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Wasserstein Dictionaries
of Persistence Diagrams

Keanu Sisouk, Julie Delon, Julien Tierny

Abstract—This paper presents a computational framework for the concise encoding of an ensemble of persistence diagrams, in the form of weighted Wasserstein barycenters of a dictionary of atom diagrams. We introduce a multi-scale gradient descent approach for the efficient resolution of the corresponding minimization problem, which interleaves the optimization of the barycenter weights with the optimization of the atom diagrams. Our approach leverages the analytic expressions for the gradient of both sub-problems to ensure fast iterations and it additionally exploits shared-memory parallelism. Extensive experiments on public ensembles demonstrate the efficiency of our approach, with Wasserstein dictionary computations in the orders of minutes for the largest examples. We show the utility of our contributions in two applications. First, we apply Wasserstein dictionaries to data reduction and reliably compress persistence diagrams by concisely representing them with their weights in the dictionary. Second, we present a dimensionality reduction framework based on a Wasserstein dictionary defined with a small number of atoms (typically three) and encode the dictionary as a low dimensional simplex embedded in a visual space (typically in 2D). In both applications, quantitative experiments assess the relevance of our framework. Finally, we provide a C++ implementation that can be used to reproduce our results.

Index Terms—Topological data analysis, ensemble data, persistence diagrams.

1 INTRODUCTION

As measurement devices and numerical techniques are becoming more and more advanced, datasets are becoming more and more complex geometrically. This geometrical complexity makes interactive exploration and analysis difficult, which challenges the interpretation of the data by the users. This motivates the creation of expressive data abstractions, capable of encapsulating the main features of interest of the data into simple representations, visually conveying the main information to the user.

Topological Data Analysis (TDA) is a family of techniques which precisely addresses this issue. It provides concise topological descriptors of the main structural features hidden in a dataset. The relevance of TDA for analyzing scalar data, its efficiency and robustness have been documented in a number of visualization tasks. Examples of successful applications include turbulent combustion, material sciences, nuclear energy, fluid dynamics, bioimaging, chemistry, or astrophysics.

Among the different topological descriptors studied in TDA (such as the merge and contour trees, the Reeb graph, the Morse-Smale complex, or the Morse-Smith complex), the Persistence Diagram [Fig. 1] is a particularly prominent example. As described in Sec. 2.1, it is a concise topological descriptor which captures the main structural features in a dataset and which assesses their individual importance. In addition to the challenge of increased geometrical complexity (discussed above), a new difficulty has recently emerged in many applications, with the notion of ensemble dataset. These representations describe a given phenomenon not only with a single dataset, but with a collection of datasets, called ensemble members.

In that context, the topological analysis of an ensemble dataset consequently results in an ensemble of corresponding topological descriptors (e.g. one persistence diagram per ensemble member).

Then, a major challenge consists in developing practical tools for such an ensemble of topological descriptors, to facilitate its processing, analysis and visualization. Such tools include compression approaches (to facilitate the manipulation of the ensemble of descriptors) or visualization methods (for instance, with planar layouts, where each point encodes a descriptor and the distance between a pair of points encodes the intrinsic differences between the corresponding descriptors).

To enable the above tools, a key research question deals with the definition of a concise, yet informative, encoding of the ensemble of descriptors. A promising research direction consists in defining a dictionary (i.e. a set of reference descriptors, or atoms), such that the topological descriptors of the ensemble can be concisely encoded by expressing them as a specific function of the atoms (e.g. a linear combination). At a technical level, this requires to accurately capture and model the implicit relations (i.e. the possible functions) which link the different descriptors of the ensemble.

A series of recent works started the exploration of this overall direction, in particular with the notion of average topological representation. These techniques can produce a topological descriptor which nicely summarizes the ensemble. However, they do not capture the implicit relations between the different topological descriptors.

This paper addresses this issue by introducing a simple and efficient approach for the estimation of linear relations between persistence diagrams on their associated Wasserstein metric space. Inspired by previous work on histograms, our approach provides a linear encoding of the input ensemble, where each diagram is represented as a weighted Wasserstein barycenter of a dictionary of automatically optimized diagrams called atom diagrams. We introduce a novel multi-scale gradient descent algorithm for the efficient resolution of the corresponding minimization problem, for which we interleave the optimization of the barycenter weights with the optimization of the atom diagrams. Extensive experiments on
public ensembles demonstrate the efficiency of our approach, with
Wasserstein dictionary computations in the orders of minutes for the
largest examples. We illustrate the relevance of our contributions
for the visual analysis of ensemble data with two applications, data
reduction (Sec. 5.1) and dimensionality reduction (Sec. 5.2).

1.1 Related Work

The literature related to our work can be classified into three main
classes: (i) uncertainty visualization, (ii) ensemble visualization, and
(iii) topological methods for ensembles.

(i) Uncertainty visualization: Data variability can be represented
in the form of uncertain datasets, by considering the data at each
point of the domain as a random variable, associated with an explicit
probability density function (PDF). The analysis and visualization
of uncertain data has been recognized as a major challenge in the
visualization community [1, 14, 49, 60, 71, 85]. Several
techniques have been proposed either dealing with the entropy of
the random variables [84], or their correlation [77] or gradient
variation [75]. The effect of data uncertainty on feature extraction
has been studied for instance for level set extraction [4, 5, 76, 81, 83, 89], for various interpolation schemes and
PDF models (e.g. Gaussian [58, 69, 70, 74] or uniform [10, 42, 96] distributions). In general, a central limitation of existing
methods for uncertain data is their dependence on a specific
PDF model (Gaussian, uniform, etc.). This challenges their usability
for ensemble data, where the PDFs estimated from the ensemble
can follow an arbitrary, unknown model. Moreover, most of these
techniques do not consider multi-modal PDFs, which are however
essential when multiple trends appear in the ensemble.

(ii) Ensemble visualization: Another approach to model data
variability consists in using ensemble datasets. In this context, the
variability is encoded by a sequence of empirical observations (i.e.
the members of the ensemble). Established techniques typically
compute geometrical objects, such as level sets or streamlines,
thereby capturing the main features for each member of the
ensemble. From there, a representative of the resulting ensemble of
generations can be computed. For this task, a few methods
have been introduced. For instance spaghetti plots [27] are used in
the case of level-set variability, more particularly for weather data
[86, 88], and box-plots [22, 103] for the variability of contours and
curves. In the case of trend variability, Hummel et al. [48]
conceived a Lagrangian framework for classification purposes in
flow ensembles. More specifically, clustering techniques have been
used to identify the main trends in ensemble of streamlines [35] and
isocontours [36]. However, only few techniques have applied this
strategy to topological objects. Favelier et al. [33] and Athawale et
al. [6] respectively introduced techniques to analyze the geometrical
variability of critical points and gradient separatrices. Overlap-
based heuristics have been studied for estimating a representative
contour tree from an ensemble [53, 105]. In the context of
ensembles of histograms, Schmitz et al. [90] introduced a dictionary
encoding approach based on optimal transport [24]. However,
this method is not directly applicable to persistence diagrams. It
focuses on a fundamentally different object (histograms). Thus,
the employed distances, geodesics and barycenters are defined
differently (in particular in an entropic form [24, 25]) and the
algorithms for their computations are drastically different (based
on Sinkhorn matrix scaling [93]). In contrast, our work focuses on
Persistence diagrams (Sec. 2.1), whose associated metric space is
also inspired from optimal transport, but with various formal and
computational specificities (Sec. 2.2). Moreover, our approach is
based on gradient descent which, from our experience, provides
better practical convergence for this kind of problems than quasi-
Newton techniques. Finally, we contribute a multi-scale progressive
optimization algorithm, which provides improved solutions in
comparison to a naive optimization.

