

A Topological Distance Between Multi-Fields Based On Multi-Dimensional Persistence Diagrams

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Abstract: The problem of computing topological distance between two scalar fields based on Reeb graphs or contour trees has been studied and applied successfully to various problems in topological shape matching, data analysis, and visualization. However, generalizing such results for computing distance measures between two multi-fields based on their Reeb spaces is still in its infancy. Towards this, in the current chapter we propose a technique to compute an effective distance measure between two multi-fields by computing a novel multi-dimensional persistence diagram (MDPD) corresponding to each of the (quantized) Reeb spaces. First, we construct a multi-dimensional Reeb graph (MDRG), which is a hierarchical decomposition of the Reeb space into a collection of Reeb graphs. The MDPD corresponding to each MDRG is then computed based on the persistence diagrams of the component Reeb graphs of the MDRG. Our distance measure extends the Wasserstein distance between two persistence diagrams of Reeb graphs to MDPDs of MDRGs. We prove that the proposed measure is a pseudo-metric and satisfies a stability property. Effectiveness of the proposed distance measure has been demonstrated in (i) shape retrieval contest data - SHREC 2010 and (ii) Pt-CO bond detection data from computational chemistry. Experimental results show that the proposed distance measure based on the Reeb spaces has more discriminating power in clustering the shapes and detecting the formation of a stable Pt-CO bond as compared to the similar measures between Reeb graphs.

Keywords: Topological Data Analysis; Multi-Field Topology; Reeb Space; MDRG; MDPD; Persistence Diagram

I. INTRODUCTION

Computing distance or similarity between a pair of shapes or data is an important problem in topological data analysis. The problem of computing distance measures using scalar topology has been studied extensively and proven useful in shape or data clustering, symmetry detection, and feature extraction [1,2]. However, not all features in a data can be described using the scalar topology. Therefore, developing new tools for computing multivariate or multi-field (consisting of multiple scalar fields) topology is indispensable [3, 4]. The Reeb space is one such topological structure that generalizes the Reeb graph, by generalizing the level set topology of a scalar field to capture the fiber topology of a multi-field [4].

Topological distances or similarities based on Reeb graphs, contour trees, and merge trees have been studied in the literature [5,6]. The persistence diagram is another important structure to capture the homological changes in the data under a filtration [7]. Bottleneck distance and its generalization Wasserstein distance are two topological distances between persistence diagrams which have been applied in various problems of topological data analysis and machine learning [8]. Recently, a stable functional distortion metric has been proposed between two Reeb graphs by Bauer et al. [9]. In the same paper, a bottleneck distance between two Reeb graphs has been introduced based on their persistence



diagrams. Moreover, it is known that the bottleneck distance is insensitive to the details of bijections between the persistence diagrams, whereas the Wasserstein distance is more appropriate to handle that [10]. However, extending such measures between two Reeb spaces is challenging as we require a multifiltration to describe the homological features of a Reeb space and no persistence diagram is known corresponding to a multifiltration. Towards this, our main contributions in the current chapter are as follows:

- **A multi-dimensional persistence diagram representation corresponding to a quantized Reeb space:** In Section I, we first decompose a quantized Reeb space or Joint Contour Net (JCN) into a multi-dimensional Reeb graph (MDRG). Then corresponding to each MDRG we define a *multi-dimensional persistence diagram* (MDPD) to capture the persistent features of the component Reeb graphs in the MDRG.
- **A distance measure between two quantized Reeb spaces:** Next, using the MDPD representation, we define a distance measure between two quantized Reeb spaces. Our distance is an extension of the distance between persistence diagrams of two Reeb graphs [9].
- **Properties of the distance measure:** We show that the proposed distance measure is a pseudo-metric and satisfies a stability property.
- **Complexity analysis:** We show the time complexity of computing the MDPD from a JCN and the complexity of computing the distance between two JCNs.
- **Applications in shape matching and data analysis:** In Section 5, we show the effectiveness of the proposed distance measure in two different domains: (i) A shape contest data SHREC 2010 - for clustering shapes and (ii) A Density Functional Theory (DFT) data from computational chemistry - for the detection of stable bond formation between Pt and CO molecules.

The chapter is organized as follows. In Section II, we discuss the related works. Section III describes the background to understand our proposed method. The main algorithm for computing the distance measure between two multi-fields, its properties, and the complexity analysis are discussed in Section IV. We show the experimental results using the proposed distance measure in Section V, which is followed by a conclusion in Section VI.

