Hyperbolic Sliced-Wasserstein via Geodesic and Horospherical Projections

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Motivation

- Data with hierarchical structure: Hyperbolic spaces [Nickel and Kiela, 2017, 2018]
  - Trees
  - Graphs [Krioukov et al., 2010, Gupte et al., 2011]
  - Words [Tifrea et al., 2018]
  - Images [Khrulkov et al., 2020]

Motivation

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Goal: develop new tools on hyperbolic spaces

- Distributions [Nagano et al., 2019]
- Neural networks [Ganea et al., 2018]
- Normalizing flows [Bose et al., 2020]
- Optimal transport (OT) [Alvarez-Melis et al., 2020, Hoyos-Idrobo, 2020]

Contribution: new OT discrepancy

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

$$W_p^p(\mu, \nu) = \inf_{\gamma \in \Pi(\mu,\nu)} \int d(x,y)^p \, \mathrm{d}\gamma(x,y), \tag{1}$$

where $\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}(M \times M),\ \pi^1_\# \gamma = \mu, \pi^2_\# \gamma = \nu\}$ and $\pi^1(x,y) = x$, $\pi^2(x,y) = y$, $\pi^1_\# \gamma = \gamma \circ (\pi^1)^{-1}$.

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 [Fatras et al., 2020]
- Sliced-Wasserstein [Rabin et al., 2011, Bonnotte, 2013] but only on Euclidean spaces

Sliced-Wassertein on $\mathbb{R}^d$

Wasserstein on $\mathbb{R}$:

$$\forall p \geq 1, \forall \mu, \nu \in \mathcal{P}_p(\mathbb{R}),\ W_p^p(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p \, \mathrm{d}u \tag{2}$$

Sliced-Wassertein on $\mathbb{R}^d$

Wasserstein on $\mathbb{R}$:

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

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

$$SW_p^p(\mu,\nu) = \int_{S^{d-1}} W_p^p(P^\theta_\# \mu, P^\theta_\# \nu) \ \mathrm{d}\lambda(\theta), \tag{3}$$

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

Sliced-Wassertein on $\mathbb{R}^d$

Wasserstein on $\mathbb{R}$:

$$\forall p \geq 1, \forall \mu, \nu \in \mathcal{P}_p(\mathbb{R}),\ W_p^p(\mu,\nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p \ \mathrm{d}u \tag{2}$$

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Properties:

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

Hyperbolic space

Hyperbolic space: Riemannian manifold of constant negative curvature

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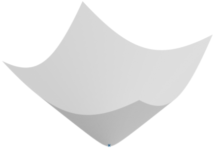
Hyperbolic space: Riemannian manifold of constant negative curvature
Different models:

- Lorentz model $\mathbb{L}^d \subset \mathbb{R}^{d+1}$

$$\mathbb{L}^d = \{(x_0, \ldots, x_d) \in \mathbb{R}^{d+1},\ \langle x, x \rangle_{\mathbb{L}} = -1, x_0 > 0\} \quad (4)$$

where

$$\forall x, y \in \mathbb{L}^d,\ \langle x, y \rangle_{\mathbb{L}} = -x_0 y_0 + \sum_{i=1}^{d} x_i y_i \quad (5)$$



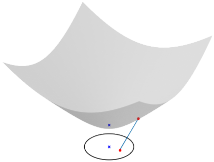
  - Origin: $x^0 = (1, 0, \ldots, 0)$
  - Geodesic distance: $d_{\mathbb{L}}(x, y) = \operatorname{arccosh}(-\langle x, y \rangle_{\mathbb{L}})$

Hyperbolic space

Hyperbolic space: Riemannian manifold of constant negative curvature
Different models:

- Lorentz model $\mathbb{L}^d \subset \mathbb{R}^{d+1}$
- Poincaré ball $\mathbb{B}^d = \{x \in \mathbb{R}^d,\ \|x\|_2 < 1\}$
    - Geodesic distance:

$$d_{\mathbb{B}}(x,y) = \operatorname{arccosh}\left(1 + 2\frac{\|x-y\|_2^2}{(1-\|x\|_2^2)(1-\|y\|_2^2)}\right)$$



$$\forall x \in \mathbb{L}^d,\ P_{\mathbb{L}\to\mathbb{B}}(x) = \frac{1}{1+x_0}(x_1,\dots,x_d)$$

$$\forall x \in \mathbb{B}^d,\ P_{\mathbb{B}\to\mathbb{L}}(x) = \frac{1}{1-\|x\|_2^2}(1+\|x\|_2^2, 2x_1,\dots,2x_d).$$

