

# Novel geometric methods for data analysis focusing on curvature and geodesics in data space

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## Part I: Data analysis using $\alpha$ and $\beta$ -metrics

- with Henry P. Wynn (London School of Economics)

## Part II: Application of metric cones to graph embedding

- with Daisuke Takehara (Accenture)

# Outline of Part I. Data Analysis Using $\alpha$ and $\beta$ -metrics

- 1 Motivation and Strategy
- 2  $\alpha$ -Metric
- 3  $\beta$ -Metric
- 4 Application

## Fréchet Mean of a Euclidean Space

Given a sample  $x_1, \dots, x_n$  in a metric space  $(X, d)$ , the intrinsic mean (Fréchet Mean) is the set of the minimizers of the Fréchet function:

$$\hat{\mu} \in \arg \min_{m \in X} \sum_{i=1}^n d(x_i, m)^2$$

For a Euclidean space, the intrinsic mean is unique since the Fréchet function  $f(m) = \sum_i \|m - x_i\|^2$  is strictly convex.

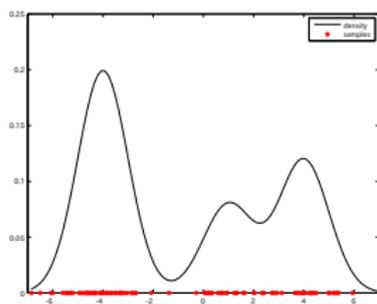
It is easy to see the intrinsic mean is equal to the sample mean  $\bar{x}$ .

In general, the less (or more negative) curvature, the less the number of (local) minima of the Fréchet function.

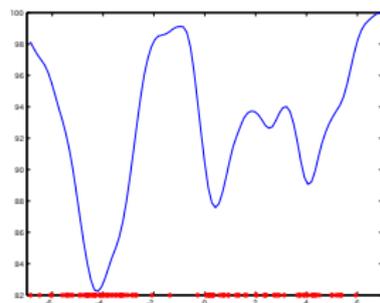
HOWEVER, this “good” behavior of the Fréchet function is not always welcome.

# Clustering

For a negatively curved space, Fréchet function  $f(m) := \sum_i d(m, x_i)^2$  is not necessarily convex and its local minima (called the Karcher means) can be used as the center of each cluster for clustering.



density function and  
its samples



$f(m)$

⇒ Controlling the curvature of the data space should play an important role in data analysis.

# Our strategy

- Ordinary data analysis (e.g. classification, regression):

Data  $X_i$  ( $i = 1, \dots, n$ ), Metric  $d$

→ Loss function  $\hat{f} \in \mathcal{F}$

(can be selected by cross validation, resampling)

→  $\hat{\theta} = \arg \min \sum_i \hat{f}(d(X_i, \theta))$

- Our approach:

Data  $X_i$  ( $i = 1, \dots, n$ ), Loss function  $f$

→ Metric  $\hat{d} \in \mathcal{D}$

(can be selected by cross validation, resampling)

→  $\hat{\theta} = \arg \min \sum_i f(\hat{d}(X_i, \theta))$

How to set the family  $\mathcal{D}$  of metrics?

⇒ by focusing on their curvature

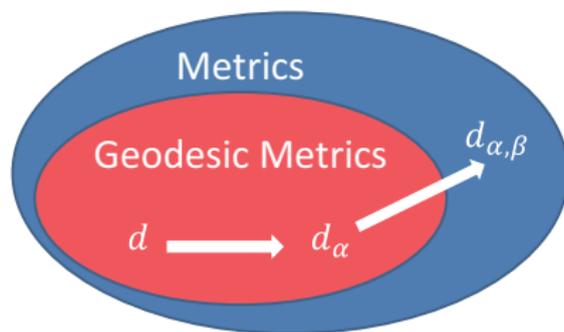
Our policy: keep the problem in geometry  
as much as possible.

## Two steps of changing metrics

A **geodesic metric space** is a metric space s.t. the distance between two points is equivalent to the shortest path length connecting them.

We can define a curvature called CAT( $k$ ) property for each geodesic metric space.

We change the metric  $d$  of the original data space, to a geodesic metric space  $d_\alpha$ , and next to a (usually non-geodesic) metric space  $d_{\alpha,\beta}$ .



# The $\alpha$ , $\beta$ -metric and $\alpha$ , $\beta$ , $\gamma$ -mean

We propose a family of metrics:

$$d_{\alpha,\beta}(x, y) = g_{\beta}(d_{\alpha}(x, y))$$

and intrinsic means:

$$\hat{\mu}_{\alpha,\beta,\gamma} = \arg \min_{m \in \mathcal{M}} \sum_{i=1}^n d_{\alpha,\beta}(x_i, m)^{\gamma}$$

$d_{\alpha}$ : a locally transformed geodesic metric ( $\alpha \in \mathbb{R}$ ), defined later

$g_{\beta}$ : a concave function corresponding to a specific kind of extrinsic means ( $\beta \in (0, \infty]$ ), defined later

$\gamma$ : for  $L_{\gamma}$ -loss ( $\gamma \geq 1$ )

# Data analysis by $\alpha$ , $\beta$ and $\gamma$

	Euclidean	$d_{\alpha,\beta}$
metrics	$d(x, y) = \ x - y\ $	$d_{\alpha\beta}(x, y) = g_{\beta}(d_{\alpha}(x, y))$
intrinsic mean	$\arg \min_{m \in \mathbb{E}^d} \sum \ x_i - m\ ^2$	$\arg \min_{m \in \mathcal{M}} \sum g_{\beta}(d_{\alpha}(x_i, m))^{\gamma}$
Fréchet variance	$\min_{m \in \mathbb{E}^d} \frac{1}{n} \sum \ x_i - m\ ^2$	$\min_{m \in \mathcal{M}} \frac{1}{n} \sum g_{\beta}(d_{\alpha}(x_i, m))^{\gamma}$
Fréchet function	$f(m) = \sum \ x_i - m\ ^2$	$f_{\alpha\beta\gamma}(m) = \sum g_{\beta}(d_{\alpha}(x_i, m))^{\gamma}$

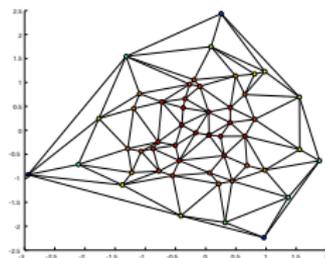
# Outline of Part I

- 1 Motivation and Strategy
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# Empirical Metric Graphs

We begin from computing empirical graphs, whose vertices are the data points. For example,

- 1 Complete graph
- 2 Delaunay graph
- 3 k-NN graphs
- 4  $\epsilon$ -NN graphs



Delaunay empirical graph

We introduce a metric on the graph by the shortest path length:

$$d(x_0, x_1) := \inf_{\gamma \in \Gamma(x_0, x_1)} \sum_{e_{ij} \in \gamma} d_{ij},$$

where  $d_{ij}$  is the length of an edge  $e_{ij}$ .

