Universität Stuttgart
IPVS – Institute for Parallel and Distributed Systems
Analytic Computing

Hyperbolic Embeddings

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Outline

- Preliminaries
- Hyperbolic Embeddings
- Embeddings Graphs with Mixed Geometries
- Future Directions

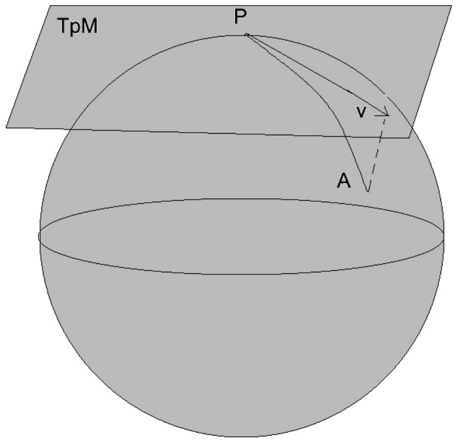
1. Preliminaries

Preliminaries

- **Manifold:** A manifold is a topological space of which each point's neighborhood can be locally approximated by R^n

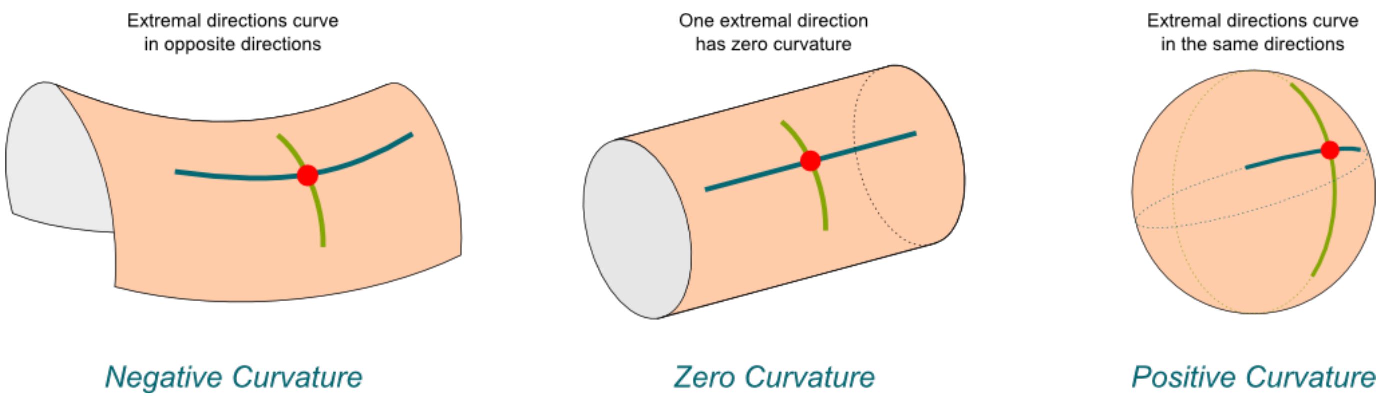
- **Tangent Space:** The tangent space T_pM of M at *p* is a n-dimensional vector space approximating *M* around *p*

- **Geodesics:** Geodesics is the the generalization of a straight line in the Euclidean space.



Curvature

- **Curvature:** how *geometric object* deviates from a *flat one*
- **Gaussian Curvature:** the product of its two *principal curvatures*

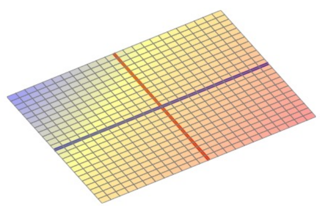
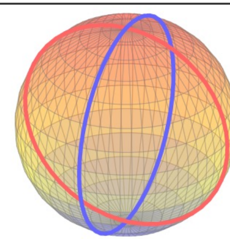
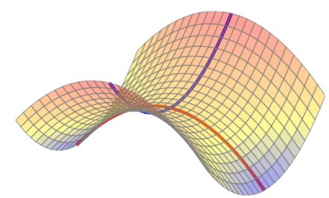
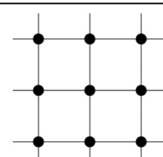
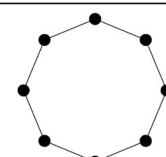
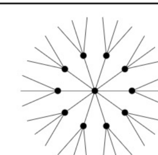


- **Sectional Curvature:** A local Gaussian curvature defined on the tangent space of point *p* *(the flat plane is the tangent space)*

Weber, Melanie, and Maximilian Nickel. "Curvature and Representation Learning: Identifying Embedding Spaces for Relational Data." *NeurIPS Relational Representation Learning* (2018).

