Linearised Optimal Transport Distances

Kantorovich Initiative

Matthew Thorpe

Joint Work with Tianji Cai (University of California Santa Barbara), Junyi Cheng (University of California Santa Barbara), Oliver Crook (University of Oxford), Mihai Cucuringu (University of Oxford), Soheil Kolouri (University of Vanderbilt), Serim Park (Twitter), Gustavo Rohde (University of Virginia), Bernhard Schmitzer (University of Götingen), Caola Schönlieb (University of Cambridge), Dejan Slepčev (Carnegie Mellon University), and Kostas Zygalakis (University of Edinburgh)

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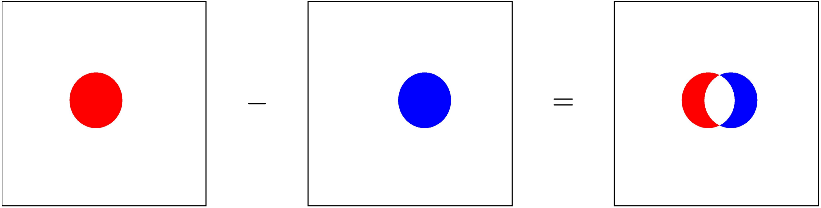
4th May 2023

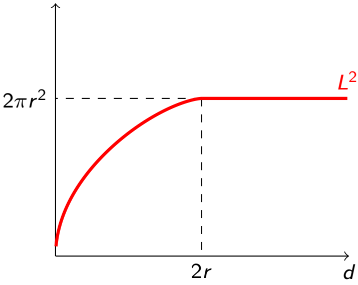
Euclidean Distances

A Euclidean distance considers a pixel-by-pixel difference.



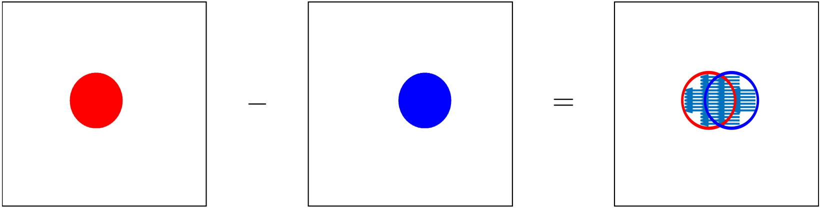
For example, the L^2 distance:

$$d_{L^2}(f,g) = \sqrt{\int_\Omega |f(x) - g(x)|^2 \, \mathrm{d}x}.$$



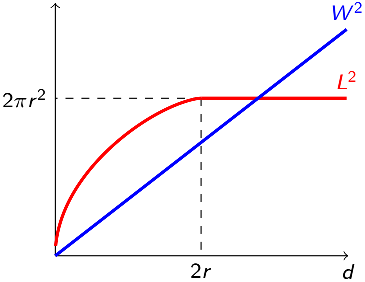
Lagrangian Distances

A Lagrangian distance considers the distance moved.



For example, the Wasserstein distance:

$$d_{W^2}(f, g) \sim \text{size of translation.}$$



Motivation

The Wasserstein distance is *great* as a distance between signals/images, because...

1. Lagrangian modelling,
2. simple to understand compared to other Lagrangian methods such as large deformation diffeomorphic metric mapping,
3. metric properties (in particular symmetry).
4. geodesics and Riemannian structure,
5. theoretical and characterising properties such as existence of optimal transport maps and optimal transport plans (under appropriate conditions).

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Solution: **linearise an unbalanced/functional optimal transport distances!**

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$$\mathrm{d}^2_{\mathrm{W}^2}(\mu,\nu) := \inf \left\{ \int_0^1 \int_\Omega \left\| \frac{\mathrm{d}\omega_t}{\mathrm{d}\rho_t}(x) \right\|^2 \mathrm{d}\rho_t(x)\,\mathrm{d}t \;:\; (\rho,\omega) \in \mathcal{CE}(\mu,\nu) \right\}$$

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Under appropriate conditions all three are equivalent.

1. Let $v_t = \frac{\mathrm{d}\omega_t}{\mathrm{d}\rho_t}$, then

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2. If $T_t^* = tT^* + (1-t)\mathrm{Id}$ is the optimal map then $\mu_t = [T_t^*]_\# \mu$ is the geodesic between μ and ν.

The Riemannian Structure of Wasserstein Spaces

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4. Hence $\mathrm{d}^2_{\mathrm{W}^2}(\mu, \nu) = \int_\Omega \|v_0\|^2 \,\mathrm{d}\mu(x)$.
5. Let $g_{\mathrm{W}^2}(\mu; u, v) = \int_\Omega u \cdot v \,\mathrm{d}\mu$, then
$$\mathrm{d}^2_{\mathrm{W}^2}(\mu, \nu) = g_{\mathrm{W}^2}(\mu; v_0, v_0).$$

The Linear Wasserstein Distance

1. Let $\mathrm{Log}_{\mathrm{W}^2}(\mu;\nu) = v_0$, so

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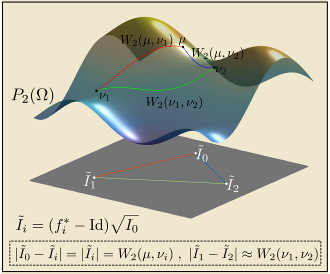

Figure credit: Soheil Kolouri.