SW on Hyperbolic space

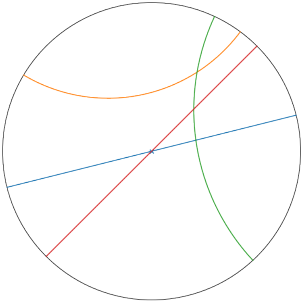
Goal: defining SW discrepancy on Hyperbolic space

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

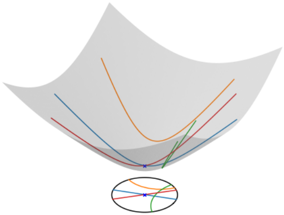
Table: SW to HSW

Geodesics

- Generalization of straight lines on manifolds: geodesics
- On $\mathbb{L}^d$, geodesics = intersection between 2-plane and $\mathbb{L}^d$
- On $\mathbb{B}^d$, geodesics = circular arcs perpendicular to the boundary S^{d-1}



(a) Geodesics on Poincaré ball.



(b) Geodesics in Lorentz model.

Wasserstein distance on geodesics

- On hyperbolic spaces, geodesic lines, *i.e.* $\gamma : \mathbb{R} \to \mathbb{L}^d$ such that

$$\forall s,t \in \mathbb{R},\ d_{\mathbb{L}}\big(\gamma(s),\gamma(t)\big) = |t-s|. \tag{6}$$

- Projection on $\mathbb{R}$: Let $v \in T_{x^0}\mathbb{L}^d = \mathrm{span}(x^0)^\perp$,

$$\forall x \in \gamma(\mathbb{R}) = \mathbb{L}^d \cap \mathrm{span}(v,x^0),\ t_{\mathbb{L}}^v(x) = \mathrm{sign}(\langle x,v\rangle) d_{\mathbb{L}}(x,x^0) \tag{7}$$

Proposition (Wasserstein distance on geodesics.)

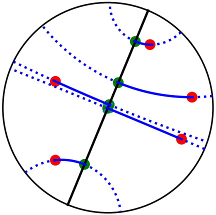
Let $v \in T_{x^0}\mathbb{L}^d \cap S^d$ and $\mathcal{G} = \mathrm{span}(x^0,v) \cap \mathbb{L}^d$ a geodesic passing through x^0. Then, for μ,ν probability measures on $\mathcal{G}$, we have

$$\begin{aligned} \forall p \geq 1,\ W_p^p(\mu,\nu) &= W_p^p(t^v_\# \mu, t^v_\# \nu) \\ &= \int_0^1 |F^{-1}_{t^v_\#\mu}(u) - F^{-1}_{t^v_\#\nu}(u)|^p \, \mathrm{d}u. \end{aligned} \tag{8}$$

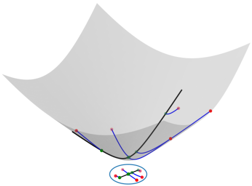
Projection along geodesics

Let $v \in T_{x^0}\mathbb{L}^d \cap S^d$, $\mathcal{G} = \mathrm{span}(x^0, v) \cap \mathbb{L}^d$ a geodesic.
Geodesic projection:

$$\begin{aligned} \forall x \in \mathbb{L}^d,\ P^v(x) &= \underset{y \in \mathcal{G}}{\mathrm{argmin}}\ d_{\mathbb{L}}(x,y) \\ &= \frac{1}{\sqrt{\langle x, x^0\rangle_{\mathbb{L}}^2 - \langle x, v\rangle_{\mathbb{L}}^2}}\big(- \langle x, x^0\rangle_{\mathbb{L}} x^0 + \langle x, v\rangle_{\mathbb{L}} v\big). \end{aligned} \tag{9}$$



(c) Along geodesics.



(d) Along geodesics.

Figure: Projection of (red) points on a geodesic (black line) in the Poincaré ball along geodesics. Projected points on the geodesic are in green.

