Hyperbolic Graph Representation Learning: A Tutorial

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Contents

1. INTRODUCTION

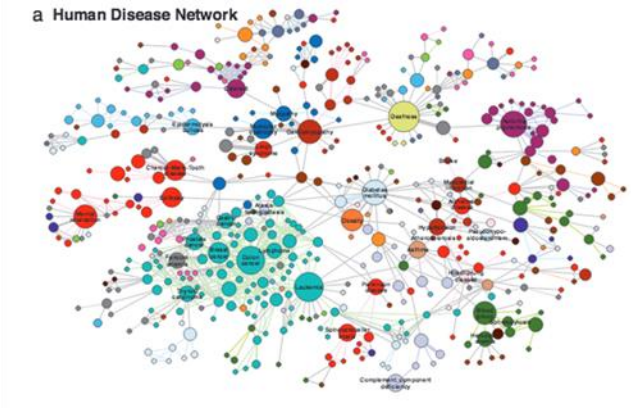
Contents

Graphs

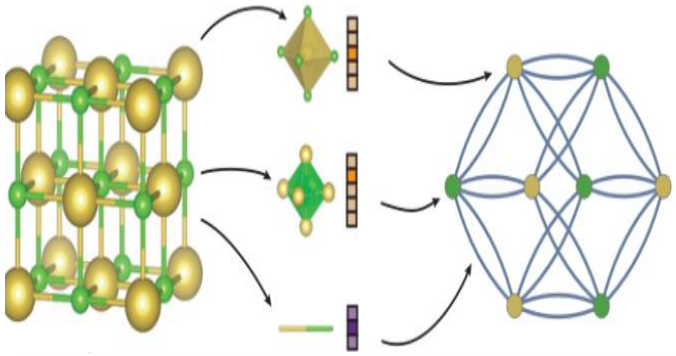
Data available in the form of graphs are ubiquitous.

Social networks

Biology network



Atom network

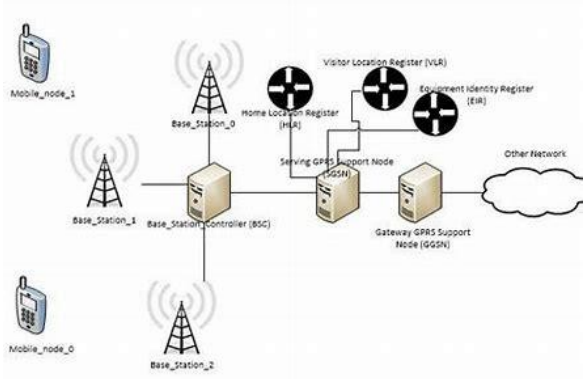


Financial networks

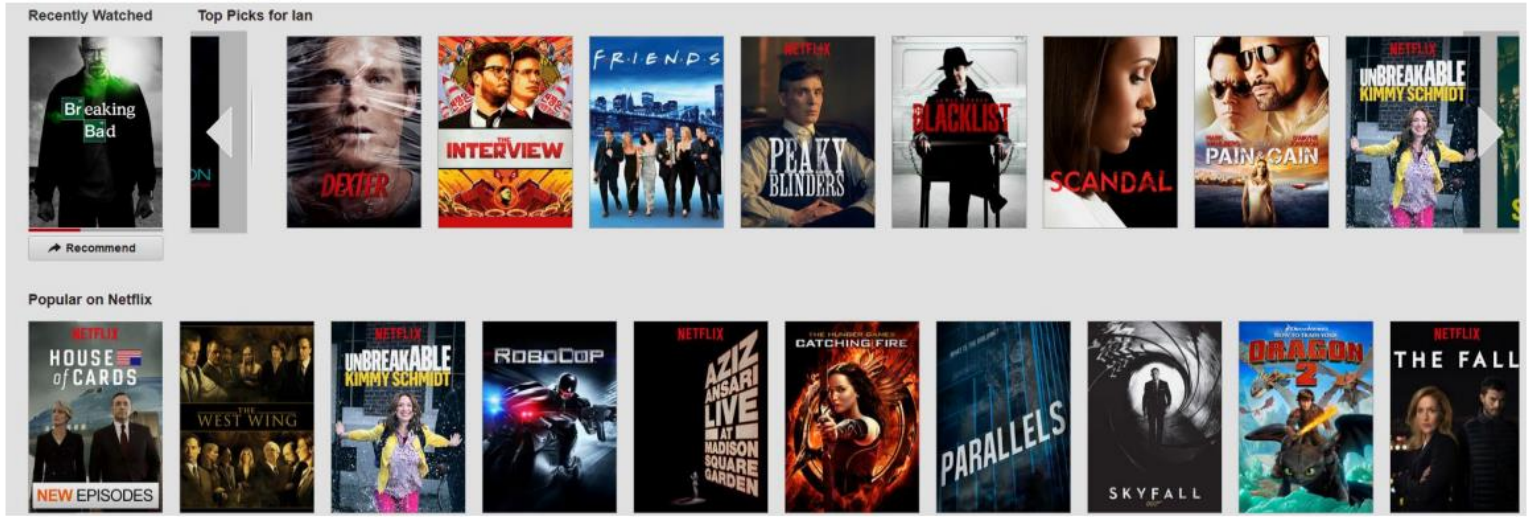
Source from Internet

Logistic networks

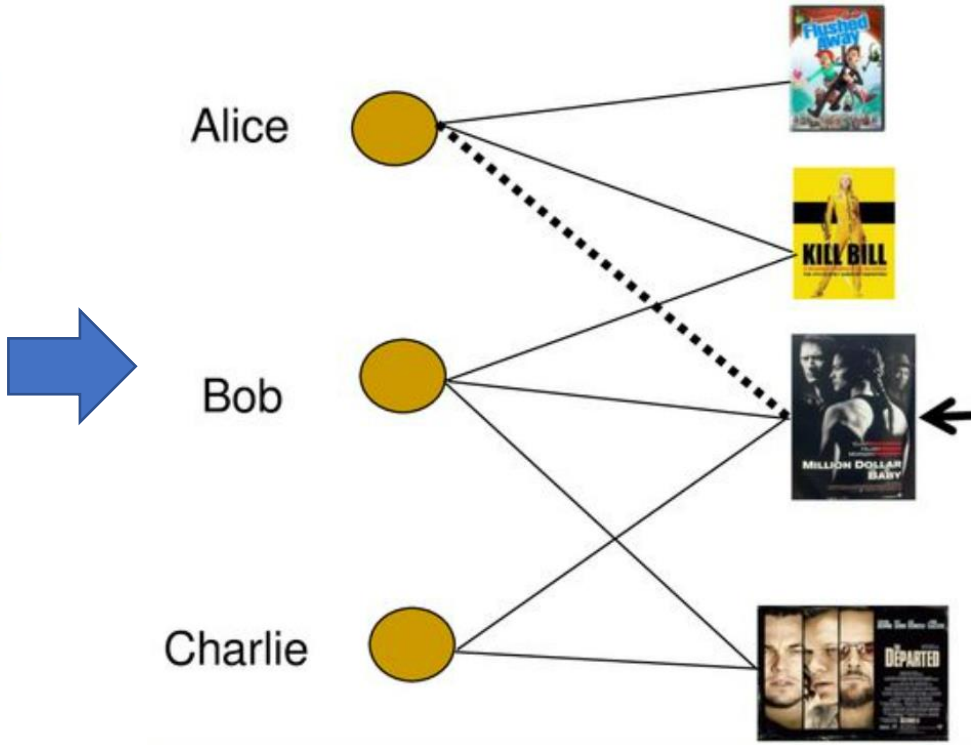
Telecom network



Recommender Systems

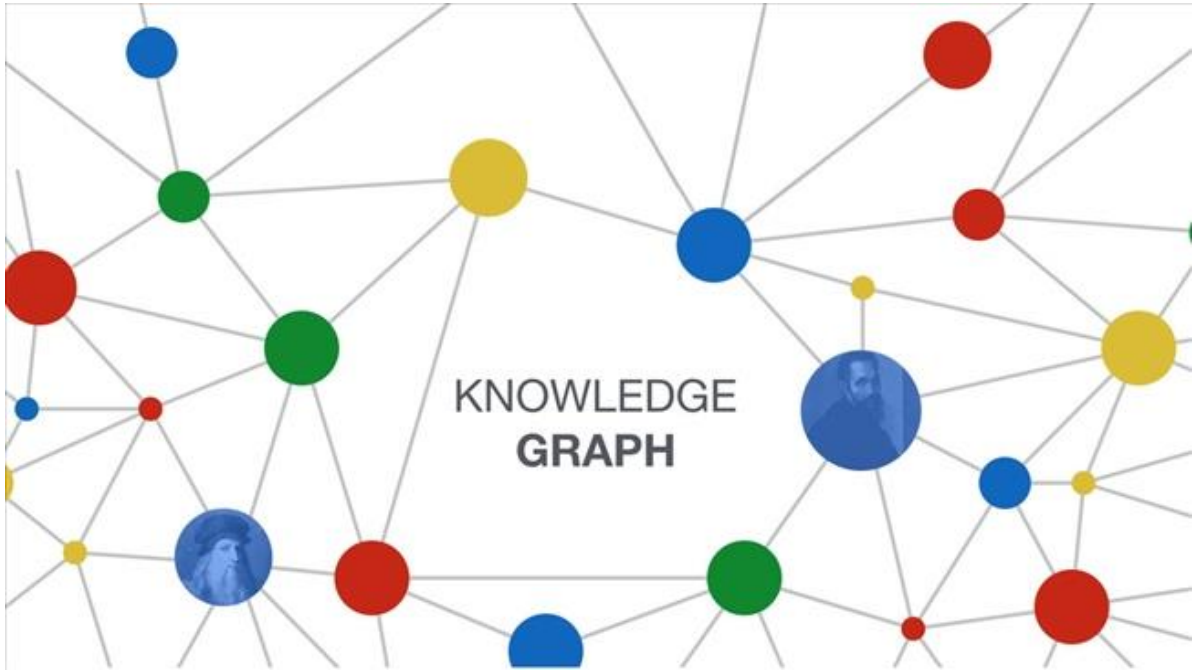


Link Prediction

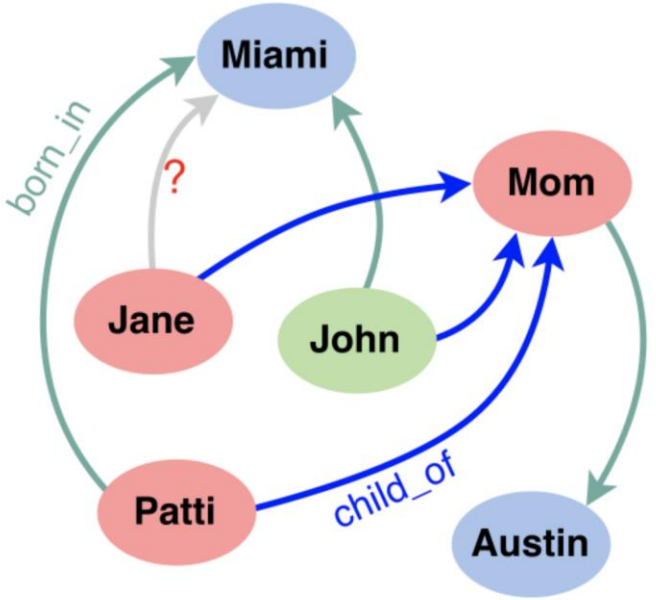


- Source from Internet

Knowledge Graph Completion

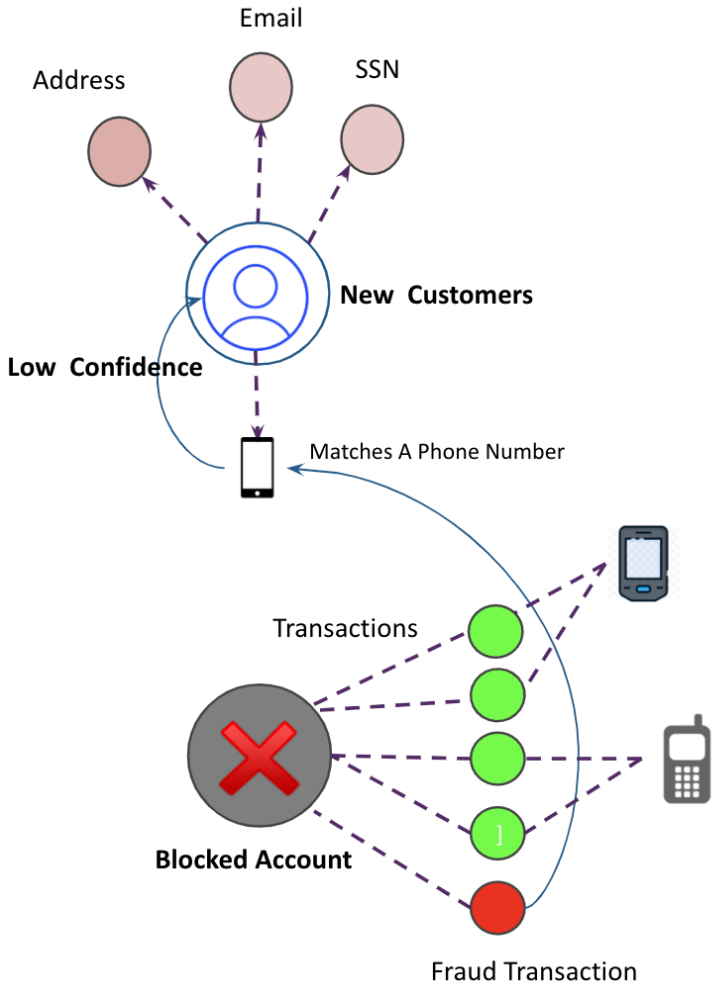


Link prediction

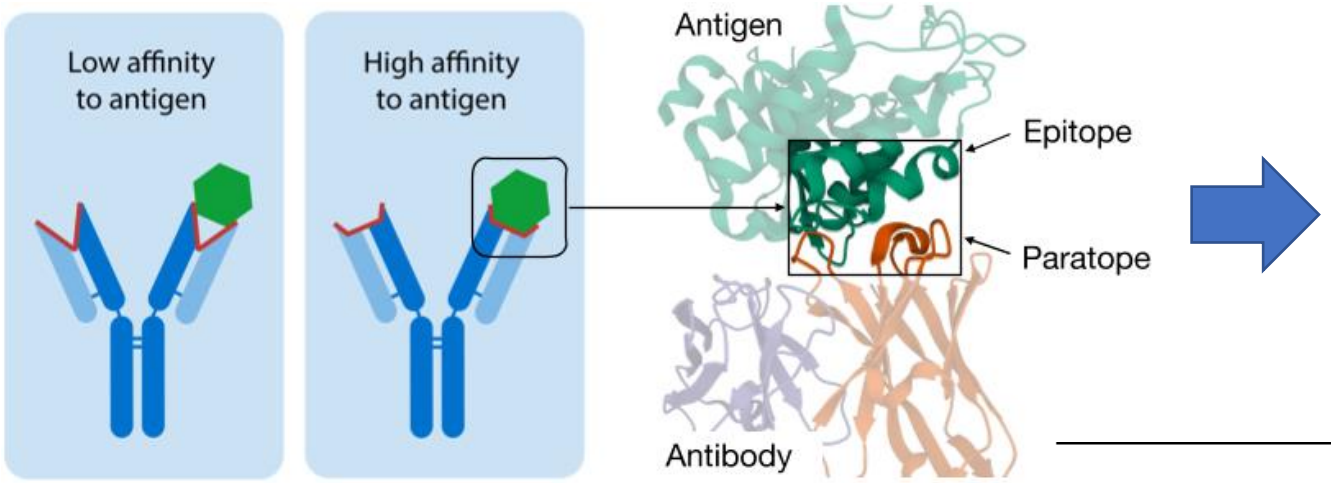


Fraud Detection

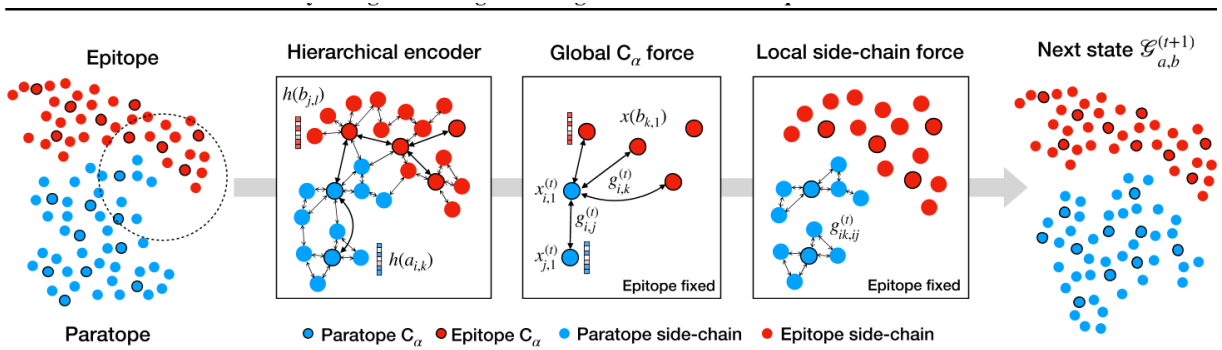
Link prediction, community detection, etc.



Antibody-Antigen Docking and Design



Graph Generation Task

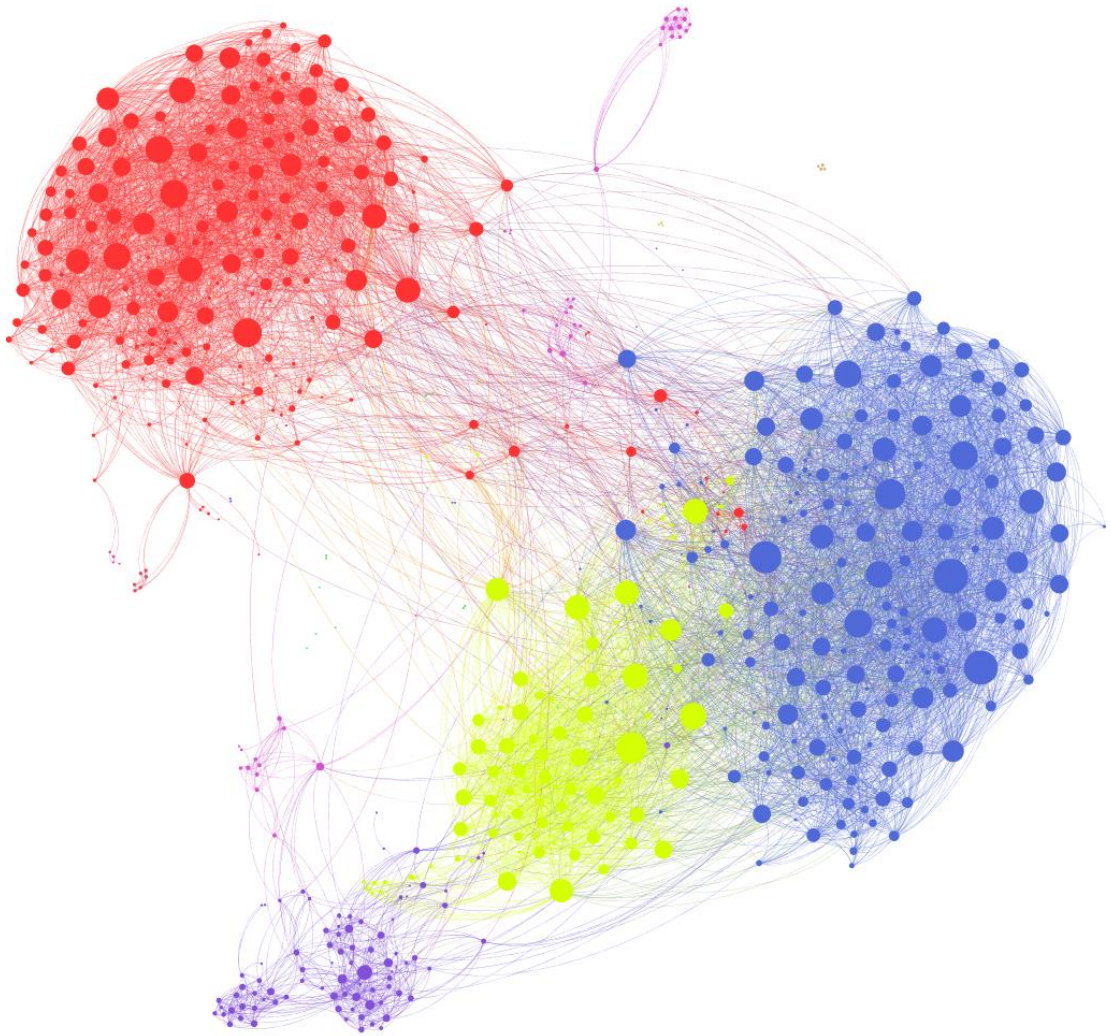


Jin W. et. al. Antibody-Antigen Docking and Design via Hierarchical Equivariant Refinement. ICML 2022

Graph Analysis and Learning

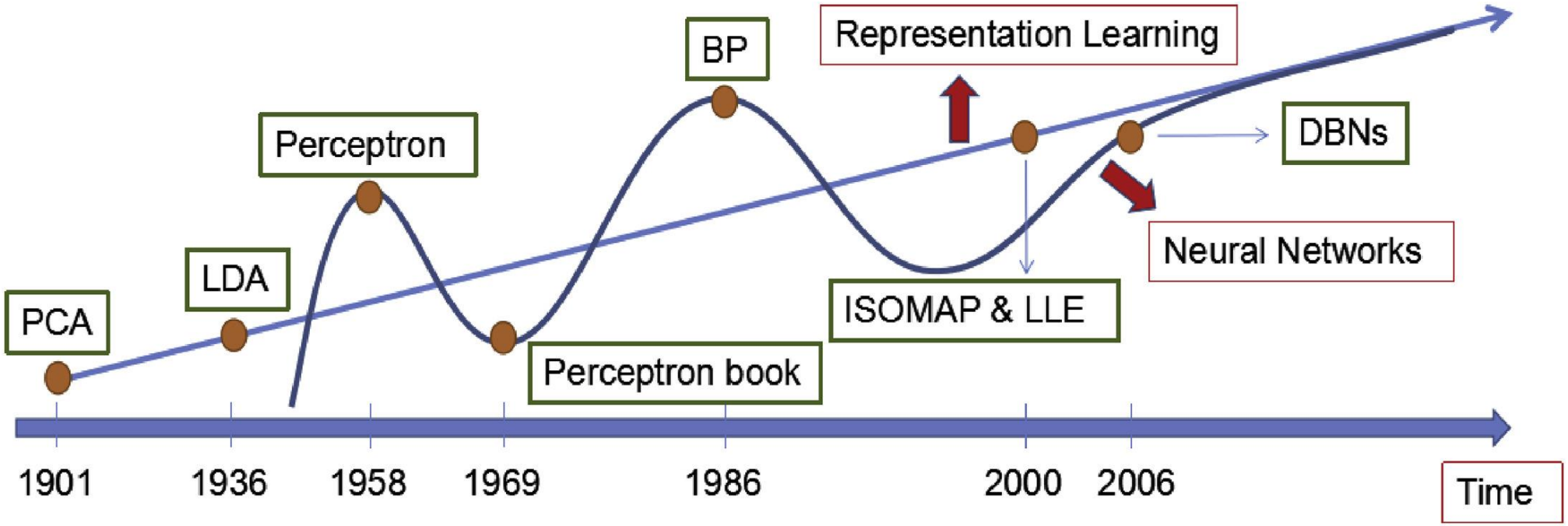
- Graph Analysis
  - Degree distribution
  - Graph diameter
  - Shortest path length
  - Sparseness
  - Curvature
  - Symmetry

- Representation Learning
  - Graph embedding
  - Graph neural network



Representation Learning

"Can we automate the learning of useful features from raw data?"



"*Deep learning algorithms seek to exploit the unknown structure in the input distribution in order to discover good representations, often at multiple levels, with higher-level learned features defined in terms of lower-level features*"

Yoshua Bengio

Representation Learning on Graph

Graph Embedding + Graph Neural Network

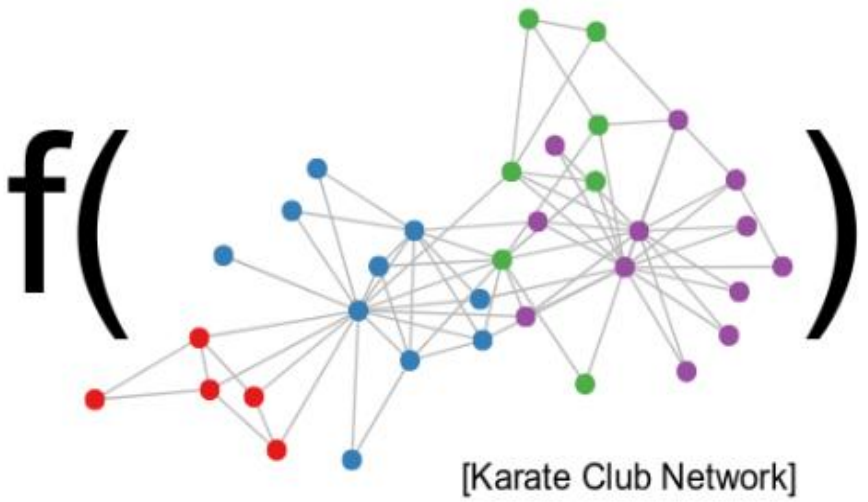
Representation Learning on Graph

Graph Embedding

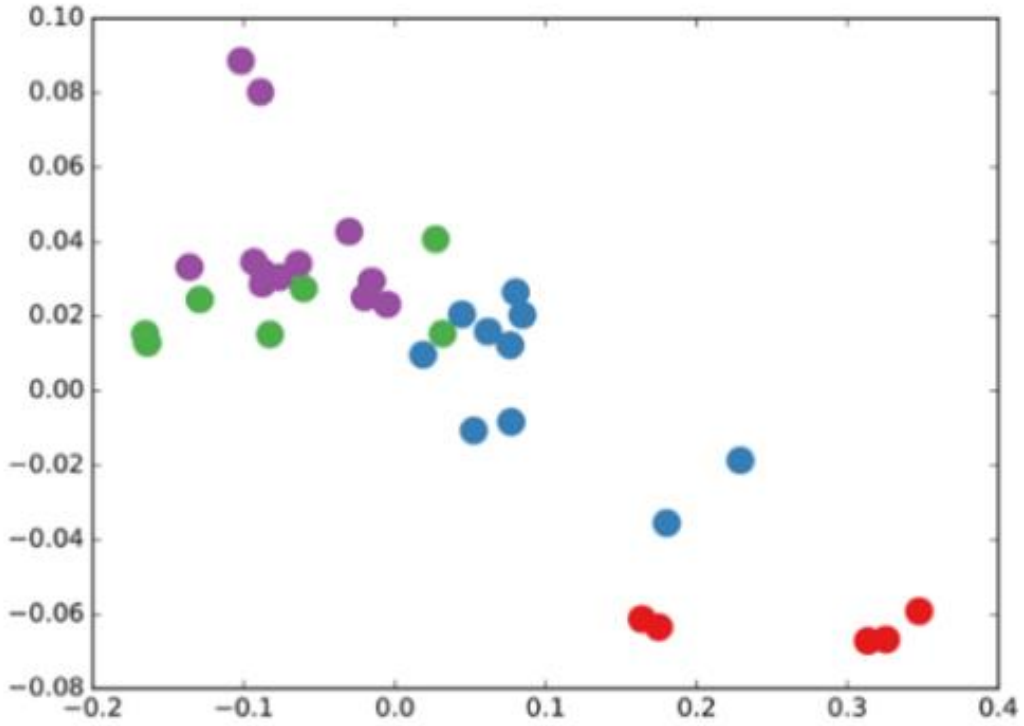
Graph Embedding

Projecting graph data into a continuum space while the graph properties are preserved.

G=(V,E)

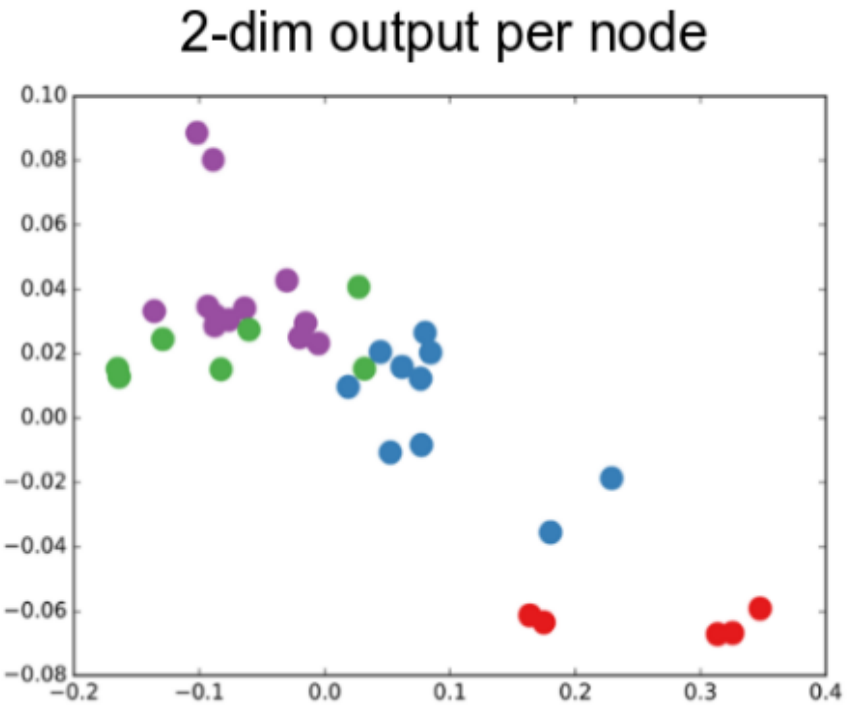


G=(V)
Vector



Graph Embedding

Goal: Perform network inference in the low-dimensional vector space



- Node importance
- Community detection
- Link prediction
- Node classification
- Network evolution
- ….

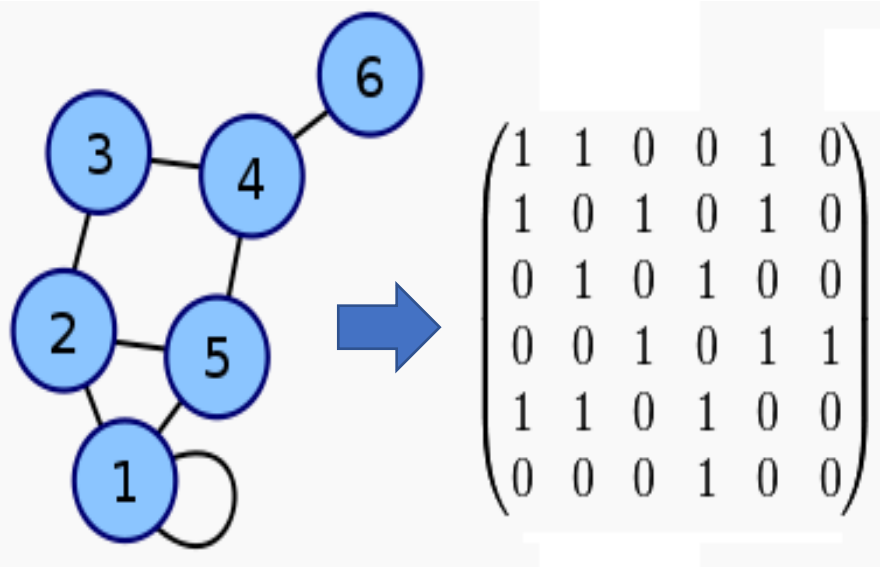
Graph vs Text

Adjacency List encoding of *edges* vs one-hot encoding of *text tokens*

Vocabulary:
Man, woman, boy, girl, prince, princess, queen, king, monarch

	1	2	3	4	5	6	7	8	9
man	1	0	0	0	0	0	0	0	0
woman	0	1	0	0	0	0	0	0	0
boy	0	0	1	0	0	0	0	0	0
girl	0	0	0	1	0	0	0	0	0
prince	0	0	0	0	1	0	0	0	0
princess	0	0	0	0	0	1	0	0	0
queen	0	0	0	0	0	0	1	0	0
king	0	0	0	0	0	0	0	1	0
monarch	0	0	0	0	0	0	0	0	1

Each word gets a 1x9 vector representation



Representing Text

Learns a vector representation for each word that maximized the probability of that word given the previous word.