## The $\alpha$ -Metric: Empirical Graph Case

$\alpha$ -metric for an empirical graph is defined by the shortest path length with powered edge lengths:

$$d_\alpha(x_0, x_1) := \inf_{\gamma \in \Gamma(x_0, x_1)} \sum_{e_{ij} \in \gamma} d_{ij}^{1-\alpha}.$$

This can be seen as an empirical approximation of

$$\tilde{d}_\alpha(x_0, x_1) := \inf_{\gamma \in \Gamma(x_0, x_1)} \int_0^1 f^{\alpha p}(z(t)) d|\gamma(t)|.$$

where  $p$  is the dimension of the original data space.

Here we use a fact, under some regularity conditions,  $d_{ij}^{-1/p}$  is an unbiased estimator of the local density and

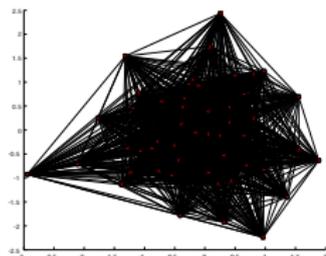
$$(d_{ij}^{-1/p})^{\alpha p} d_{ij} = d_{ij}^{1-\alpha}.$$

## Some facts about the $\alpha$ -metric

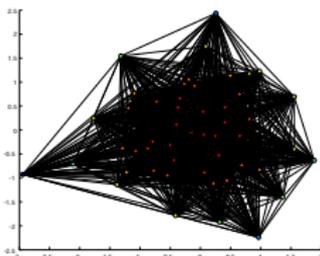
- Stochastic convergence of the empirical version  $d_\alpha$  to a continuous version  $\tilde{d}_\alpha$  has been proved by Hwang, et al.(2016) under some condition.
- Geodesic subgraphs computed using  $\alpha$ -metric are a special case of “Pathfinder networks” used mainly in areas of Psychology.

# Ex: Geodesic subgraphs (starting from the complete graph)

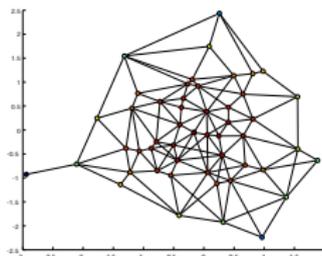
A geodesic subgraph is computed by removing edges that cannot be used in any geodesics.



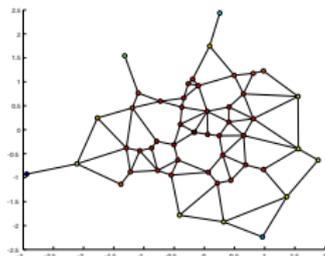
(a)  $\alpha = 1$



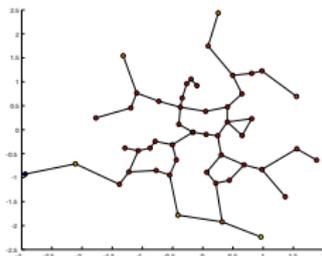
(b)  $\alpha = 0$



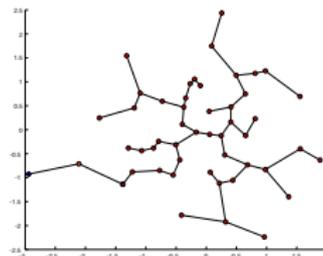
(c)  $\alpha = -0.3$



(d)  $\alpha = -1$



(e)  $\alpha = -5$



(f)  $\alpha = -30$

In K. and Wynn (2020), we proved the following facts under some conditions:

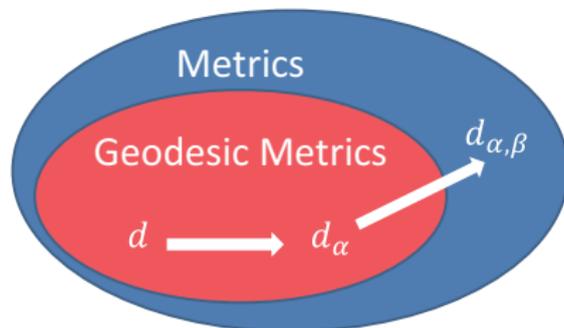
- The edge set of a geodesic subgraph of an  $\alpha$ -empirical graph becomes smaller as  $\alpha$  decreases.
- Each geodesic subgraph becomes a tree (minimum spanning tree) for sufficiently small  $\alpha$ .
- The curvature of a geodesic subgraph decreases as  $\alpha$  decreases in the sense of CAT( $k$ ) property and finally becomes CAT(0).

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## Further metric transformation by $\beta$

We next introduce a parameter  $\beta$  to change a geodesic metric  $d_\alpha$  to a (not necessarily geodesic) metric  $d_{\alpha,\beta}$ .



# $\beta$ -Metric

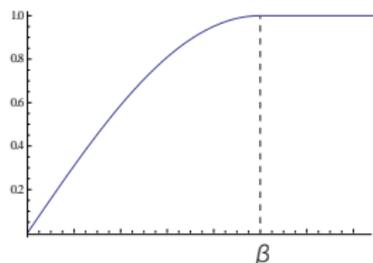
Let  $(X, d)$  be a geodesic metric space.

For  $\beta > 0$ , transform the metric  $d$  as

$$d_\beta(x_0, x_1) = g_\beta(d(x_0, x_1))$$

where

$$g_\beta(z) = \begin{cases} \sin\left(\frac{\pi z}{2\beta}\right), & \text{for } 0 \leq z \leq \beta, \\ 1, & \text{for } z > \beta. \end{cases}$$



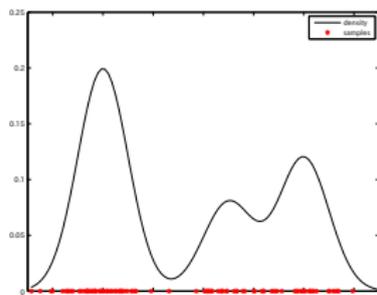
For  $\beta = \infty$ ,  $d_\beta = d$ .

$d_\beta$  satisfies the triangle inequality and becomes a metric but not necessarily a geodesic metric.

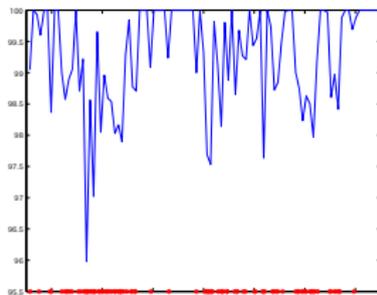
**$d_\beta$ -mean:**  $\hat{\mu}_\beta = \arg \min_{m \in X} \sum_i g_\beta(d(x_i, m))^2$ .