Constant (Sectional) Curvature Manifold (CCM)

Table 1: Properties of model spaces with constant sectional curvature κ.

	Euclidean $\mathbb{R}^d$	**Spherical** $\mathbb{S}^d$	**Hyperboloid** $\mathbb{H}^d$
Space	$\mathbb{R}^n$	$\{x \in \mathbb{R}^{n+1} : \langle x, x \rangle = 1\}$	$\{x \in \mathbb{R}^{n+1} : \langle x, x \rangle = -1, x_0 > 0\}$
$\langle u, v \rangle$	$\sum_{i=1}^{n} u_i v_i$	$\sum_{i=1}^{n} u_i v_i$	$-u_0 v_0 + \sum_{i=1}^{n} u_i v_i$
$d(u, v)$	$\sqrt{\langle u - v, u - v \rangle}$	$\mathrm{arccos}(\langle u, v \rangle)$	$\mathrm{arccosh}(-\langle u, v \rangle)$
Curvature	$\kappa = 0$	$\kappa = 1$	$\kappa = -1$
Sum of angles	π	$> \pi$	$< \pi$
Circle length	$C(r) = 2\pi r$	$C(r) = 2\pi \sin r$	$C(r) = 2\pi \sinh r$
Disc area	$A(r) = 2\pi r^2/2$	$A(r) = 2\pi(1 - \cos r)$	$A(r) = 2\pi(\cosh r - 1)$
Principle Curvatures			
Characteristic Graph			

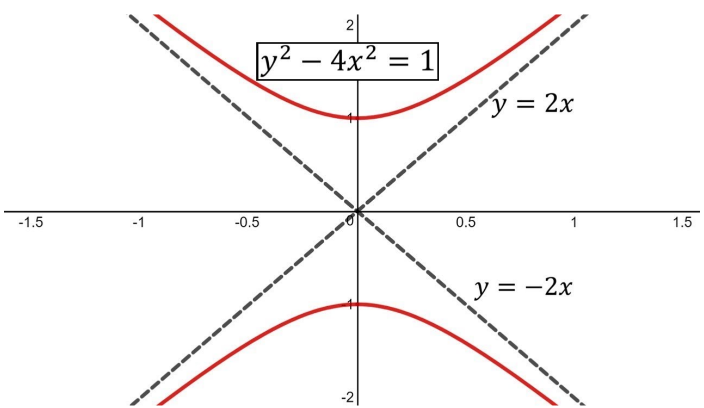
Weber, Melanie, and Maximilian Nickel. "Curvature and Representation Learning: Identifying Embedding Spaces for Relational Data." *NeurIPS Relational Representation Learning* (2018).

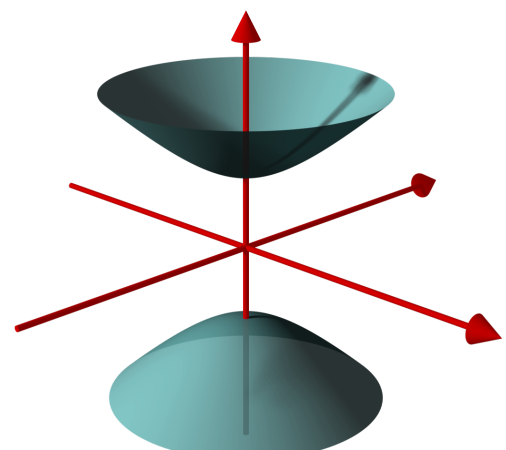
Lorentz Model

- The Lorentz model L^n of an n-dimensional hyperbolic space is a manifold embedded in the n-dimensional Minkowski space.

$$\mathbb{L}^n = \{x = (x_0, \ldots, x_n) \in \mathbb{R}^{n+1} :< x, x >_{\mathbb{L}} = -1, x_0 > 0\}$$

$$< x, y >_{\mathbb{L}} = x^T \mathfrak{g}^L y = -x_0 y_0 + \sum_{i=1}^{n} x_i y_i, x \text{ and } y \in \mathbb{R}^{n+1}$$



