

# Non-linear Embeddings in Hilbert Simplex Geometry

Frank Nielsen  Sony CSL  
Sony Computer Science Laboratories Inc

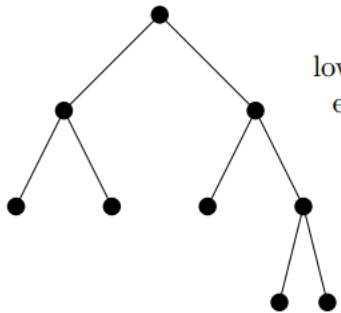
Ke Sun    
CSIRO Data 61

2023

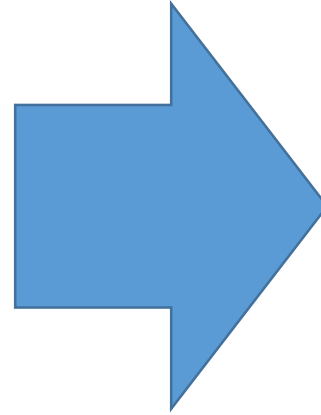
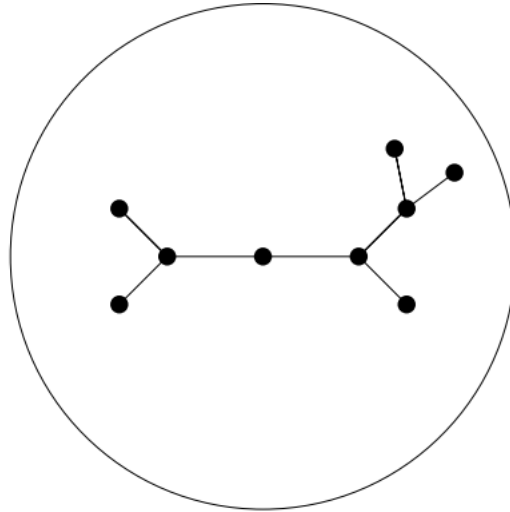
arXiv:2203.11434  
ICML TAG-ML'23

# Embedding discrete hierarchical structures in hyperbolic spaces: Continuous representations

Discrete tree/hierarchies



low-distortion  
embedding



Downstream tasks

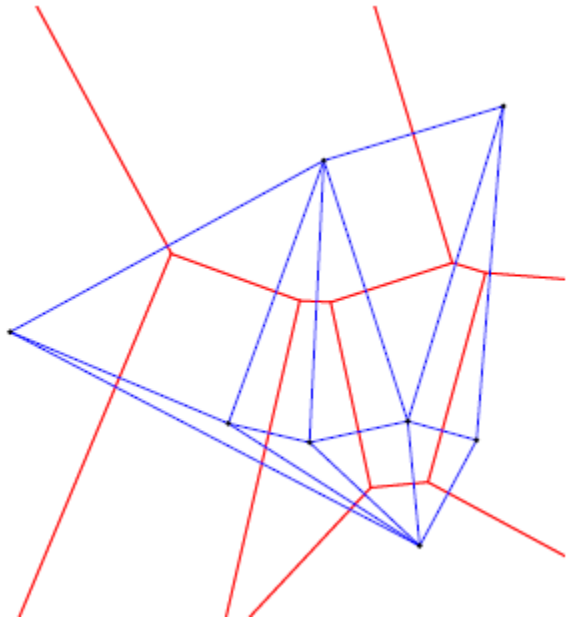
Hierarchical structure  
(not embedded)

Embedded  
(hyperbolic model, e.g. Klein disk model)

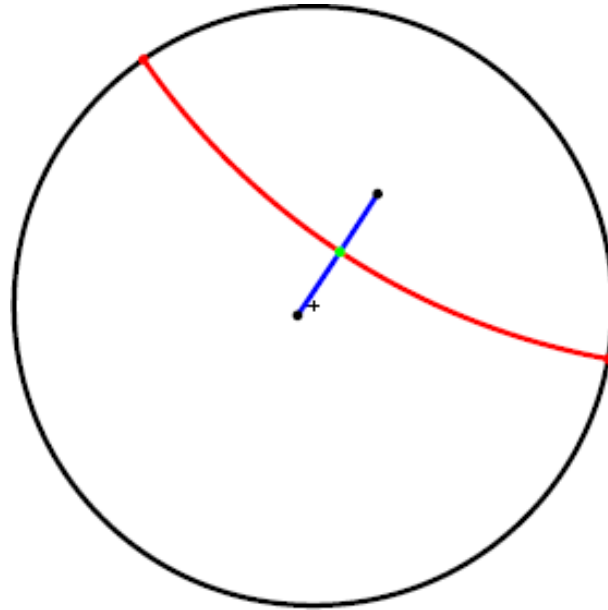
**Theorem: One can embed *any weighted edge tree* as a *Delaunay graph* of embedded tree nodes in *hyperbolic geometry* with *arbitrary small distortion***

Sarkar, Low distortion delaunay embedding of trees in hyperbolic plane  
International symposium on graph drawing, 2011

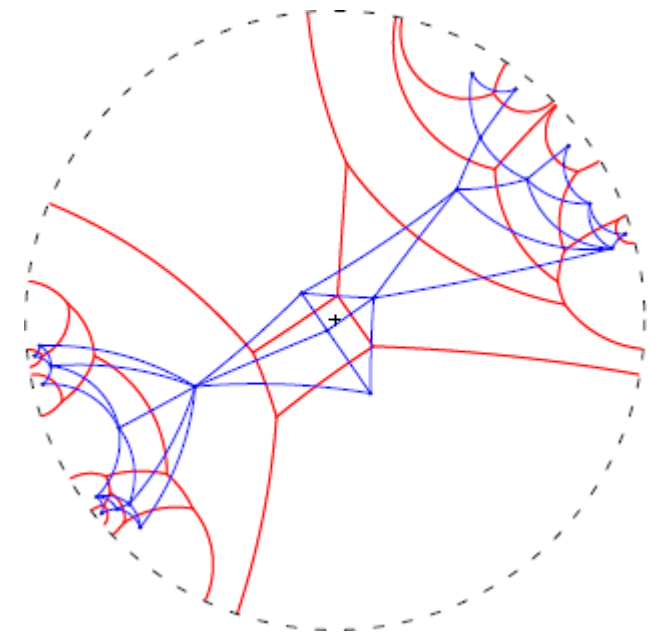
# Hyperbolic Voronoi diagram/Delaunay complex



Ordinary **Voronoi/Delaunay**



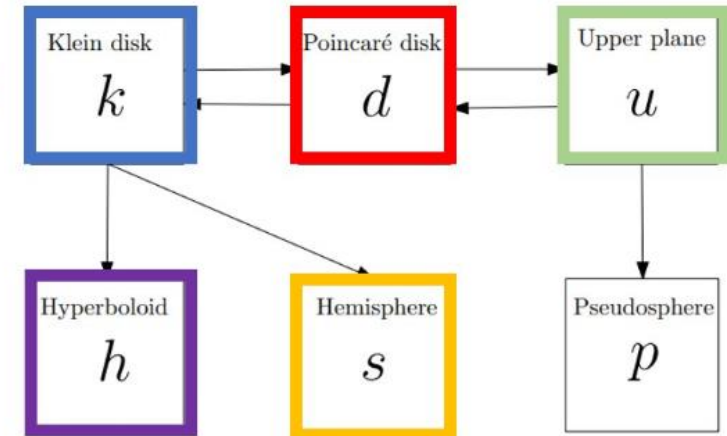
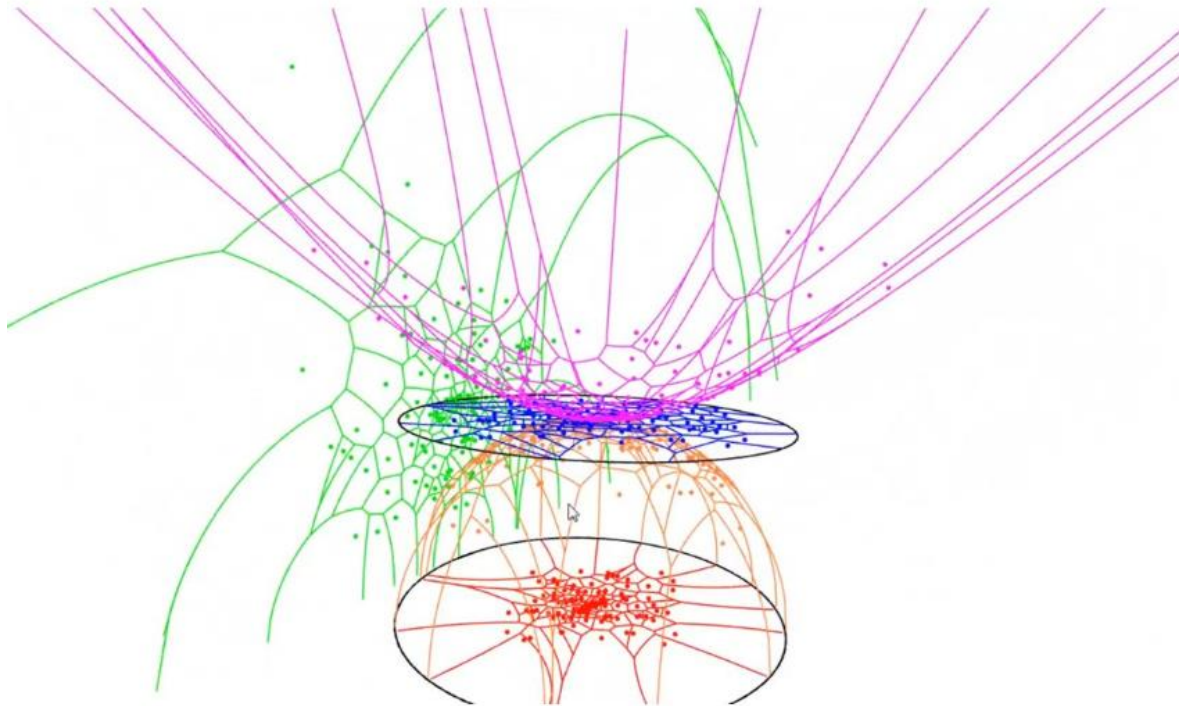
Poincaré **bisector/geodesic**



Poincaré **Voronoi/Delaunay**

On Voronoi diagrams on the information-geometric Cauchy manifolds  
Entropy 22.7 (2020)

# Various models of hyperbolic geometry



$$\begin{aligned}
 k \rightarrow h &: \frac{1}{\sqrt{1-\|k\|^2}}(k_1, k_2, 1) \\
 k \rightarrow d &: \frac{1-\sqrt{1-\|k\|^2}}{\|k\|^2}(k_1, k_2) \\
 d \rightarrow k &: \frac{2}{1+\|d\|^2}(d_1, d_2) \\
 d \rightarrow u &: \frac{i(1+d)}{1-d} \\
 u \rightarrow d &: \frac{u-i}{u+i} \\
 k \rightarrow s &: \frac{1}{\sqrt{1-\|k\|^2}}(k_1, k_2) \\
 u \rightarrow p &: \left( \frac{1}{u_2} \cos \frac{u_1}{M}, \frac{1}{u_2} \sin \frac{u_2}{M}, \operatorname{arccosh}(u_2) - \sqrt{1 - \frac{1}{u_2^2}} \right)
 \end{aligned}$$