# $\beta$ and clustering

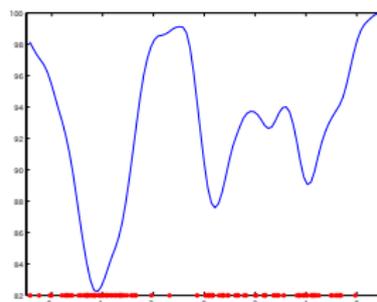
$f(m) = \sum_i g_\beta(|x_i - m|)^2$  with various  $\beta$ :



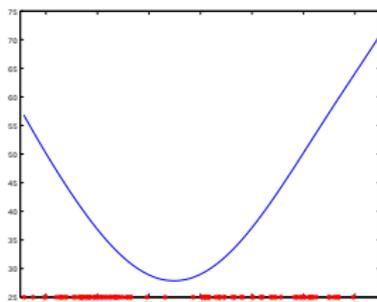
(a) Density function



(b)  $\beta = 0.1$



(c)  $\beta = 1$



(d)  $\beta = 10$

## Can $\beta$ -metric be explained by curvature?

$d_\beta$ -mean: 
$$\hat{\mu}_\beta = \arg \min_{m \in X} \sum_i g_\beta(d(x_i, m))^2.$$

Fréchet function on the  $d_\beta$  metric space behaves similar to positively curved space.

But the curvature (i.e. CAT( $k$ ) property) can not be defined for non geodesic metric spaces.

The  $d_\beta$ -mean can be redefined as an **extrinsic mean** when the data space is embedded in a geodesic metric space called a “metric cone”.

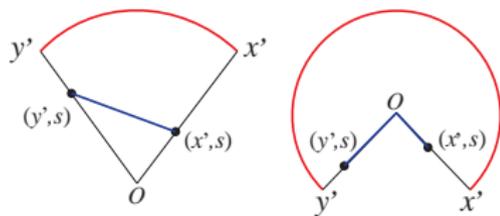
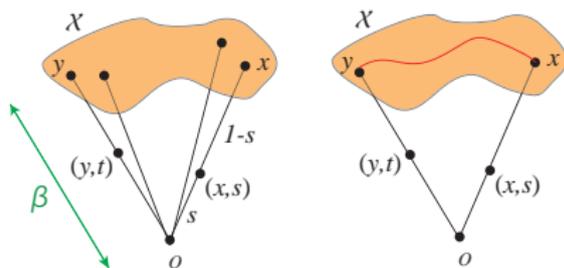
# Metric Cone

$\mathcal{X}$ : a geodesic metric space

A **metric cone**  $\tilde{\mathcal{X}}_\beta$  with  $\beta > 0$  is a (truncated) cone  $\mathcal{X} \times [0, 1] / \mathcal{X} \times \{0\}$  with a metric

$$\tilde{d}_\beta((x, s), (y, t)) = \sqrt{t^2 + s^2 - 2ts \cos(\pi \min(d_{\mathcal{X}}(x, y)/\beta, 1))}$$

for any  $(x, s), (y, t) \in \tilde{\mathcal{X}}_\beta$ .

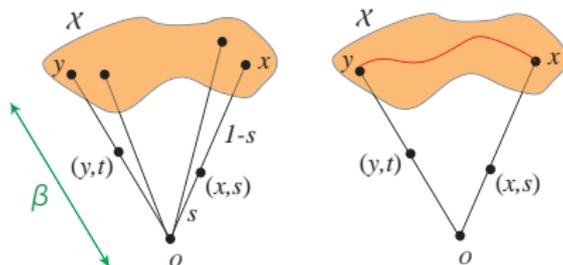


The  $d_\beta$ -mean can be redefined as an extrinsic mean when the data space is embedded in a “metric cone”.

# Extrinsic Mean in Metric Cone

Merits of embedding in a metric cone:

- Curvature of embedding space can be tuned by  $\beta$  in the sense of CAT( $k$ ) property (K. and Wynn(2020)) and Riemannian sense (Takehara and K.(2021)).
- The embedding space is only 1-dimensional higher than the original data space.
- Every geodesic metric space can be embedded. (Remark this is not true for embedding in a Euclidean space, e.g.  $d_\alpha$  metric spaces.)



## The $\alpha, \beta, \gamma$ -mean: Summary

We proposed a class of the intrinsic means:

$$\hat{\mu}_{\alpha, \beta, \gamma} = \arg \min_{m \in \mathcal{M}} \sum_i g_{\beta}(d_{\alpha}(x_i, m))^{\gamma}$$

and corresponding Fréchet variances:

$$V_{\alpha, \beta, \gamma} = \min_{m \in \mathcal{M}} \frac{1}{n} \sum_i g_{\beta}(d_{\alpha}(x_i, m))^{\gamma}.$$

The Fréchet function can be used for clustering.

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## Application: Clustering

Data: five kinds of data from UCI Machine Learning Repository (iris, wine, ionosphere, breast cancer, yeast)

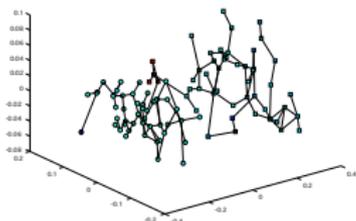
- The clustering error by k-means method decreases significantly by selecting an adequate value.

-  $\alpha \in \{-5.0, -4.8, \dots, 0.8, 1\}$  and  
 $\beta \in \{2^{-3}, 2^{-2}, \dots, 2^6, \infty\}$ .

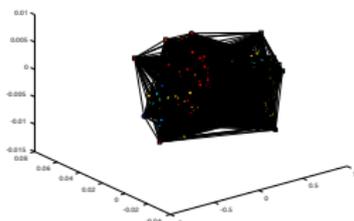
data set	k-means with $d_{\alpha,\beta}$			Euclid
	$\hat{\alpha}$	$\hat{\beta}$	$r^*$	$r$
(i) iris	-4.4	0.125	0.0333	0.1067
(ii) wine	0.8	8	0.2753	0.2978
(iii) ionosphere	-5.0	16	0.0798	0.2877
(iv) cancer	0.8	16	0.0914	0.1459
(v) yeast	-0.6	2	0.4447	0.4515

# Application: Clustering

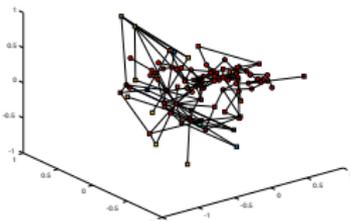
- The structure of the “optimal” geodesic graphs differs depending on the data:



(a) iris ( $\hat{\alpha} = -5.0, \hat{\beta} = 0.125$ )



(b) wine ( $\hat{\alpha} = 0.8, \hat{\beta} = 4$ )



(c) ionosphere ( $\hat{\alpha} = -3.2, \hat{\beta} = 8$ )

**Figure 1:** The geodesic graph of each data set with an optimum value of  $\alpha$  and  $\beta$  for a randomly selected 100 sub-samples.