Input: one hot encoded vector

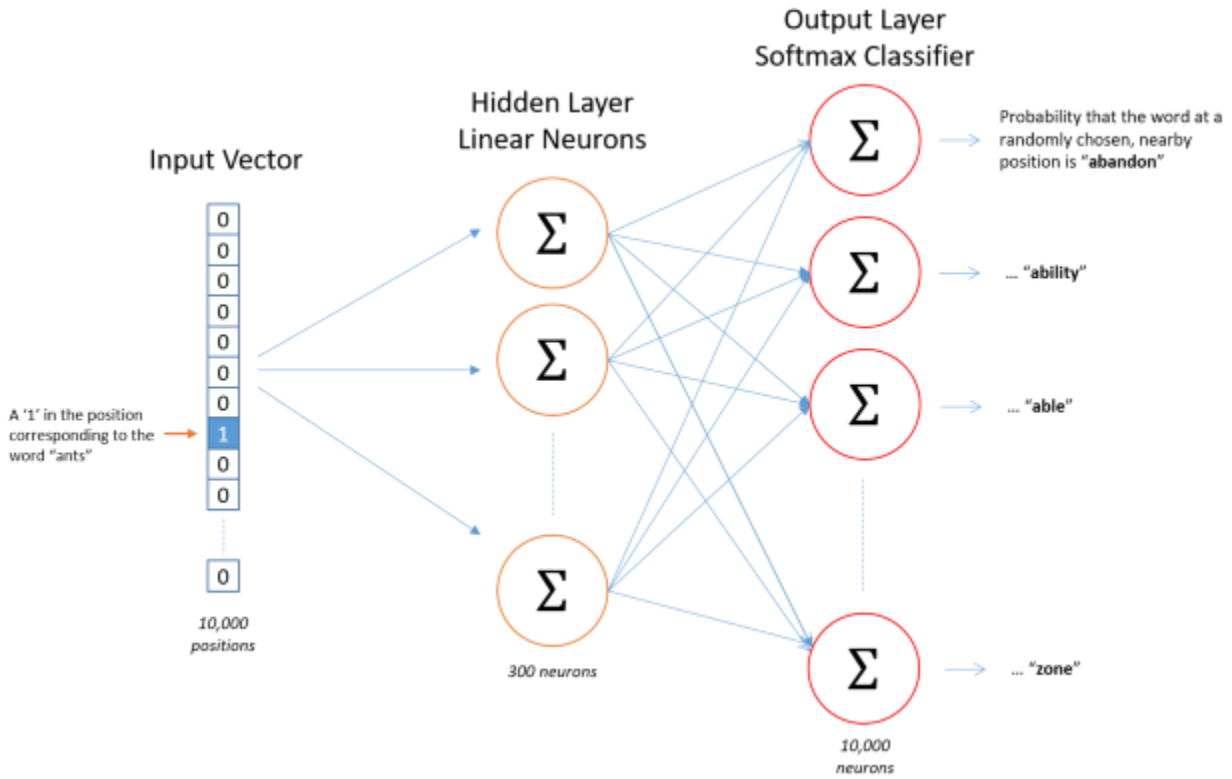


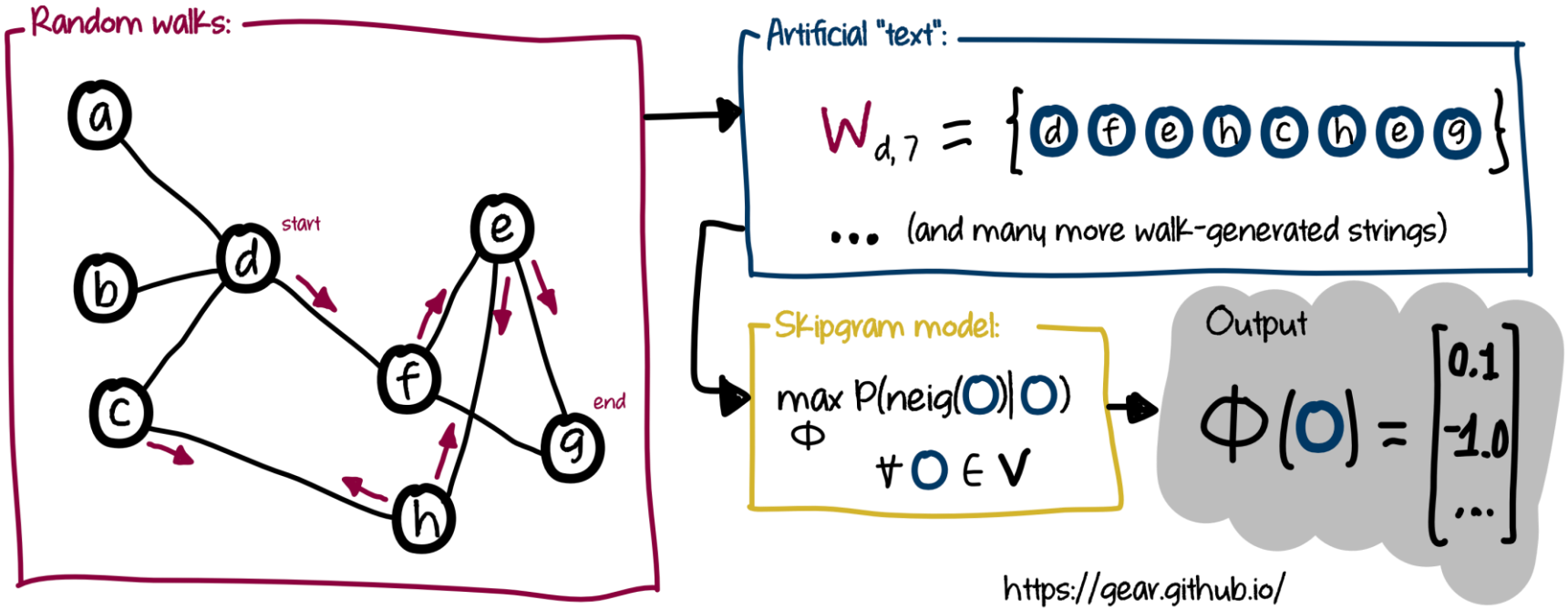
Illustration of SkipGram

Output: probability for each word in the corpus

https://towardsdatascience.com/word2vec-skip-gram-model-part-1-intuition-78614e4d6e0b

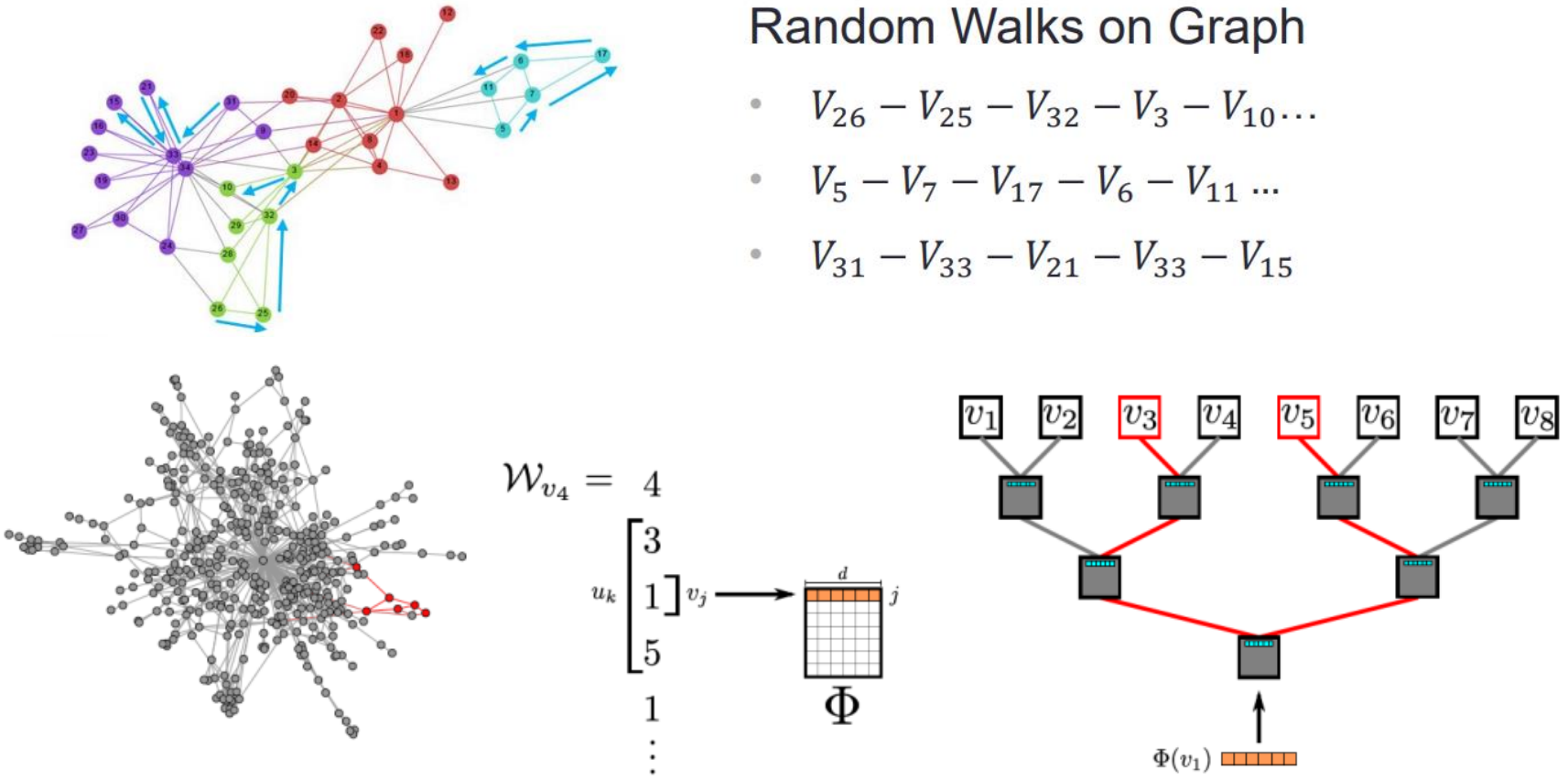
Representing Graph

- How should we represent a node in a graph mathematically?
- Can we mimic word embedding?
  - Treat each node treat as a word
  - Neighborhood around the node as the context window



Deep Walk

- Exploit truncated random walks to define neighborhoods of a node

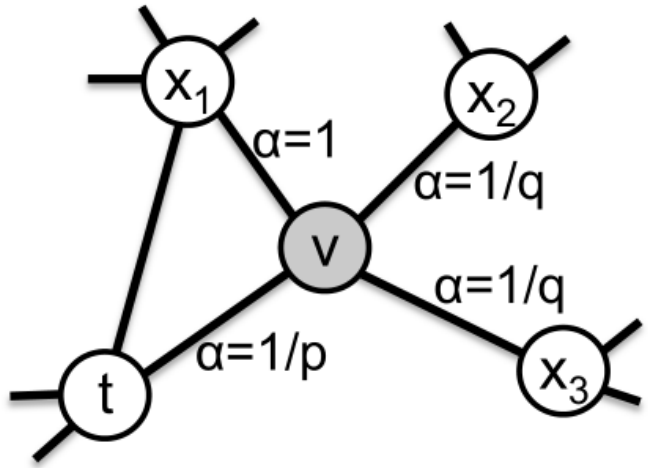


(a) Random walk generation. (b) Representation mapping. (c) Hierarchical Softmax.

B. Perozzi et al. Deepwalk: Online learning of social representations. KDD 2014

Node2vec

- Generate representations of nodes in the graph via 2nd order (biased) random walk.



- Apply a bias factor alpha to reweigh the edge weights depending on the previous state

$$\alpha_{pq}(t,x) = \begin{cases} \frac{1}{p} & \text{if } d_{tx} = 0 \\ 1 & \text{if } d_{tx} = 1 \\ \frac{1}{q} & \text{if } d_{tx} = 2 \end{cases}$$

- Second order transition probability:

$$p(u|v,t) = \frac{\alpha_{pq}(t,u)w(u,v)}{\sum_{u' \in \mathcal{N}_v} \alpha_{pq}(t,u')w(u',v)}$$

Grover, Aditya, and Jure Leskovec. "node2vec: Scalable feature learning for networks." KDD 2016

Graph Embedding Summary

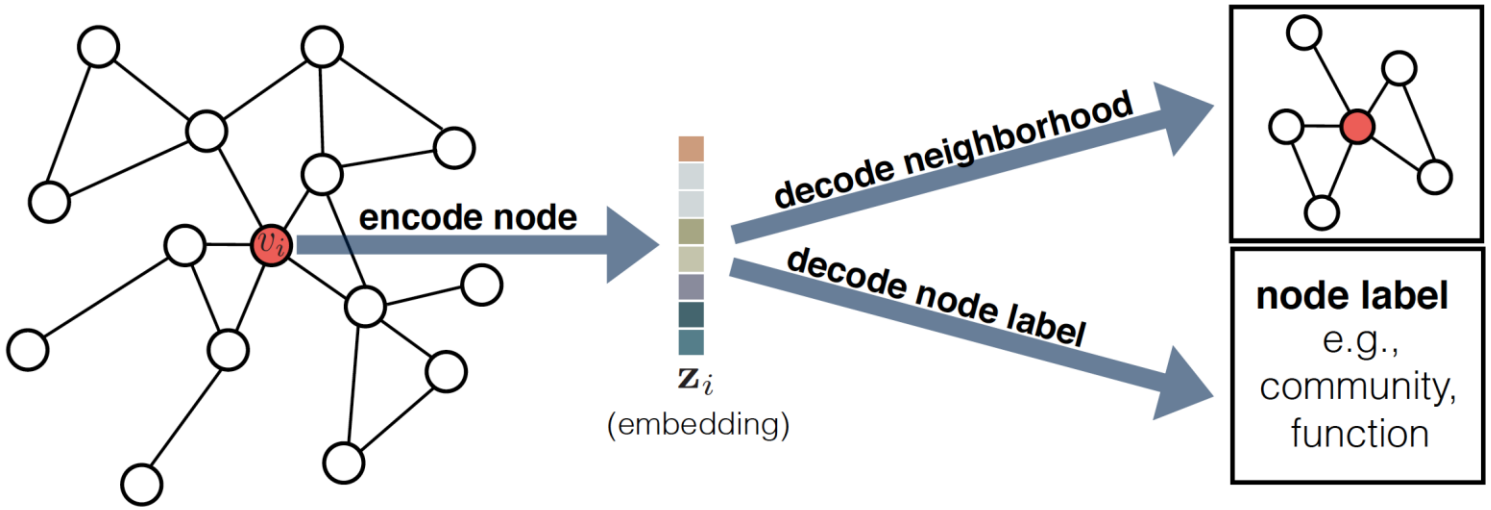
- Many different methods:
  - Matrix Factorization
  - Random walk
  - Others

Category	Year	Published	Method	Time Complexity	Properties preserved
Factorization	2000	Science[26]	LLE	$O(\|E\|d^2)$	1^{st} order proximity
	2001	NIPS[25]	Laplacian Eigenmaps	$O(\|E\|d^2)$	
	2013	WWW[21]	Graph Factorization	$O(\|E\|d)$	
	2015	CIKM[27]	GraRep	$O(\|V\|^3)$	$1 - k^{th}$ order proximities
	2016	KDD[24]	HOPE	$O(\|E\|d^2)$	
Random Walk	2014	KDD[28]	DeepWalk	$O(\|V\|d)$	
	2016	KDD[29]	*node2vec*	$O(\|V\|d)$	$1 - k^{th}$ order proximities, structural equivalence

Hamilton, W. L. et.al. Representation Learning on Graphs: Methods and Applications. 2017

Graph Embedding Summary

- Most techniques consist of:

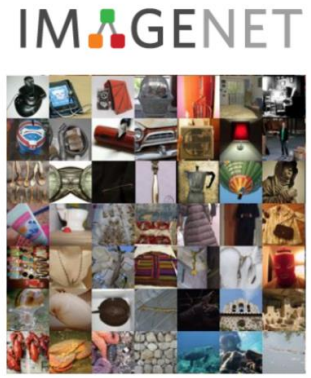


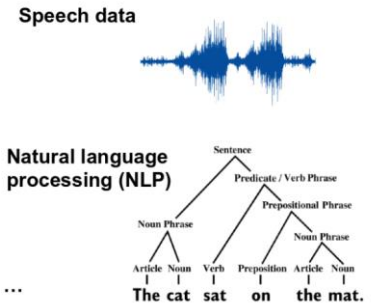
- A pairwise similarity function measures the similarity between nodes
- An encoder function to generate the node embedding
- A decoder function to reconstruct pairwise similarity
- A loss function to measure the quality of the pairwise reconstructions

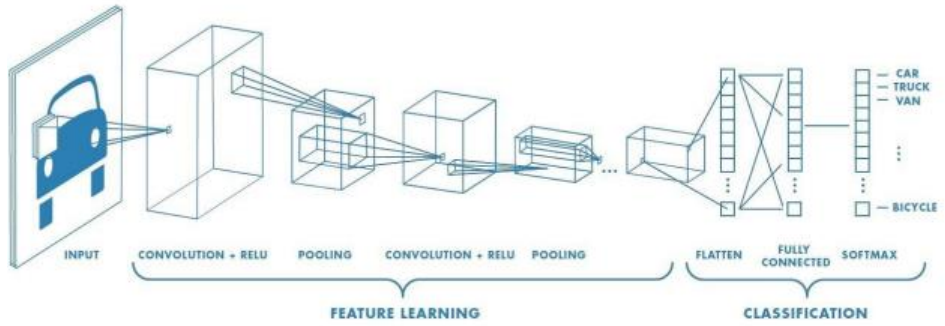
Hamilton, W. L. et.al. Representation Learning on Graphs: Methods and Applications. 2017

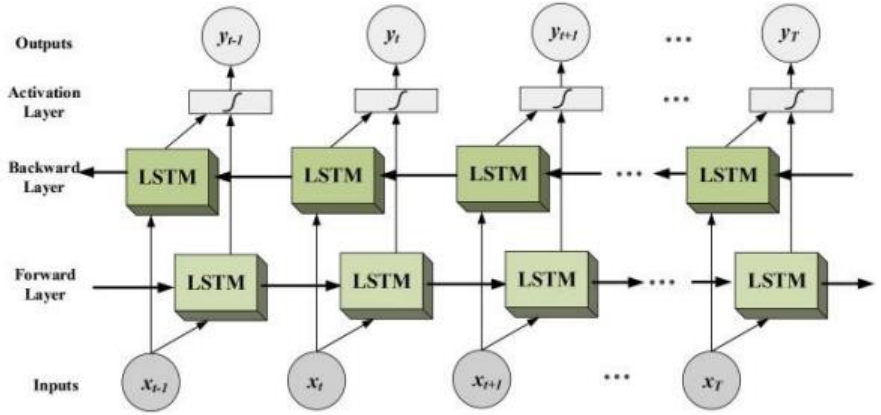
Graph Neural Network

Graph Neural Network

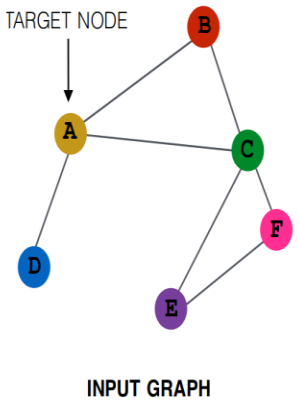


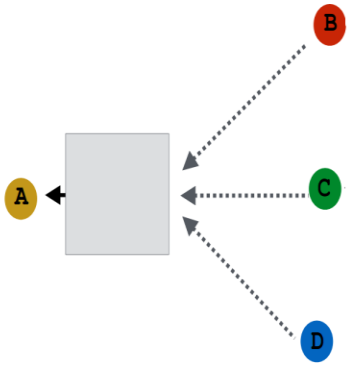






Graph Neural Network

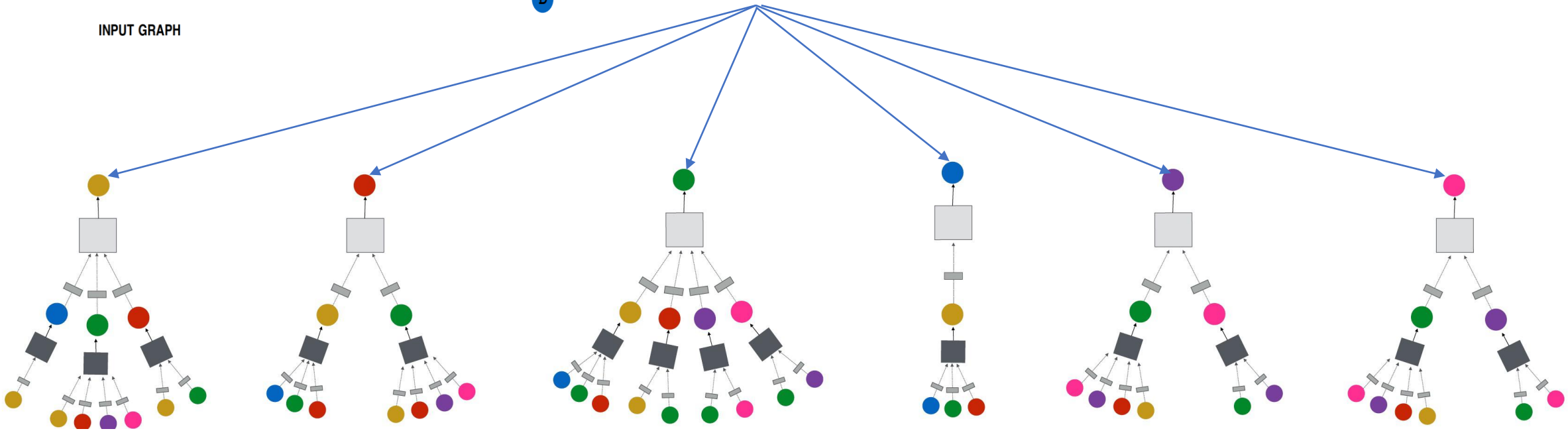




a. Neighborhood aggregation
b. Information propagation

$$H^{(l+1)} = f(H^{(l)}, A)$$

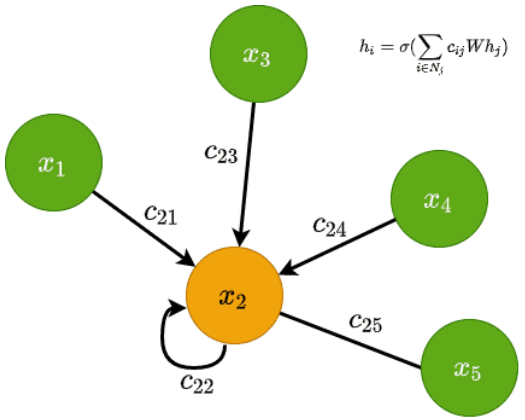
Every node defines a computation graph

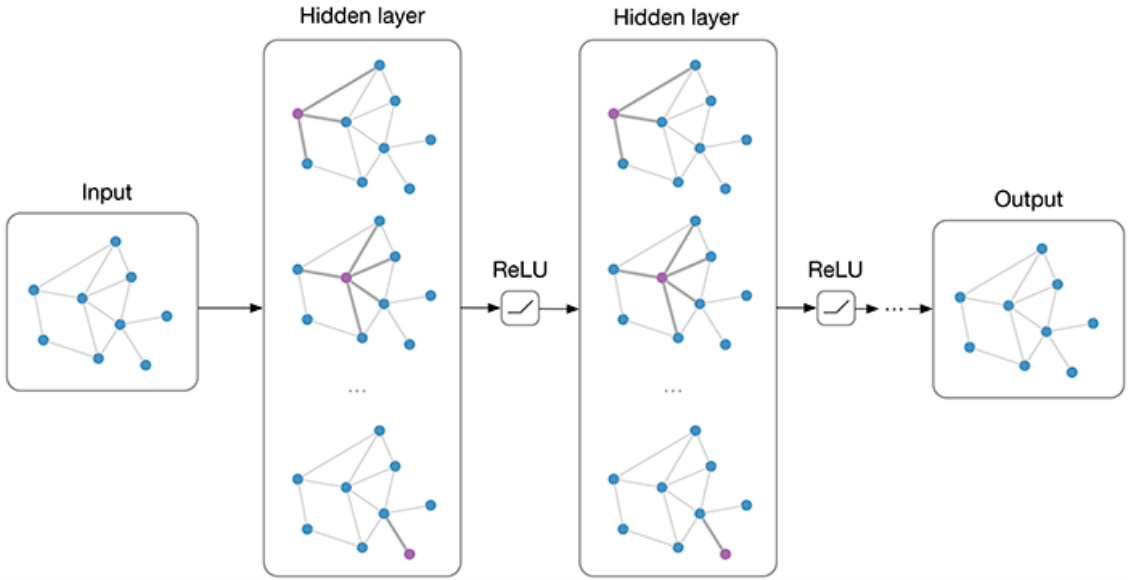


GCN

- Deal with the representation of a graph in the spectral domain
- Aggregate info from neighborhood via the normalized Laplacian matrix

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)})$$





- Spectral method & Transductive learning
  - Easy to apply
  - Conduct on the entire graph and computationally inefficient

T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. ICLR, 2017.

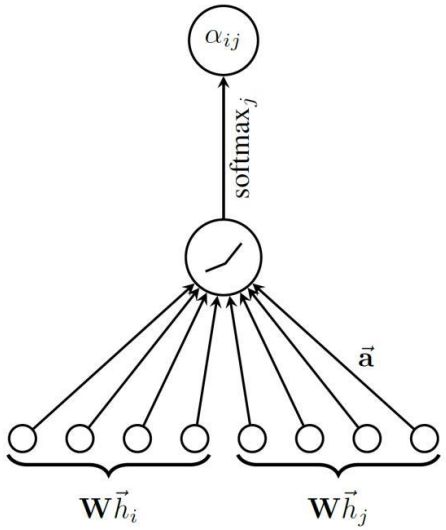
GAT

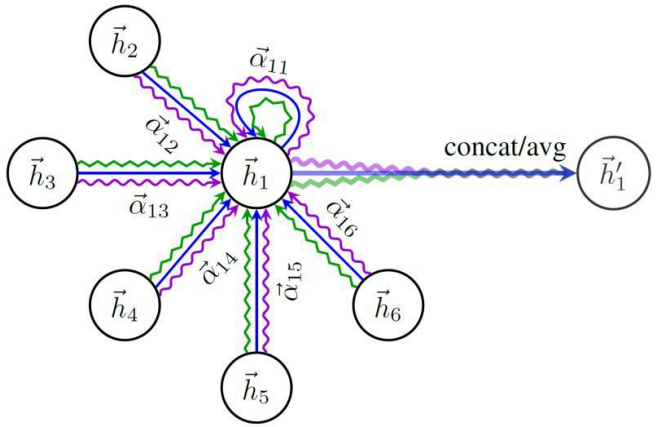
- Aggregate info from neighborhood via attention mechanism

$$a_{ij} = attention(h_i, h_j)$$

$$a_{ij} = \frac{exp(a_{ij})}{\sum_{k \in N_i} exp(a_{ik})}$$

$$h_i^{(l)} = \sigma(\sum_{i \in N_j} a_{ij} W h_j)$$



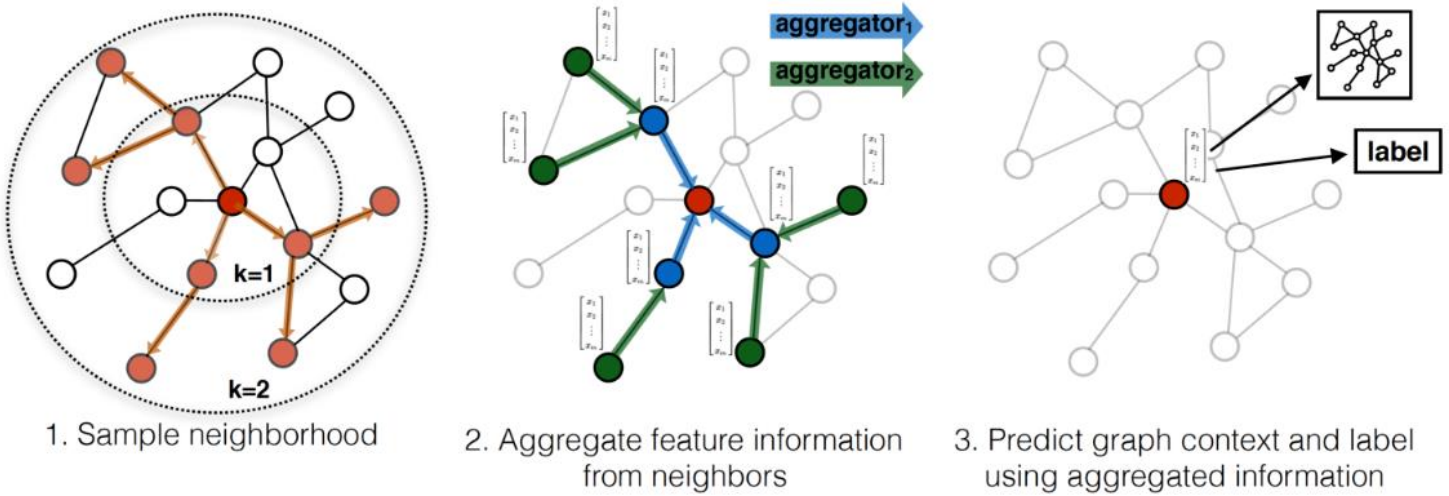


- Spatial method
- More flexible to handle multisource graph inputs

Veličković, Petar, et al. "Graph Attention Networks." ICLR. 2018.

GraphSAGE

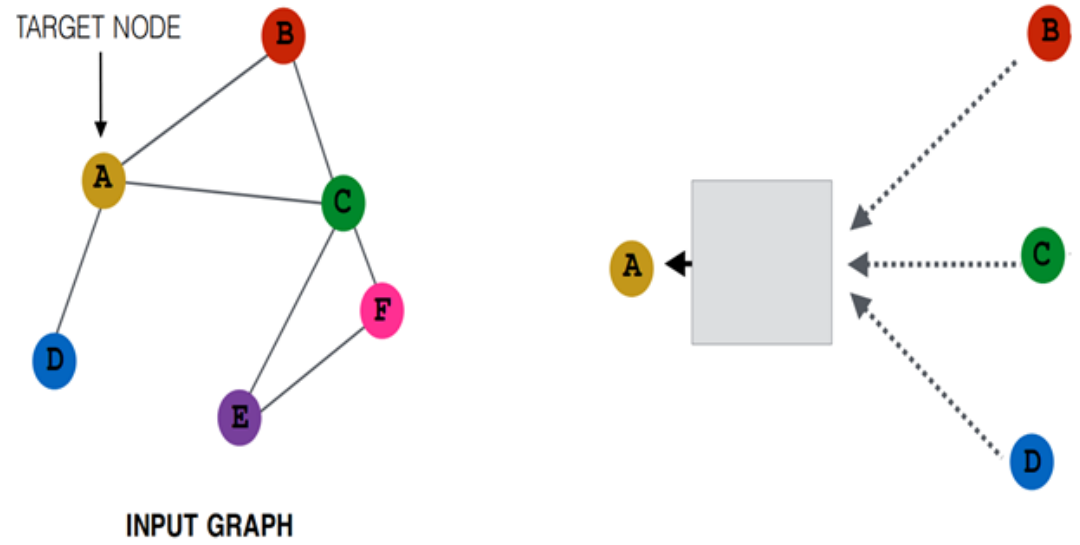
- Sample a subset of node to conduct propagation
- Generalized aggregation: any differentiable function that maps set of vectors to a single vector



- Spatial method with inductive capability

T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. ICLR, 2017.

Summary of GNNs

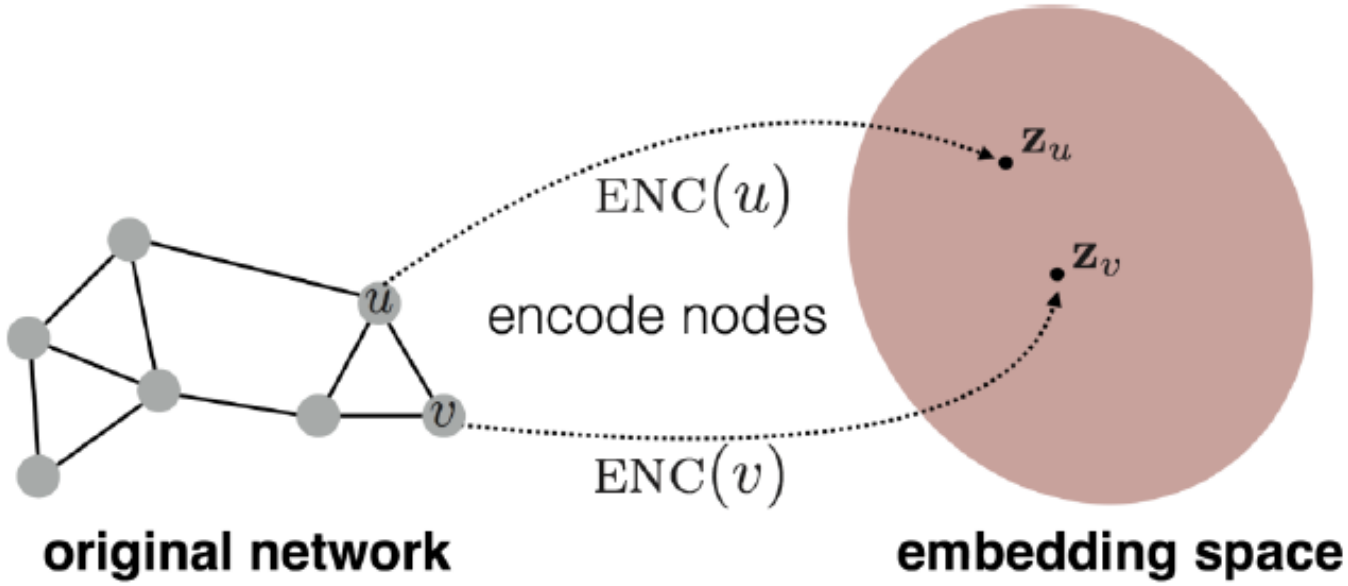


- Characteristics of GNNs
  - Information aggregation and prorogation
  - Trained via end-to-end manner according to downstream task
    - Supervised or semi-supervised
  - Utilize graph structure and node features simultaneously

Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www, WWW 2018

Pipeline for Graph Learning

- **Step 1:** Obtain edge or/and node information , possibly with some augmentation
- **Step 2**: Use a parameterized encoder to map nodes in the graph(s) to an embedding space
- **Step 3**: Make predictions on nodes, edges or graphs based on embeddings
- **Step 4**: Compute loss and optimize the parameters

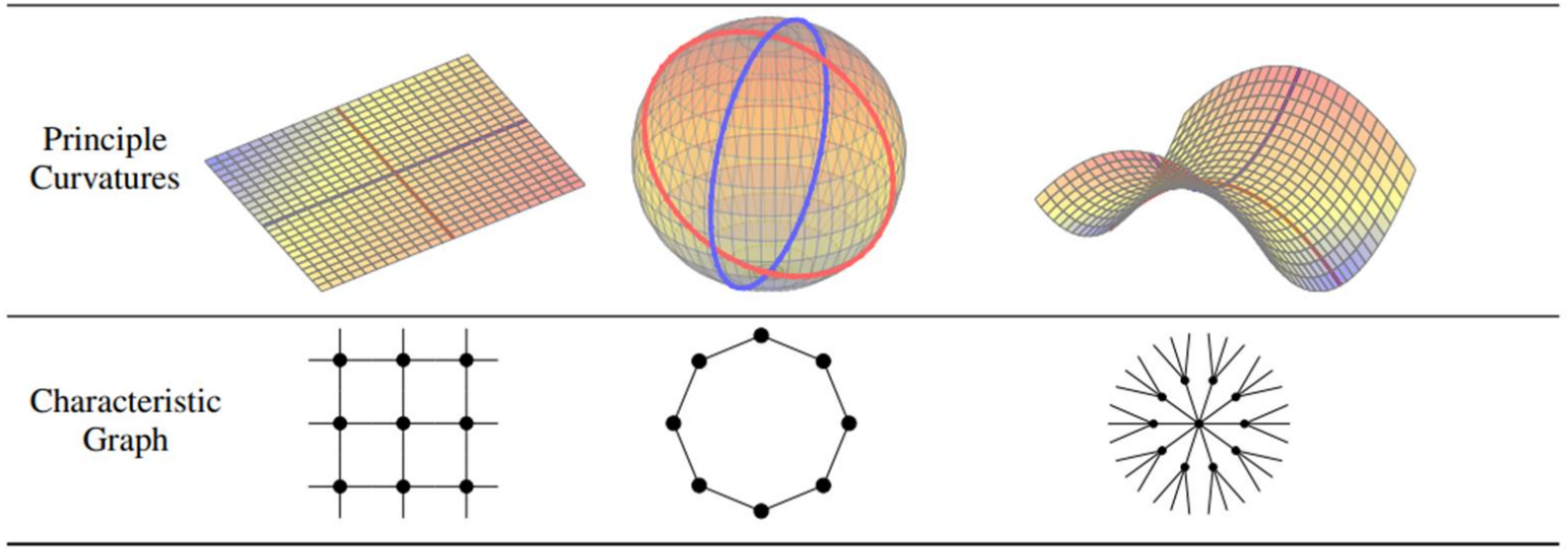


- Graph G = (V, E)
- V: Node set,
- E: Edge set
- f_G: Mapping function
- Z: Node embedding

Rex Ying. Introduction on Graph Representation Learning: A Geometric Perspective. 2022

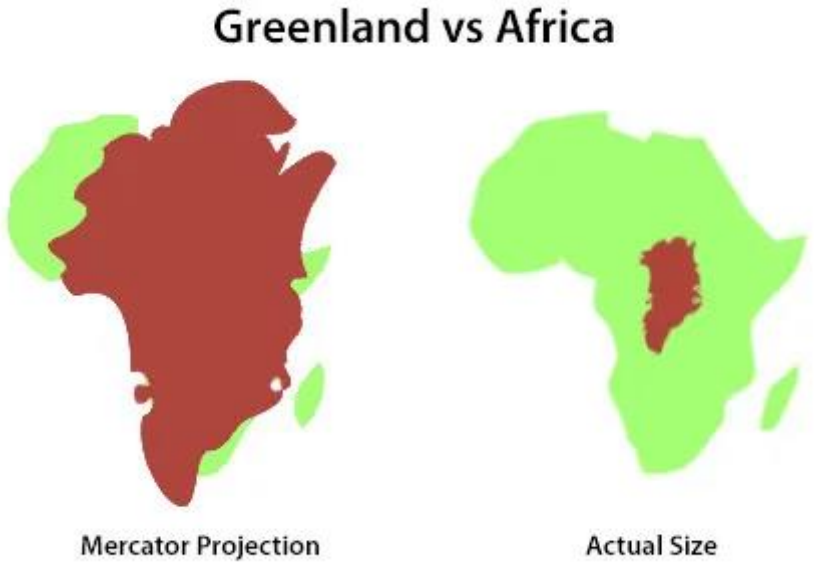
Where to Learn Graphs?

