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SFB F68
Tomography Across the Scales

Technische Universität Berlin

Sliced Optimal Transport on the Sphere

Michael Quellmalz | TU Berlin | CSIP 2023
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Joint work with Robert Beinert and Gabriele Steidl

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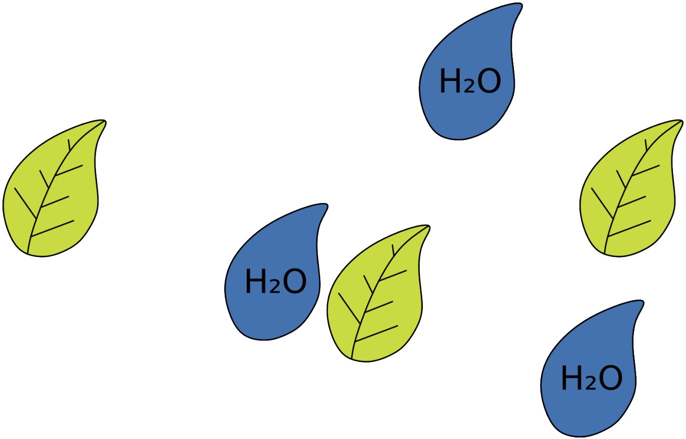
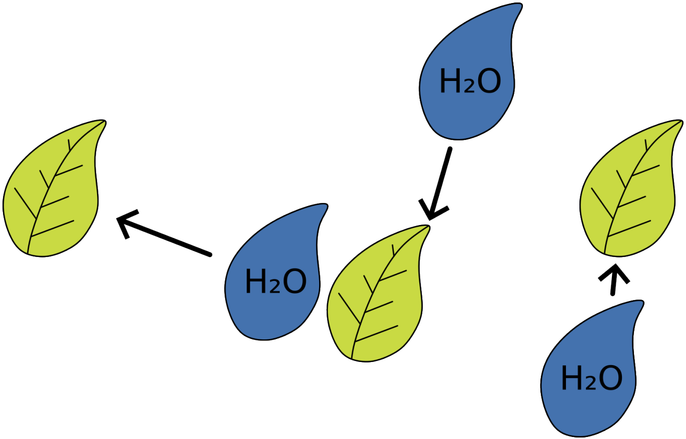
Content

Introductory Example: Water Your Plants Optimal Transport Style



Images Courtesy of Florian Beier (TU Berlin)