(iii) Topological methods for ensembles: To analyze the relations
between the persistence diagrams of an ensemble, several key
low level notions are required, such as the notion of distance
and barycenters between diagrams, for which we review the
literature here. Inspired by optimal transport [50, 63], the
Wasserstein distance between persistence diagrams [29] (Sec. 2.2)
has been extensively studied [22, 23]. It relies on a bipartite
assignment problem, for which exact [64] and approximate [8, 52] implementations are available in open-source [98]. Based
on this distance, several approaches have explored the possibility
to define a representative diagram of an ensemble of persistence
diagrams, with the notion of Wasserstein barycenter. Turner et
al. [100] introduced the first approach for the computation of
such a barycenter. Lacombe et al. [55] presented an approach
based on entropic transport [24, 25]. However, it requires a
pre-vectorization step which is subject to several parameters, and
which is not conducive to visualization tasks (features can no
longer be individually tracked beyond the pre-vectorization step). In
contrast, Vidal et al. [102] introduced a vectorization-free approach
which maintains the feature assignments explicitly. It is based on
a progressive scheme, which greatly accelerates computation in
practice. These concepts have been recently investigated for other
topological descriptors, such as merge trees [79, 106]. Recently,
several authors have investigated another compact representation
of ensembles of topological descriptors, via a basis of representative
descriptors. For instance, Li et al. [57] introduce a vectorization
for merge trees, which was subsequently used by matrix sketching
procedures [104] to create a basis of representative merge trees.
In contrast, our work focuses on persistence diagrams (which
can encode different features). Also, it directly operates on the
Wasserstein metric space of persistence diagrams, thereby avoiding
the typical technical difficulties associated with vectorizations (e.g.
quantization and/or linearization artifacts, potential stability issues,
possible inaccuracies in vectorization reversal, etc.). Pont et al.
[80] introduced the notion of principal geodesic analysis of merge
trees (and persistence diagrams), with the same overall goal of
characterizing the relations between the topological descriptors of
an ensemble. In this work, we introduce a different formulation of
the problem, which is both simpler (based on the construction of
weighted Wasserstein barycenters) and more flexible (our
optimization is not subject to complicated constraints such as
gesdics orthogonality). This results in a simpler implementation
and slightly faster computations (Sec. 6).

1.2 Contributions

This paper makes the following new contributions:

1) A simple approach for the linear encoding of Persistence
Diagrams: We formulate the linear encoding of an ensemble
of persistence diagrams on their associated Wasserstein
metric space as a dictionary optimization (Sec. 3), which
simply optimizes, simultaneously, (i) the barycentric weights
(Sec. 3.2) and (ii) the atoms of the dictionary (Sec. 3.3).

2) A multi-scale algorithm for the computation of a Wasserstein
dictionary of Persistence Diagrams: We introduce a novel,
efficient algorithm for the optimization of the above dictionary encoding problem. Our algorithm leverages the analytic expressions of the gradient of both of the above sub-problems, to ensure fast iterations. Moreover, in comparison to a naive optimization, our algorithm reaches solutions of improved energy thanks to a multi-scale strategy. Finally, we leverage shared-memory parallelism to further improve performances.

3) An application to data reduction: We present an application to data reduction (Sec. 5.1), where the persistence diagrams of the input ensemble are significantly compressed, by solely storing their barycentric weights as well as the atom diagrams.

4) An application to dimensionality reduction: We present an application to dimensionality reduction (Sec. 5.2), by embedding each input diagram as a point within a 2D view, based on its weights relative to a Wasserstein dictionary composed of three atoms (thereby defining a 2-simplex).

5) Implementation: We provide a C++ implementation of our algorithms that can be used for reproducibility purposes.

2 PRELIMINARIES

This section presents the theoretical elements needed for the formalization of our work. We introduce the topological data representation that we use - the persistence diagram (Sec. 2.1) - and its associated metric (Sec. 2.2). Then we define the notion of Wasserstein barycenter of persistence diagrams (Sec. 2.3), which is a core component of our approach (Sec. 3).

2.1 Persistence diagrams

Each input ensemble member is given in the form of a piecewise linear (PL) scalar field \( f : \mathcal{M} \to \mathbb{R} \) defined on a PL \((d,\mathcal{M})\)-manifold \(\mathcal{M}\), with \(d,\mathcal{M} \leq 3\) for our applications. Given an isovalue \(w \in \mathbb{R}\), we denote \(f_{\leq w}^{-1}(w) = f^{-1}((\infty, w])\) the sub-level set of \(f\) at \(w\). As \(w\) increases, the topolgy of \(f_{\leq w}^{-1}\) changes at specific points of \(\mathcal{M}\), called "critical points". Critical points are classified by their index \(\mathcal{F}\): 0 for minima, 1 for 1-saddles, \(d,\mathcal{M} - 1\) for \((d,\mathcal{M} - 1)\)-saddles, and \(d,\mathcal{M}\) for maxima (in practice, \(f\) is enforced to contain only isolated, non-degenerate critical points [31], [32]). According to the Elder rule [29], each topological feature of \(f_{\leq w}^{-1}(w)\) (e.g. a connected component, a cycle, a void) can be associated with a pair of critical points \((c, c')\) (with \(f(c) < f(c')\) and \(\mathcal{F}_{c} = \mathcal{F}_{c'} - 1\)), corresponding to its birth and death during the sweep of the data by \(w\) (from \(-\infty\) to \(+\infty\)). Such a pair \((c, c')\) is called a persistence pair.

For instance, when two connected components of \(f_{\leq w}^{-1}(w)\) meet at a critical point \(c'\), the younger one (created last) dies, leaving the oldest one (created first) survive. Then, the critical points are represented visually as 2D bar codes where the horizontal axis encodes the birth of a feature (noted \(b = f(c)\)) and where the vertical axis encodes its lifespan and death (noted \(d = f(c')\)). This representation is called the Persistence Diagram, noted \(X\). In the diagram, salient features stand out from the diagonal and small-amplitude noise is typically located near the diagonal, as shown in Fig. 1. In the remainder, we enumerate the points of \(X\) with indices such that \(X = \{x^1, \ldots, x^K\}\) and we note \(IX = \{1, \ldots, K\}\) the set of indices (i.e. the set of all integers going from 1 to \(K\)).