# Example: Rainfall Data (1)

Data:

Daily precipitation data of 9 regions in UK since 1931  
(UK Met office Hadley Centre observation data)

Target:

Check if the variance throughout each year changed

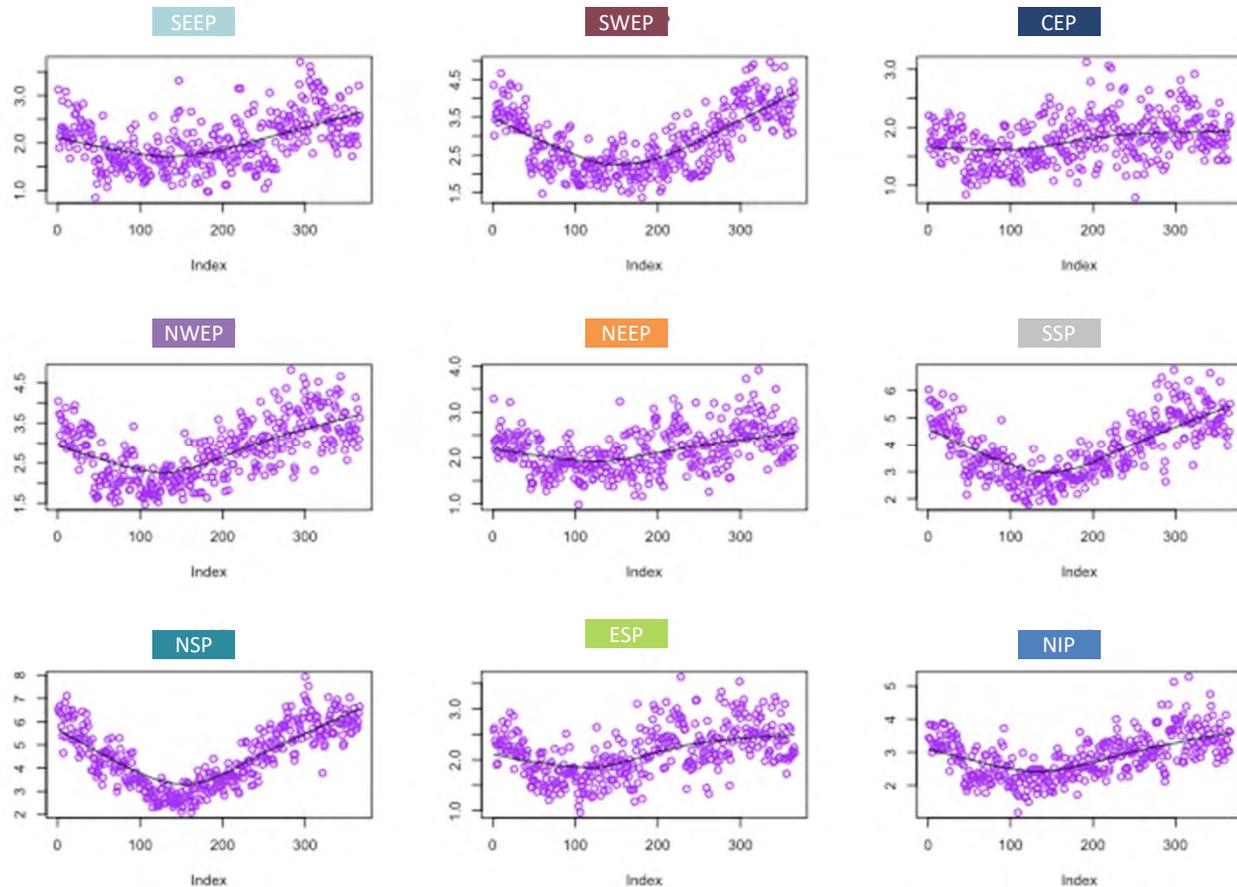
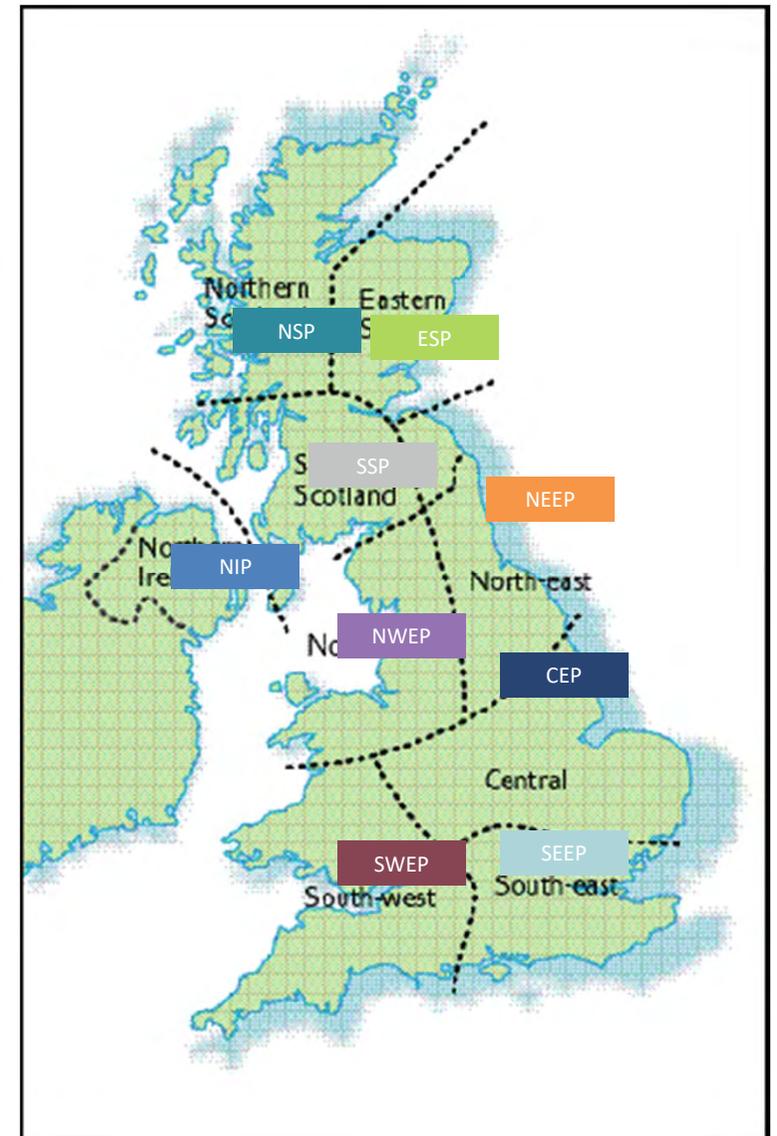
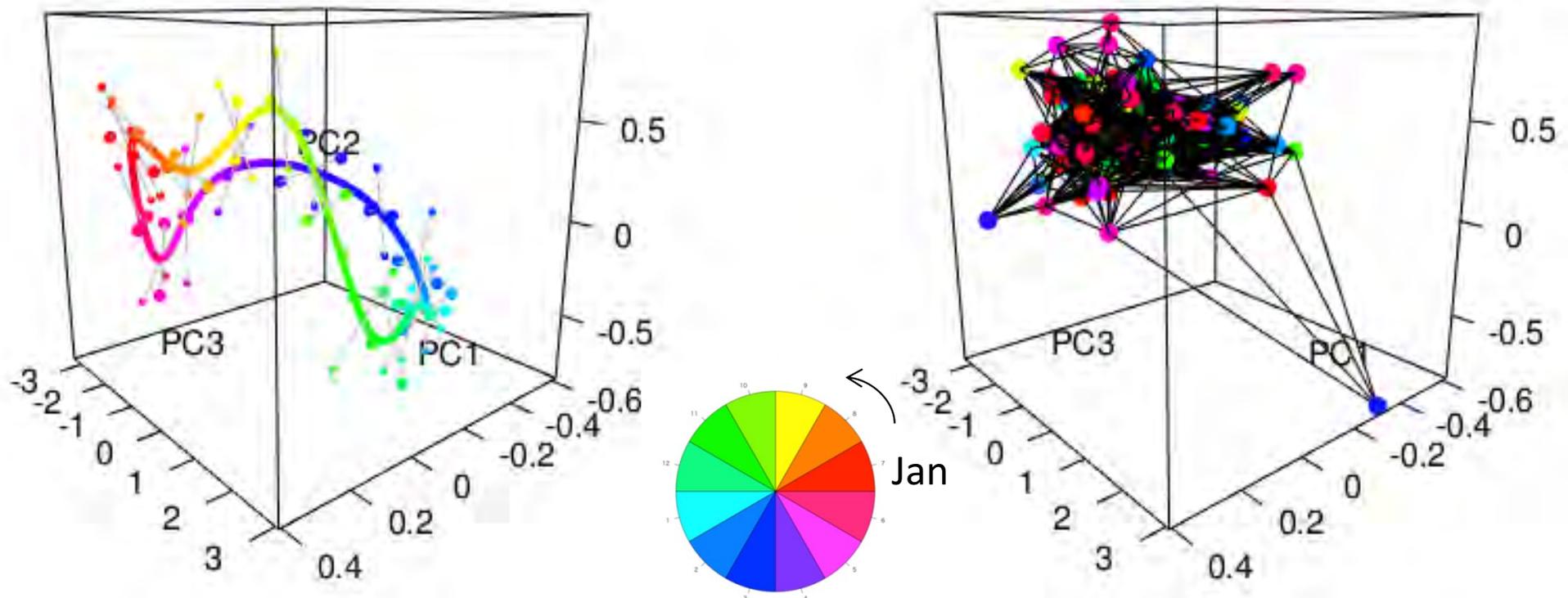


