

Spherical Sliced-Wasserstein

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Motivation

Goal of Optimal Transport: Transport mass in an optimal way

$$W_c(\mu, \nu) = \min_{T \# \mu = \nu} \int c(x, T(x)) \, d\mu(x) \quad (1)$$

- Coupling
- Value of the min

Widely use nowadays in Machine Learning

- Generative Models (*e.g.* WGAN [Arjovsky et al., 2017])
- Domain Adaptation [Courty et al., 2016]
- ...

Data generally lie on manifolds, *e.g.* on the sphere $S^{d-1} = \{x \in \mathbb{R}^d, \|x\|_2 = 1\}$:

- Directional data, meteorology, cosmology...
- Also used as embeddings for VAEs, Self-supervised learning...

Wasserstein Distance

Definition (Wasserstein distance)

Let M be a Riemannian manifold endowed with the Riemannian distance d , $p \geq 1$, $\mu, \nu \in \mathcal{P}_p(M)$, then

$$W_p^p(\mu, \nu) = \inf_{\gamma \in \Pi(\mu, \nu)} \int d^p(x, y) \, d\gamma(x, y), \quad (2)$$

where $\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}(M \times M) \mid \pi_{\#}^1 \gamma = \mu, \pi_{\#}^2 \gamma = \nu\}$ and $\pi^1(x, y) = x$, $\pi^2(x, y) = y$, $\pi_{\#}^1 \gamma = \int \pi^1(x, y) \, d\gamma(x, y)$.

Numerical approximation: Linear program $O(n^3 \log n)$ [Peyré et al., 2019]

Proposed Solutions:

- Entropic regularization + Sinkhorn $O(n^2)$ [Cuturi, 2013]
- Minibatch estimator [Fratras et al., 2020]
- Sliced-Wasserstein [Rabin et al., 2011b, Bonnotte, 2013] but only on Euclidean spaces

Sliced-Wasserstein on \mathbb{R}^d

Wasserstein on \mathbb{R} :

$$\text{for } p \geq 1, \mu, \nu \in \mathcal{P}_p(\mathbb{R}), W_p^p(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p du \quad (3)$$

Sliced-Wasserstein on \mathbb{R}^d

Wasserstein on \mathbb{R} :

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Definition (Sliced-Wasserstein [[Rabin et al., 2011b](#)])

Let $\mu, \nu \in P_p(\mathbb{R}^d)$,

$$SW_p^p(\mu, \nu) = \int_{S^{d-1}} W_p^p(P_\#^\theta \mu, P_\#^\theta \nu) d\lambda(\theta), \quad (4)$$

where $P^\theta(x) = \langle x, \theta \rangle$, λ uniform measure on S^{d-1} .

Sliced-Wasserstein on \mathbb{R}^d

Wasserstein on \mathbb{R} :

$$\forall p \geq 1, \forall \mu, \nu \in \mathcal{P}_p(\mathbb{R}), W_p^p(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p du \quad (3)$$

Definition (Sliced-Wasserstein [[Rabin et al., 2011b](#)])

Let $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$,

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where $P^\theta(x) = \langle x, \theta \rangle$, λ uniform measure on S^{d-1} .

Properties:

- Distance
- Topologically equivalent to the Wasserstein distance
- Monte-Carlo approximation in $O(Ln \log n)$

Radon Transform

Definition (Radon Transform)

Let $f \in L^1(\mathbb{R}^d)$, then the Radon transform $R : L^1(\mathbb{R}^d) \rightarrow L^1(\mathbb{R} \times S^{d-1})$ is defined as

$$\forall \theta \in S^{d-1}, \forall t \in \mathbb{R}, Rf(t, \theta) = \int_{\mathbb{R}^d} f(x) \mathbb{1}_{\langle hx, \theta \rangle = t} dx. \quad (5)$$

Definition (Back-projection operator)