Geodesic Hyperbolic Sliced-Wasserstein

Definition (Geodesic Hyperbolic Sliced-Wasserstein)

Let $p \geq 1$, $\mu, \nu \in \mathcal{P}_p(\mathbb{L}^d)$,

$$GHSW_p^p(\mu, \nu) = \int_{T_{x^0}\mathbb{L}^d \cap S^d} W_p^p(t^v_\# P^v_\# \mu, t^v_\# P^v_\# \nu)\ \mathrm{d}\lambda(v). \tag{10}$$

	SW	HSW
Closed-form of W	Line	Geodesic
Projection	$P^\theta(x) = \langle x, \theta \rangle$	$P^v(x)$
Integration	S^{d-1}	$T_{x^0}\mathbb{L}^d \cap S^d \cong S^{d-1}$

Table: Comparison SW-HSW

A second projection

- Geodesic projection:

$$\langle x, \theta \rangle \theta = \underset{y \in \mathrm{span}(\theta)}{\operatorname{argmin}} \|x - y\|_2 \tag{11}$$

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- Coordinate point of view

$$\langle x, \theta \rangle = \lim_{t \to \infty} \ \big(t - \|x - t\theta\|_2 \big) \tag{12}$$

- Busemann function:

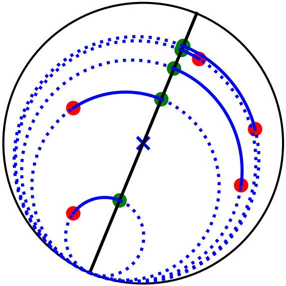
$$B_\gamma(x) = \lim_{t \to \infty} \ \big(d(x, \gamma(t)) - t \big). \tag{13}$$

Proposition (Busemann function on hyperbolic space.)

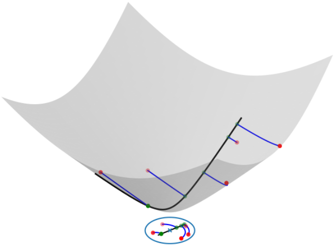
- *On* $\mathbb{L}^d$*:* $\forall v \in T_{x^0}\mathbb{L}^d \cap S^d, \ \forall x \in \mathbb{L}^d, \ B_v(x) = \log(-\langle x, x^0 + v \rangle_{\mathbb{L}})$
- *On* $\mathbb{B}^d$*:* $\forall \tilde{v} \in S^{d-1}, \ \forall x \in \mathbb{B}^d, \ B_{\tilde{v}}(x) = \log\left(\frac{\|\tilde{v} - x\|_2^2}{1 - \|x\|_2^2} \right)$

Projection along horospheres

- Projection along the level sets of B_v
- Level sets $=$ horospheres
- Tend to better preserve the distances [Chami et al., 2021]



(a) Along horospheres.



(b) Along horospheres.

Figure: Projection of (red) points on a geodesic (black line) in the Poincaré ball along geodesics or horospheres (in blue). Projected points on the geodesic are in green.

Projection along horospheres

- Projection along the level sets of B_v
- Level sets = horospheres
- Tend to better preserve the distances [Chami et al., 2021]

Proposition (Horospherical projection)

1. *Let $v \in T_{x^0}\mathbb{L}^d \cap S^d$ be a direction and $\mathcal{G} = \mathrm{span}(x^0, v) \cap \mathbb{L}^d$ the corresponding geodesic passing through x^0. Then, for any $x \in \mathbb{L}^d$, the projection on $\mathcal{G}$ along the horosphere is given by*

$$\tilde{P}^v(x) = \frac{1+u^2}{1-u^2}x^0 + \frac{2u}{1-u^2}v, \tag{14}$$

where $u = \frac{1+\langle x, x^0+v\rangle_{\mathbb{L}}}{1-\langle x, x^0+v\rangle_{\mathbb{L}}}$.

