Symmetric Spaces For Graph Embeddings: A Finsler-Riemannian Approach

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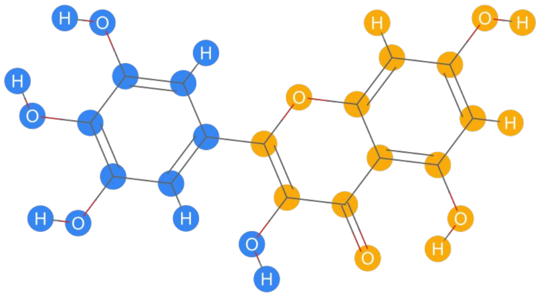
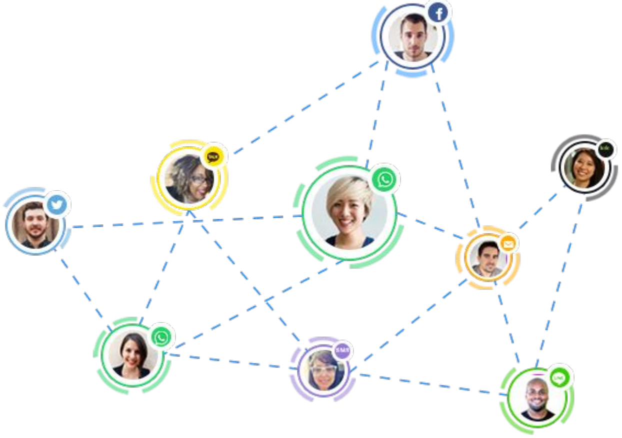
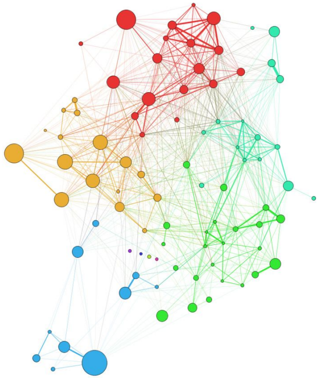
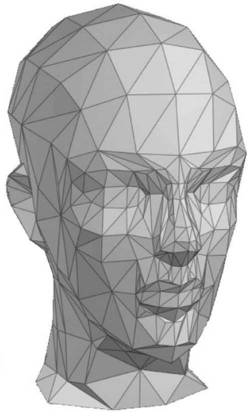
Graphs are ubiquitous!

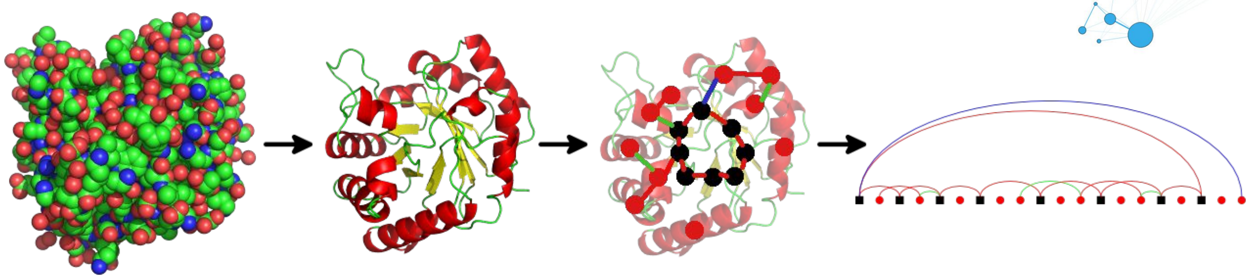
- Social networks
- Proteins
- Molecules
- Genes
- Internet
- And many more!



