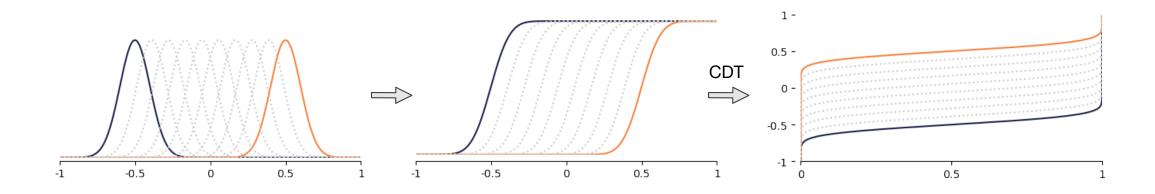
Transport transforms for signal analysis and machine learning

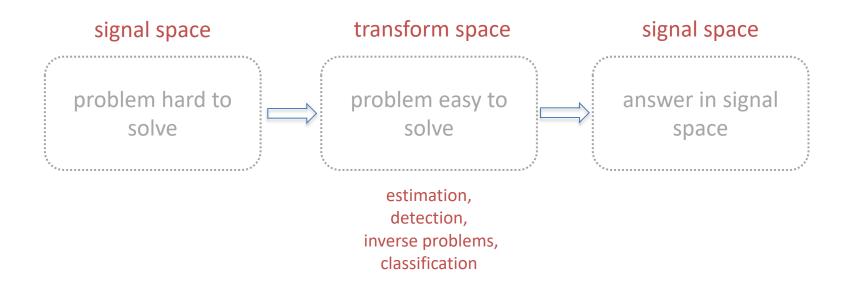
Gustavo K. Rohde

Imaging and Data Science Laboratory

imagedatascience.com/transport github.com/rohdelab/PyTransKit



Transport Transforms



[Wang, Slepcev, Basu, Ozolek, Rohde, IJCV 2013]
[Kolouri, Tosun, Ozolek, Rohde, Pattern Recognition 2016]
[Kolouri, Park, Rohde, IEEE TIP, 2016]
[Park, Kolouri, Kundu, Rohde, ACHA 18]
[Rubaiyat et al, IEEE TSP, 20]
[Aldroubi, Li, Rohde, SaSiDa, 21]
[Shifat-E-Rabbi et al, Rohde, JMIV 21]
[Aldroubi et al, AIMS Foundations of Data Science, 22]

Fourier transform:

forward

$$\hat{s}(\omega) = \int s(t)e^{-jwt}dt$$

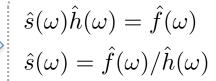
$$\hat{s}(\omega) = \int s(t)e^{-jwt}dt$$
 $s(t) = \frac{1}{2\pi} \int \hat{s}(\omega)e^{k\omega t}d\omega$

$$\int s(u)h(t-u)du = f(t) \implies \hat{s}(\omega)\hat{h}(\omega) = \hat{f}(\omega)$$

$$\hat{s}(\omega) = \hat{f}(\omega)/\hat{h}(\omega)$$

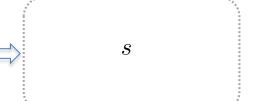
signal domain

difficult to solve



transform domain

easier to solve



signal domain

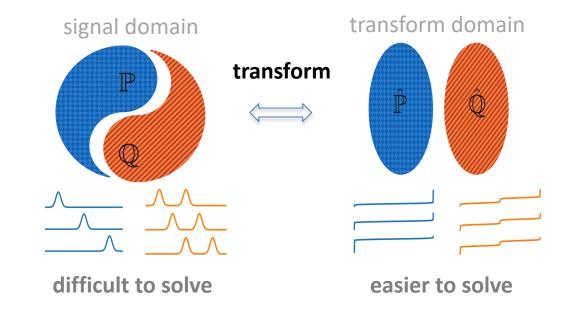
New signal transform

forward

$$\hat{s}(x) := S^{-1}(x)$$

inverse

$$s(t) = \frac{d}{dt}(\hat{s})^{-1}$$



Outline

- 1D case
 - CDT, SCDT
 - Connections with optimal transport
- N-D case
 - R-CDT, LOT
 - Connections with optimal transport
 - Related work

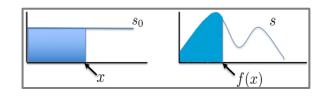
1-D Transport transform

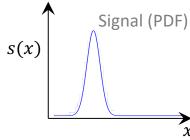
cumulative distribution transform (CDT)

Let $s(x), s_0(x) > 0$ and $\int s(x)dx = \int s_0(x)dx = 1$ (PDFs)

Consider a map f(x), such that

$$\int_{-\infty}^{x} s_0(u) du = \int_{-\infty}^{f(x)} s(u) du$$





[Park, Kolouri, Kundu, Rohde, ACHA 2018]

antiderivative

$$S_0(x) = S(f(x)) \Longrightarrow f(x) = S^{-1}(S_0(x))$$
transform of S

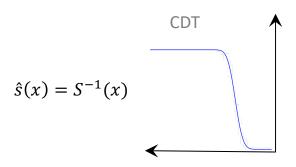
S(x) CDF

Eg.: Let $s_0 = \chi_{[0,1]}$. Then, $S_0(x) = x$ and $f(x) = S^{-1}(x)$.

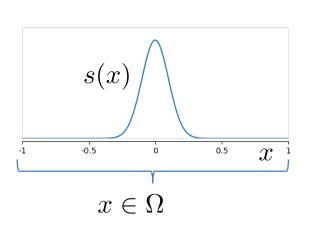
transform equations

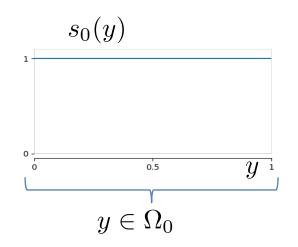
$$\hat{s}(x) := S^{-1}(x) \quad \text{forward}$$

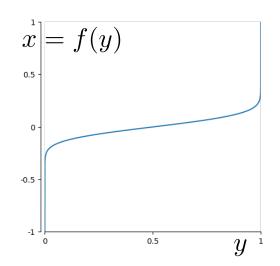
$$s(x) = \left(\hat{s}^{-1}(x)\right)' \quad \text{inverse}$$

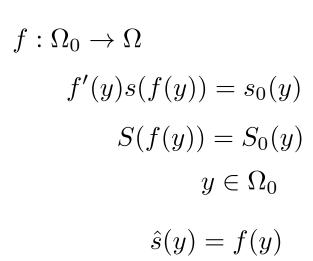


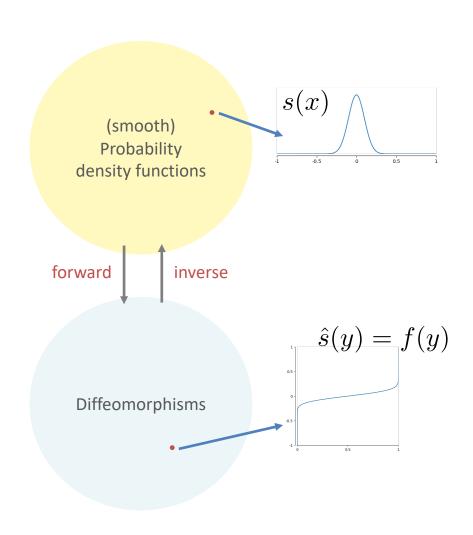
CDT: invertible (nonlinear) signal transform