Minkowski/Lorentz model is well-suited for optimization since the domain is unconstrained

Visualizing hyperbolic Voronoi diagrams, Symp. Computational Geometry 2014  
 Representation tradeoffs for hyperbolic embeddings, ICMLR 2018

# Outline and contributions

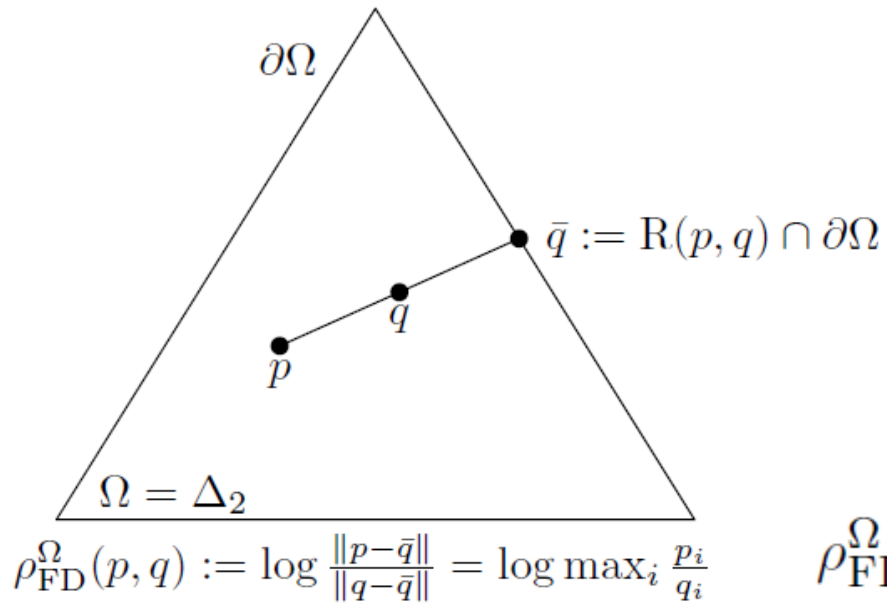
- Present **Hilbert simplex geometry** (HSG) for embeddings of graphs

## Contributions:

- Simple proof of **monotonicity** of Hilbert distance
- **Connection** of Hilbert distance with Aitchison distance
- **Differentiable approximation** of Hilbert distance for machine learning
- Application to **non-linear HSG embedding**: experimentally fast, robust, and competitive

# Funk and Hilbert distance

- Consider an **open bounded** convex set  $\Omega$  of a space (eg open standard simplex)
- Funk asymmetric distance (weak distance satisfies the triangular inequality):



Independent of the chosen norm since

$$\rho_{\text{HG}}^{\Omega}(p, q) = \rho_{\text{HG}}^{\Omega_{pq}}(p, q)$$

$$\Omega_{pq} := \Omega \cap (pq)$$

$$\rho_{\text{FD}}^{\Omega}(p, q) \neq \rho_{\text{FD}}^{\Omega}(q, p)$$

- Hilbert metric distance (1895) is the symmetrization of Funk distance:

$$\begin{aligned} \rho_{\text{HG}}^{\Omega}(p, q) &:= \rho_{\text{FD}}^{\Omega}(p, q) + \rho_{\text{FD}}^{\Omega}(q, p), \\ &= \begin{cases} \log \frac{\|p-\bar{q}\| \|q-\bar{p}\|}{\|p-\bar{p}\| \|q-\bar{q}\|}, & p \neq q, \\ 0 & p = q. \end{cases} = \log \frac{\max_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}{\min_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}} \end{aligned}$$

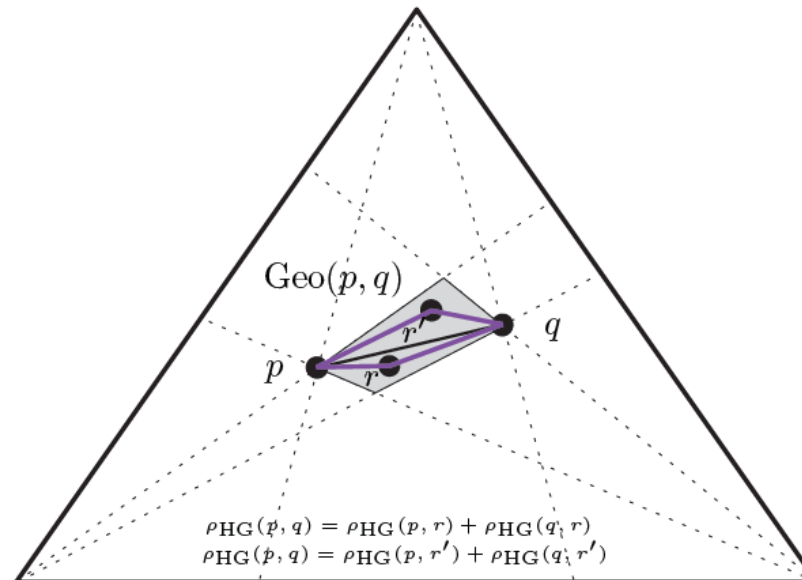
# Hilbert distance: The log cross-ratio metric

$$\rho_{\text{HG}}^{\Omega}(p, q) = \begin{cases} \log \text{CR}(\bar{p}, p; q, \bar{q}), & p \neq q \\ 0 & p = q \end{cases}$$

A **metric distance** which satisfies the triangle inequality:

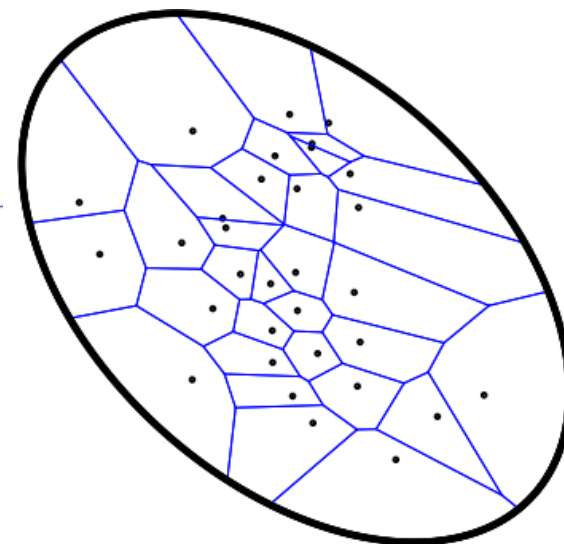
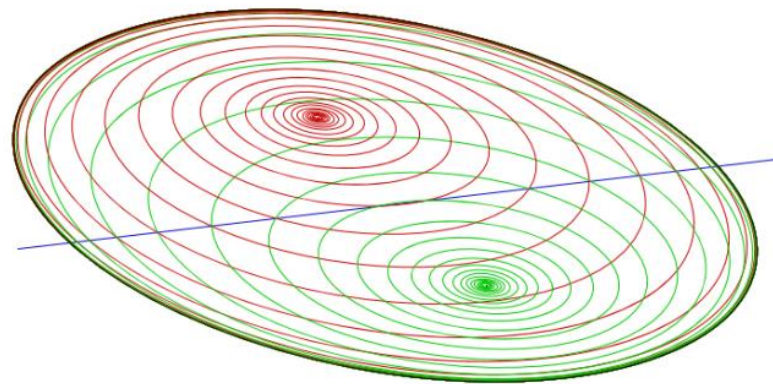
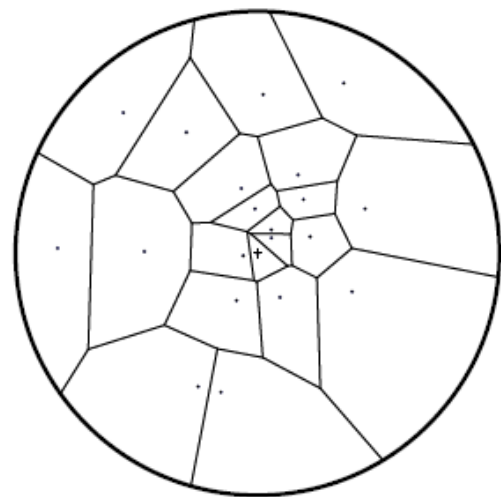
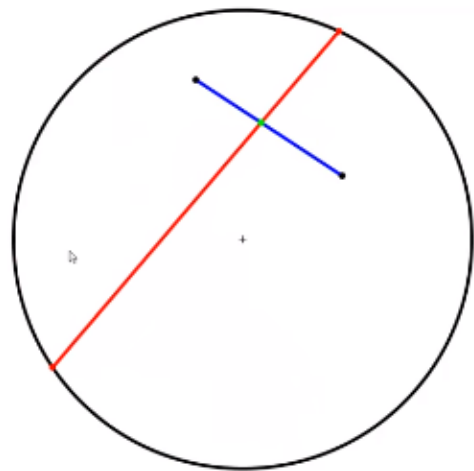
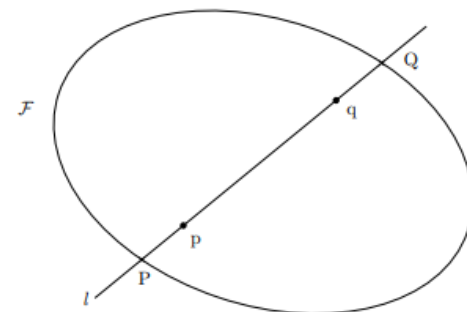
$$\forall r \in [pq], \quad \rho_{\text{HG}}^{\Omega}(p, q) = \rho_{\text{HG}}^{\Omega}(p, r) + \rho_{\text{HG}}^{\Omega}(r, q)$$

**Straight lines are geodesics** but geodesics are not unique:



# Hilbert geometry generalizes Klein and Cayley projective geometries

- When  $\Omega = \text{Open disk}$   $\rightarrow$  Klein geometry
- When  $\Omega = \text{Open ellipsoid}$   $\rightarrow$  Cayley-Klein geometry
- When  $\Omega = \text{Open convex with smooth boundary}$   $\rightarrow$  hyperbolic-type Finsler geometry



Klein

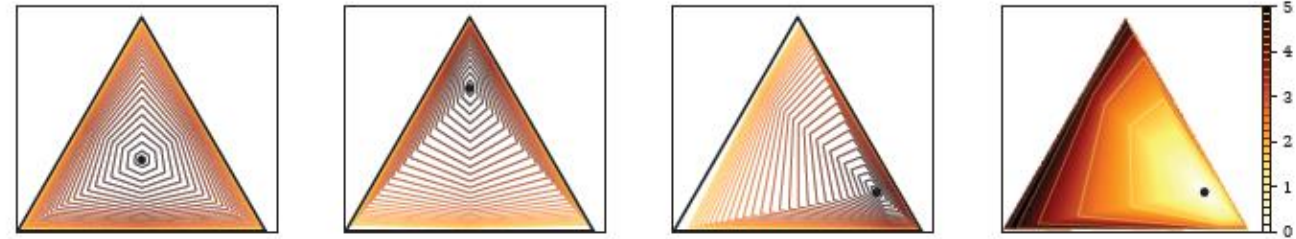
$$\text{arccosh} \left( \frac{1 - \langle p, q \rangle}{\sqrt{1 - \langle p, p \rangle} \sqrt{1 - \langle q, q \rangle}} \right)$$