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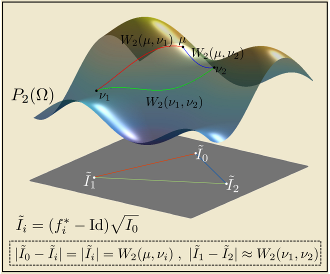

$$\mathrm{d}_{\mathrm{W}^2,\mu,\mathrm{lin}}(\mu_1,\mu_2) = \|\mathrm{Log}_{\mathrm{W}^2}(\mu;\mu_1) - \mathrm{Log}_{\mathrm{W}^2}(\mu;\mu_2)\|_{\mathrm{L}^2(\mu)}.$$

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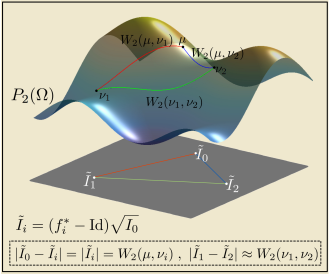

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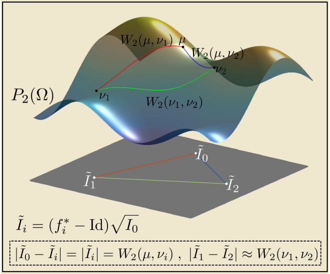

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4. **Linear Optimal Transport Assumption:**

$$\mathrm{d}_{\mathrm{W}^2}(\mu_1,\mu_2) \approx \mathrm{d}_{\mathrm{W}^2,\mu,\mathrm{lin}}(\mu_1,\mu_2) = \|P_{\mathrm{W}^2,\mu,\mathrm{lin}}(\mu_1) - P_{\mathrm{W}^2,\mu,\mathrm{lin}}(\mu_2)\|_{\mathrm{L}^2(\mu)}.$$

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Approximate Numerical Method

1. Solve the Kantorovich formulation to find π^* (e.g. Sinkhorns algorithm)

$$\mathrm{d}^2_{\mathrm{W}^2}(\mu,\nu) := \min_{\pi\in\Pi(\mu,\nu)} \int_{\Omega\times\Omega} |x-y|^2 \,\mathrm{d}\pi(x,y).$$

2. Extract T^* the optimal Monge map from $\pi^* = (\mathrm{Id}\times T^*)_{\#}\mu$

$$\mathrm{d}^2_{\mathrm{W}^2}(\mu,\nu) := \inf_{T\,:\,T_{\#}\mu=\nu} \int_{\Omega} |x-T(x)|^2 \,\mathrm{d}\mu(x).$$

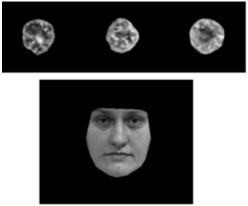
3. Compute the velocity map at time $t=0$, i.e. $v_0 = T^* - \mathrm{Id}$

$$\mathrm{d}^2_{\mathrm{W}^2}(\mu,\nu) = \int_{\Omega} \|v_0\|^2 \,\mathrm{d}\mu(x).$$

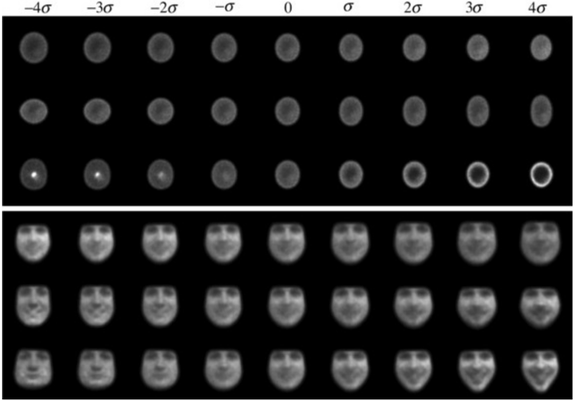
Road map:

$$\nu \quad\mapsto\quad \pi^* \quad\mapsto\quad T^* \quad\mapsto\quad v_0.$$

Example Data:



Principle Component Analysis on Linear Embedding:



Source: Wang, Slepčev, Basu, Ozolek and Rohde, *A Linear Optimal Transportation Framework for Quantifying and Visualizing Variations in Sets of Images*, International Journal of Computer Vision 101(2):254–269, 2013.