Introductory Example: Water Your Plants Optimal Transport Style



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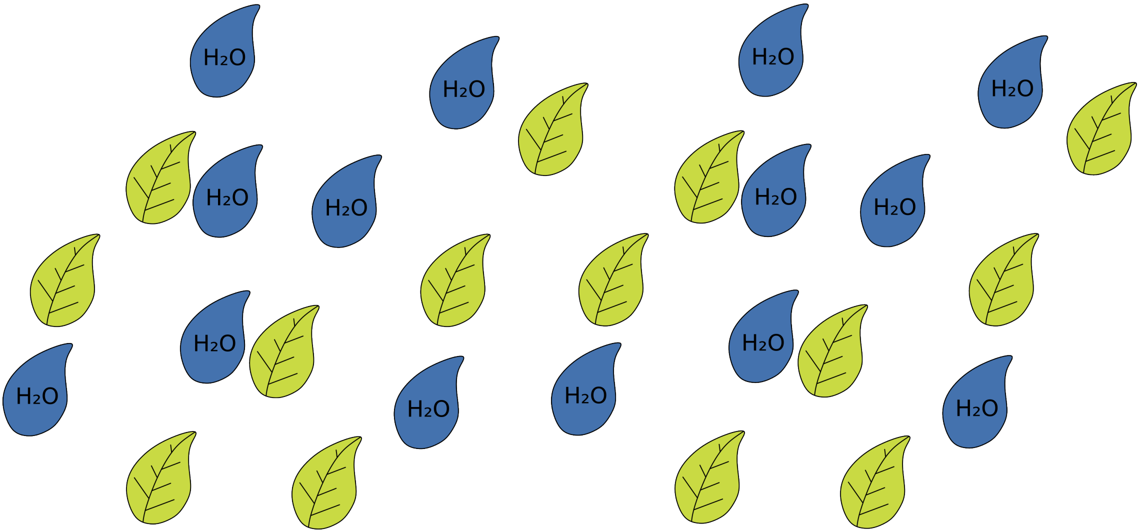
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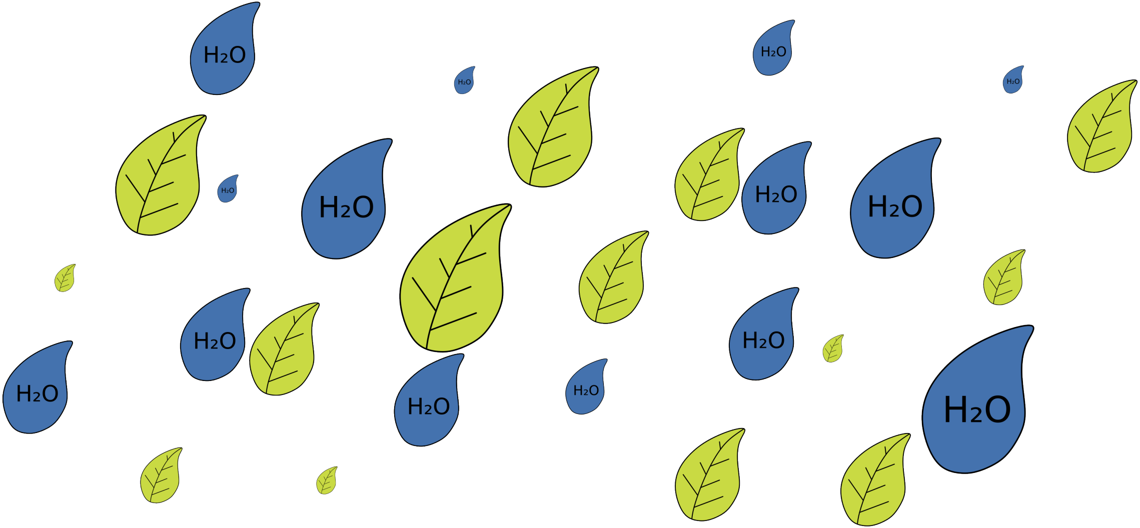
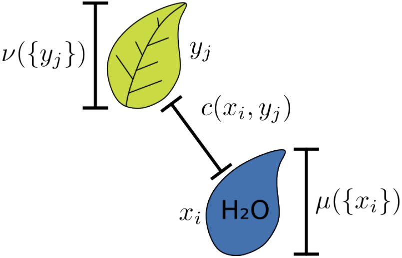
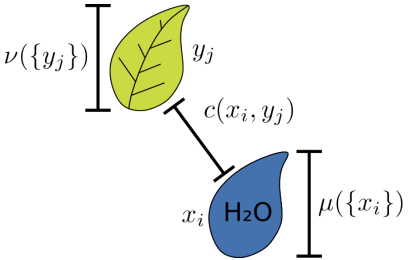

H2O

Kantorovich Problem



- positions water: $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^2$
- positions plants: $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n \in \mathbb{R}^2$
- cost between $\boldsymbol{x}_i$ and $\boldsymbol{y}_j$: $c(\boldsymbol{x}_i, \boldsymbol{y}_j) \in [0, \infty)$
- amount of water at $\boldsymbol{x}_i$: $\mu(\{\boldsymbol{x}_i\}) \in [0, 1]$
- demand of plant $\boldsymbol{y}_j$: $\nu(\{\boldsymbol{y}_j\}) \in [0, 1]$
- water moved from $\boldsymbol{x}_i$ to $\boldsymbol{y}_j$: transport plan $\pi_{i,j}$

Kantorovich Problem



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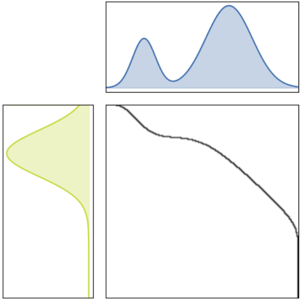
- Kantorovich Optimal Transport (OT) problem (1942):

$$\min_{\pi \in \mathbb{R}^{n \times m}_{\geq 0}} \left\{ \sum_{i=1}^{n} \sum_{j=1}^{m} \underbrace{c(\boldsymbol{x}_i, \boldsymbol{y}_j)\pi_{i,j}}_{\text{weighted transport-costs between } \boldsymbol{x}_i \text{ and } \boldsymbol{y}_i} : \sum_{j=1}^{m} \pi_{i,j} = \mu_i, \sum_{i=1}^{n} \pi_{i,j} = \nu_j \right\}$$

where $\mu_i = \mu(\{\boldsymbol{x}_i\})$, $\nu_j = \nu(\{\boldsymbol{y}_j\})$.