Cayley-Klein

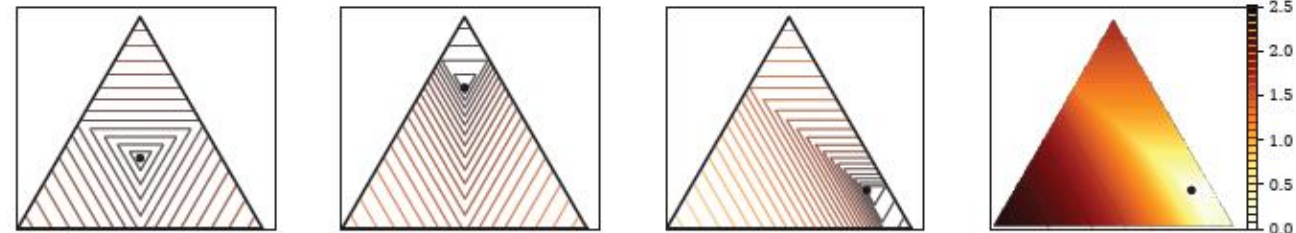


# Funk and Hilbert balls

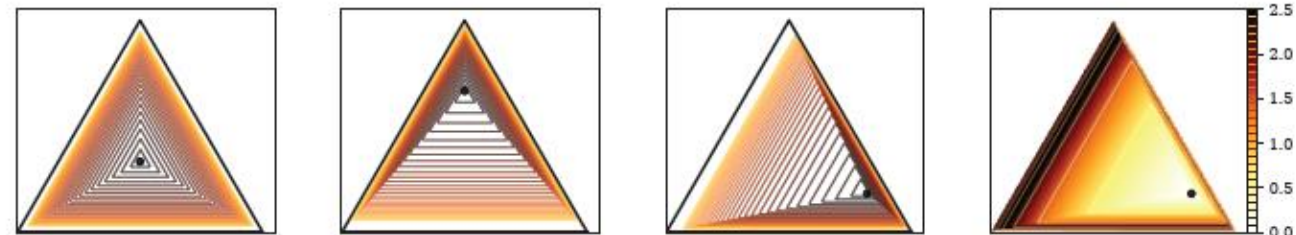
- Hilbert balls have  
Euclidean **hexagonal shapes**



(a)  $\rho_{HG}(p, c)$



(b)  $\rho_{FD}(p, c)$

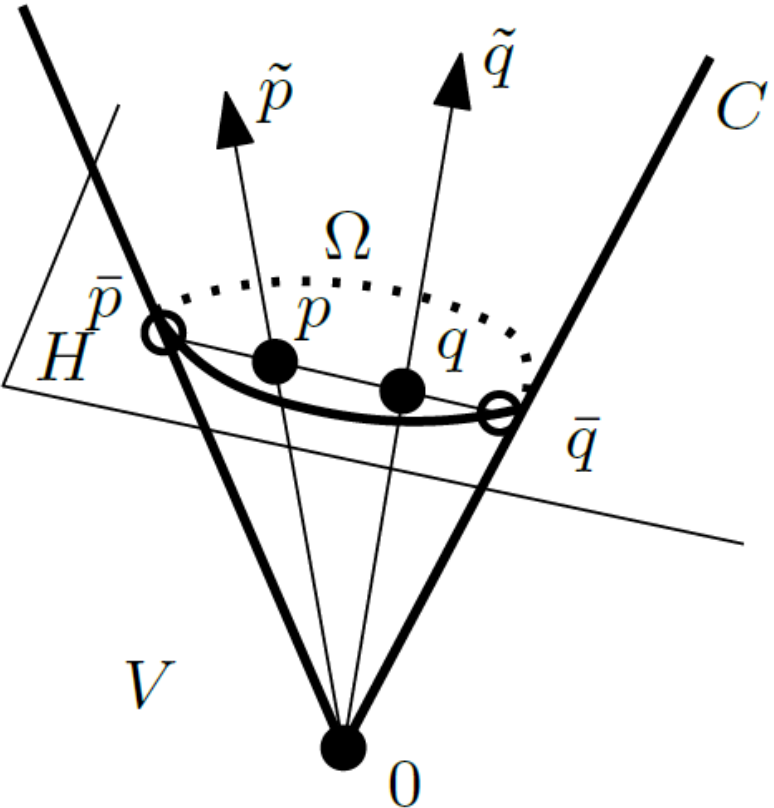


(c)  $\rho_{FD}(c, p)$

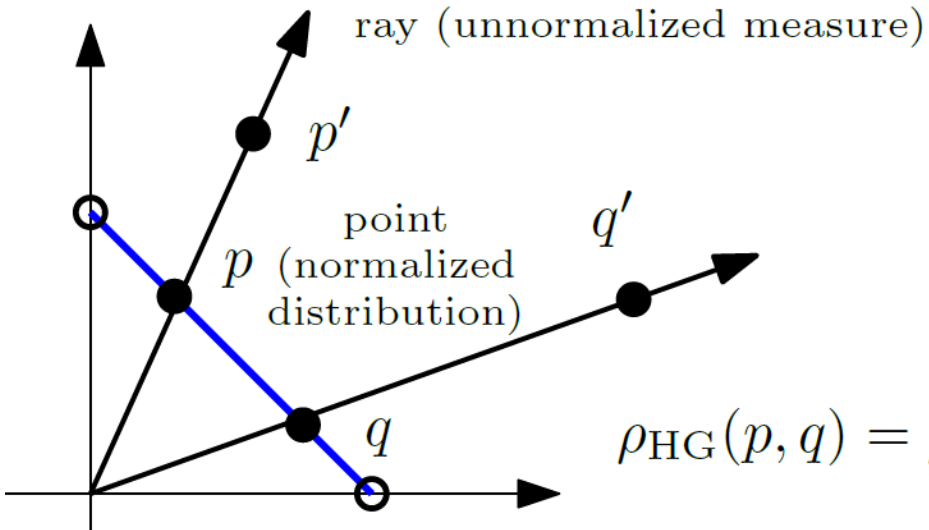
On balls in a Hilbert polygonal geometry, SoCG 2017

# Hilbert: Metric vs Projective distance

- Metric distance on an open **bounded convex** set  $\Omega$  of  $d$ -dim space
- Projective distance on the **pointed cone**  $C$  defined by homothets  $\lambda\Omega$  in  $\text{dim } d$
- distances between points vs pseudo-distance between rays



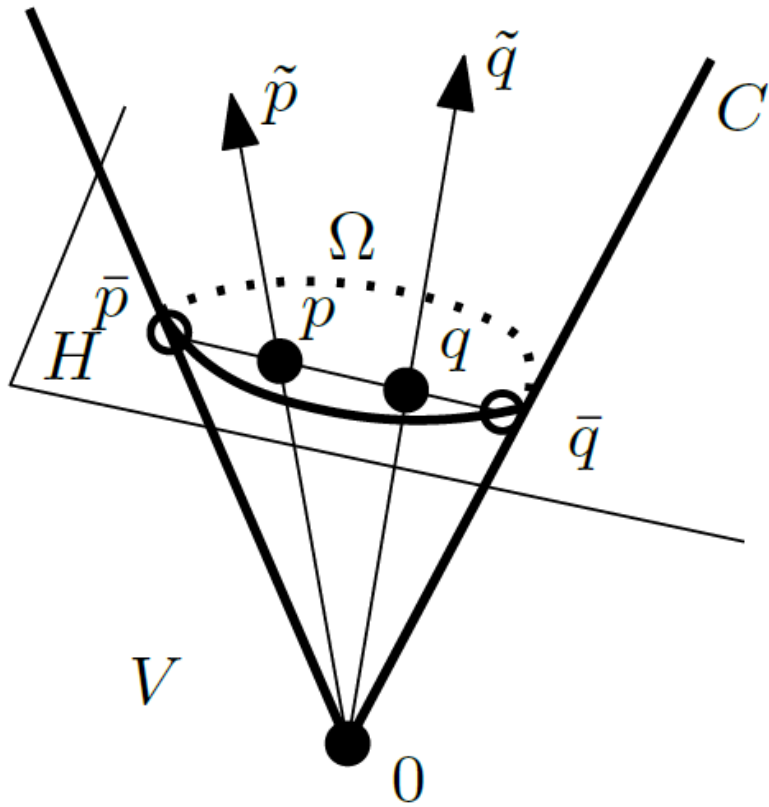
$\Omega = \text{standard simplex}$   
 Positive orthant cone  $\mathbb{R}^2$



$$\rho_{\text{HG}}(p, q) = \rho_{\text{HG}}(p', q')$$

$$\rho_{\text{HG}}(p, q) = \log \frac{\max_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}{\min_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}$$

# Hilbert projective distance in a cone



Cone:  $C = \{(\lambda, x) : \lambda \in \mathbb{R}_{>0}, x \in \Omega\}$

Cone defines a partial ordering:  $p \preceq_C q \Leftrightarrow q - p \in C$

Projective Hilbert distance:  $\rho_{\text{HG}}^C(p, q) = \log \frac{M(p, q)}{m(p, q)}$

where  $M(p, q) = \inf\{\lambda \in \mathbb{R}_{>0} : p \preceq_C \lambda q\}$

$m(p, q) = \sup\{\lambda \in \mathbb{R}_{>0} : \lambda q \preceq_C p\}$

Projective distance:  $\rho_{\text{HG}}^C(p, q) = \rho_{\text{HG}}^C(\alpha p, \beta q), \quad \alpha, \beta > 0$

which becomes a metric distance on  $\Omega$ :  $\rho_{\text{HG}}^\Omega(p, q) = \rho_{\text{HG}}^C(p, q), \quad \forall p, q \in \Omega$

# Monotone distances

- Let  $T$  be a map. A distance is **monotone** or **strictly monotone** iff

$$\rho(T(p), T(q)) \leq \rho(p, q), \quad \forall p, q \quad \rho(T(p), T(q)) < \rho(p, q), \quad \forall p \neq q$$

- In information geometry, the separable monotone "distances" are precisely the **f-divergences** when  $d > 2$ .

- Theorem: **Funk distance and Hilbert simplex distance are non-separable monotone distances**

- Contraction theorem (Birkhoff, 1957):  $\rho_{\text{HG}}(Ap, Aq) \leq \tanh\left(\frac{1}{4}\Delta(A)\right) \rho_{\text{HG}}(p, q)$ .