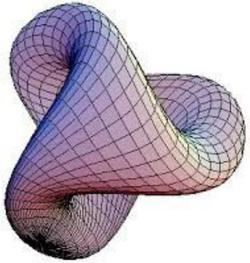




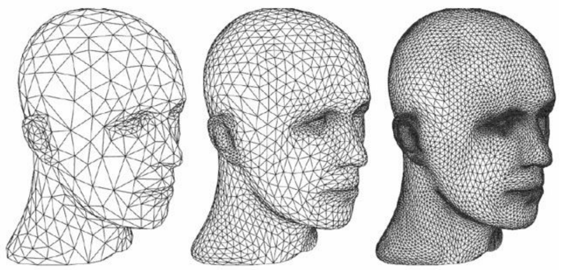


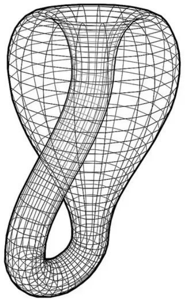


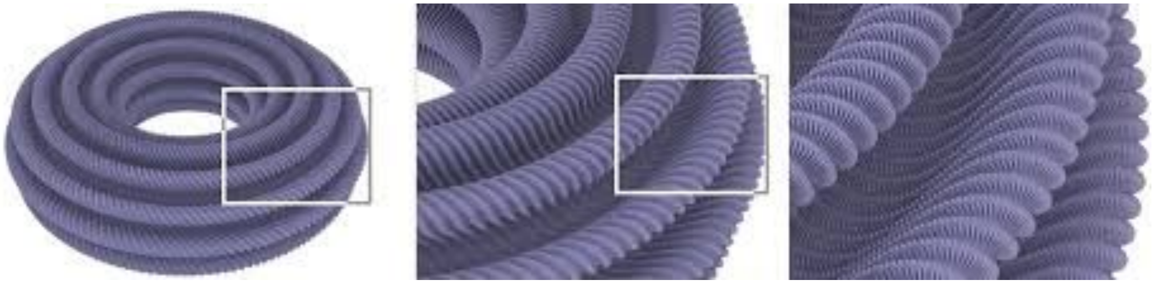
Graphs are non-Euclidean!



- Approach: embed graph into a Euclidean space
- Graphs typically exhibit non-Euclidean features
- Richer manifold structure needed
- The choice of a metric space where to embed the data is a powerful inductive bias

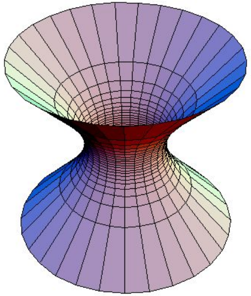


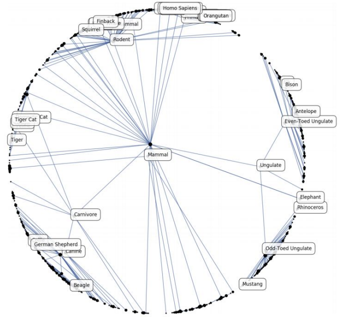


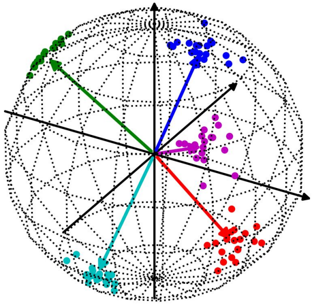


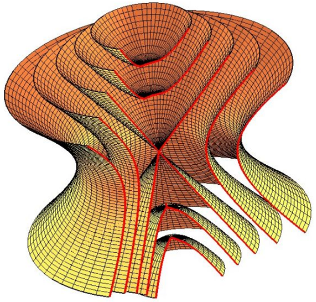
Previous Work

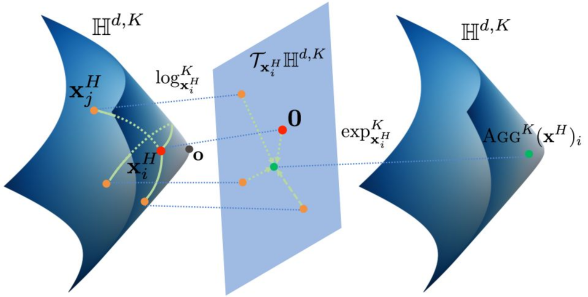
- Hyperbolic spaces
  Krioukov et al., 2009; Chamberlain et al., 2017; Nickel & Kiela, 2017, 2018; Sala et al., 2018; Ganea et al., 2018.
- Spherical spaces
  Wilson et al., 2014; Liu et al., 2017; Xu & Durrett, 2018; Meng et al., 2019; Defferrard et al., 2020
- Different curvatures combined
  Chami et al., 2019; Bachmann et al., 2020; Grattarola et al., 2020
- Cartesian products of spaces
  Gu et al., 2019; Tifrea et al., 2019; Skopek et al., 2020
- Symmetric Positive Definite matrices and Grassmannian manifolds
  Huang & Gool, 2017; Huang et al., 2018; Cruceru et al., 2020











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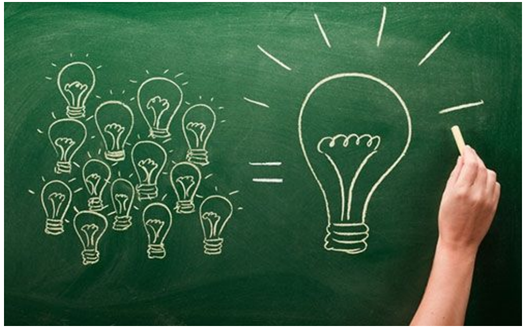
These are all **symmetric spaces!!!**