CDT properties: composition

Composition: s(x) $x \in \Omega$ $\hat{s}(y)$ $y \in \Omega_0$ what is the CDT of $s_g(x) = g'(x)s(g(x)), x \in \Omega_g$?

$$\int_{-\infty}^{\widehat{s}(y)} s(u)du = \int_{-\infty}^{\widehat{s}_g(y)} s_g(u)du = \int_{-\infty}^{y} s_0(u)du$$

$$\int_{-\infty}^{\widehat{s}(y)} s(u) du = \int_{-\infty}^{\widehat{s}_g(y)} g'(u) s(g(u)) du \qquad \text{change of variables} \quad g(u) = v \quad g'(u) du = dv$$

$$\int_{-\infty}^{\widehat{s}(y)} s(u) du = \int_{-\infty}^{g(\widehat{s}_g(y))} s(v) dv \quad \Longrightarrow \quad g(\widehat{s}_g(x)) = \widehat{s}(x) \implies \widehat{s}_g(x) = g^{-1}(\widehat{s}(x)) \text{ or, } \widehat{s}_g = g^{-1} \circ \widehat{s}$$

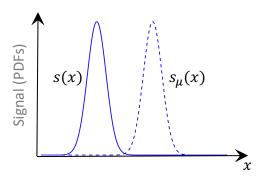
Conclusion: the CDT of $s_g(x)=g'(x)s(g(x)), x\in\Omega_g$ is given by: $\widehat{s}_g(y)=g^{-1}(\widehat{s}(y)), y\in\Omega_0$

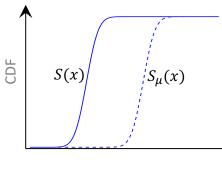
CDT Properties

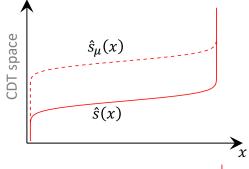
Translation

$$s_{\mu}(x) = s(x - \mu)$$

$$\hat{s}_{\mu}(x) = \hat{s}(x) + \mu$$



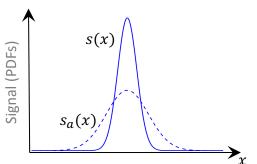


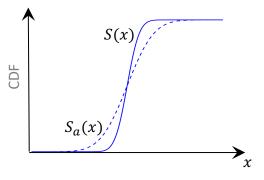


Scaling

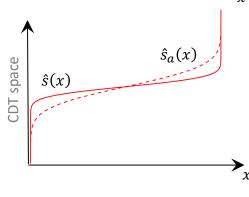
$$s_a(x) = as(ax)$$

$$\hat{s}_a(x) = \frac{\hat{s}(x)}{a}$$





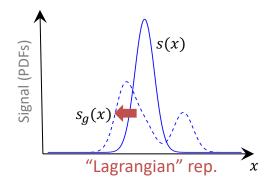
 \rightarrow_{χ}

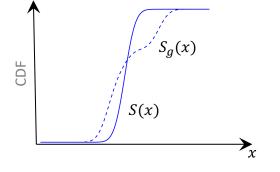


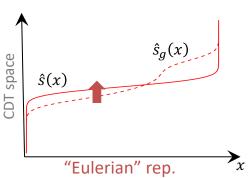
Composition

$$s_g(x) = g'(x)s(g(x))$$

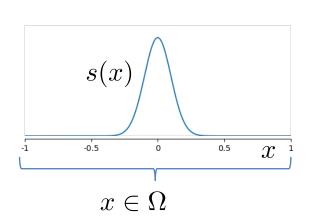
$$\hat{s}_g(x) = g^{-1}(\hat{s}(x))$$

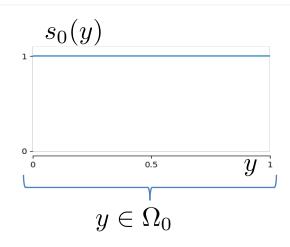


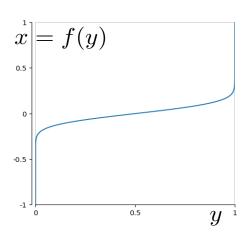




1D optimal transport







Integrate: $S(f(y)) = S_0(y)$ $y \in \Omega_0$ Differentiate: $f'(y)s(f(y)) = s_0(y)$

Mapping function $f:\Omega_0\to\Omega$ is unique.

Matching (optimal transport) cost:

Monge
$$(f) = \int_{\Omega_0} |f(y) - y|^2 s_0(y) dy$$

$$\hat{s}(y)$$

Squared Wasserstein distance $W_2^2(s,s_0)$

$$W_2^2(s,s_0)$$

Claim:
$$W_2^2(s_1, s_2) = \|(\hat{s_1} - \hat{s_2})\sqrt{s_0}\|_2^2$$

Proof:

Let
$$\hat{s}_1$$
 transform of s_1 that is

$$\hat{s}_2$$
 transform of s_2

$$\hat{s}'_1(y)s_1(\hat{s}_1(y)) = \hat{s}'_2(y)s_2(\hat{s}_2(y)) = s_0(y) \quad y \in \Omega_0 \quad \hat{s}_1 : \Omega_0 \to \Omega_1$$

$$y \in \Omega_0 \quad \hat{s}_1 : \Omega_0 \to \Omega$$

Let
$$s_1(x) = h'(x)s_2(h(x))$$
 that is $\hat{s}_1 = h^{-1} \circ \hat{s}_2 \longrightarrow \hat{s}_2 = h \circ \hat{s}_1$

that is
$$\hat{s}_1 = h^-$$

$$\rightarrow \hat{s}_2 = h \circ \hat{s}_1$$

$$W_2^2(s_1, s_2) = \int_{\Omega_1} (x - h(x))^2 s_1(x) dx$$

$$x = \hat{s}_1(y)$$

$$W_2^2(s_1, s_2) = \int_{\hat{s}_1^{-1}(\Omega_1)} (\hat{s}_1(y) - h(\hat{s}_1(y)))^2 s_1(\hat{s}_1(y)) \hat{s}_1'(y) dy$$

use:
$$\hat{s}_1:\Omega_0\to\Omega_1$$

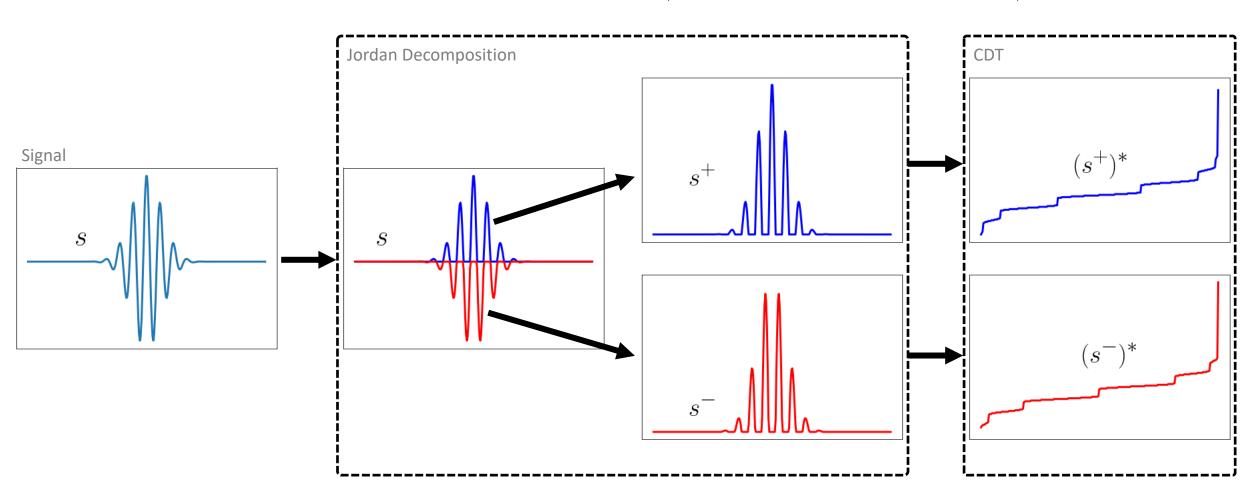
$$\hat{s}_1'(y)s_1(\hat{s}_1(y))=s_0(y)$$