- The quality of embeddings crucially depends on whether the geometry of the learning space matches the dataset.
- What embedding space geometry is optimal for data?



Curvature and Representation Learning: Identifying Embedding Spaces for Relational Data

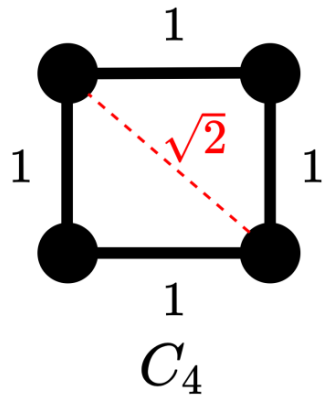
Constraints of Euclidean Geometry



- Many times, we have data lies on non-Euclidean manifold

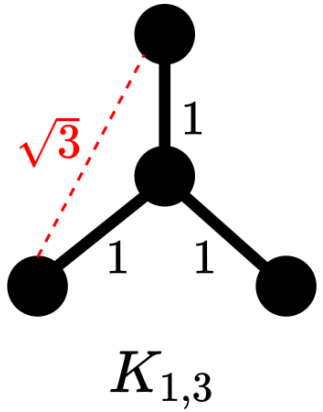
Constraints of Euclidean Geometry

- Cannot embed large classes of graph w/ low distortion or w/o loss of information
  - E.g. cycles, trees



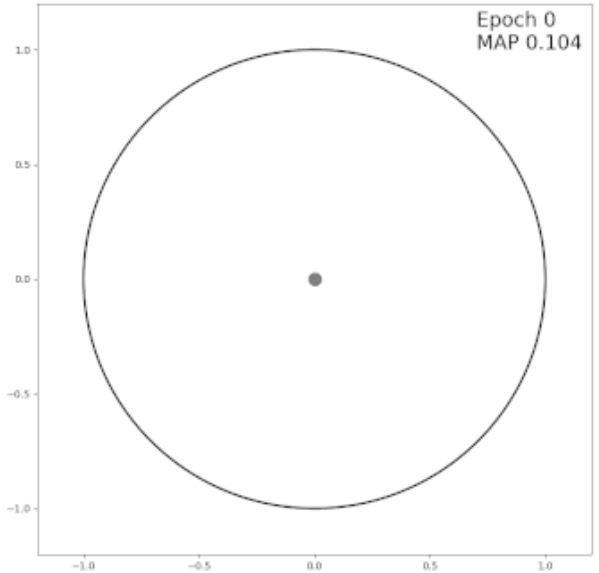
C_4

Distortion $\sqrt{2}$



$K_{1,3}$

Distortion $^{2}/_{\sqrt{3}}$

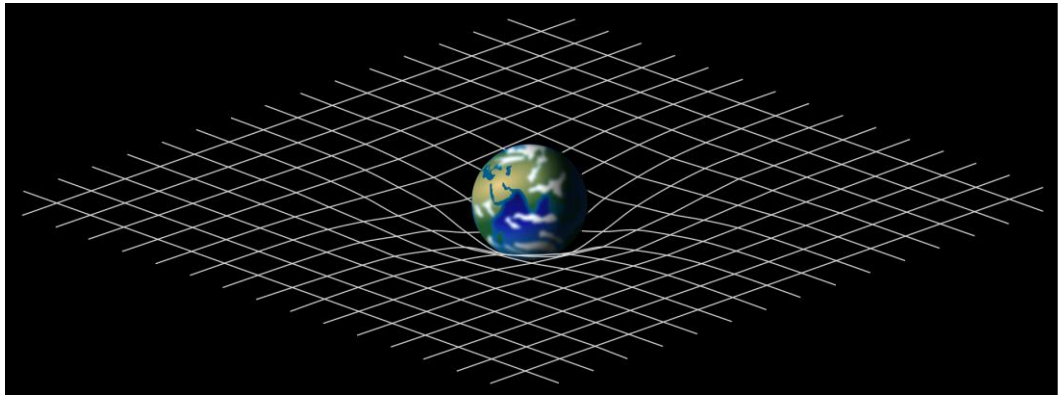


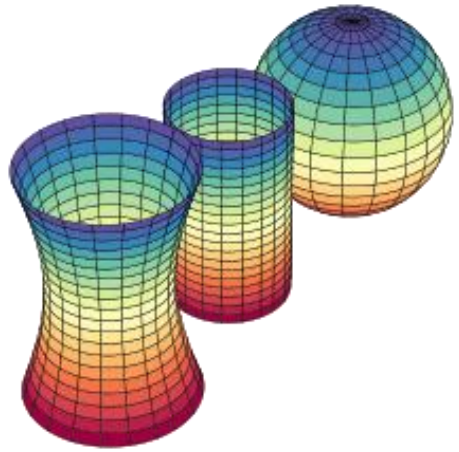
- Graph distance $d_G(i,j)$= "shortest path from i to j"

https://people.csail.mit.edu/oct/ctgnn_slides.pdf

Riemannian Geometry

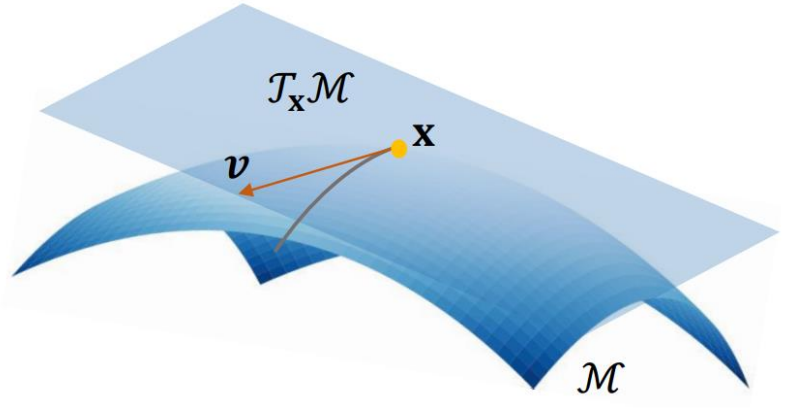
- Manifolds: high dimensional surface that looks locally-Euclidean
- Riemannian Manifold
  - Equipped with
    - *Inner product* $\langle .,. \rangle$: metric space
    - *Tangent space* $\mathcal{T}_x$: an $\mathbb{R}^n$ that approximates the manifold at any point x
  - Curvature: how much the surface deviates from being a plane
  - Geodesic: shortest path in manifold
    - Analogous to straight lines in $\mathbb{R}^n$





Tangent Spaces

- Tangent Space:
  - T_pM= space of speed vectors of all curves that go through a point x on the manifold
  - A vector space with the same dimension as the manifold

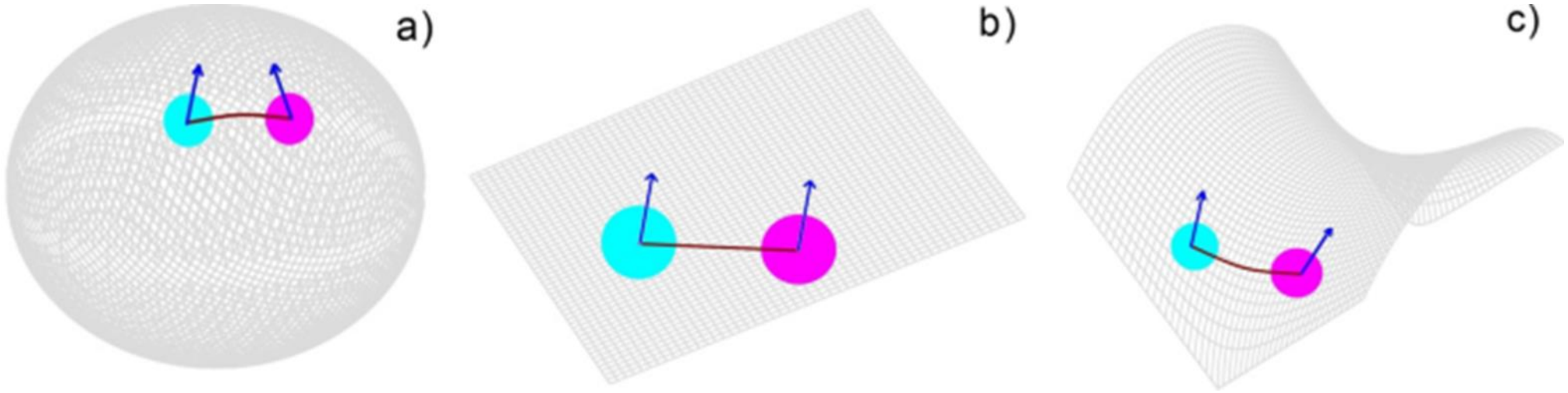


- *Exp* & *Log* Maps:
  - $exp_p: T_pM \rightarrow M$
  - $log_p: M \rightarrow T_pM$

(1) Map to tangent space
(2) Solve problem in the tangent space
(3) Map back to the manifold

Curvature

- A geometric property: Flatness of an object
- Geometric intuition: Measure for growth rate of volume of distance ball→ "geodesic dispersion"



Positive Curvature

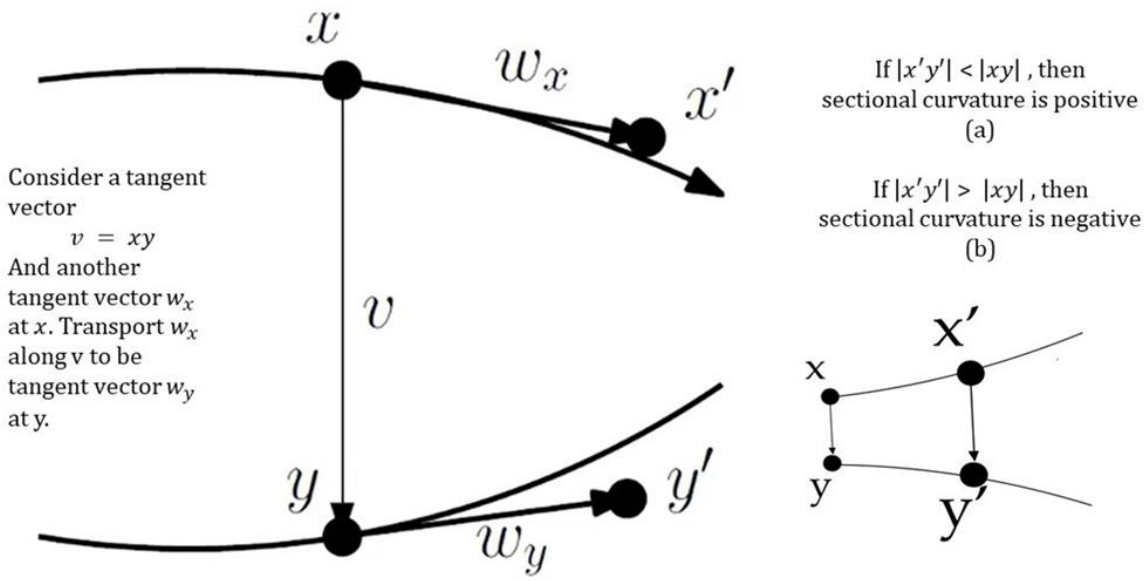
Flat Curvature

Negative Curvature

Eidi M, Jost J. Ollivier ricci curvature of directed hypergraphs[J]. Scientific Reports, 2020, 10(1): 1-14

Sectional Curvature & Ricci Curvature

- Consider a tangent vector $v = xy$ and another tangent vector w_x at x. Transport w_x along v to be a tangent vector w_x at y.

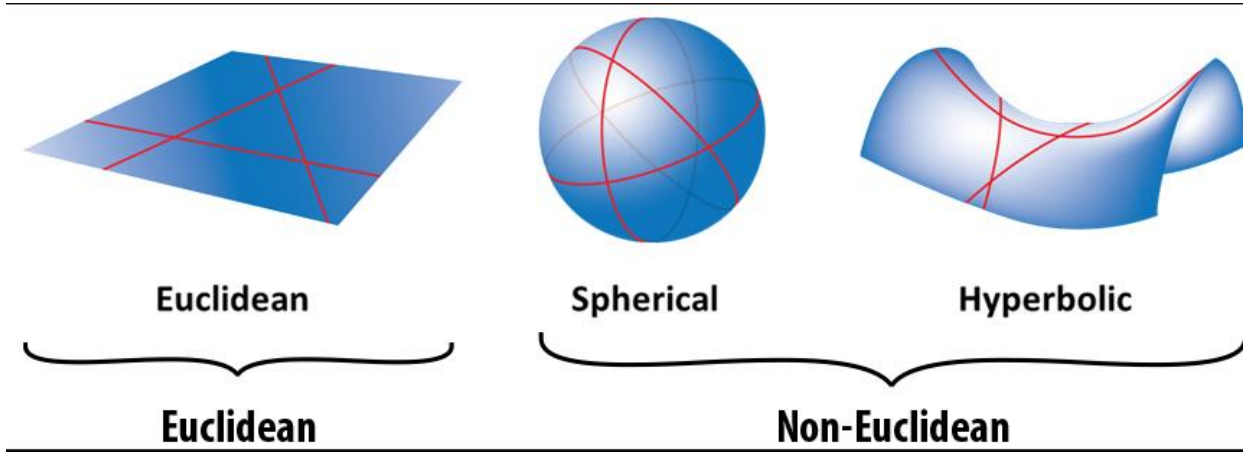


- Ricci Curvature: averaging over all directions w

Ni, Chien-Chun, et al. "Ricci curvature of the internet topology." *2015 IEEE conference on computer communications (INFOCOM)*. IEEE, 2015.

Geodesic Distance

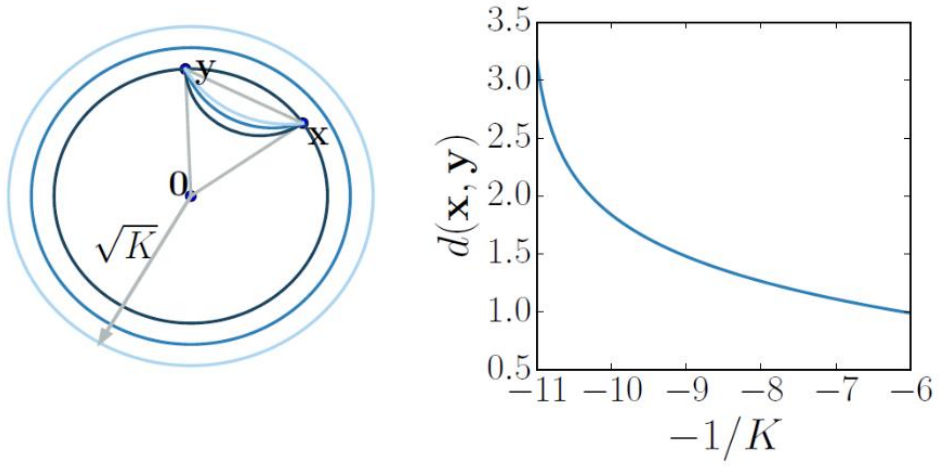
- Geodesic: Shortest path in the manifold



http://drmarkliu.com/noneuclidean

Geodesic Distance

- The more negative the curvature:
  - The more geodesic bends inward
  - Distance between two given points also increases

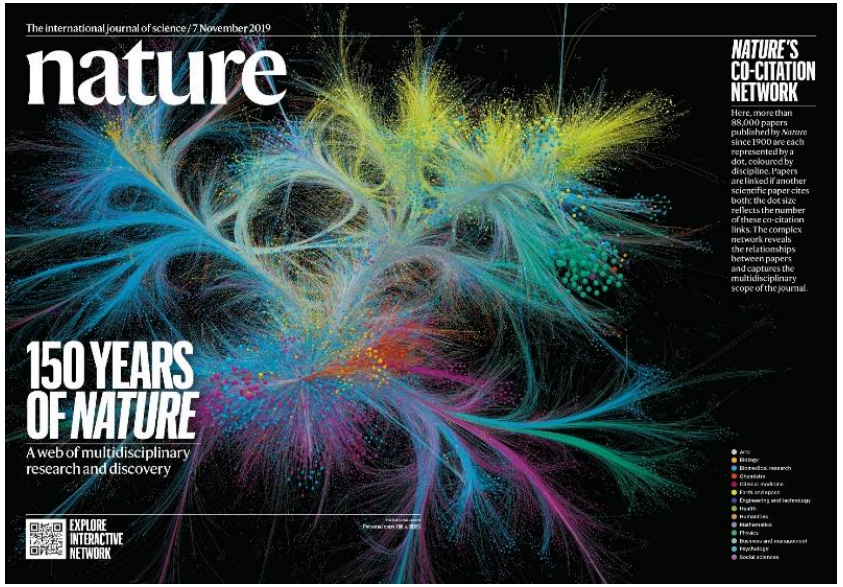


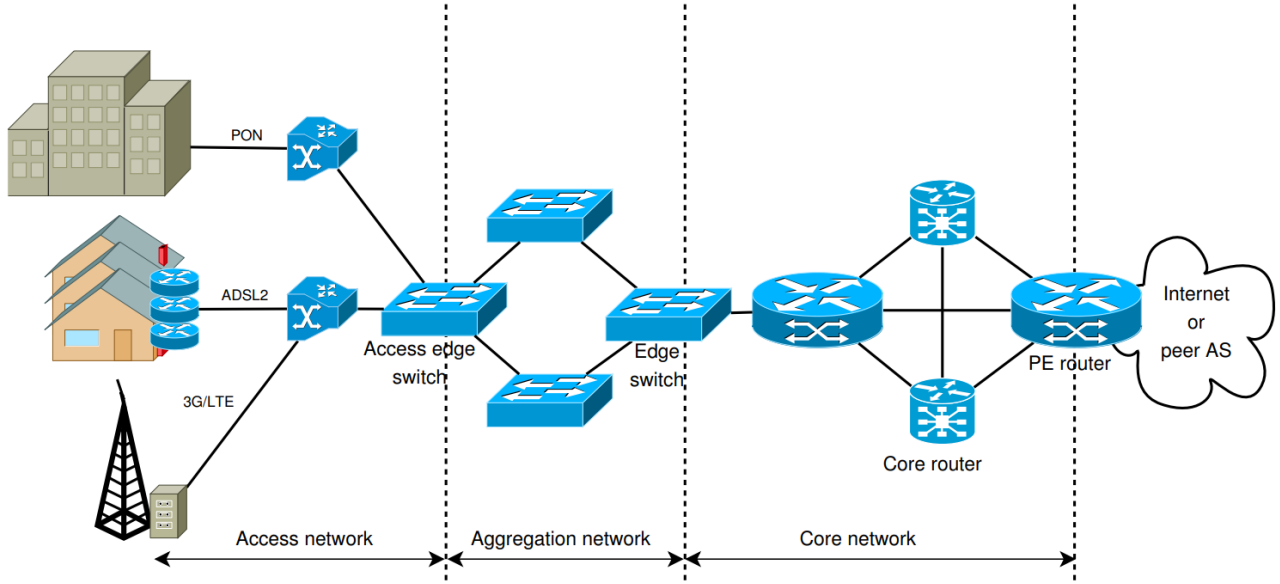
Dark blue: high curvature boundary and geodesics
Light blue: low curvature boundary and geodesics

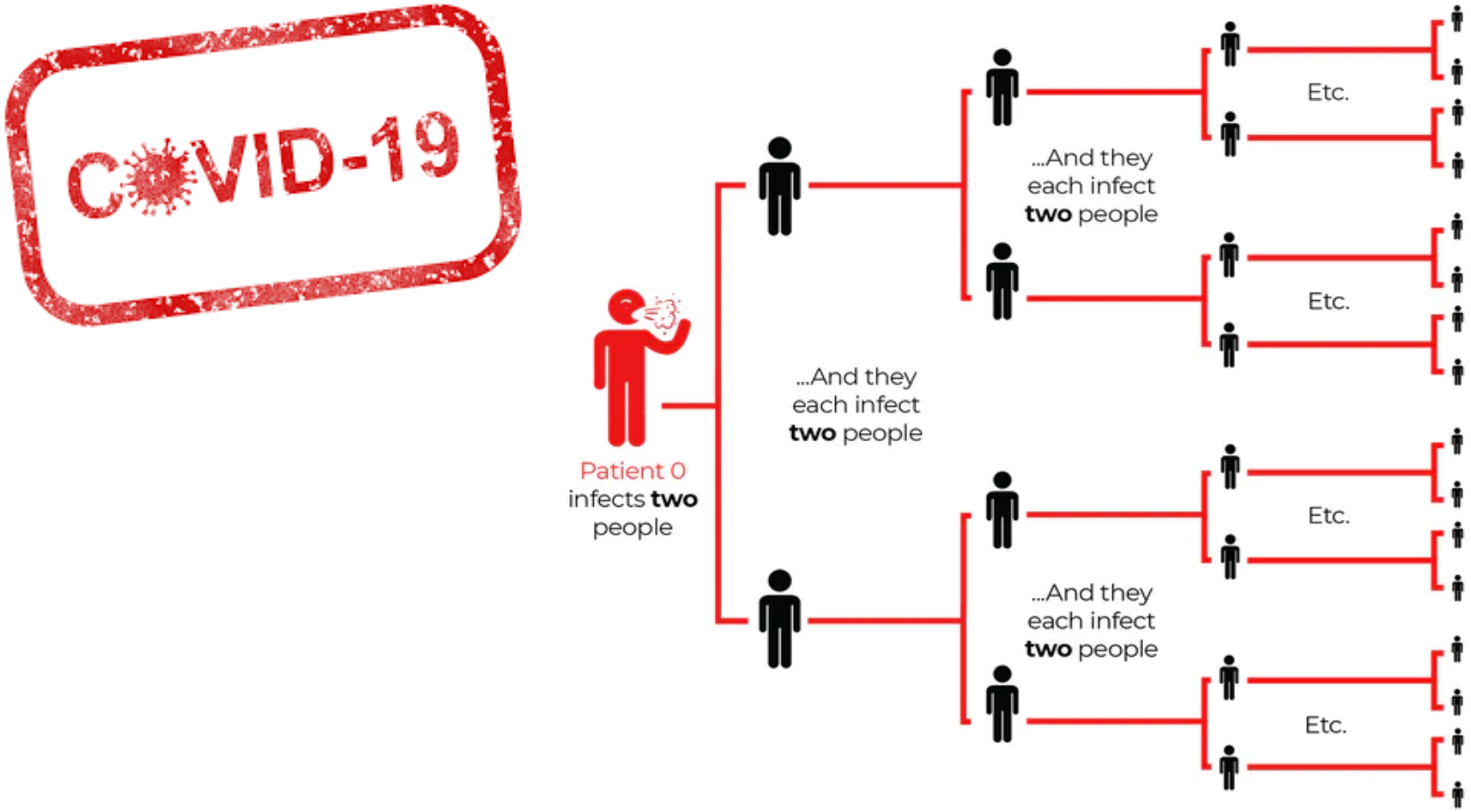
Hyperbolic Graph Convolutional Neural Networks, NeurIPS 2019

Why Hyperbolic Space?

- Many network are with tree-like structures or power-law distributed.

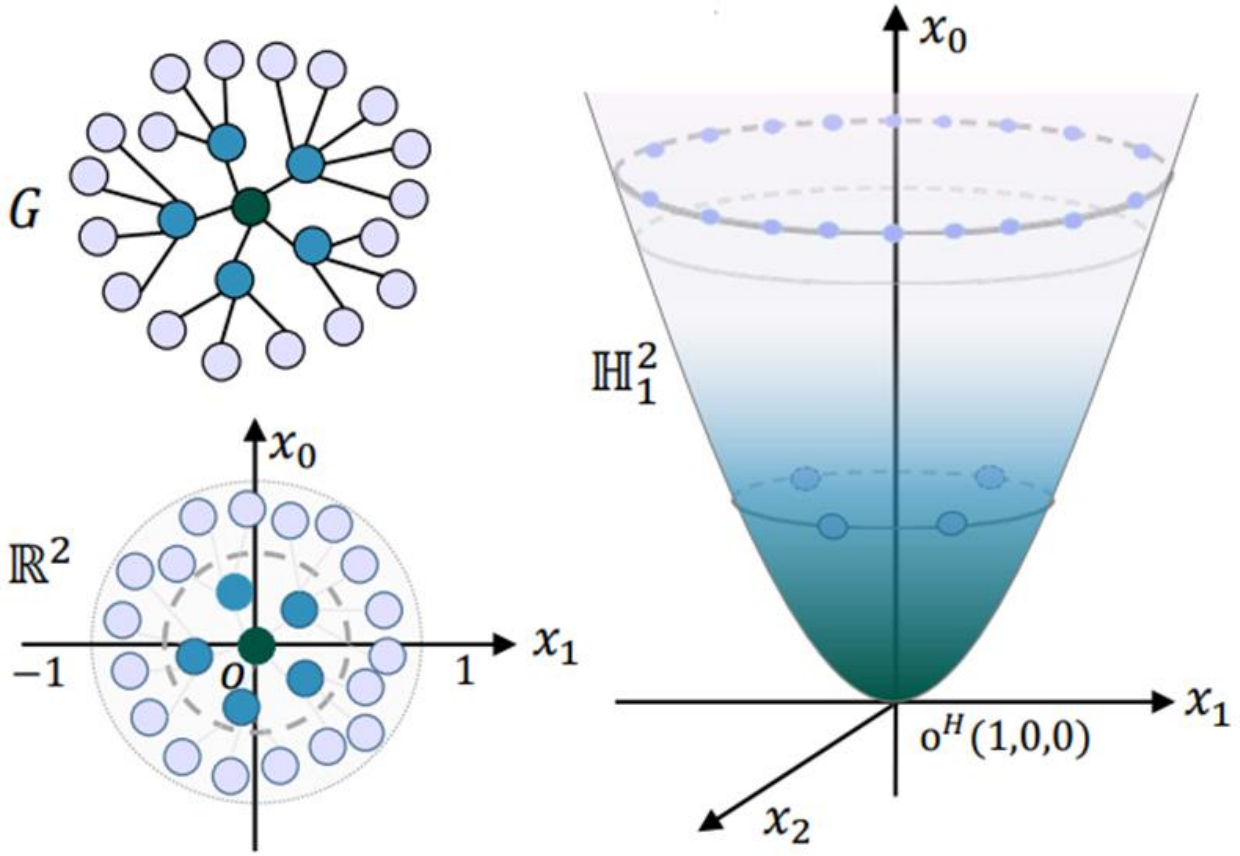






Nodes are exponentially increasing and hierarchical arranged.

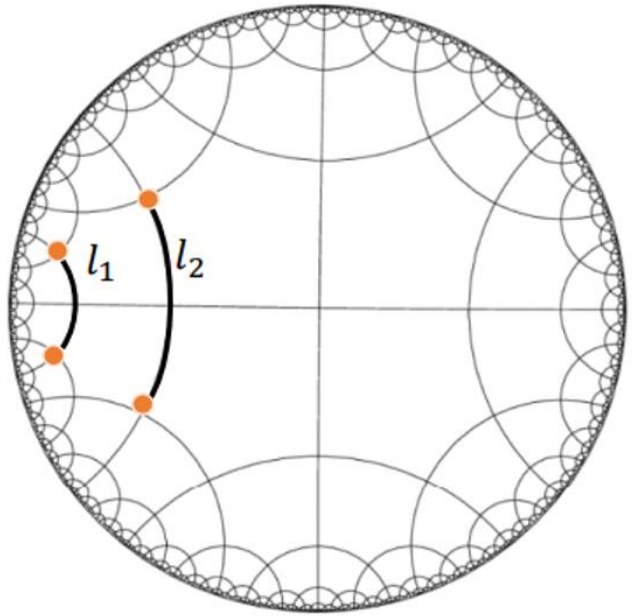
- Figure source: https://labblog.uofmhealth.org/rounds/how-scientists-quantify-intensity-of-an-outbreak-like-covid-19



(1) Acts as a geometric prior for hierarchical structures / tree graphs / heavy tailed distributions (e.g. scale-free, power-law). *

$$V_n^{\mathbb{E}}(r) = \frac{\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)} r^n.$$

$$V_n^{\mathbb{H}}(r) \sim \frac{\mathrm{Vol}\left(\mathbb{S}^n\right)}{2^{n-1}} e^{(n-1)r}, as \quad r \to \infty.$$

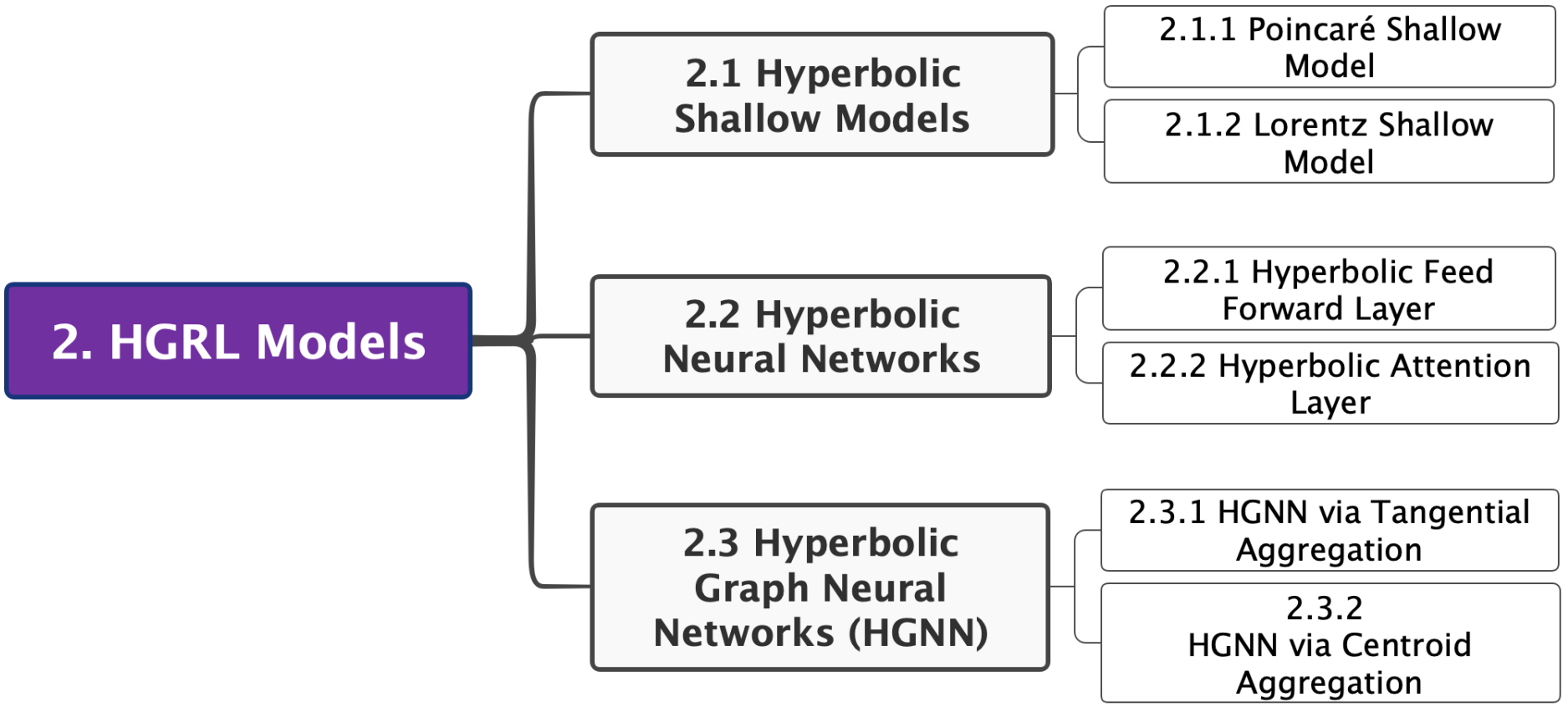


(2) Larger embedding space ---smaller embedding dimension and fewer parameter

2. Hyperbolic Graph Representation Learning (HGRL)

Contents

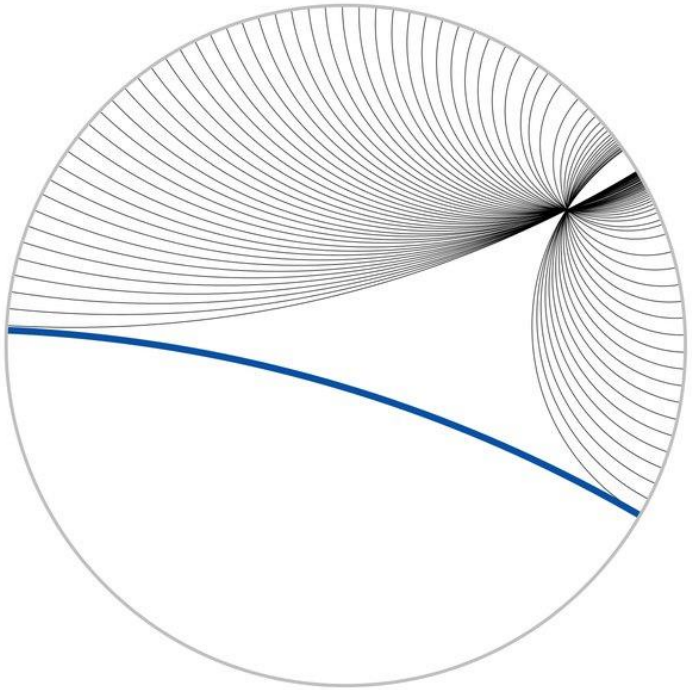
2. HYPERBOLIC GRAPH REPRESENTATION LEARNING (HGRL)



Backgrounds

Hyperbolic Geometry

- A non-Euclidean geometry that reject the validity of Euclid's fifth, the "parallel", postulate.



