Geodesic Properties of a Generalized Wasserstein Embedding for Time Series Analysis

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Abstract
Transport-based metrics and related embeddings (transforms) have recently been used to model signal classes where nonlinear structures or variations are present. In this paper, we study the geodesic properties of time series data with a generalized Wasserstein metric and the geometry related to their signed cumulative distribution transforms in the embedding space. Moreover, we show how understanding such geometric characteristics can provide added interpretability to certain time series classifiers, and be an inspiration for more robust classifiers.

1. Introduction
Transport-based distances, such as Wasserstein distances (Villani, 2003), have been shown to be an effective tool in signal analysis and machine learning applications including image retrieval (Rubner et al., 2000) and registration (Haker et al., 2004), modeling biological morphology (Ozolek et al., 2014; Basu et al., 2014), comparing probability distributions (Arjovsky et al., 2017), and providing good low-dimensional embeddings of image manifolds (Hamm et al., 2022), to name a few. The success of transport-based distances are in part due to their ability to incorporate information of spatial or time deformations naturally structured in signals (Kolouri et al., 2017). For example, they are observed to correctly recover biologically interpretable and statistically significant differences (Basu et al., 2014) and quantify semantic differences between distributions that correlate well with human perception (Rubner et al., 2000).

Within the set of problems in data science, modeling of time series data is considered a challenging problem. Deformation-based methods such as dynamic time warping (Abanda et al., 2019; Lines & Bagnall, 2015) have been shown successful in enabling the comparison of time series data more meaningfully. In addition to being able to align features from two different time series, Wasserstein-type distances are also true distances that can allow for a low-dimensional representation of dynamical systems in which time series can be classified and statistically analyzed (Muskulus & Verduyn-Lunel, 2011). In recent years, many transport transform-based techniques have been developed to leverage Wasserstein distances and linearized ($L^2$) embeddings to facilitate the application of many standard data analysis (Kolouri et al., 2017). In particular, the cumulative distribution transform (CDT), based on the 1D Wasserstein embedding, was introduced in (Park et al., 2018) as a means of classifying normalized non-negative signals, and has been extended to general signed signals via the the signed cumulative distribution transform (SCDT) in (Aldroubi et al., 2022).

Wasserstein embeddings based on the cumulative distribution transform (CDT) (Park et al., 2018; Rubaiyat et al., 2020; Aldroubi et al., 2022) have recently emerged as a robust, computationally efficient, and accurate end-to-end classification method for time series (1D signal) classification. They are particularly effective for classifying data emanating from physical processes where signal classes can be modeled as observations of a particular set of template signals under some unknown, possibly random, temporal deformation or transportation (Park et al., 2018; Shifat-E-Rabbi et al., 2021; Rubaiyat et al., 2022b). Efforts have been made to explain the success of these models by understanding the geometry of the transform embedding space (Park et al., 2018; Aldroubi et al., 2021; Moosmüller & Cloninger, 2020), where embedding properties and conditions when the data class becomes convex and linearly separable in the transform space are studied. In a nutshell, the template-deformation-based generative models capture the nonlinear structure of signals and the nonlinear transport transforms render signal classes that are nonlinear and non-convex into convex sets in transform embedding space (see Figure 1).

As the CDT (Park et al., 2018) is defined for probability measures (or their associated density functions) which are non-negative and normalized, in this manuscript we elucidate the geometry of general time series (signed, non-normalized) with a generalized Wasserstein metric in the SCDT embedding space with a $L^2$-type metric. In addition to the convexity and isometric embedding properties of the SCDT (Aldroubi et al., 2022), which are shared by the CDT, we look at the geodesic properties of the SCDT and illustrate the differences between geometry of data in
CDT and SCDT space. In particular, the SCDT embedding $\tilde{S} \subseteq (L^2(s_0) \times \mathbb{R})^2$ is not a geodesic space while geodesics exist between signals in a generative model (see Figure 1). As a preliminary application, we provide an interpretation of the nearest (transform) subspace classifiers proposed in (Rubaiyat et al., 2022a; b) through visualizing paths between the test signals and their projections to various subspaces. In particular, we illustrate that using the training samples, these classifiers “correctly” generate a (local) subspace that models the generative clusters (see (9)) to which the given test signals belong. We hypothesise this knowledge can lead to the design of more efficient and accurate pattern recognition tools and added interpretability of various classifiers.

Figure 1. Space of time series with a generalized Wasserstein metric (top) and its embedding $\tilde{S}$ (bottom) are not geodesic spaces while geodesics exist between any pair of signals in the same generative cluster $S_{p,G}$. Here $\tilde{S}$ is represented as the faces of the polyhedron (see Remark 2.7 and 2.8) and its ambient space $(L^2(s_0) \times \mathbb{R})^2$ is represented as the open cube.

Throughout the manuscript, we work with $L^1$ signals $s$ with finite second moments, $^1$ where $\Omega_s \subseteq \mathbb{R}$ is the bounded domain over which $s$ is defined. We denote $S$ as the set of $L^1$ signals with finite second moments and $S_1$ as the set of non-negative $L^1$-normalized signals in $S$ and $\|s\|$ as the $L^1$-norm of $s$.

2. Transport Transforms and Geometric Properties of Time Series

We give a brief overview of the CDT and SCDT and their associated embedding properties in Section 2.1 and present the main theorems about the geodesic properties of time series with respect to a generalized Wasserstein metric and the geometry of the SCDT embedding in Section 2.2.