2.2 Wasserstein distance

To evaluate the distance between two diagrams, a typical pre-processing step consists in augmenting each diagram, by including the diagonal projection of all the off-diagonal points of the other diagram. To illustrate that, let us consider \(X_1 = \{x^1_1, \ldots, x^1_K\}\) and \(X_2 = \{x^2_1, \ldots, x^2_K\}\). Given an off-diagonal point \(x\) (i.e. \(b < d\)), let \(\Delta x\) be its diagonal projection, specifically: \(\Delta x = (\frac{b + d}{2}, \frac{b + d}{2})\). Let \(P_1\) and \(P_2\) be the sets of the diagonal projections of the points of \(X_1\) and \(X_2\) respectively. Then, \(X_1\) and \(X_2\) are augmented into \(X'_1\) and \(X'_2\) by considering \(X'_1 = X_1 \cup P_2\) and \(X'_2 = X_2 \cup P_1\). This ensures that \(|X'_1| = |X'_2| = K\) (which eases distance evaluation).

Specifically, we consider in the remainder that the notations \(X_1\) and \(X_2\) refer to augmented diagrams (i.e. \(|X_1| = |X_2| = K\)).

Then, given two persistence diagrams \(X_1\) and \(X_2\) the \(L^2\)-Wasserstein distance between them is defined as:

\[
W(X_1, X_2) = \min_{\psi, \{i_1, \ldots, i_K\}} \sum_{k=1}^{K} \sum_{j=1}^{K} c(x^1_j, x^2_k)^{\psi(j)},
\]

where \(\psi\), the matching, is a bijection of the index set \(IX\) towards itself (i.e. \(\psi\) is a permutation of \(IX\)). This bijection matches one
will call in the remainder dictionary (Fig. 3) – or Fréchet mean – of the dictionary based on an iterative optimization, where each point in the dictionary diagrams. This can be done since theapsulation distance as a cost function (Sec. 2.2), this 

assignment 

\[ E_F(B) = \sum_{i=1}^{m} \lambda_i W^2(a_i, B) \]

\( \lambda \) is such that \( \lambda_i \geq 0 \) and \( \sum_{i=1}^{m} \lambda_i = 1 \). We denote \( \Sigma_m \) the simplex of such vectors. Intuitively, \( Y(\lambda, D) \) is a diagram which minimizes the above linear combination, given \( \lambda \), of its squared Wasserstein distances to the diagrams of the dictionary \( D \).

The computation of the barycenter \( Y(\lambda, D) \) requires generalizing the pairwise augmentation described in Sec. 2.2. Specifically, each non-diagonal point of each dictionary diagram \( a_i \) is projected to the diagonal of all the other dictionary diagrams \( a_j \) (with \( i \neq j \)). After this first augmentation, each dictionary diagram \( a_i \) contains \( K = \sum_{i=1}^{m} |a_i| \) points (where \( |a_i| \) is the number of non-diagonal points in \( a_i \)). Then \( Y(\lambda, D) \) is typically initialized on the dictionary diagram \( a_i \) which initially minimizes the Fréchet energy \( E_F \). Let \( |Y(\lambda, D)| = |a_i| \) be the number of non-diagonal points of \( a_i \). Then, all the non-diagonal points of all the atoms are projected on the diagonal of \( Y(\lambda, D) \), and reciprocally, all the non-diagonal points of \( Y(\lambda, D) \) are projected on the diagonal of each atom. Thus, at this stage, after this second augmentation, each dictionary diagram \( a_i \) and the candidate barycenter \( Y(\lambda, D) \) contains \( K = \sum_{i=1}^{m} |a_i| + |Y(\lambda, D)| \) points (mostly on the diagonal).

Next, we optimize \( Y(\lambda, D) \) in practice with the approach by Vidal et al. [102], which provides a time-efficient approximation of the original algorithm by Turner et al. [100]. Similar to Turner et al., it is based on an iterative optimization, where each iteration includes an Assignment step, followed by an Update step. Specifically, the Assignment step computes the optimal assignments \( \psi \) between the candidate \( Y(\lambda, D) \) and each dictionary diagram \( a_i \). Next, the Update step minimizes the Fréchet energy \( E_F \) under the current assignments \( \psi \). Since the \( L^2 \)-Wasserstein distance considers the Euclidean distance as a cost function (Sec. 2.2), this minimization is achieved by simply placing each point of \( Y(\lambda, D) \) at the arithmetic mean in the birth/death space of its assigned points in the dictionary diagrams. This can be done since the arithmetic mean minimizes the Fréchet energy defined respectively to Euclidean distances (more sophisticated Update procedures, e.g. based on an optimization routine, would need to be derived for other distances in the birth/death space). After this Update step, the subsequent Assignment further improves the assignments \( \psi \), hence decreasing the Fréchet energy constructively at each iteration.

The approach by Vidal et al. [102] revisits this framework by integrating tailored approximations throughout the computation. Specifically, it approximates the optimal assignments \( \psi \) with the fast Auction optimization [8] (instead of the traditional, yet prohibitive, Munkres algorithm [24]). Further, it improves performance with a mechanism called price memorization, which enables the initialization of the Auction optimization with the assignments \( \psi \) computed in the previous Assignment step. This allows the barycenter optimization to resume the assignment optimization instead of re-computing it from scratch at each iteration. This approach also includes a strategy for the adaptive increase of the accuracy parameter of the Auction optimization, allowing for fast assignments in the early iterations of the barycenter algorithm, and slower but more accurate assignments towards its convergence.

3 WASSERSTEIN DICTIONARY ENCODING

This section formalizes our approach for the Wasserstein dictionary encoding of an ensemble of persistence diagrams. Sec. 3.1 provides an overview of our approach, which interleaves barycentric weight optimization \( (\lambda) \) with atom optimization \( (D) \). Finally, Secs. 3.2 and 3.3 detail the gradient estimation for both sub-problems.

3.1 Overview

Let \( \{X_1, \ldots, X_N\} \) be the input ensemble of \( N \) persistence diagrams. The goal of our approach is to jointly optimize two sub-problems:

- Optimize a set \( D \) of \( m \) reference persistence diagrams, called the atoms of the Wasserstein dictionary \( D \);
- Optimize for each input diagram \( X_n \) a vector of \( m \) barycentric weights \( \lambda_n \in \Sigma_m \), in order to accurately approximate \( X_n \) with a Wasserstein barycenter \( Y(\lambda_n, D) \) (Sec. 2.2).

This can be formalized as a joint optimization, where one wishes to find the optimal barycentric weights \( \Lambda^* = \lambda_1^*, \ldots, \lambda_N^* \) and the optimal Wasserstein dictionary \( D^* = \{a_1^*, \ldots, a_m^*\} \) (with \( m \ll N \)), in order to minimize the following dictionary energy:

\[ E_D(\Lambda, D) = \sum_{n=1}^{N} W^2(\{Y(\lambda_n, D)\}, X_n). \]

Our overall strategy for optimizing Eq. 2 consists in iteratively interleaving two sub-optimizations:

1. For a fixed dictionary \( D \), the set of barycentric weights \( \Lambda \) is optimized with one step of gradient descent (Sec. 3.2);
2. For a fixed set of barycentric weights \( \Lambda \), the dictionary \( D \) is optimized with one step of gradient descent (Sec. 3.3).