In hyperbolic space, there are at least two lines that parallel a line through a given point.

https://en.wikipedia.org/wiki/Poincar%C3%A9_disk_model

Backgrounds

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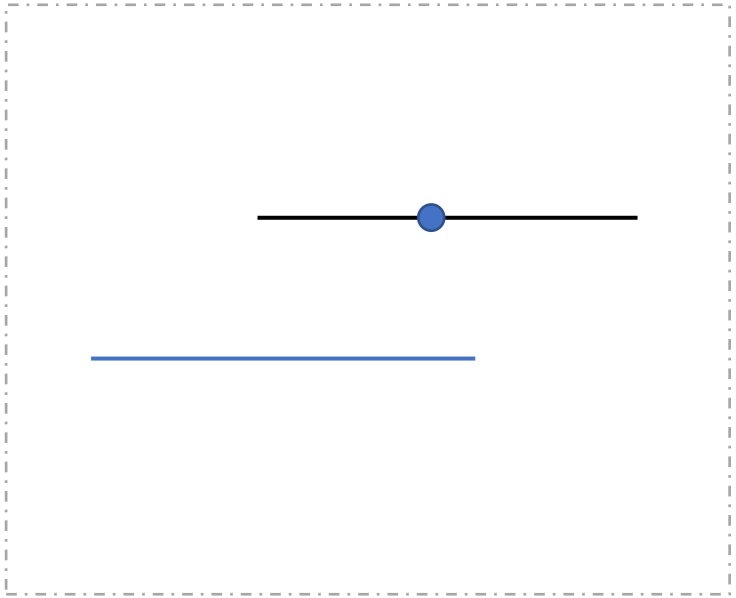
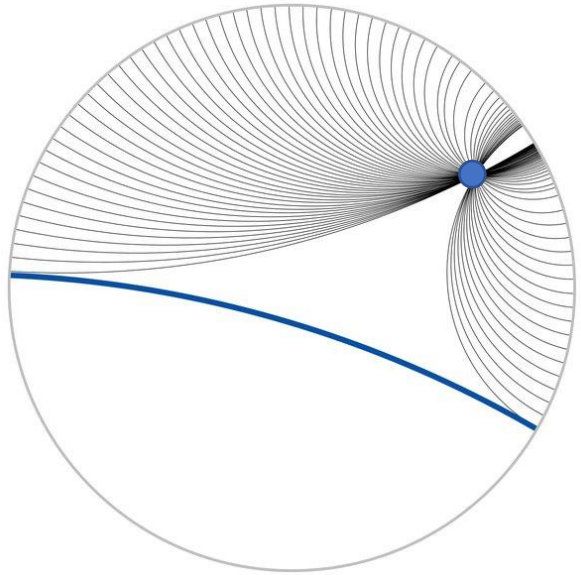


In Euclidean space, there is only one line that paralls a line through a given point.

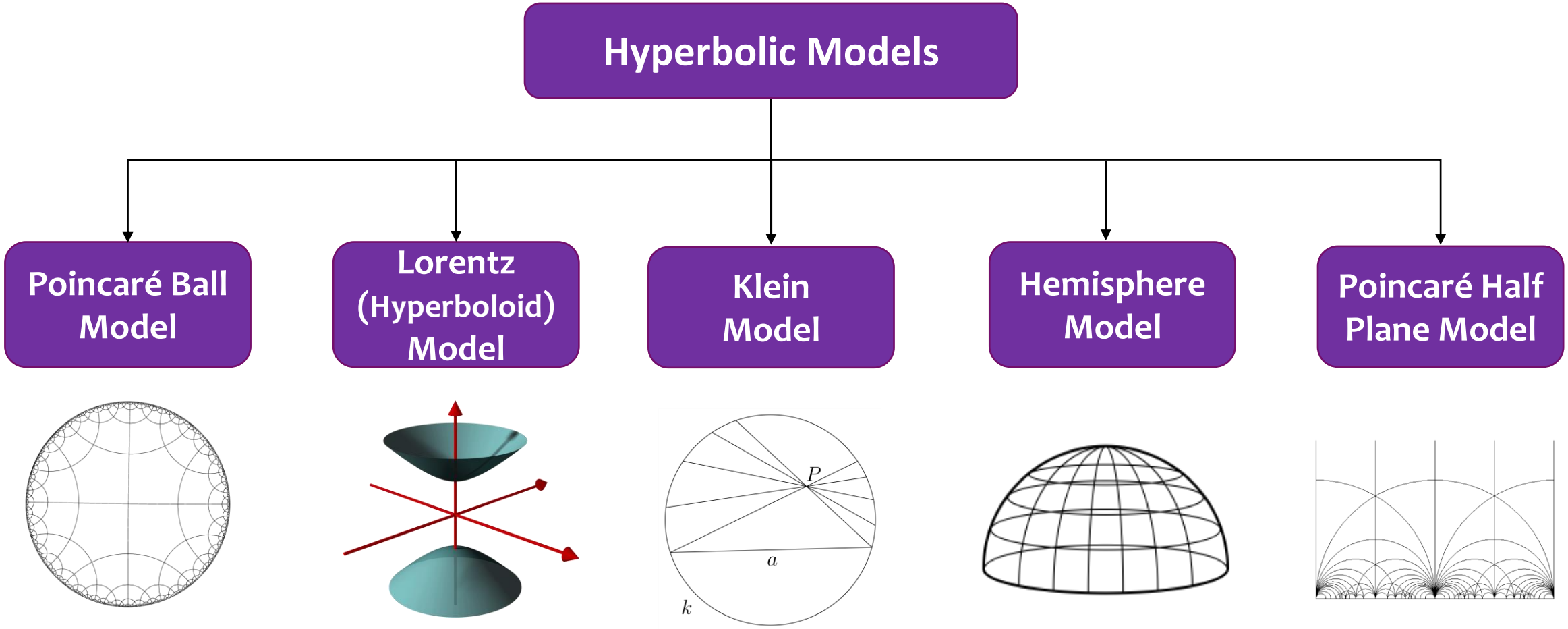


In hyperbolic space, there are at least two lines that parallel a line through a given point.

https://en.wikipedia.org/wiki/Poincar%C3%A9_disk_model

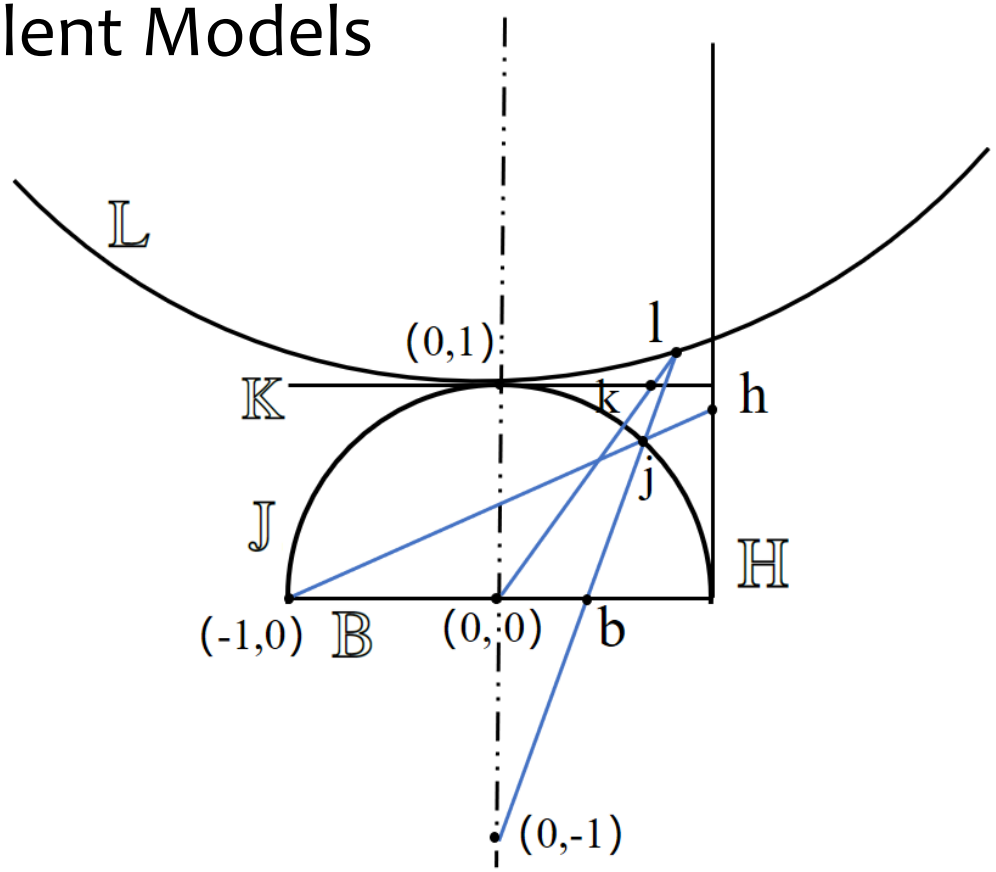
Backgrounds

Mathematical Models for Hyperbolic Geometry



Backgrounds

Isometrically Equivalent Models

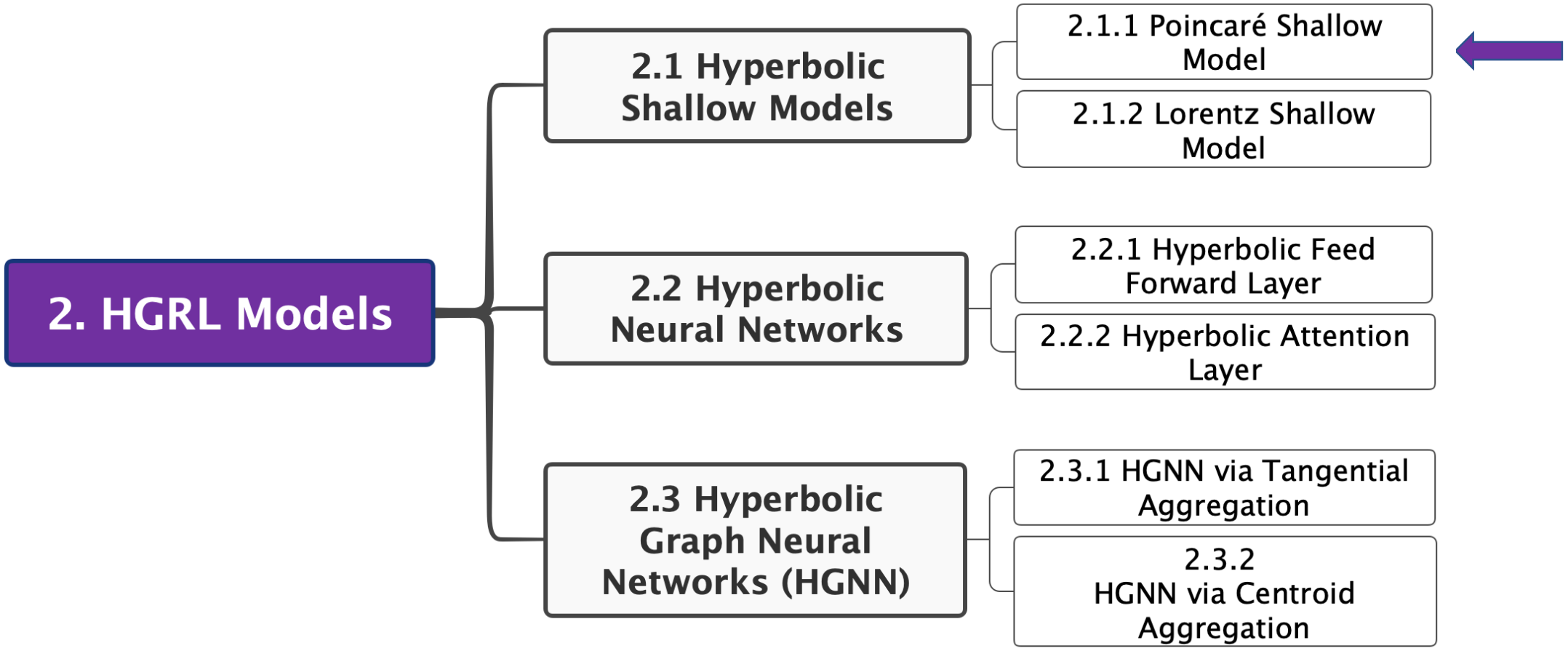


𝕃: Lorentz Model
𝕂: Klein Model
𝕁: Hemisphere model
𝔹: Poincaré Model
ℍ: Poincaré half plane Model

The five hyperbolic models are isometrically equivalent and the points h, b, j, k, l can be thought of as the same point in the hyperbolic space.

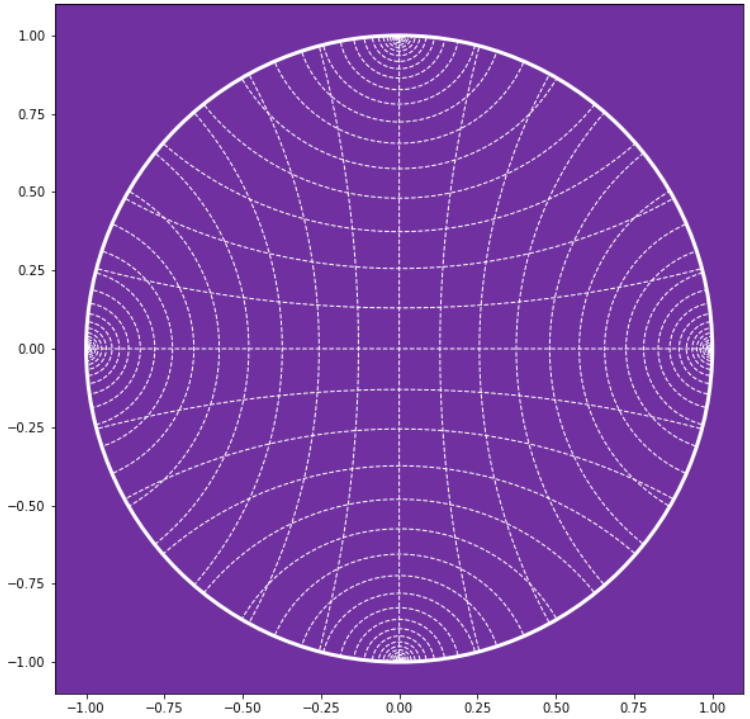
Peng, Wei, et al. "Hyperbolic deep neural networks: A survey." *arXiv preprint arXiv:2101.04562* (2021).

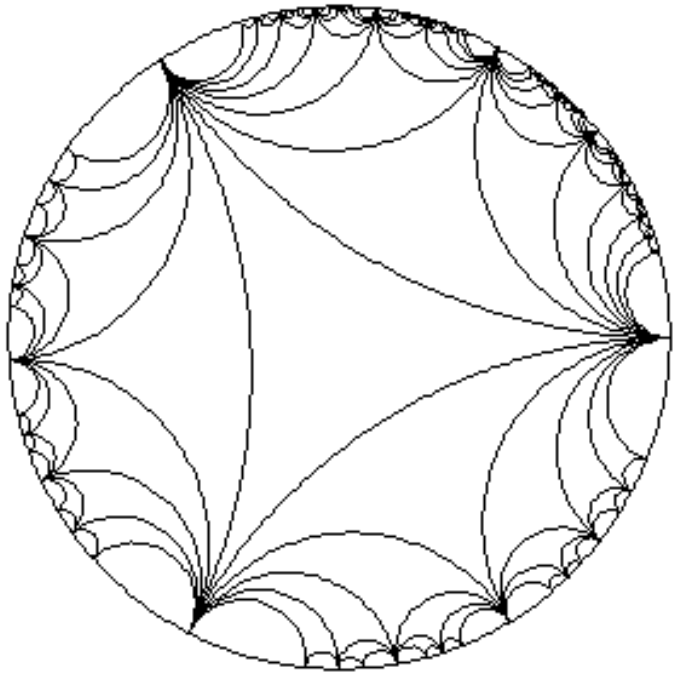
2.1 Hyperbolic Shallow Models

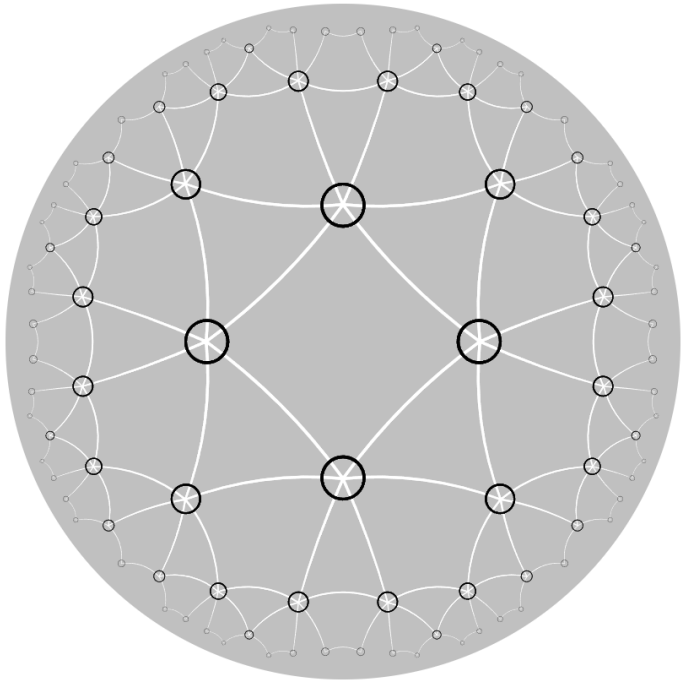


2.1.1 Poincaré Shallow Model

Poincaré Ball Model







Radius proportional to K (inverse of curvature), Open ball (exclude boundary)
In the right two figure, each triangle/circle has the same area.

https://mathworld.wolfram.com/PoincareHyperbolicDisk.html

2.1.1 Poincaré Shallow Model

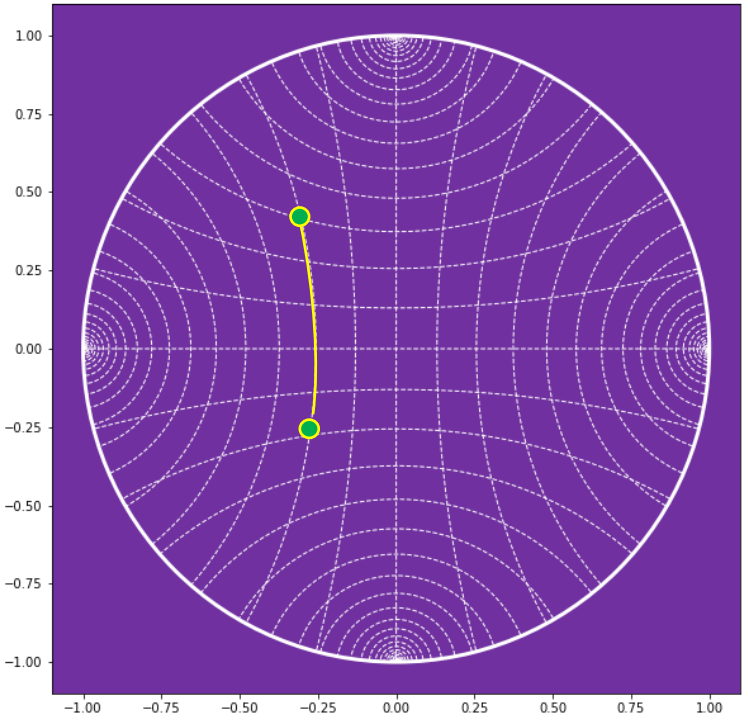
Poincaré Ball Model (Intuitive Visualization)

❖ **Definition** $\mathcal{B}^d = \{x \in \mathbb{R}^d \big| ||x|| < 1\}$,

where $||x|| = \sqrt{\sum_{i=1}^{d} x_i^2}$, a Euclidean norm.

❖ **Distance** between $u, v \in \mathcal{B}^d$:

$$d_{\mathcal{B}}(u,v) = arcosh\left(1 + 2 \cdot \frac{||u-v||^2}{(1-||u||^2)(1-||v||^2)}\right).$$



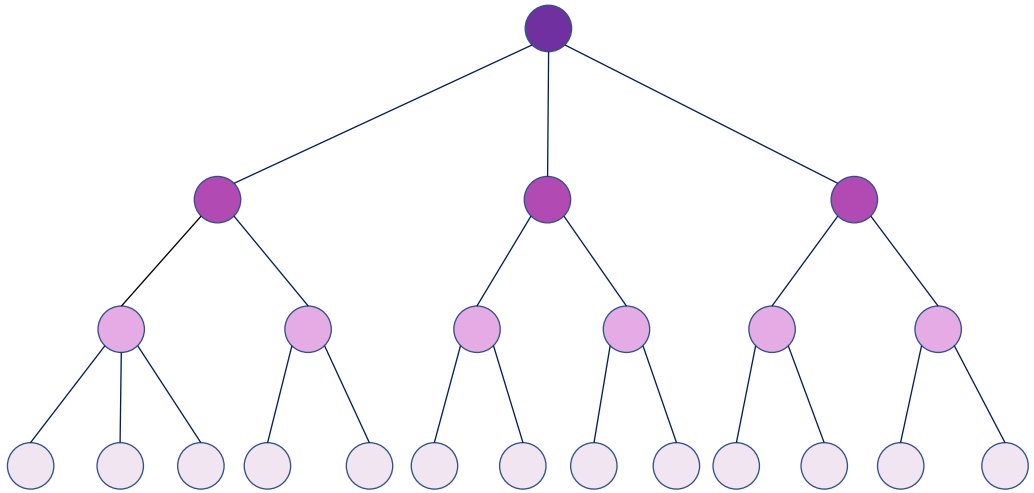
2-dimensional Poincaré ball

2.1.1 Poincaré Shallow Models

Poincaré Shallow Embedding

❖ **Problem** We have a tree-like graph with set of vertices $\mathcal{N} = \{\boldsymbol{x}_i\}_i^n$, and we want to find embeddings $\Theta = \{\boldsymbol{\theta}_i\}_i^n$, that they

- capture the similarity between vertices (including semantics and structures)
- encode the latent hierarchical structure
- have feasible runtime and memory complexity



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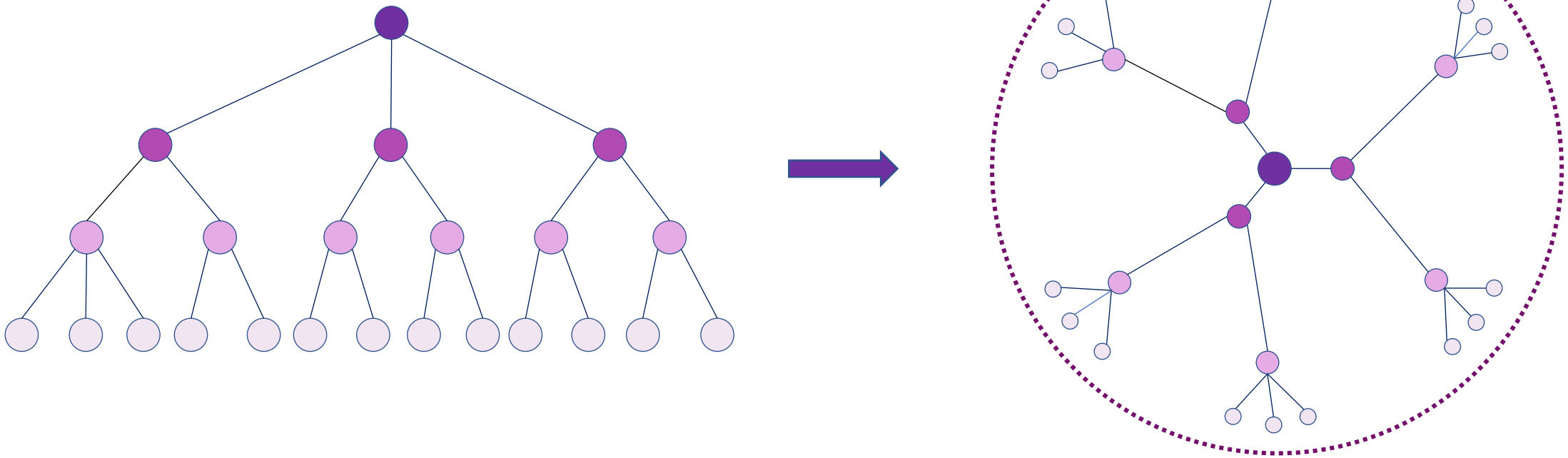


2.1.1 Poincaré Shallow Models

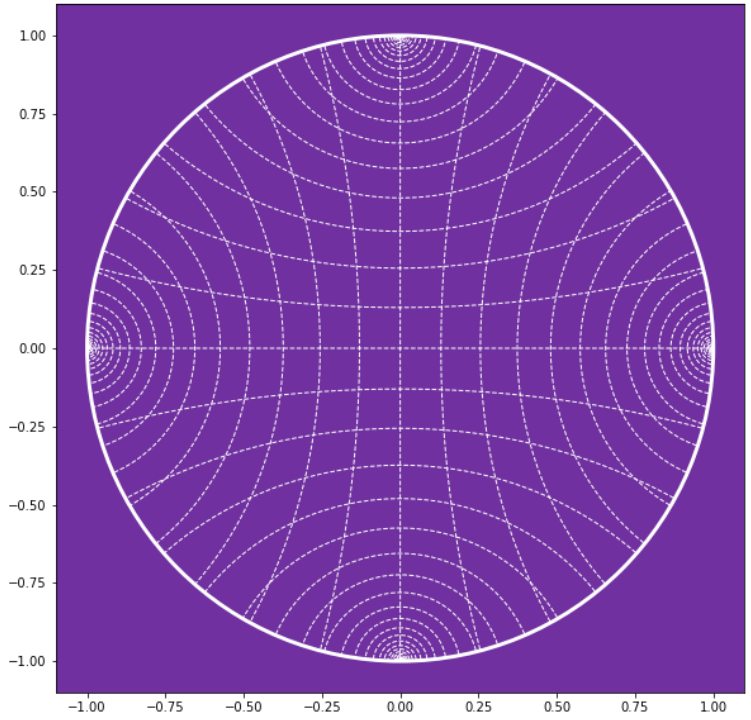
Poincaré Shallow Embedding

❖**Objective**

$$\Theta^* \leftarrow argmin_{\theta}\, L(\Theta),$$

$$\boldsymbol{s.t.} \forall \boldsymbol{\theta_i} \in \boldsymbol{\Theta}: \left|\left|\boldsymbol{\theta_i}\right|\right| < 1$$

where $L(\boldsymbol{\theta})$ is task-specific loss function.



2-dimensional Poincaré ball

Poincaré Shallow Embedding

1. **Initialization**: all node are projected to Poincaré Ball.
   1) Without node feature: randomly using uniform distribution
   2) With node feature: using exponential map

2. **Update** $\Theta: \boldsymbol{\theta_{t+1}} \rightarrow \text{proj}\left(\boldsymbol{\theta_t} - \eta_t \cdot \frac{\left(1-\left|\left|\boldsymbol{\theta_t}\right|\right|^2\right)^2}{4}\boldsymbol{\nabla_E}\right)$

where

$$\boldsymbol{\Delta_E} = \frac{\boldsymbol{\partial L(\theta_t)}}{\boldsymbol{\partial\left(d(\theta_t, x)\right)}} \cdot \frac{\boldsymbol{\partial d(\theta_t, x)}}{\boldsymbol{\partial \theta_t}} \qquad \text{proj}(\boldsymbol{\theta_t}) = \begin{cases} \frac{\boldsymbol{\theta_t}}{\left|\left|\boldsymbol{\theta_t}\right|\right|} - \boldsymbol{\epsilon\ if}\ \left|\left|\boldsymbol{\theta_t}\right|\right| \geq \mathbf{1} \\ \boldsymbol{\theta_t} \quad \boldsymbol{otherwise} \end{cases}$$

Nickel, Maximillian, and Douwe Kiela. "Poincaré embeddings for learning hierarchical representations." *NeurIPS* 30 (2017).

Poincaré Shallow Embedding

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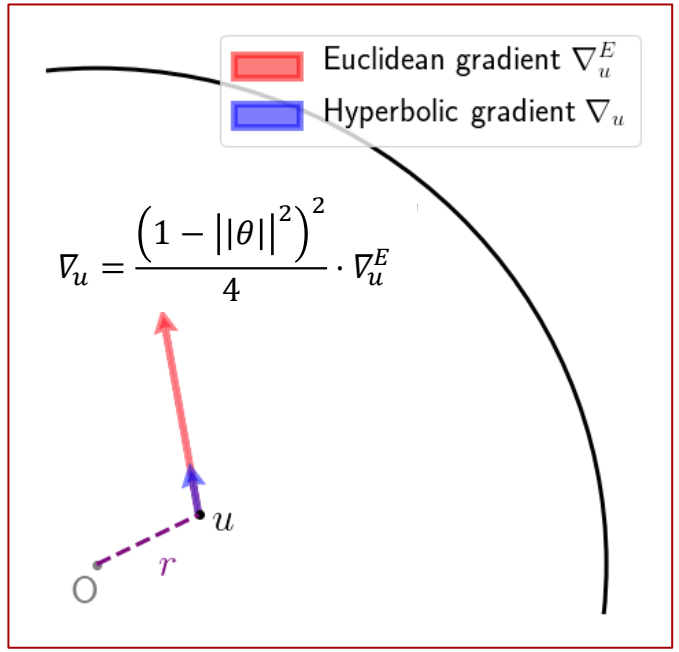

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Nickel, Maximillian, and Douwe Kiela. "Poincaré embeddings for learning hierarchical representations." *NeurIPS* 30 (2017).