2.1. The Signed Cumulative Distribution Transform and a Generalized Wasserstein Metric

The Cumulative Distribution Transform (CDT) was introduced in (Park et al., 2018) for non-negative $L^1$-normalized functions. In particular, given non-negative signals $s$ and $s_0$ (a fixed reference) with $\|s\|_1 = \|s_0\|_1 = 1$, the CDT $s^*$ of $s$ is defined as the optimal transport map $^2$ between reference $s_0$ and $s$, which is the unique non-decreasing map (Santambrogio, 2015)

$$s^* = F^1_s \circ F_{s_0},$$

where $F_{s_0}$ is the cumulative distribution function of $s_0$ and $F^1_s(x) := \inf\{t \in \mathbb{R} : F(t) \geq x\}$ is the generalized inverse of $F_s$. $^3$ In particular, $(s^*)_2 s_0 = s$ and $s^*$ minimizes the Wasserstein-2 cost $d_{W^2}(s_0, s) := \sqrt{\int_{\Omega} \min(x - T(x), 2s_0(x)) dx}$ between $s_0$ and $s$. It is well-known (Santambrogio, 2015) that $(S_1, d_{W^2}(-, \cdot))$ is a geodesic space with the constant-speed geodesic between $s$ and $\tilde{s}$ given by for $\alpha \rightarrow \rho_\alpha = (1 - \alpha)id + \alpha T^*$, where $T^*$ is the optimal transport map between $s$ and $\tilde{s}$ in $S_1$ and $\alpha \in [0, 1]$. Moreover, the CDT defines an isometric embedding from the space of non-negative normalized signals $(S_1, d_{W^2})$ to the transform space $(S^*_1, L^2(s_0))$ (cf. (Villani, 2003)), i.e.,

$$d_{W^2}(s_1, s_2) = \|s_1^* - s_2^*\|_{L^2(\mu_0)}$$

where $S^*_1$ is the set of CDTs of signals in $S_1$.

Now for a (non-zero) signed signal, the Jordan decomposition (Royden & Fitzpatrick, 1988) is applied to $s(t) = s^+(t) - s^-(t),$ where $s^+(t)$ and $s^-(t)$ are the absolute values of the positive and negative parts of the signal $s(t)$. Given a fixed $L^1$-normalized positive reference signal $s_0$ defined on $\Omega_{s_0}$, the signed cumulative distribution transform (SCDT) (Aldroubi et al., 2022) of $s(t)$ is then defined as the

$^1$The fact that $s_0$ and $s$ have finite second moments guarantees the existence of a unique optimal transport map between them.

$^2$If $F_s$ is strictly increasing on $\Omega_s$, then $F^1_s = F_s^{-1}$.

$^3$Here $s^+(t)$ and $s^-(t)$ can be seen as the density functions of corresponding measures in the Jordan decomposition of the measure $\mu_s$ associated with $s$ where $d\mu_s(x) := s(x)dx$. 

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We first present a sufficient condition on a pair of signals $s_1, s_2$.

### 2.2 Geodesic Properties

Let $s_1, s_2$ be time series to its transform space $S$. A generalized Wasserstein-2 distance between two signals can be defined as follows:

$$D_S(s_1, s_2) := d^2_W(\frac{\|s_1^+\|}{\|s_1\|}, \frac{\|s_2^+\|}{\|s_2\|}) + d^2_W(\frac{\|s_1^-\|}{\|s_1\|}, \frac{\|s_2^-\|}{\|s_2\|})$$

where $(\frac{\|s^+\|}{\|s\|}, \frac{\|s^-\|}{\|s\|})$ is the CDT (defined in eqn. (1)) of the normalized signal $\frac{\|s\|}{\|s\|}$. To simplify notations, from now on, for non-negative signals (e.g., $s^+$), its CDT is defined as the CDT of its normalized version, i.e., we denote $(\frac{\|s^+\|}{\|s\|})$ simply as $(s^+)$. Equivalently, (3) becomes $\tilde{s} = ((s^+)^+, (s^+) , (s^-)^-, (s^-)^-)$. Like the CDT, the SCGD is invertible with the inverse transform (see A.5 for more details) given by

$$s = \|s^+\| ((s^+) s_0) - \|s^-\| ((s^-) s_0).$$

Similarly, a generalized Wasserstein-2 distance between two time series can be defined as follows:

$$D_S(s_1, s_2) := \left|d^2_W(\frac{\|s_1^+\|}{\|s_1\|}, \frac{\|s_2^+\|}{\|s_2\|}) + d^2_W(\frac{\|s_1^-\|}{\|s_1\|}, \frac{\|s_2^-\|}{\|s_2\|})\right|^2$$

where the second-to-last equality follows from the embedding property (2) of the CDT. Hence the SCGD also defines an isometry (embedding) from the space $(S, D_S(\cdot, \cdot))$ of time series to its transform space $\tilde{S} = \|\cdot\|_{L^2(s_0) \times \mathbb{R}}$.

### 2.2 Geodesic Properties

We first present a sufficient condition on a pair of signals under which a geodesic exists between them.

**Theorem 2.1.** Fix a reference signal $s_0 \in S$. Given a signal $s \in S$ and a strictly increasing differentiable function $g : \mathbb{R} \to \mathbb{R}$, there is a constant speed geodesic between $s$ and $\tilde{s} := g' \circ g$. In particular, the geodesic $\tilde{s} := g' \circ g$ is given by

$$\tilde{s} = [(1 - \alpha)(s^+)^+ + \alpha(s^+) \|s^+\|] (\|s^+\|^2 + \alpha(s^+) \|s^+\|) s_0 - [(1 - \alpha)(s^-)^- + \alpha(s^-) \|s^-\|] (\|s^-\|^2 + \alpha(s^-) \|s^-\|) s_0.$$  

**Proof.** It suffices to show that given $\alpha_1, \alpha_2 \in [0, 1]$, $D_S(p_{\alpha_1}, p_{\alpha_2}) = |\alpha_1 - \alpha_2| D_S(s_1, s_2)$. By the composition property of the CDT (see A.4), $(s^+) = g^{-1} \circ (s^+)$. Hence we have that

$$(1 - \alpha)(s^+)^+ + \alpha(s^+) \|s^+\| = (1 - \alpha) g' + \alpha g^{-1} \circ (s^+)\|s^+\|.$$  

Since $(1 - \alpha) g' + \alpha g^{-1}$ is strictly increasing and $(s^+) s_0 \perp (s^+) s_0$ (see A.5), it follows that $(1 - \alpha)(s^+)^+ + \alpha(s^+) \|s^+\| s_0 = (1 - \alpha)(s^+)^+ + \alpha(s^+) \|s^+\| s_0$ (see Lemma 5.4 in Aldroubi et al., 2022). By the inverse formula in Proposition A.3, it is hard to see that the expression in (8) is the Jordan decomposition of $p_{\alpha}$, i.e.,

$$p_{\alpha} = [(1 - \alpha)(s^+)^+ + \alpha(s^+) \|s^+\|] (\|s^+\|^2 + \alpha(s^+) \|s^+\|) s_0.$$  