$$\hat{s}_2=h\circ\hat{s}_1$$

$$W_2^2(s_1, s_2) = \int_{\Omega_0} (\hat{s}_1(y) - \hat{s}_2(y))^2 s_0(y) dy = \|(\hat{s}_1 - \hat{s}_2)\sqrt{s_0}\|_2^2$$

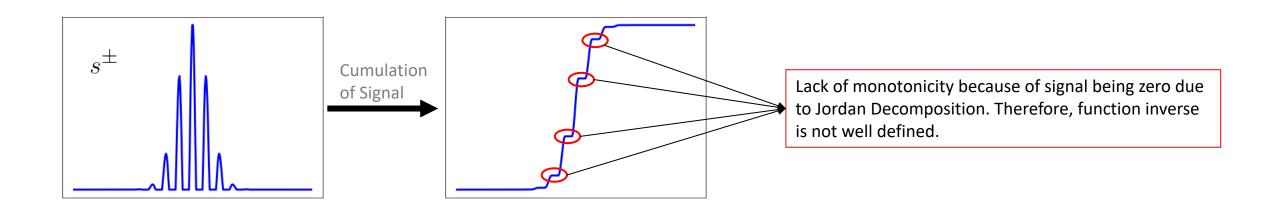
Signed Cumulative Distribution Transform (SCDT)

$$\hat{s} = ((s^+)^*, ||s^+||_{L_1}, (s^-)^*, ||s^-||_{L_1})$$

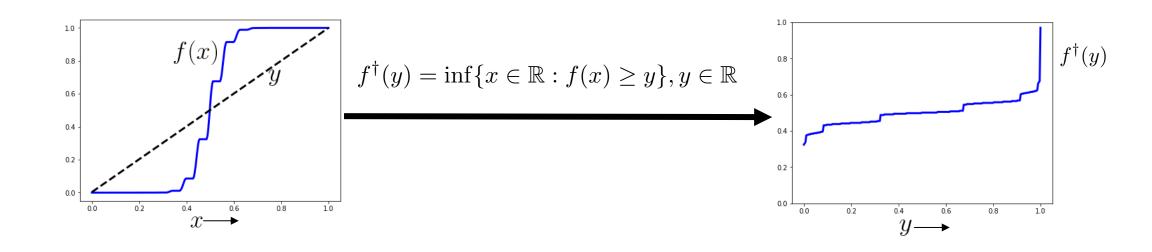


Aldroubi, Diaz Martin, Medri, Rohde, Thareja, The Signed Cumulative Distribution Transform for 1D signal analysis and classification, AIMS Foundations of Data Science, 2022

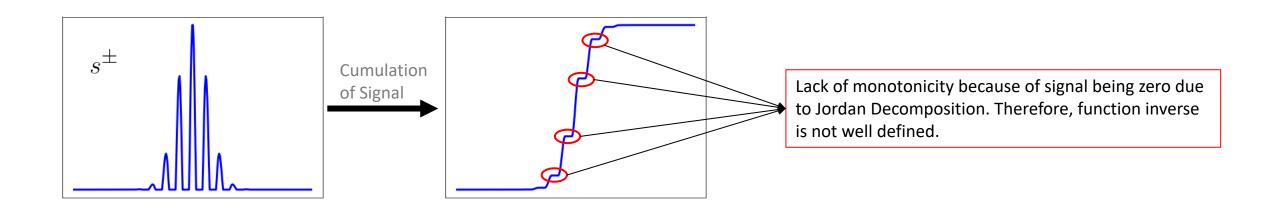
Generalized Inverse to Calculate SCDT



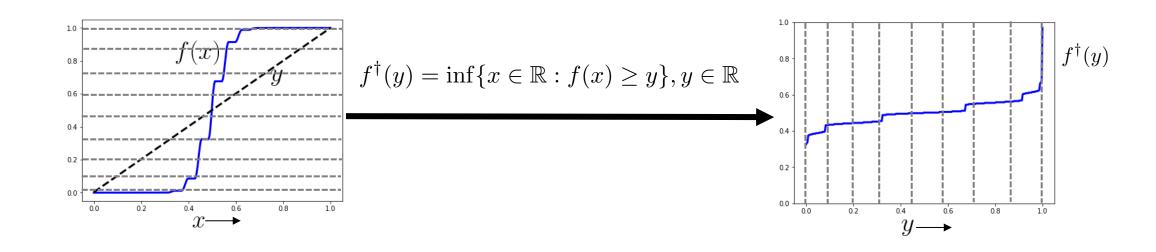
Generalized Inverse:



Generalized Inverse to Calculate SCDT



Generalized Inverse:



Signed Cumulative Distribution Transform (SCDT)

Forward:

$$\hat{s} = ((s^+)^*, ||s^+||_{L_1}, (s^-)^*, ||s^-||_{L_1})$$

Inverse:

$$s(t) = \|s^{+}\|_{L_{1}} \left((s^{+})^{*^{\dagger}}(t) \right)' s_{0}((s^{+})^{*^{\dagger}}(t)) - \|s^{-}\|_{L_{1}} \left((s^{-})^{*^{\dagger}}(t) \right)' s_{0}((s^{-})^{*^{\dagger}}(t))$$

Composition:

$$s_g = g's \circ g \implies \widehat{s}_g = (g^{-1} \circ (s^+)^*, ||s^+||_{L_1}, g^{-1} \circ (s^-)^*, ||s^-||_{L_1})$$

Convexity:

Let
$$\mathbb{S} = \{s_j | s_j = g_j' \varphi \circ g_j, \forall g_j \in \mathcal{G}\}$$
 $\widehat{\mathbb{S}} = \{\widehat{s}_j : s_j \in \mathbb{S}\} \text{ convex IFF } \mathcal{G}^{-1} = \{g_j^{-1} : g_j \in \mathcal{G}\} \text{ convex.}$

for any reference S_0

New metric/distance:

$$D_S^2(s_1, s_2) := \|\hat{s}_2 - \hat{s}_2\|_{(L^2 \times \mathbb{R}^2)} = W_2^2(s_1^+, s_2^+) + W_2^2(s_1^-, s_2^-) + \lambda(\|s_1^+|_{L_1} - \|s_2^+|_{L_1})^2 + \lambda(\|s_1^-|_{L_1} - \|s_2^-|_{L_1})^2$$

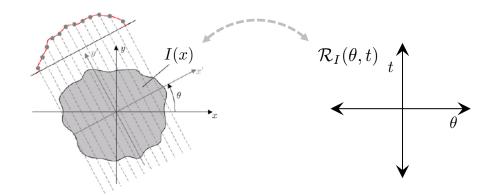
Aldroubi, Diaz Martin, Medri, Rohde, Thareja, The Signed Cumulative Distribution Transform for 1D signal analysis and classification, AIMS Foundations of Data Science, 2022