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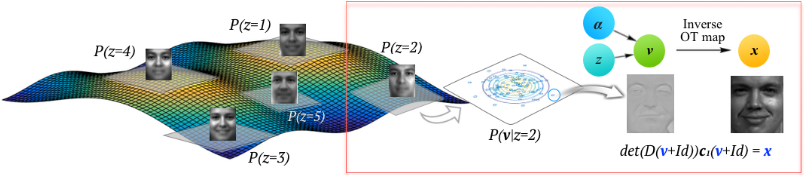

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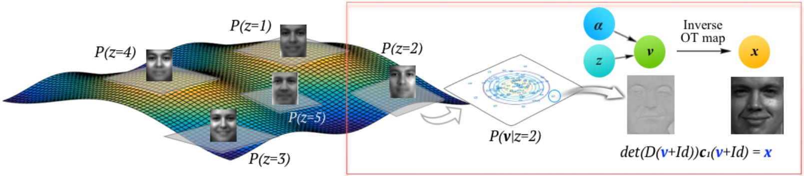

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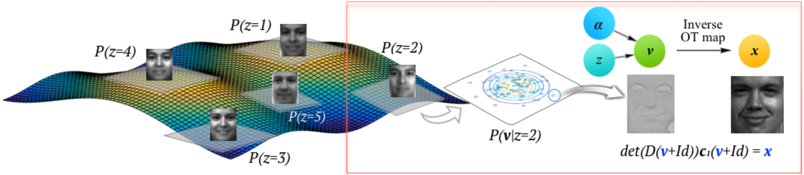

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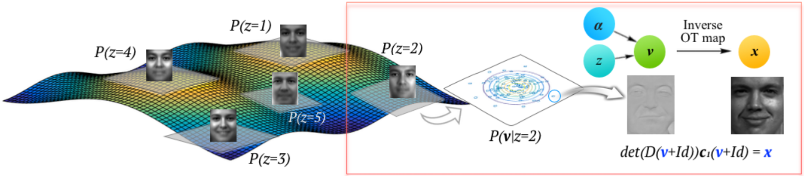
    1. Cluster the data $\{\mu_i\}_{i=1}^n$ into K groups.



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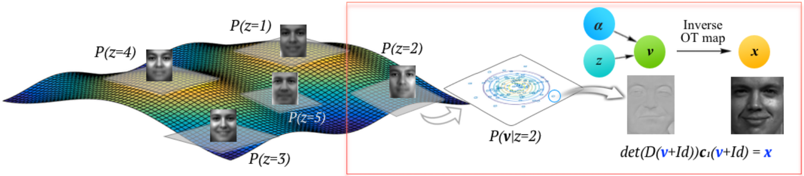

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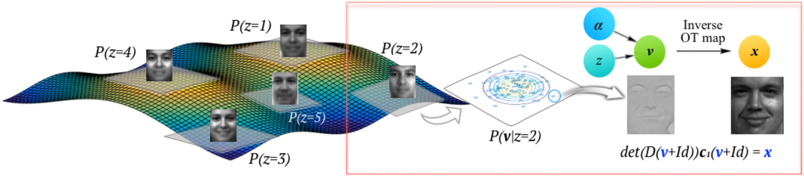

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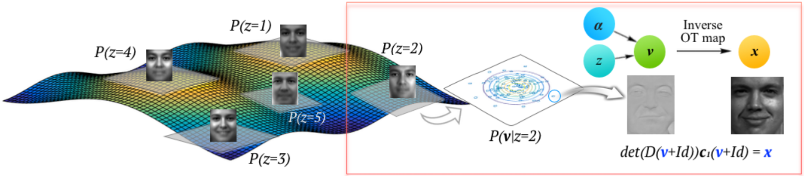
    3. At each of the K centres model the tangent space by a Gaussian with mean m_k and covariance W_k.
    4. To generate a new data point (i) sample a cluster centre $k \in \{1, \ldots, K\}$, then (ii) sample a tangent vector $v \sim N(m_k, W_k)$, finally (iii) create a new image by pushing forward the cluster centre ν_k by the transport map $T = v + \mathrm{Id}$.



Are we Learning New Images?

1. Top row, all 19 original images.
2. Second and third rows, generated images.

Source: Park and T., *Representing and Learning High Dimensional Data with the Optimal Transport Map from a Probabilistic Viewpoint*, CVPR, 2018.

Unbalanced Optimal Transport via Benamou–Brenier

1. Recall the continuity equation:

$$(\rho, \omega) \in \mathcal{CE}(\mu, \nu) \Leftrightarrow \frac{\partial \rho}{\partial t} + \nabla_x \omega = 0, \rho_0 = \mu, \rho_1 = \nu.$$

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4. The Hellinger–Kantorovich distance:

$$\mathrm{d}^2_{\mathrm{HK}}(\mu,\nu):=\inf_{(\rho,\omega,\zeta)\in\mathcal{CES}(\mu,\nu)}\int_0^1\int_\Omega\left(\left\|\frac{\mathrm{d}\omega_t}{\mathrm{d}\rho_t}\right\|^2+\frac{1}{4}\left(\frac{\mathrm{d}\zeta_t}{\mathrm{d}\rho_t}\right)^2\right)\mathrm{d}\rho_t\,\mathrm{d}t.$$

Soft Marginal Kantorovich Form

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$$\mathrm{KL}(\mu|\nu) = \int \varphi\left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu}\right)\,\mathrm{d}\nu$$

if $\mu \ll \nu$ and where $\varphi(s) = s\log(s) - s + 1$.