II. RELATED WORK

Various similarity and distance measures between scalar fields have been studied to analyze topological features in data. This has been facilitated by the development of tools for capturing topological features, such as contour trees, merge trees, Reeb graphs, extremum graphs, and persistence diagrams. A survey paper by Yan et al. [11] discusses various topological descriptors for the comparison of scalar fields. Various techniques for matching shapes based on topological features have been developed by different groups. Hilaga et al. [5] studied the matching of shapes by using a data-structure called multi-resolution Reeb graph. Zhang et al. [12] proposed a similarity measure based on dual-contour trees and applied it in the classification of protein structures into different categories. Fabio et al. [13] proposed an edit distance between Reeb graphs and showed its stability. Various distance measures between Reeb graphs such as functional distortion metric [9] and interleaving distance [14] have been developed which are stable under small perturbations of functions. However, the generalization of these techniques to multi-fields is a challenging task. Persistent Homology [15-16] provided a topological descriptor for capturing the persistent homological features of high-dimensional datasets based on persistence diagram. Cohen-Steiner et al. [18] proposed the bottleneck distance between persistence diagrams and proved it to be stable. Carriere et al. [17] showed that, locally, the bottleneck distance between Reeb graphs is as discriminative as the functional distortion and interleaving distances. Dey et al. [19] developed a stable distance measure between metric graphs based on persistence diagrams. Favelier et al. [20] proposed a persistence based framework for analysing clusters and trend variability in ensemble data.

Multi-field topology, being richer than scalar topology, captures more prominent features leading to a better understanding of data. Singh et al. proposed a *mapper* data-structure to capture the topology of high dimensional point cloud data. Edelsbrunner et al. proposed an algorithm for computing the Reeb space. Huettnerberger et al. extended the notion of topological structures for multi-fields based on the Pareto optimality and Pareto dominance, and demonstrated



their applicability in fluid-flow simulations. Carr et al. proposed the Joint Contour Net (JCN), which is a quantized approximation of the Reeb space. Duke et al. showed the effectiveness of JCN in visualizing nuclear scission using multivariate density functional theory (DFT) data. Chattopadhyay et al. proposed the multi-dimensional Reeb graph (MDRG), which is a hierarchical decomposition of the Reeb space into a set of Reeb graphs in different dimensions and applied this structure for multivariate topology simplification. Dey et al. developed the multi-scale mapper (MSM), which is a tower of simplicial complexes connected by simplicial maps, and proved its bottleneck-stability. Agarwal et al. proposed a distance between multi-fields based on their fiber-component distributions. Recently, Ramamurthi et al. proposed a similarity measure between multi-resolution Reeb spaces, and showed its effectiveness in detecting prominent features in multivariate DFT data. In Section 5, we compare the proposed method with distances based on fiber-component distributions, MSMs, and MRSs.

The theory of multiparameter persistence [17, 18] deals with the extension of one parameter persistence to multiparameter based on persistence modules. A survey paper by Botnan et al. [14] gives a good overview of the recent developments in this direction. Recently, Dey et al. [15] presented an algorithm for the decomposition of the multiparameter persistence module into indecomposables, which are the counterparts of the bars in the case of one-parameter persistence modules. However, the time complexity for computing the decomposition of a multiparameter persistence module corresponding to a simplicial filtration consisting of $|s|$ simplices, is at least $O(|s|^4)$. To address this issue, Loiseaux et al. introduced a technique that can compute an approximate decomposition for multiparameter persistence modules in lesser time. Some invariants of persistence modules have been developed, such as the Hilbert function, the rank invariant, and multigraded Betti numbers. Scaramuccia et al. introduced a technique for computing multiparameter persistent homology based on *discrete MorseTheory*. Carrière et al. developed a descriptor for multiparameter persistence modules by generalizing the *persistence image* of a persistence diagram.

III. PERSISTENCE DIAGRAM AND REEB GRAPH

The persistence diagram is a topological descriptor that captures the topology of a scalar field f through a multiset of points in $\mathbb{R}^2$, where $\mathbb{R} = \mathbb{R} \cup \infty$. Each point in a persistence diagram of a fixed dimension encodes the birth and death of a homological feature of that dimension. In particular, connected components are 0-dimensional features and loops are 1-dimensional features. A point (a, b) in a persistence diagram indicates that a homological feature is born at ' a ' and dies at ' b ', and its persistence is given by $b - a$. We refer the reader to Appendix B.2 for a detailed description of persistence diagrams.

The persistence diagram corresponding to the Reeb graph of a scalar field is useful in identifying significant features from the Reeb graph. Consider the metaphor of a mountain range, where elevation on earth can be taken as a scalar field [2]. Then each peak corresponds to an arc in the Reeb graph, and a point in the associated persistence diagram. The persistence of a point indicates the prominence of the peak, i.e. the height of its summit above the lowest contour line which encompasses it but doesn't enclose a higher peak. In particular, peaks with higher prominence correspond to points with higher persistence. Further, the persistence diagram provides a compact representation for a Reeb graph, and the computation of distances between Reeb graphs based on their persistence diagrams is more tractable than directly comparing Reeb graphs.