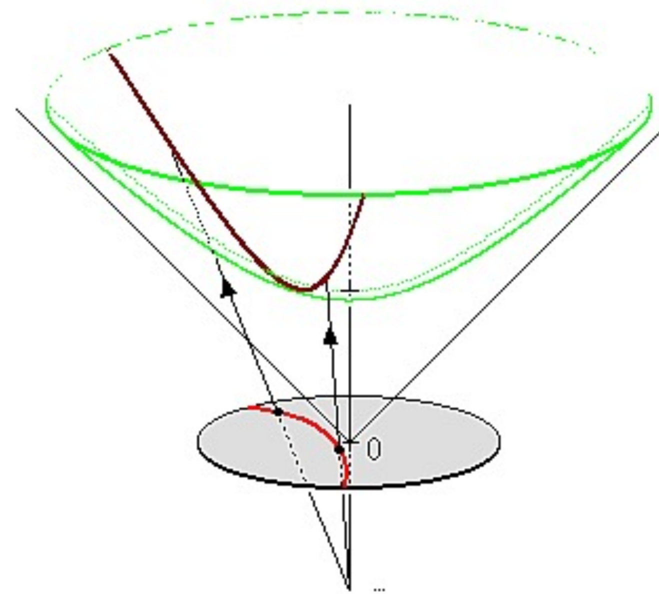


Poincare Ball Model

- The Poincare Ball model B^n is given by projecting each point of L^n on to the hyperplane x_0=0

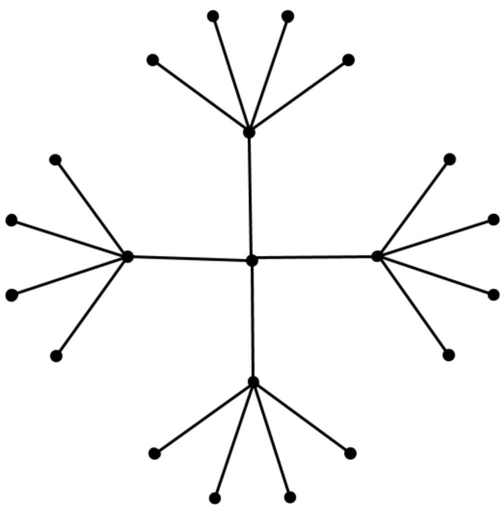
$$\mathbb{B}^n = \{x \in \mathbb{R}^n : ||x|| < 1\}$$

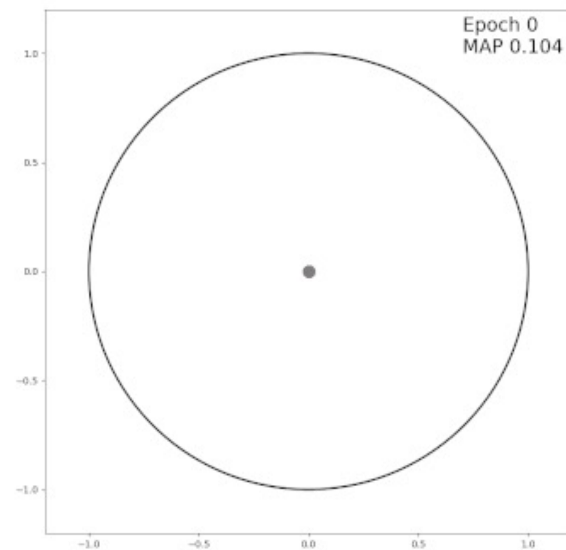
$$\mathfrak{g}^B = \lambda_x^2 \mathfrak{g}^E \qquad \lambda_x = \frac{2}{1-||x||^2}$$