Then, this sequence of two sub-procedures is iterated until a pre-defined stopping condition is reached (Sec. 4.2).

Finally, the output of our approach is the optimized Wasserstein dictionary \( D^* \) (a set of \( m \) atom diagrams) and, for each input diagram \( X_n \), a vector of weights \( \lambda_n^* \in \Sigma_m \), which can be interpreted as the barycentric coordinates of \( X_n \) in \( D^* \), (thus capturing linear relations between the input diagrams on the Wasserstein dictionary).

3.2 Weight optimization

This section details the optimization of the barycentric weights \( \Lambda = \lambda_1, \ldots, \lambda_N \). Let \( D = \{a_1, \ldots, a_m\} \) be a fixed dictionary of atom diagrams, with \( m > 0 \). Let \( X \) be a diagram of the input ensemble. For a given set of weights \( \lambda = (\lambda_1, \ldots, \lambda_m) \), let \( Y(\lambda) = \{y^1(\lambda), \ldots, y^K(\lambda)\} \) be its barycentric approximation, relative to \( D \) (i.e. each point \( y^i(\lambda) \) of \( Y(\lambda) \) approximates a point in \( X \)).

We recall that after augmentation (Sec. 2.3), \( Y(\lambda) \) and the atoms contain \( \sum_{i=1}^{m} |a_i| + |Y(\lambda)| \) points each, where \( |a_i| \) and \( |Y(\lambda)| \) denote the number of non-diagonal points in \( a_i \) and \( Y(\lambda) \) respectively.
where A step of the corresponding gradient descent is illustrated in Fig. 4.

Then, by exploiting Eq. 4,

\[ E_K(t) = \text{argmin}_{\gamma} \sum \sum_{i=1}^{m} |a_i| + |y(\lambda_i)| + |x| \]

where \( K \) is the size of \( Y(\lambda) \) and \( m \) is the number of points in \( X \) that matches to \( Y(\lambda) \) (one point per atom \( a_i \)), under the optimal assignments \( \phi \) (i.e. minimizing Eq. 1).

For a fixed set of assignments \( \phi_1, \ldots, \phi_m \), the Wasserstein distance (Eq. 1) between \( X \) and its approximation \( Y(\lambda) \) is then:

\[ E_W(\lambda) = W^2(Y(\lambda), X) = \sum_{i=1}^{K} c(\phi(i), x) \]

where \( \psi \) denotes the optimal assignment (Eq. 1) between \( X \) and its approximation \( Y(\lambda) \). When \( \psi(i) \) and \( \phi(j) \) are not both diagonal points, the cost \( c(\psi(i), \phi(j)) \) is given by their squared Euclidean distance in the birth/death space (it is zero otherwise, see Sec. 2.2).

Then, by exploiting Eq. 4, \( E_W(\lambda) \) can be re-written as:

\[ E_W(\lambda) = W^2(Y(\lambda), X) = \sum_{i=1}^{K} \| \sum_{i=1}^{m} \lambda_i \phi(i) - x \|^2 \]

Intuitively, this energy measures the error (in terms of Wasserstein distance) induced by approximating the input diagram \( X \) with its barycentric approximation \( Y(\lambda) \). In Eq. 5 it is computed for each \( j \text{th} \) point \( y(\lambda) \) of the diagram \( Y(\lambda) \), by considering the birth/death distances between the points \( y(\lambda) \) maps to, in the input hand and in the input diagram \( X \) on the other.

Then, by applying the chain rule on Eq. 5 the gradient of the weight energy (Eq. 3) is given by:

\[ \nabla E_W(\lambda) = 2 \sum_{i=1}^{m} \sum_{j=1}^{K} \left[ \begin{array}{c} a_i \phi(j) - x_{\psi(j)} \\ \phi(j) - x_{\psi(j)} \end{array} \right] \left( \lambda_i \phi(j) - x_{\psi(j)} \right) \]

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where \( \Pi_{\mathcal{W}}(\lambda) \) is the projection onto the simplex of admissible barycentric weights (i.e. positive and summing to 1, c.f. Sec. 2.2).

Since \( \nabla E_W(\lambda) \) is L-Lipschitz (see the computation details in Appendix A), a gradient step will guarantee an energy decrease as long as:

\[ \sum_{j=1}^{K} \left\| \phi(j) - x_{\psi(j)} \right\| < \frac{1}{L} \]

Overall, for a given input diagram \( X \), each iteration \( t \) of gradient descent for the optimization of \( E_W \) consists in the following steps:

1. Computing the Wasserstein barycenter \( Y(\lambda) \) (Sec. 2.3);
2. Computing the Wasserstein distance \( W^2(Y(\lambda), X) \) (Eq. 3);
3. Estimating the gradient \( \nabla E_W(\lambda) \) (Eq. 6);
4. Applying one step \( \rho(\lambda) \) of gradient descent (Eq. 7).
A step of the corresponding gradient descent is illustrated in Fig. 5.

Given the set of optimal matchings \( \phi_1, \ldots, \phi_m \) between \( Y(\mathcal{D}) \) and the \( m \) atoms, the \( j^{th} \) point of \( Y(\mathcal{D}) \), noted \( y^j(\mathcal{D}) \), is given by:

\[
\forall j \in \{1, \ldots, K\}, \quad y^j(\mathcal{D}) = \sum_{i=1}^{m} \lambda_i a_i^{\phi(j)}.
\]

This expression is identical to Eq. 4 (Sec. 3.2). However, \( y^j \) now depends on \( \mathcal{D} \), which is the variable of the current optimization. Then, the gradient of \( y^j(\mathcal{D}) \) with regard to \( \mathcal{D} \) is simply given by:

\[
\nabla y^j(\mathcal{D}) = [\lambda_1 \cdots \lambda_m]^T. \tag{8}
\]

For a fixed set of assignments \( \phi_1, \ldots, \phi_m \), the Wasserstein distance (Eq. 1) between \( X \) and its approximation \( Y(\lambda) \) is then:

\[
E_A(\mathcal{D}) = W^2(\text{Y}(\mathcal{D}), X) = \sum_{j=1}^{K} \sum_{i=1}^{m} (y^j(\mathcal{D}) - x^i)^2.
\]