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3. Then, (Liero, Mielke and Saveré (2018))

$$\mathrm{d}^2_{\mathrm{HK}}(\mu,\nu) = \inf_{\pi\in\mathcal{M}_+(\Omega^2)} \left\{ \int_{\Omega^2} c\,\mathrm{d}\pi + \mathrm{KL}(P_{1\#}\pi|\mu) + \mathrm{KL}(P_{2\#}\pi|\nu) \right\}.$$

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$$\mathrm{d}^2_{\mathrm{HK}}(\mu,\nu) = \inf_{\pi\in\mathcal{M}_+(\Omega^2)} \left\{ \int_{\Omega^2} c\,\mathrm{d}\pi + \mathrm{KL}(P_{1\#}\pi|\mu) + \mathrm{KL}(P_{2\#}\pi|\nu) \right\}.$$

4. Furthermore, there exists π^*, T^* and $\tilde{\mu}$ such that $\pi^* = (\mathrm{Id}\times T^*)_{\#}\tilde{\mu}$ is optimal.

PARENTAL
ADVISORY
EXPLICIT CONTENT

Warning: Long (and uninformative) equations are present on the next slide.

Hellinger–Kantorovich Geodesics via Optimal Plans

Let $\mu, \nu \in \mathcal{M}_+(\Omega)$, π^* optimal and T^* be the Monge map $\pi^* = (\mathrm{Id} \times T^*)_\# \tilde{\mu}$. Let $\tilde{\mu} = P_{1\#}\pi^*$, $\tilde{\nu} = P_{2\#}\pi^*$ and write

$$\mu = u\tilde{\mu} + \mu^\perp \qquad \nu = w\tilde{\nu} + \nu^\perp.$$

Then a geodesic is given by

$$\begin{aligned}
\tilde{\rho}_t &= X\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right)_\# \left[M\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right) \tilde{\mu}\right] \\
\rho_t &= \tilde{\rho}_t + (1-t)^2\mu^\perp + t^2\nu^\perp \\
\omega_t &= X\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right)_\# \left[M\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right) \frac{\partial X}{\partial t}\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right) \tilde{\mu}\right] \\
\tilde{\zeta}_t &= X\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right)_\# \left[\frac{\partial M}{\partial t}\left(t; \cdot, u(\cdot), T^*(\cdot), w \circ T^*(\cdot)\right) \tilde{\mu}\right] \\
\zeta_t &= \tilde{\zeta}_t - 2(1-t)\mu^\perp + 2t\nu^\perp.
\end{aligned}$$

where

$$\begin{aligned}
M(t) &= (1-t)^2 m_0 + t^2 m_1 + 2t(1-t)\sqrt{m_0 m_1}\cos\|x_0 - x_1\| \\
\varphi(t) &= \cos^{-1}\left(\frac{(1-t)\sqrt{m_0} + t\sqrt{m_1}\cos(\|x_0 - x_1\|)}{\sqrt{M(t)}}\right) \\
X(t) &= x_0 + \frac{x_1 - x_0}{\|x_0 - x_1\|}\varphi(t).
\end{aligned}$$

Time Independent Benamou–Brenier Form

Thm: Let $\mu, \nu \in \mathcal{M}_+(\Omega)$ and $\pi^* = (\mathrm{Id} \times T^*)_\# \tilde{\mu}$ be optimal. Let (ρ, ω, ζ) be the geodesics constructed on the previous slide. Set for $t \in [0, 1)$:

$$v_t = \frac{\mathrm{d}\omega_t}{\mathrm{d}\rho_t} \qquad\qquad \alpha_t = \frac{\mathrm{d}\tilde{\zeta}_t}{\mathrm{d}\rho_t} - 2(1-t)\frac{\mathrm{d}\mu^\perp}{\mathrm{d}\rho_t}.$$

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Then

$$v_0(x) = \begin{cases} \frac{T^*(x)-x}{\|T^*(x)-x\|}\sqrt{\frac{w(T^*(x))}{u(x)}}\sin(\|T^*(x)-x\|) & \tilde{\mu}\text{-a.e.}, \\ 0 & \mu^\perp\text{-a.e.}, \end{cases}$$

$$\alpha_0(x) = \begin{cases} 2\left(\sqrt{\frac{w(T^*(x))}{u(x)}}\cos(\|T^*(x)-x\|) - 1\right) & \tilde{\mu}\text{-a.e.}, \\ -2 & \mu^\perp\text{-a.e.} \end{cases}$$