**Jiao, Information measures: the curious case of the binary alphabet, IEEE Transactions on Information Theory 60.12 (2014)**

# Aitchison distance:

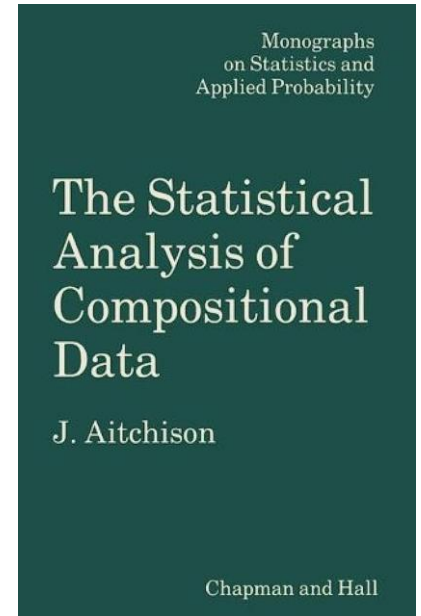
## Another non-separable monotone distance

- Often used in COmpositional Data Analysis (CODA)

$$\rho_{\text{Aitchison}}(p, q) := \sqrt{\sum_{i=1}^d \left( \log \frac{p_i}{G(p)} - \log \frac{q_i}{G(q)} \right)^2}$$

where  $G$  is the geometric mean

$$G(p) = \left( \prod_{i=1}^d p_i \right)^{\frac{1}{d}} = \exp \left( \frac{1}{d} \sum_{i=1}^d \log p_i \right)$$



Erb and Ay, The information-geometric perspective of Compositional Data Analysis

Advances in Compositional Data Analysis: Festschrift in Honour of Vera Pawlowsky-Glahn, 2021.

# HSG: Isometry to a vector space (Normed Hilbert)

- The only Hilbert geometries isometric to vector spaces are obtained with open simplex domains:  $(\Delta_d, \rho_{\text{HG}}) \cong (V_d, \|\cdot\|_{\text{NH}})$

- Slanted hyperplane:  $V_d = \{v \in \mathbb{R}^d : \sum_{i=1}^d v_i = 1\} \subset \mathbb{R}^d$

- Isometric mapping:  $v : p = (p_1, \dots, p_d) \in \Delta_d \rightarrow v(p) = (v_1, \dots, v_d) \in V_d$

$$v_i = \frac{1}{d} \left( (d-1) \log p_i - \sum_{j \neq i} \log p_j \right) = \log p_i - \frac{1}{d} \sum_{j=1}^d \log p_j = \log \frac{p_i}{G(p)}$$

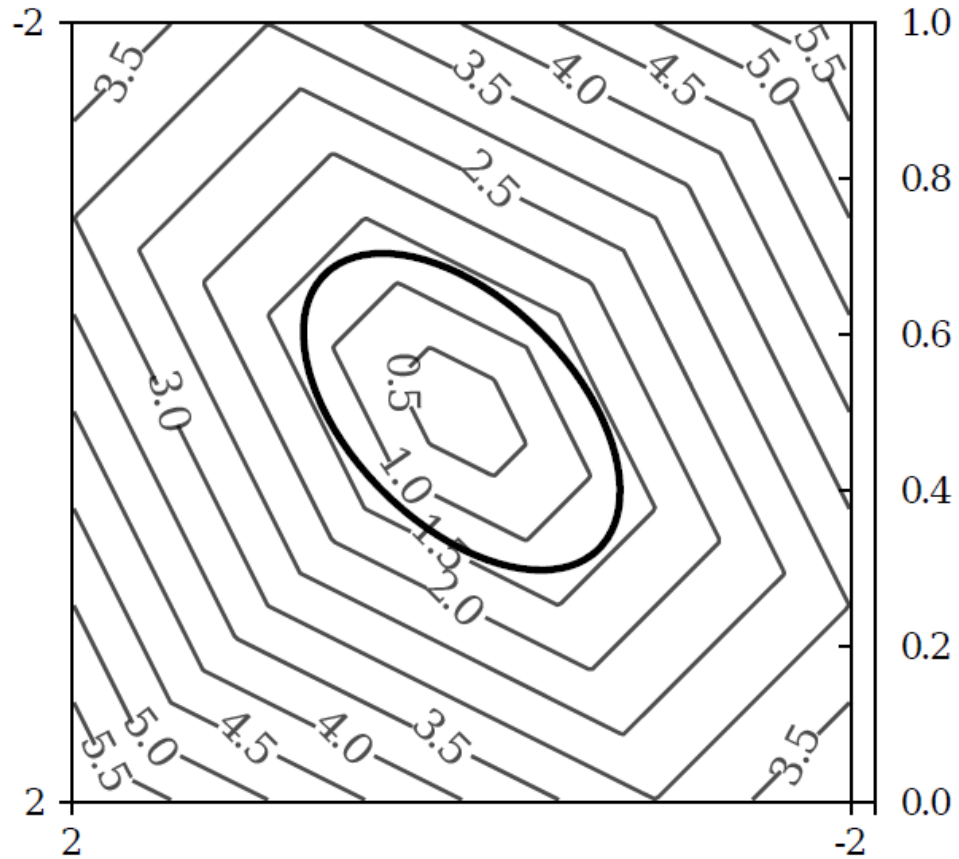
- Norm/unit ball in vector space:

$$B_V = \{v \in V_d : |v_i - v_j| \leq 1, \forall i \neq j\} = \{v \in V_d : \|v\|_{\text{NH}} \leq 1\}$$

- Distance:  $\rho_V(v, v') = \|v - v'\|_{\text{NH}} = \inf \{\tau \in \mathbb{R}_{>0} : v' \in \tau(B_V \oplus \{v\})\}$

$$\text{Minkowski sum of sets: } A \oplus B = \{a + b : a \in A, b \in B\}$$

# Symmetric polytope norm NH



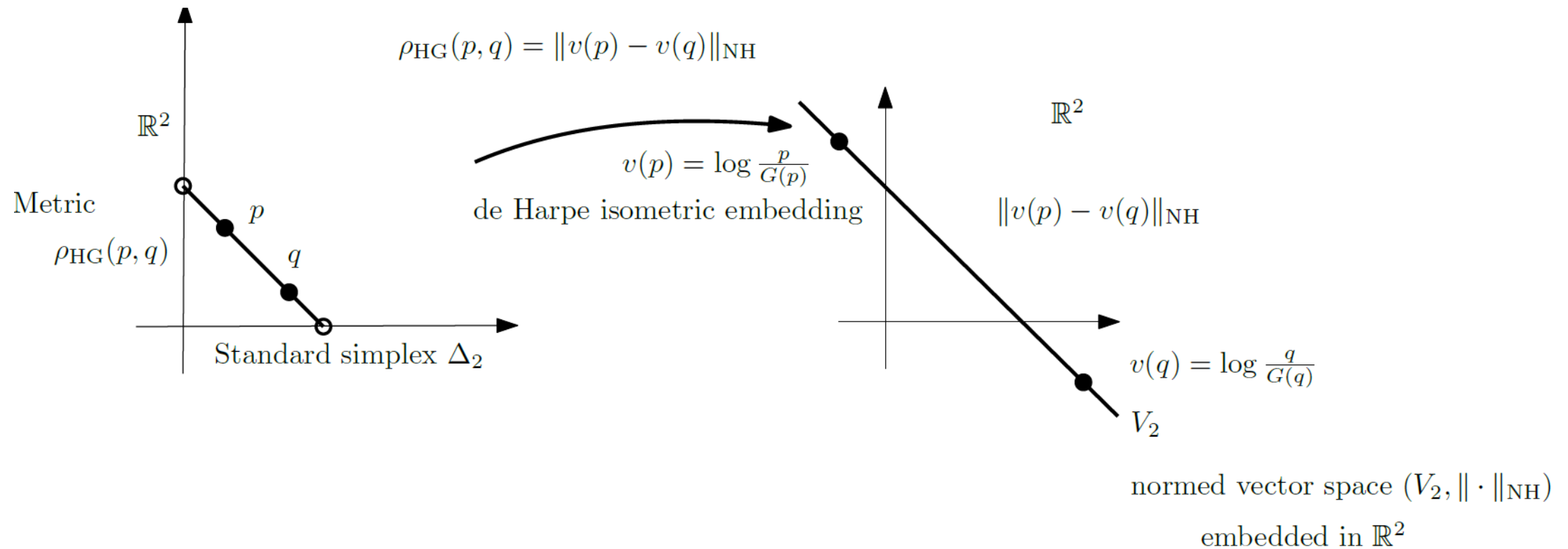
Visualized on the slanted plane  $V_2$ :

$$V_d = \{v \in \mathbb{R}^d : \sum_{i=1}^d v_i = 1\} \subset \mathbb{R}^d$$

$$B_V = \{v \in V_d : |v_i - v_j| \leq 1, \forall i \neq j\} = \{v \in V_d : \|v\|_{NH} \leq 1\}$$

de la Harpe, P. On Hilbert's metric for simplices.  
In Geometric Group Theory, volume 1, 1991

# HSG isometry to a normed space



$$v_i = \frac{1}{d} \left( (d-1) \log p_i - \sum_{j \neq i} \log p_j \right) = \log p_i - \frac{1}{d} \sum_{j=1}^d \log p_j = \log \frac{p_i}{G(p)}$$



# Logarithmic mapping and variation semi-norm

**Logarithmic representation:**  $l(p) = (\log p_1, \dots, \log p_d) \in \mathbb{R}^d$

**Hilbert distance as normed distance:**  $\rho_{\text{HG}}(p, q) = \|v(p) - v(q)\|_{\text{NH}} = \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{NH}}$

**Hilbert projective distance as semi-normed variation distance:**

$$\rho_{\text{HG}}(p, q) = \max_i \log \frac{p_i}{q_i} - \min_i \log \frac{p_i}{q_i} \quad (\text{log monotone increasing: } \log \max = \max \log, \log \min = \min \log)$$

$$= \left\| \log \frac{p}{q} \right\|_{\text{var}}$$

$$= \|l(p) - l(q)\|_{\text{var}}$$

$$= \|l(\alpha p) - l(\beta q)\|_{\text{var}}, \forall \alpha, \beta$$

$$= \|l(\alpha p) - l(\beta q)\|_{\text{var}}, \alpha = \frac{1}{G(p)}, \beta = \frac{1}{G(q)}$$