Let \( \mathcal{D}^j = [a_1^{\phi(j)}, \ldots, a_m^{\phi(j)}]^T \) be the \((m \times 2)\)-matrix formed by the atom points matching to a given point \( y^j(\mathcal{D}) \) of \( Y(\mathcal{D}) \), via the fixed assignments \( \phi_1, \ldots, \phi_m \). Specifically, the \( j^{th} \) line of this matrix refers to the point \( a_i^{\phi(j)} \) in the atom \( a_i \) where \( y^j(\mathcal{D}) \) maps to (via the optimal assignment \( \phi_j \)). For this line, the two columns of the matrix encode the birth/death coordinates of the point \( a_i^{\phi(j)} \). Then, the pointwise atom energy of \( y^j(\mathcal{D}) \), noted \( e_A(\mathcal{D}^j) \), is given by:

\[
e_A(\mathcal{D}^j) = \left\| \sum_{i=1}^{m} \lambda_i (a_i^{\phi(j)} - x^i)^2 \right\|^2. \tag{9}
\]

Now that the gradient of the pointwise atom energy is available (Eq. 10), we can proceed to a step of gradient descent. Specifically, at the iteration \( t + 1 \) (noted \( \mathcal{D}^j_{t+1} \)) obtained by a step \( \rho_{\mathcal{D}} \) from the same matrix at the iteration \( t \) (noted \( \mathcal{D}^j_t \)) along the gradient:

\[
\mathcal{D}^j_{t+1} = \Pi_{\mathcal{D}} (\mathcal{D}^j_t - \rho_{\mathcal{D}} \nabla e_A(\mathcal{D}^j_t)), \tag{11}
\]

where \( \Pi_{\mathcal{D}} \) projects each atom point to an admissible region of the 2D birth/death space (i.e. above the diagonal and within the global scalar field range). Since \( \nabla e_A \) is \( L \)-Lipschitz (see the computation details in Appendix B), a gradient step will guarantee an energy decrease as long as: \( \rho_{\mathcal{D}} < 4(m - 1)^{-1} \cdot L^{-1} \).

Now, that in order to control the final size \( S_m \) of the dictionary \( \mathcal{D} \), after each iteration of atom optimization, each atom \( a_i \) is thresholded by removing its \( \mathcal{K} = (mK - S_m) \) least persistent points (at the subsequent optimization iteration, all diagrams will be re-augmented again in a pre-process, as detailed in Sec. 3.2).

Overall, for a given input diagram \( X \), each iteration \( t \) of gradient descent for the optimization of \( E_A \) consists in the following steps:

1. Computing the Wasserstein barycenter \( Y(\mathcal{D}_t) \) (Sec. 2.3);
2. Computing the Wasserstein distance \( W^2(\text{Y}(\mathcal{D}_t), X) \) (Eq. 3);
3. For each point \( y^j(\mathcal{D}) \) of \( Y(\mathcal{D}) \):
   a) Estimating the gradient \( \nabla e_A(\mathcal{D}^j) \) (Eq. 10);
   b) Applying one step \( \rho_{\mathcal{D}} \) of gradient descent on \( \mathcal{D}^j_d \) (Eq. 11);
4. Remove the \( \mathcal{K} \) least persistent points from each atom \( a_i \).

\section{Algorithm}

This section presents our overall algorithm for the resolution of the optimization formulated in Sec. 3. Sec. 4.1 details our initialization strategy. Our overall multi-scale scheme is presented in Sec. 4.2. Finally, shared-memory parallelism is discussed in Sec. 4.3.

\subsection{Initialization}

Our strategy for the initialization of the Wasserstein dictionary \( \mathcal{D} \), illustrated in Fig. 6, is inspired by the celebrated \textit{k-means++} strategy [21]. Specifically, we iteratively select the \( m \) atoms among the \( N \) input diagrams. At the first iteration, we select as first atom the diagram which maximizes the sum of its Wasserstein distances (Eq. 1) to all the input diagrams (cyan point in Fig. 6). Next, each iteration selects as the next atom the diagram which maximizes the sum of its Wasserstein distances to all the previously selected atoms. This process stops when the desired number of atoms, \( m \),
Wasserstein barycenter optimization. Specifically, given an input
would occur for instance with a per-ensemble normalization).
would prevent the capture of variability in data ranges within the
which ensures that the non-atom points can indeed be expressed
(for instance by dividing it by 2 at each resolution), but the best
experimental results were obtained for the above decrease strategy.
The multi-resolution is illustrated in Fig. 7. In our experiments,
consider finer resolutions (taken from the
experimental results were obtained for the above decrease strategy.
Note that alternative strategies were considered for decreasing
the most salient features of the data. As detailed in Sec. 6.2, this
the optimization on the most persistent pairs, which correspond to
In real-life data, persistence diagrams tend to contain many low-
these are uniformly initialized (i.e. to 1
initial barycentric approximations. As for the barycentric weights,
point set, this initialization strategy has the nice property that it
line) are considered in the optimization.

4.2 Multi-scale optimization algorithm
In real-life data, persistence diagrams tend to contain many low-
persistence features, which essentially encode the noise in the data (see Fig. 1 right). In this section, we present a multi-scale
optimization strategy which addresses this issue by prioritizing
the optimization on the most persistent pairs, which correspond to
the most salient features of the data. As detailed in Sec. 6.2, this
strategy leads the optimization to solutions of improved energy in
comparison to a naive (non-multi-scale) approach.

Our multi-scale strategy consists in iterating our optimization
procedure by progressively increasing the resolution (in terms of persistence) of the input diagrams. This is inspired by the
progressive strategy by Vidal et al. [102] for the problem of
Wasserstein barycenter optimization. Specifically, given an input
diagram $X$, let $\Delta f$ be the span in scalar values in the corresponding
ensemble member $f$ (i.e. $\Delta f = \max_{v \in \mathbb{R}} f(v) - \min_{v \in \mathbb{R}} f(v)$). Given a threshold $\tau \in [0, 1]$, we note $X_\tau = \{x \in X | d_x - b_x \geq \tau \Delta f\}$
the version of $X$ at resolution $\tau$. It is a subset of $X$ which contains
persistence pairs whose relative persistence is above $\tau$. Note
that the input diagrams are not normalized by persistence, which
would prevent the capture of variability in data ranges within the
ensemble. Instead, we normalize the above persistence threshold, by
expressing it as a fraction $\tau \in [0, 1]$ of the scalar field range $\Delta f$.

Then, our multi-scale optimization will first consider the
input diagrams at a resolution $\tau_0$ and then will progressively
consider finer resolutions $\tau_1, \ldots, \tau_r$ until the full diagrams are
considered at $\tau_r = 0$. This multi-resolution strategy, based on
a per-diagram normalized persistence threshold ($\tau \in [0, 1]$) prevents
diagrams from being empty in the early resolutions in case of
large variations in data range within the ensemble (which would
occur for instance with a per-ensemble normalization). The
multi-resolution is illustrated in Fig. 7. In our experiments,
we set $\tau_0 = 0.2$ and decrease $\tau$ by 0.05 at each resolution (i.e. $\tau_1 = 0.15, \tau_2 = 0.10, \tau_3 = 0.05, \tau_4 = 0$). At each resolution,
the solution for the previous resolution is used as an initialization.
Note that alternative strategies were considered for decreasing $\tau$
(for instance by dividing it by 2 at each resolution), but the best
experimental results were obtained for the above decrease strategy.