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and

$$\mathrm{d}^2_{\mathrm{HK}}(\mu, \nu) = \int_\Omega \left(\|v_0\|^2 + \frac{1}{4}(\alpha_0)^2\right) \mathrm{d}\mu + \|\nu^\perp\|.$$

Linear Hellinger–Kantorovich Distance

1. One can show that $\tilde{\mu}, \mu^\perp \perp \nu^\perp$, so $\mu \perp \nu^\perp$.

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3. Let $\mathrm{Log}_{\mathrm{HK}}(\mu;\nu) = (v_0, \alpha_0)$, so

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$$\mathrm{d}_{\mathrm{HK},\mu,\mathrm{lin}}(\mu_1, \mu_2) = \|\mathrm{Log}_{\mathrm{HK}}(\mu; \mu_1) - \mathrm{Log}_{\mathrm{HK}}(\mu; \mu_2)\|_{\mathrm{L}^2(\mu)}.$$

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$$P_{\mathrm{HK},\mu,\mathrm{lin}}(\mu_i) = \mathrm{Log}_{\mathrm{HK}}(\mu; \mu_i).$$

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6. **Linear Hellinger–Kantorovich Assumption:**

$$\mathrm{d}_{\mathrm{HK}}(\mu_1, \mu_2) \approx \mathrm{d}_{\mathrm{HK},\mu,\mathrm{lin}}(\mu_1, \mu_2) = \|P_{\mathrm{HK},\mu,\mathrm{lin}}(\mu_1) - P_{\mathrm{HK},\mu,\mathrm{lin}}(\mu_2)\|_{\mathrm{L}^2(\mu)}.$$

Approximate Numerical Method

1. Solve the Kantorovich formulation to find π^* (e.g. Sinkhorns algorithm)

$$\mathrm{d}^2_{\mathrm{HK}}(\mu,\nu) = \inf_{\pi \in \mathcal{M}_+(\Omega^2)} \left\{ \int_{\Omega^2} c \,\mathrm{d}\pi + \mathrm{KL}(P_{1\#}\pi|\mu) + \mathrm{KL}(P_{2\#}\pi|\nu) \right\}.$$

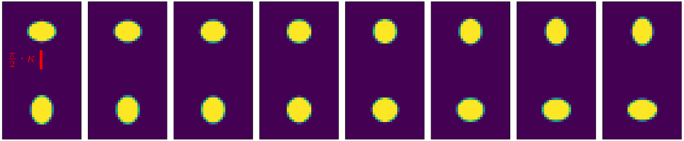
2. Extract T^* the optimal Monge map from $\pi^* = (\mathrm{Id} \times T^*)_{\#}\tilde{\mu}$ and the densities u, w.
3. Compute the velocity and growth maps at time $t = 0$, i.e. v_0, α_0 using the previous theorem

$$\mathrm{d}^2_{\mathrm{HK}}(\mu,\nu) = \int_{\Omega} \left(\|v_0\|^2 + \frac{1}{4}(\alpha_0)^2 \right) \mathrm{d}\mu.$$

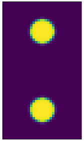
Road map:

$$\nu \quad \mapsto \quad \pi^* \quad \mapsto \quad (T^*, u, w) \quad \mapsto \quad (v_0, \alpha_0).$$

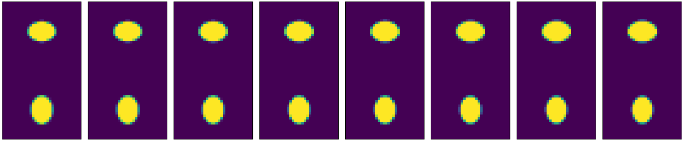
A Toy Example: Data and Barycentres



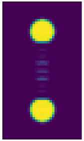
(a) samples for different elongations p_1 (sizes p_2 fixed)



(c) HK barycenter

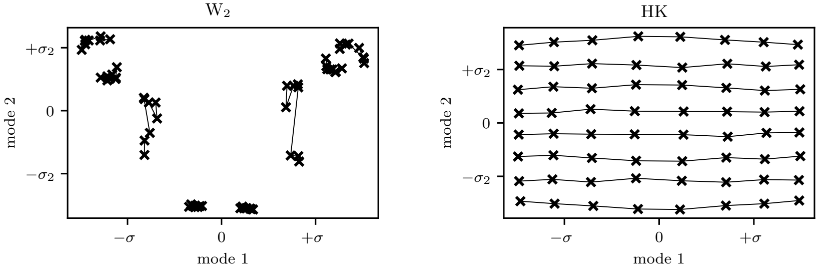


(b) samples for different sizes p_2 (elongations p_1 fixed)