Fig: precipitation plot for 85 years



## Example: Rainfall Data (2)



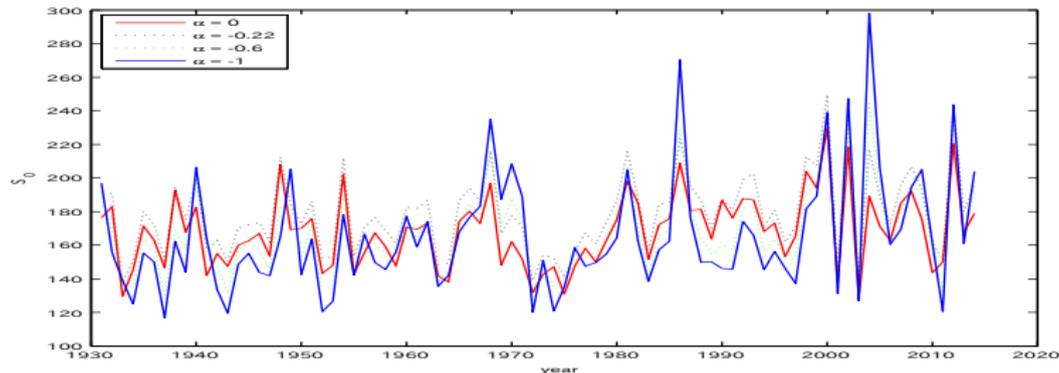
Annual cycle structure of the average of the 85 years

The geodesic graph of 1986,  
 $\alpha = -0.6$

- Precipitation data has some annual cyclic structure.
- The geodesic subgraph and the corresponding generalized variance are expected to reflect such geometric structure.

# Application: Rainfall Data

Time series of “variance”  $s_0^2 := \left\{ \min_i \sum_j d_\alpha(x_i, x_j)^2 \right\}^{1/(1-\alpha)}$  are plotted for  $\alpha = 0$  (red solid line),  $-0.22$  (black dashed line) and  $-1$  (blue solid line).



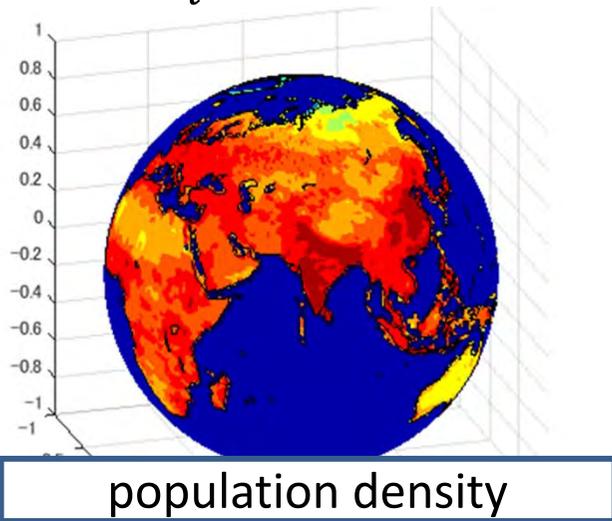
This generalized “variance” is expected to detect change of another type of volatility incorporating spacio-temporal geometrical structure of the precipitation data.