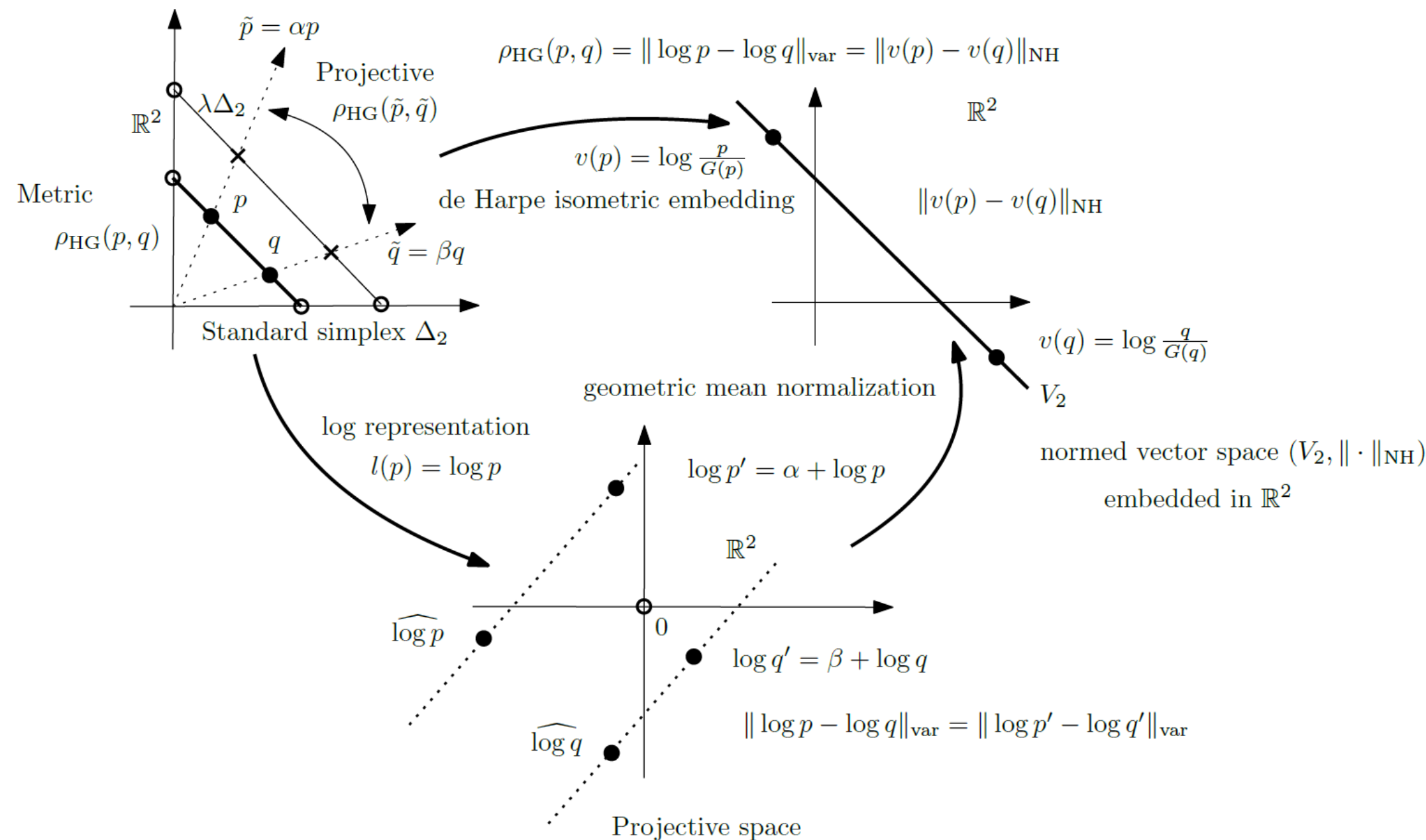
$$= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{var}}$$

**variation semi-norm:**

$$\|x\|_{\text{var}} := \max_i x_i - \min_i x_i = \|x\|_{+\infty} - \|x\|_{-\infty}$$

$$\|(\lambda, \dots, \lambda)\|_{\text{var}} = 0, \quad \forall \lambda \in \mathbb{R}$$

# Metric/projective Hilbert simplex/pos. orthant distance



# Relationship between HSG and Aitchison

Logarithm mapping normalized by **homogeneous geometric mean**:

$$\forall \lambda > 0, \quad \log \frac{p}{G(p)} = \log \frac{\lambda p}{G(\lambda p)}$$

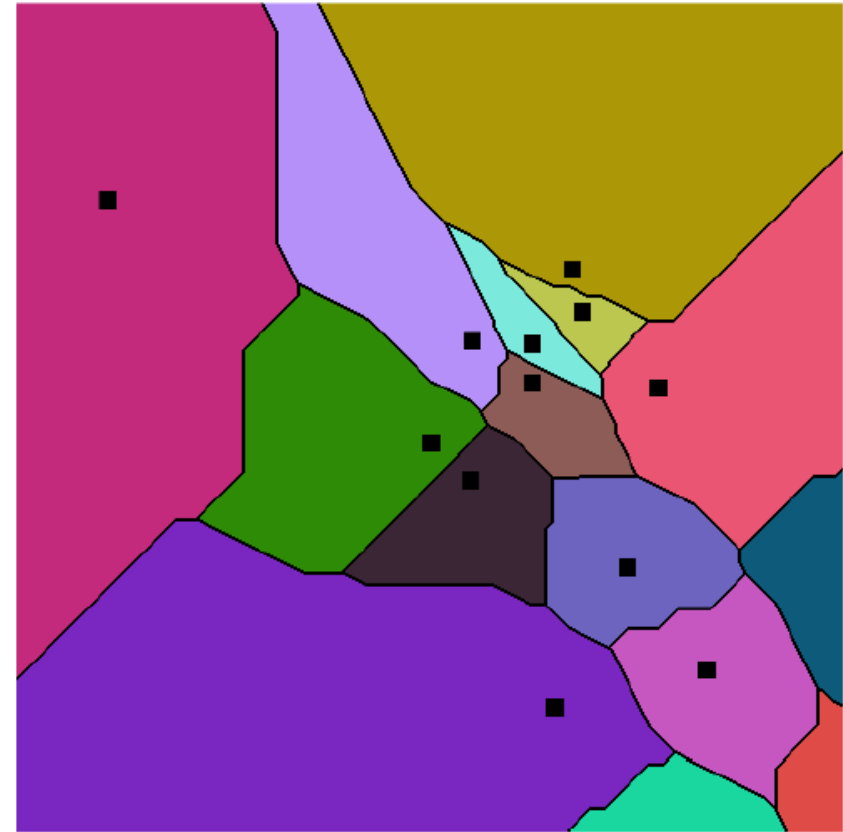
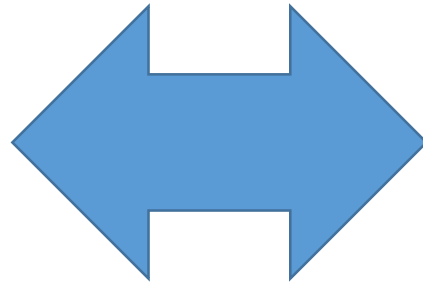
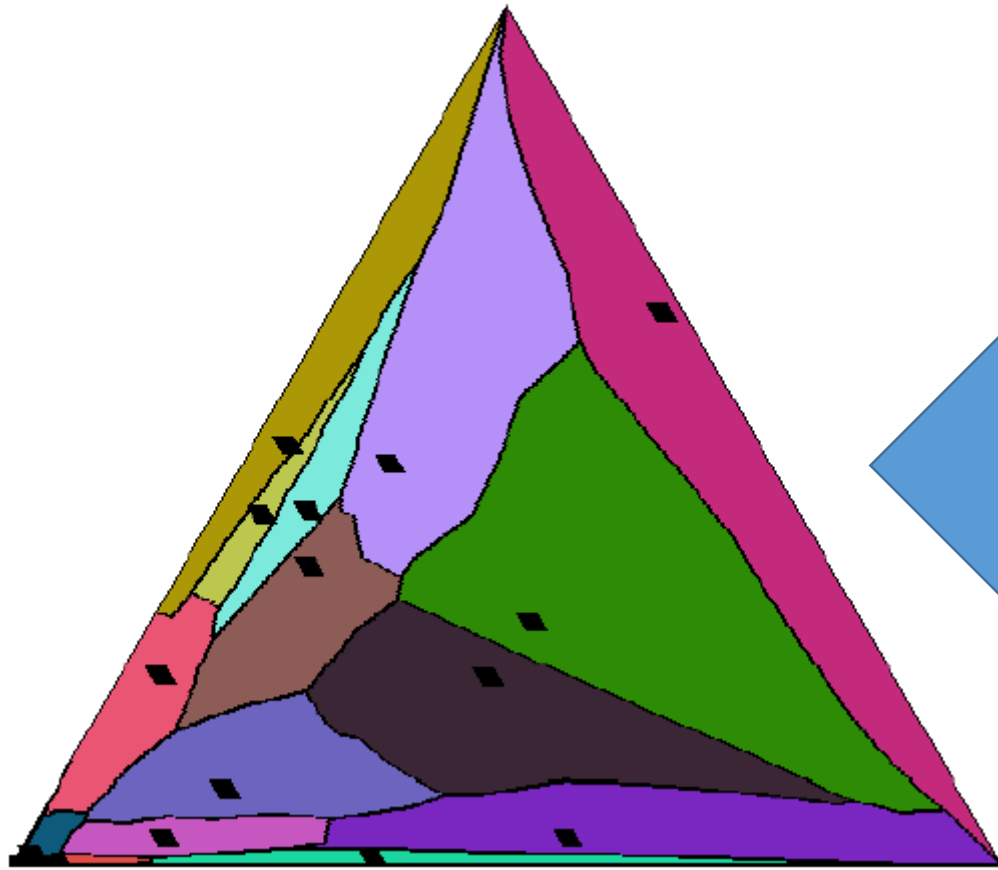
Hilbert distance:

$$\begin{aligned} \rho_{\text{HG}}(p, q) &= \|v(p) - v(q)\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{var}} \end{aligned}$$

Aitchison distance:

$$\begin{aligned} \rho_{\text{Aitchison}}(p, q) &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_2 \\ \rho_{\text{Aitchison}}(p, q) &:= \sqrt{\sum_{i=1}^d \left( \log \frac{p_i}{G(p)} - \log \frac{q_i}{G(q)} \right)^2} \end{aligned}$$

# Hilbert simplex Voronoi diagrams



$$\rho_{\text{HG}}(p, q) = \log \frac{\max_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}{\min_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}$$

$$\begin{aligned} \rho_{\text{HG}}(p, q) &= \|v(p) - v(q)\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{var}} \end{aligned}$$

# Differentiable approximation of Hilbert simplex distance

- max and min operations in Hilbert simplex distance are not differentiable
- **log-sum-exp** (LSE) commonly used in ML to approximate max operator
- We approximate Hilbert simplex distance by **differentiable function**:

$$\tilde{\rho}_{\text{LSE}^T}(p, q) = \frac{1}{T} \log \left( \sum_i \left( \frac{p_i}{q_i} \right)^T \right) \left( \sum_i \left( \frac{q_i}{p_i} \right)^T \right)$$

with guarantees

$$\rho_{\text{HG}}(p, q) + 2\epsilon_1(r, T) \leq \tilde{\rho}_{\text{LSE}^T}(p, q) \leq \rho_{\text{HG}}(p, q) + 2\epsilon_2(r, T)$$

where

$$\epsilon_1(x, T) := \frac{1}{T} \log [1 + (d - 1) \exp(-T\|x\|_{\text{var}})]$$