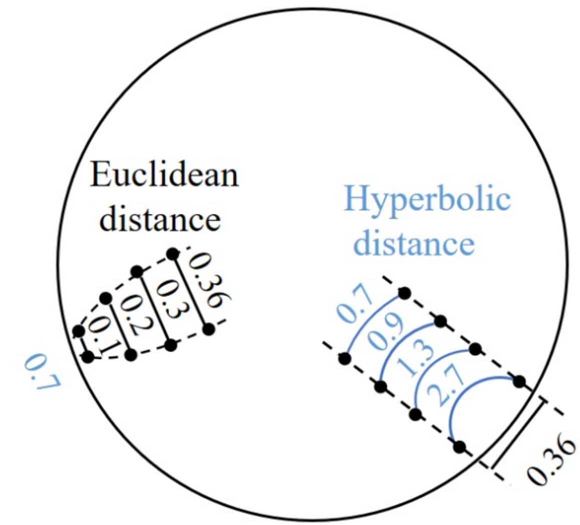


2. Hyperbolic Embeddings

Hyperbolic Embeddings for Tree-like data



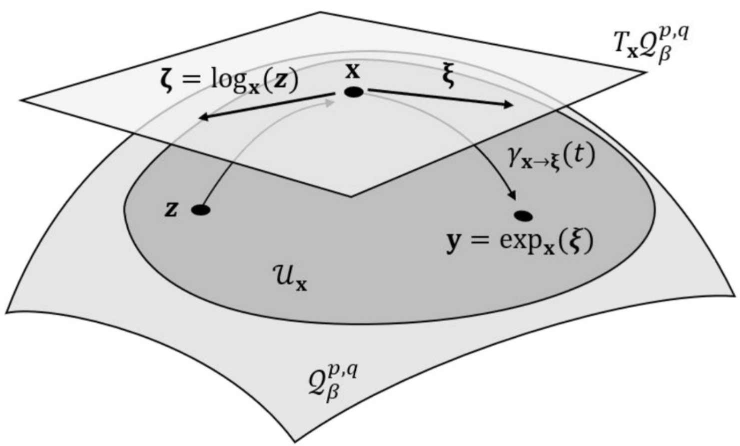




Hyperbolic Embedding—Operations

- **Vector operations:** multiplications, addition, etc.
- **Neural operations:** pooling function, concatenation, etc.

- Moving the operations into the tangent space

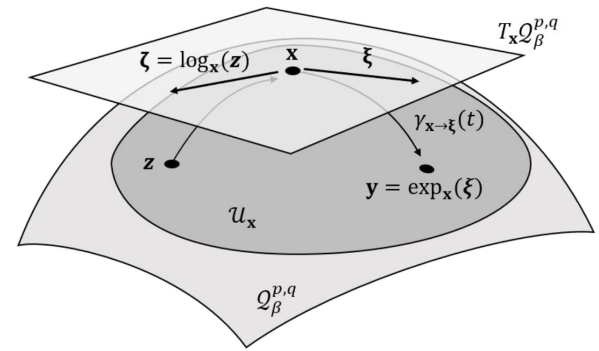


- **Exponential map**
- **Logarithm map**

Operations

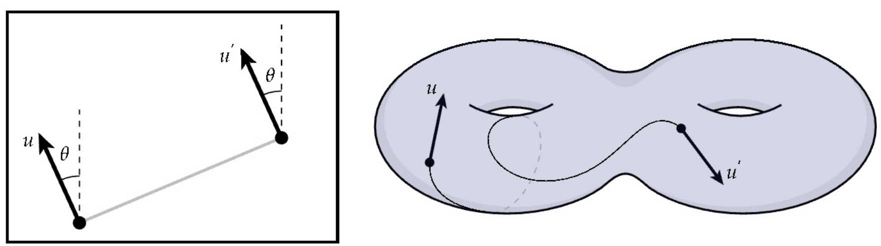
- Matrix multiplication (e.g. neural transformation)

$$W \otimes^K \mathbf{x}^H := \exp_{\mathbf{o}}^K(W \log_{\mathbf{o}}^K(\mathbf{x}^H)),$$



- Addition (e.g. TransE)

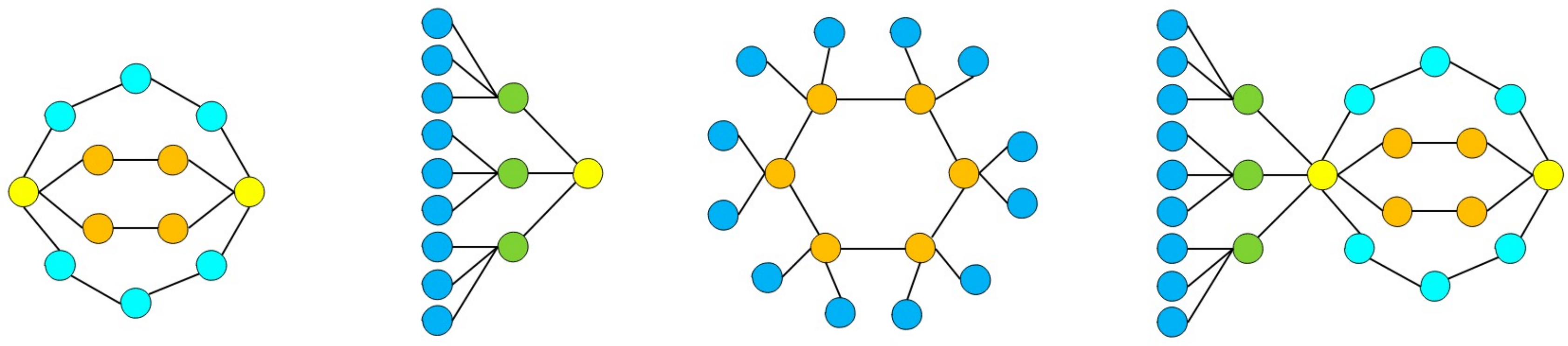
$$\mathbf{x}^H \oplus^K \mathbf{b} := \exp_{\mathbf{x^H}}^K(P_{\mathbf{o}\to\mathbf{x}^H}^K(\mathbf{b})).$$