# Example: Clustering of Populations on the earth

$X_i$ : a person on the earth

$y$ : a point on the earth

$$f_\beta(y) = \sum_i g_\beta(\|X_i - y\|)^2$$



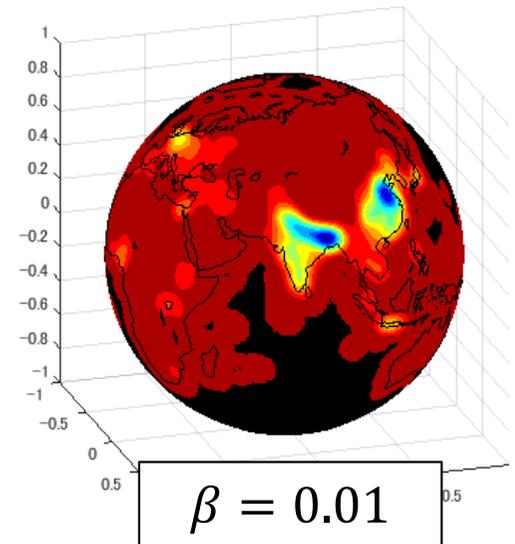
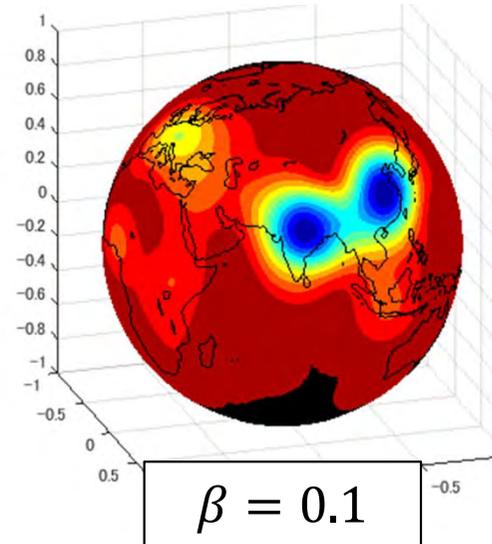
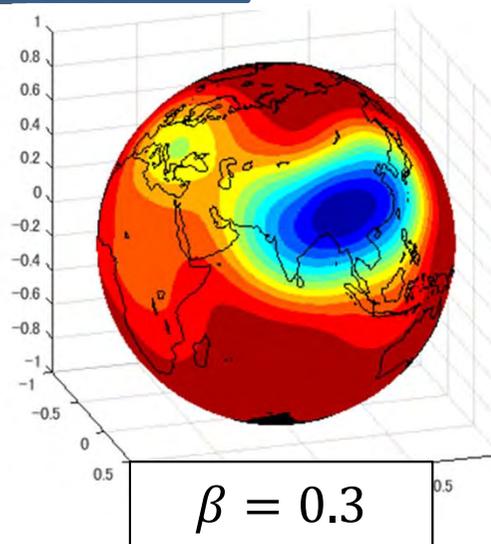
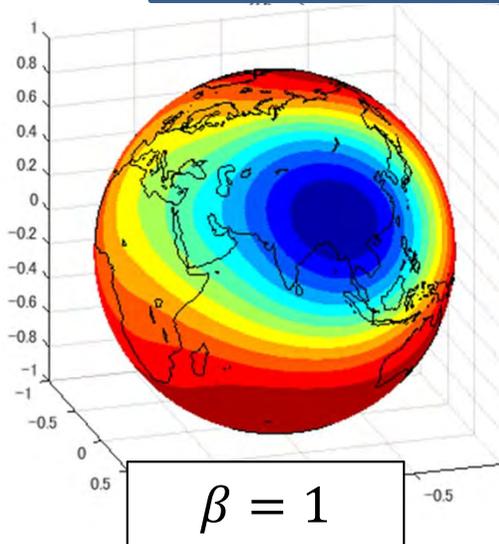
$\beta = 1$ : Embedding into a Euclidean space

↓ Let  $\beta$  smaller

Curvature of the embedding metric cone becomes more positive

↓

Local minima of  $f_\beta$  increases and are applicable to clustering



- Hwang, Sung Jin, Steven B. Damelin, and Alfred O. Hero III. (2016), “Shortest Path through Random Points.” *The Annals of Applied Probability: An Official Journal of the Institute of Mathematical Statistics* 26 (5): 2791–2823.
- Kobayashi, K. and H. Wynn, (2020), Empirical geodesic graphs and  $CAT(k)$  metrics for data analysis, *Statistics and Computing*, 30(1), 1-18.
- Mckenzie, D. and Damelin, S. (2019). Power weighted shortest paths for clustering Euclidean data. arXiv preprint arXiv:1905.13345.

## Part II

# Application of metric cones to graph embedding

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collaboration with **Daisuke Takehara (Accenture)**

Boston-Keio-Tsinghua2023 2023/06/30

# Original problem setting

**True model (unknown):** A finite directed acyclic graph  $G = (E, V)$  whose vertex corresponds to a data.

## Input:

- an undirected finite graph  $\bar{G} = (\bar{E}, V)$  without weights
- a metric space  $M$  with a "height" coordinate  $h_M : M \rightarrow \mathbb{R}_{\geq 0}$

## Output:

- a "representation of hierarchy": i.e. an embedding  $\varphi : V \rightarrow M$  s.t.  $h_M(\varphi(V))$  is consistent to the directions of  $E$ .

The problem does not make sense without further conditions.

**Here we assume  $G$  is a rooted tree or approximately a rooted tree.**

## Example data and task

- Social Networks

**Input:** Tweets of a buzz topic (w/o time stamps)

**Output:** Estimated time order (and time intervals) of the tweets

- Chemical/Biological reactions

**Input:** List of substance pairs whose interactions have been experimentally observed

**Output:** Estimated direction and timing of each interaction

E.g., the Poincaré embeddings are applied to extract hierarchical structures from biological cell data (Kilmovskaia et al., 2020).

- The Poincaré embedding (Nickel and Kiela, 2017) is a method for learning hierarchical representations of symbolic data by embedding them into a hyperbolic space (Poincaré ball).
- The Poincaré embeddings were reported “outperforming Euclidean embeddings significantly on data with latent hierarchies, both in terms of representation capacity and in terms of generalization ability.”

# Poincaré ball

The Poincaré embeddings embed data points(= vertices) to a **Poincaré ball**.