π	1/4	1/4	1/2	μ
1/2 =	1/8 +	1/4 +	1/8	
1/4	1/8	0	1/8	
1/4	0	0	1/4	
ν				

Kantorovich Problem (Formulation with Measures)



- $\mathcal{P}(\mathbb{X})$ probability measures on compact metric space $\mathbb{X}$
- $P_1(x, y) := x$ projection to the first component
- Pushforward of $f\colon \mathbb{X} \to \mathbb{Y}$ and $\mu \in \mathcal{P}(\mathbb{X})$ is

$$f_{\#}\mu := \mu \circ f^{-1} \in \mathcal{P}(\mathbb{Y})$$

- $\mu \in \mathcal{P}(\mathbb{X})$, $\nu \in \mathcal{P}(\mathbb{Y})$

$$\min_{\pi \in \mathcal{P}(\mathbb{X}\times\mathbb{Y})} \left\{ \int_{\mathbb{X}\times\mathbb{Y}} c(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\pi(\boldsymbol{x}, \boldsymbol{y}) : P_{1\#}\pi = \mu, P_{2\#}\pi = \nu \right\}$$

- If $\mathbb{X}, \mathbb{Y} \subset \mathbb{R}^d$ and $c(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|_2^p$, the minimum is the Wasserstein-p distance

$$W_p^p(\mu, \nu) := \min_{\pi \in \mathcal{P}(\mathbb{X}\times\mathbb{Y})} \left\{ \int_{\mathbb{X}\times\mathbb{Y}} \|\boldsymbol{x} - \boldsymbol{y}\|_2^p \mathrm{d}\pi(\boldsymbol{x}, \boldsymbol{y}) : P_{1\#}\pi = \mu, P_{2\#}\pi = \nu \right\}$$

Wasserstein Barycenters

[Agueh Carlier 2011]

- $\mu_i \in \mathcal{P}(\mathbb{R}^d)$ and $t_i \in [0,1]$, $i = 1, \ldots, N$ with $\sum_{i=1}^N t_i = 1$
- Wasserstein Barycenter

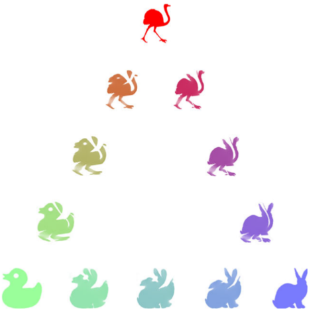
$$\operatorname*{argmin}_{\nu \in \mathcal{P}(\mathbb{R}^d)} \sum_{i=1}^{N} t_i \, \mathrm{W}_2^2(\mu_i, \nu)$$

- For $N = 2$ inputs, a barycenter $\hat{\nu}$ can be computed by

$$\hat{\nu} = \sum_{(\boldsymbol{x}_1, \boldsymbol{x}_2) \in \mathrm{supp}(\hat{\pi})} \hat{\pi}(\{(\boldsymbol{x}_1, \boldsymbol{x}_2)\}) \delta_{\{t_1 \boldsymbol{x}_1 + t_2 \boldsymbol{x}_2\}}, \qquad \text{(McCann Interpolation)}$$

where $\hat{\pi}$ solves $W_2(\mu_1, \mu_2)$

- Wasserstein distances and barycenters on $\mathbb{R}^d$ are computationally expensive



Wasserstein barycenters between 3 measures
[Bonneel Rabin Peyré Pfister 2015]

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Sliced Optimal Transport on $\mathbb{R}^d$

[Rabin Peyré Delon Bernot 2012] [Kolouri Park Rohde 2016]

- Absolutely continuous measure $\mu \in \mathcal{P}_{\mathrm{ac}}(\mathbb{R}^d)$ with density f_μ, i.e.

$$\mu(A) = \int_A f_\mu(x)\,\mathrm{d}x \qquad \forall A \in \mathcal{B}(\mathbb{R}^d)$$

- Radon transform

$$\mathcal{R}_{\boldsymbol{\theta}} f(t) := \int_{\boldsymbol{\theta}^\top \boldsymbol{x} = t} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \quad \boldsymbol{\theta} \in \mathbb{S}^{d-1},\ t \in \mathbb{R}$$

- Sliced Wasserstein distance

$$\mathrm{SW}_p^p(\mu,\nu) := \int_{\mathbb{S}^{d-1}} \mathrm{W}_p^p(\mathcal{R}_{\boldsymbol{\theta}} f_\mu, \mathcal{R}_{\boldsymbol{\theta}} f_\nu)\,\mathrm{d}\boldsymbol{\xi}$$

- Integral over Wasserstein distances of one-dimensional measures (density functions)

OT on $\mathbb{R}$

[Vilani 03] [Peyre Cuturi 19]