Hence

$$D_S^2(p_{\alpha_1}, p_{\alpha_2}) = D_S^2(p_{\alpha_1}, p_{\alpha_2}) + D_S^2(p_{\alpha_1}, p_{\alpha_2}) + |\alpha_1 - \alpha_2|^2 D_S^2(s_0, s_0) = |\alpha_1 - \alpha_2|^2 D_S^2(s_0, s_0) = |\alpha_1 - \alpha_2|^2 \| (1 - \alpha)_1 (s^+) \|_{L^2(s_0)}^2 + |\alpha_1 - \alpha_2|^2 (\|s^+ \| - \|s^-\|)^2,$$

where the second-to-last equality follows from the fact that $p_{\alpha}^2 = (1 - \alpha_1) (s^+)^+ + \alpha_1 (s^+)^+$, $i = 1, 2$ (see A.5 for more details).

**Remark 2.2.** The same conclusion holds if $\tilde{s} := \lambda g' \circ g$ for any constant $\lambda > 0$ and $g$ strictly increasing and differentiable.

**Corollary 2.3.** Let $G = \{g : \mathbb{R} \to \mathbb{R} : g \text{ is strictly increasing and differentiable}\}$ and $p \in S$. Consider the following template-deformation based generative model (Park et al., 2018)

$$S_{p, G} := \{g \cdot p \circ g : g \in G\}.$$  

Then for any two signals in $S_{p, G}$, a unique constant-speed geodesic exists with respect to the generalized Wasserstein-2 metric defined in (6).
2.3 Examples of Geodesics

Proof. Let \( p_i = g_i^1 p \circ g_i \in S_{p,G}, i = 1, 2 \). It follows that \( p_2 = (g_1^{-1} \circ g_2) p_1 \circ (g_1^{-1} \circ g_2) \). Since \( g_1^{-1} \circ g_2 \) is also strictly increasing, by Theorem 2.1, there exists a constant speed geodesic between \( p_1 \) and \( p_2 \).

Remark 2.4. More generally, one can show the existence of geodesics between pairs of signals in any subset \( U \) of \( S \) such that \( U \) is convex, the proof of which is presented in A.1. By the convexity property of the SCDT (Aldroubi et al., 2022), \( \hat{S}_{p,G} \) is convex if and only if \( G^{-1} \) is convex. Hence Corollary 2.3 can be seen as a special case of Proposition A.1 since the set \( G = G^{-1} \) is convex for \( G = \{ g : \mathbb{R} \rightarrow \mathbb{R} : g \) is strictly increasing and differentiable \}.

Next we show that a geodesic may not exist between arbitrary two signals in \( S \) with the generalized Wasserstein metric.

Theorem 2.5. The metric space \((S, D_S(\cdot, \cdot))\) is not a geodesic space.

Proof. Recall that a metric space is geodesic means that for any two given elements, there exists a path between such that the length of the path equals the distance between them. We prove this theorem by giving an example where the length of any path between some \( s_1, s_2 \in S \) is larger than their distance \( D_S(s_1, s_2) \). Let \( s_1 = \mathbb{I}_{[-1,0]} - \mathbb{I}_{[0,1]} \) and \( s_2 = \mathbb{I}_{[0,1]} - \mathbb{I}_{[-1,0]} \). Assume by contradiction that there is a path \( \gamma : [0,1] \rightarrow S \) where \( \gamma_0 = s_1 \) and \( \gamma_1 = s_2 \) such that \( \text{Len}(\gamma) = D_S(s_1, s_2) \). By the embedding property (7) of the SCDT, it follows that \( \tilde{\gamma}_\alpha(\alpha \in [0,1]) \) defines a geodesic in \( \hat{S} \subseteq (L^2(s_0) \times \mathbb{R})^2 \). Since the space \( (L^2(s_0) \times \mathbb{R})^2 \) is uniquely geodesic (see A.6), then \( \tilde{\gamma}_\alpha = (1 - \alpha)\tilde{s}_1 + \alpha\tilde{s}_2 \). Let \( \tilde{s}_1 = (f_{11}^+, 1, f_{11}^-, 1) \in \hat{S} \) and it is not hard to see that \( \tilde{s}_2 = (f_{12}^+, 1, f_{12}^-, 1) \). Hence \( \tilde{\gamma}_{1/2} := (f_{12}^{1/2} + f_{12}^{1/2} - f_{12}^{1/2}, 1) \) is a contradiction to the fact that \( \tilde{\gamma}_{1/2} \in \hat{S} \) (since by definition \( f_{12}^{1/2} > 0 \) and \( f_{12}^{1/2} > 0 \) should be mutually singular, see A.5).

Remark 2.6. Using the fact that the space \( (L^2(s_0) \times \mathbb{R})^2 \) is uniquely geodesic, one can show that if the geodesic in \((S, D_S(\cdot, \cdot))\) exists between two signals \( s \) and \( \tilde{s} \), it should be of the form (8).

Remark 2.7. Observing from Proposition A.1, it is not hard to see that \( \hat{S} \) is not convex. This is in contrast to the fact the embedding CDT space \( S^1 \) is convex (Aldroubi et al., 2021).

Remark 2.8. The set \( G \) in Corollary 2.3 is a group with the group operation being composition and defines an equivalence relation in \( S \) via \( s \sim \tilde{s} \) if and only if \( \tilde{s} = g \circ s \) for some \( g \in G \). It follows that \( S \) can be partitioned into disjoint clusters \( \bigcup_i S_{p_i,G} \) (see (9)). Hence by Remark 2.4 \( \hat{S} \) can be partitioned as a union of convex subsets \( \bigcup_i \hat{S}_{p_i,G} \).

3Here \( \mathbb{I}_{[a,b]} \) denotes the indicator function of interval \([a,b] \).