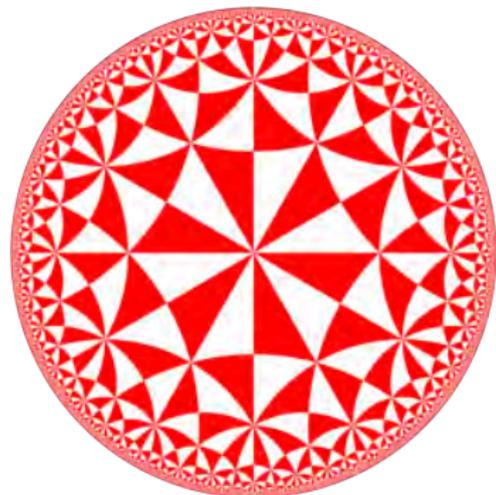
The Poincaré ball is a ball  $B^d := \{\mathbf{x} \in \mathbb{R}^d \mid \|\mathbf{x}\| < 1\}$  with a metric

$$g_{\mathbf{x}} := \left( \frac{2}{1 - \|\mathbf{x}\|^2} \right)^2 g^E.$$

The corresponding distance function becomes

$$d(\mathbf{u}, \mathbf{v}) = \arccos \left( 1 + 2 \frac{\|\mathbf{u} - \mathbf{v}\|^2}{(1 - \|\mathbf{u}\|^2)(1 - \|\mathbf{v}\|^2)} \right).$$

The Poincaré ball is a hyperbolic space and has a negative constant curvature.



M.C. Escher's hyperbolic tiling  
from Wikipedia

# Poincaré embedding 1

The Poincaré embeddings learn the embedding of an undirected graph  $G$  by maximizing the following objective function:

$$L(\varphi) = \sum_{(u,v) \in E} \log \frac{\exp(-d(\varphi(u), \varphi(v)))}{\sum_{v' \in N(u)} \exp(-d(\varphi(u), \varphi(v')))}$$

where  $N(u) := \{v' \in V \mid (u, v') \notin E\}$  and  $d$  denotes the distance function on a Poincaré ball.

## Poincaré embedding 2

The maximization of the objective function is done by the stochastic gradient descent on Riemannian manifolds (Riemannian SGD).

Euclidean SGD updates:

$$\mathbf{u} \leftarrow \mathbf{u} - \eta \nabla_{\mathbf{u}} L(\mathbf{u}),$$

Riemannian SGD updates:

$$\mathbf{u} \leftarrow \exp_{\mathbf{u}}(-\eta \nabla_{\mathbf{u}}^R L(\mathbf{u})).$$

Here  $\eta = \eta_t > 0$  is a learning rate.

With the metric matrix of the embedding space (now, the Poincaré ball) as  $g_{\mathbf{u}}$  at  $\mathbf{u}$ , the gradient on the Riemannian manifold  $\nabla_{\mathbf{u}}^R L(\mathbf{u})$  is a scaled Euclidean gradient:

$$\nabla_{\mathbf{u}}^R L(\mathbf{u}) = g_{\mathbf{u}}^{-1} \nabla_{\mathbf{u}} L(\mathbf{u}).$$



# Pros and Cons of Poincaré embedding

## Pros

- In experiments, embedding in a Poincaré ball works better than a Euclidean Space.
- The negative curvature of Poincaré balls suits the graph embedding problem, especially for tree-like networks.

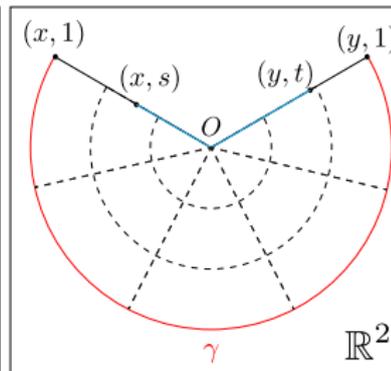
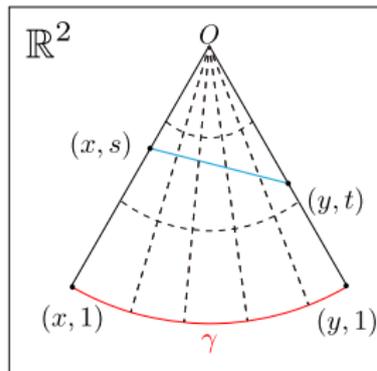
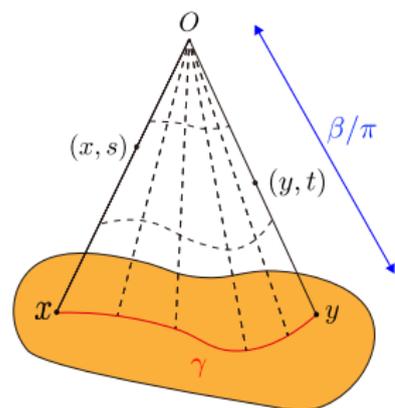
## Cons

- It requires much more computational costs compared to the Euclidean embedding.
- The model does not have much flexibility thus we cannot select a model suitable to each graph structure.
- Especially the curvature of the Poincare ball is fixed and cannot be controlled.
- The computed hierarchical relation is not invariant under isometric transformations (e.g. the Möbius transformation).

# Our proposed method: Cone embedding 1

In Takehara and K. (2023), we proposed the **Cone embedding**, a method embedding a graph into a **metric cone**.

We first use another embedding algorithm to embed a graph into a Riemannian space (called “original embedding space”), and next optimize the height parameters.



## Our proposed method: Cone embedding 2

The distance function on a metric cone is

$$\bar{d}_\beta((x, s), (y, t)) := \beta \sqrt{t^2 + s^2 - 2ts \cos(\pi \min(d_Z(x, y)/\beta, 1))}.$$

The corresponding metric matrix at non-apex points is

$$\bar{g}(x, r) = \begin{pmatrix} r^2 \pi^2 g(x) & 0 \\ 0 & \beta^2 \end{pmatrix}.$$

Thus we use the Riemannian SGD updates with this metric:

$$\mathbf{u} \leftarrow \exp_{\mathbf{u}}(-\eta \nabla_{\mathbf{u}}^R L(\mathbf{u})).$$

$$\nabla_{\mathbf{u}}^R L(\mathbf{u}) = \bar{g}_{\mathbf{u}}^{-1} \nabla_{\mathbf{u}} L(\mathbf{u}).$$

## Uniformly variable curvatures

The Ricci curvatures  $\tilde{R}_{\alpha\gamma}$  and the scalar curvature  $\tilde{R}$  at  $(x, s)$  become

$$\begin{aligned}\tilde{R}_{\alpha\gamma} &= R_{\alpha\gamma} - \pi^2(n-1)\beta^{-2}\bar{g}_{\alpha\gamma}, \\ \tilde{R}_{\alpha 0} = \tilde{R}_{0\gamma} = \tilde{R}_{00} &= 0, \quad \tilde{R} = \{\pi^{-2}R - n(n-1)\beta^{-2}\}s^{-2}\end{aligned}$$

- The scalar curvature and the Ricci curvatures become more negative than (a constant times of) the corresponding original curvatures for  $\beta < \infty$  and  $n \geq 2$ .
- $\beta$  changes the curvatures uniformly thus we can control the curvatures by tuning  $\beta$ .
- The closer to the apex, i.e. the smaller the value of  $s$ , the greater the change of the scalar curvature.