2.1.1 Results on Poincaré Ball

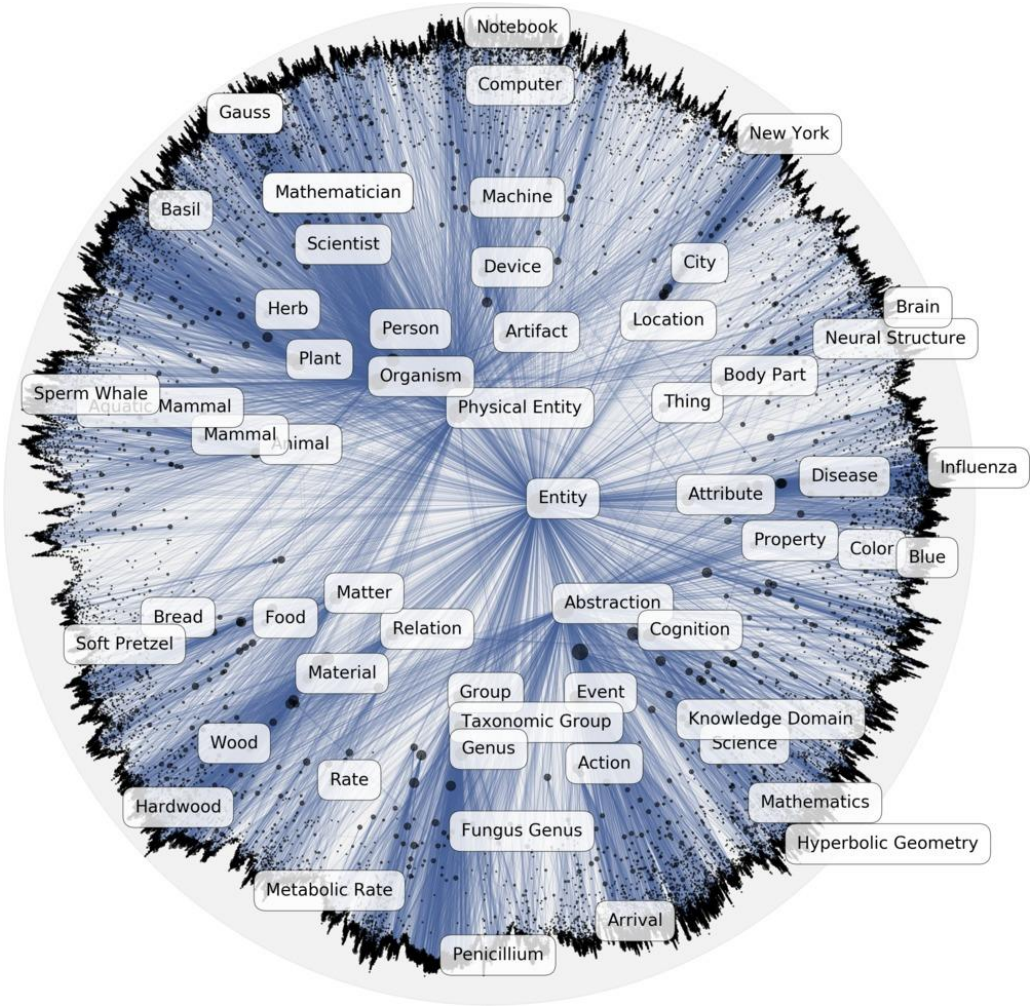
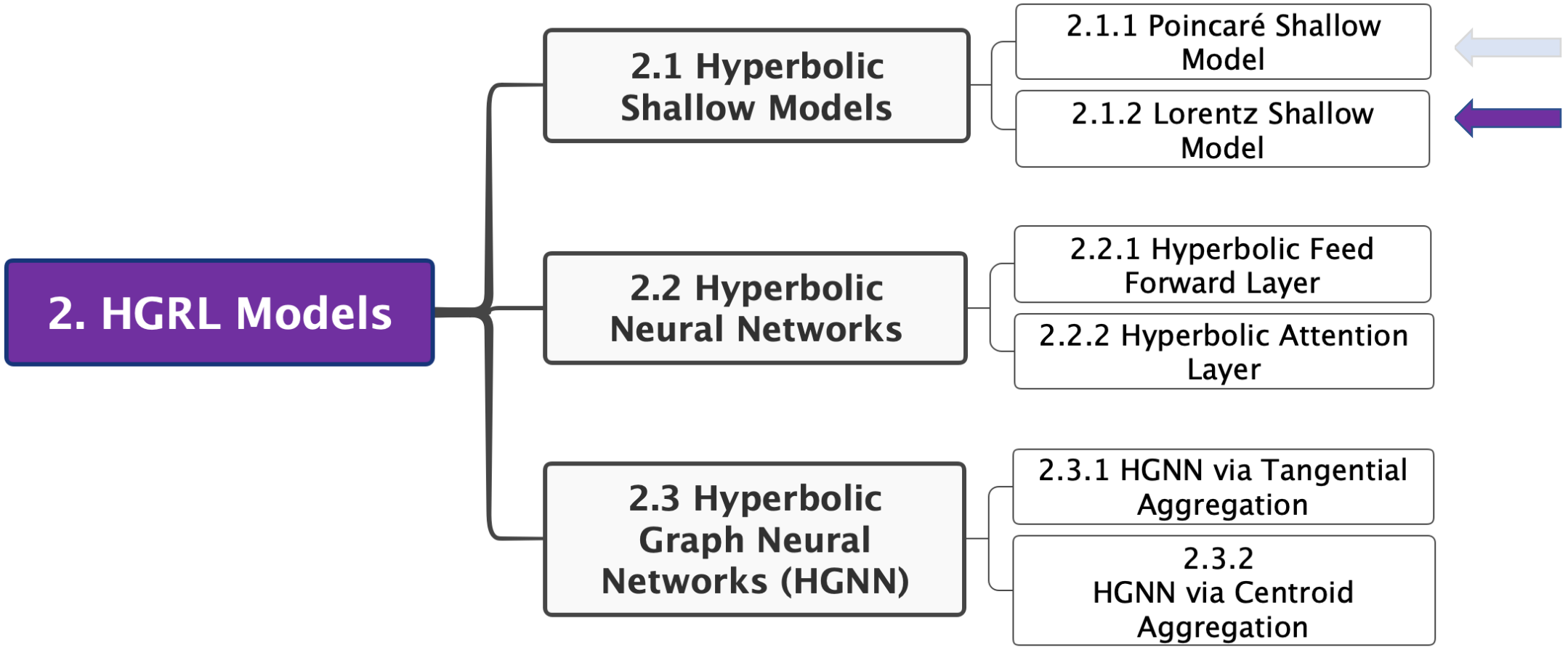


Table: Experimental results on the transitive closure of the WORDNET noun hierarchy. Highlighted cells indicate the best Euclidean embeddings as well as the Poincaré embeddings which achieve equal or better results. Bold numbers indicate absolute best results.

			Dimensionality					
			5	10	20	50	100	200
WORDNET Reconstruction	**Euclidean**	Rank	3542.3	2286.9	1685.9	1281.7	1187.3	1157.3
		MAP	0.024	0.059	0.087	0.140	0.162	0.168
	Translational	Rank	205.9	179.4	95.3	92.8	92.7	91.0
		MAP	0.517	0.503	0.563	0.566	0.562	0.565
	Poincaré	Rank	4.9	4.02	3.84	3.98	3.9	**3.83**
		MAP	0.823	0.851	0.855	0.86	0.857	**0.87**
WORDNET Link Pred.	**Euclidean**	Rank	3311.1	2199.5	952.3	351.4	190.7	81.5
		MAP	0.024	0.059	0.176	0.286	0.428	0.490
	Translational	Rank	65.7	56.6	52.1	47.2	43.2	40.4
		MAP	0.545	0.554	0.554	0.56	0.562	0.559
	Poincaré	Rank	5.7	**4.3**	4.9	4.6	4.6	4.6
		MAP	0.825	0.852	0.861	**0.863**	0.856	0.855

Nickel, Maximillian, and Douwe Kiela. "Poincaré embeddings for learning hierarchical representations." *NeurIPS* 30 (2017).

2.1.2 Lorentz Shallow Models



2.1.2 Lorentz Shallow Models

Lorentz Model

(Numerically more stable, simpler formula)

❖**Definition** $\mathcal{L}^d = \{x \in \mathbb{R}^{d+1} : < x, x >_{\mathcal{L}} = -1, x_0 > 0\}$,

where $< x, y >_{\mathcal{L}} := -x_0 y_0 + x_1 y_1 + \cdots + x_d y_d$.

Time-like

Space-like

❖**Distance** between $u, v \in \mathcal{L}^d$:

$$d_{\mathcal{L}}(u, v) = arcosh(- < x, y >_{\mathcal{L}}).$$

2.1.2 Lorentz Shallow Models

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Time-like Space-like

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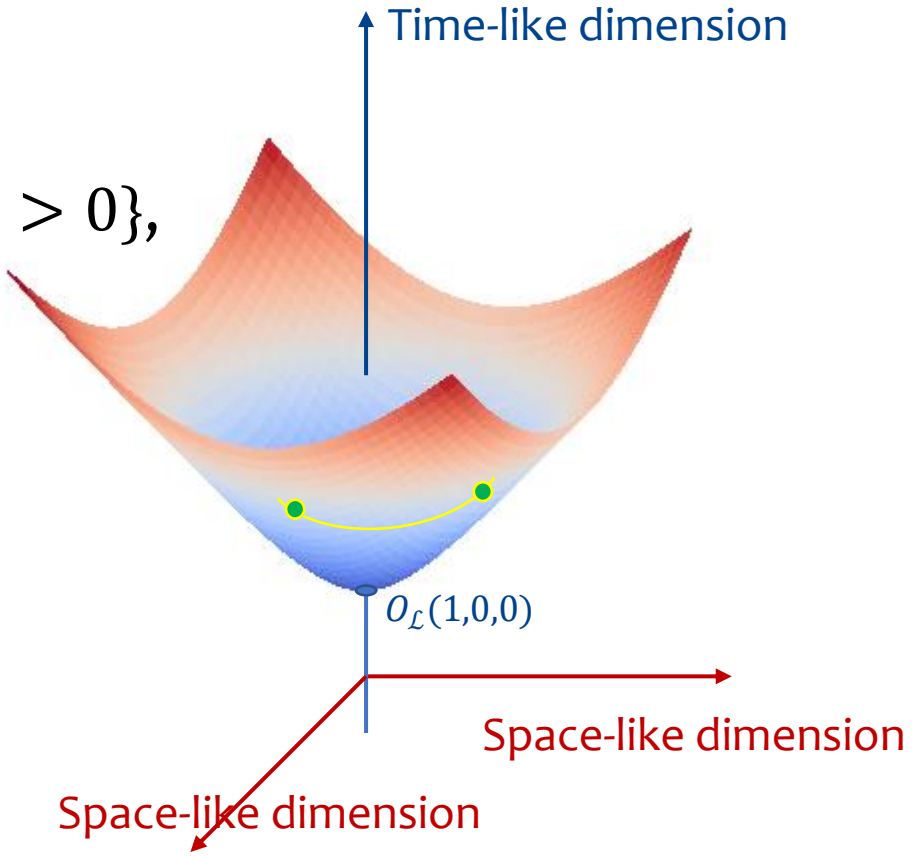


2-dimensional Lorentz Model

2.1.2 Lorentz Shallow Models

Lorentz Shallow Embedding

❖ **Problem** We have a tree-like graph with set of vertices $\mathcal{N} = \{x_i\}_i^n$, and we want to find embeddings $\Theta = \{\theta_i\}_i^n$, that they

- capture the similarity between vertices (including semantics and structure);
- encode the latent hierarchical structure;
- have feasible runtime and memory complexity.

2.1.2 Lorentz Shallow Models

Lorentz Shallow Embedding

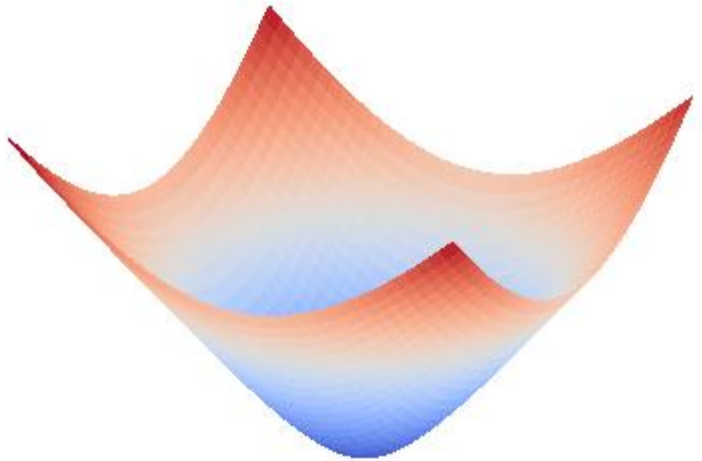
❖ **Objective**

$$\theta^* \leftarrow \arg min_\theta \, L(\boldsymbol{\Theta}),$$

$$s.t. \; \forall \boldsymbol{\theta_i} \in \boldsymbol{\Theta}: \boldsymbol{\theta_i} \in \mathcal{L}^{\boldsymbol{d}}$$

$$\boldsymbol{\theta_{i,0}^2 + \theta_{i,1}^2 + \cdots + \theta_{i,d}^2 = -1}$$

where $L(\theta)$ is task-specific loss function.



2-dimensional Lorentz Model

2.1.2 Lorentz Shallow Models

Lorentz Shallow Embedding

1. **Initialization:** all node are projected to Lorentz Model.
   1) Without node feature: randomly using uniform distribution
   2) With node feature: using exponential map
2. **Update Θ :** $\theta_{t+1} \rightarrow exp_{\theta_t}(-\eta_t \cdot \mathrm{grad} f(\theta_t))$,

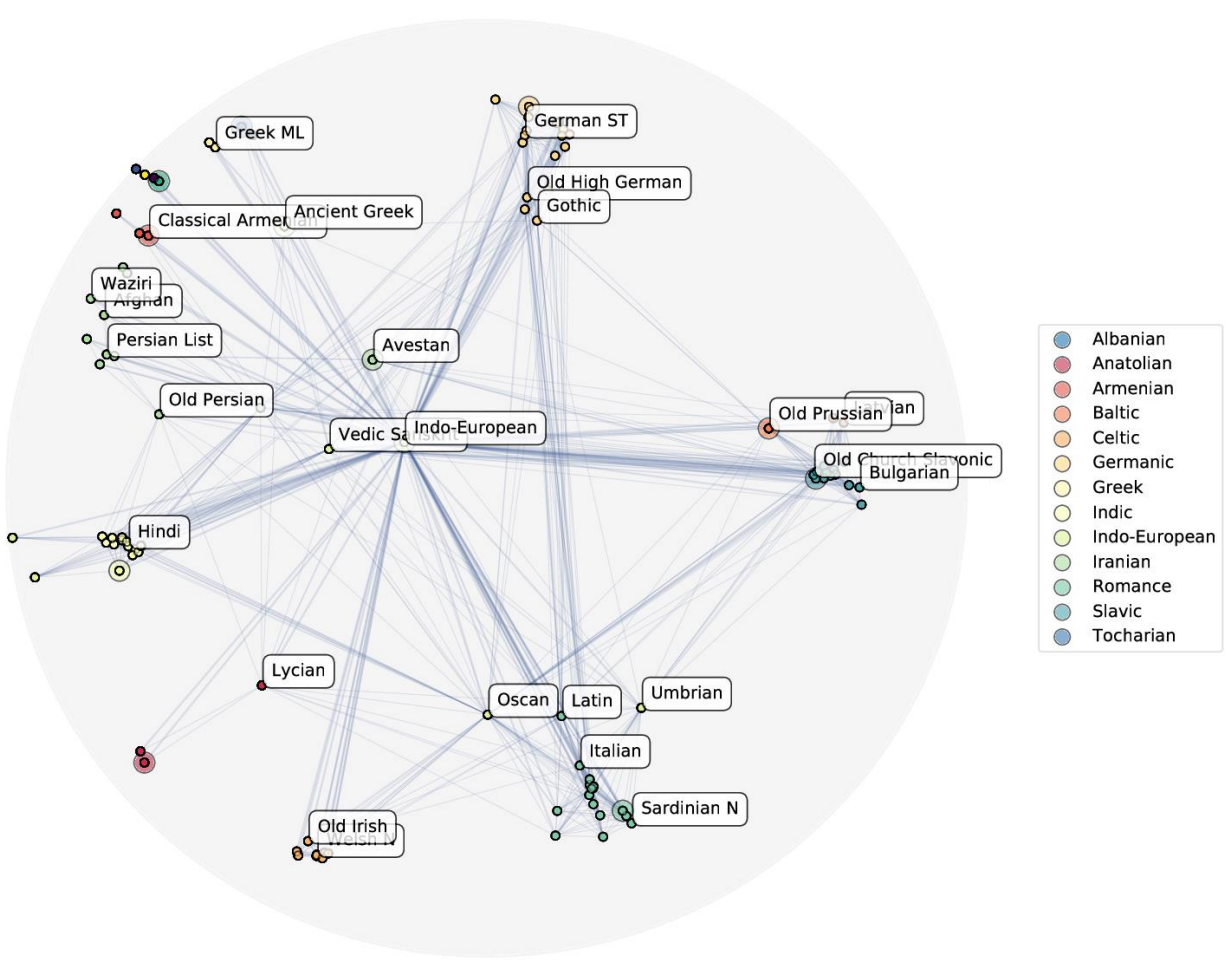
Where $\mathrm{grad}\, f(\theta_t) \in \mathcal{T}_\theta \mathcal{M}$ denotes the Riemannian gradient and η denotes the learning rate.

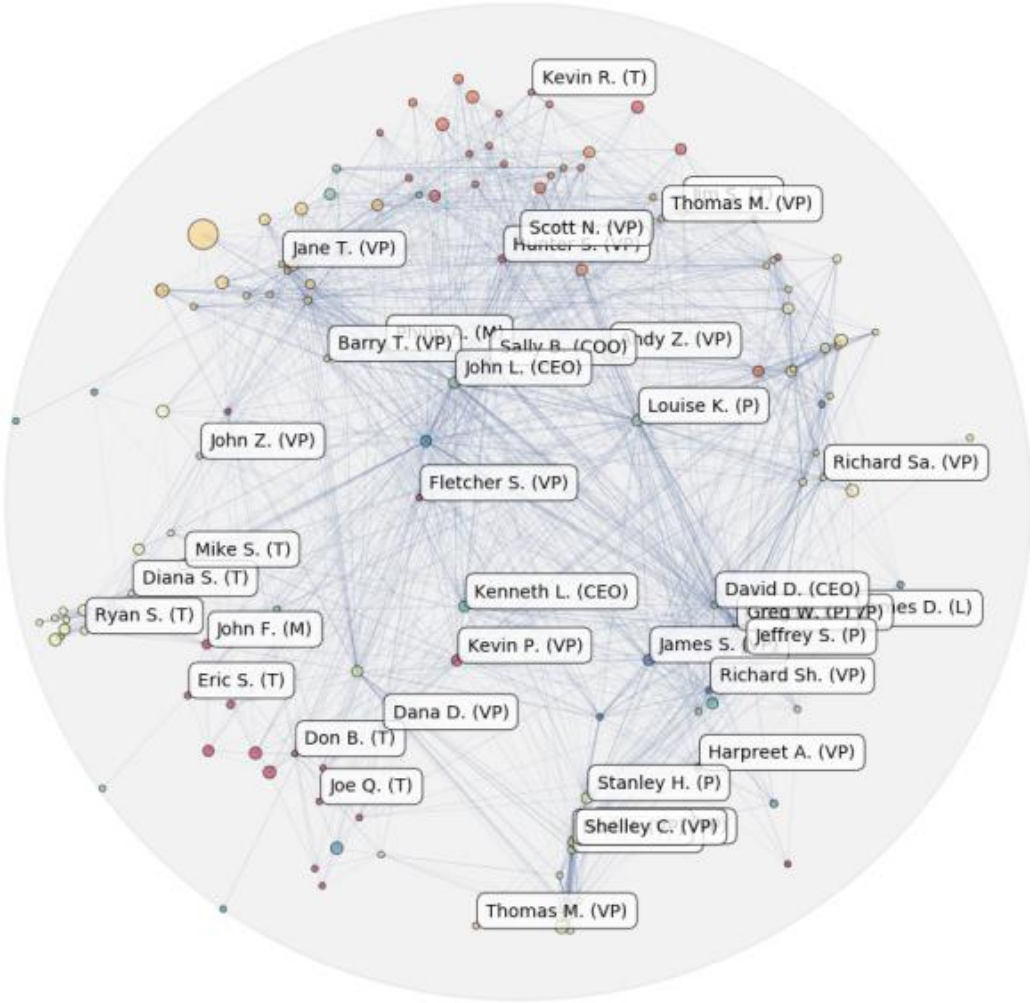
Algorithm 1 Riemannian Stochastic Gradient Descent

Input Learning rate η, number of epochs T.
for $t = 1, \ldots, T$

$$\begin{aligned} \boldsymbol{h}_t &\leftarrow g_{\theta_t}^{-1} \nabla f(\theta_t) \\ \mathrm{grad}\, f(\theta_t) &\leftarrow \mathrm{proj}_{\theta_t}(\boldsymbol{h}_t) \\ \theta_{t+1} &\leftarrow \exp_{\theta_t}(-\eta\, \mathrm{grad}\, f(\theta_t)) \end{aligned}$$

2.1.2 Results on Lorentz Model





https://mnick.github.io/project/geometric-representation-learning/

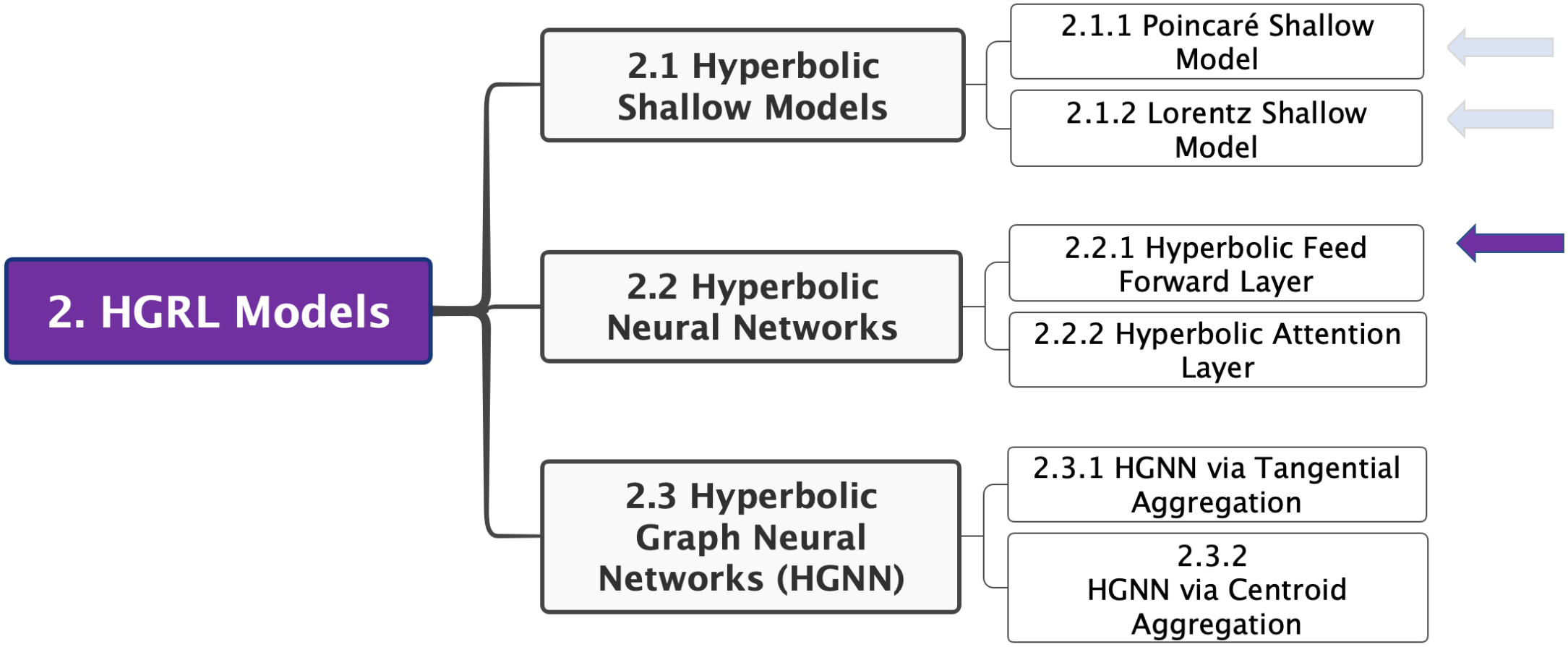
Summary

Concepts and functions for hyperbolic geometry

- ❖ Hyperbolic Models
- ❖ Manifold and Metric
- ❖ Induced Distance Function
- ❖ Exponential and Logarithmic Maps
- ❖ Parallel Transport

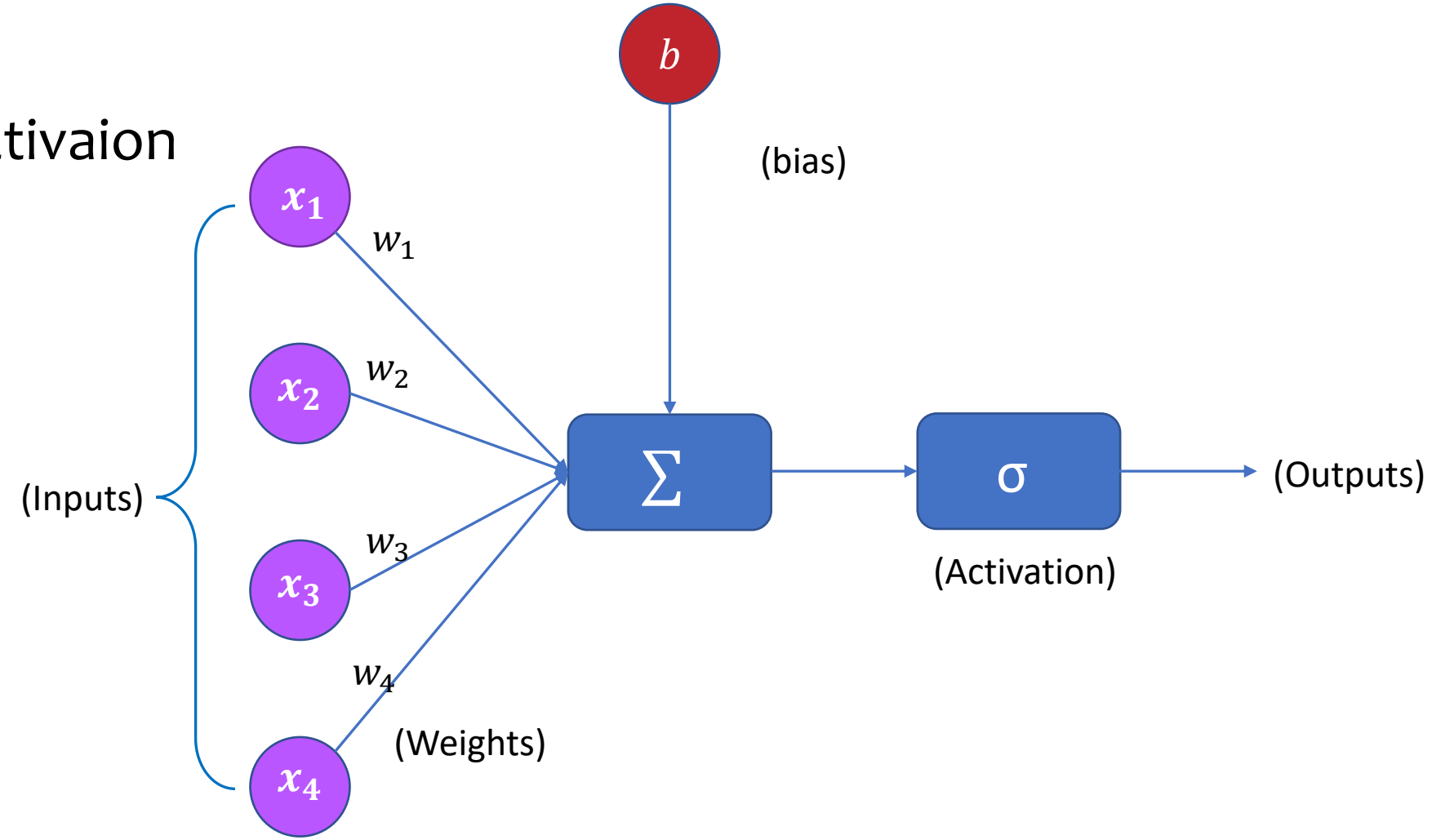
	Poincaré Ball Model	**Lorentz Model**
Manifold	$\mathcal{B}_c^n = \{x \in \mathbb{R}^n : \langle \mathbf{x}, \mathbf{x} \rangle_2 < -1/c\}$	$\mathcal{L}_c^n = \left\{\mathbf{x} \in \mathbb{R}^{n+1} : \langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{L}} = 1/c\right\}$
Metric	$g_{\mathbf{x}}^{\mathcal{B}_c^n} = (\lambda_{\mathbf{x}}^c)^2 g^{\mathrm{E}^n}$ where $\lambda_{\mathbf{x}}^c = \frac{2}{1+c\|\mathbf{x}\|_2^2}$ and $g^{\mathrm{E}^n} = \mathbf{I}_n$	$g_{\mathbf{x}}^{\mathcal{L}_c^n} = \eta$, where η is I except $\eta_{0,0} = -1$
Induced distance	$d_{\mathcal{B}}^c(\mathbf{x}, \mathbf{y}) = \frac{1}{\sqrt{\lvert c \rvert}} \cosh^{-1}\left(1 - \frac{2c\|\mathbf{x}-\mathbf{y}\|_2^2}{(1+c\|\mathbf{x}\|_2^2)(1+c\|\mathbf{y}\|_2^2)}\right)$	$d_{\mathcal{L}}^c(\mathbf{x}, \mathbf{y}) = \frac{1}{\sqrt{\lvert c \rvert}} \cosh^{-1}\left(c\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}\right)$
Logarithmic map	$\log_{\mathbf{x}}^c(\mathbf{y}) = \frac{2}{\sqrt{\lvert c \rvert}\lambda_{\mathbf{x}}^c} \tanh^{-1}\left(\sqrt{\lvert c \rvert}\, \lVert -\mathbf{x} \oplus_c \mathbf{y} \rVert_2\right) \frac{-\mathbf{x} \oplus_c \mathbf{y}}{\lVert -\mathbf{x} \oplus_c \mathbf{y} \rVert_2}$	$\log_{\mathbf{x}}^c(\mathbf{y}) = \frac{\cosh^{-1}(c\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}})}{\sinh\left(\cosh^{-1}(c\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}})\right)} \left(\mathbf{y} - c\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}} \mathbf{x}\right)$
exponential map	$\exp_{\mathbf{x}}^c(\mathbf{v}) = \mathbf{x} \oplus_c \left(\tanh\left(\sqrt{\lvert c \rvert} \frac{\lambda_{\mathbf{x}}^c \lVert \mathbf{v} \rVert_2}{2}\right) \frac{\mathbf{v}}{\sqrt{\lvert c \rvert} \lVert \mathbf{v} \rVert_2}\right)$	$\exp_{\mathbf{x}}^c(\mathbf{v}) = \cosh\left(\sqrt{\lvert c \rvert} \lVert \mathbf{v} \rVert_{\mathcal{L}}\right) \mathbf{x} + \mathbf{v} \frac{\sinh\left(\sqrt{\lvert c \rvert} \lVert \mathbf{v} \rVert_{\mathcal{L}}\right)}{\sqrt{\lvert c \rvert} \lVert \mathbf{v} \rVert_{\mathcal{L}}}$
Parallel transport	$PT_{\mathbf{x} \to \mathbf{y}}^c(\mathbf{v}) = \frac{\lambda_{\mathbf{x}}^c}{\lambda_{\mathbf{y}}^c} \operatorname{gyr}[\mathbf{y}, -\mathbf{x}]\mathbf{v}$	$PT_{\mathbf{x} \to \mathbf{y}}^c(\mathbf{v}) = \mathbf{v} - \frac{c\langle \mathbf{y}, \mathbf{v} \rangle_{\mathcal{L}}}{1+c\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}}(x + \mathbf{y})$