Extension to 2d, 3d, ...: Radon Cumulative distribution transform (R-CDT)

Radon Transform

Forward

$$\mathcal{R}_{I}(\theta, t) = \int I(x)\delta(t - \omega \cdot x)dx$$
$$\omega = [\sin \theta, \cos \theta]^{T}$$



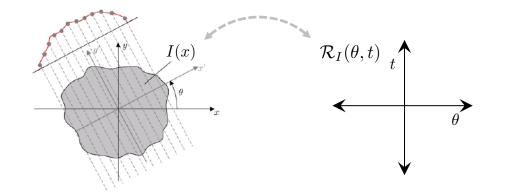
Extension to 2d, 3d, ...: Radon Cumulative distribution transform (R-CDT)

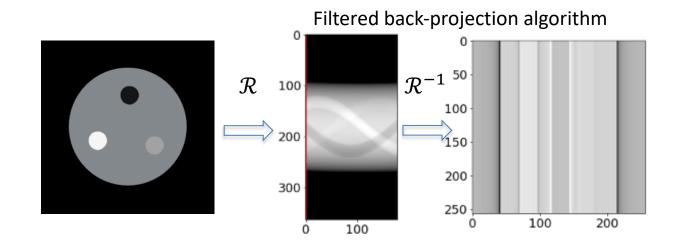
Radon Transform



$$\mathcal{R}_{I}(\theta, t) = \int I(x)\delta(t - \omega \cdot x)dx$$
$$\omega = [\sin \theta, \cos \theta]^{T}$$

Inverse
$$\mathcal{R}_I^{-1}(x) = \int_{\mathbb{S}^{d-1}} (\mathcal{R}I(\cdot,\theta) * \eta(\cdot)) \circ (x \cdot \theta) d\theta$$





Extension to 2d, 3d: Radon Cumulative distribution transform (R-CDT)

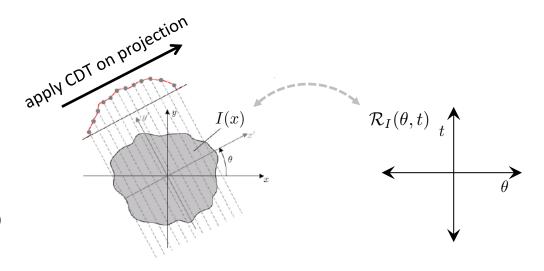
Radon Transform

Forward

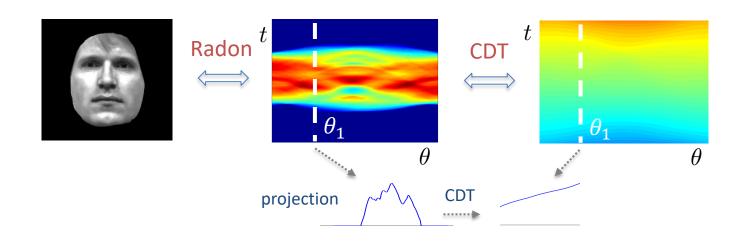
$$\mathcal{R}_{I}(\theta, t) = \int I(x)\delta(t - \omega \cdot x)dx$$
$$\omega = [\sin \theta, \cos \theta]^{T}$$

Inverse

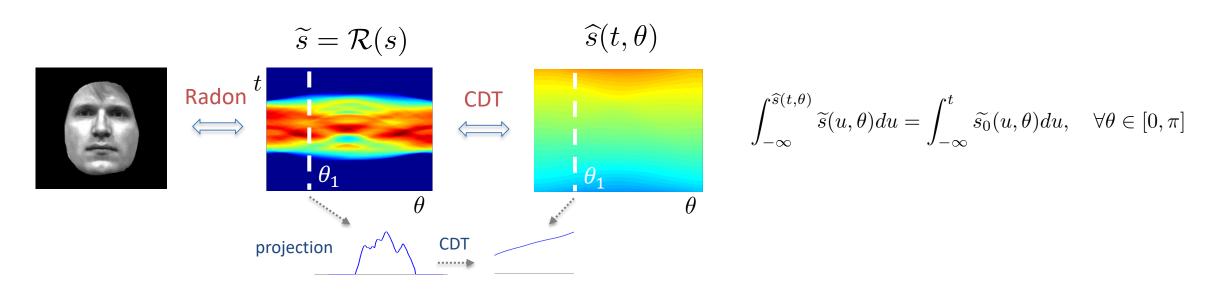
Inverse
$$\mathcal{R}_I^{-1}(x) = \int_{\mathbb{S}^{d-1}} (\mathcal{R}I(\cdot,\theta) * \eta(\cdot)) \circ (x \cdot \theta) d\theta$$



Radon Cumulative Distribution Transform



Radon Cumulative distribution transform (R-CDT)



Inverse:
$$s(\mathbf{x}) = \mathcal{R}^{-1} \left(\frac{\partial \widehat{s}^{-1}(t,\theta)}{\partial t} \widetilde{s_0} \left(\widehat{s}^{-1}(t,\theta), \theta \right) \right)$$

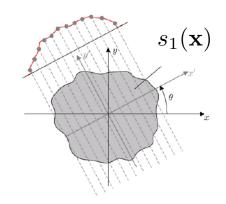
Composition:

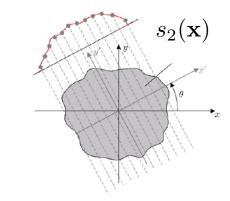
Let
$$s_{g^{\theta}}(\mathbf{x}) = \mathcal{R}^{-1}\left(\frac{\partial \widehat{s}^{-1}(g^{\theta}(t), \theta)}{\partial t} \widetilde{s_0}\left(\widehat{s}^{-1}(g^{\theta}(t), \theta), \theta\right)\right)$$

Then $\widehat{s}_{g^{\theta}}(t, \theta) = (g^{\theta})^{-1}(\widehat{s}(t, \theta))$

Sliced Wasserstein Distance

$$SW_2^2(s_1, s_2) = \int_{\Omega_{\widetilde{s}_0}} \int_0^{\pi} (\widehat{s}_1(t, \theta) - \widehat{s}_2(t, \theta))^2 \widetilde{s}_0(t, \theta) d\theta dt$$



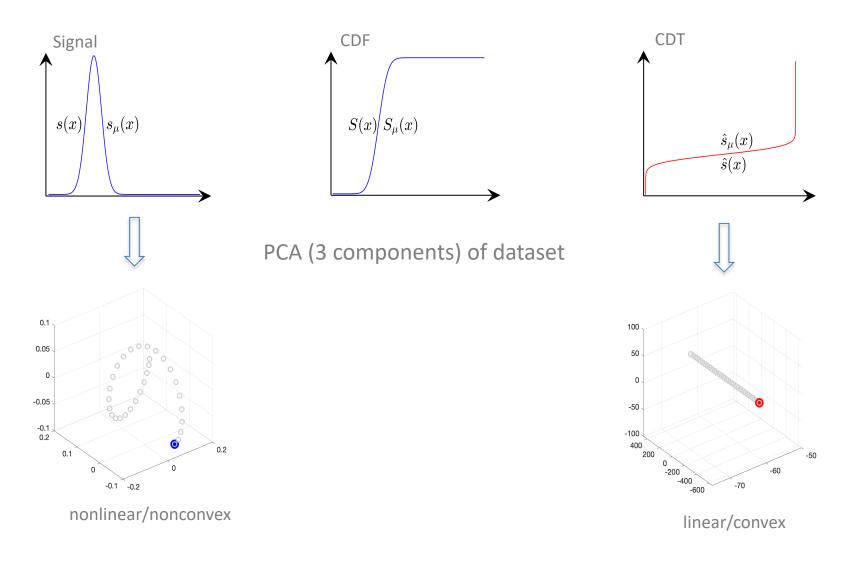


Sliced Wasserstein Embedding:

$$SW_2^2(s_1,s_2) = \left| \left| (\widehat{s}_1 - \widehat{s}_2) \sqrt{\widetilde{s_0}} \right| \right|_{L^2(\Omega_{\widetilde{s}_0})}^2$$
R-CDT