Algorithm 1: Multi-scale Wasserstein Dictionary Optimization.

| Input: | Set of persistence diagrams $\{X_1, \ldots, X_N\}$; |
| Output 1: | Wasserstein Dictionary $\mathcal{D}$; |
| Output 2: | Barycentric weights $\lambda_1^*, \ldots, \lambda_N^*$; |
| for $r \in \{0, \ldots, r\}$ do |
| if $\tau = \tau_0$ then |
| Initialization Sec. 4.1; |
| while $E_D$ (Eq. 2) decreases do |
| for $n \in \{1, \ldots, N\}$ do |
| Perform a gradient step $\rho_n^{\lambda_n}$ along $VE_{\lambda_n}$ relative to $X_n$ Sec. 3.2; |
| end |
| for $n \in \{1, \ldots, N\}$ do |
| Perform a gradient step $\rho_{\lambda_n}$ along $VE_{\lambda_n}$ relative to $X_n$ Sec. 3.3; |
| end |

Alg. 1 summarizes our overall approach. For each sub-
optimization (i.e. weight and atom optimization), although each
gradient step is guaranteed to decrease the corresponding energy
(see the end of Secs. 3.2 and 3.3), this is only true for fixed assignments (between a diagram $X$ and its barycentric
approximation as well as between the barycentric approximation and the atoms). Since the assignments can change along the
iterations of the optimization, the overall energy $E_D$ (Eq. 2)
may increase between consecutive iterations. Hence, pragmatic
stopping conditions need to be considered. In practice, if $E_D$ has
not decreased for more than 10 iterations, we return the solutions $\lambda^*$ and $\mathcal{D}$, reached by the optimization with the lowest energy $E_D$.

4.3 Parallelism
Our approach can be trivially parallelized with shared-memory
parallelism. First, its most computationally demanding task, the $N$
barycentric approximations of the input diagrams can be computed
independently. Thus, for each barycentric approximation, we use
one parallel task per input diagram. Next, the estimation of the gradient of $E_{\lambda}$ (Sec. 3.2) is done on a per input diagram basis,
independently. Thus, we use one parallel task per input diagram. Regarding the estimation of the gradient of $E_{\lambda}$ (Sec. 3.3), given a
barycentric approximation $Y(\mathcal{D})$ of an input diagram $X$, each of its points $y(\mathcal{D})$ defines independently a pointwise version of the
gradient of the atom energy (see the last paragraph of Sec. 3.3).
Thus, we use one parallel task per point $y(\mathcal{D})$ of a barycentric
approximation $Y(\mathcal{D})$ of an input diagram $X$.

5 Applications
This section illustrates the utility of our approach in concrete visualization tasks: data reduction and dimensonality reduction.

5.1 Data reduction
Like any data representation, persistence diagrams can benefit from
lossy compression. This can be useful in in-situ [17] use-cases, where
time-steps are represented on permanent storage with topological
signatures [17]. In such scenarios, lossy compression is useful to
facilitate the manipulation (i.e. storage and transfer) of the resulting
ensemble of persistence diagrams. We present now an application to
data reduction where the input ensemble of persistence diagrams is
compressed, by only storing to disk:
(i) the Wasserstein dictionary of persistence diagrams $\mathcal{D}$, and
(ii) the $N$ barycentric weights $\lambda_1^*, \ldots, \lambda_N^*$.

The compression quality can be controlled with two input
parameters (i) the number of atoms $m$ and (ii) the maximum $S_m$
Fig. 8. Visual comparison (left) between the input persistence diagrams (top insets, saddle-maximum persistence pairs only) and our compressed diagrams (bottom insets, Sec. 5.1, saddle-maximum persistence pairs only) for three members of the *Isabel* ensemble (one member per ground-truth class). For each member, the sphere color encodes the matching between the input and the compressed diagrams (for the meaningful persistence pairs, above 10% of the function range). This visual comparison shows that the main features of the diagrams (encoding the main hurricane wind gusts in the data) are well preserved by the data reduction, especially for the members coming from the cluster 2, for which a lower relative reconstruction error ($Err$) can be observed. The planar overview of the ensemble (right) generated by our dimensionality reduction (Sec. 5.2) enables the visualization of the relations between the different diagrams of the ensemble. Specifically, this illustration shows a larger disparity for two clusters.

Fig. 9. Visual comparison (left) between the input persistence diagrams (top insets) and our compressed diagrams (bottom insets, Sec. 5.1) for four members of the *Ionization front (3D)* ensemble (one member per ground-truth class). The color encoding is the same as in Fig. 8. This visual comparison shows that the main features of the diagrams (the extremities of the ionization front) are well preserved by the data reduction, especially for the members coming from the clusters 2 and 3, for which a lower reconstruction error ($Err$) can be observed. The planar overview of the ensemble (right) generated by our dimensionality reduction (Sec. 5.2) enables the visualization of the relations between the diagrams of the ensemble. Specifically, it shows a larger disparity for the clusters 0 and 1 (spread out purple and pink spheres), which are also the most difficult to reconstruct.

The reconstruction error (given by the energy $E_D$, Eq. 2) will be minimized for large values of both parameters, while the compression factor will be maximized for low values. In our data reduction experiments, we set the number of atoms $m$ to the number of ground-truth classes of each ensemble, as documented in the ensemble descriptions [79]. Moreover, we set $S_m$ to $c_f^{-1} \sum_{i=1}^{N} |X_n|$, where $c_f$ is a target compression factor and $|X_n|$ is the number of non-diagonal points in the input diagram $X_n$ (see Sec. 6.2 for a quantitative evaluation).

Fig. 8 (left) provides a visual comparison between the diagram compressed with this strategy (bottom insets) and the original diagram (top insets), for three members of the *Isabel* ensemble. This experiment shows that diagrams can be significantly compressed ($c_f = 5.49$), while still faithfully encoding the main features of the data. Fig. 9 (left) provides a similar visual comparison for the *Ionization front (3D)* ensemble ($c_f = 2.9$).

We have applied our data reduction approach to topological clustering [102], where the main trends within the ensemble are identified by clustering the ensemble members based on their persistence diagrams. For the large majority of our test ensembles, the outcome of the clustering algorithm [102] was identical when used with the input diagrams or our compressed diagrams (Sec. 6.3 documents a counter-example). This confirms the viability and utility of our data reduction scheme.

### 5.2 Dimensionality reduction

Our framework can also be used to generate low-dimensional layouts of the ensemble, for its global visual inspection. Specifically, we generate 2D planar layouts by using $m = 3$ atoms and by embedding our Wasserstein dictionary $D^*$ as a triangle in the plane, such that its edge lengths are equal to the Wasserstein distances between the corresponding atoms. Next, each diagram $X$ of the input ensemble is embedded as a point in this triangle by using its barycentric weights $\lambda^*$ as barycentric coordinates.