2. *Let $\tilde{v} \in S^{d-1}$ be an ideal point. Then, for all $x \in \mathbb{B}^d$,*

$$\tilde{P}^{\tilde{v}}(x) = \left(\frac{1-\|x\|_2^2 - \|\tilde{v}-x\|_2^2}{1-\|x\|_2^2 + \|\tilde{v}-x\|_2^2}\right)\tilde{v}. \tag{15}$$

Horospherical Hyperbolic Sliced-Wasserstein

Definition (Horospherical Hyperbolic Sliced-Wasserstein)

Let $p \geq 1$, $\mu, \nu \in \mathcal{P}_p(\mathbb{L}^d)$,

$$HHSW_p^p(\mu, \nu) = \int_{S^{d-1}} W_p^p(t^v_\# \tilde{P}^v_\# \mu, t^v_\# \tilde{P}^v_\# \nu) \, \mathrm{d}\lambda(v). \tag{16}$$

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

$$HHSW_p^p(\mu, \nu) = \int_{S^{d-1}} W_p^p(t^{\tilde{v}}_\# \tilde{P}^{\tilde{v}}_\# \mu, t^{\tilde{v}}_\# \tilde{P}^{\tilde{v}}_\# \nu) \, \mathrm{d}\lambda(\tilde{v}). \tag{17}$$

Proposition

Let $\mu, \nu \in \mathcal{P}(\mathbb{B}^d)$ and denote $\tilde{\mu} = (P_{\mathbb{B}\to\mathbb{L}})_\# \mu$, $\tilde{\nu} = (P_{\mathbb{B}\to\mathbb{L}})_\# \nu$. Then,

$$\forall p \geq 1, \; HHSW_p^p(\mu, \nu) = HHSW_p^p(\tilde{\mu}, \tilde{\nu}). \tag{18}$$

Summary

	SW	GHSW	HHSW
Closed-form of W	Line	Geodesic	Geodesic
Projection along	Straight line	Geodesic	Horosphere
Integration	S^{d-1}	S^{d-1}	S^{d-1}
Distance	Yes	Pseudo	Pseudo

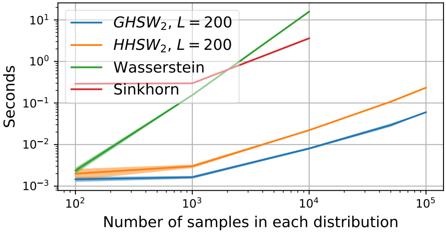
Table: Comparison SW-HSW

HHSW/GHSW distances? Rely on related Radon transform injectivity.

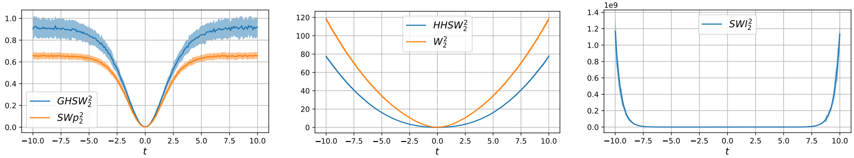
Runtime Comparisons

Method	Complexity
Wasserstein + LP	$O(n^3 \log n)$
Sinkhorn	$O(n^2)$
GHSW	$O(Ln(d + \log n))$
HHSW	$O(Ln(d + \log n))$

Table: Complexity



Let $\mu = \mathcal{G}(x^0, I_d)$, $\nu_t = \mathcal{G}(x_t, I_d)$ where $x_t = \cosh(t)x^0 + \sinh(t)v$.



(a) SW on Poincaré, GHSW (b) HHSW and Wasserstein (c) SW on Lorentz

Figure: Comparison of the Wasserstein distance (with the geodesic distance as cost), GHSW, HHSW and SW between Wrapped Normal distributions.

Goal:

$$\underset{\mu}{\operatorname{argmin}}\ HSW_2^2(\mu,\nu),$$

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.

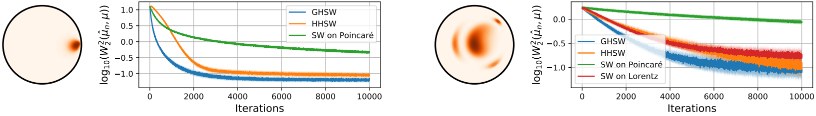
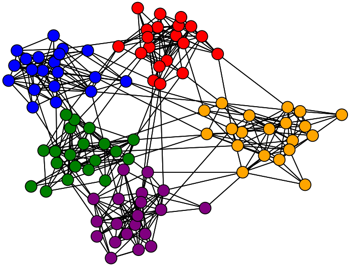


Figure: Target distribution and evolution of the log 2-Wasserstein between the target and the gradient flow of GHSW, HHSW and SW. On the left, the target is a WND and on the right, a mixture of 4 WNDs.