Data Geometry

Consider the data set generated by a signal and all of its translates

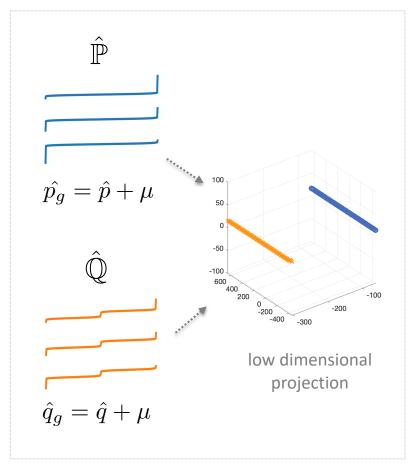


Signal classes: algebraic generative model

signal space

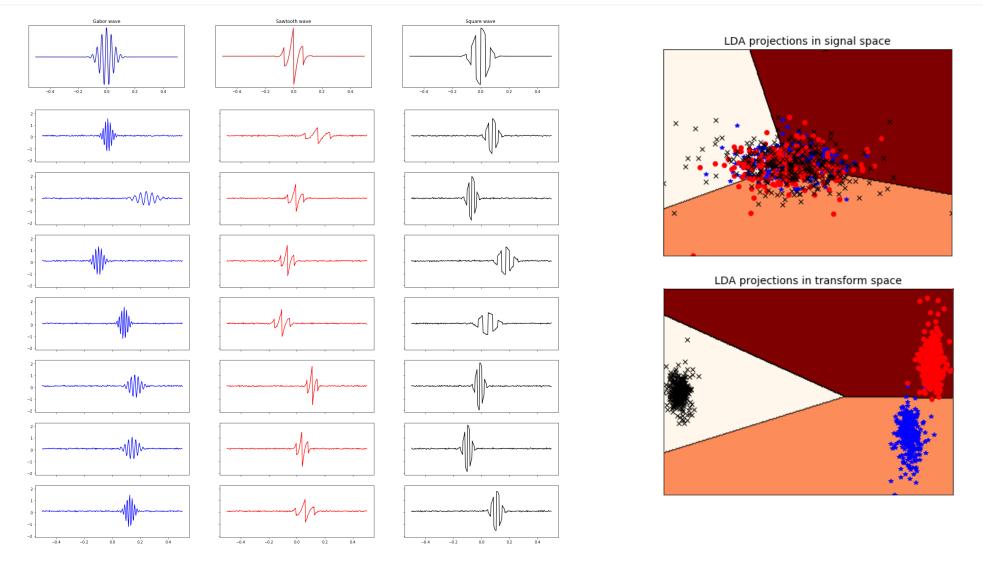
<u>Class</u> template 1 p_0 $\mathbb{P} = \{ p_g | p_g(x) = g'(x) p_0(g(x)) \}$ 0.05 -0.05 Class Q $q_0(x-\mu)$ -0.1 » 0.1 template 2 q_0 -0.2 -0.2 low dimensional projection $\mathbb{Q} = \{ q_g | q_g(x) = g'(x)q_0(g(x)) \}$

transform space



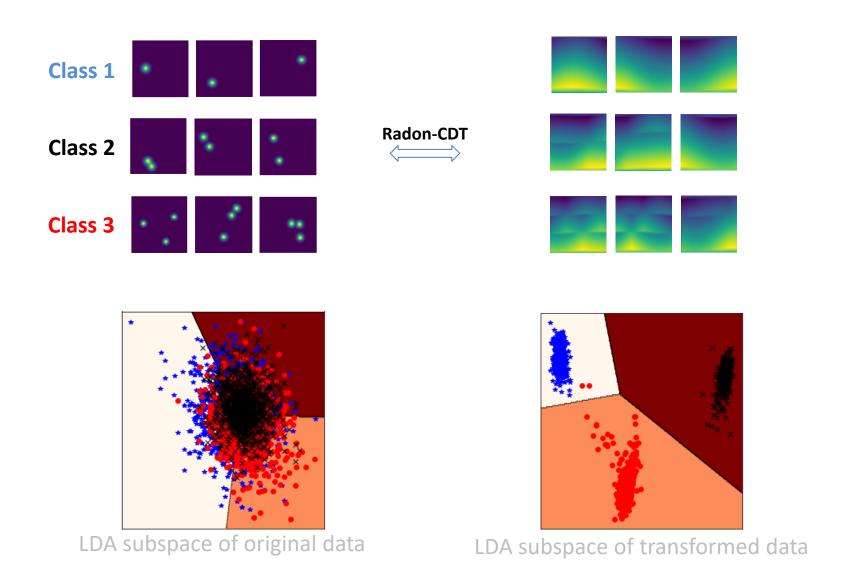
"confound" $g \in \mathcal{C}$ e.g.: translation $g(x) = x - \mu$

SCDT & linear separability



Aldroubi, Diaz Martin, Medri, Rohde, Thareja, The Signed Cumulative Distribution Transform for 1D signal analysis and classification, AIMS Foundations of Data Science, 2022

2D Example (R-CDT)



CDT: linear separation theorem

Consider signal classes:

$$\mathbb{P} = \{p_g: g \in \mathcal{C}\} \text{ and } \mathbb{Q} = \{q_g: g \in \mathcal{C}\}$$
 where
$$p_g(x) = g'(x)p_0(g(x))$$

$$p_g(x) = g'(x)q_0(g(x))$$

$$\mathbb{P} \cap \mathbb{Q} = \emptyset$$

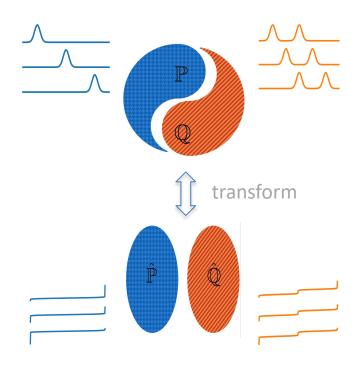
Theorem:

 $\hat{\mathbb{P}}$, $\hat{\mathbb{Q}}$ will be *convex* iff \mathcal{C}^{-1} is convex.

for any reference $\,s_0\,$ does not require knowledge of $\,p_0\,\,q_0\,$

Corollary: $\hat{\mathbb{P}}$, $\hat{\mathbb{Q}}$ linearly separable if \mathcal{C}^{-1} is convex.