- Absolutely continuous measure $\mu \in \mathcal{P}_{\mathrm{ac}}(\mathbb{R})$
- Cumulative distribution function $F_\mu(x) := \mu((-\infty, x])$
- Quantile function $F_\mu^{-1}(r) := \min\{x \in \mathbb{R} : F_\mu(x) \geq r\}$, $r \in [0,1]$
- Wasserstein distance

$$W_p^p(\mu, \nu) = \int_0^1 |\tilde{F}_\mu^{-1}(r) - \tilde{F}_\nu^{-1}(r)|^p \,\mathrm{d}r$$

- Unique OT plan

$$\pi = (\mathrm{Id}, T^{\mu,\nu})_{\#}\mu \quad \text{with} \quad T^{\mu,\nu}(x) := F_\nu^{-1}(F_\mu(x)), \quad x \in \mathbb{R}$$

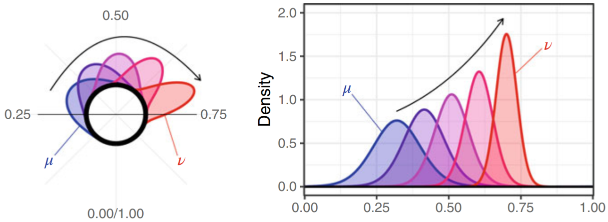
OT on the Circle

[Delon Salomon Sobolevski 2010] [Rabin Delon Gousseau 2011]

- Circle $\mathbb{T} := \mathbb{R}/(2\pi\mathbb{Z})$
- Idea: Cut $\mathbb{T}$ at the right position to get an OT problem on the interval
- Wasserstein distance

$$W_p^p(\mu,\nu) = \min_{\theta \in \mathbb{R}} \int_0^1 |\tilde{F}_\mu^{-1}(r) - (\tilde{F}_\nu - \theta)^{-1}(r)|^p \, \mathrm{d}r$$

- Compute optimal θ via bisection



Barycenters of measures μ, ν on $\mathbb{T}$, see [Hundrieser Klatt Munk 2022]

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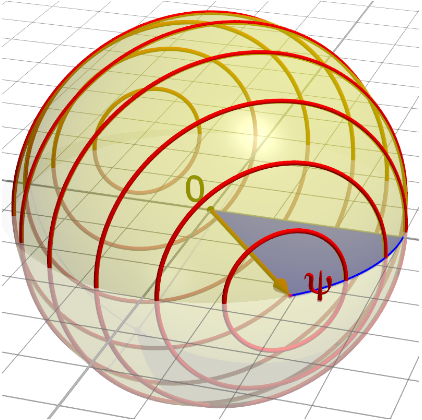
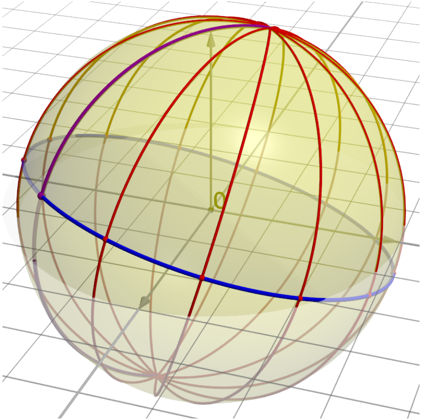
Sliced OT on the Sphere $\mathbb{S}^2 := \{\boldsymbol{\xi} \in \mathbb{R}^3 : \|\boldsymbol{\xi}\| = 1\}$

Vertical Slices (“egg cutter”)



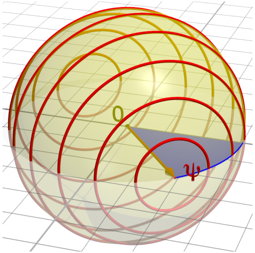
Semicircles (“orange segments”)



Vertical Slices

- Slicing operator for fixed $\psi \in \mathbb{T} \sim [0, 2\pi)$

$$\mathcal{S}_\psi \colon \mathbb{S}^2 \to [-1,1], \qquad \mathcal{S}_\psi(\boldsymbol{\xi}) \coloneqq \boldsymbol{\xi}^\top (\cos\psi, \sin\psi, 0),$$



- Circle

$$\mathcal{S}_\psi^{-1}(t) = \{\boldsymbol{\xi} \in \mathbb{S}^2 : \mathcal{S}_\psi(\boldsymbol{\xi}) = t\}, \qquad t \in [-1,1],$$

is the intersection of $\mathbb{S}^2$ and the plane with normal ψ and distance t from the origin.