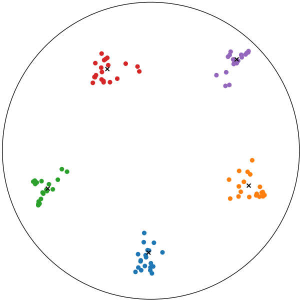
Graph Clustering

- Embed a graph as $\nu \in \mathcal{P}(\mathbb{B}^d)$
- Fit a mixture:

$$\underset{(\mu_k)_k,(\Sigma_k)_k,(\alpha_k)_k}{\mathrm{argmin}} \quad HSW\left(\nu, \sum_k \alpha_k \mathcal{G}(\mu_k, \Sigma_k)\right) \tag{19}$$



(a) SBM



(b) SBM embedded

Figure: Fit of a mixture of WND on a SBM. Cross in black denote the centers learned.

Classification with Prototypes

- $(x_i, y_i)_{i=1}^n$ training set, $y_i \in \{1, \dots, C\}$, $\forall c \in \{1, \dots, C\}$, p_c prototype.
- $\forall i,\ z_i = \exp_0\big(f_\theta(x_i)\big)$
- Loss:

$$\ell(\theta) = \frac{1}{n}\sum_{i=1}^n B_p(z_i) + \lambda HSW\left(\frac{1}{n}\sum_{i=1}^n \delta_{z_i}, \frac{1}{C}\sum_{c=1}^C \mathcal{G}(\alpha_c p_c, \beta I_d)\right) \tag{20}$$

Table: Test accuracy.

	CIFAR10			CIFAR100			
Dimensions	2	3	4	3	5	10	50
Busemann	91.2	92.2	92.2	49.0	54.6	59.1	**65.8**
GHSW	**91.61**	**92.48**	**92.29**	**54.78**	**60.94**	**62.72**	59.22
HHSW	91.32	92.34	91.92	54.29	60.67	62.14	63.17

Conclusion

- SW discrepancies on hyperbolic spaces
- Application to different ML tasks

Future works

- Statistical analysis
- Distance?
- Applications: persistent diagrams...

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Thank you!

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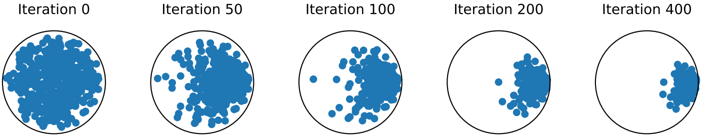
Gradient Flows

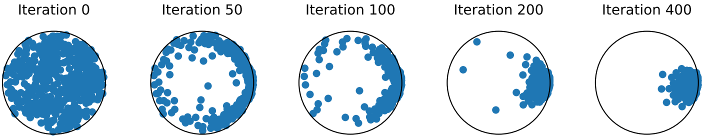
Goal:

$$\underset{\mu}{\operatorname{argmin}} \;\; HSW_2^2(\mu, \nu),$$

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) With geodesic projection.



(b) With horospherical projection.

Figure: Evolution of the particles along the gradient flow of HSW (with geodesic or horospherical projection).

Document Classification

- Each document = distribution of words
- Embed words in $\mathbb{B}^{100}$
- Compute the matrix of distances and use k-NN

Table: Document classification accuracy with k-NN ($k=5$).

	W	W_ϵ	SWp	SWl	GHSW	HHSW
Movie Reviews	**71.5**	60.5	65	65.5	**69.3**	58.8
Twitter	$\mathbf{69.7_{\pm 0.7}}$	-	$67.2_{\pm 0.5}$	$\mathbf{67.3_{\pm 2.3}}$	$66.6_{\pm 1.1}$	$63.8_{\pm 1}$
BBCSport	$\mathbf{94.7}_{\pm 1.1}$	$\mathbf{89.8_{\pm 0.5}}$	$\mathbf{89.8}_{\pm 1.4}$	$89.8_{\pm 0.8}$	$89.4_{\pm 1.5}$	$75.6_{\pm 1.7}$