2.3. Examples of Geodesics

In this section, we give two examples (Figure 2) where a unique geodesic exists between the given signals and two examples (Figure 3) where a geodesic does not exist. By Remark 2.6, the geodesic \( p_\alpha \) for \( \alpha \in [0,1] \) is of the form (8) when it exists. In the case when a geodesic does not exist, we plot a path in \( S \) according to (8). For a geodesic \( p_\alpha \) with \( p_0 = s \) and \( p_1 = \tilde{s} \), it follows by definition that \( \sum_{i=1}^n D_S(p_{\alpha_{i-1}, p_\alpha}) = D_S(s, \tilde{s}) \) for \( 0 < \alpha_0 < \alpha_1 < \cdots < \alpha_n = 1 \); while \( \sum_{i=1}^n D_S(p_{\alpha_{i-1}, p_\alpha}) > D_S(s, \tilde{s}) \) if \( \alpha \not\rightarrow p_\alpha, \alpha \in [0,1] \) is not a geodesic path.

In particular, in the following plots the signals \( p_{\alpha_i} \) where \( \alpha_i = \frac{1}{4}, i = 0, \cdots, 4 \) are presented and distances \( D_i := D_S(p_{\alpha_{i-1}, p_{\alpha_i}}), i = 1, 2, 3, 4 \) and \( D := D_S(s, \tilde{s}) \) are shown.

Figure 2. Examples of geodesics: (top) the geodesic between the zero signal and \( s(t) = \sin(2\pi t)\mathbb{I}_{[0,1]}(t) \) where \( p_\alpha(t) = \sin(2\pi \alpha t)\mathbb{I}_{[0,1]}(t) \). (bottom) the geodesic between \( s(t) = -\sin(3\pi t)\mathbb{I}_{[0,1]}(t) \) and \( \tilde{s} = g' \circ g \) where \( g(t) = t^2 \). In both examples, \( D = \sum_{i=1}^4 D_i \).

Figure 3. Examples where geodesics do not exist: (top) signal path \( p_\alpha \) defined by (8) between \( s = -\mathbb{I}_{[0,5]} + \mathbb{I}_{[5,1]} \) and \( \tilde{s} = \mathbb{I}_{[0,5]} - \mathbb{I}_{[5,1]} \); for this path \( D = .71 \ll \sum_{i=1}^4 D_i = 2.48 \). (bottom) signal path \( p_\alpha \) defined by (8) between \( s \) and \( \tilde{s} = s \circ g \) where \( g(t) = t^2 \) and \( s(t) = -\sin(3\pi t)\mathbb{I}_{[0,1]}(t) \). Note the \( \tilde{s} \) here differs from that in second example of Figure 2 (there is no normalizing term \( g'(t) \) here); for path \( D = .27 \ll \sum_{i=1}^4 D_i = .49 \).

4By a direct computation (see A.8), we have that the geodesic is given by \( p_\alpha(t) = \frac{\sin(t^2)}{t} \) for \( \alpha \in (0,1] \) and \( p_0 := 0 \).
3. A Preliminary Application: Interpreting the SCDT Subspace Classifier

In this section, we attempt to utilize the preliminary geodesic properties discussed above to partially interpret the decisions made by the SCDT subspace classifiers proposed in (Rubaiyat et al., 2022b) and (Rubaiyat et al., 2022a), which were shown to achieve very high accuracy in classifying segmented time series events.

3.1. SCDT Subspace Classifiers

The signed cumulative distribution transform (SCDT) combined with a subspace classifier has recently been shown very effective in classifying time series data (Rubaiyat et al., 2022b,a). In (Rubaiyat et al., 2022b), the authors employed a nearest subspace search technique in SCDT space to classify time series events that follow a certain generative model: \( S^{(c)} = \left\{ s_j^{(c)} | s_j^{(c)} = g_j^{(c)}, g_j \in G_j^{(c)}, j = 1, \ldots, N \right\} \), where \( s_j^{(c)} \) is a signal in class \( c \) deformed from \( \varphi^{(c)} \) (a template pattern corresponding to class \( c \)), and \( G_j^{(c)} \) denotes a set of increasing deformations of a specific kind (e.g. translation, scaling, etc.). In the embedding (transform) space, each signal class is hypothesized to be modeled well by the containing subspace \( V^{(c)} = \text{span}(S^{(c)}) \), and the corresponding classifier searches for the nearest subspace to the test sample to predict its class label.

An extension of the SCDT nearest subspace approach was proposed in (Rubaiyat et al., 2022a), where a more general multi-template generative model was used, assuming that a signal class is generated from a set of templates under some unknown deformations. Formally, the multi-template generative model for signal class \( c \) is defined to be the set: \( S^{(c)} = \bigcup_{m=1}^{M_c} S_m^{(c)} G_m^{(c)} \), where \( S_m^{(c)} G_m^{(c)} = \left\{ s_j^{(c)} | s_j^{(c)} = g_j^{(c)}, g_j \in G_j^{(c)} \right\} \) and \( G_j^{(c)} = \left\{ \sum_{i=1}^{k} \alpha_i t_i, \alpha_i \geq 0 \right\} \) lies in a linear space of deformations. Each signal class is hypothesized to be modeled well by a union of subspaces \( \bigcup_{m=1}^{M_c} V_m^{(c)} \) in the embedding (transform) space, where \( V_m^{(c)} = \text{span}(S_m^{(c)} G_m^{(c)}) \). The corresponding classifier searches for the nearest local subspace \( V_m^{(c)} \) to the test sample to predict the class label.

3.2. Interpretation of the SCDT Subspace Classifiers

As explained in the section above, the SCDT subspace classifiers search for the nearest subspace \( V_m^{(c)} \) (Rubaiyat et al., 2022b) or local subspace \( \hat{V}_m^{(c)} \) (Rubaiyat et al., 2022a) to a given test signal in SCDT (embedding) space. In particular, for the nearest subspace classifier, it can be shown that under certain assumptions, \( d^2(\hat{s}, \hat{V}^{(c)}) < d^2(\hat{s}, \hat{V}^{(p)}) \) for \( s \in S^{(c)} \) and \( p \neq c \), where \( d^2(\cdot, \cdot) \) denotes the \( L^2 \)-metric. Similar properties hold for the nearest local subspace classifier. The class labels are then predicted by searching for the (local) subspace with the smallest distance to the test signal.