The back-projection operator $R : C_0(\mathbb{R} \times S^{d-1}) \rightarrow C_0(\mathbb{R}^d)$ is defined as

$$\forall g \in C_0(\mathbb{R} \times S^{d-1}), \forall x \in \mathbb{R}^d, Rg(x) = \int_{S^{d-1}} g(\langle hx, \theta \rangle, \theta) d\theta. \quad (6)$$

$$Rf, R(Rf) = f, R(Rg) = g$$

Radon Transform of Measures and Link with SW

- Radon transform of a measure $\mu \in \mathcal{P}(\mathbb{R}^d)$ defined as the measure $R\mu$ such that $\int_{\mathbb{R}^{d-1}} g \, dR\mu = \int_{\mathbb{R}^d} g \, d\mu$.
- Disintegration of $R\mu \in \mathcal{P}(\mathbb{R}^{d-1})$ w.r.t. λ : $R\mu = \int K \, d\lambda$
- [Bonneel et al., 2015, Proposition 6]: For λ -ae $\theta \in S^{d-1}$, $K(\theta, \cdot) = P_{\theta}^{\#} \mu$

$$\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d), \quad SW_p^p(\mu, \nu) = \int_{S^{d-1}} W_p^p((R\mu)^{\theta}, (R\nu)^{\theta}) \, d\lambda(\theta). \quad (7)$$

Interest: If R injective, SW is a distance.

SW on the Sphere

Goal: defining SW discrepancy on the sphere taking care of geometry of the manifold

	SW	SSW
Closed-form of W	Line	?
Projection	$P^\theta(x) = \langle x, \theta \rangle$?
Integration	S^{d-1}	?

Table: SW to SSW

SW on the Sphere

Goal: defining SW discrepancy on the sphere taking care of geometry of the manifold

	SW	SSW
Closed-form of W	Line	?
Projection	$P^\theta(x) = \langle x, \theta \rangle$?
Integration	S^{d-1}	?

Table: SW to SSW

- Generalization of straight lines on manifolds: geodesics
- On S^{d-1} , geodesics = great circles

Wasserstein on the Circle

Let $\mu, \nu \in P(S^1)$ where $S^1 = \mathbb{R}/\mathbb{Z}$.

- Parametrize S^1 by $[0, 1[$
- $\forall x, y \in [0, 1[, d_{S^1}(x, y) = \min(|x - y|, 1 - |x - y|)$
- For a cost function $c(x, y) = h(d_{S^1}(x, y))$ with $h : \mathbb{R} \rightarrow \mathbb{R}^+$ increasing and convex
- $\delta\mu, \nu \in P(S^1)$, [Rabin et al., 2011a]

$$W_c(\mu, \nu) = \inf_{\alpha \in \mathcal{A}} \int_0^1 h(|F_\mu^{-1}(t) - (F_\nu \circ \alpha)^{-1}(t)|) dt. \quad (8)$$

- To find α : binary search [Delon et al., 2010]

Particular Cases

- For $h = \text{Id}$, [Hundrieser et al., 2021]

$$W_1(\mu, \nu) = \int_0^1 j_{F_\mu}(t) \quad F_\nu(t) \quad \text{LevMed}(F_\mu \quad F_\nu) j \, dt, \quad (9)$$

where

$$\text{LevMed}(f) = \inf \left\{ t \in \mathbb{R}, \beta(fx \in [0, 1[, f(x) \quad tg) \quad \frac{1}{2} \right\}. \quad (10)$$

- For $h(x) = x^2$ and $\nu = \text{Unif}(S^1)$,

$$W_2^2(\mu, \nu) = \int_0^1 j_{F_\mu}^{-1}(t) \quad t \quad \hat{\alpha} j^2 \, dt \quad \text{with} \quad \hat{\alpha} = \int x \, d\mu(x) \quad \frac{1}{2}. \quad (11)$$

In particular, if $x_1 < \dots < x_n$ and $\mu_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$, then

$$W_2^2(\mu_n, \nu) = \frac{1}{n} \sum_{i=1}^n x_i^2 \quad \left(\frac{1}{n} \sum_{i=1}^n x_i \right)^2 + \frac{1}{n^2} \sum_{i=1}^n (n+1 \quad 2i)x_i + \frac{1}{12}. \quad (12)$$

Sliced-Wasserstein on the Sphere

- Great circle: Intersection between 2-plane and S^{d-1}
- Parametrize 2-plane by the Stiefel manifold

$$\mathbb{V}_{d,2} = \{U \in \mathbb{R}^{d \times 2}, U^T U = I_2\}$$

- Projection on great circle C : For a.e. $x \in S^{d-1}$,

$$P^C(x) = \operatorname{argmin}_{y \in C} d_{S^{d-1}}(x, y),$$

where $d_{S^{d-1}}(x, y) = \arccos(\langle x, y \rangle)$.