- Vertical slice transform [Gindikin Reeds Shepp 1994] [Zangerl Scherzer 2010]

$$\mathcal{V}f(\psi, t) \coloneqq \frac{1}{|\mathbb{S}^2|\sqrt{1-t^2}} \int_{\mathcal{S}_\psi^{-1}(t)} f(\boldsymbol{\xi}) \,\mathrm{d}s(\boldsymbol{\xi}), \quad \psi \in \mathbb{T},\ t \in (-1,1)$$

- Restriction $\mathcal{V}_\psi \coloneqq 2\pi\, \mathcal{V}(\psi, \cdot)$ transforms a function on $\mathbb{S}^2$ to many functions on $[-1,1]$
- Singular value decomposition of $\mathcal{V}$ is known [Hielscher Q. 2015]

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Vertical Slices (Definition for Measures)

We generalize the **vertical slice transform** $\mathcal{V}_\psi$ for measures by

$$\mathcal{V}\colon \mathcal{M}(\mathbb{S}^2) \to \mathcal{M}(\mathbb{T} \times [-1,1]), \qquad \mu \mapsto T_\#(u_\mathbb{T} \times \mu) \quad \text{with} \quad T(\psi, \boldsymbol{\xi}) := (\psi, \mathcal{S}_\psi(\boldsymbol{\xi})),$$
$$\mathcal{V}_\psi\colon \mathcal{M}(\mathbb{S}^2) \to \mathcal{M}([-1,1]), \qquad \mu \mapsto (\mathcal{S}_\psi)_\# \mu = \mu \circ \mathcal{S}_\psi^{-1}.$$

where $u_\mathbb{T}$ is the normalized Lebesgue measure on $\mathbb{T}$.

Theorem (absolutely continuous measures)

For $f \in L^1(\mathbb{S}^2)$,

$$\mathcal{V}[f\sigma_{\mathbb{S}^2}] = (\mathcal{V}f)\,\sigma_{\mathbb{T}\times[-1,1]},$$

where σ is the Lebesgue measure.

Theorem

The vertical slice transform $\mathcal{V}\colon \mathcal{M}_{\mathrm{sym}}(\mathbb{S}^2) \to \mathcal{M}(\mathbb{T} \times [-1,1])$ is injective, where

$$\mathcal{M}_{\mathrm{sym}}(\mathbb{S}^2) := \{\mu \in \mathcal{M}(\mathbb{S}^2) : \langle \mu, f\rangle = \langle \mu, \check{f}\rangle\, \forall f \in C(\mathbb{S}^2)\}, \quad \check{f}(\boldsymbol{x}) = f(x_1, x_2, -x_3),$$

Semicircle transform

- Spherical coordinates $\Phi\colon \mathbb{T} \times [0,\pi] \to \mathbb{S}^2$,

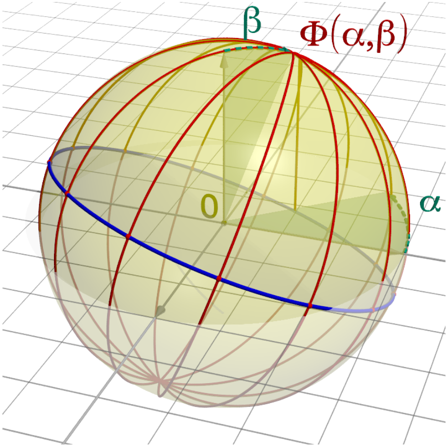
$$\Phi(\varphi,\vartheta) \coloneqq (\cos\varphi \, \sin\vartheta,\ \sin\varphi \, \sin\vartheta,\ \cos\vartheta) \in \mathbb{S}^2$$

- Rotation group
  $\mathrm{SO}(3) \coloneqq \{\boldsymbol{Q} \in \mathbb{R}^{3\times 3} : \boldsymbol{Q}^\top \boldsymbol{Q} = I,\ \det \boldsymbol{Q} = 1\}$
- Euler angles

$$\Psi(\alpha,\beta,\gamma) \coloneqq R_3(\alpha) R_2(\beta) R_3(\gamma) \in \mathrm{SO}(3),$$

  where $R_i(\alpha)$ is the rotation around the i-th axis with angle α
- Normalized semicircle transform $\mathcal{W}$ of $f\colon \mathbb{S}^2 \to \mathbb{R}$

$$\mathcal{W}f(\alpha,\beta,\gamma) \coloneqq \frac{1}{4\pi} \int_0^\pi f(\Psi(\alpha,\beta,0)\,\Phi(\gamma,\vartheta)) \sin\vartheta \,\mathrm{d}\vartheta$$



- Restriction $\mathcal{W}_{\alpha,\beta} f \coloneqq 4\pi \, \mathcal{W}f(\alpha,\beta,\cdot)$
- Unnormalized semicircle transform (without $\sin\vartheta$) due to [Groemer 1998]