2.2 Hyperbolic Neural Networks



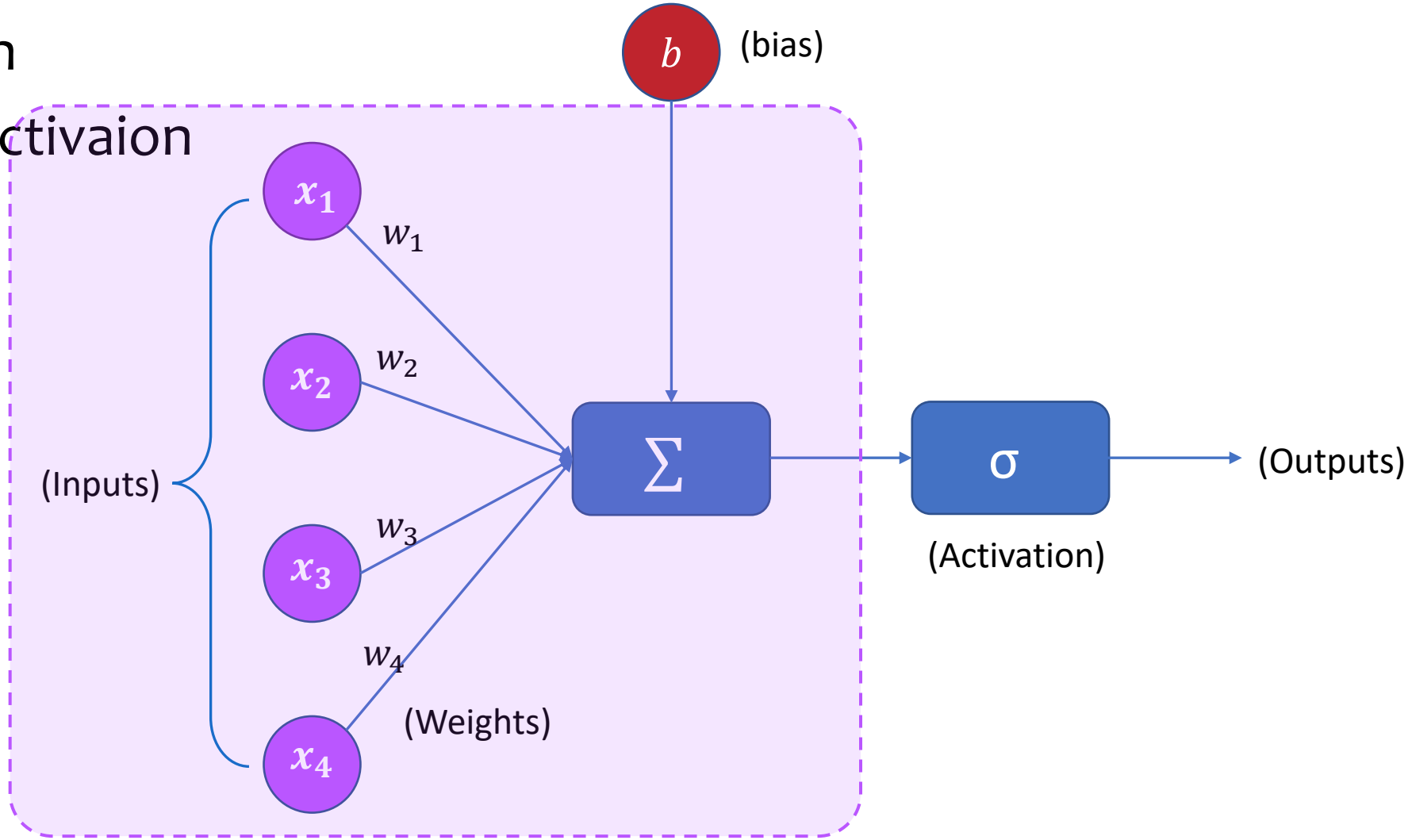
2.2.1 Feed Forward Layer

- Matrix-vector Multiplication
- Bias Addition
- Non-linear Activaion



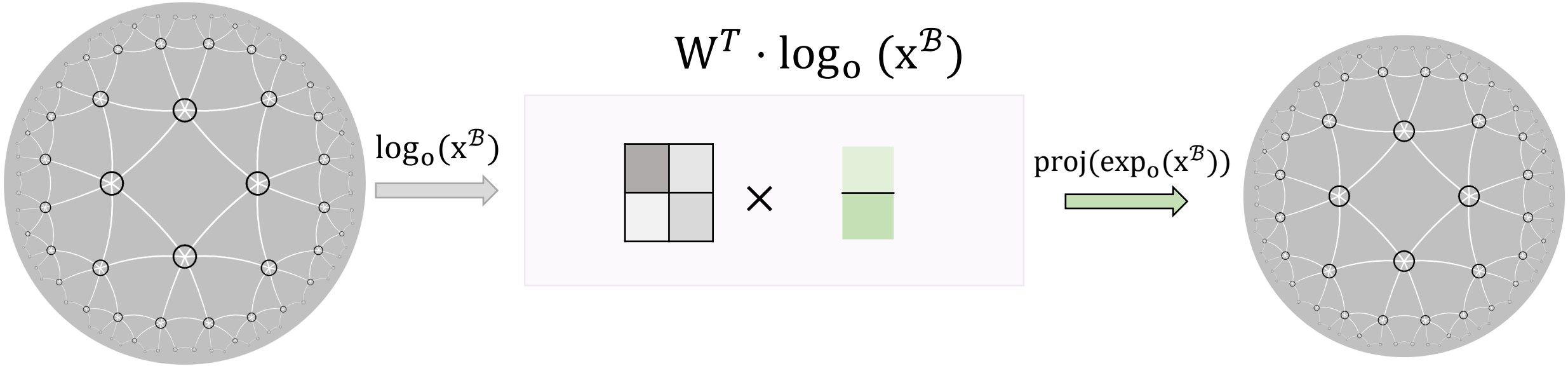
2.2.1 Feed Forward Layer

- **Matrix-vector Multiplication**
- Bias Addition
- Non-linear Activaion



2.2.1 Hyperbolic Feed Forward Layer

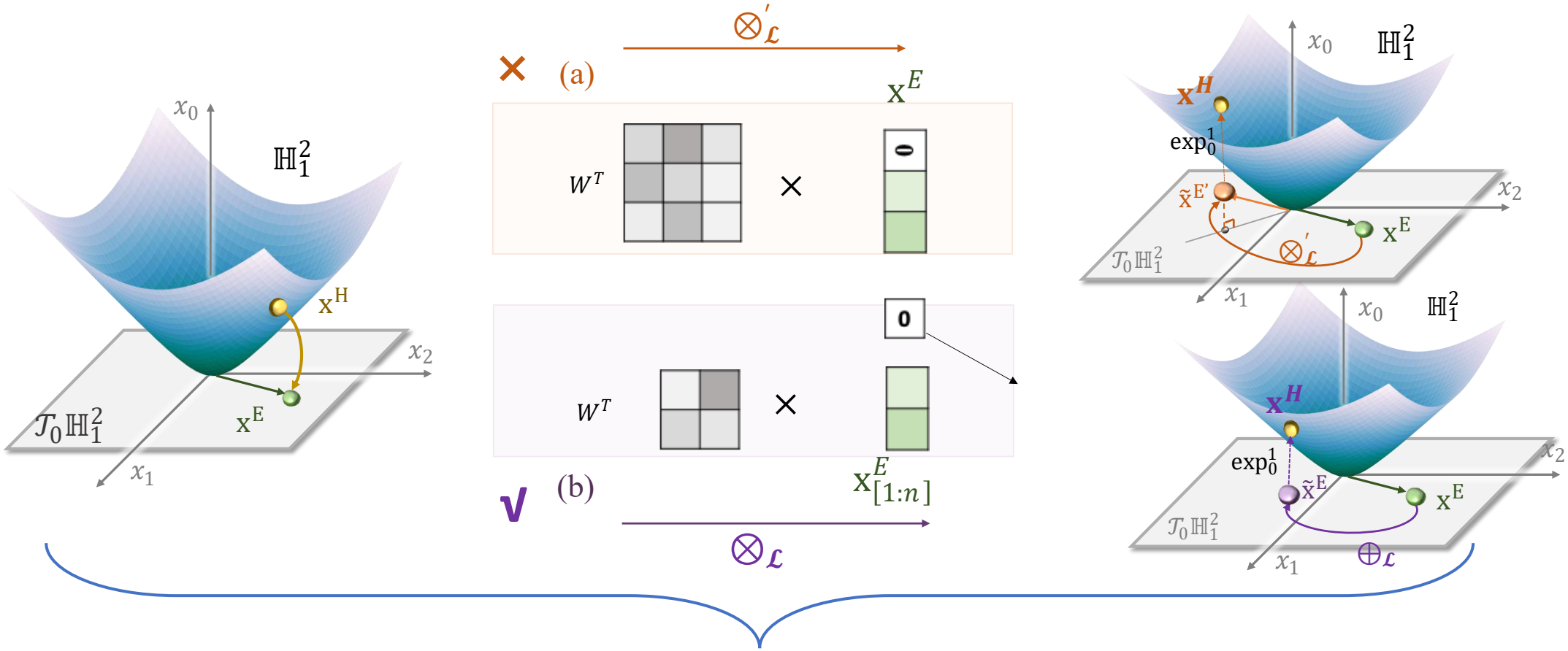
- Hyperbolic Matrix-vector Multiplication on Poincaré Ball Model



$$\text{Hyperbolic Matrix Multiplication}: W \otimes_{\mathcal{B}} x^{\mathcal{B}} = \text{proj}(\exp_{\mathbf{o}}(W^{\mathrm{T}} \log_o(x^{\mathcal{B}})))$$

2.2.1 Hyperbolic Feed Forward Layer

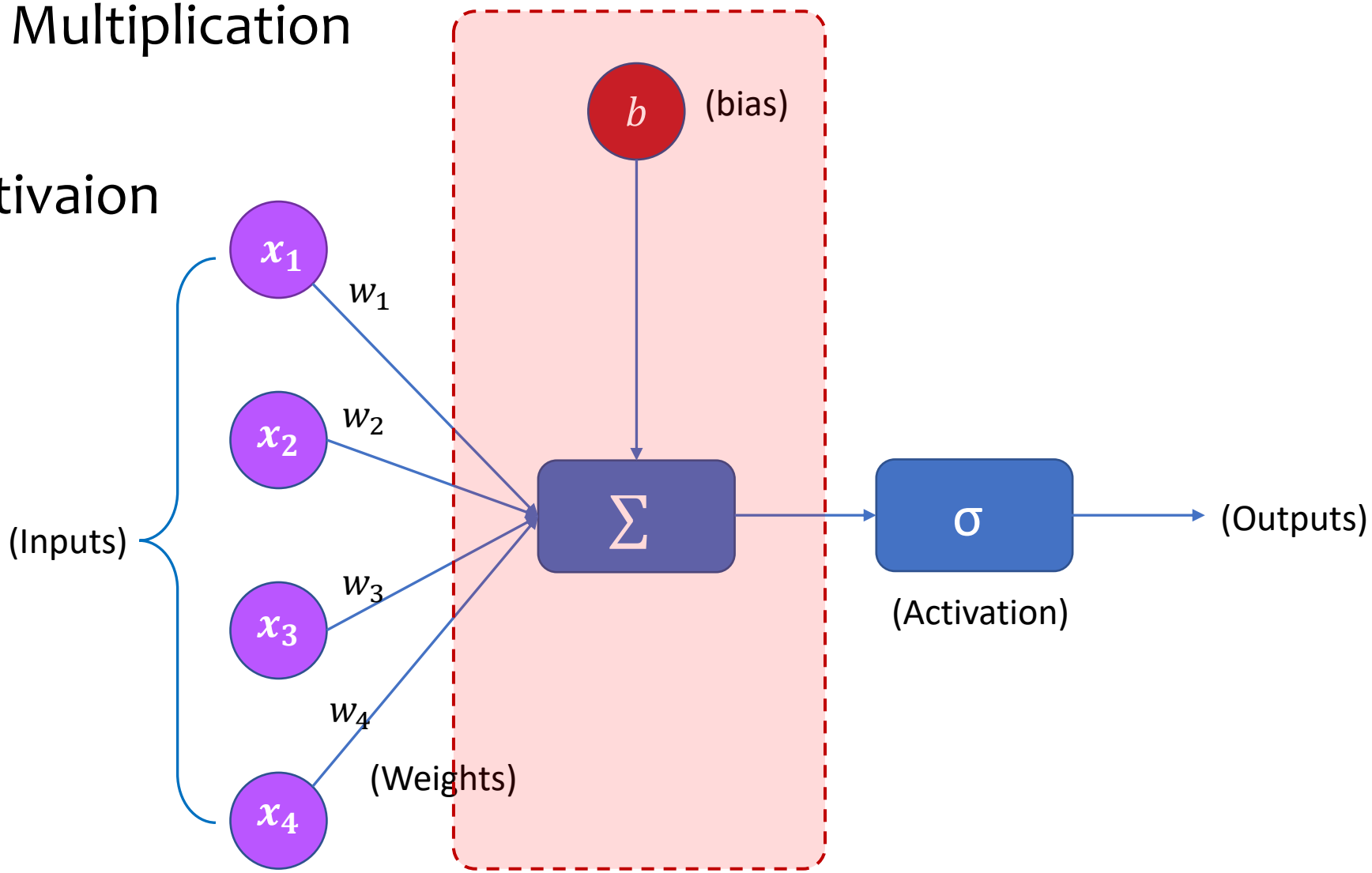
- Hyperbolic Matrix-vector Multiplication on Lorentz Model



$$\text{Hyperbolic Matrix Multiplication}: W \otimes_{\mathcal{B}} x^{\mathcal{B}} = \text{proj}(\exp_{\mathbf{o}}([\mathbf{0}: W^{\mathrm{T}} \log_{\mathrm{o}}(x^{\mathcal{B}}_{[1:n]}))))$$

2.2.1 Hyperbolic Feed Forward Layer

- Matrix-vector Multiplication
- **Bias Addition**
- Non-linear Activaion



2.2.1 Hyperbolic Feed Forward Layer

- Bias addition on Poincaré Ball Model and Lorentz Model

  - In Euclidean Space

$$x \leftarrow x + b$$

  - In Hyperbolic Space

$$x^H \leftarrow x^H \oplus b = \exp_{x^H}\left(P_{0 \to x^H}(\log_0(b))\right)$$

Fig: https://imgur.com/gallery/tqplYeT

2.2.1 Hyperbolic Feed Forward Layer

- Bias addition on Poincaré Ball Model and Lorentz Model

  - In Euclidean Space

$$x \leftarrow x + b$$

  - In Hyperbolic Space

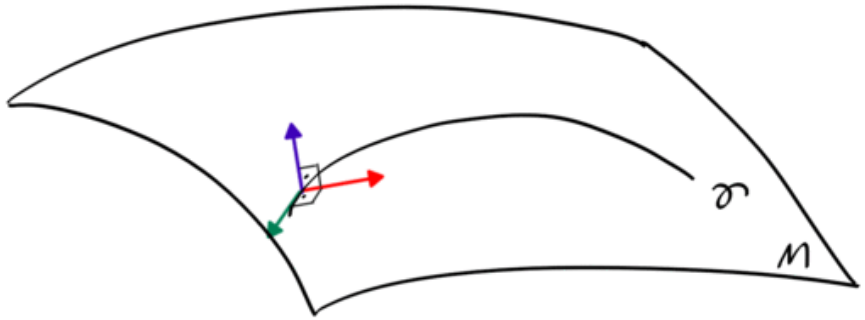


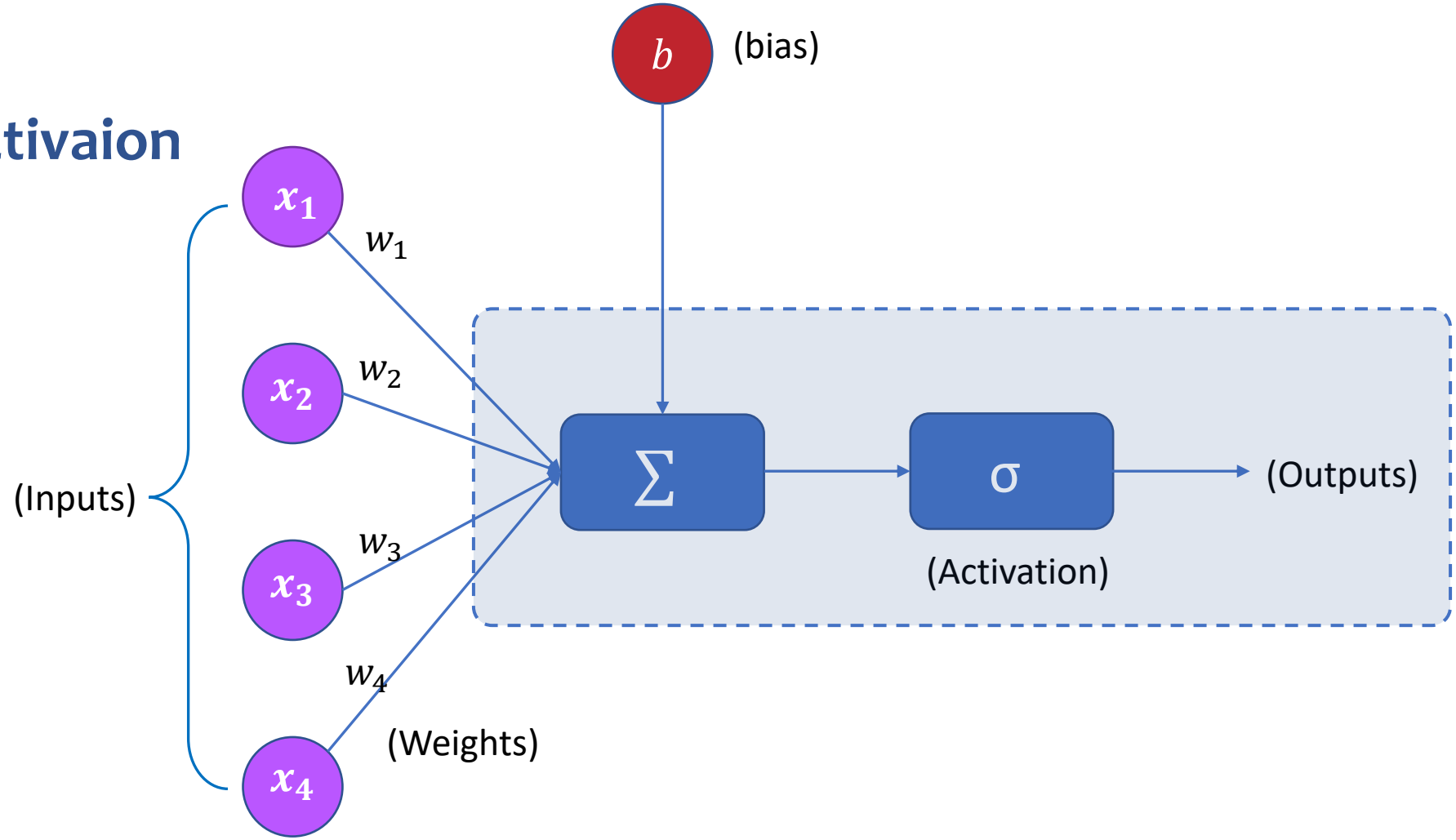
Fig: Parallel Transport

$$x^H \leftarrow x^H \oplus b = \exp_{x^H}\left(P_{0 \to x^H}(\log_0(b))\right)$$

Fig: https://imgur.com/gallery/tqplYeT

2.2.1 Hyperbolic Feed Forward Layer

- Matrix-vector Multiplication
- Bias Addition
- **Non-linear Activaion**



2.2.1 Hyperbolic Feed Forward Layer

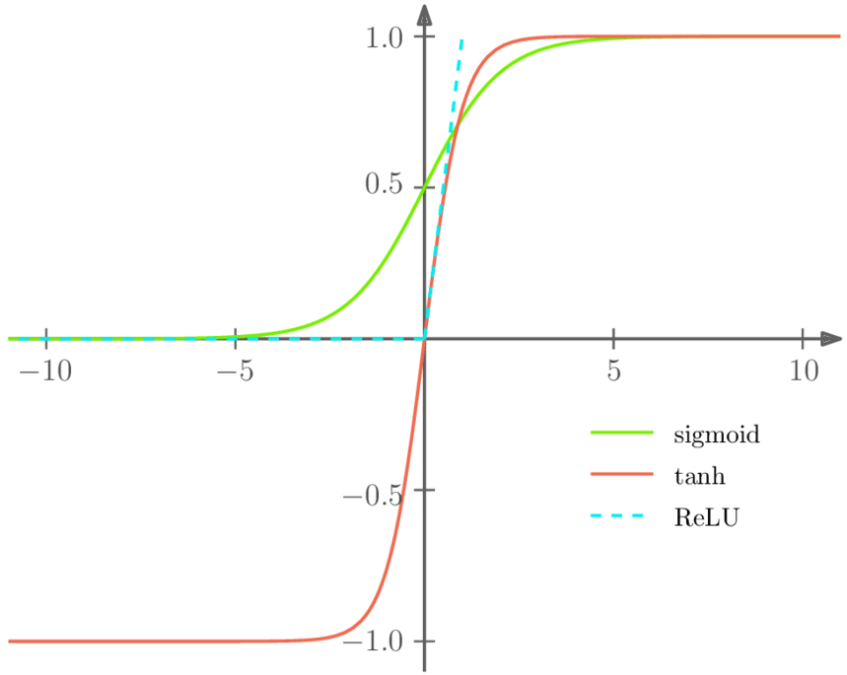
- Non-linear Activation on Poincaré Ball Model and Lorentz Model

  - In Euclidean Space

$$x \leftarrow f(x)$$

  - In Hyperbolic Space

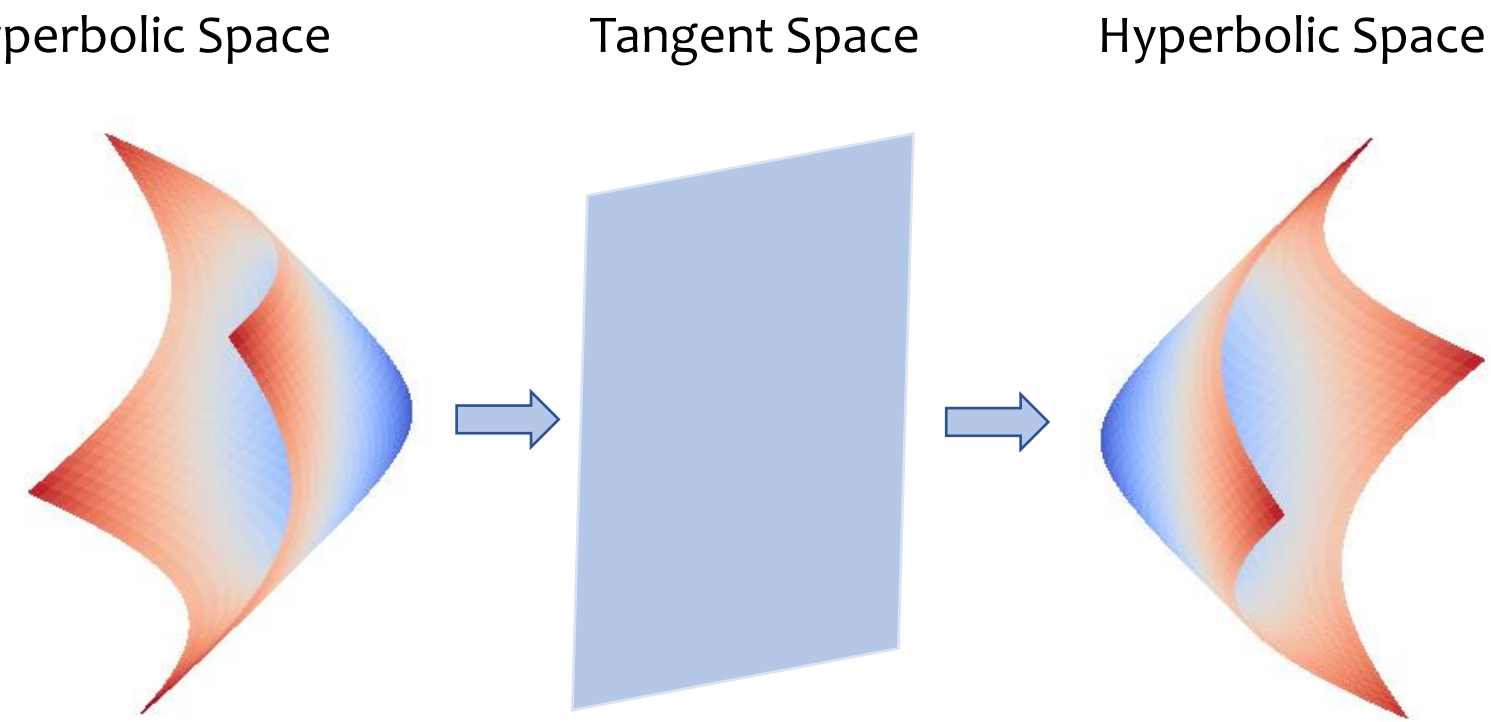
$$x^H \leftarrow f(x^H)$$



$$\text{Update}^{K_{l-1},K_l}(x^H) := \exp_0^{K_l}\left(f\left(\log_0^{K_{l-1}}(x^H)\right)\right)$$

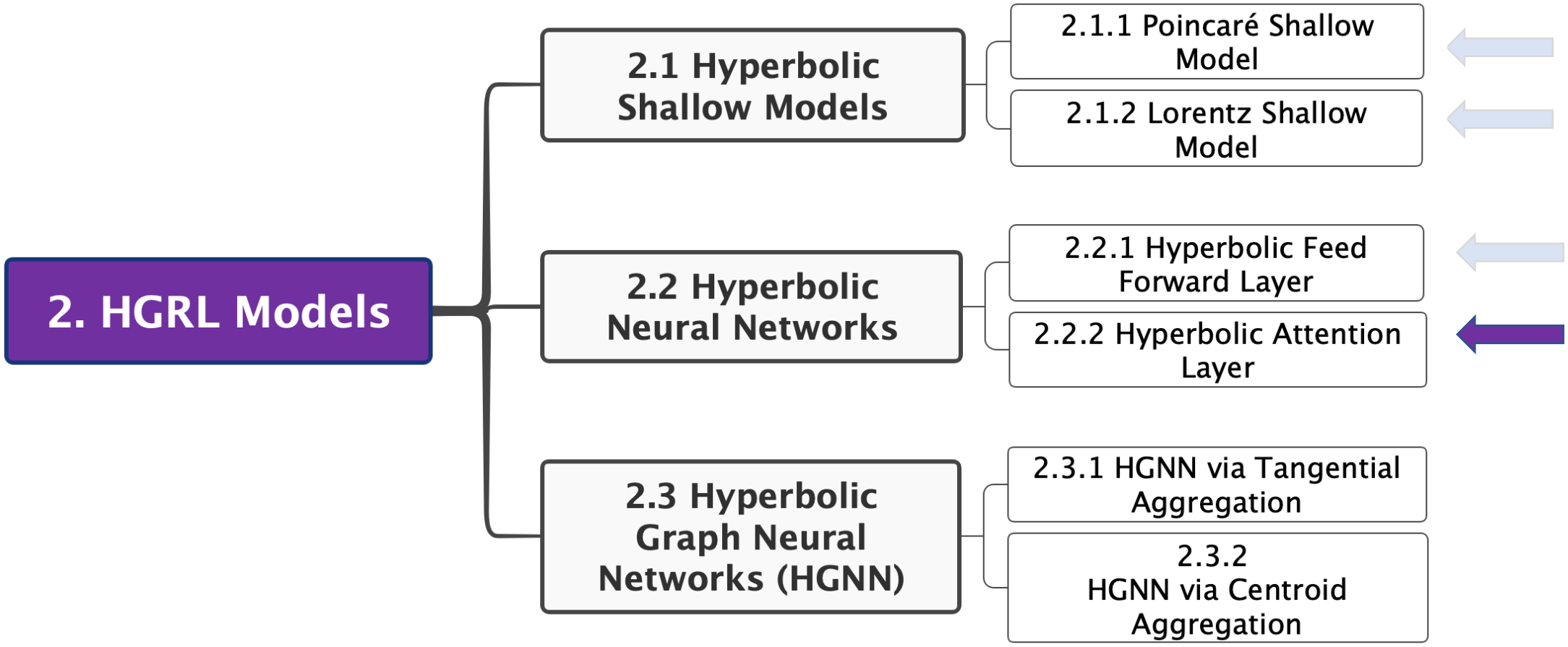
Fig: https://imgur.com/gallery/tqplYeT

2.2.1 Uniform Paradim



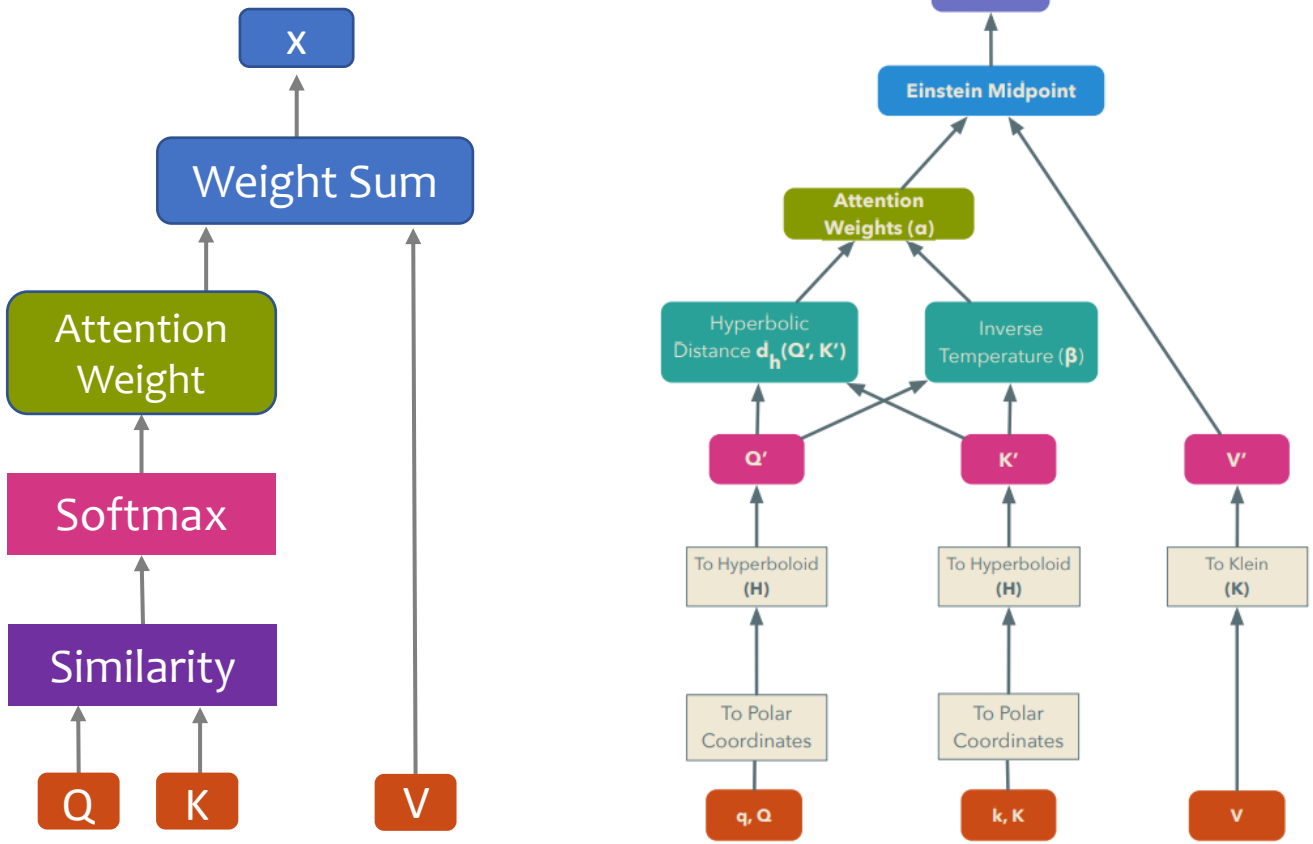
- Hyperbolic space to tangent space
- Operations on tangent space
- Tangent space to Hyperbolic space

2.2 Hyperbolic Neural Networks



2.2 Hyperbolic Neural Networks

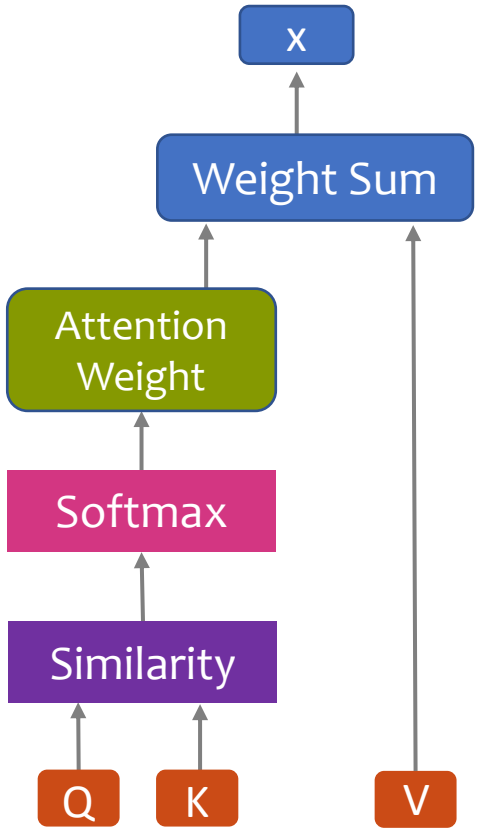
- Hyperbolic Attention Layer

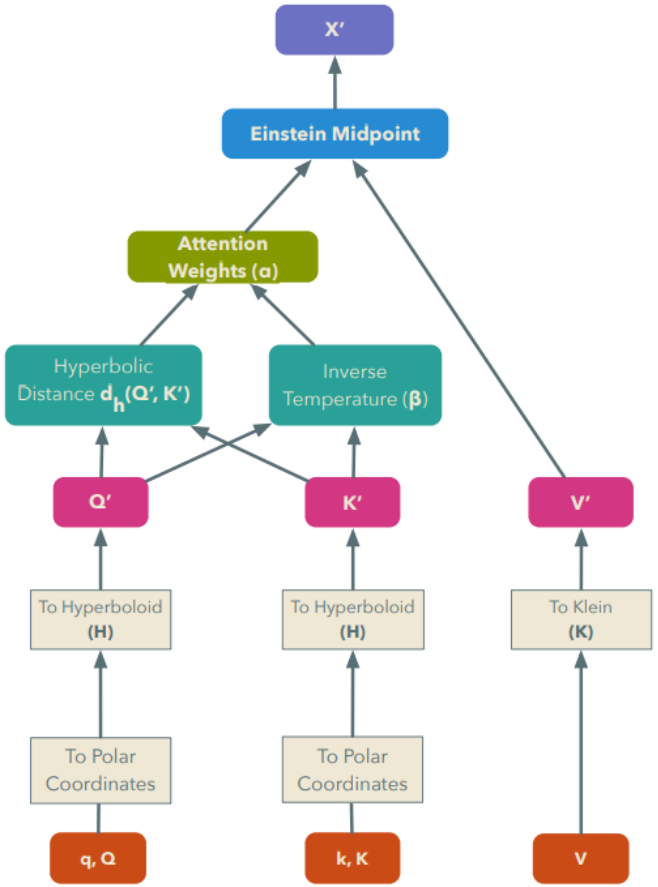


Gulcehre, Caglar, et al. "Hyperbolic attention networks." *arXiv preprint arXiv:1805.09786* (2018).