- For $U \in \mathbb{V}_{d,2}$, $C = \operatorname{span}(UU^T) \cap S^{d-1}$,

$$\begin{aligned} P^U(x) &= U^T \operatorname{argmin}_{y \in C} d_{S^{d-1}}(x, y) \\ &= \frac{U^T x}{\|U^T x\|_2}. \end{aligned}$$

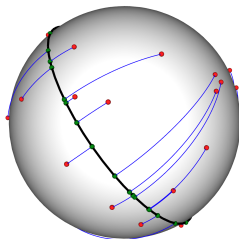


Figure: Illustration of the geodesic projections on a great circle (in black). In red, random points sampled on the sphere. In green the projections and in blue the trajectories.

Spherical Sliced-Wasserstein

Definition (Spherical Sliced-Wasserstein)

Let $p \geq 1$, $\mu, \nu \in \mathcal{P}_p(S^{d-1})$ absolutely continuous w.r.t. Lebesgue measure,

$$SSW_p^p(\mu, \nu) = \int_{\mathbb{V}_{d,2}} W_p^p(P_{\#}^U \mu, P_{\#}^U \nu) d\sigma(U), \quad (13)$$

with σ the uniform distribution over $\mathbb{V}_{d,2}$.

	SW	SSW
Closed-form of W	Line	(Great)-Circle
Projection	$P^\theta(x) = \langle x, \theta \rangle$	$P^U(x) = \frac{U^T x}{\ U^T x\ _2}$
Integration	S^{d-1}	$\mathbb{V}_{d,2}$

Table: Comparison SW-SSW

A New Spherical Radon Transform

Question: Is SSW a distance?

Definition (Spherical Radon Transform)

Let $f \in L^1(S^{d-1})$, then we define a Spherical Radon transform $\tilde{R} : L^1(S^{d-1}) \rightarrow L^1(S^1 \times \mathbb{V}_{d,2})$ as

$$\forall z \in S^1, \forall U \in \mathbb{V}_{d,2}, \tilde{R}f(z, U) = \int_{S^{d-1}} f(x) \mathbb{1}_{fz = P^U(x)} g dx. \quad (14)$$

Definition (Back-projection operator)

The back-projection operator $R : C_0(S^1 \times \mathbb{V}_{d,2}) \rightarrow C_b(S^{d-1})$ is defined as for a.e. $x \in S^{d-1}$,

$$\tilde{R}g(x) = \int_{\mathbb{V}_{d,2}} g(P^U(x), U) d\sigma(U). \quad (15)$$

For all $f \in L^1(S^{d-1})$, $g \in C_0(S^1 \times \mathbb{V}_{d,2})$,

$$\int_{S^1 \times \mathbb{V}_{d,2}} \tilde{R}f, g = \int_{S^{d-1}} hf, \tilde{R}g. \quad (16)$$

Spherical Radon Transform of Measures

Define the Radon transform of $\mu \in \mathcal{M}(S^{d-1})$ as $\tilde{R}\mu$ such that

$$g \in C_0(S^1 \times \mathbb{V}_{d,2}), \int_{S^1 \times \mathbb{V}_{d,2}} g(z, U) d(\tilde{R}\mu)(z, U) = \int_{S^{d-1}} \tilde{R} g(x) d\mu(x). \quad (17)$$

Disintegration: $\tilde{R}\mu = \int \sigma_U (\tilde{R}\mu)^U$

Proposition

Let $\mu \in \mathcal{M}(S^{d-1})$, then for σ -almost every $U \in \mathbb{V}_{d,2}$, $(\tilde{R}\mu)^U = P_{\#}^U \mu$.

$$g_{\mu, \nu} \in P_{p,ac}(S^{d-1}), \int_{\mathbb{V}_{d,2}} W_p^p((\tilde{R}\mu)^U, (\tilde{R}\nu)^U) d\sigma(U). \quad (18)$$

SSW distance?