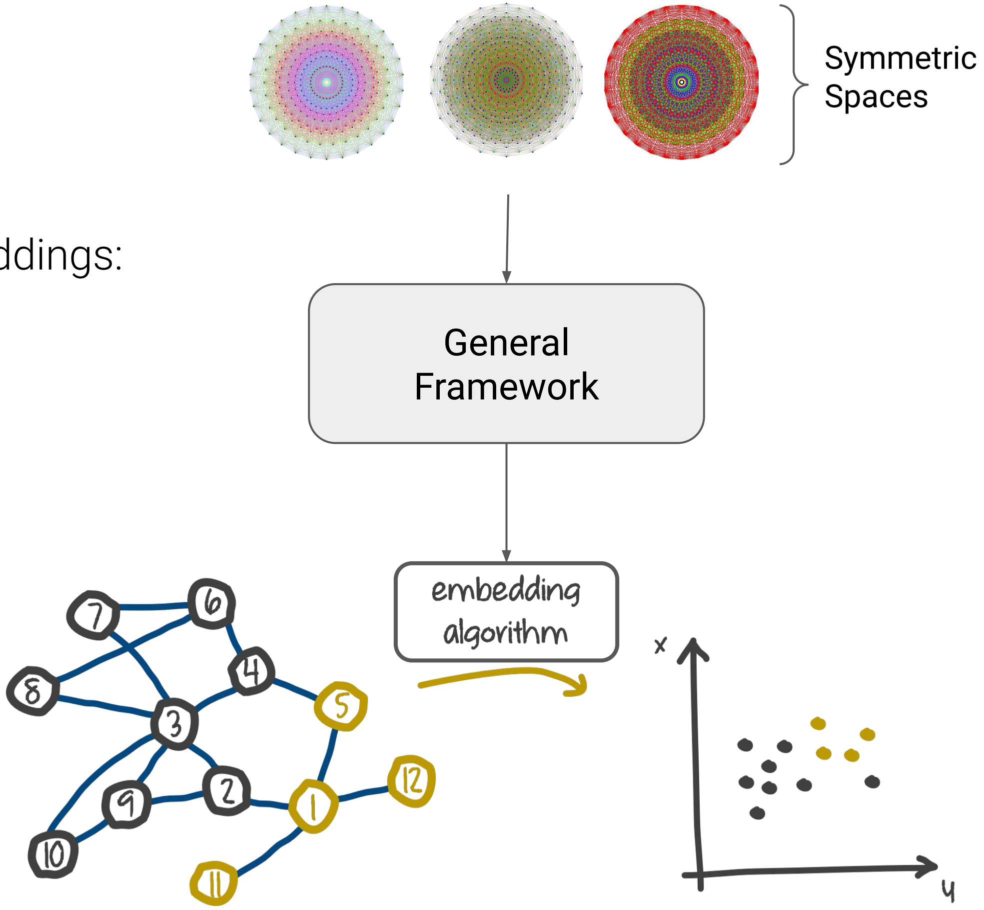
A **unified framework** in which to encompass these various examples is still missing

We Propose!

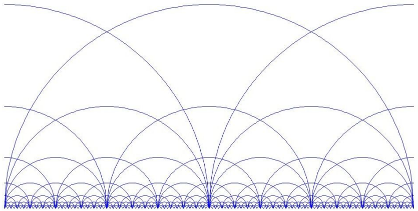
Systematic use of **symmetric spaces** in representation learning

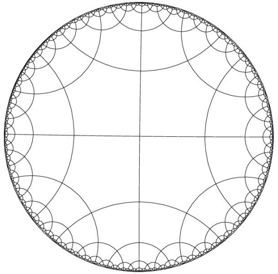
- **General framework** to learn graph embeddings:
  - Choose a space to represent nodes
  - How to measure distances
  - How to compute gradient

- Concrete implementation of the framework with **Siegel Spaces**



Siegel Spaces

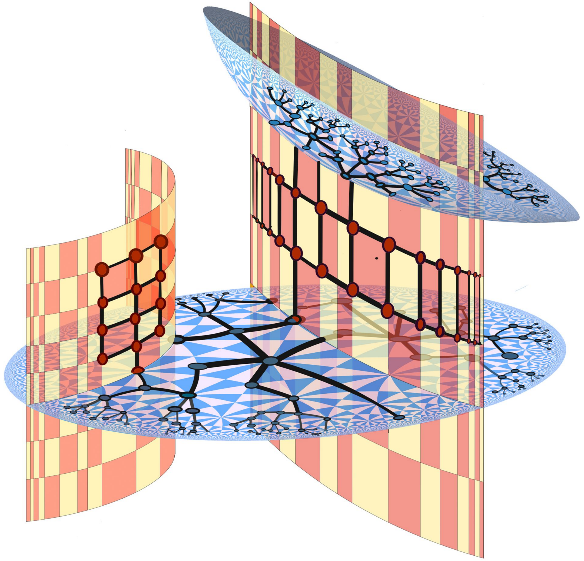




- A family of non-compact symmetric spaces of **non-positive** curvature

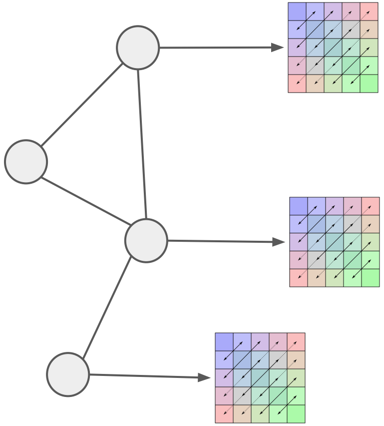
- Generalization of hyperbolic plane

- Rich geometry:
    - Euclidean subspaces
    - Hyperbolic subspaces
    - Products of Euclidean x Hyperbolic
    - Copies of SPD matrix spaces