The persistent homological features of a Reeb graph RG_f can be encoded in 0- and 1-dimensional persistence diagrams [6]. The 0-th ordinary persistence diagram $Dg_0(RG_f)$ encodes the birth and death of sublevel set components in a filtration. The 0th extended persistence diagram $ExDg_0(RG_f)$ captures the range of the function f and the 1-st extended persistence diagram $ExDg_1(RG_f)$ captures the loops in RG_f . We use the notation $PD_0(RG_f)$ to denote the union of $Dg_0(RG_f)$ and $ExDg_0(RG_f)$, excluding the point with infinite persistence in $Dg_0(RG_f)$. Finally, we obtain a single persistence diagram $PD(RG_f)$ by taking the union of $PD_0(RG_f)$ and $ExDg_1(RG_f)$ which is used for computing the multi-dimensional persistence diagram. Figure 1 illustrates the construction of $PD(RG_f)$ from a Reeb graph. We refer the reader for further details on the construction of the persistence diagrams corresponding to a Reeb graph.



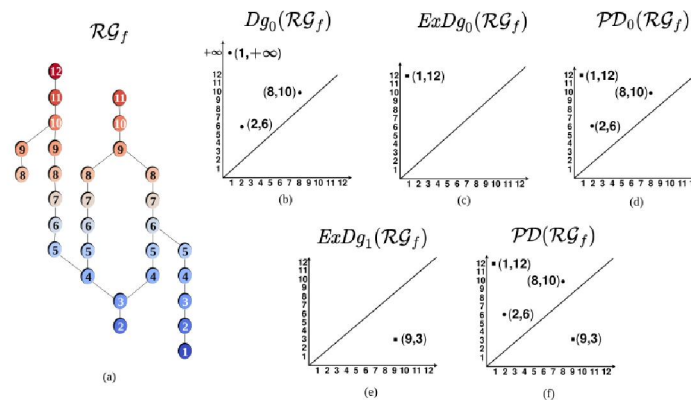


Figure 1 Reeb graph of a real-valued function f .

IV. PROPOSED ALGORITHM

Analysing persistent features in data across multiple parameters can yield deeper insights into it. For instance, consider investigating temperature patterns in mountain ranges. The temperature at a particular point depends both on its latitude and elevation (altitude). The latitude influences the angle of sunlight it receives. Locations near the equator receive sunlight more directly, resulting in higher temperatures. Conversely, the polar regions receive sunlight at a more oblique angle, which generally leads to cooler temperatures. Similarly, as altitude increases, temperature typically decreases.

Consequently, mountaintops are generally cooler than their bases. The persistence diagram corresponding to the Reeb graph of the elevation field captures peaks along with their prominence. A point (a, b) in the persistence diagram represents a peak with base altitude a and summit altitude b . Within the altitudes spanning between a and b , the variation of latitudes along various peaks can be captured by persistence diagrams (of the Reeb graphs) corresponding to the latitudes. The persistent features of both the altitude and latitude can jointly be represented in an MDPD. This consolidated representation can then be utilized in examining how temperature depends on both of these parameters.

Consider the MDRG of the bivariate field $\mathbf{f} = (f_1, f_2)$, denoted by $\text{MDRG}\mathbf{f}$, as defined in equation. $\text{MDRG}\mathbf{f}$ consists of Reeb graphs $\text{RG}f_1$ and $\text{RG}f_2$ for $p \in \text{RG}f_1$. We obtain the persistence diagram $\text{PD}(\text{RG}f_1)$ corresponding to $\text{RG}f_1$ and the persistence diagram $\text{PD}(\text{RG}f_2)$ corresponding to $\text{RG}f_2$ for each $p \in \text{RG}f_1$, as described in Section 4.3.5. For a birth-death point $x_1 = (a_1, b_1) \in \text{PD}(\text{RG}f_1)$, its *persistence interval* is defined as $pl(x_1) = [\min\{a_1, b_1\}, \max\{a_1, b_1\}]$. We note, $\text{PD}(\text{RG}f_1)$ consists of both 0- and 1-dimensional persistent features. For 0-dimensional persistent features, birth is less than death, whereas, birth is greater than death for 1-dimensional persistent features. Intuitively, an MDPD corresponding to an MDRG of a bivariate field, captures the persistent features of its Reeb graphs in various dimensions, jointly. More explicitly, with each persistent feature x_1 in the persistence diagram corresponding to the Reeb graph in the first dimension, the MDPD associates the persistent features of the second-dimensional Reeb graphs that occur within the life span of x_1 .