$$\epsilon_2(x, T) := \frac{1}{T} \log [d - 1 + \exp(-T\|x\|_{\text{var}})]$$

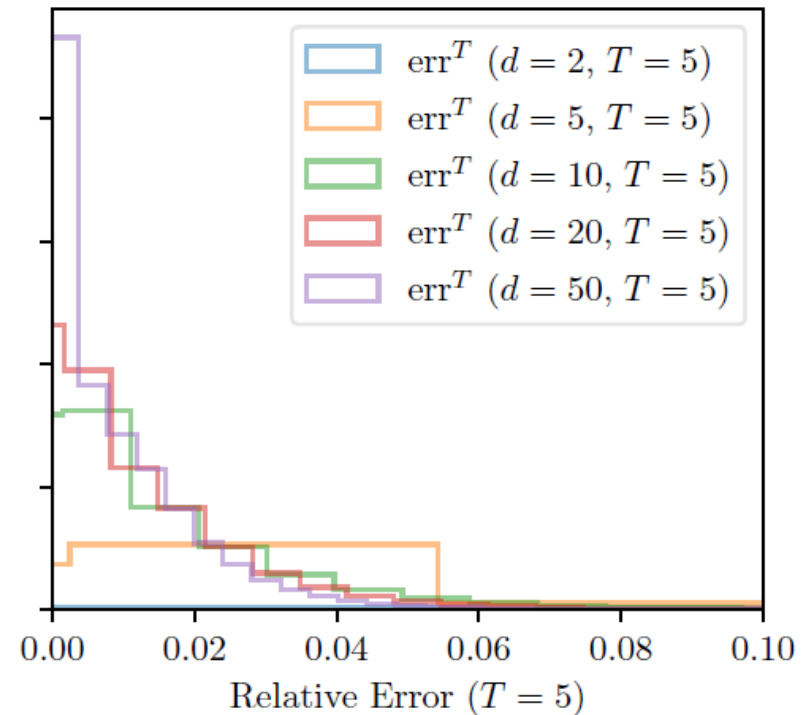
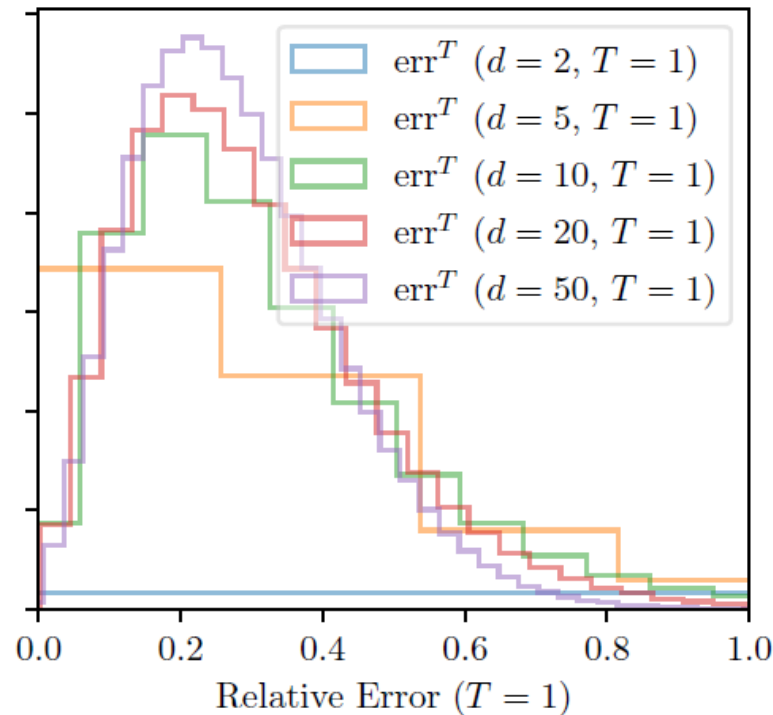
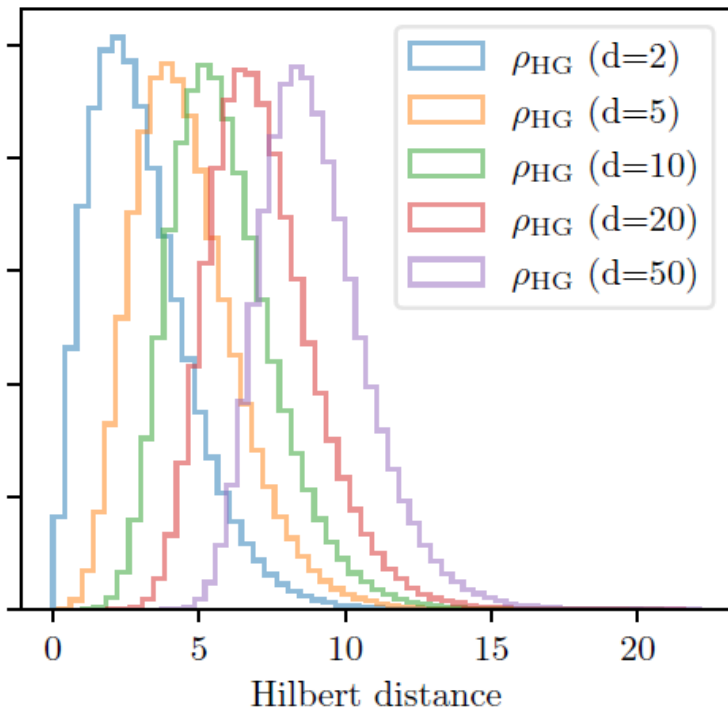
The larger  $T$ , the better the approximation:  $0 < \epsilon_1(x, T) \leq \epsilon_2(x, T) \leq \frac{1}{T} \log d$

Guaranteed bounds on information-theoretic measures of univariate mixtures using piecewise log-sum-exp inequalities. *Entropy* 18.12 (2016)

# Differentiable approximation: Experiments

$10^6$  pairs of points randomly sampled inside the  $d$ -dimensional standard simplex

We measure: 
$$\text{err}^T(p, q) := \frac{\tilde{\rho}_{\text{LSE}^T}(p, q) - \rho_{\text{HG}}(p, q)}{\rho_{\text{HG}}(p, q)}$$



# Non-linear embeddings: Evaluation metrics

Remark: When  $(M_1, \rho_1)$  isometric to  $(M_2, \rho_2)$   $\leftrightarrow$  same representation power

Loss associated to a **distance matrix**  $[D_{ij}]$  (e.g., calculated from weighted graphs):

$$\ell(\mathcal{D}, \mathcal{M}^d) := \inf_{\mathbf{Y} \in (\mathcal{M}^d)^n} \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n (\mathcal{D}_{ij} - \rho_{\mathcal{M}}(\mathbf{y}_i, \mathbf{y}_j))^2$$

or use **row-stochastic probability matrix**  $[P_{ij}]$  (loss in manifold learning/graph embedding):

$$\ell(\mathcal{P}, \mathcal{M}^d) := \inf_{\mathbf{Y} \in (\mathcal{M}^d)^n} \frac{1}{n} \sum_{i=1}^n \sum_{j:j \neq i} \mathcal{P}_{ij} \log \frac{\mathcal{P}_{ij}}{q_{ij}(\mathbf{Y})}$$

empirical average of the KL divergence between pmf  $P_i$  and  $q_i$

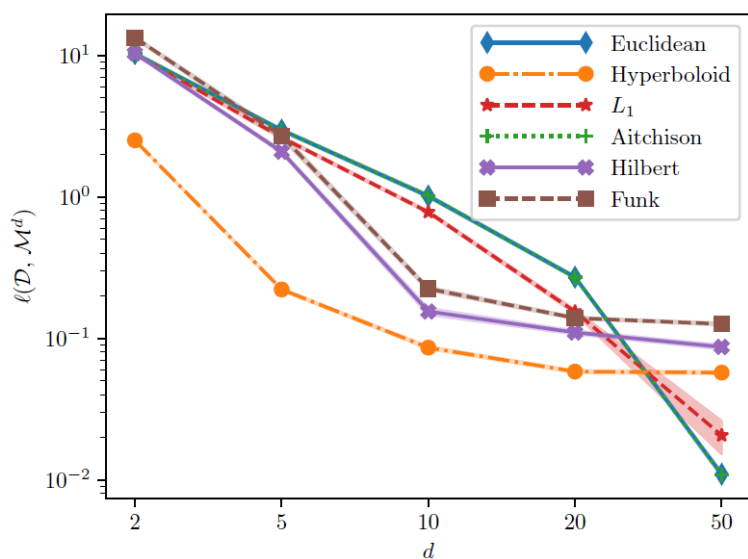
$$q_{ij}(\mathbf{Y}) := \frac{\exp(-\rho_{\mathcal{M}}^2(\mathbf{y}_i, \mathbf{y}_j))}{\sum_{j:j \neq i} \exp(-\rho_{\mathcal{M}}^2(\mathbf{y}_i, \mathbf{y}_j))}$$

heat kernel

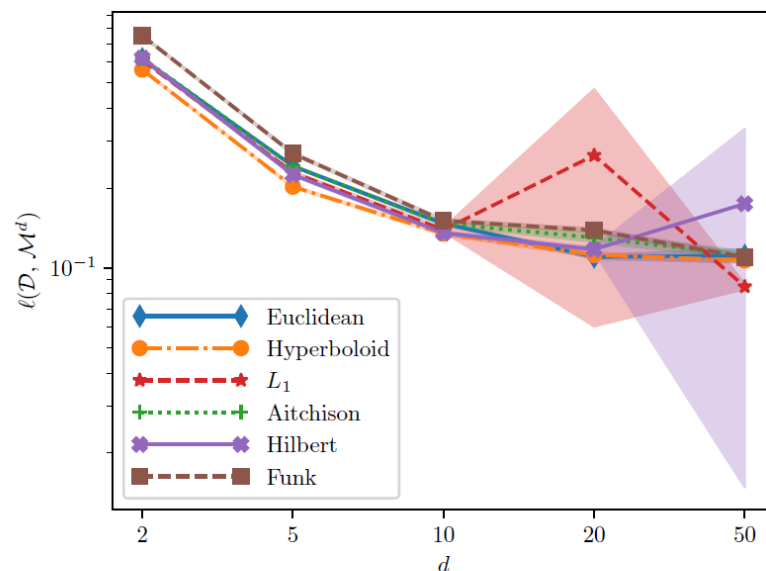
# Non-linear embeddings: Results (MSE)

Use Adam local optimizer [Kingma & Ba, 2015]

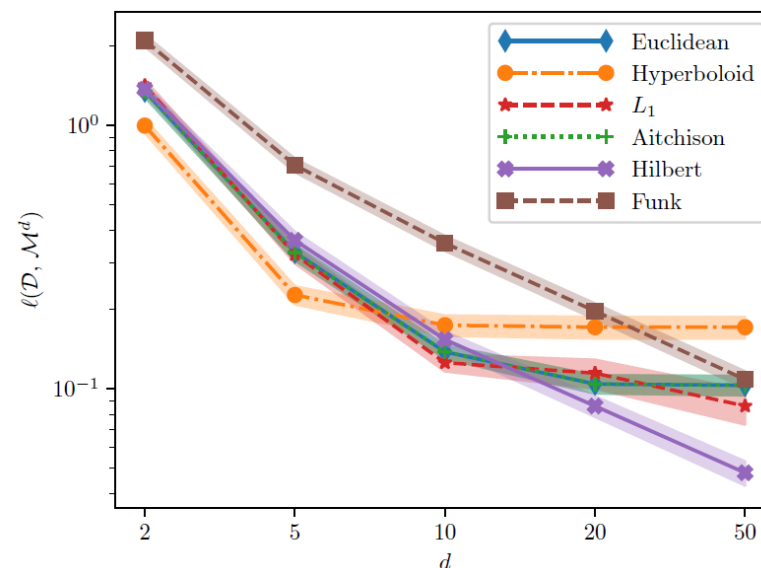
Repeat 10 different instances to get standard deviation shown in color bands