- $\delta\mu, \nu \geq P_p(S^{d-1})$, $SSW_p(\mu, \nu) = 0$, $SSW_p(\mu, \nu) = SSW_p(\nu, \mu)$,
 $\mu = \nu \Rightarrow SSW_p(\mu, \nu) = 0$
- Triangular inequality: $\delta\mu, \nu, \alpha \geq P_p(S^{d-1})$,

$$\begin{aligned} SSW_p(\mu, \nu) &= \left(\int_{\mathbb{V}_{d,2}} W_p^p(P_{\#}^U \mu, P_{\#}^U \nu) \, d\sigma(U) \right)^{\frac{1}{p}} \\ &\quad \left(\int_{\mathbb{V}_{d,2}} (W_p(P_{\#}^U \mu, P_{\#}^U \alpha) + W_p(P_{\#}^U \alpha, P_{\#}^U \nu))^p \, d\sigma(U) \right)^{\frac{1}{p}} \\ &\quad \left(\int_{\mathbb{V}_{d,2}} W_p^p(P_{\#}^U \mu, P_{\#}^U \alpha) \, d\sigma(U) \right)^{\frac{1}{p}} \\ &\quad + \left(\int_{\mathbb{V}_{d,2}} W_p^p(P_{\#}^U \alpha, P_{\#}^U \nu) \, d\sigma(U) \right)^{\frac{1}{p}} \\ &= SSW_p(\mu, \alpha) + SSW_p(\alpha, \nu). \end{aligned} \tag{19}$$

- Distance if $SSW_p(\mu, \nu) = 0 \Rightarrow \mu = \nu$,
i.e. for σ -ae U , $(\tilde{R}\mu)^U = (\tilde{R}\nu)^U \Rightarrow \mu = \nu$, i.e. \tilde{R} injective

Properties of the Spherical Radon Transform

- \tilde{R} related to Hemispherical transform H [Rubin, 2003] on S^{d-2} , where for $f \in L^1(S^{d-2})$,

$$\forall x \in S^{d-2}, Hf(x) = \int_{S^{d-2}} f(y) \mathbb{1}_{\langle x, y \rangle > 0} dy. \quad (20)$$

Proposition

$\ker(\tilde{R}) = \{f \mu \in M_{\text{even}}(S^{d-1}), \forall H \in G_{d,d-1}, \mu(H \cap S^{d-1}) = 0\}$,

where $\mu \in M_{\text{even}}$ if for all $f \in C(S^{d-1})$, $\int f d\mu = \int f \circ i d\mu$, $f_+ = (f(x) + f(-x))/2$.

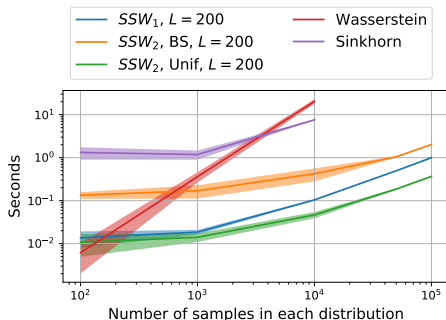
Proposition

Let $p \geq 1$, SSW_p is a pseudo-distance on $P_p(S^{d-1})$.

Runtime Comparisons

Method	Complexity
Wasserstein + LP	$O(n^3 \log n)$
Sinkhorn	$O(n^2)$
SSW_2 + BS	$O(L(n + m)(d + \log(\frac{1}{\epsilon})) + Ln \log n + Lm \log m)$
SSW_1	$O(L(n + m)(d + \log(n + m)))$
SSW_2 + Unif	$O(Ln(d + \log n))$

Table: Complexity

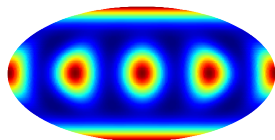


Gradient Flows

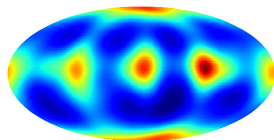
Goal:

$$\operatorname{argmin}_{\mu} SSW_2^2(\mu, \nu),$$

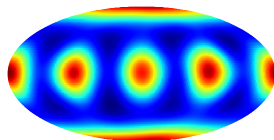
where we have access to ν through samples, *i.e.* $\hat{\nu}_m = \frac{1}{m} \sum_{j=1}^m \delta_{y_j}$ with $(y_j)_j$ i.i.d samples of ν .