To see this: $\widehat{\mathbb{P}} = \{g^{-1}(\widehat{p}(y)) | g^{-1} \in \mathcal{C}^{-1}\}$ $\widehat{\mathbb{Q}} = \{g^{-1}(\widehat{q}(y)) | g^{-1} \in \mathcal{C}^{-1}\}$ convex iff \mathcal{C}^{-1} convex



[Park, Kolouri, Kundu, Rohde, ACHA 18]
[Aldroubi, Li, Rohde, SaSiDa, 21]
[Shifat-E-Rabbi, ..., Rohde, JMIV 21]
[Aldroubi et al, AIMS Foundations of Data Science, 22]

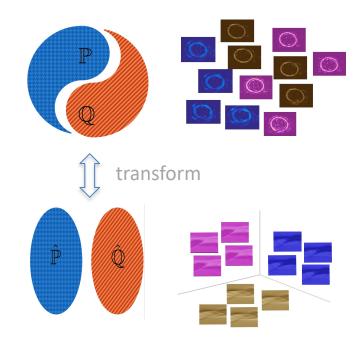
R-CDT: linear separation theorem

Consider signal classes:

$$\begin{split} \mathbb{P} &= \{p_g: g \in \mathcal{C}\} \text{ and } \mathbb{Q} = \{q_g: g \in \mathcal{C}\} \end{split}$$
 where
$$\begin{aligned} p_g &= \mathcal{R}^{-1} \left(\left(g^\theta \right)' \widetilde{p_0} \circ g^\theta \right) \\ q_g &= \mathcal{R}^{-1} \left(\left(g^\theta \right)' \widetilde{q_0} \circ g^\theta \right) \\ \mathbb{P} \cap \mathbb{Q} &= \emptyset \end{aligned}$$

Theorem:

 $\hat{\mathbb{P}}$, $\hat{\mathbb{Q}}$ will be *linearly separable* if \mathcal{C}^{-1} is convex. for any reference s_0 does not require knowledge of p_0 q_0



[Park, Kolouri, Kundu, Rohde, ACHA 18]
[Aldroubi, Li, Rohde, SaSiDa, 21]
[Shifat-E-Rabbi, ..., Rohde, JMIV 21]
[Aldroubi et al, AIMS Foundations of Data Science, 22]

Linear Optimal Transport (LOT)

Wasserstein space $(P(\Omega), W_2)$ is a Riemannian manifold



$$f_{\alpha}(x) = (1 - \alpha)x + \alpha f(x)$$

$$s_0(x) = D_f(x)s_1(f(x)), \ f = \nabla \phi = \hat{s}_1$$

Linear optimal transport (LOT):

[Wang, Slepcev, Basu, Ozolek, Rohde, IJCV 13]

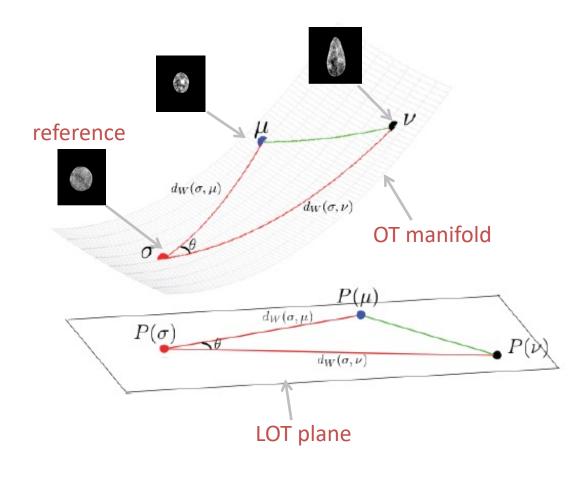
projection (invertible):

$$P(s) = \hat{s}$$

LOT distance:

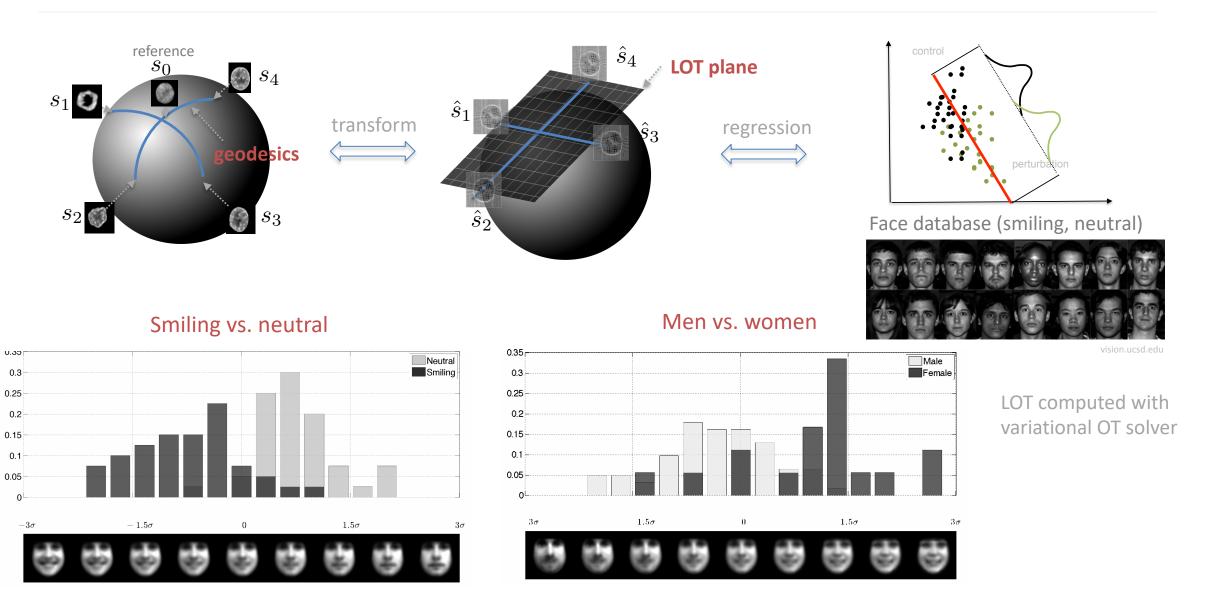
$$||P(s_1)\sqrt{s_0} - P(s_2)\sqrt{s_0}||^2$$

CDT is simply LOT projection



Azimuthal equidistant projection

Linear Optimal Transport (LOT)



Convexity property of CDT (1D):

Recall that for $\mathbb{P}(p,\mathcal{C})=\{p_g=g'p\circ g:g\in\mathcal{C}\}$ (p - template, \mathcal{C} - a set of increasing diffeomorphisms), $\hat{\mathbb{P}}$ is convex for every p iff \mathcal{C}^{-1} is convex.

Key: composition property $\widehat{p}_g = g^{-1} \circ \widehat{p}$

Corollary: If $\mathcal C$ is a convex group, the transform space is partitioned equivalent classes $\bigcup\limits_{p}\widehat{\mathbb P}(p,\mathcal C)$, where each $\widehat{\mathbb P}(p,\mathcal C)$ is convex.