- Excellent device for learning embeddings of complex networks:
    - They **automatically adapt** to dissimilar graphs without a priori knowledge of their internal structure

Points in the Space

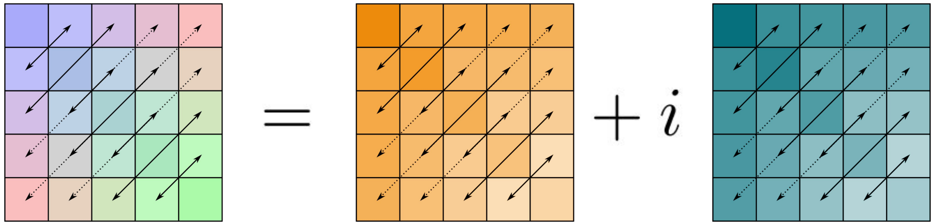


- Each point is represented as a **symmetric matrix** with coefficients in the **complex numbers** $\mathbb{C}$

- Complex variable representation:

$$Z = X + iY \in \mathrm{Sym}(n, \mathbb{C})$$

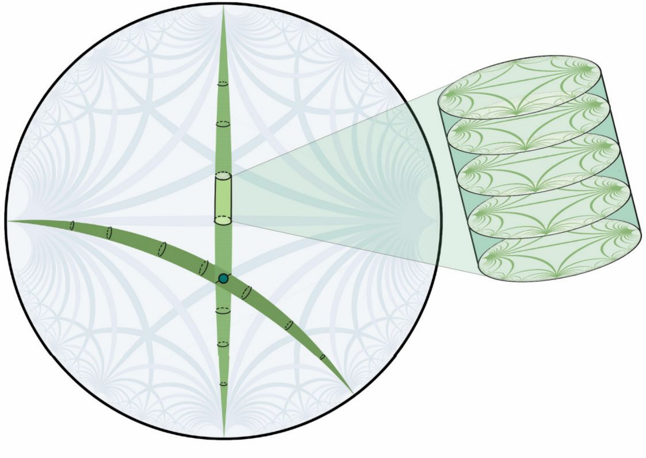
$$Z \qquad X = \Re(Z) \qquad Y = \Im(Z) \in \mathrm{Sym}(n, \mathbb{R})$$



Models of Siegel Spaces

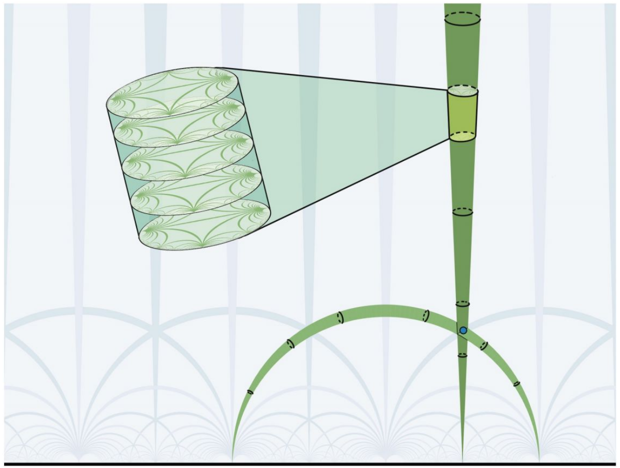
- Bounded domain model:
  - Generalizes the Poincaré disk

$$\mathcal{B}_n := \{Z \in \mathrm{Sym}(n, \mathbb{C}) |\ \mathrm{Id} - Z^* Z \gg 0\}$$

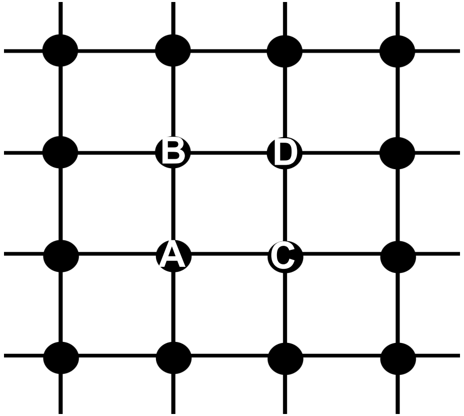


- Siegel upper half space model:
  - Generalizes the upper half plane model of the hyperbolic plane