In this paper, we provide a preliminary interpretation of the subspace classifiers using a synthetic dataset and a real dataset StarLightCurves (Rebbapragada et al., 2009) hosted by the UCR time series classification archive (Dau et al., 2018). In particular, we present a visualization of the paths between a test signal and its projections onto the subspaces associated with different classes. The projection \( \hat{s} \) of a test signal \( s \) onto the subspace \( \hat{V}^{(c)} \) associated with class \( c \) is defined in the sense that \( \hat{\hat{s}} := P_{\hat{V}^{(c)}} \hat{s} \), where \( P_{\hat{V}^{(c)}} \) denotes the \( L^2 \)-projection operator to the subspace \( \hat{V}^{(c)} \).

If the classifier can successfully model a subspace (using training data) that contains a test signal \( s \), then the projection \( \hat{\hat{s}} = s \). In practice, we observe that the path defined by (8) between a test signal \( s \) and its projection \( \hat{s} \) to a subspace associated with the same class as \( s \) consists of signals of similar shapes (or looks like a geodesic lying in the same class) and \( s \approx \hat{s} \). On the other hand, the path between \( s \) and its projection to a subspace associated with a different class seems to exhibit unpredictable behavior.

**Experiment 1:** For this experiment, we created a synthetic dataset of three classes consisting of scaled and translated signals of three template signals: Gabor wave, apodized sawtooth wave, and apodized square wave, respectively (shown in Figure 4). The training samples were generated following the generative model given by: \( S^{(c)} = \{ g \varphi^{(c)} | g \in G \} \), where \( G = \{ g = \omega t + \tau, \omega > 0, \tau \in \mathbb{R} \} \) and \( \varphi^{(c)}(t) \) denotes the template corresponding to class \( c \) (see Figure 4). Here the test sample (not present in training set) follows the generative model for class 1 (Gabor wave). The signal paths \( p_m \) between the test signal and its projections onto three subspaces formed via the subspace classifier (Rubaiyat et al., 2022b) are shown in Figure 5. We observe that the projection onto class 1 resembles the test signal and the corresponding path looks like a geodesic (i.e., the ratio \( \sum_{i=1}^{k} D_i / D \approx 1 \)), indicating the subspace \( \hat{V}^{(1)} \) generated by the subspace classifier contains the SCDTs of the test signal \( s \) and its cluster \( S_{s,G} \). However the paths from the test signal \( s \) to the nearest subspace classifier, it can be shown that under certain assumptions, \( d^2(\hat{s}, \hat{V}^{(c)}) < d^2(\hat{s}, \hat{V}^{(p)}) \) for \( s \in S^{(c)} \) and \( p \neq c \), where \( d^2(\cdot, \cdot) \) denotes the \( L^2 \)-metric. Similar properties hold for the nearest local subspace classifier. The class labels are then predicted by searching for the (local) subspace with the smallest distance to the test signal.

In this paper, we provide a preliminary interpretation of the subspace classifiers using a synthetic dataset and a real dataset StarLightCurves (Rebbapragada et al., 2009) hosted by the UCR time series classification archive (Dau et al., 2018). In particular, we present a visualization of the paths between a test signal and its projections onto the subspaces associated with different classes. The projection \( \hat{s} \) of a test signal \( s \) onto the subspace \( \hat{V}^{(c)} \) associated with class \( c \) is defined in the sense that \( \hat{\hat{s}} := P_{\hat{V}^{(c)}} \hat{s} \), where \( P_{\hat{V}^{(c)}} \) denotes the \( L^2 \)-projection operator to the subspace \( \hat{V}^{(c)} \).

If the classifier can successfully model a subspace (using training data) that contains a test signal \( s \), then the projection \( \hat{\hat{s}} = s \). In practice, we observe that the path defined by (8) between a test signal \( s \) and its projection \( \hat{s} \) to a subspace associated with the same class as \( s \) consists of signals of similar shapes (or looks like a geodesic lying in the same class) and \( s \approx \hat{s} \). On the other hand, the path between \( s \) and its projection to a subspace associated with a different class seems to exhibit unpredictable behavior.

**Experiment 1:** For this experiment, we created a synthetic dataset of three classes consisting of scaled and translated signals of three template signals: Gabor wave, apodized sawtooth wave, and apodized square wave, respectively (shown in Figure 4). The training samples were generated following the generative model given by: \( S^{(c)} = \{ g \varphi^{(c)} | g \in G \} \), where \( G = \{ g = \omega t + \tau, \omega > 0, \tau \in \mathbb{R} \} \) and \( \varphi^{(c)}(t) \) denotes the template corresponding to class \( c \) (see Figure 4). Here the test sample (not present in training set) follows the generative model for class 1 (Gabor wave). The signal paths \( p_m \) between the test signal and its projections onto three subspaces formed via the subspace classifier (Rubaiyat et al., 2022b) are shown in Figure 5. We observe that the projection onto class 1 resembles the test signal and the corresponding path looks like a geodesic (i.e., the ratio \( \sum_{i=1}^{k} D_i / D \approx 1 \)), indicating the subspace \( \hat{V}^{(1)} \) generated by the subspace classifier contains the SCDTs of the test signal \( s \) and its cluster \( S_{s,G} \). However the paths from the test signal \( s \) to the nearest subspace classifier, it can be shown that under certain assumptions, \( d^2(\hat{s}, \hat{V}^{(c)}) < d^2(\hat{s}, \hat{V}^{(p)}) \) for \( s \in S^{(c)} \) and \( p \neq c \), where \( d^2(\cdot, \cdot) \) denotes the \( L^2 \)-metric. Similar properties hold for the nearest local subspace classifier. The class labels are then predicted by searching for the (local) subspace with the smallest distance to the test signal.
signal to its projections onto the other two classes contain signals that belong to neither classes and seem to exhibit unpredicted patterns.

Figure 5. Signal path \( p_\alpha \) defined by eq. (8) between a test sample \( s \) from class 1 and its projections \( \tilde{s}^{(1)}, \tilde{s}^{(2)} \) associated with the subspaces obtained by the subspace classifier (Rubaiyat et al., 2022b) corresponding to the three classes, respectively. Note that the distance \( D \) between \( s \) and \( \tilde{s}^{(2)} \) (i.e., \( D_S(s, \tilde{s}^{(1)}) \)) is the smallest, and hence the classifier predicts the correct label.