Theorem (singular value decomposition) [Q. Beinert Steidl 2023]

The normalized semicircle transform fulfills

$$\mathcal{W} Y_n^k = \mathrm{w}_n Z_n^k, \quad n \in \mathbb{N}_0,\ k \in \{-n, \dots, n\},$$

with the singular values $\mathrm{w}_n := \|\mathcal{W} Y_n^k\|_{L^2(\mathbb{S}^2)} \in \mathcal{O}(n^{-1/2})$ and the orthonormal functions

$$Z_n^k := \mathrm{w}_n^{-1} \sum_{j=-n}^{n} \lambda_n^j \, \overline{D_n^{k,j}} \in L^2(\mathrm{SO}(3)),$$

where $\lambda_0^0 := 2(4\pi)^{-3/2}$ and, for $n \in \mathbb{N}$ and $j \in \{1, \dots, n\}$ with $n + j$ even,

$$\lambda_n^j := \frac{(-1)^j}{4\pi} \sqrt{\frac{2n+1}{4\pi} \frac{(n-j)!}{(n+j)!}} \, \frac{j\,(n-2)!!\,(n+j-1)!!}{(n-j)!!\,(n+1)!!} \begin{cases} 2: & n \text{ even}, \\ \pi: & n \text{ odd}, \end{cases}$$

$\lambda_n^{-j} := (-1)^j \lambda_n^j$, and $\lambda_n^j = 0$ otherwise. Here Y_n^k denote the spherical harmonics and $D_n^{k,j}$ the rotational harmonics (Wigner D-functions). Moreover, there are constants $C_1, C_2 > 0$ such that
$C_1\ (n+1)^{-1/2} \le \mathrm{w}_n \le C_2\ (n+1)^{-1/2} \quad \forall n \in \mathbb{N}_0.$

Semicircle Transform of Measures

For $\Phi(\alpha, \beta) \in \mathbb{S}^2$, we define the **azimuth operator**

$$\mathcal{A}_{\alpha,\beta} \colon \mathbb{S}^2 \to \mathbb{T}, \quad \mathcal{A}_{\alpha,\beta}(\boldsymbol{\xi}) \coloneqq \operatorname{azi}(\Psi(\alpha, \beta, 0)^{\mathrm{T}} \boldsymbol{\xi}),$$

where azi denotes the first component of the inverse of the spherical coordinate transform Φ, i.e.

$$\operatorname{azi}(\Phi(\varphi, \theta)) = \varphi \quad \forall \varphi, \theta.$$

We generalize the (restricted) **semicircle transform** $\mathcal{W}_{\alpha,\beta}$ by

$$\begin{aligned} \mathcal{W}_{\alpha,\beta} \colon \mathcal{M}(\mathbb{S}^2) \to \mathcal{M}(\mathbb{T}), &\qquad \mu \mapsto (\mathcal{A}_{\alpha,\beta})_{\#}\mu = \mu \circ \mathcal{A}_{\alpha,\beta}^{-1}. \\ \mathcal{W} \colon \mathcal{M}(\mathbb{S}^2) \to \mathcal{M}(\mathrm{SO}(3)), &\qquad \mu \mapsto (T_{\mathcal{W}})_{\#}(u_{\mathbb{S}^2} \times \mu) \quad \text{with} \quad T_{\mathcal{W}}(\Phi(\alpha, \beta), \boldsymbol{\xi}) \coloneqq \Psi(\alpha, \beta, \mathcal{A}_{\alpha,\beta}(\boldsymbol{\xi})). \end{aligned}$$

Theorem (injectivity)

The normalized semicircle transform is injective $\mathcal{M}(\mathbb{S}^2) \to \mathcal{M}(\mathrm{SO}(3))$.

Sliced Spherical Wasserstein Distances

Definition

Let $p \in [1, \infty)$ and $\mu, \nu \in \mathcal{M}(\mathbb{S}^2)$. We define the **vertical sliced Wasserstein distance**

$$\mathrm{VSW}_p^p(\mu, \nu) := \frac{1}{2\pi} \int_0^{2\pi} \mathrm{W}_p^p(\mathcal{V}_\psi \mu, \mathcal{V}_\psi \nu) \, \mathrm{d}\psi$$

and the **semicircular sliced Wasserstein distance**

$$\mathrm{SSW}_p^p(\mu, \nu) := \int_{\mathbb{S}^2} \mathrm{W}_p^p(\mathcal{W}_{\alpha,\beta} \mu, \mathcal{W}_{\alpha,\beta} \nu) \, \mathrm{d}u_{\mathbb{S}^2}(\Phi(\alpha, \beta)),$$

which are integrals over Wasserstein distances on $[-1, 1]$ and $\mathbb{T}$, respectively.