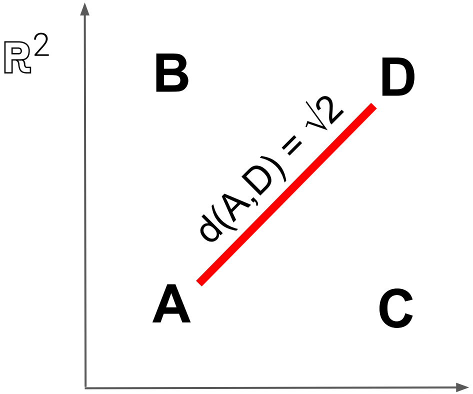
$$\mathcal{S}_n := \{Z = X + iY \in \mathrm{Sym}(n, \mathbb{C}) |\ Y \gg 0\}$$



Finsler Distances

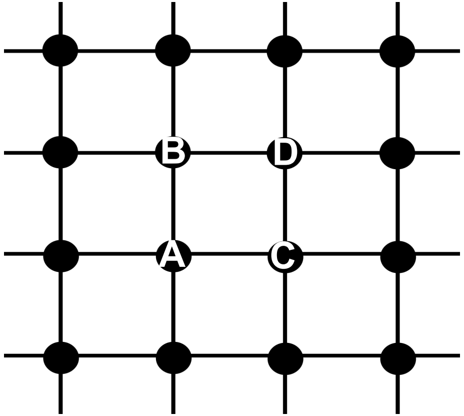


We embed a 2D grid in an Euclidean plane $\mathbb{R}^2$



- Distances are distorted!
  - $d_G(A,D) = 2$ **!=** $d_{\mathbb{R}}(A,D) = \sqrt{2}$
- Length minimizing paths are **unique**

Finsler Distances



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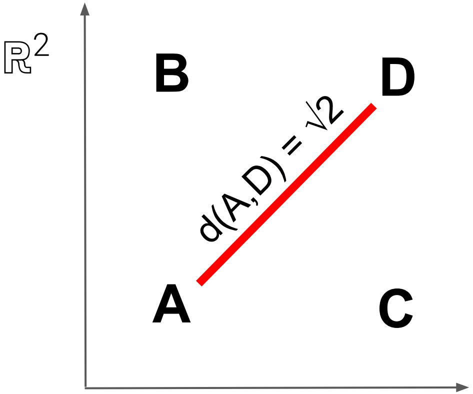
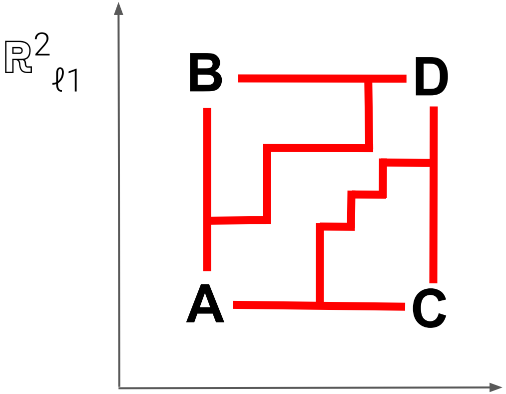
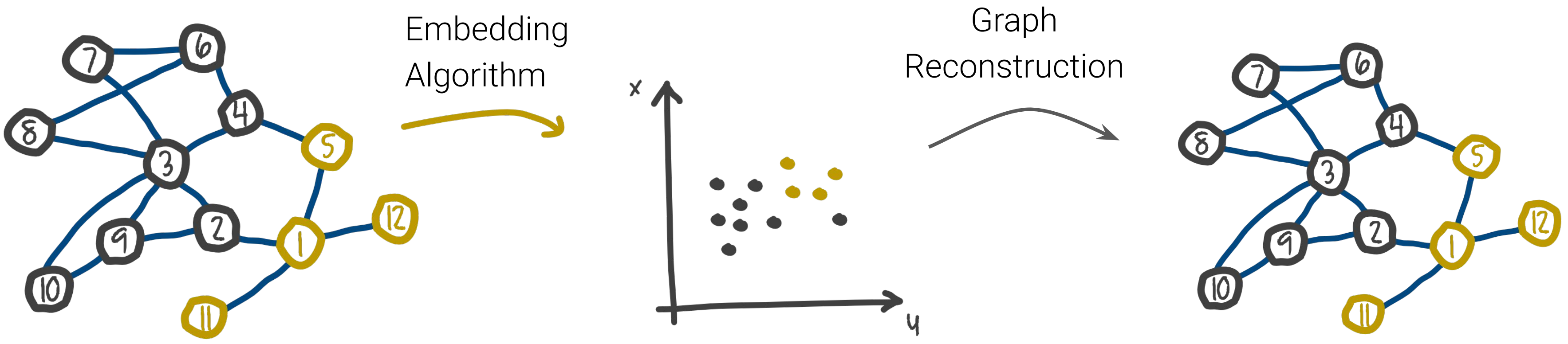




- Distances are distorted!
  - $d_G(A,D) = 2$ **!=** $d_{\mathbb{R}}(A,D) = \sqrt{2}$
- Length minimizing paths are **unique**