**Experiment 2:** We conducted a similar experiment with a very noisy signals which seem to belong to neither classes.

**Remark 3.1.** Given the stark differences between the path from a signal to its projection associated with a subspace of its own class and that to its projection associated with a subspace of a different class, one may consider using

![Figure 6. Samples from two classes in the StarLightCurves dataset](Figure 6. Samples from two classes in the StarLightCurves dataset)

![Figure 7. Signal path \( p_\alpha \) defined by eq. (8) between a test sample \( s_j \) and its projections \( \tilde{s}^{(i)}_j \) \((i, j = 1, 2)\) in the local subspaces obtained by the subspace classifier (Rubaiyat et al., 2022a) corresponding to two classes, respectively. Note that in the top panel the distance \( D \) between \( s_1 \) and \( \tilde{s}^{(2)}_1 \) (i.e., \( D_S(s_1, \tilde{s}^{(1)}_1) \)) is smaller, and in the bottom panel the distance \( D \) between \( s_2 \) and \( \tilde{s}^{(2)}_2 \) is smaller. Hence the local classifier predicts the correct labels in both cases.

In this preliminary study, we look into the geometry of time series with respect to a generalized Wasserstein metric and its embedding in a linear space. In particular, a geodesic may not exist between two arbitrary time series in \( S \) but exists between signals within the same generative cluster (see (9)). We utilize this knowledge to show whether the (local) subspaces formed by the training samples via the SCDT subspace classifiers do a good job in modeling the signal classes conforming to certain generative modeling assumptions. We illustrate it by visualizing the paths between random test signals and their projections onto the corresponding subspaces associated with different classes and observe that there is a path resembling a geodesic from a test signal to its projection in the subspace associated with the same class of the test signal. This shows some preliminary evidence that the classifiers produce a “good” subspace that models the corresponding generative clusters to which the test signals belong. In the future, we are interested in quantitative (numerical) characterization of geodesics for real/noisy data in the hope of building more robust models.
and classifiers for time series events.

References

Abanda, A., Mori, U., and Lozano, J. A. A review on distance based time series classification. *Data Mining and Knowledge Discovery*, 33(2):378–412, 2019.

Aldroubi, A., Li, S., and Rohde, G. K. Partitioning signal classes using transport transforms for data analysis and machine learning. *Sampling Theory, Signal Processing, and Data Analysis*, 19(1):1–25, 2021.

Aldroubi, A., Martin, R. D., Medri, I., Rohde, G. K., and Thareja, S. The signed cumulative distribution transform for 1-D signal analysis and classification. *Foundations of Data Science*, 2022.

Arjovsky, M., Chintala, S., and Bottou, L. Wasserstein generative adversarial networks. In *International conference on machine learning*, pp. 214–223. PMLR, 2017.

Basu, S., Kolouri, S., and Rohde, G. K. Detecting and visualizing cell phenotype differences from microscopy images using transport-based morphometry. *Proceedings of the National Academy of Sciences*, 111(9):3448–3453, 2014.

Bridson, M. R. and Haefliger, A. *Metric spaces of non-positive curvature*, volume 319. Springer Science & Business Media, 2013.

Dau, H. A., Keogh, E., Kamgar, K., Yeh, C.-C. M., Zhu, Y., Gharghabi, S., Ratanamahatana, C. A., Yanping, Hu, B., Begum, N., Bagnall, A., Mueen, A., Batista, G., and Hexagon-ML. The UCR time series classification archive, October 2018. https://www.cs.ucr.edu/~eamonn/time_series_data_2018/.

Haker, S., Zhu, L., Tannenbaum, A., and Angenent, S. Optimal mass transport for registration and warping. *International Journal of computer vision*, 60(3):225–240, 2004.

Hamm, K., Henscheid, N., and Kang, S. Wassmap: Wasserstein isometric mapping for image manifold learning. *arXiv preprint arXiv:2204.06645*, 2022.

Kolouri, S., Park, S. R., Thorpe, M., Slepcev, D., and Rohde, G. K. Optimal mass transport: Signal processing and machine-learning applications. *IEEE signal processing magazine*, 34(4):43–59, 2017.

Lines, J. and Bagnall, A. Time series classification with ensembles of elastic distance measures. *Data Mining and Knowledge Discovery*, 29(3):565–592, 2015.

Moosmüller, C. and Cloninger, A. Linear optimal transport embedding: Provable wasserstein classification for certain rigid transformations and perturbations. *arXiv preprint arXiv:2008.09165*, 2020.

Muskulus, M. and Verduyn-Lunel, S. Wasserstein distances in the analysis of time series and dynamical systems. *Physica D: Nonlinear Phenomena*, 240(1):45–58, 2011.

Ozolek, J. A., Tosun, A. B., Wang, W., Chen, C., Kolouri, S., Basu, S., Huang, H., and Rohde, G. K. Accurate diagnosis of thyroid follicular lesions from nuclear morphology using supervised learning. *Medical image analysis*, 18(5):772–780, 2014.

Park, S. R., Kolouri, S., Kundu, S., and Rohde, G. K. The cumulative distribution transform and linear pattern recognition. *Applied and computational harmonic analysis*, 45:616–641, 2018.

Rubaiyat, A. H. M., Protopapas, P., Brodley, C. E., and Alcock, C. Finding anomalous periodic time series. *Machine learning*, 74(3):281–313, 2009.

Royden, H. L. and Fitzpatrick, P. *Real analysis*, volume 32. Macmillan New York, 1988.

Rubaiyat, A. H. M., Hallam, K. M., Nichols, J. M., Hutchinson, M. N., Li, S., and Rohde, G. K. Parametric signal estimation using the cumulative distribution transform. *IEEE Transactions on Signal Processing*, 68:3312–3324, 2020.

Rubaiyat, A. H. M., Li, S., Yin, X., Rabbi, M. S. E., Zhuang, Y., and Rohde, G. K. End-to-end signal classification in signed cumulative distribution transform space. *arXiv preprint arXiv:2205.00348*, 2022a.

Rubaiyat, A. H. M., Shifat-E-Rabbi, M., Zhuang, Y., Li, S., and Rohde, G. K. Nearest subspace search in the signed cumulative distribution transform space for 1d signal classification. In *ICASSP 2022-2022 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pp. 3508–3512. IEEE, 2022b.