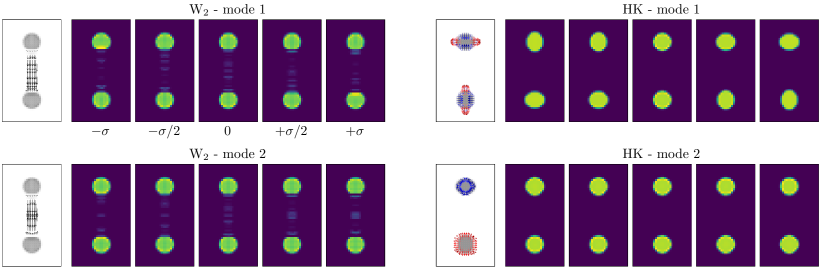


(d) W_2 barycenter

A Toy Example: 2D PCA Projection



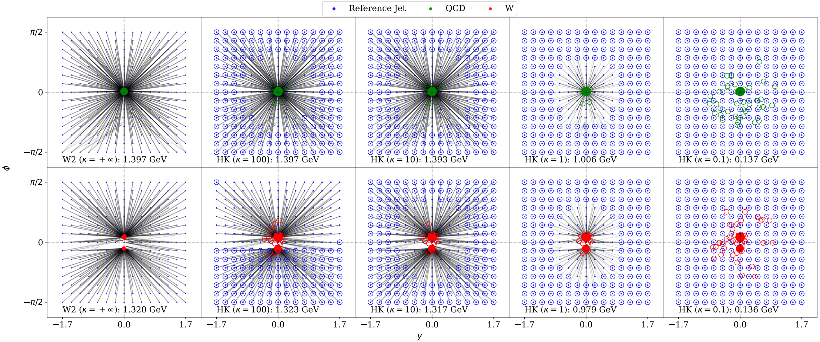
A Toy Example: Dominant Eigenmodes



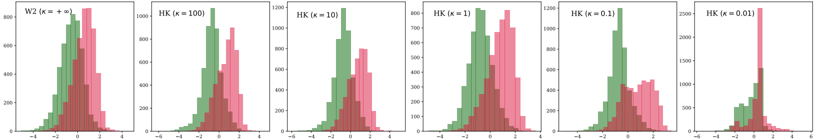
For each mode, the quiver plot on the left shows the initial velocity field v_0, for HK the color of the arrows encodes α_0 (blue means decrease, red increase of mass). The five images on the right visualize the exponential map evaluated between $-\sigma$ and σ where σ denotes the standard deviation along the considered mode.

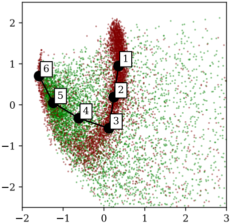
Collider Events: Data

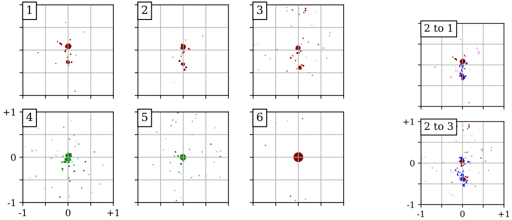
Aim: Jet tagging. In particular, can we label W boson jets and QCD (quark or gluon) jets from a simulated dataset of particle collider events observed in the rapidity-azimuth plan (i.e. $\Omega \subset \mathbb{R}^2$).



Collider Events: LDA and PCA







Collider Events: Labelling

Table: Results for the W vs. QCD jet tagging task using LDA, kNN and SVM on the (unbalanced) linearized OT embeddings for various length scale parameters κ ($\kappa = +\infty$ denotes balanced the Wasserstein distance).

	length scale κ	$+\infty$	100	10	5	1	0.7	0.5	0.3	0.1	0.05	0.01
LDA	**AUC**	0.694	0.733	0.746	0.747	0.752	0.751	0.748	0.760	**0.765**	0.763	0.642
	TPR	0.684	0.684	0.703	0.721	0.724	0.740	0.736	0.692	0.704	0.731	**0.770**
	FPR	0.296	0.218	0.211	0.226	0.220	0.239	0.239	**0.171**	0.174	0.205	0.486
	run time	several seconds										
kNN	**AUC**	0.821	0.818	0.819	0.818	0.829	0.841	**0.849**	0.847	0.821	0.772	0.671
	TPR	0.771	0.763	0.768	0.763	0.760	0.791	0.798	0.809	**0.821**	0.783	0.733
	FPR	0.128	0.127	0.130	0.126	0.102	0.110	**0.100**	0.114	0.181	0.238	0.390
	hyperpar. k	30	20	30	20	10	20	10	20	10	10	30
	run time	1.5 hours										
SVM	**AUC**	0.842	0.842	0.842	0.841	0.849	0.851	**0.856**	0.853	0.845	0.806	0.694
	TPR	0.817	0.819	0.817	0.819	0.823	0.829	**0.832**	0.829	0.788	0.741	0.787
	FPR	0.133	0.134	0.134	0.137	0.126	0.127	0.120	0.124	**0.099**	0.128	0.401
	hyperpar. C	1	1	1	1	1	1	1	1	1	10	10
	hyperpar. γ	100	100	100	100	100	100	100	100	1000	1000	100000
	run time	5 hours										