SSW was defined in [Bonet Berg Courty Septier Drumetz Pham 2023]

Theorem (metric properties) [Q. Beinert Steidl 2023]

Let $p \in [1, \infty)$. The vertical sliced Wasserstein distance VSW_p is a metric on $\mathcal{M}_{\mathrm{sym}}(\mathbb{S}^2)$, and the semicircular Wasserstein distance SSW_p is a metric on $\mathcal{M}(\mathbb{S}^2)$.

Invariance to Rotations

Theorem

Let $p \in [1, \infty)$. The vertical sliced Wasserstein distance VSW_p is invariant to rotations $\boldsymbol{R}_3$ around the vertical axis, i.e., for all $\mu, \nu \in \mathcal{M}(\mathbb{S}^2)$ and $\alpha \in \mathbb{T}$,

$$\mathrm{VSW}_p(\mu, \nu) = \mathrm{VSW}_p(\mu \circ \boldsymbol{R}_3(\alpha), \nu \circ \boldsymbol{R}_3(\alpha)).$$

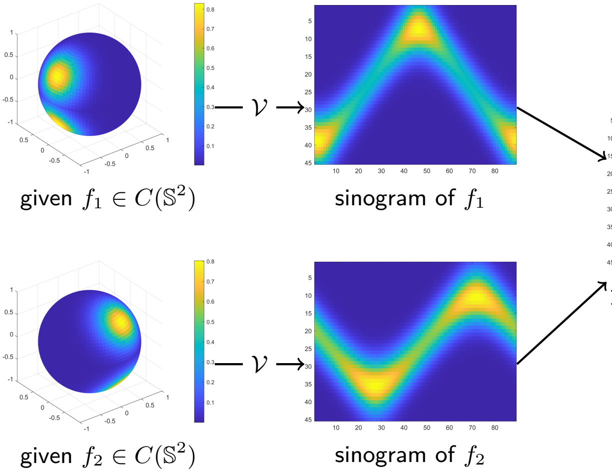
Theorem

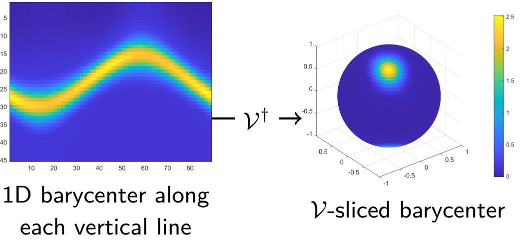
Let $p \in [1, \infty)$. The semicircular sliced Wasserstein distance SSW_p is rotationally invariant, i.e., for all $\mu, \nu \in \mathcal{M}(\mathbb{S}^2)$ and $\boldsymbol{Q} \in \mathrm{SO}(3)$,

$$\mathrm{SSW}_p(\mu, \nu) = \mathrm{SSW}_p(\mu \circ \boldsymbol{Q}, \nu \circ \boldsymbol{Q}).$$

Content

Sliced (Radon) barycenter





- Compute pseudoinverse $\mathcal{V}^\dagger$ via SVD
- Quadrature on $\mathrm{SO}(3)$ [Graef Potts 2011]

Inversion of $\mathcal{W}$ by Variational Approach

- Barycenter of probability measures is again probability measure
- $\mathcal{W}^\dagger g$ might be negative even if $g \geq 0$, therefore not a probability density
- Find approximate solution f of the inversion problem $\mathcal{W} f = g$ via

$$\operatorname*{argmin}_{\substack{f \geq 0 \\ \int_{\mathbb{S}^2} f = 1}} \mathrm{KL}(\mathcal{W} f, g) + \rho\, \mathrm{KL}(f, 1),$$

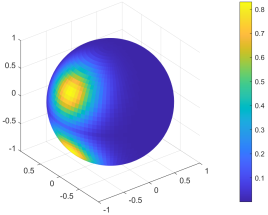
  with the Kullback–Leibler (KL) divergence

$$\mathrm{KL}(f, \tilde{f}) := \langle f, \log f - \log \tilde{f} \rangle + \langle \tilde{f} - f, 1 \rangle$$