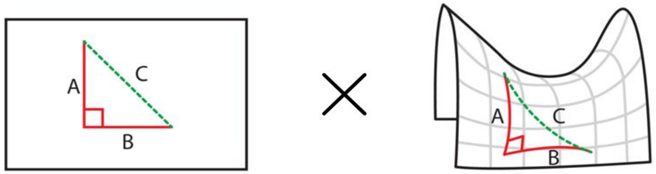
- Distances are **not** distorted!
  - $d_G(A,D) = 2$ **==** $d_{\ell 1}(A,D) = 2$
- Geodesics are **not unique!**

Experiments on Graph Reconstruction

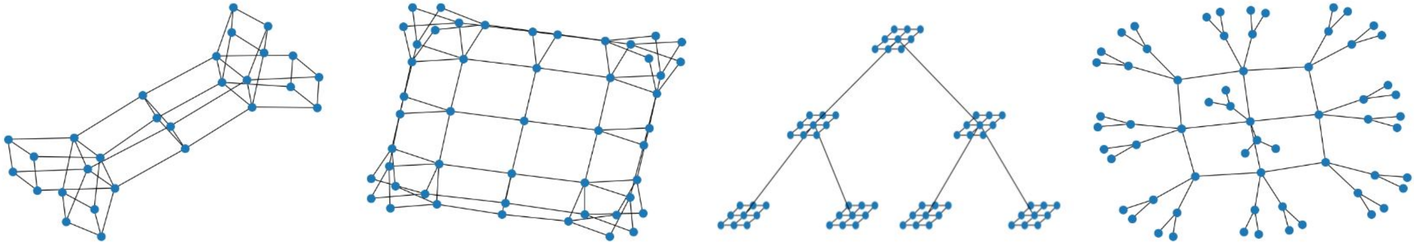


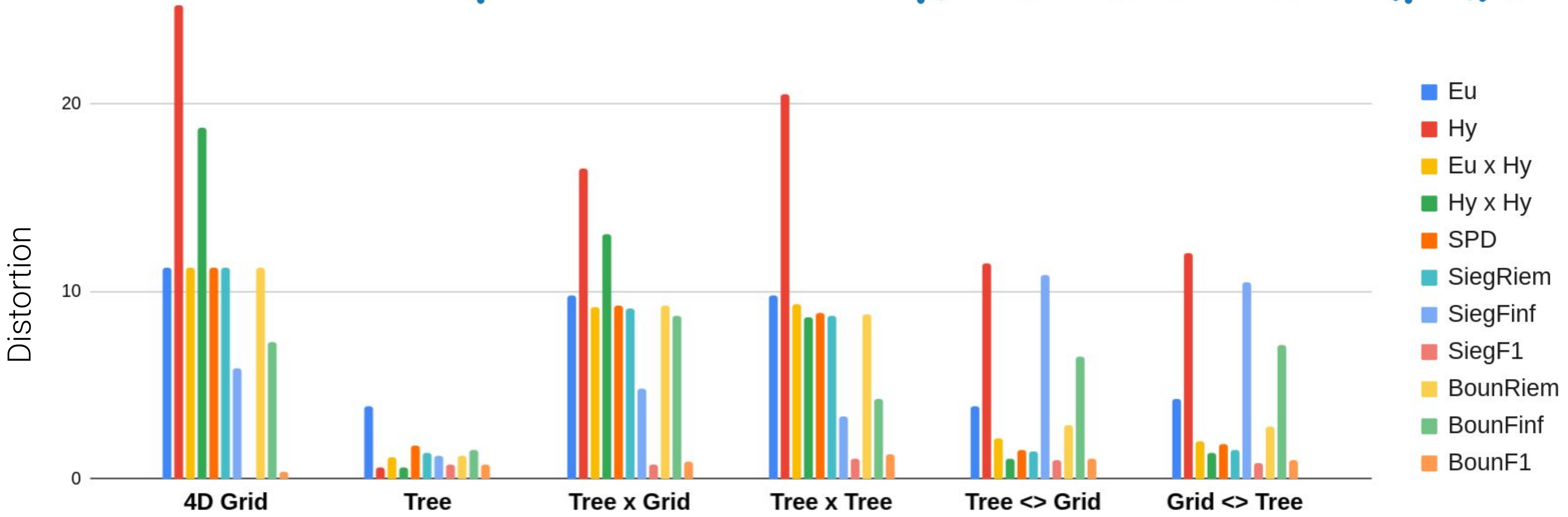
- Metrics
  - Global and local metric

- Model Baselines
  - Euclidean, Hyperbolic
  - Cartesian product thereof
  - SPD