TL^p Definition

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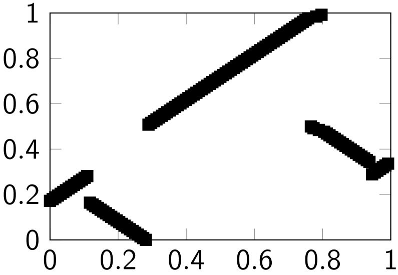
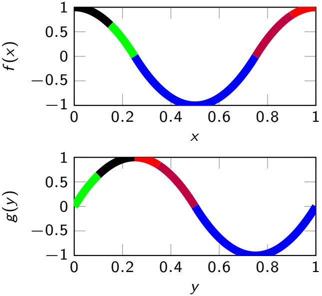
5. TL^p definition (Monge formulation):

$$\mathrm{d}^p_{\mathrm{TL}^p}((f,\mu),(g,\nu)) = \inf_{T:T_{\#}\mu=\nu} \int_X |x - T(x)|^p + |f(x) - g(T(x))|^p \,\mathrm{d}\mu(x).$$

A Simple Example

For example consider the functions $f(x) = \cos(2\pi x)$ and $g(y) = \sin(2\pi y)$ defined on $[0, 1]$ with the uniform measure. The optimal plan using the TL^2 distance is given below.





Relationship Between TL^p and OT: via the Cost Function

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2. So TL^p is a special case of OT with cost function $c(x,y;f,g) = |x-y|^p + |f(x) - f(y)|^p$.

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4. This includes Cuturi's entropy regularised approach (Sinkhorn algorithm).

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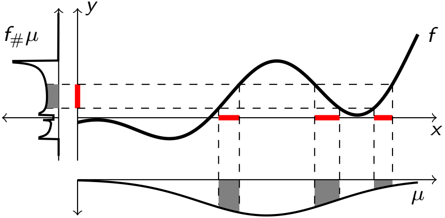

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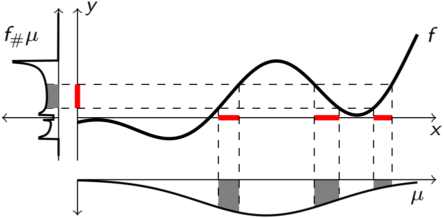
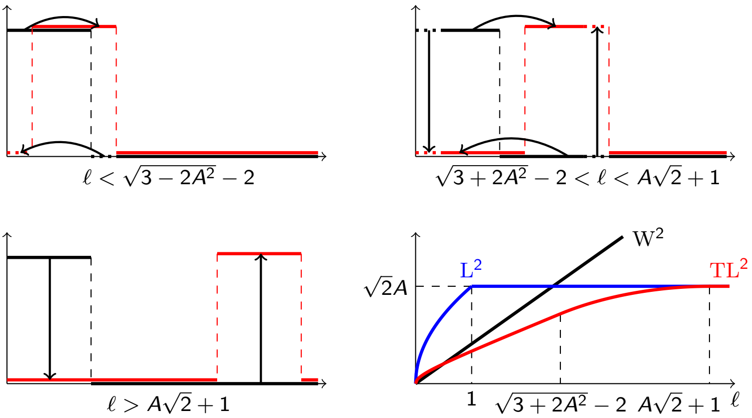


3. In which case we have

$$\mathrm{d}^p_{\mathrm{TL}^p}((f,\mu),(g,\nu)) = \min_{T:T_{\#}\tilde{\mu}=\tilde{\nu}} \int_{X\times\mathbb{R}} |\tilde{x} - T(\tilde{x})|^p \,\mathrm{d}\tilde{\mu}(\tilde{x}).$$

TL^p Translations

TL^2 transport between $f(x) = A\chi_{[0,1]}$ and $g(x) = f(x-\ell)$ with the uniform measure.



TL^p Properties: Summary

1. Signals can be negative and not all of the same size (i.e. not integrate to the same value).
2. Can discriminate between fast oscillating signals (true for L^p, false for W^p).
3. Can track translations for further than L^p (but not as far as W^p).
4. Existing numerical methods for OT are available.
5. The distance defines a metric.
6. We have the existence of plans.
7. Maps exist in the discrete case when $\mu = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ and $\nu = \frac{1}{n}\sum_{j=1}^n \delta_{y_j}$.
8. Disadvantages: no geodesics, not complete.