(a) 100 random points in  $\mathbb{R}^{100}$



(b) Erdős-Rényi graphs  $G(n, p)$  ( $n = 200, p = 0.2$ )



(c) Barabási-Albert graphs  $G(n, m)$  ( $n = 200, m = 2$ )

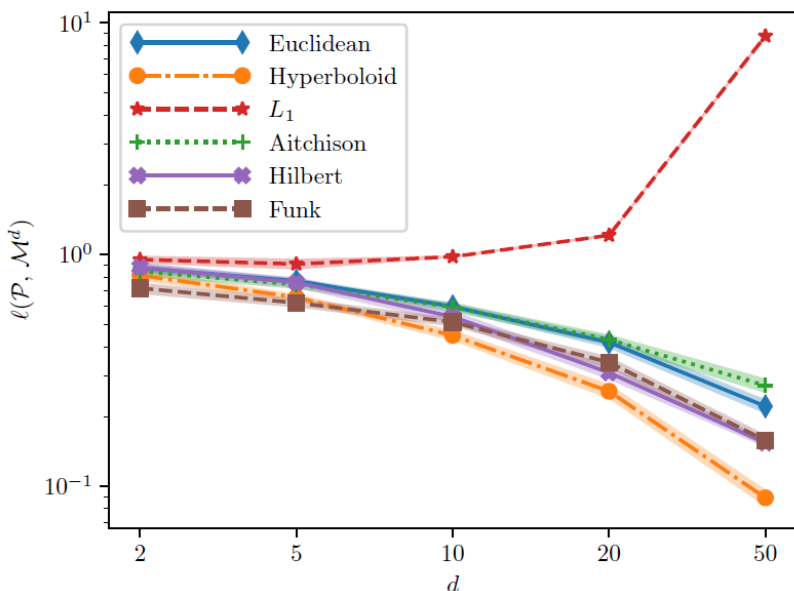
Hilbert simplex geometry  
is the winner  
for discrete graphs

The larger the embedding dimension, the better!

**Hilbert & hyperbolic hyperboloid geometries experimentally performed best**

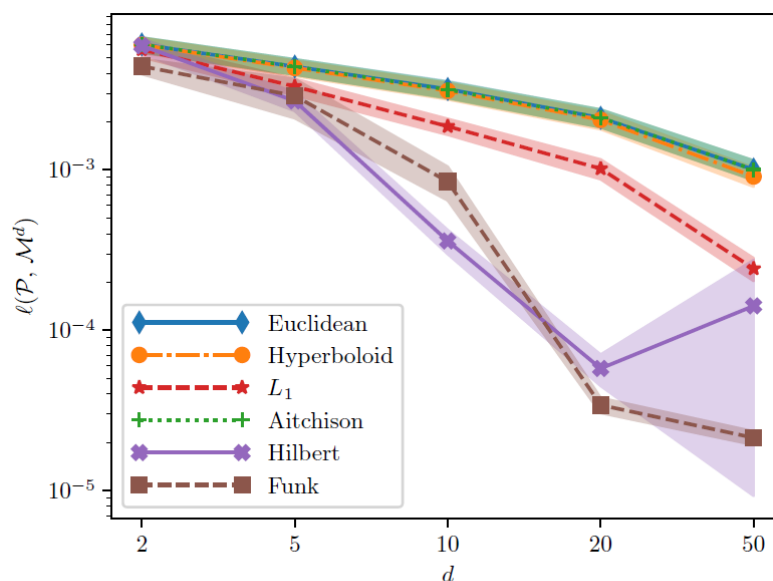


# Non-linear embeddings: Results (empirical KLD)



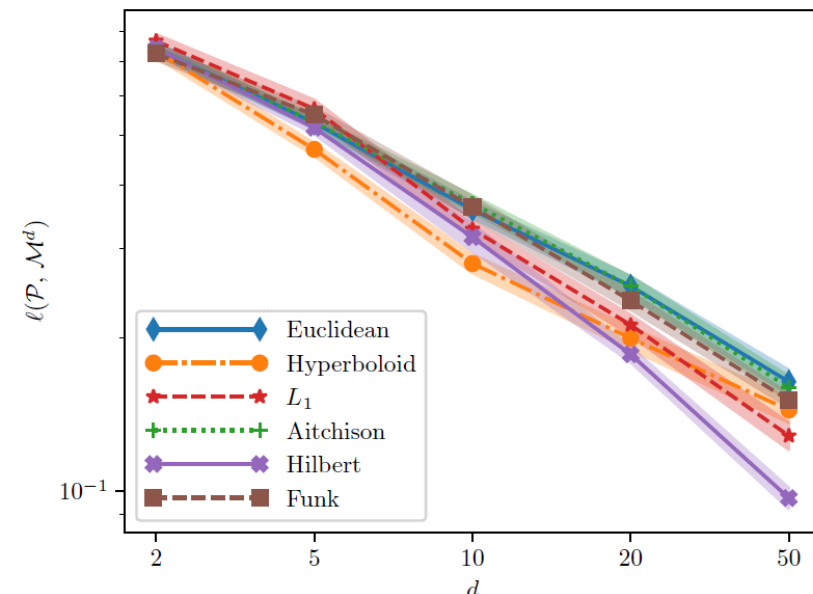
(a) 100 random points in  $\mathbb{R}^{100}$

hyperbolic geometry  
is the winner for continuous data



(b) Erdős-Rényi graphs  $G(n, p)$  ( $n = 200, p = 0.2$ )

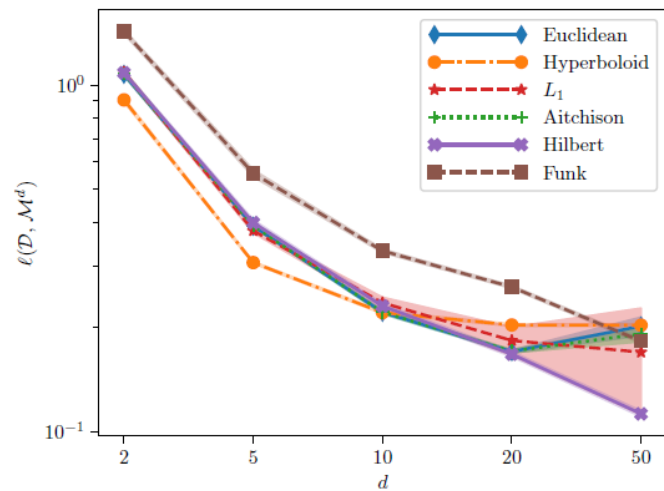
Funk geometry also  
good for embedding!



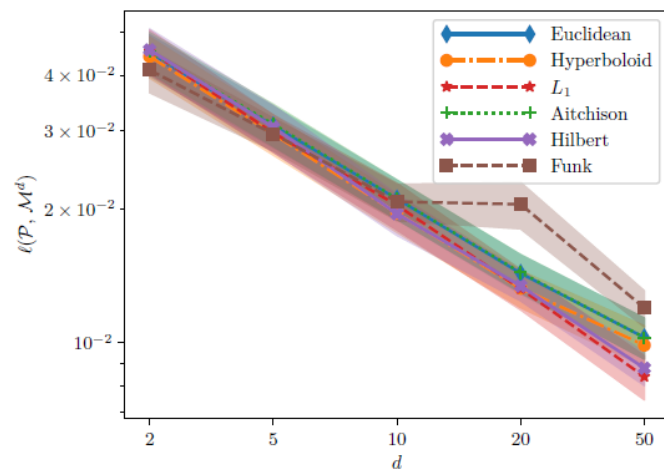
(c) Barabási-Albert graphs  $G(n, m)$  ( $n = 200, m = 2$ )

Hilbert simplex geometry  
is the winner  
for discrete graphs

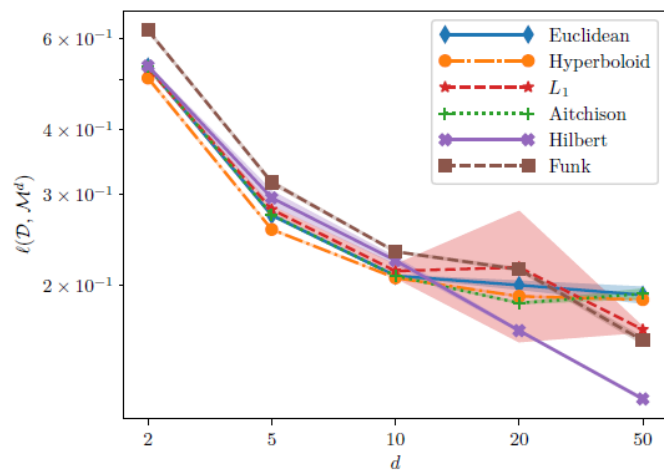
# Non-linear embeddings: Comparative results



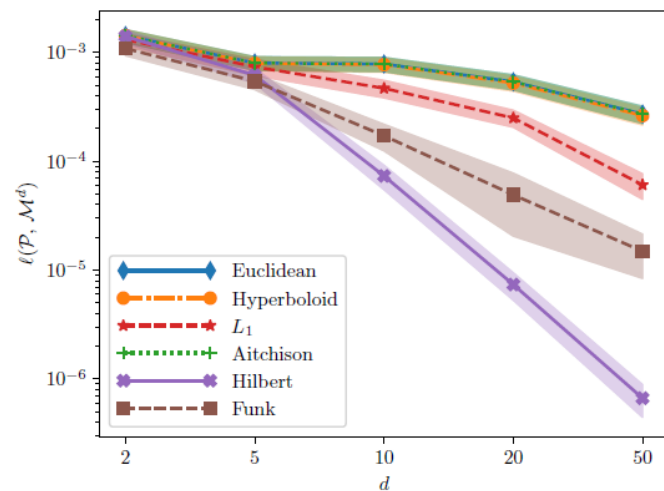
(a)  $\ell(\mathcal{D}, \mathcal{M}^d)$  ( $n = 200, p = 0.05$ )



(b)  $\ell(\mathcal{P}, \mathcal{M}^d)$  ( $n = 200, p = 0.05$ )



(c)  $\ell(\mathcal{D}, \mathcal{M}^d)$  ( $n = 200, p = 0.5$ )



(d)  $\ell(\mathcal{P}, \mathcal{M}^d)$  ( $n = 200, p = 0.5$ )

Embedding losses against  $d$  (Erdős–Rényi random graph  $G(n, p)$ ).