Algorithm: Construct-MDPD

Input: PL bivariate field $\mathbf{f} = (f_1, f_2): M \rightarrow \mathbb{R}^2$

Output: Multi-Dimensional Persistence Diagram $\text{MDPD}\mathbf{f}$

1. Compute $\text{RG}f_1 \leftarrow \text{ReebGraph}(f_1)$
2. Initialize $\text{MDPD}\mathbf{f} \leftarrow \emptyset$
3. For each point $p_1 \in \text{RG}f_1$ do
4. Identify contour C_p corresponding to p_1



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5. Define restricted field:
    $\tilde{f}_2p1 \leftarrow f_2 \mid C_p$ 
6. Compute component Reeb graph:
    $RGp1 \leftarrow \text{ReebGraph}(\tilde{f}_2p1)$ 
7. Compute persistence diagram:
    $PDp1 \leftarrow \text{PersistenceDiagram}(RGp1)$ 
8. For each persistence pair  $(b,d) \in PDp1$  do
9. Add  $(p1,b,d)$  to  $MDPDF$ 
10. End For
11. End For
12. Return  $MDPDF$ 

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V. EXPERIMENTAL RESULTS

The accuracy of a distance measure is measured based on the standard evaluation techniques Nearest Neighbour (NN), First Tier (FT), Second Tier (ST), E-measure, and Discounted Cumulative Gain (DCG). These techniques take a distance matrix consisting of the distances between all pairs of shapes as input and return a value between 0 and 1, where higher values indicate better accuracy. We provide a short description of these measures here and refer the readers to Shilane et al. [10], for more details. NN is the percentage of the closest matches that belong to the same query class. FN and SN represent the percentage of the number of models belonging to the query class that appear within the top K retrieved models. For FN, K is set as $|C| - 1$ and for SN, K is set as $2 \cdot (|C| - 1)$, where $|C|$ is the size of the query class. For each query model in class C and any number of retrieved models K , precision represents the percentage of the number of retrieved models belonging to class C , while recall indicates the ratio of the number of models in class C returned within the K retrieved models.

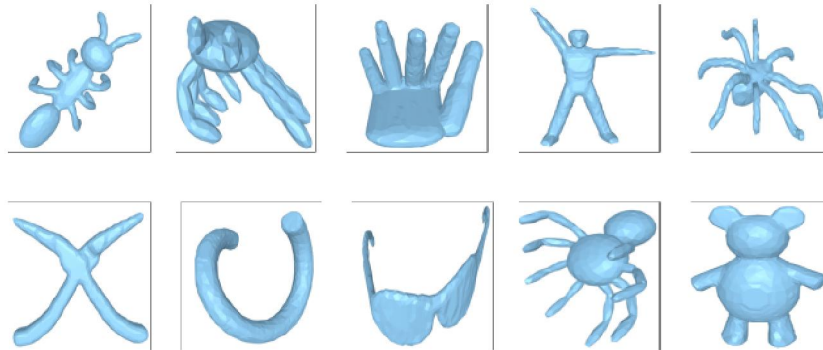


Figure 2: Collection of shapes from SHREC 2010.



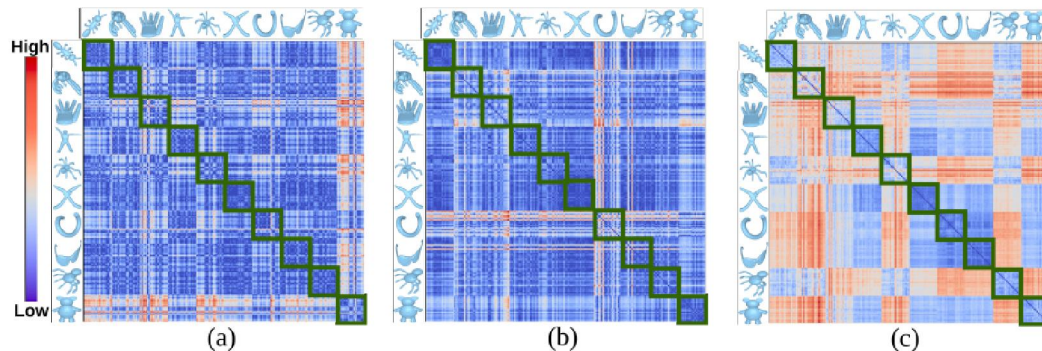


Figure 3: Wasserstein distance between all pairs of shapes in SHREC 2010 dataset. (a) Distance matrix computed using Reeb graphs of μ_n . (b) Distance matrix computed using Reeb graphs of $d2n$. (c) Distance matrix computed using the MDRG of the bivariate field $(\mu_n, d2n)$. later in the list.

