epsilon^2}) = \epsilon \). This example proves that there exist configurations of diagrams so that \( \hat{E} \) has arbitrary bad local minima.

One could argue that when initialized to one of the input diagram (as suggested in (Turner et al., 2014)), the algorithm will not get stuck to the orange diagram. Fig. 9b provide a configuration involving three diagrams with two points each where the algorithm will always get stuck in a bad local minimum when initialized with any of the three diagrams. The analysis is similar to previous statement.

Figure 9: Example of simple configurations in which the B-Munkres algorithm will converge to arbitrarily bad local minima

(a) Example of arbitrary bad local minima of \( \hat{E} \). Blue point and green point represent our two diagrams of interest. Red point is a global minimizer of \( \hat{E} \). The two orange points give a diagram which is a local minimizer of \( \hat{E} \) achieving an energy arbitrary higher (relatively) than the one of the red diagram (as \( \epsilon \) goes to 0).

(b) Failing configuration for B-Munkres algorithm. Three diagrams (red, blue, green) along with the output of Turner et al algorithm (purple) when initialized on the green diagram (we have a similar result by symmetry when initialized on any other diagram).