When the original space is a geodesic metric space, similar results in the sense of CAT( $k$ ) property were proved in K. and Wynn(2020).

# Identifiability 1

The Cone embedding has identifiability of hierarchical values from the learnt metrics that the Poincaré embedding does not satisfy.

Assume the original embedding space  $Z$  is a Riemannian manifold, and let  $X$  be the metric cone of  $Z$  with a parameter  $\beta > 0$ .

We assume that each data point  $z_i \in Z$  ( $i = 1, \dots, n$ ) has its specific “height”  $t_i \in [0, 1]$  in the metric cone  $X$ .

Our proposed method embeds data points into a metric cone based on the estimated distances  $\tilde{d}_\beta(x_i, x_j)$  ( $i, j = 1, \dots, n$ ) and tries to compute the heights  $t_1, \dots, t_n$  as a measure of the hierarchy level.

However, it is not evident if these heights are identifiable only from the information of the original data points in  $Z$  and the distances  $\tilde{d}_\beta(x_i, x_j)$  ( $i, j = 1, \dots, n$ ) in the metric cone.

## Identifiability 2

### Theorem 1 (Theorem 1 of Takehara and K. (2023))

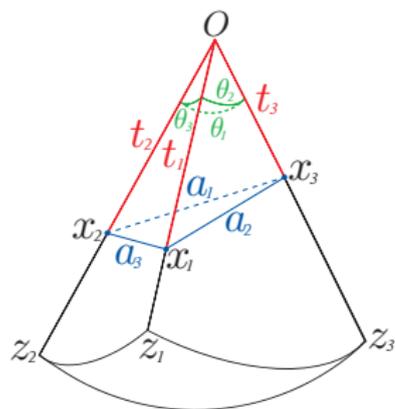
- (a) *Let  $n \geq 3$  and assume that  $z_1, \dots, z_n$  are not all aligned on a geodesic in  $Z$ . Then, the heights  $t_1, \dots, t_n$  are “identifiable” up to at most four candidates.*
- (b) *Let  $n \geq 4$  and assume  $z_1, \dots, z_n$  and  $t_1, \dots, t_n$  take “general” positions and heights, respectively. Then, the heights  $t_1, \dots, t_n$  are identifiable uniquely.*
- (c) *If  $d_Z(z_i, z_j) \geq \beta/2$  for all  $i, j = 1, \dots, n$ ,  $i \neq j$ , then the heights  $t_1, \dots, t_n$  are identifiable uniquely.*

See Takehara and K. (2023) for the definition of “identifiable” and “general”.

# Identifiability 3

Comments on the proof)

- For  $n = 3$ , the problem becomes an elementary geometrical problem.
- We used algebraic approach and evaluate the number of solutions of a quadratic polynomial system using the Gröbner basis.
- For  $n \geq 4$ , the system becomes overdetermined.



$$\begin{aligned}t_2^2 + t_3^2 - 2t_2t_3 \cos \theta_1 &= a_1^2, \\t_3^2 + t_1^2 - 2t_3t_1 \cos \theta_2 &= a_2^2, \\t_1^2 + t_2^2 - 2t_1t_2 \cos \theta_3 &= a_3^2.\end{aligned}$$

# Experiments

We evaluate the proposed method in two experiments:

- E1 embedding graphs (coauthors' network of academic papers),
- E2 embedding taxonomies (WordNet).

For every vertex  $u$ , we rank  $\{\tilde{d}_\beta(u, v) \mid v \in V\}$  and an index MR(mean ranking) is computed as the difference from the ranking of  $u$  and the mean ranking of  $v$ s adjacent to  $u$ .

Mean average precisions(MAP) are also compared<sup>1</sup>.

In E2, the following score is used instead of  $\tilde{d}_\beta(u, v)$ :

$$\text{score}(\text{is-a}((u, s), (v, t))) = -(1 + \alpha(s - t))d(u, v)$$

where  $\alpha = 10^3$ .

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<sup>1</sup>Average precision is similar to AUC (AUROC) but using a plot of precision (not specificity) as a function of sensibility. MAP is the mean of APs over  $u$ .

# Experimental results 1

Table 1: Embedding accuracy for WordNet

		dimension			
		10	20	50	100
Euclidean	MR	1471.70	232.88	2.51	1.82
	MAP	0.070	0.122	0.838	0.899
Poincare	MR	<b>19.94</b>	<b>19.62</b>	19.47	19.36
	MAP	<b>0.528</b>	<b>0.534</b>	0.537	0.538
Our Model (Metric Cone)	MR	1401.28	209.11	<b>2.30</b>	<b>1.79</b>
	MAP	0.052	0.126	<b>0.853</b>	<b>0.902</b>



# Experimental results 3

Table 2: Results of GrQc embedding into low-dimensional space

Model	eval.	2	3	4	5	6	7	8	9
Euclid.	MR	88.99	37.17	17.15	9.42	5.78	4.27	3.42	3.18
	MAP	0.375	0.488	0.600	0.719	0.842	0.929	0.983	0.998
Metric Cone	MR	72.35	26.39	14.50	8.65	5.50	4.16	3.40	3.18
	MAP	0.450	0.551	0.614	0.726	0.851	0.935	0.986	0.998

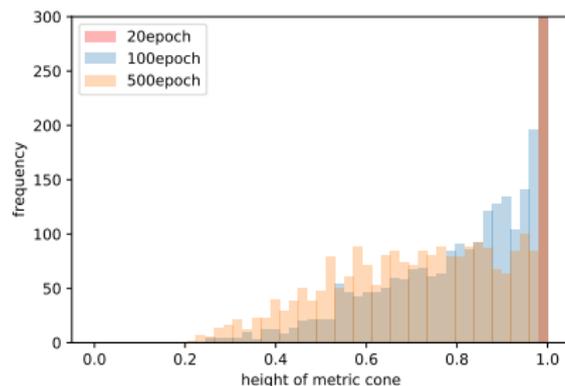


Figure 1: Changes in the distribution of the heights of data points

## Summary: Merits of cone embeddings

- We provide an indicator of hierarchical information that is both geometrically and intuitively natural to interpret.
- The model can inherit the merits of the original embedding method. Thus it can suit each graph structure more flexibly.
- Computation for cone embeddings is light since it optimizes only one coordinate variable per each data point.
- The curvatures of the embedding space can be controlled by parameter  $\beta$ .
- The hierarchical relation is determined uniquely by the distances between the data points under mild conditions.

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