Rubaiyat, A. H. M., Tomasi, C., and Guibas, L. J. The earth mover’s distance as a metric for image retrieval. *International journal of computer vision*, 40(2):99–121, 2000.

Santambrogio, F. Optimal transport for applied mathematicians. *Birkäuser, NY*, 55(58-63):94, 2015.

Shifat-E-Rabbi, M., Yin, X., Rubaiyat, A. H. M., Li, S., Kolouri, S., Aldroubi, A., Nichols, J. M., and Rohde, G. K. Radon cumulative distribution transform subspace modeling for image classification. *Journal of Mathematical Imaging and Vision*, pp. 1–19, 2021.

Villani, C. *Topics in Optimal Transportation*. Number 58. American Mathematical Soc., 2003.
A. Appendix

A.1. An additional proposition

Proposition A.1. Let $U \subseteq S$ such that $\hat{U}$ is a convex subset of $\hat{S}$. Then there exists a unique constant speed geodesic with respect to $D_S(\cdot, \cdot)$ between any two signals in $U$.

Proof. Let $u, w \in U$. Since $\hat{U}$ is convex, $(1 - \alpha)\hat{u} + \alpha\hat{w} \in \hat{U} \subseteq \hat{S}$ for any $\alpha \in [0, 1]$. Since the SCDT is a bijection between $S$ and $\hat{S}$ (see A.4), there exists a unique $u_\alpha \in U$ such that $\hat{u}_\alpha = (1 - \alpha)\hat{u} + \alpha\hat{w}$ for any $\alpha \in [0, 1]$. Note that $u_0 = u$ and $u_1 = w$. By the embedding property (7) of the SCDT, we have that

\[
D_S(u_{\alpha_1}, u_{\alpha_2}) = \|\hat{u}_{\alpha_1} - \hat{u}_{\alpha_1}\|_{L^2(s_0) \times \mathbb{R}}^2
\]

\[
= |\alpha_1 - \alpha_2| \|\hat{u} - \hat{w}\|_{L^2(s_0) \times \mathbb{R}}^2
\]

\[
= |\alpha_1 - \alpha_2| D_S(u, w),
\]

which shows that $\alpha \mapsto u_\alpha$ defines a constant speed geodesic in $U$. \hfill \Box

A.2. Push-forward of density functions

The push-forward operator is more generally defined for measures. Here we present its analog for the associated density functions. Given a $L^1$-normalized density function $s : \Omega_s \to \mathbb{R}$ ($s \geq 0$) and a (measurable) map $T : \mathbb{R} \to \mathbb{R}$, the push forward density function $T_\sharp s \in L^1(\mathbb{R})$ is defined via

\[
\int_B (T_\sharp s)(y)dy = \int_{T^{-1}(B) \cap \Omega_s} s(t)dt,
\]

for any measurable set $B \subseteq \mathbb{R}$.

A.3. A characterization of the CDT

The following fact is a corollary of Theorem 2.9 in (Santambrogio, 2015).

Proposition A.2. Given $s_1, s_2 \in S_1$, there exists a unique optimal transport map $T^*$ (i.e., a map such that $T_\sharp^* s_1 = s_2$ which minimizes the Wasserstein-2 cost) between them given by the non-decreasing map

\[
T^* = F_{s_2}^\dagger \circ F_{s_1}.
\]

On the other hand, if $T^* : \Omega_{s_1} \to \Omega_{s_2}$ is a non-decreasing map such that $T_\sharp^* s_1 = s_2$, it follows that $T^*$ is the optimal transport map between $s_1$ and $s_2$.

A.4. The composition property of the CDT and SCDT

Let $g : \mathbb{R} \to \mathbb{R}$ be a strictly increasing and differentiable function. Here we present the formulas for the transform (CDT or SCDT) of $s_g := g^* s \circ g$ for some $s \in S$.

For $s \in S_1$, the composition property for the CDT is given by (Park et al., 2018)

\[
s_g^* = g^{-1} \circ s^*.
\]

For $s \in S$ such that $\|s^+\| \neq 0$ and $\|s^-\| \neq 0$, the composition property for the SCDT is given by (Aldroubi et al., 2022)

\[
\hat{s}_g = \left( g^{-1} \circ (s^+)^*, \|s^+\|, g^{-1} \circ (s^-)^*, \|s^-\| \right).
\]

Similarly, for $s$ such that $\hat{s} = \left( (s^+)^*, \|s^+\|, 0, 0 \right)$ or $\hat{s} = \left( 0, 0, (s^-)^*, \|s^-\| \right)$ or $s = 0$, $\hat{s}_g$ is given by $\left( g^{-1} \circ (s^+)^*, \|s^+\|, 0, 0 \right)$ and $\left( 0, 0, g^{-1} \circ (s^-)^*, \|s^-\| \right)$ and $(0, 0, 0, 0)$, respectively.
A.5. On invertibility of the SCDT

Let $s_0 \in S_1$ be a $L^1$-normalized positive signal supported on $\Omega_0$ and let $s \in S$. Then by the definition of the CDT and Jordan decomposition, it is not hard to see that $(s^+)^*_{\Omega_0}s_0 \perp (s^-)^*_{\Omega_0}s_0$ since $(s^+)^*_{\Omega_0}s_0 = s^+$ and $(s^-)^*_{\Omega_0}s_0 = s^-$. Here “$\perp$” means that the measure with density $(s^+)^*_{\Omega_0}s_0$ and the measure with density $(s^-)^*_{\Omega_0}s_0$ are mutually singular. In particular, there exists $\Omega_+$ and $\Omega_-$ such that $\Omega_+ = \Omega_+ \cup \Omega_- \subset S$ with $\int_{\Omega_+} s^+(x)dx = 0$ and $\int_{\Omega_-} s^-(x)dx = 0$.

The following fact is a special case of Theorem 2.7 in (Aldroubi et al., 2022).