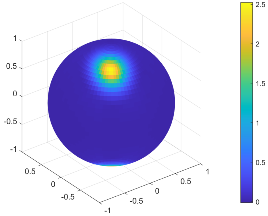
  for $f, \tilde{f} \geq 0$ with $f(x) = 0$ whenever $\tilde{f}(x) = 0$ and $0 \log 0 := 0$.
- Primal-dual splitting [Chambolle Pock 2016] yields converging iteration

$$\boldsymbol{f}^{k+1} := \operatorname{proj}_\Delta\big(\boldsymbol{f}^k - \tau \mathcal{W}^* \boldsymbol{y}_1^k - \tau \boldsymbol{y}_2^k\big), \qquad \tilde{\boldsymbol{f}}^{k+1} := \boldsymbol{f}^{k+1} + \theta(\boldsymbol{f}^{k+1} - \boldsymbol{f}^k),$$

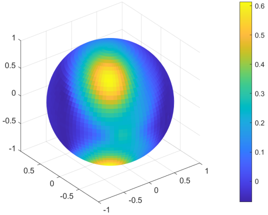
$$\boldsymbol{y}_1^{k+1} := \operatorname{prox}_{\sigma\, \mathrm{KL}^*(\cdot, \boldsymbol{g})}\big(\boldsymbol{y}_1^k + \sigma \mathcal{W} \tilde{\boldsymbol{f}}^{k+1}\big), \qquad \boldsymbol{y}_2^{k+1} := \operatorname{prox}_{\sigma(\rho\, \mathrm{KL})^*(\cdot, \boldsymbol{1})}\big(\boldsymbol{y}_2^k + \sigma\, \tilde{\boldsymbol{f}}^{k+1}\big).$$



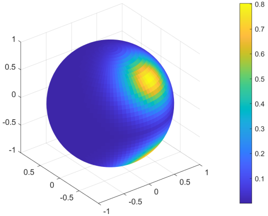
(a) Given measure μ
(van Mises–Fischer distribution)



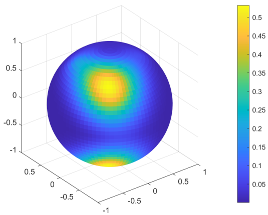
(b) $\mathcal{V}$-sliced barycenter (0.01 s)



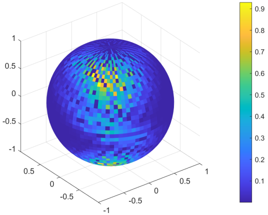
(c) $\mathcal{W}$-sliced barycenter (3.2 s)



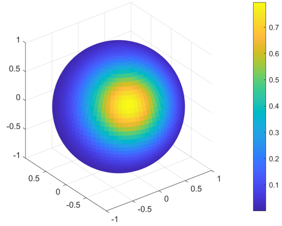
(d) Given measure ν



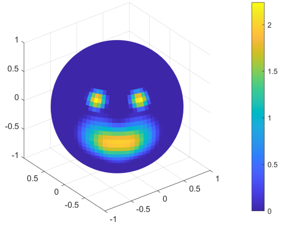
(e) Regularized Wasserstein barycenter (PythonOT, 19 s)



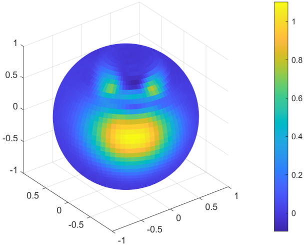
(f) Unregularized Wasserstein barycenter (PythonOT, 33 h)



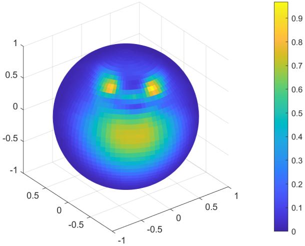
(a) Density of vMF distribution μ



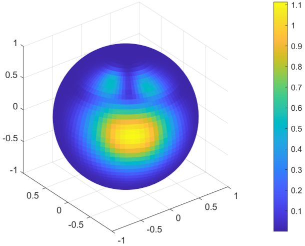
(b) Density of ν (quadratic spline)



(c) $\mathcal{W}$-sliced barycenter with Moore–Penrose inverse



(d) $\mathcal{W}$-sliced barycenter with regularized inverse



(e) Regularized Wasserstein barycenter

Conclusions

- We defined the vertical slice and normalized semicircle transform, and generalized them to measures.
- For absolutely continuous measures, the generalized and initial definitions coincide
- We showed an SVD of the normalized semicircle transform, which provides an approach for numerical computations and inversion.
- The normalized semicircle transform is injective for measures, hence the sliced Wasserstein distance fulfills the properties of a metric.

M Quellmalz, R Beinert, G Steidl. Sliced optimal transport on the sphere. *Inverse Problems* 39, 2023.

Future

- Modify vertical slice transform to support any direction (not just on the equator)
- Other manifolds, $\mathbb{S}^d$ or $\mathrm{SO}(3)$

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Thank you for your attention!