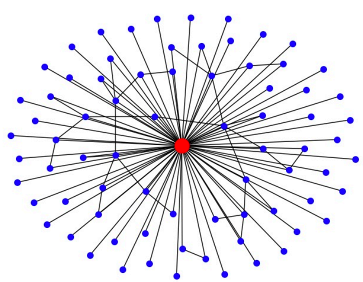
Parallel Transport

3. Embeddings Graphs with Mixed Geometries

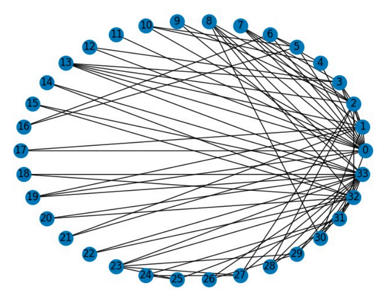
Embeddings Graphs with Mixed Geometry



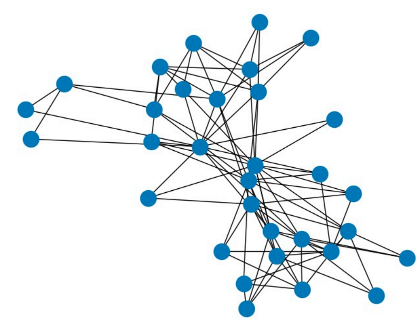
(a) Cycle (b) Tree (c) Cycle-Tree (balanced) (d) Cycle-Tree (unbalanced)