**Proposition A.3.** Given a fixed a $L^1$-normalized positive signal reference signal $s_0 \in S_1$ supported on $\Omega_0$. Then for any tuple $(f, a, g, b)$ satisfying

$$f \sharp s_0 \perp g \sharp s_0,$$

where $f, g \in L^2(s_0)$ are non-decreasing $s_0$-a.e. and $a, b > 0$, there is a unique $s \in S$ such that $s = (f, a, g, b)$ given by the following inverse formula

$$s = af_\sharp s_0 - bg_\sharp s_0. \quad (15)$$

Moreover, the unique inverses for tuples of the forms $(f, a, 0, 0)$, $(0, 0, g, b)$ and $(0, 0, 0, 0)$ are $af \sharp s_0$, $bg \sharp s_0$ and the zero signal respectively.

**Remark A.4.** From the above proposition, we see that the SCDT defines a bijection from $S$ to $\hat{S}$ via $s \mapsto \hat{s}$ and $\hat{S} = \{\hat{s} : s \in S\} = \{(f, a, g, b) : f, g \in L^2(s_0) \text{ non-decreasing } s_0 \text{-a.e.}, f \sharp s_0 \perp g \sharp s_0, a, b > 0\} \cup \{(f, a, 0, 0) : f \in L^2(s_0) \text{ non-decreasing } s_0 \text{-a.e., } a > 0\} \cup \{(0, 0, g, b) : g \in L^2(s_0) \text{ non-decreasing } s_0 \text{-a.e., } b > 0\} \cup \{(0, 0, 0, 0)\}$.

A.6. Length of a path and geodesics in metric spaces

Let $(V, d)$ be a metric space and $p : [0, 1] \to V$ be a curve (path) in $V$. Then the length of $p$ is defined by:

$$\text{Len}(p) := \sup \left\{ \sum_{i=0}^{n-1} d(p(\alpha_i), p(\alpha_{i+1})) : n \geq 1, 0 = \alpha_0 < \alpha_1 < \cdots < \alpha_n \right\}. \quad (16)$$

A curve $p : [0, 1] \to V$ between $v$ and $w$ in $V$ is called a geodesic if it is a length-minimizing curve:

$$\text{Len}(p) = \min \{\text{Len}(\gamma) : \gamma : [0, 1] \to V, \gamma(0) = v, \gamma(1) = w\}. \quad (17)$$

Moreover, it is called a constant-speed geodesic if

$$d(p(\alpha), p(\beta)) = |\alpha - \beta|d(p(0), p(1)), \quad \forall \alpha, \beta \in [0, 1]. \quad (18)$$

A metric space $(V, d)$ is said to be a geodesic space if for any $v, w \in V$, there exists a curve $p : [0, 1] \to V$ with $p(0) = v$ and $p(1) = w$ such that $d(v, w) = \text{Len}(p)$. Indeed, this curve $p$ is a geodesic between $v$ and $w$.

A.7. Uniqueness of geodesics in normed spaces with strictly convex norms

We present the following property of strictly convex spaces (see Proposition 1.6 in (Bridson & Haefliger, 2013)):

**Lemma A.5.** Every normed vector space $V$ is a geodesic space. It is uniquely geodesic if and only if the unit ball in $V$ is strictly convex (in the sense that if $u$ and $w$ are distinct vectors of norm 1, then $\|u - v\| < 1$ for all $\alpha \in (0, 1)$. The geodesic between $v, w \in V$ is given by $\alpha \mapsto (1 - \alpha)v + \alpha w$ for $\alpha \in [0, 1]$. \[\]

**Corollary A.6.** Let $s_0 \in S_1$. The space $(L^2(s_0) \times \mathbb{R})^2 = \{(f, a, g, b) : f, g \in L^2(s_0), a, b \in \mathbb{R}\}$ of tuples endowed with the 2-norm $\|(f, a, b, c)^2 := \sqrt{\|f\|^2_{L^2(s_0)} + a^2 + \|g\|^2_{L^2(s_0)} + b^2}$ is uniquely geodesic, with the unique geodesic between $(f_0, a_0, g_0, b_0)$ and $(f_1, a_1, g_1, b_1)$ given by $f_\alpha = (1 - \alpha)(f_0, a_0, g_0, b_0) + \alpha(f_1, a_1, g_1, b_1)$ with $\alpha \in [0, 1]$. \[\]
A.8 Geodesics between the zero signal and an arbitrary signal

Let $s \in S$. There exists a unique constant-speed geodesic in $(S, D_S(\cdot, \cdot))$ between 0 and $s$ given by $p_\alpha(t) = s(\frac{1}{\alpha} t)$ for $\alpha \in (0, 1]$ and $p_0 := 0$. By direct computation, for $\alpha_1, \alpha_2 \in (0, 1]$,

$$D_S^2(p_{\alpha_1}, p_{\alpha_2}) = \| (p_{\alpha_1}^+) - (p_{\alpha_2}^+) \|^2 + \| (p_{\alpha_1}^-) - (p_{\alpha_2}^-) \|^2 + \left( \| (p_{\alpha_1}^+) - \| (p_{\alpha_2}^+) \| \right)^2 + \left( \| (p_{\alpha_1}^-) - \| (p_{\alpha_2}^-) \| \right)^2$$

$$= \| \alpha_1 (s^+) - \alpha_2 (s^+) \|^2_{L^2(s_0)} + \| \alpha_1 (s^-) - \alpha_2 (s^-) \|^2_{L^2(s_0)} + \left( \alpha_1 \| s^+ \| - \alpha_2 \| s^- \| \right)^2 + \left( \alpha_1 \| s^- \| - \alpha_2 \| s^+ \| \right)^2$$

$$= (\alpha_1 - \alpha_2)^2 \left( \| (s^+) \|^2_{L^2(s_0)} + \| (s^-) \|^2_{L^2(s_0)} + \| s^+ \|^2 + \| s^- \|^2 \right)$$

$$= (\alpha_1 - \alpha_2)^2 \left( (0, 0, 0, 0) - \left( (s^+)^*, \| s^+ \|, (s^-)^*, \| s^- \| \right) \right)^2_{(L^2(s_0) \times \mathbb{R})^2}$$

$$= (\alpha_1 - \alpha_2)^2 D_S^2(0, s),$$

where the second equality follows from the composition property of the SCDT. Similarly one can verify that $D_S(0, p_\alpha) = \alpha D_S(0, s)$ for $\alpha \in [0, 1]$. 