Note: group $\mathcal C$ defines an equivalence relation by $p \sim_{\mathcal C} q$ iff $q \in \mathbb P(p,\mathcal C)$ i.e., $\widehat{\mathbb P}(p,\mathcal C) \cap \widehat{\mathbb P}(q,\mathcal C) \neq \emptyset \Rightarrow \widehat{\mathbb P}(p,\mathcal C) = \widehat{\mathbb P}(q,\mathcal C)$

Given a subgroup $\mathcal{C}_1\subseteq\mathcal{C}$, each $\widehat{\mathbb{P}}(p,\mathcal{C})$ can be further partitioned into a collection of convex sets

Examples of convex groups:

- scaling group: $\{\alpha \text{ id} : \alpha > 0\}$
- translation group: $\{g_{\mu}(x) = x \mu : \mu \in \mathbb{R}\}$
- affine group: $\{g_{\alpha,\mu}(x) = \alpha x \mu : \alpha > 0, \mu \in \mathbb{R}\}$
- Fixed point group: $\{f: f(x_0) = x_0: f \text{ is an increasing diffeomorphism}\}, x_0 \in \mathbb{R}$
- It can be shown there are uncountable many distinct convex subgroups

[Aldroubi, Li, Rohde, SaSiDa, 21]

Convexity property of LOT (n-D)

Unlike the 1-d case, the convexity of $\widehat{\mathbb{P}}(p,\mathcal{C})$ does not follow from the convexity of \mathcal{C}^{-1} using the same proof techniques since the composition property does not hold in general

Let
$$\mathcal{P}_d := \{p : \mathbb{R}^d \to \mathbb{R}^+ \mid \operatorname{supp}(p) = \Omega_p \text{ is compact}, \int_{\mathbb{R}^d} p(x) dx = 1\}$$
 be the set of non-negative normalized signals on \mathbb{R}^d

Theorem: Let $d \geq 2$ and $\mathcal{W}_p \subseteq \mathcal{F}_d$ be a set of deformations. If $\widehat{p}_g = g^{-1} \circ \widehat{p}$ holds for all $g \in \mathcal{W}_p$, then $\widehat{\mathbb{P}}(p, \mathcal{W}_p)$ is convex if the set \mathcal{W}_p^{-1} is convex.

Theorem: Let $d \geq 2$ and $\mathcal{W} \subseteq \mathcal{F}_d$ be a set of deformations. If for any $p \in \mathcal{P}_d$, $\widehat{p}_g = g^{-1} \circ \widehat{p}$ holds all $g \in \mathcal{W}$ then $\mathcal{W} \subseteq \mathcal{H}_a := \{h(x) = ax + u : a > 0, u \in \mathbb{R}^d\}$, i.e., if the composition property holds regardless of p, \mathcal{W} has to be a subset of compositions of translation and scaling diffeomorphisms.

Remark: one can relax the condition $p \in \mathcal{P}_d$ above to hold on a subset of \mathcal{P}_d and enlarge \mathcal{W} .

Open questions: Can one derive the convexity of $\widehat{\mathbb{P}}(p,\mathcal{W})$ from the convexity of \mathcal{W}^{-1} without the composition property being true for all $g \in \mathcal{W}$? Are there other conditions one can impose on the model $\mathbb{P}(p,\mathcal{W})$ other than \mathcal{W}^{-1} being convex so that $\widehat{\mathbb{P}}(p,\mathcal{W}_p)$ is convex?

[Aldroubi, Li, Rohde, SaSiDa, 21]

A relaxation in dimension d=2

Definition 4.8 (Restrictive sets of transformations and PDFs).

(16)
$$\mathcal{H}_r = \left\{ h(x,y) := \frac{1}{2} \begin{bmatrix} f'(x+y) + g'(x-y) \\ f'(x+y) - g'(x-y) \end{bmatrix} \mid f, g \in \mathcal{R} \right\}$$

where $\mathcal{R} = \{ f \in C^2(\mathbb{R}) \mid f' \text{ is a strictly increasing bijection on } \mathbb{R} \}.$

(17)
$$\mathcal{P}_r := \{ p \in \mathcal{P}_2 : |\det J_h| (p \circ h) = r \text{ for some } h \in \mathcal{H}_r \}.$$

Note: \mathcal{H}_r is a convex group .

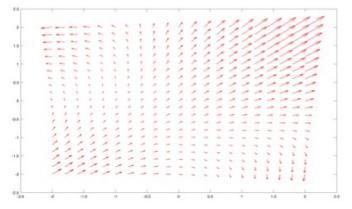


FIGURE 6. A vector field h on a grid $[-2,2] \times [-2,2]$ generated with $f'(t) = t + 0.1t^2$ and g'(t) = t.

Theorem 4.10. For any $p \in \mathcal{P}_r$, we have $\widehat{p}_h = h^{-1} \circ \widehat{p}$ for any $h \in \mathcal{H}_r$ where $p_h = |\det J_h| \cdot p \circ h$.

Note: here the generating template r for \mathcal{P}_r is the same as reference r for computing the LOTs

Example 2. Let $\mathcal{R}_s = \{f(t) = at^2 + bt \mid a > 0, b \in \mathbb{R}\}$ and $\mathcal{H}_s = \{h(x,y) = \frac{1}{2}\nabla (f(x+y) + g(x-y)) \mid f,g \in \mathcal{R}_s\}$

By direct computation, it is easy to see that every $h \in \mathcal{H}_s$ is of the form

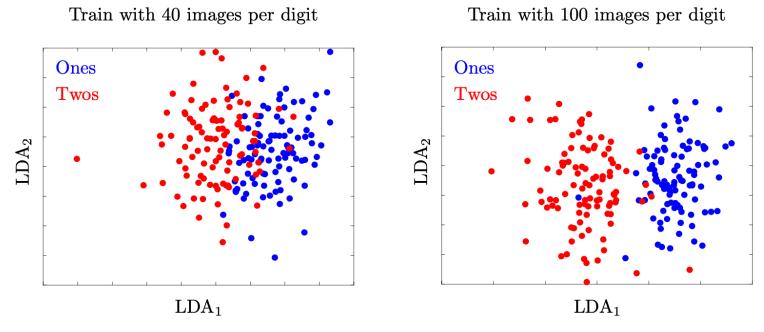
(20)
$$h(x,y) = (a_1 + a_2) \begin{bmatrix} x \\ y \end{bmatrix} + (a_1 - a_2) \begin{bmatrix} y \\ x \end{bmatrix} + \begin{bmatrix} b_1 - b_2 \\ b_1 + b_2 \end{bmatrix},$$

a convex group of diffeomorphisms under the composition operation.

and vice versa, where $a_1, a_2 > 0$ and $b_1, b_2 \in \mathbb{R}$. Equivalently, $h(x, y) = A \begin{bmatrix} x \\ y \end{bmatrix} + u$, where $A = \begin{bmatrix} a_1 + a_2 & a_1 - a_2 \\ a_1 - a_2 & a_1 + a_2 \end{bmatrix}$ and $u = \begin{bmatrix} b_1 - b_2 \\ b_1 + b_2 \end{bmatrix}$. It is not difficult to show that \mathcal{H}_s is

[Moosmüller, Cloninger, 21] Linear Optimal Transport Embedding: Provable Wasserstein classification for certain rigid transformations and perturbations https://arxiv.org/abs/2008.09165

- explored settings when LOT embeds family of distributions into linearly separable sets
- linear separability: if $\mathcal{P} = \{\mu_i : y_i = 1\}$ are ϵ -perturbations of shifts and scalings of μ and $\mathcal{Q} = \{\nu_i : y_i = -1\}$ are are ϵ -perturbations of shifts and scalings of ν , and \mathcal{P} and \mathcal{Q} have a small minimal distance depending on ϵ , then \mathcal{P} and \mathcal{Q} are linearly separable in the LOT embedding space.
- provided conditions when the LOT distance between two measures is nearly isometric to the Wasserstein distance



LDA embedding plots for the MNIST classification of digits 1 and 2 using LOT.

figure credit: Moosmüller et al.