Barabási-Albert network



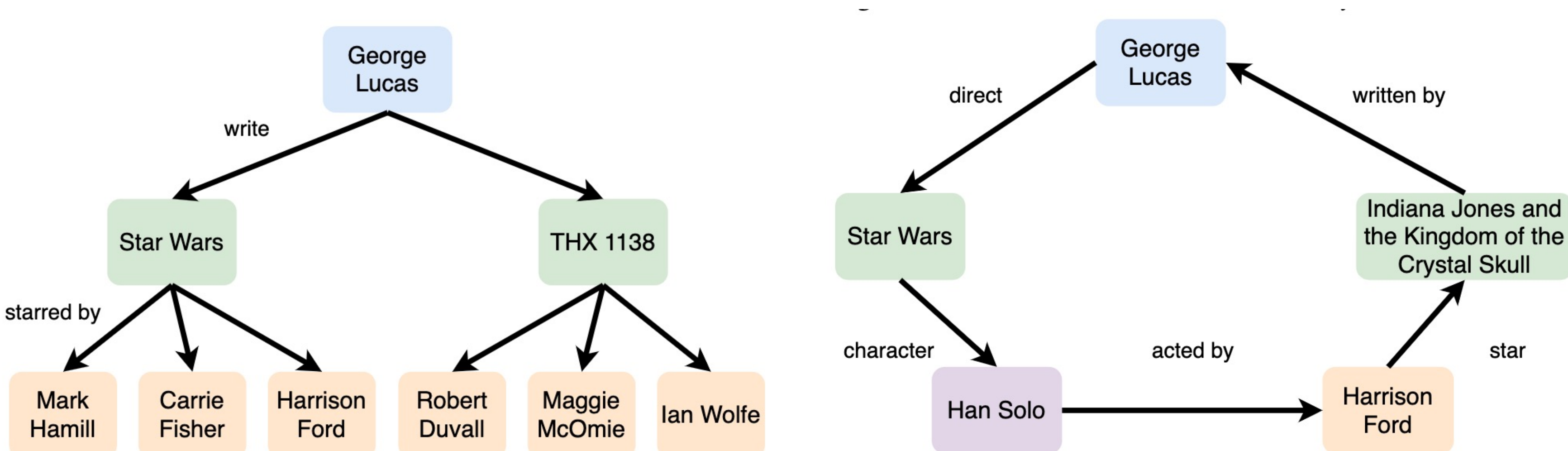
Zachary’s karate club



Knowledge Graphs

Embeddings Graphs with Mixed Geometry

- Tree & Cycle in KGs

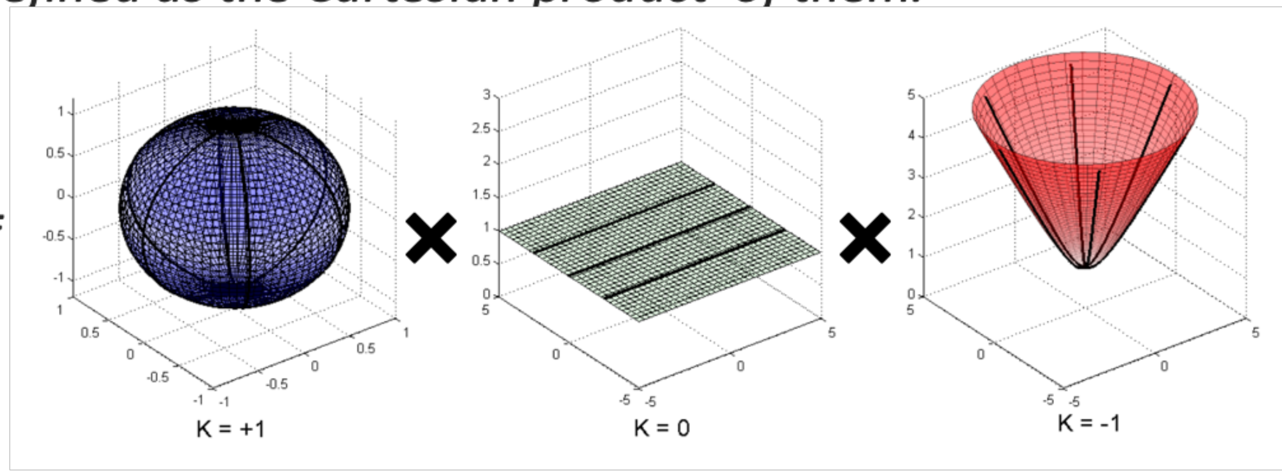


Embeddings with Mixed Geometry

- Solution: Learning Embedding in Product (Manifold) Space

  Product Manifold: *Given a sequence of smooth manifolds, the product manifold space is defined as the Cartesian product of them.*