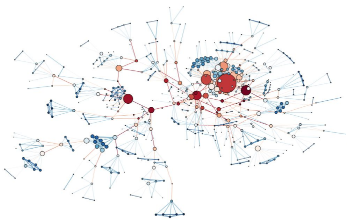
Synthetic Graphs

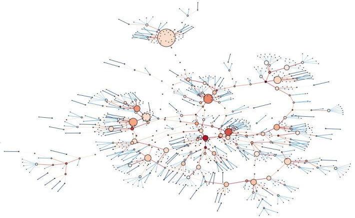


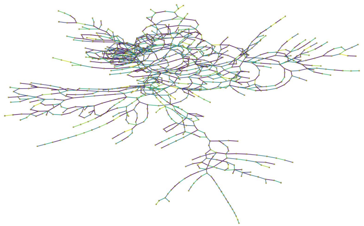


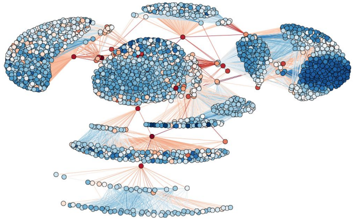
- The **Riemannian metric performs on par** with the best matching geometric spaces
- Siegel space with **Finsler metrics significantly outperform** the baselines in most graphs

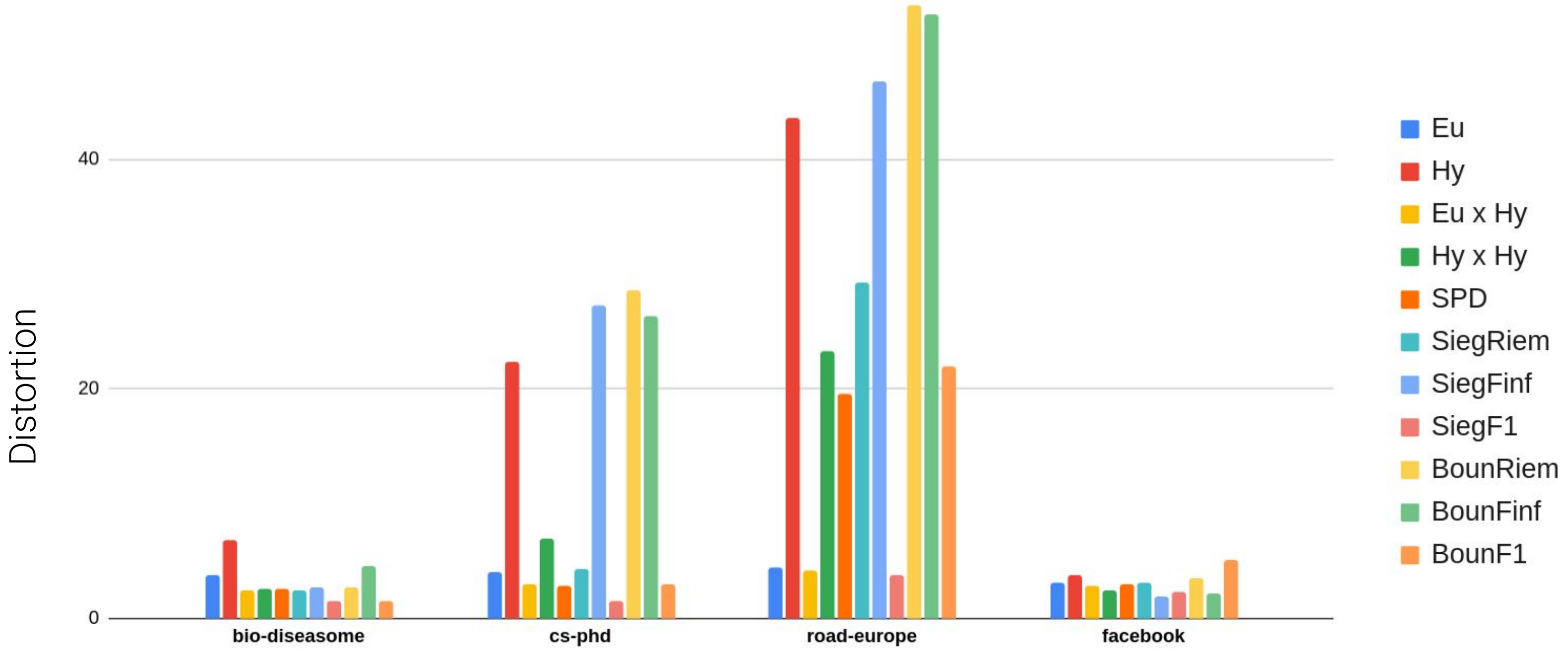
Real-World Datasets





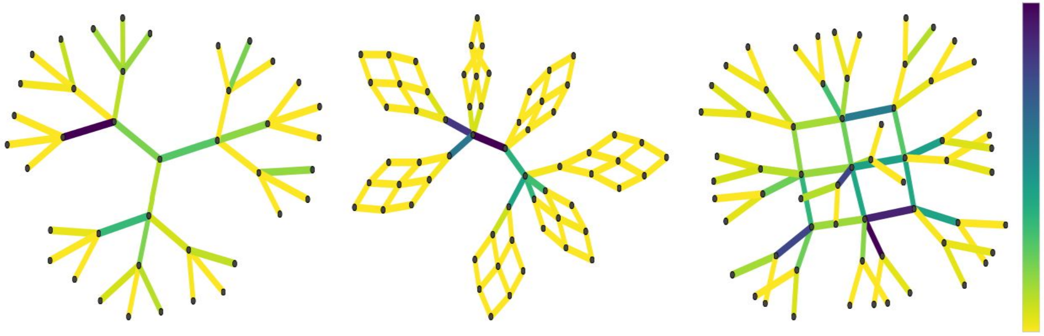




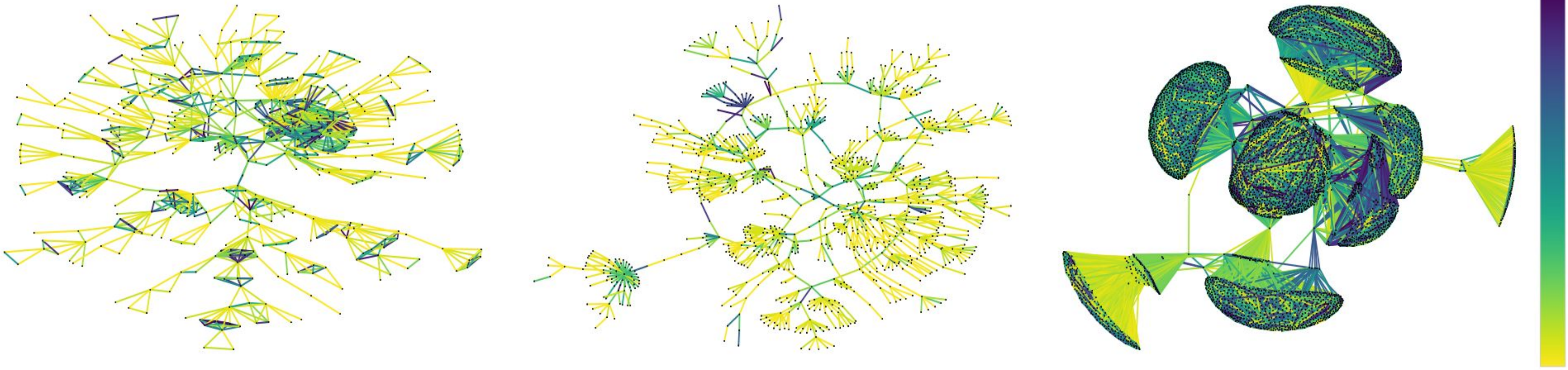


- Models with Finsler (One) metrics **outperform all baselines** 🏆
- **Strong reconstruction capabilities** of RSS for real-world data 💪

Structure Analysis



- The **vector-valued distance** can be leveraged to find structure in graphs.
- The model distinguishes tree-like and grid-like edges



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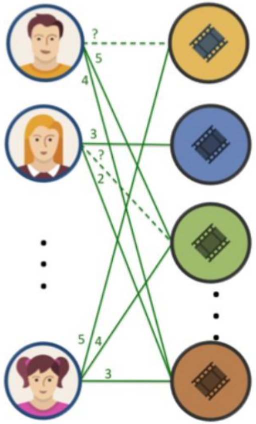
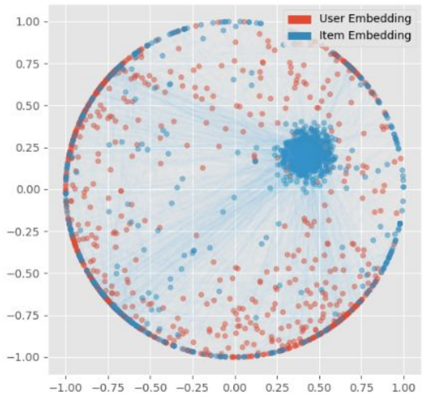
More Applications

- Downstream tasks:
    - Recommender Systems
    - Node classification



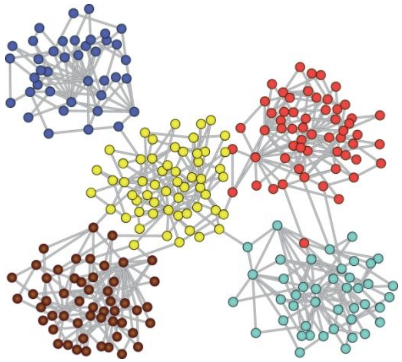


- Embeddings capture **structural properties** of the datasets useful for the task

- Downstream tasks can profit from the **enhanced graph representation capacity**

- **Flexibility** of the method

- **Integration** of RSS embeddings with classical Euclidean network layers



Summary

- General framework for embeddings in **symmetric spaces**
  - **Finsler Metrics**: better representation capacities
  - **Vector-valued distance**: tool for graph analysis

- Implementation on Siegel spaces
  - **Matrix models** of hyperbolic plane
  - **Ties or outperforms** constant-curvature baselines on three different tasks
  - It **does not require** any previous assumption on geometric features of the graph
  - Approach offers **flexibility** and enhanced **representation capacity**