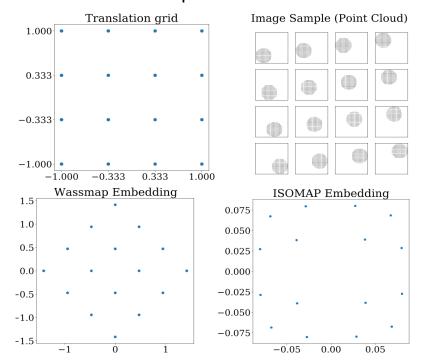
[Hamm, Henscheid, Kang, 22] Wassmap: Wasserstein Isometric Mapping for Image Manifold Learning https://arxiv.org/abs/2204.06645

Proposed a variant of ISOMAP called Wassmap, where classical multi-dimensional scaling (MDS) is applied to

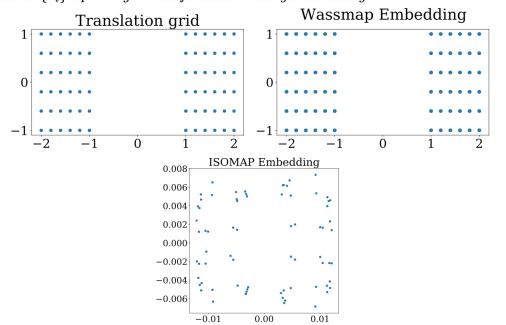
Algorithm 3.1 Functional Wasserstein Isometric Mapping (Functional Wassmap)

- 1: **Input:** Probability measures $\{\mu_i\}_{i=1}^N \subset \mathbb{W}_2(\mathbb{R}^m)$; embedding dimension d
- 2: Output: Low-dimensional embedding points $\{z_i\}_{i=1}^N \subset \mathbb{R}^d$
- 3: Compute pairwise Wasserstein distance matrix $W_{ij} = W_2^2(\mu_i, \mu_j)$
- 4: $B = -\frac{1}{2}HWH$, where $(H = I \frac{1}{N}\mathbb{1}_N)$ 5: (Truncated SVD): $B_d = V_d\Lambda_dV_d^T$
- 6: $z_i = (V_d \Lambda_d^{\frac{1}{2}})(i,:)$, for i = 1, ..., N
- 7: Return: $\{z_i\}_{i=1}^N$
- Recover manifold parametrizations

pairwise Wasserstein distances of data



THEOREM A. Let $\Theta \subset \mathbb{R}^d$ be a parameter set that generates a smooth submanifold $\mathcal{M}(\Theta) \subset \mathbb{W}_2(\mathbb{R}^m)$ such that $(\mathcal{M}, \mathcal{W}_2)$ is isometric up to a constant to $(\Theta, |\cdot|_{\mathbb{R}^d})$. If $\{\theta_i\}_{i=1}^N \subset \Theta$, and $\{\mu_{\theta_i}\}_{i=1}^N \subset \mathcal{M}$ are the corresponding measures on the manifold, then the Functional Wassmap Algorithm (Algorithm 3.1) with embedding dimension d recovers $\{\theta_i\}$ up to rigid transformation and global scaling.



- studied the local linearization of the Hellinger–Kantorovich distance via its Riemannian structure.
- Hellinger–Kantorovich distance defines a metric for non-negative measures which allows for the creation/destruction of mass within the optimal transport framework and can be seen as a particular variant of an 'unbalanced' transport problem

DEFINITION 3.1 (Continuity equation with source). For $\mu_0, \mu_1 \in \mathcal{M}(\Omega)$ we denote by $\mathcal{CES}(\mu_0, \mu_1)$ the set of solutions for the continuity equation with source on $[0,1] \times \Omega$, i.e. the set of triplets of measures $(\rho, \omega, \zeta) \in \mathcal{M}([0,1] \times \Omega)^{1+d+1}$ where ρ interpolates between μ_0 and μ_1 and that solve

$$\partial_t \rho + \operatorname{div} \omega = \zeta$$

[Beier, Beinert, Steidl, 21] On a linear Gromov–Wasserstein distance https://arxiv.org/pdf/2112.11964.pdf

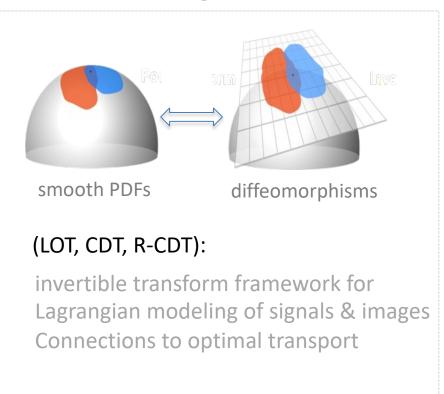
- Gromov-Wasserstein (GW) distance is invariant under translation and rotation, is practical for applications such as shape comparison
- defined a generalized LOT based on barycentric projection maps of transport plans, which coincides with LOT when the reference (base) measure is absolutely continuous
- defined a notion of generalized linear Gromov-Wasserstein (gLGW) distance to alleviate computational cost of GW

[Nenna, Pass, 22] Transport type metrics on the space of probability measures involving singular base measures

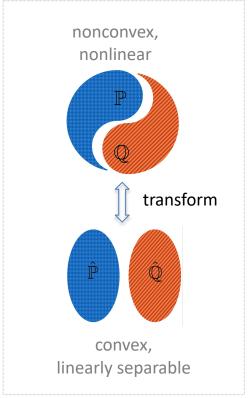
- $\bullet \quad \text{Semi-metric inspired by generalized geodesics} \quad W_{\nu}(\mu_1,\mu_0) := \sqrt{\inf_{\gamma \in \mathcal{P}(X \times X \times X) \mid \gamma_{yx_i} \in \Pi_{opt}(\mu_i,\nu), i=0,1} \int_{X \times X \times X} |x_0 x_1|^2 d\gamma(y,x_0,x_1)}.$
- the base measure ν can be singular, e.g., concentrated on a lower dimensional manifold -- related to the <u>unequal</u> <u>dimensional OT</u>; If ν is concentrated on a line segment <u>layerwise-Wasserstein metric</u>; LOT distance can be seen as a special case
- If ν abs. continuous w.r.t Lebesgue, $W_{\nu}(\mu_0,\mu_1)=\int_{\mathbb{R}^n}|\tilde{T}_0(y)-\tilde{T}_1(y)|^2d\nu(y)$ -- LOT
- If $u=\delta_{\mathcal{Y}}$, $W^2_{
 u}(\mu_0,\mu_1)=\inf_{\pi\in\Pi(\mu_0,\mu_1)}\int_{X imes X}|x_0-x_1|^2d\pi(x_0,x_1)$ standard Wasserstein

Summary: Transport & other Lagrangian Transforms

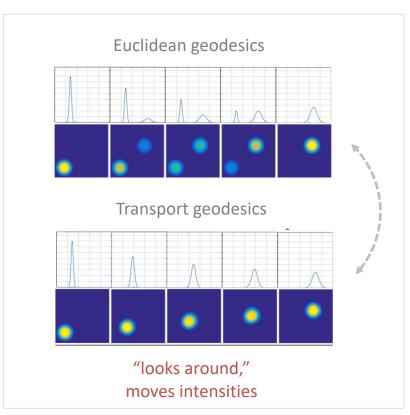
Nonlinear signal transform



Properties



Intuition



Imagedatascience.com/transport