2.2 Hyperbolic Neural Networks

- Hyperbolic Attention Layer





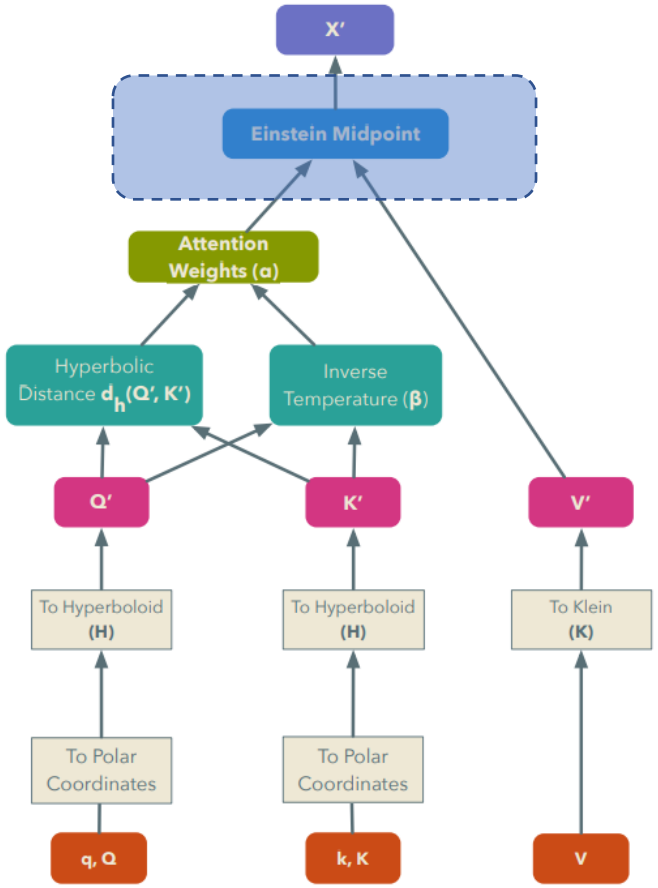
Final Results x:

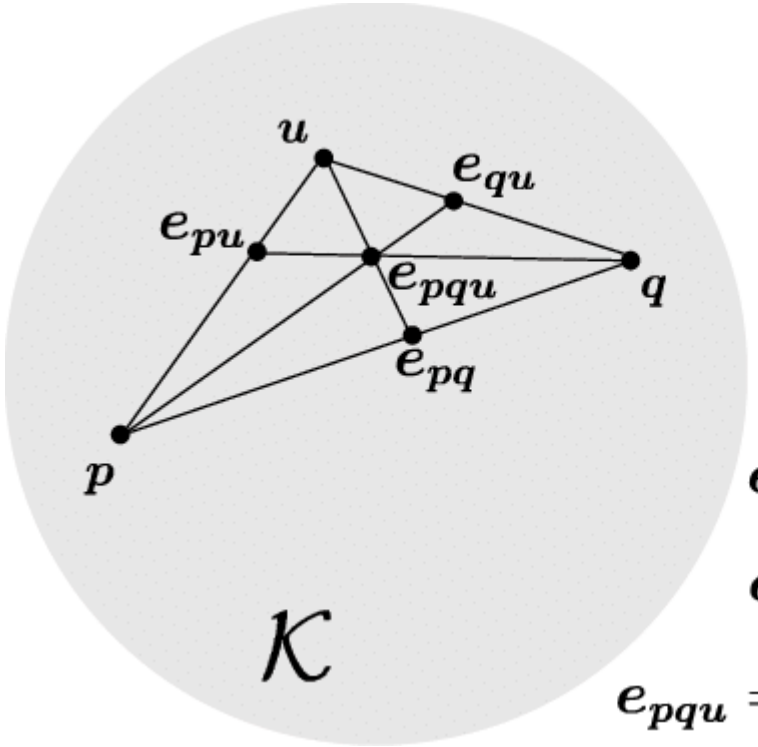
$$\mathrm{x}' = \sum_j \left[\frac{\alpha_{ij}\gamma(\boldsymbol{v}_{ij})}{\sum_\ell \alpha_{i\ell}\gamma(\boldsymbol{v}_{i\ell})} \right] \boldsymbol{v}_{ij}$$

Attention Weights:

$$\alpha(\mathbf{q_i}, \mathbf{k_i}) = f(-\beta \mathrm{d_h}(\mathbf{q_i}, \mathbf{k_j}) - \mathrm{c})$$

Einstein Midpoint





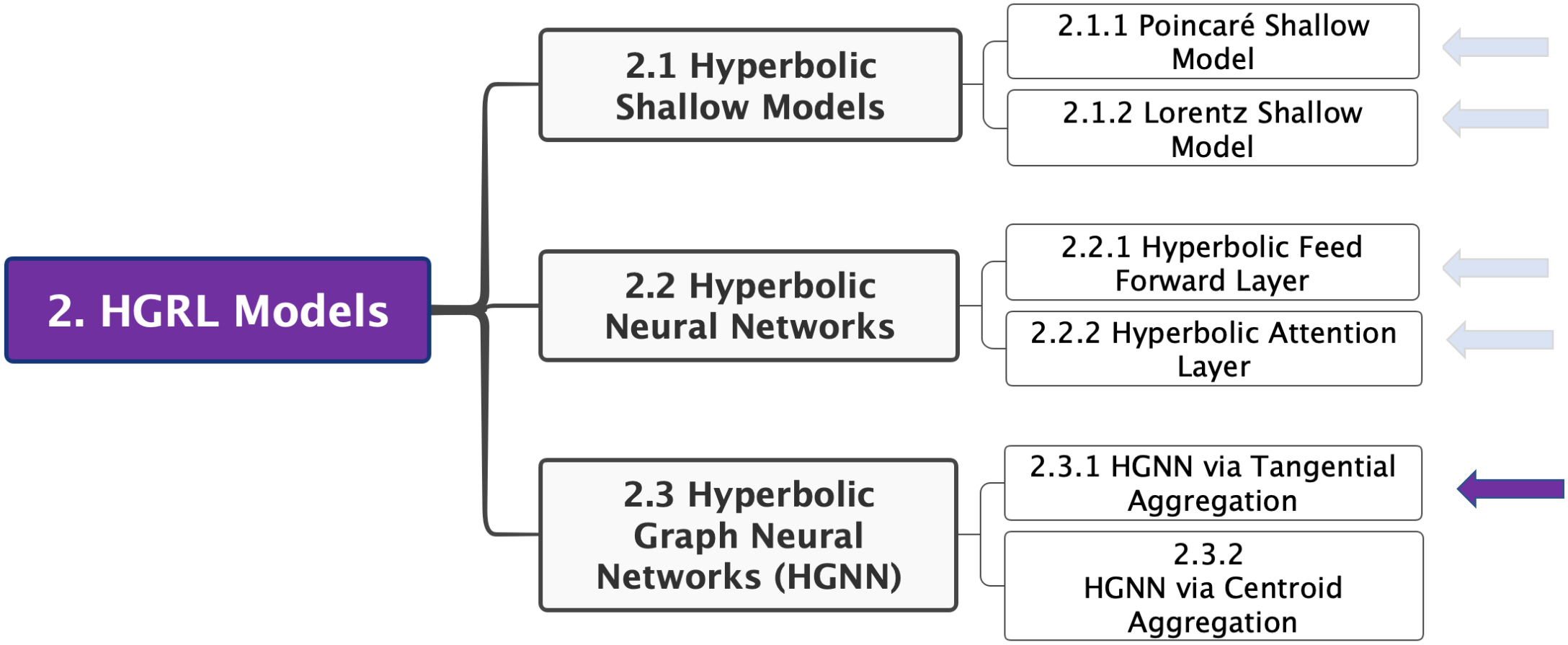
$$e_{pq} = \frac{\gamma_p p + \gamma_q q}{\gamma_p + \gamma_q}$$

$$e_{pu} = \frac{\gamma_p p + \gamma_u u}{\gamma_p + \gamma_u}$$

$$e_{qu} = \frac{\gamma_q q + \gamma_u u}{\gamma_q + \gamma_u}$$

$$e_{pqu} = \frac{\gamma_p p + \gamma_q q + \gamma_u u}{\gamma_p + \gamma_q + \gamma_u}$$

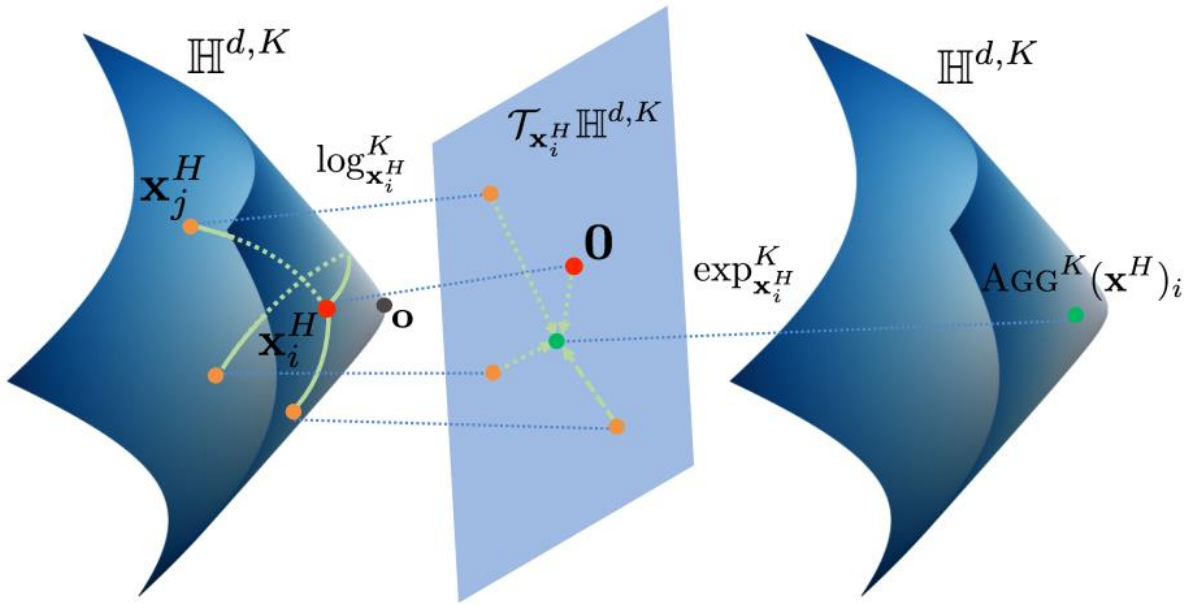
2.2 Hyperbolic Neural Networks



2.3 HGNN via Tangential Aggregation

- Hyperbolic Graph Convolutional Neural Networks
  - Feature Transformation (**Message**)
  - Neighborhood Aggregation (**Aggregation**)
  - Non-linear Activation (**Update**)

- $\boldsymbol{h}_i^{l,H} = \mathrm{Msg}(\boldsymbol{x}_i^{l-1,H})$
- $\boldsymbol{y}_i^{l,H} = \mathrm{AGG}^{K_{l-1}}(\boldsymbol{h}^{l,H})_i$
- $\boldsymbol{x}_i^{l,H} = \mathrm{Update}^{K_{l-1},K_l}(\boldsymbol{y}_i^{l,H})$



Chami, Ines, et al. "Hyperbolic graph convolutional neural networks." NeurIPS (2019).

2.3 HGNN via Tangential Aggregation

- Input Transformation: $x^{0,H} := \exp_0^K\left((0, x^{0,E})\right)$

- **Message:**

$$\boldsymbol{h}_i^{l,H} = \left(W^l \otimes^{K_{l-1}} \boldsymbol{x}_i^{l-1,H}\right) \oplus^{K_{l-1}} \boldsymbol{b}^l$$

$$W \otimes^K \boldsymbol{x}^H := \exp_0^K(W \log_0^K(\boldsymbol{x}))$$

$$\boldsymbol{x}^H \oplus \boldsymbol{b} := \exp_{x^H}^K\left(P_{o \to x^H}^K(\boldsymbol{b})\right)$$

- **Aggregation:**

$$\mathrm{AGG}(\boldsymbol{x}^H)_i := \exp_{\boldsymbol{x}_i^H}^{\mathrm{K}}\Big(\sum_{j \in N(j)} w_{ij} \log_{\boldsymbol{x}_i^H}^{\mathrm{K}}(\boldsymbol{x}_j^H)\Big)$$

Attention weights

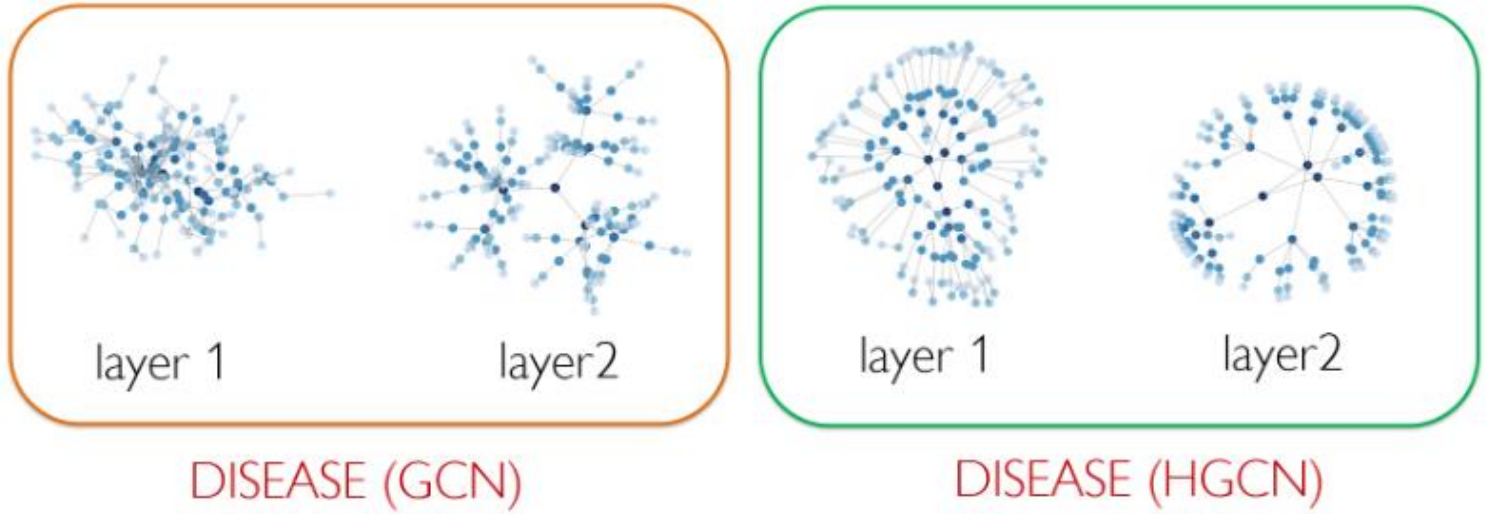
- **Update:**

Trainable curvature

$$\mathrm{Update}^{K_{l-1}, K_l}(x^H) := \exp_0^{K_l}\left(\sigma\left(\log_{\mathrm{o}}^{K_{l-1}}(x^H)\right)\right)$$

Chami, Ines, et al. "Hyperbolic graph convolutional neural networks." NeurIPS (2019).

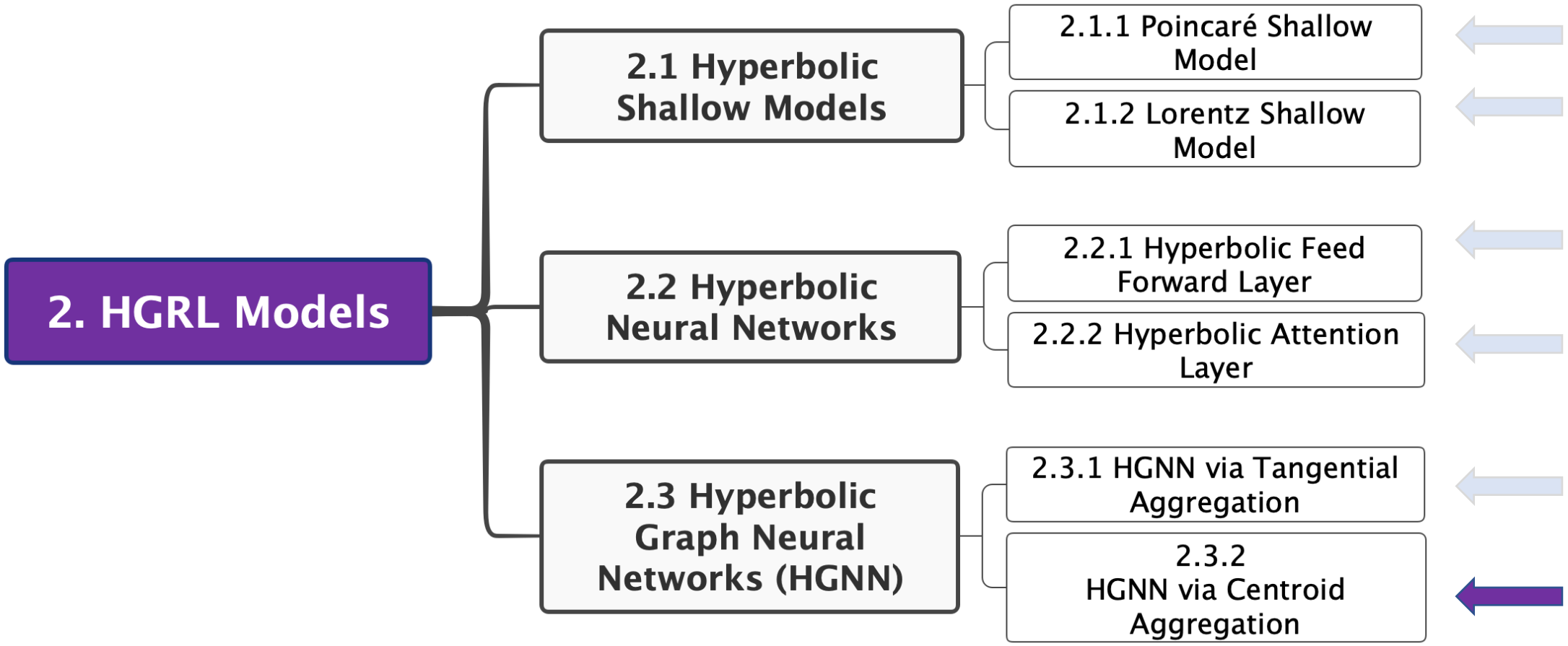
2.3 HGNN via Tangential Aggregation



The above show that the 1st layer and 2nd layer embedding for both GCN and HGCN.

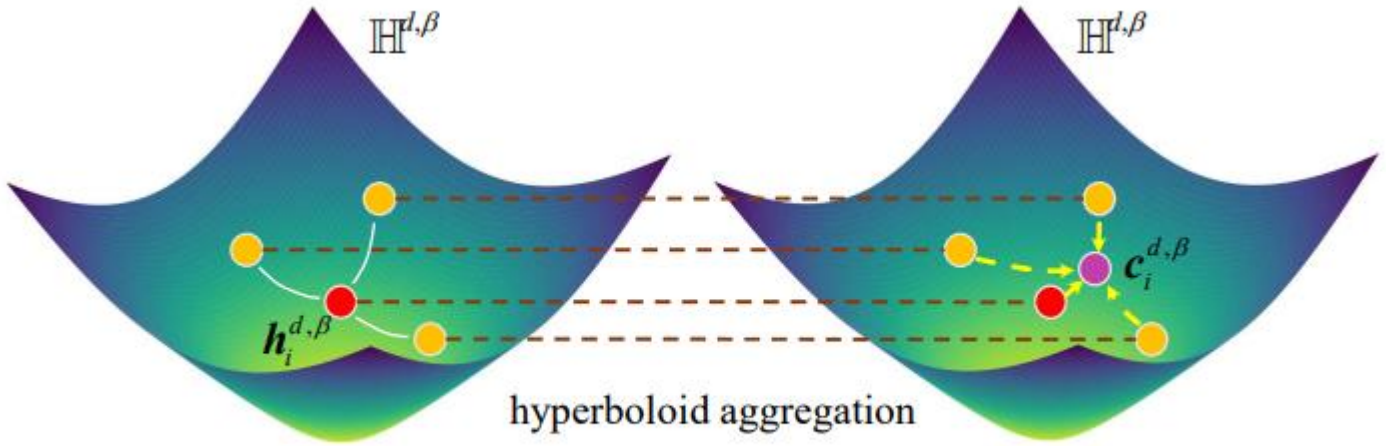
HGCN can map the nodes to embeddings of different hyperbolic space with different curvature at each layer, resulting in low distortion embedding for hierarchical data.

Chami, Ines, et al. "Hyperbolic graph convolutional neural networks." NeurIPS (2019).


2. HGRL Models
2.1 Hyperbolic Shallow Models
2.1.1 Poincaré Shallow Model
2.1.2 Lorentz Shallow Model
2.2 Hyperbolic Neural Networks
2.2.1 Hyperbolic Feed Forward Layer
2.2.2 Hyperbolic Attention Layer
2.3 Hyperbolic Graph Neural Networks (HGNN)
2.3.1 HGNN via Tangential Aggregation
2.3.2 HGNN via Centroid Aggregation

2.3 HGNN via Centroid Aggregation

- Hyperbolic Graph Neural Networks
  - Feature Transformation
  - Neighborhood Aggregation
  - Non-linear Activation



(b) Hyperbolic aggregation on hyperboloid model via centroid

Zhang, Yiding, et al. "Lorentzian graph convolutional networks." *The WebConf*. 2021.

2.3 HGNN via Centroid Aggregation

- Input Transformation: $x^{0,H} := \exp_0^K\left((0, x^{0,E})\right)$
- **Message:**

$$\boldsymbol{h}_i^{l,H} = \left(W^l \otimes^{K_{l-1}} \boldsymbol{x}_i^{l-1,H}\right)$$

$$W \otimes^K \boldsymbol{x}^H := \exp_0^K\left(\left(0, \mathrm{W}\log_0^K\left(\boldsymbol{x}_{[1:n]}\right)\right)\right)$$

- **Aggregation:**

$$\mathrm{AGG}(\boldsymbol{x}^H)_i := \frac{\sum_{j\in N(i)} w_{ij} x_j^H}{|\|\sum_{j\in N(i)} w_{ij} x_j^H\|_{\mathcal{L}}|}$$

Edge weights/attention weights

- **Update:**

Trainable curvature

$$\mathrm{Update}^{K_{l-1},K_l}(x^H) := \exp_0^{K_l}\left(0, \sigma\left(\log_{\mathrm{o}}^{K_{l-1}}\left(x_{[1;n]}^H\right)\right)\right)$$

Zhang, Yiding, et al. "Lorentzian graph convolutional networks." *The WebConf*. 2021.

Table 4: AUC (%) for link prediction task. The best results are marked by bold numbers.

Dataset	dimension	deepwalk	poincaréEmb	GraphSage	GCN	GAT	HGCN	κGCN	HAT	LGCN
Disease $\delta_{avg} = 0.00$	8	57.3±1.0	67.9±1.1	65.4±1.4	76.9±0.8	73.5±0.8	84.1±0.7	85.3±0.8	83.9±0.7	**89.2±0.7**
	16	55.2±1.7	70.9±1.0	68.1±1.0	78.2±0.7	73.8±0.6	91.2±0.6	92.0±0.5	91.8±0.5	**96.6±0.6**
	32	49.1±1.3	75.1±0.7	69.5±0.6	78.7±0.5	75.7±0.3	91.8±0.3	94.5±0.6	92.3±0.5	**96.3±0.5**
	64	47.3±0.1	76.3±0.3	70.1±0.7	79.8±0.5	77.9±0.3	92.7±0.4	95.1±0.6	93.4±0.4	**96.8±0.4**
USA $\delta_{avg} = 0.16$	8	91.5±0.1	92.3±0.2	82.4±0.8	89.0±0.6	89.6±0.9	91.6±0.8	92.0±0.6	92.7±0.8	**95.3±0.2**
	16	92.3±0.0	93.6±0.2	84.4±1.0	90.2±0.5	91.1±0.5	93.4±0.3	93.3±0.6	93.6±0.6	**96.3±0.2**
	32	92.5±0.1	94.5±0.1	86.6±0.8	90.7±0.5	91.7±0.5	93.9±0.2	93.2±0.3	94.2±0.6	**96.5±0.1**
	64	92.5±0.1	95.5±0.1	89.3±0.3	91.2±0.3	93.3±0.4	94.2±0.2	94.1±0.5	94.6±0.6	**96.4±0.2**
Amazon $\delta_{avg} = 0.20$	8	96.1±0.0	95.1±0.4	90.4±0.3	91.1±0.6	91.3±0.6	93.5±0.6	92.5±0.7	94.8±0.8	**96.4±1.1**
	16	96.6±0.0	96.7±0.3	90.8±0.5	92.8±0.8	92.8±0.9	96.3±0.9	94.8±0.5	96.9±1.0	**97.3±0.8**
	32	96.4±0.0	96.7±0.1	92.7±0.2	93.3±0.9	95.1±0.5	97.2±0.8	94.7±0.5	97.1±0.7	**97.5±0.3**
	64	95.9±0.0	97.2±0.1	93.4±0.4	94.6±0.8	96.2±0.2	97.1±0.7	95.3±0.2	97.3±0.6	**97.6±0.5**
Cora $\delta_{avg} = 0.35$	8	86.9±0.1	84.5±0.7	87.4±0.4	87.8±0.9	87.4±1.0	91.4±0.5	90.8±0.6	91.1±0.4	**92.0±0.5**
	16	85.3±0.8	85.8±0.8	88.4±0.6	90.6±0.7	93.2±0.4	93.1±0.4	92.6±0.4	93.0±0.3	**93.6±0.4**
	32	82.3±0.4	86.5±0.6	88.8±0.4	92.0±0.6	93.6±0.3	93.3±0.3	92.8±0.5	93.1±0.3	**94.0±0.4**
	64	81.6±0.4	86.7±0.5	90.0±0.1	92.8±0.4	93.5±0.3	93.5±0.2	93.0±0.7	93.3±0.3	**94.4±0.2**
Pubmed $\delta_{avg} = 0.36$	8	81.1±0.1	83.3±0.5	86.1±1.1	86.8±0.7	87.0±0.8	94.6±0.2	93.5±0.5	94.4±0.3	**95.4±0.2**
	16	81.2±0.1	85.1±0.5	87.1±0.4	90.9±0.6	91.6±0.3	96.1±0.2	94.9±0.3	96.2±0.3	**96.6±0.1**
	32	76.4±0.1	86.5±0.1	88.2±0.5	93.2±0.5	93.6±0.2	96.2±0.2	95.0±0.3	96.3±0.2	**96.8±0.1**
	64	75.3±0.1	87.4±0.1	88.8±0.5	93.6±0.4	94.6±0.2	96.5±0.2	94.9±0.5	96.5±0.1	**96.9±0.0**
Citeseer $\delta_{avg} = 0.46$	8	80.7±0.3	79.2±1.0	85.3±1.6	90.3±1.2	89.5±0.9	93.2±0.5	92.6±0.7	93.1±0.3	**93.9±0.6**
	16	78.5±0.5	79.7±0.7	87.1±0.9	92.9±0.7	92.2±0.7	94.3±0.4	93.8±0.4	93.6±0.5	**95.4±0.5**
	32	73.1±0.4	79.8±0.6	87.3±0.4	94.3±0.6	93.4±0.4	94.7±0.3	93.5±0.5	94.2±0.5	**95.8±0.3**
	64	72.3±0.3	79.6±0.6	88.1±0.4	95.4±0.5	94.4±0.3	94.8±0.3	93.8±0.5	94.3±0.2	**96.4±0.2**

Zhang, Yiding, et al. "Lorentzian graph convolutional networks." *The WebConf*. 2021.

3. Applications

Contents

3.1 HGRL for Recommendation Systems

- Recommender System are Everywhere

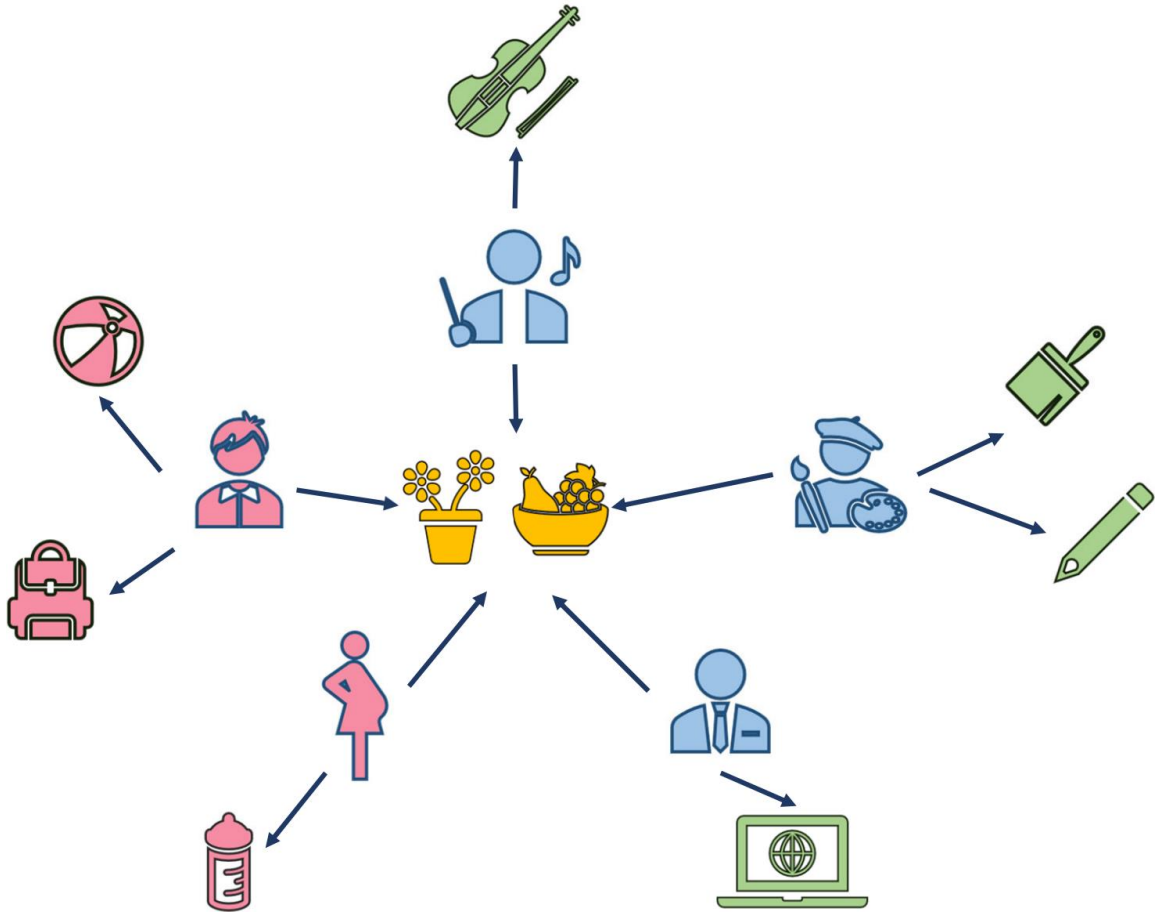
Music Recommendation

Products Recommendation

News Recommendation

3.1 HGRL for Recommendation Systems

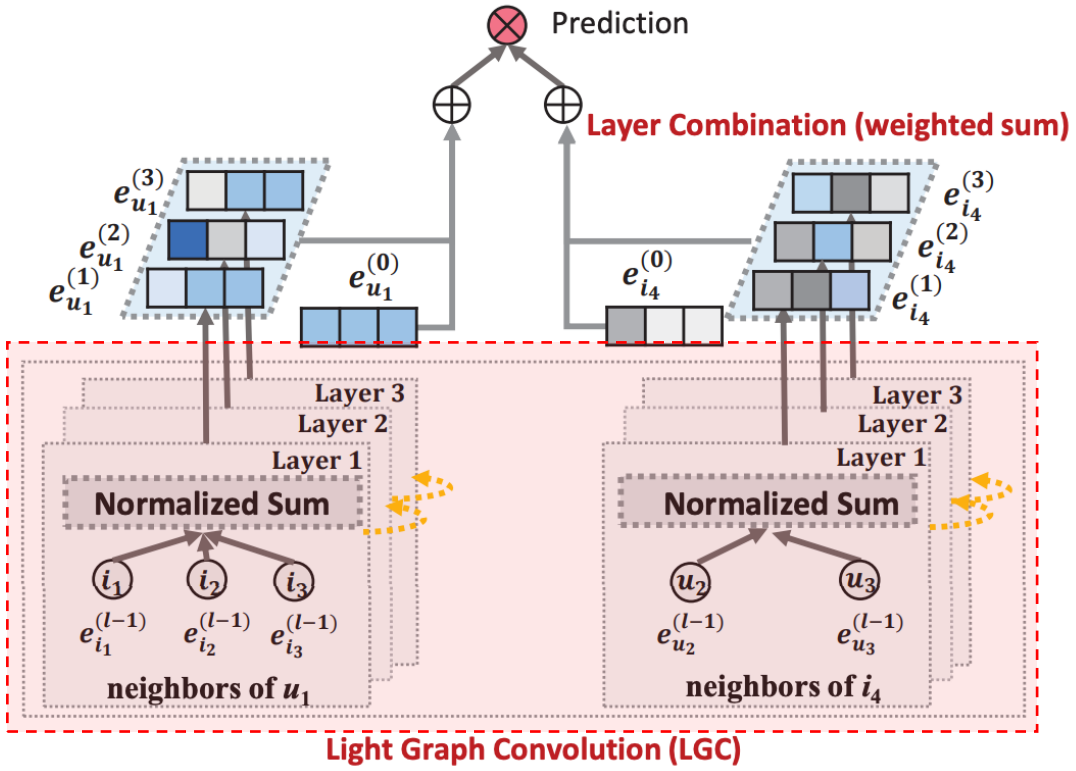
- User-item Networks



Users and items are nodes and the interactions are edges.

3.1 HGRL for Recommendation Systems

- GNN for User-item Network Modeling *in Euclidean Space*



$$\mathbf{e}_u^{(k+1)} = \sum_{i \in \mathcal{N}_u} \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_i|}} \mathbf{e}_i^{(k)},$$

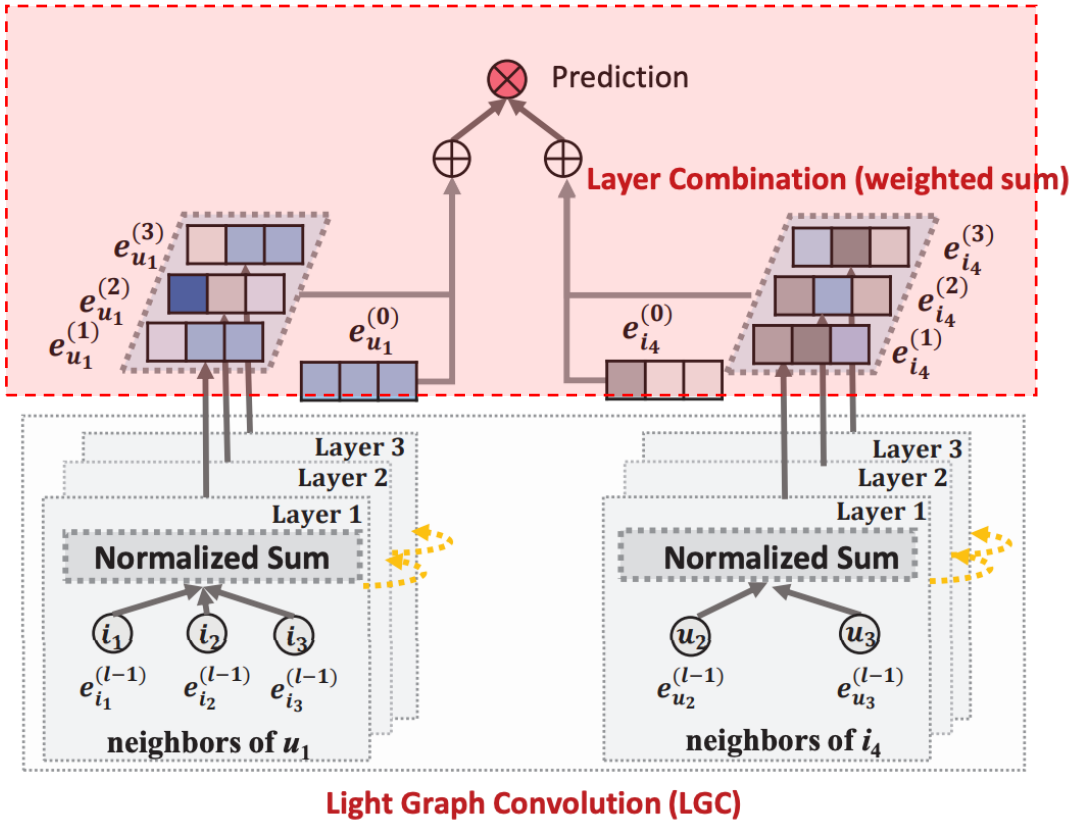
$$\mathbf{e}_i^{(k+1)} = \sum_{u \in \mathcal{N}_i} \frac{1}{\sqrt{|\mathcal{N}_i|}\sqrt{|\mathcal{N}_u|}} \mathbf{e}_u^{(k)}.$$

Note: where $\mathbf{e}_u^k$ and $\mathbf{e}_i^k$ respectively denote the refined embedding of user u and item i after k layers propagation. N_u denotes the set of items that are interacted by user u, N_i denotes the set of users that interact with item i.