Linear TL^2 Distance

- Fix a reference point $(f, \mu) \in \mathrm{TL}^2$ and let T^* is the TL^2-optimal transport map between (f, μ) and (g, ν). I.e. $T^*_{\#}\mu = \nu$ and

$$\mathrm{d}^2_{\mathrm{TL}^2}((f, \mu), (g, \nu)) = \int_X |x - T^*(x)|^2 + |f(x) - g(T^*(x))|^2 \,\mathrm{d}\mu(x).$$

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- Assume $\mu = \frac{1}{N} \sum_{k=1}^N \delta_{z_k}$ then we define

$$P_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}(g, \nu) = (P_1(g, \nu), P_2(g, \nu)) \in \mathbb{R}^{2N}$$
$$[P_1(g, \nu)]_k = T^*(z_k) - z_k$$
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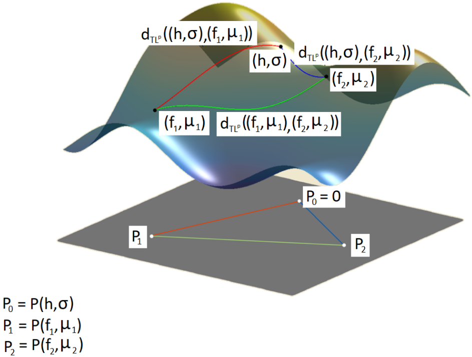
- The linear TL^2 distance

$$\mathrm{d}_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}((g,\nu),(h,\omega)) = \|P_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}(g,\nu) - P_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}(h,\omega)\|_{\ell^2}.$$

Properties of Linear TL^2

- If $\nu = \frac{1}{N}\sum_{k=1}^{N} \delta_{x_k}$ then $P_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}(g,\nu) \in \ell^2$.
- $P_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}(f,\mu) = \underline{0}$.
- $\mathrm{d}_{\mathrm{TL}^2,(f,\mu),\mathrm{lin}}((f,\mu),(g,\nu)) = \mathrm{d}_{\mathrm{TL}^2}((f,\mu),(g,\nu))$.



Spatially Correlated Histogram Specification

Histogram Specification: The problem of matching one histogram $\varphi(y) := f_{\#}\mu(y) = \frac{1}{N}\{x : f(x) = y\}$ with another ψ, i.e. find a map $T : X \to Y$ such that $\psi = T_{\#}\varphi$.

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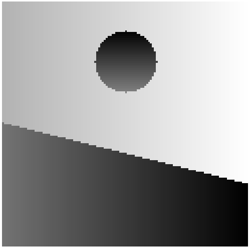
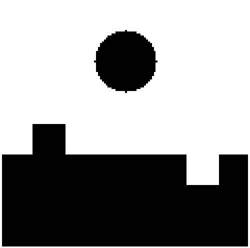
W^2 Solution: (For greyscale images) define histograms φ, ψ from the images and let T be the optimal Monge map between them. The recoloured image is $\hat{f} = g \circ T$.

TL^2 Solution: Let T be the TL^2 optimal map between (f, μ) and (g, ν) (f, g may be RGB images).

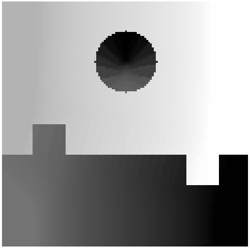
Histogram Specification: Synthetic



(a) Exemplar image.



(b) Original image to be shaded.



(c) The TL^2 solution.

(a) Exemplar image.

(b) Original image to be coloured.

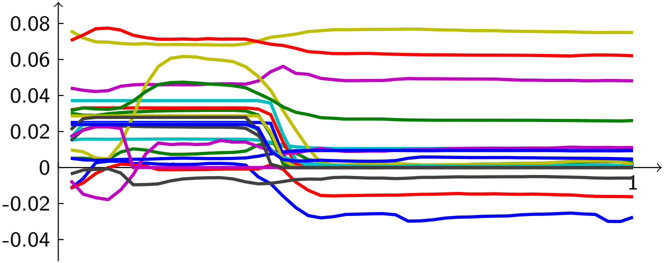
(c) TL^2 solution.

(d) W^2 solution.

(e) Reinhard, Ashikhmin, Gooch and Shirley's method.

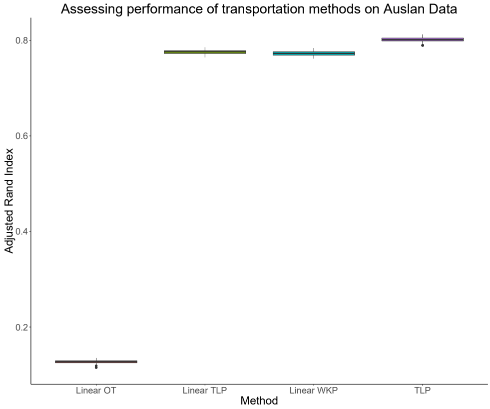
(f) Pitié and Kokaram's method.

1. The AUSLAN data set is a set of 95 words ‘spoken’ by a native AUSLAN (Australian sign language) using 22 sensors on a cyberglove.
2. 27 signals in each class, so a total of 2565 signals.



AUSLAN Results

Accuracy:



Computation time:

Method	Linear W^2	Linear TL^2	Linear $\mathrm{TW}^{k,p}$	TL^p
CPU times (seconds)	12.1	13.0	13.5	91200

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Thank you for listening!

People worry that computers will get too smart and take over the world, but the real problem is that they're too stupid and they've already taken over the world.

— Pedro Domingos