The SHREC 2010 dataset consists of 200 watertight shapes classified into 10 categories. A sample of the shapes is shown in Figure 2. Each of the meshes is simplified into 2000 faces. First, we show the significance of the proposed distance between MDRGs of bivariate fields over the Wasserstein distance between Reeb graphs of scalar fields in differentiating between various classes of shapes in this dataset.

Table 1: SHREC 2010 dataset: Performance of the Wasserstein distance between Reeb graphs of scalar fields and the Wasserstein distance between MDRGs of the bivariate field.

Fields	NN	1-Tier	2-Tier	e-Measure	DCG
μ_n	0.2100	0.2308	0.3942	0.2580	0.5520
$d2_n$	0.2700	0.2039	0.3484	0.2290	0.5444
$(\mu_n, d2_n)$	0.9000	0.6076	0.8084	0.5661	0.8677

We compare the performance of the proposed method using the bivariate field $(\mu_n, d2n)$ with the performances using the bivariate fields obtained from Heat Kernel Signature (HKS) and Wave Kernel Signature (WKS). The HKS at a point on the shape is defined as the amount of heat that remains after time t . In our experiment, Table 1: SHREC 2010 dataset: Comparison of Wasserstein distance between persistence diagrams of MSMs, approximate matching distance between bi-filtered JCNs, distance between fiber-component distributions, distance between MRSs, and Wasserstein distance between MDRGs using the bivariate field $(\mu_n, d2n)$.

Table 2 Comparative Analysis of Different Method

Methods	NN	1-Tier	2-Tier	e-Measure	DCG
MSM	0.5500	0.3374	0.5166	0.3529	0.6580
MatchingDistance	0.1700	0.1121	0.2187	0.1288	0.4715
Histogram	0.6600	0.3347	0.4908	0.3325	0.6874
MRS	0.7600	0.4634	0.6682	0.4596	0.7740
MDRG	0.9000	0.6076	0.8084	0.5661	0.8677

Table 3: SHREC 2010 dataset: Performance of the bivariate fields obtained from HKS, WKS, and the bivariate field $(\mu_n, d2n)$, based on the Wasserstein distance between MDRGs.

Fields	NN	1-Tier	2-Tier	e-Measure	DCG
HKS	0.8500	0.5150	0.7095	0.4914	0.8000
WKS	0.7700	0.3871	0.5421	0.3745	0.7336
$(\mu_n, d2_n)$	0.9000	0.6076	0.8084	0.5661	0.8677



we consider a bivariate field by computing the HKS corresponding to the first two values of t , in the discrete temporal domain. The WKS represents the average probabilities of measuring quantum particles of different energy levels at a point in the shape. In our experiment, we consider the WKS corresponding to the two smallest energy levels as a bivariate field. We assess the performance of HKS and WKS using the standard evaluation measures, and the results are presented in Table 3. It can be seen that the proposed method using the bivariate field ($\mu_n, d2n$) is more effective than HKS and WKS.

VI. CONCLUSION

In this chapter, we have proposed the multi-dimensional persistence diagram corresponding to an MDRG of a quantized Reeb space. Based on this, we have developed a novel distance measure between two multi-fields by extending the Wasserstein distance between two Reeb graphs. The proposed distance measure is a pseudo-metric and is shown to satisfy a stability property. We observed the discriminating power of the proposed method in the SHREC 2010 dataset. Its effectiveness is also shown in a computational chemistry dataset through the detection of the stable bond formation between Pt and CO molecules. The proposed method is seen to perform better as compared to other related topological techniques in the literature. However, the MDRG and consequently the MDPD structures corresponding to a multi-field depend on the field orderings, although the overall topology of the Reeb space, they capture, remains the same. However, to define a topological distance between two multi-fields or Reeb spaces that is independent of the field orderings one needs to find a generalization of the persistence diagram for a multi-filtration which is an open problem. Furthermore, the worst-case time complexity of computing the Wasserstein distance using the Hungarian algorithm is cubic on the number of points in the persistence diagrams. One can try using the Auction algorithm to improve the performance which should be addressed in a future work. We note, computing the multi-dimensional persistent features of a Reeb space dispensing with the quantization of the joint contour net is a challenging open problem. In the next chapter, we introduce an algorithm for computing a net-like structure corresponding to the Reeb space of a piecewise-linear bivariate field which is independent of the range quantization.

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