  Product Manifold =

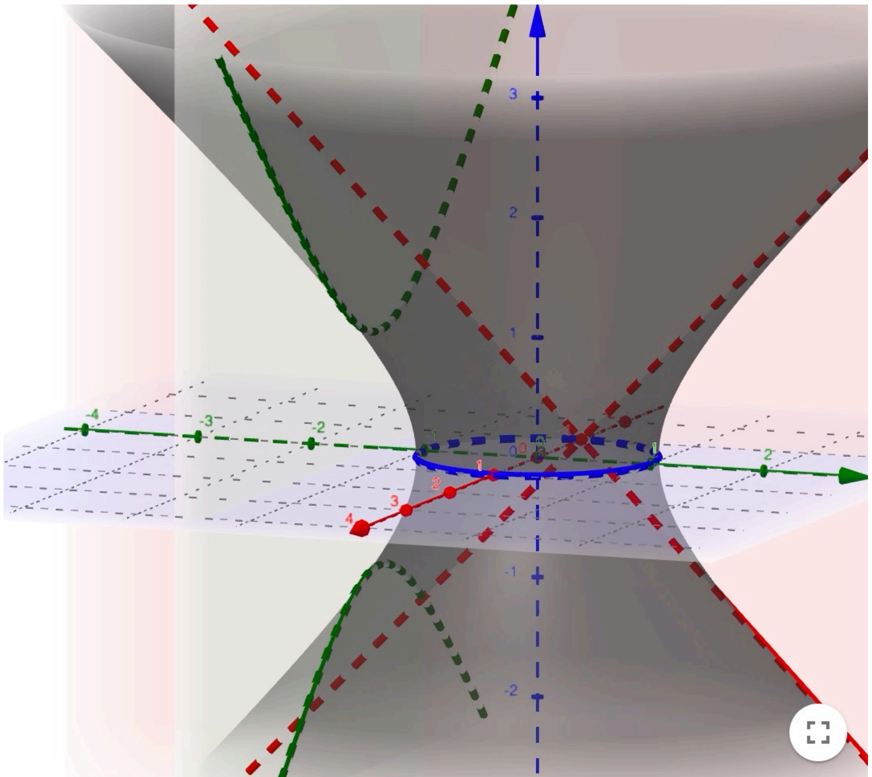


  Distance:

$$d^2(p_1, p_2) = d^2_{H_1}(p_1, p_2) + d^2_{H_2}(p_1, p_2) + \ldots + d^2_{S_1}(p_1, p_2) + \ldots + d^2_E(p_1, p_2).$$

Semi-Riemannian Embeddings

- Semi-Riemannian manifold fits graphs containing cycles and trees



$$\Omega^{1,2}_{K=-1}: -x_1^2 - x_2^2 + x_3^2 = -1$$

- Space-like geodesic: sphere properties
- Time-like geodesic: hyperbolic properties
- Light-like geodesic: Euclidean properties

Future Directions

- **Applications**
  - GNNs , KG completions, NLP, Recommendation Systems, Computer Vision, Clustering.
  - More applications

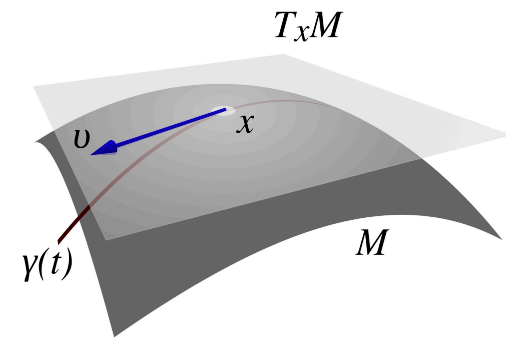
- **Theoretical**
  - Identifying the geometric prior for graphs
  - Defining model-specific operations
  - Defining operations directly on the manifolds

Thank you

Riemannian manifold

- **Riemannian manifold** *(M, g)* is a smooth manifold $M \subseteq R^n$ equipped with a metric *g,* a smoothly varying function defined on the **tangent space**

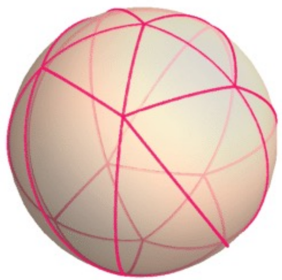
$$g_{\mathbf{x}} : \mathcal{T}_{\mathbf{x}}\mathcal{M} \times \mathcal{T}_{\mathbf{x}}\mathcal{M} \to \mathbb{R}.$$

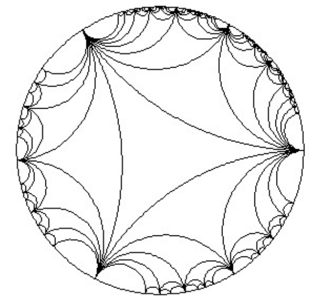


- The metric *g* induces *distance*, *angle*
- The metric should be:

(i) **symmetric** if $g(v, w) = g(w, v)$ for all $v, w \in T_pM$;
(ii) **nondegenerate** if $g(v, w) = 0$ for all $w \in T_pM$ implies $v = 0$;
(iii) **positive definite** if $g(v, v) > 0$ for all $v \in T_pM \setminus \{0\}$.

Constant Curvature Manifolds (CCM)





- S_K^n: $\{x \in \mathrm{R}^{\mathrm{n}}$: $x_1^2 + x_2^2$+…+ x_n^2=K (K>0)}
- Metric: Euclidean inner product
- $< x, y >_2 = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n$
- Positive curvature (K>0，1/K)

- H_K^n: $\{x \in \mathrm{R}^{\mathrm{n}}$: $-x_1^2 + x_2^2$+…+ x_n^2=K (K<0)}
- Metric: Lorentz (Minkowski) inner product
- $< x, y >_{\mathcal{L}} = -x_1 y_1 + x_2 y_2 + \cdots + x_n y_n$
- Negative curvature (K<0)