As illustrated in Figs. 8 (right) and 9 (right), our dimensionality reduction provides a planar overview of the ensemble which groups
6 RESULTS

This section presents experimental results obtained on a computer with two Xeon CPUs (3.2 GHz, 2x10 cores, 96GB of RAM). The input persistence diagrams were computed with the Discrete Morse Sandwich algorithm [41]. We implemented our approach in C++ (with OpenMP), as modules for TTK [58], [12]. Experiments were run on the benchmark of public ensembles [78] described in [79], which includes simulated and acquired 2D and 3D ensembles from previous work and past SciVis contests [68]. The considered type of persistence pairs (i.e. the index of the corresponding critical points, Sec. 2.1) was selected on a per-ensemble basis, depending on the features of interest present in the ensemble. All types of pairs (i.e. minimum-saddle pairs, saddle-saddle pairs and saddle-maximum pairs) were considered for the following ensembles: Cloud processes, Isabel, Starting Vortex, Sea Surface Height, Vortex Street. Only the persistence pairs including extrema were considered for the ensembles Ionization front (2D) and Ionization front (3D). Finally, only the persistence pairs containing maxima were considered for the remaining ensembles: Asteroid Impact, Dark Matter, Earthquake, Viscous Fingering, Volcanic Eruptions.

6.1 Time performance

The most computationally expensive part of our approach is the computation of the N Wasserstein barycenters, for which we use the algorithm by Vidal et al. [102]. Each iteration of barycenter optimization approximatively requires $O(mK^2)$ steps in practice (where K is the size of the augmented diagrams, cf. Sec. 2.2). As discussed in Sec. 4.3, each barycenter is computed in parallel. The evaluations of the gradient of the weight energy (Sec. 3.2) and the atom energy (Sec. 3.3) both require $O(NmK)$ steps. As described in Secs. 3.2 and 3.3, both evaluations can be run in parallel.

Table 1 evaluates the practical time performance of our multiscale algorithm for the optimization of the Wasserstein dictionary. In sequential, the runtime is roughly a function of the number of input diagrams (N) as well as their average size ($|X|$). The parallelization of our algorithm (with 20 cores) induces a significant speedup (up to 18 for the largest ensembles), resulting in an average execution time below 5 minutes, which we consider to be an acceptable pre-processing time, prior to interactive exploration. In comparison to the principal geodesic analysis of persistence diagrams (Tab. 1 of [80]), on a per ensemble basis, our approach is 1.56 times faster on average (on the same hardware).

6.2 Framework quality

Table 2 reports compression factors and average relative reconstruction errors for our application to data reduction (Sec. 5.1). For each ensemble, the compression factor is the ratio between the storage size of the input diagrams and that of the Wasserstein dictionary $\mathcal{D}$, (the m atoms, of average size $|a|$, plus the N sets of barycentric weights). The relative reconstruction error is obtained by considering the Wasserstein distance between an input diagram and its barycentric approximation, divided by the maximum pairwise Wasserstein distance observed in the input ensemble. Then this relative reconstruction error is averaged over all the diagrams of the ensemble. Tab. 2 compares a naive optimization (Sec. 3) to our multi-scale strategy (Sec. 4.2). Specifically, for a given ensemble, the same target compression factor was used for both approaches (by imposing the same upper boundary on the total size of the atoms, Sec. 5.1). Tab. 2 shows that our multi-scale strategy (Sec. 4.2) enables the optimization to progress towards better solutions, as assessed by the improvement in reconstruction error of 30% on average. In comparison to the principal geodesic analysis of persistence diagrams (Appendix D of [80]), for the same compression factors, the error induced by our approach is on average 1.79 times larger. However, our approach is simpler, more flexible (our optimization is not subject to restrictive constraints, such as geodesic orthogonality) and slightly faster (Sec. 6.1).

Fig. 10 provides a visual comparison between the 2D layouts obtained with our approach on the Isabel ensemble and those obtained with two typical dimensionality reduction techniques, namely MDS [54] and tSNE [101], directly applied on the distance matrix obtained by computing the Wasserstein distance between all the pairs of input diagrams. For a given technique, to quantify the diagrams of the ensemble, Tab. 2 compares a naive optimization (Sec. 3) to our multi-scale strategy (Sec. 4.2). Specifically, for a given ensemble, the same target compression factor was used for both approaches (by imposing the same upper boundary on the total size of the atoms, Sec. 5.1). Tab. 2 shows that our multi-scale strategy (Sec. 4.2) enables the optimization to progress towards better solutions, as assessed by the improvement in reconstruction error of 30% on average. In comparison to the principal geodesic analysis of persistence diagrams (Appendix D of [80]), for the same compression factors, the error induced by our approach is on average 1.79 times larger. However, our approach is simpler, more flexible (our optimization is not subject to restrictive constraints, such as geodesic orthogonality) and slightly faster (Sec. 6.1).

![Fig. 10. Comparison between the 2D layouts obtained with our approach (W2-Dict) and those obtained with two typical dimensionality reduction techniques, namely MDS [54] and tSNE [101], directly applied on the distance matrix obtained by computing the Wasserstein distance between all the pairs of input diagrams. For a given technique, to quantify](image-url)
Fig. 11. Comparison between the 2D layouts obtained with our approach (W2-Dict) and these obtained with typical dimensionality reduction approaches (W2-MDS [54], W2-tSNE [101]) on a challenging ensemble. In this example (Asteroid Impact), the presence of an outlier (time step of the actual impact, red entry in the distance matrix, left) challenges cluster preservation. While W2-tSNE provides the best cluster preservation scores (NMI/ARI), it fails at visually depicting the outlier (red circle) as being far away from the other ensemble members. In contrast, W2-MDS and W2-Dict do a better job at isolating this outlier (red circle), with W2-Dict providing slightly improved cluster preservation scores (NMI/ARI).

Table 3

<table>
<thead>
<tr>
<th>Dataset</th>
<th>W2-MDS</th>
<th>W2-tSNE</th>
<th>W2-Dict</th>
</tr>
</thead>
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<tr>
<td>Asteroid Impact (3D)</td>
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<td>0.86</td>
<td>0.49</td>
</tr>
<tr>
<td>Dark Matter (3D)</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Earthquake (3D)</td>
<td>0.65</td>
<td>0.65</td>
<td>0.65</td>
</tr>
<tr>
<td>Ionization Front (3D)</td>
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<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Isabel (3D)</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Viscous Fingering (3D)</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Cloud Processes (2D)</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Ionization Front (2D)</td>
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<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Sea Surface Height (2D)</td>
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<td>1.00</td>
</tr>
<tr>
<td>Starting Vortex (2D)</td>
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<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Street Vortex (2D)</td>
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<td>1.00</td>
</tr>
<tr>
<td>Volcanic Eruption (2D)</td>
<td>0.66</td>
<td>1.00</td>
<td>0.66</td>
</tr>
</tbody>
</table>

Fig. 12 reports the evolution of the normalized energy $E_D$ along the optimization for all test ensembles, for the naive optimization strategy (Sec. 3), by using a number of atoms equal to the number of ground-truth classes (cf. our application to data reduction, Sec. 5.1). In this figure, the energy is normalized on a per ensemble basis, based on its initial value. This figure shows that the energy does decrease for most ensembles, but still with large oscillations due to the non-convex nature of the dictionary energy $E_D$. In contrast, the energy evolution with our multi-scale strategy (Fig. 13) results in much less oscillations, which indicates the ability of this strategy to help the optimization explore in a more stable manner the locally convex areas of the energy (Appendix D discusses a counter-example). Specifically, in Fig. 13, one can observe sequences of discontinuous decrease patterns, characterized by an abrupt drop followed by a plateau. Each of these patterns corresponds to one persistence scale of our multi-scale strategy (this is particularly apparent on the Cloud Processes ensemble).