# Summary

- Proposed **differentiable approximation** of Hilbert distance
- Presented **Hilbert simplex geometry** for graph embeddings via distance matrices using Adam optimizer
- Results for **non-linear embeddings**: Hilbert/Funk simplex geometry is experimentally fast, robust, and competitive compared to  $L_1$ ,  $L_2$ , Aitchison and hyperbolic hyperboloid embeddings
- Proved the **monotonicity** of Funk and Hilbert distances
- Shown a **connection** between Hilbert distance and Aitchison distance via the normalized logarithmic representation of standard simplex points

# Erdős–Rényi random graph datasets $G(n,p)$

Graph with  $n$  nodes constructed by connecting nodes randomly  
An edge  $E_{ij}$  is included in the graph with probability  $p$   
(independently from other edges)

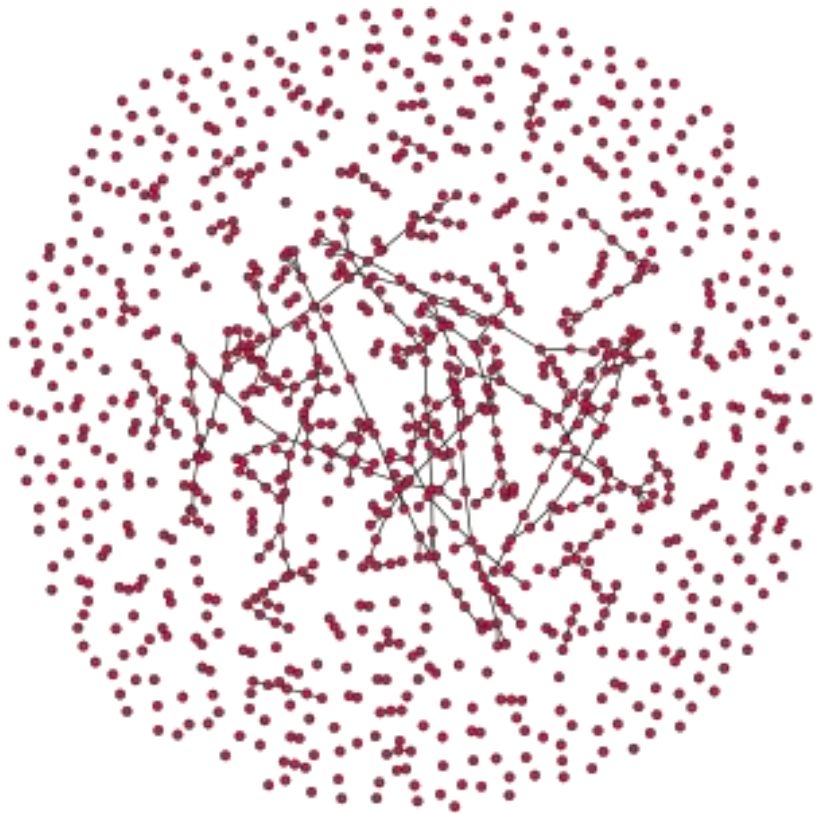


Image courtesy of Wikipedia

Caption:

"An Erdős–Rényi–Gilbert graph with 1000 vertices at the critical edge probability  $p=1/(n-1)$  showing a large component and many small ones"

# Barabási–Albert random graph datasets $G(n,m)$

- Generating random scale-free networks with power-law degree distributions
- Preferential attachment  $m$ :
  - the more connected a node is, the more likely it is to receive new links.
- Begins with an initial connected network of  $m_0$  vertices.
- Add vertices incrementally: A new vertex  $v$  is connected to already existing vertex  $v_i$  with probability  $\frac{\text{deg}(v_i)}{\sum_j \text{deg}(v_j)}$

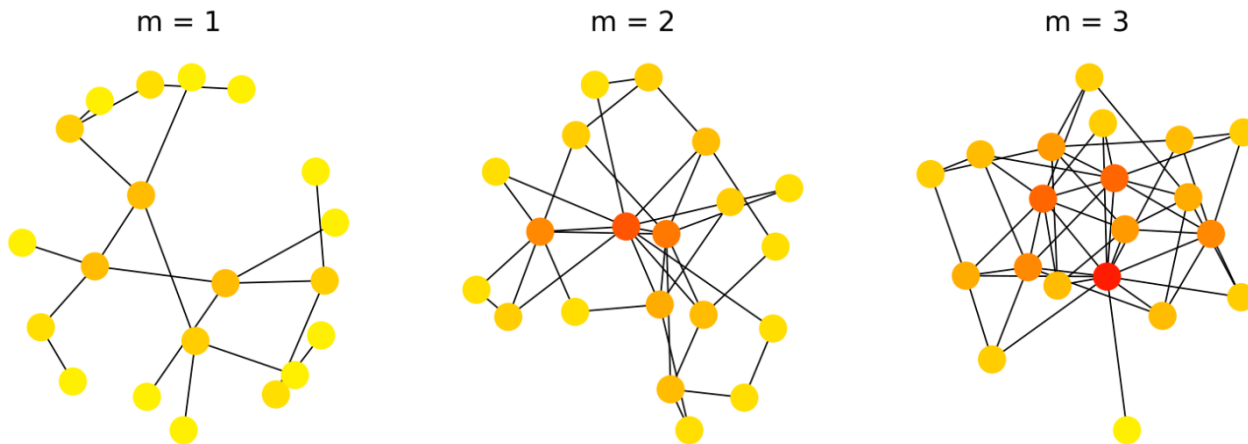


Image courtesy of Wikipedia

Caption:

"Display of three graphs generated with the Barabasi-Albert (BA) model. Each has 20 nodes and a parameter of attachment  $m$  as specified. The color of each node is dependent upon its degree (same scale for each graph)."

# References

- **Clustering in Hilbert's projective geometry: The case studies of the probability simplex and the ellipsope of correlation matrices**, *Geometric structures of information* (2019)
- **Non-linear Embeddings in Hilbert Simplex Geometry**, *Topology, Algebra, and Geometry in Machine Learning Workshop (ICML TAGML'23)*, *arXiv:2203.11434* (2022)
- Home page: <https://franknielsen.github.io/HSG/>

# Non-linear Embeddings in Hilbert Simplex Geometry

- Hilbert distance on the simplex:

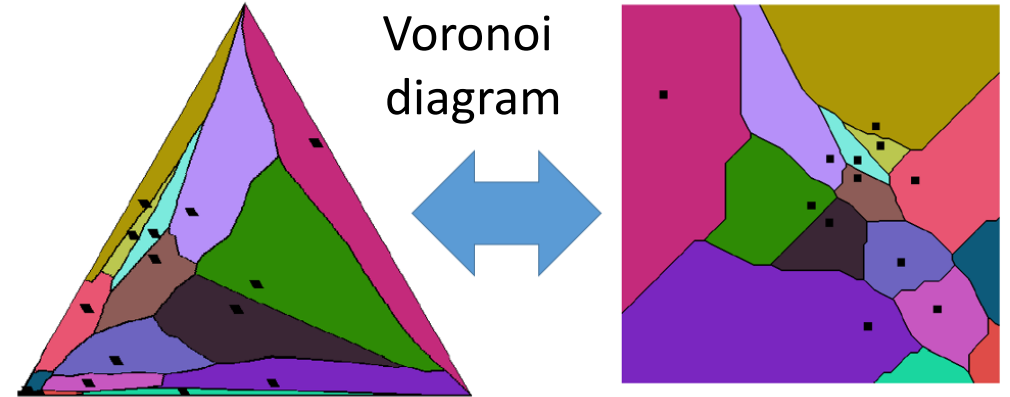
$$\rho_{\text{HG}}(p, q) = \log \frac{\max_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}{\min_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}$$

- Hilbert simplex geometry is isometric to normed vector space:

HD is projective distance on the positive orthant cone.

- Differentiable approximation of the Hilbert distance:

$$\tilde{\rho}_{\text{LSE}^T}(p, q) = \frac{1}{T} \log \left( \sum_i \left( \frac{p_i}{q_i} \right)^T \right) \left( \sum_i \left( \frac{q_i}{p_i} \right)^T \right)$$



$$\rho_{\text{HG}}(p, q) = \log \frac{\max_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}{\min_{i \in \{1, \dots, d\}} \frac{p_i}{q_i}}$$

$$\begin{aligned} \rho_{\text{HG}}(p, q) &= \|v(p) - v(q)\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{NH}} \\ &= \left\| \log \frac{p}{G(p)} - \log \frac{q}{G(q)} \right\|_{\text{var}} \end{aligned}$$

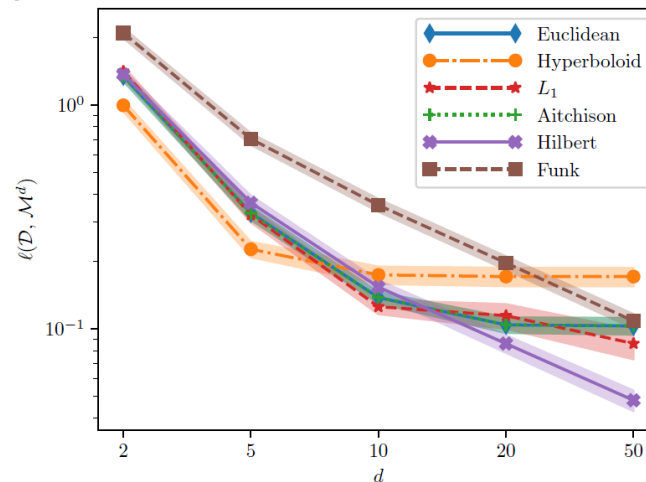
- Loss functions for embedding distance matrices:

$$\ell(\mathcal{D}, \mathcal{M}^d) := \inf_{\mathbf{Y} \in (\mathcal{M}^d)^n} \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n (\mathcal{D}_{ij} - \rho_{\mathcal{M}}(\mathbf{y}_i, \mathbf{y}_j))^2$$

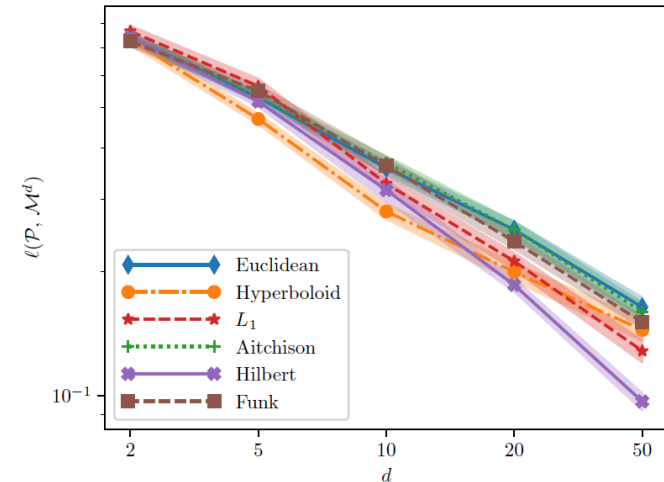
or empirical average Kullback-Leibler divergence:

$$\ell(\mathcal{P}, \mathcal{M}^d) := \inf_{\mathbf{Y} \in (\mathcal{M}^d)^n} \frac{1}{n} \sum_{i=1}^n \sum_{j:j \neq i} \mathcal{P}_{ij} \log \frac{\mathcal{P}_{ij}}{q_{ij}(\mathbf{Y})}$$

$$q_{ij}(\mathbf{Y}) := \frac{\exp(-\rho_{\mathcal{M}}^2(\mathbf{y}_i, \mathbf{y}_j))}{\sum_{j:j \neq i} \exp(-\rho_{\mathcal{M}}^2(\mathbf{y}_i, \mathbf{y}_j))}$$



(c) Barabási-Albert graphs  $G(n, m)$  ( $n = 200, m = 2$ )



(c) Barabási-Albert graphs  $G(n, m)$  ( $n = 200, m = 2$ )