(a) Target: Mixture of vMF



(b) KDE estimate of the MLP



(c) KDE estimate of 500 particles

Figure: Minimization of SSW with respect to a mixture of vMF.

Variational Inference

Goal:

$$\operatorname{argmin}_{\mu} \text{SSW}_2^2(\mu, \nu),$$

where we know the density of ν up to a constant.

Algorithm SWVI [Yi and Liu, 2021]

Input: V a potential, K the number of iterations of SWVI, N the batch size, ℓ the number of MCMC steps

Initialization: Choose q_{θ} a sampler

for $k = 1$ **to** K **do**

 Sample $(z_i^0)_{i=1}^N \sim q_{\theta}$

 Run ℓ MCMC steps starting from $(z_i^0)_{i=1}^N$ to get $(z_j^{\ell})_{j=1}^N$

 // Denote $\hat{\mu}_0 = \frac{1}{N} \sum_{j=1}^N \delta_{z_j^0}$ and $\hat{\mu}_{\ell} = \frac{1}{N} \sum_{j=1}^N \delta_{z_j^{\ell}}$

 Compute $J = \text{SSW}_2^2(\hat{\mu}_0, \hat{\mu}_{\ell})$

 Backpropagate through J w.r.t. θ

 Perform a gradient step

end for

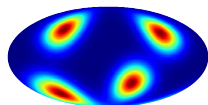
Variational Inference

Goal:

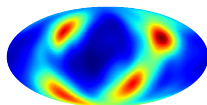
$$\operatorname{argmin}_{\mu} \operatorname{SSW}_2^2(\mu, \nu),$$

where we know the density of ν up to a constant.

- Use SSW instead of SW
- Use Normalizing flows + MCMC on the sphere



(a) Target distribution



(b) Density learned

Figure: Amortized SSWVI with a normalizing flow *w.r.t.* a mixture of vMF.

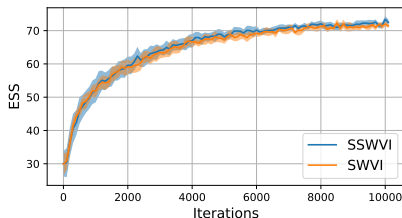


Figure: Comparison of the ESS between SWVI et SSWVI with the mixture target (mean over 10 runs).

Wasserstein Autoencoders



Figure: Autoencoder with spherical latent space.

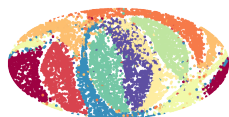
SSWAE:

$$L(f, g) = \int c(x, g(f(x))) d\mu(x) + \lambda SSW_2^2(f\#\mu, p_Z), \quad (21)$$

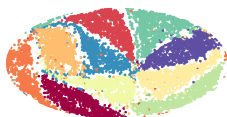
Much interest in using a spherical latent space [Davidson et al., 2018, Xu and Durrett, 2018], e.g. uniform.

SSWAE:

$$L(f, g) = \int c(x, g(f(x))) d\mu(x) + \lambda SSW_2^2(f\#\mu, p_Z), \quad (22)$$



(a) SWAE



(b) SSWAE

Figure: Latent space of SWAE and SSWAE for a uniform prior on S^2 .

Table: FID (Lower is better).

Method / Prior	Unif(S^{10})
SSWAE	14.91 ± 0.32
SWAE	15.18 ± 0.32
WAE-MMD IMQ	18.12 ± 0.62
WAE-MMD RBF	20.09 ± 1.42
SAE	19.39 ± 0.56
Circular GSWAE	15.01 ± 0.26

Wasserstein Autoencoders

SSWAE:

$$L(f, g) = \int c(x, g(f(x))) d\mu(x) + \lambda SSW_2^2(f\#\mu, p_Z), \quad (23)$$



(a) SSWAE



(b) SWAE



(c) SAE

Figure: Samples generated with Sliced-Wasserstein Autoencoders with a uniform prior on S^{10} .

Conclusion

- First SW discrepancy on manifolds
- Good performance on ML tasks

Future works

- SW on hyperbolic spaces
- Statistical analysis

- First SW discrepancy on manifolds
- Good performance on ML tasks

Future works

- SW on hyperbolic spaces
- Statistical analysis

Thank you!

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