Fig. 14 provides a closer comparison between the two strategies on a selection of four ensembles. The Cloud Processes ensemble is an example where the naive optimization reaches a solution of slightly lower energy. For the other ensembles, our multi-scale strategy leads to solutions of much lower energy, visually confirming the conclusions of Tab. 2. In this figure, one can also observe the characteristic decrease patterns discussed above, particularly apparent on the Ionization Front (3D) ensemble, which correspond to the distinct scales of our multi-scale strategy.
6.3 Limitations

Similarly to other optimization problems based on topological descriptors \cite{79, 80, 100, 102}, our energy is not convex. Additionally, as shown in Fig. 12, the interleaving of the weight optimization (Sec. 3.2) with atom optimization (Sec. 3.3) can even lead to oscillations in the energy. As discussed in Sec. 6.2, our multi-scale strategy (Sec. 4.2) greatly mitigates both issues, with a more stable optimization than a naive approach (Sec. 3), which leads to relevant solutions which are exploitable in the applications (Sec. 5). However, we have found one example in our test ensembles (the Sea Surface Height ensemble), where our multi-scale strategy reached solutions which were arguably worse than these obtained with a naive solution, as described in details in Fig. 15. In this example, the most persistent features in the diagrams are not particularly discriminative for the separation of the ground-truth classes. On the contrary, the variations between these classes seem mostly encoded by the low persistence features: in Fig. 15 clear separations in the distance matrices between the ground-truth classes only start to occur in the latest persistence scales (dashed sub-matrices, top right inset). This counter-intuitive observation goes against the rule of thumb traditionally used in topological data analysis, which states that the most persistent pairs encode the most important features in the data. For this example, when applying our framework to dimensionality reduction, the non-discriminative aspect of the early persistence scales eventually lead our multi-scale strategy towards a local minium which does not separate the ground-truth classes well (planar layout, bottom left) in
comparison to the naive strategy (planar layout, bottom right). Thus, for this ensemble, we reported dimensionality reduction results (Tab. 3, Appendix C) obtained with the naive optimization. In general, this means that when users are confronted with ensembles where the most persistent pairs are not the most responsible for data variability (hence class separation), the naive optimization may need to be considered additionally as it might provide solutions which better encode the ground-truth classes.

Finally, as detailed in Appendix D, the presence of clear outliers can also challenge our optimization, especially when the selected number of atoms equals the number of ground-truth classes. Then, in this case, the best dictionary encoding will consequently be obtained by increasing the number of atoms, specifically, by considering that each outlier forms a singleton class.

7 Conclusion

In this paper, we presented an approach for the encoding of linear relations between persistence diagrams, given the Wasserstein metric. Specifically, we introduced a dictionary-based representation of an ensemble of persistence diagrams, inspired by previous work on histograms [90]. We first documented a naive optimization which interleaves the optimization of the barycentric weights of the input diagrams with the optimization of the atoms of the dictionary (Sec. 3). Then, we presented a multi-scale strategy (Sec. 4.2) leading to more stable optimizations and relevant solutions (Sec. 6.2). We demonstrated the utility of our contributions in applications (Sec. 5) to data reduction and dimensionality reduction, where the visualizations generated by our framework enable the visual identification of the main trends in the ensembles (Figs. 8, 9), and the quick identification of outliers (Fig. 11). In contrast to previous work on persistence diagram encoding [80], our framework is simpler, less constrained and slightly faster in practice.

A natural direction for future work is the extension of our framework to other topological descriptors such as Reeb graphs or Morse-Smale complexes. However, this requires the definition of key geometrical tools, such as geodesic or barycenter computation algorithms, which is still an active research problem. We believe our framework for the dictionary encoding of persistence diagrams is an interesting practical step for the analysis of collections of persistence diagrams. In the future, we will continue our investigation of the adaptation of tools from optimal transport to the analysis of ensembles of topological descriptors, as we believe it can become a key solution in the long term for the advanced analysis of large-scale ensembles.

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References


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We suppose the optimal matchings to be constant, thus we write $\nabla$. This also shows that $\nabla$. For the following part we denote $H_j = \sum_{i=1}^{m} \lambda_i (a_i^{(j)} - \psi^{(j)})$. The Hessian then writes as $H = H(\lambda) = 2 \sum_{j=1}^{K} (H^j)^T H^j$. This shows that $\lambda \mapsto W^2(Y(\lambda), X)$ is convex. Indeed for $u \in \mathbb{R}^m$ we have:

$$u^T H u = 2 \sum_{j=1}^{K} u^T (H^j)^T (H^j) u = 2 \sum_{j=1}^{K} \|H^j u\|^2 \geq 0$$

This also shows that $\nabla E_W$ is $L$-Lipschitz with $L = \|H\|$. For numerical reasons, we bound $L$ as follows:

$$L = \|H\| = 2 \sum_{j=1}^{K} \|H^j\|^2 \geq 2 \sum_{j=1}^{K} \|H^j\|^2 = 2 \sum_{j=1}^{K} \|H^j\|^2.$$ 

Thus for our algorithm, we consider the following gradient step:

$$\rho \leq \left(2 \sum_{j=1}^{K} \|H^j\|^2\right)^{-1}.$$
Fig. 16. Comparison of the planar layouts for typical dimensionality reduction techniques on all our test ensembles. The color encodes the classification ground-truth [79]. For each quality score, the best value appears bold. For the Sea Surface Height ensemble, the naive optimization procedure has been used (cf. Sec. 6.3 of the main manuscript).

Optimization results in few oscillations and a consistent energy decrease (yellow curve). This indicates that the outlier member (light purple) should be interpreted as a singleton class and that the best dictionary encoding will consequently be obtained with 4 atoms.
Fig. 17. Evolution of the (normalized) energy $E_D$ along the optimization (top curves), with our multi-scale strategy, for the Volcanic eruption ensemble, for distinct initializations. The ground-truth classification of this ensemble contains 3 classes [79], including one outlier (light purple entry in the bottom views, from left to right: terrain view of the data, aggregated birth/death space, distance matrix). A clear energy increase can be observed when considering the entire ensemble (black curve), while a more characteristic oscillating behavior occurs when discarding the outlier (green curve). When initializing the optimization with 4 atoms (1 per class, plus 1 for the outlier), the optimization results in few oscillations and a consistent energy decrease (yellow curve).