Xiangnan He, et al. "Lightgcn: Simplifying and powering graph convolution network for recommendation." SIGIR. 2020.

3.1 HGRL for Recommendation Systems

- GNN for User-item Network Modeling *in Euclidean Space*



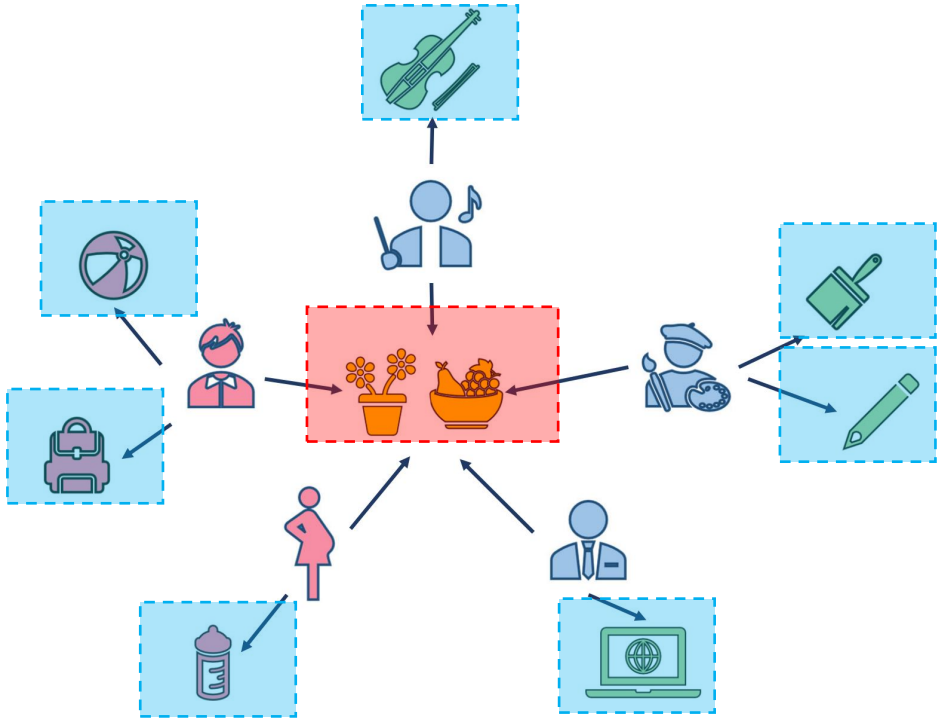
$$\hat{y}_{ui} = \mathbf{e}_u^T \mathbf{e}_i,$$

Note: The model prediction is defined as the inner product of user and item final representations.

Xiangnan He, et al. "Lightgcn: Simplifying and powering graph convolution network for recommendation." SIGIR. 2020.

3.1 HGRL for Recommendation Systems

- User-item Networks



(plotted by Jiahong Liu)

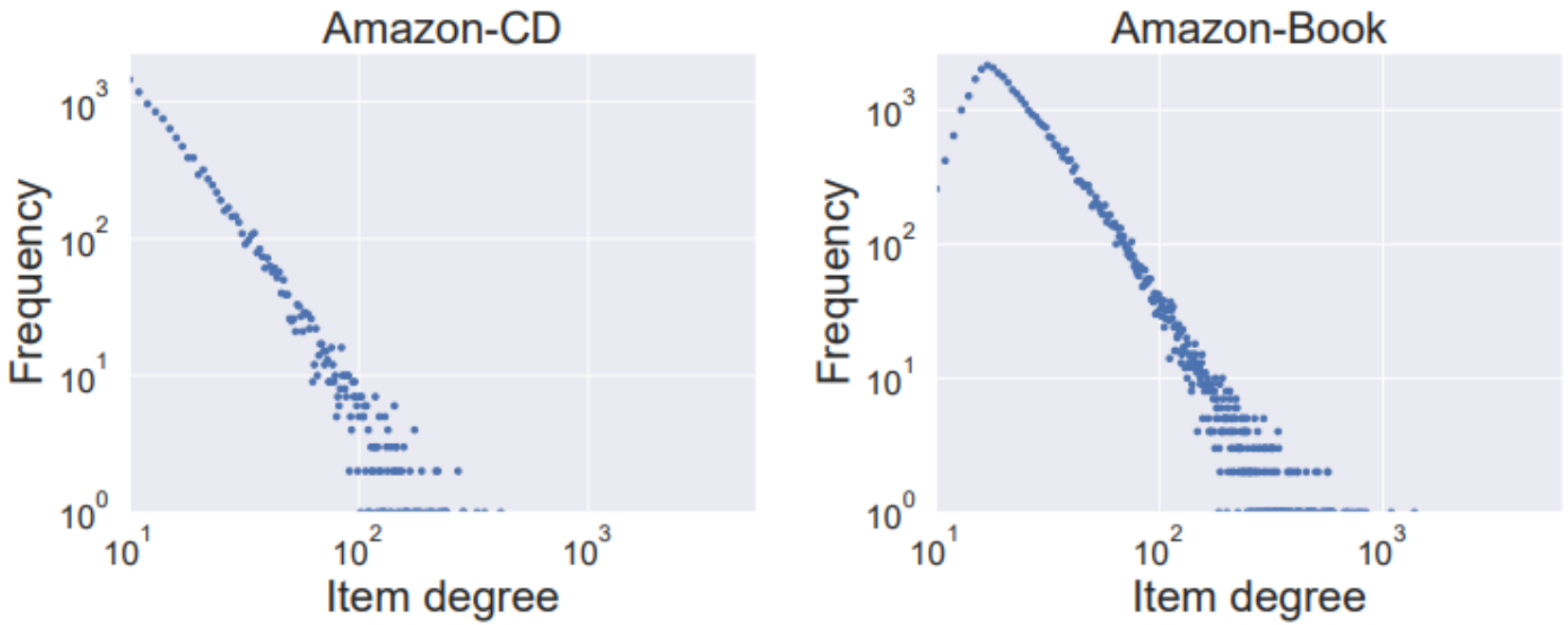
Note: Popular items are competitive while the long-tail item reflects personalized preference or something new.

The popular items are in the minority, whereas the individualized or unpopular items are in the majority.

Menglin Yang, et.al. Hyperbolic Informative Collaborative Filtering. KDD 2022

3.1 HGRL for Recommendation Systems

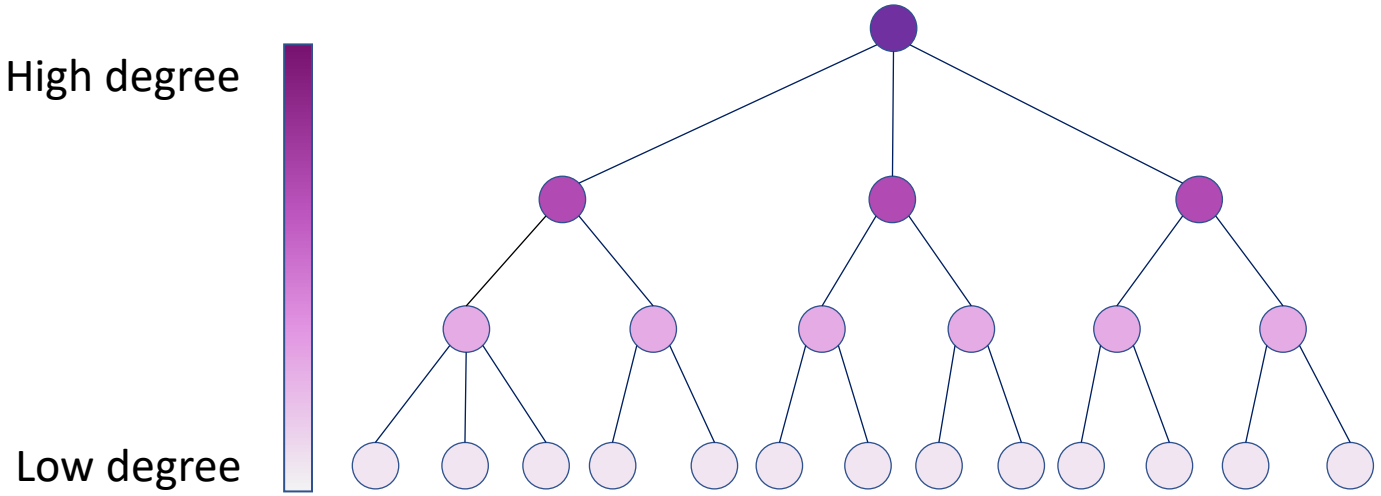
- Degree Distribution



Power-law distribution !!!

Menglin Yang, et al. HRCF: Enhancing collaborative filtering via hyperbolic geometric regularization. *Proceedings of the ACM Web Conference 2022*.

3.1 HGRL for Recommendation Systems



Tree-like structure (Power-law distribution)

Note:

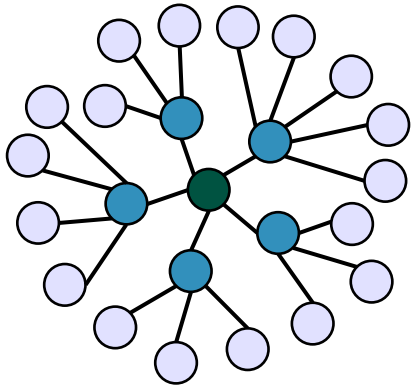
High degree nodes are liked by the majority which indicates their popularity is high.

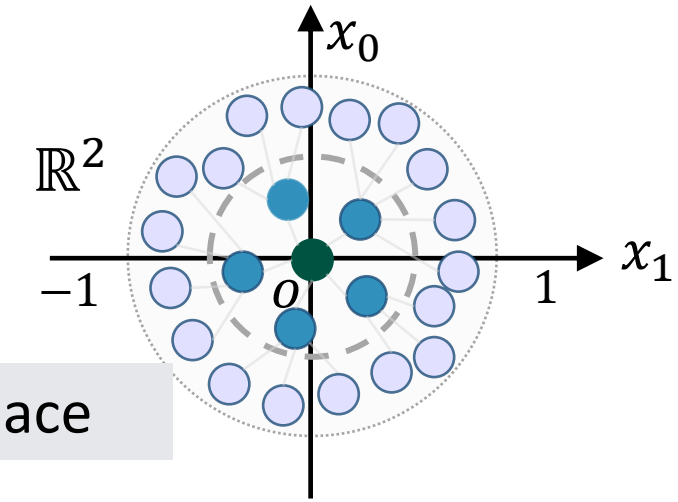
Low degree nodes are liked by the minority which demonstrates **their popularity is low.**

3.1 HGRL for Recommendation Systems

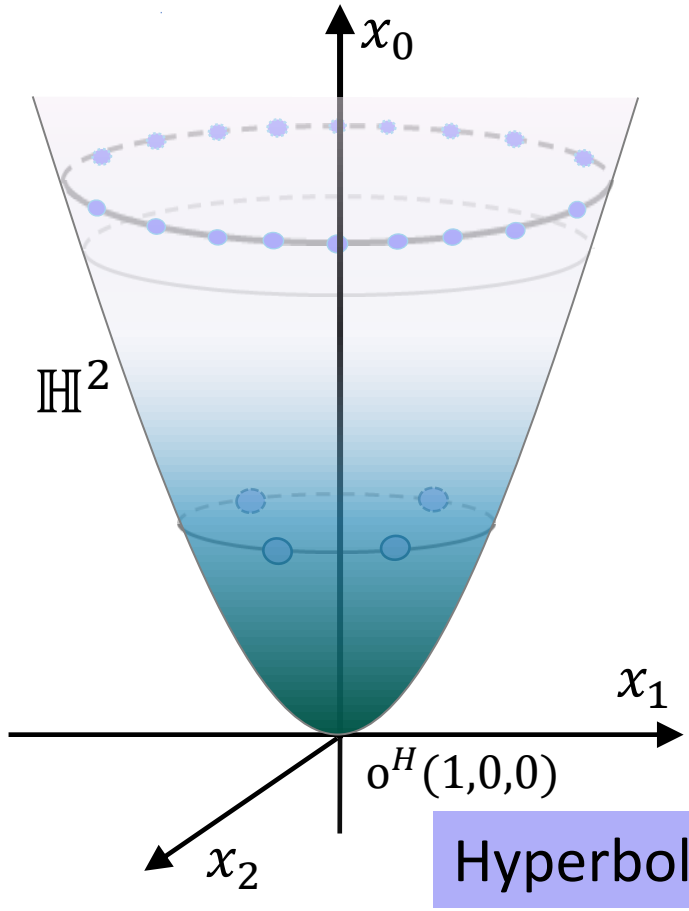
- Embedding Tree-like Graphs

Tree-like G





Euclidean space

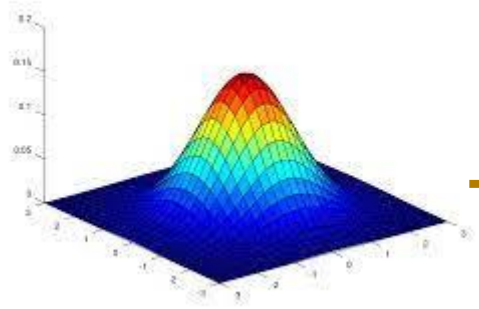


Hyperbolic space

Menglin Yang, et al. HRCF: Enhancing collaborative filtering via hyperbolic geometric regularization. The WebConf 2021

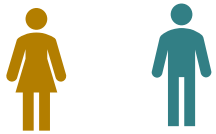
3.1 HGRL for Recommendation Systems

- Hyperbolic Embedding Initializing Layer



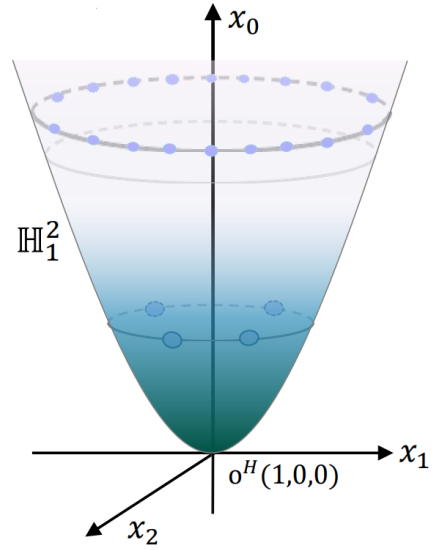
Multivariate Gaussian Distribution

Items' initialized embedding



Users' initialized embedding

$\mathcal{T}_o\mathbb{H}$



$N(\mathbf{0}, \sigma\boldsymbol{I})$

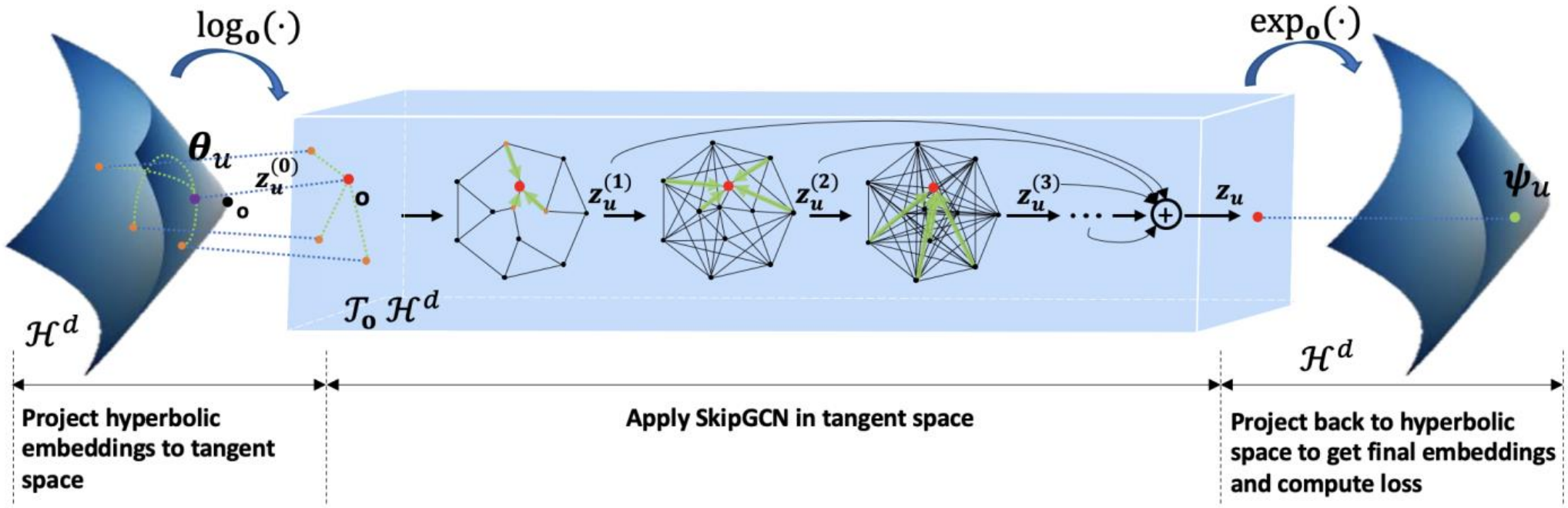
Item: $\mathrm{x}_i \sim N(\mathbf{0}, \sigma\boldsymbol{I})$
User: $\mathrm{x}_u \sim N(\mathbf{0}, \sigma\boldsymbol{I})$

Item: $(0, \mathrm{x}_i)$
User: $(0, \mathrm{x}_u)$

Item: $\mathrm{x}_\mathrm{i}^\mathrm{H} = \exp_\mathrm{o}(0, \mathrm{x}_\mathrm{i})$
User: $\mathrm{x}_\mathrm{i}^\mathrm{H} = \exp_\mathrm{o}(0, \mathrm{x}_\mathrm{u})$

3.1 HGRL for Recommendation Systems (WWW'21)

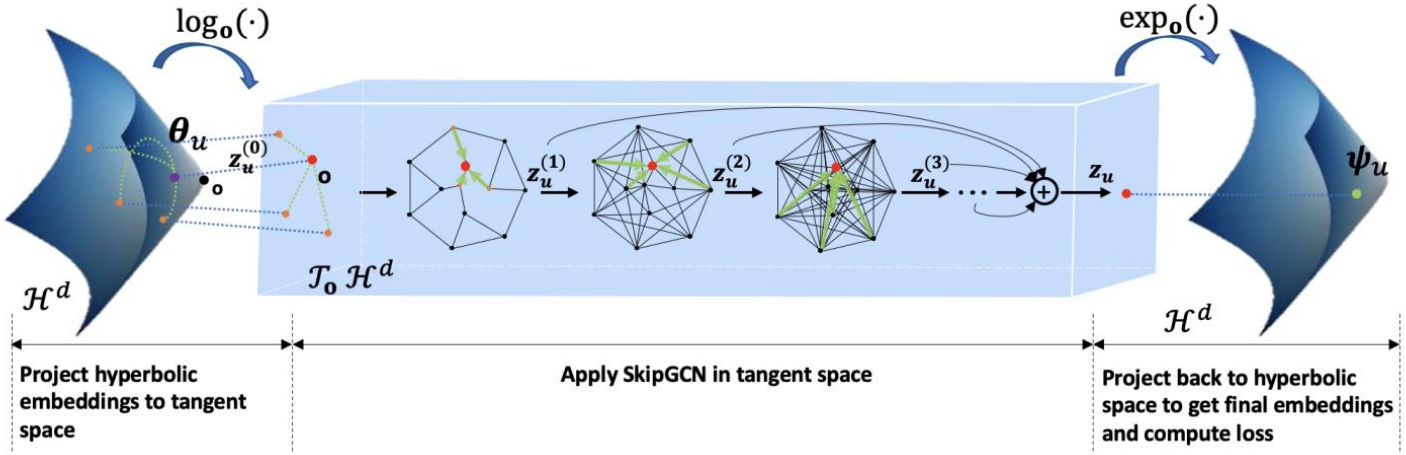
- Hyperbolic Embedding Initializing Layer
- Hyperbolic Message Aggregation



Sun, Jianing, et al. "Hgcf: Hyperbolic graph convolution networks for collaborative filtering." *Proceedings of the Web Conference 2021*.

3.1 HGRL for Recommendation Systems (WWW'21)

- Hyperbolic Embedding Initializing Layer
- Hyperbolic Message Aggregation
- Loss Function

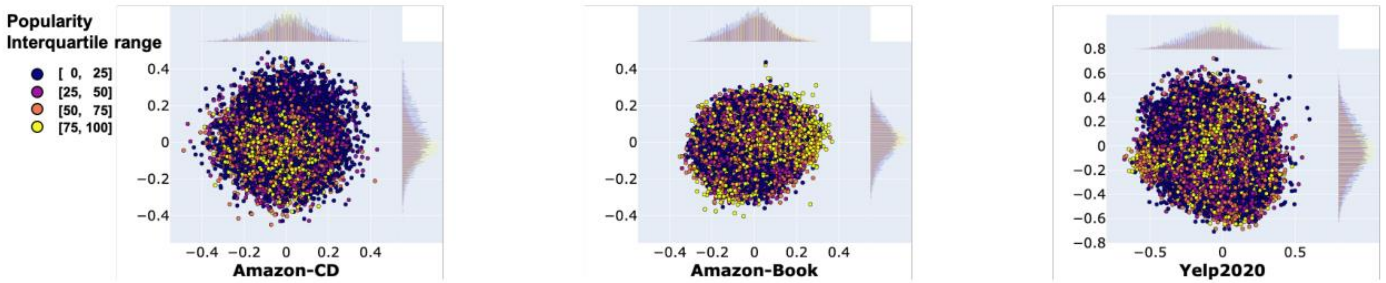


Loss Function

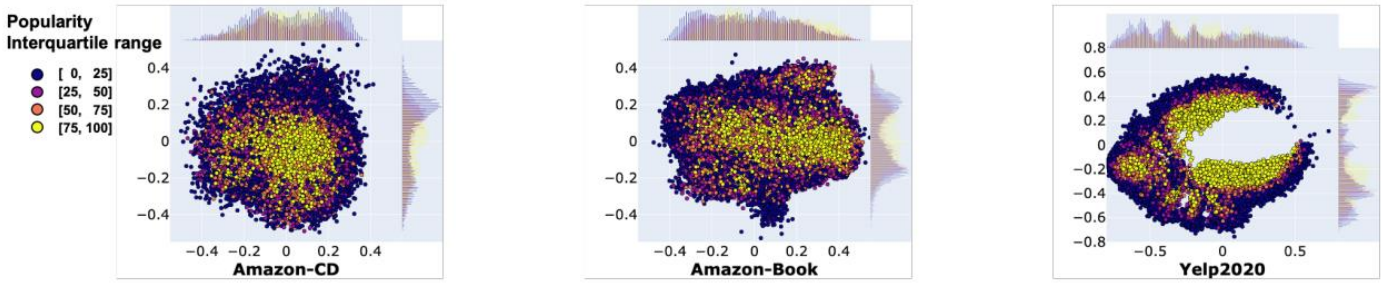
$$L_{\text{margin}}(u,i,j) = \max(d_{\mathcal{L}}(\mathbf{e}_u^H, \mathbf{e}_i^H)^2 - d_{\mathcal{L}}(\mathbf{e}_u^H, \mathbf{e}_j^H)^2 + m, 0)$$

Sun, Jianing, et al. "Hgcf: Hyperbolic graph convolution networks for collaborative filtering." *The WebConf 2021*

3.1 HGRL for Recommendation Systems (WWW'21)



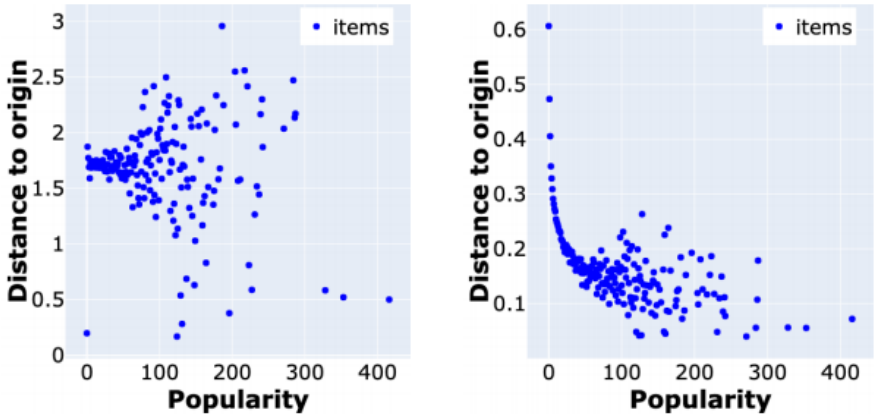
(a) Item embeddings **before** the graph convolution layers.



(b) Item embeddings **after** the graph convolution layers.

- After the graph convolution layers, a clear hierarchy appears according to popularity.
- In the Amazon datasets this hierarchy is reflected in an almost circular way with the most popular items at the center and the less popular ones away from it.

- BPR tends to cluster less popular items at specific distance from the origin.
- HGCF on the other hand has a clear exponential trend where distance to the origin increases exponentially for less popular items



(a) BPR (b) HGCF

Sun, Jianing, et al. "Hgcf: Hyperbolic graph convolution networks for collaborative filtering." *The WebConf 2021*

3.1 HGRL for Recommendation Systems (WSDM '22)

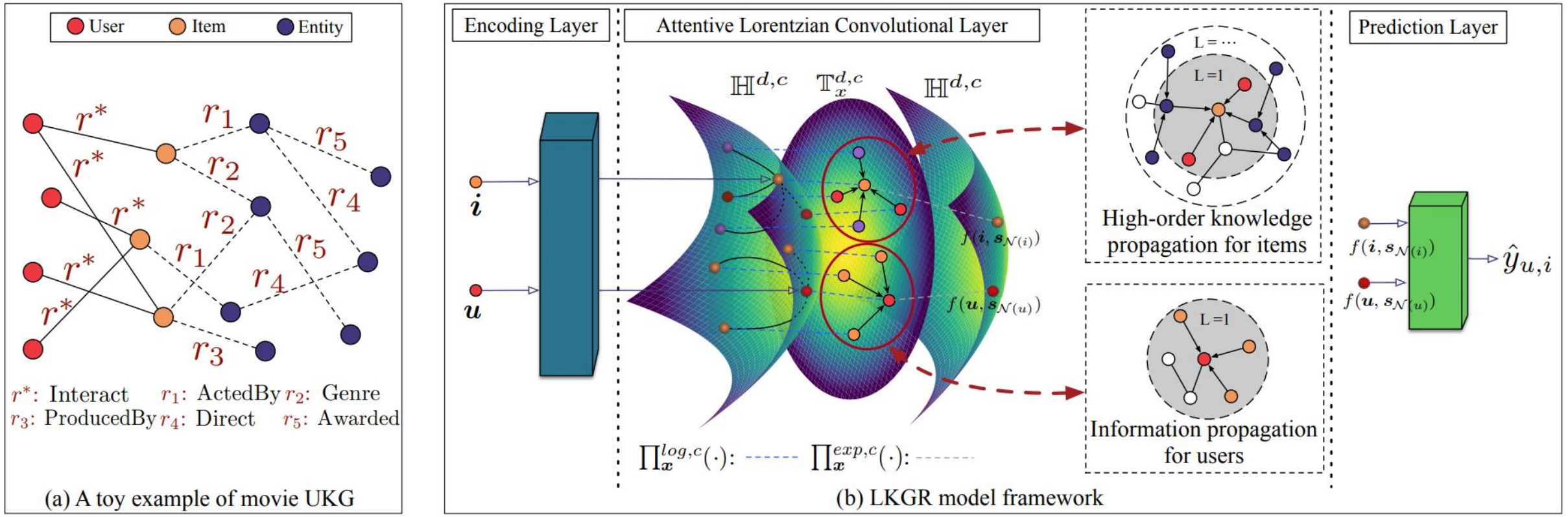
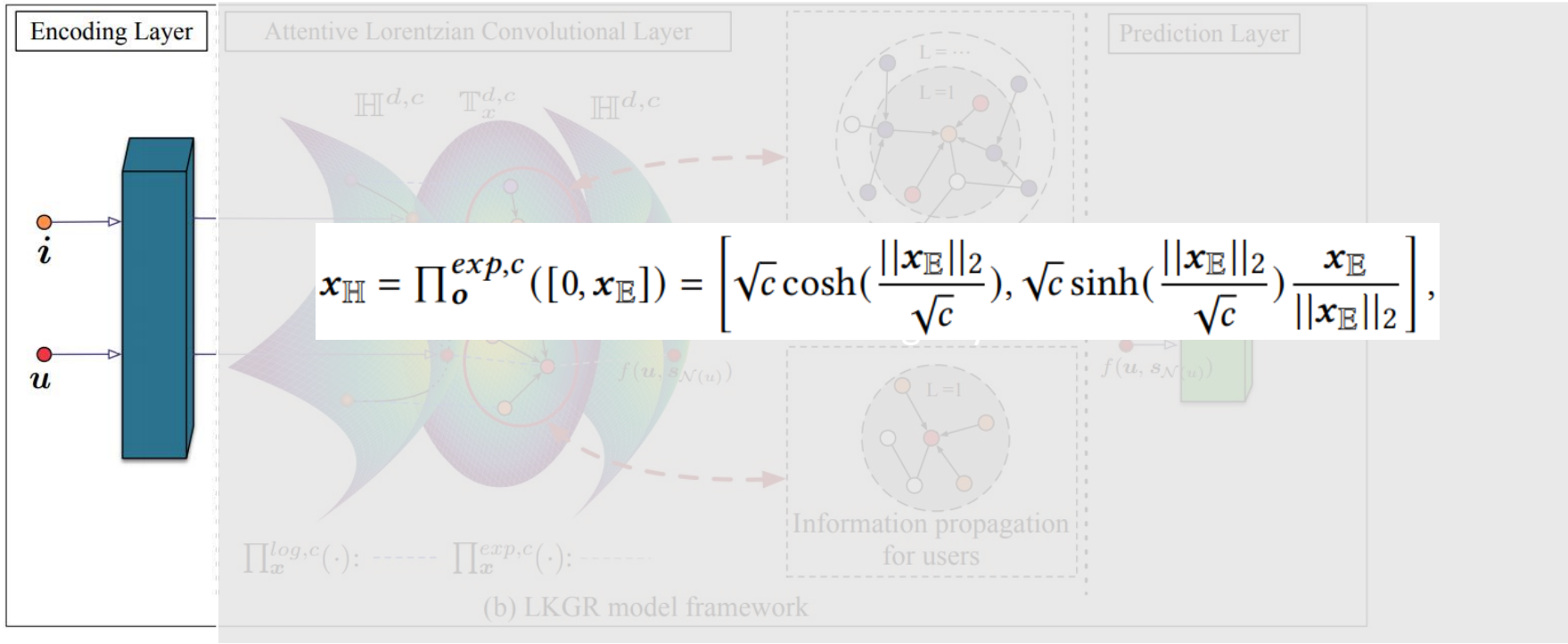


Figure 2: (a) The tripartite graph modeling users, items and KG entities. (b) Illustration of the proposed LKGR model.

Chen, Yankai, et al. "Modeling Scale-free Graphs with Hyperbolic Geometry for Knowledge-aware Recommendation." WSDM '22.

3.1 HGRL for Recommendation Systems (WSDM '22)

- **Encoding Layer**

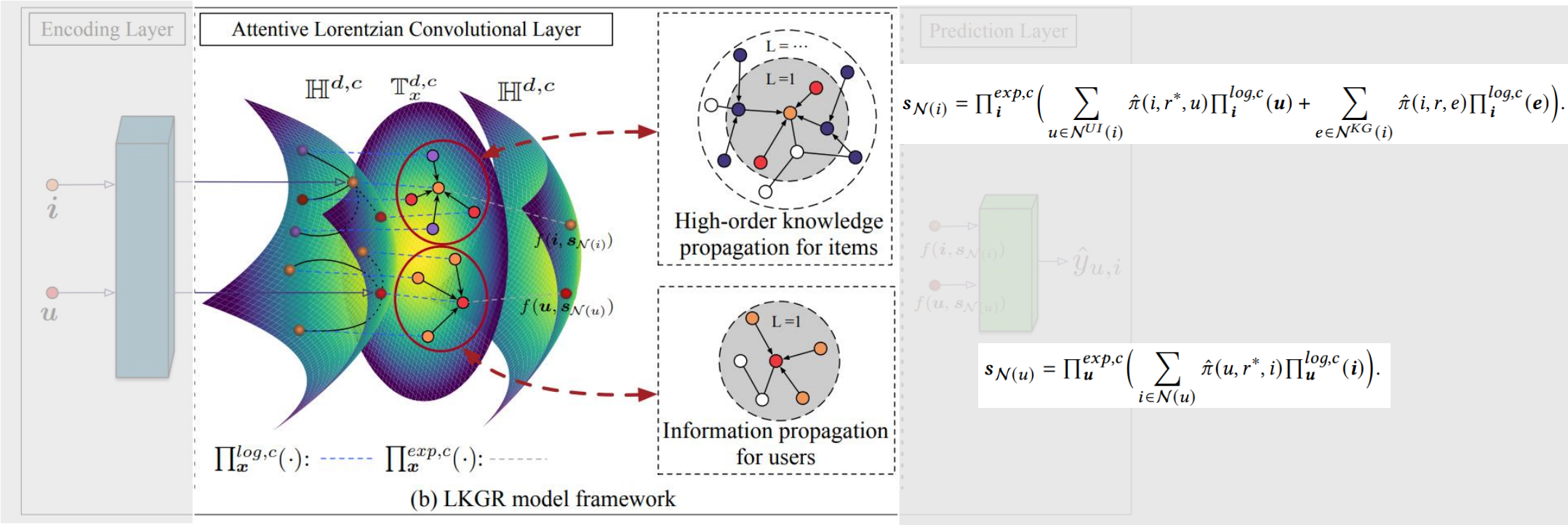


$$x_{\mathbb{H}} = \prod_o^{exp,c}([0, x_{\mathbb{E}}]) = \left[\sqrt{c}\cosh\left(\frac{||x_{\mathbb{E}}||_2}{\sqrt{c}}\right), \sqrt{c}\sinh\left(\frac{||x_{\mathbb{E}}||_2}{\sqrt{c}}\right)\frac{x_{\mathbb{E}}}{||x_{\mathbb{E}}||_2}\right],$$

Chen, Yankai, et al. "Modeling Scale-free Graphs with Hyperbolic Geometry for Knowledge-aware Recommendation." WSDM '22.

3.1 HGRL for Recommendation Systems (WSDM '22)

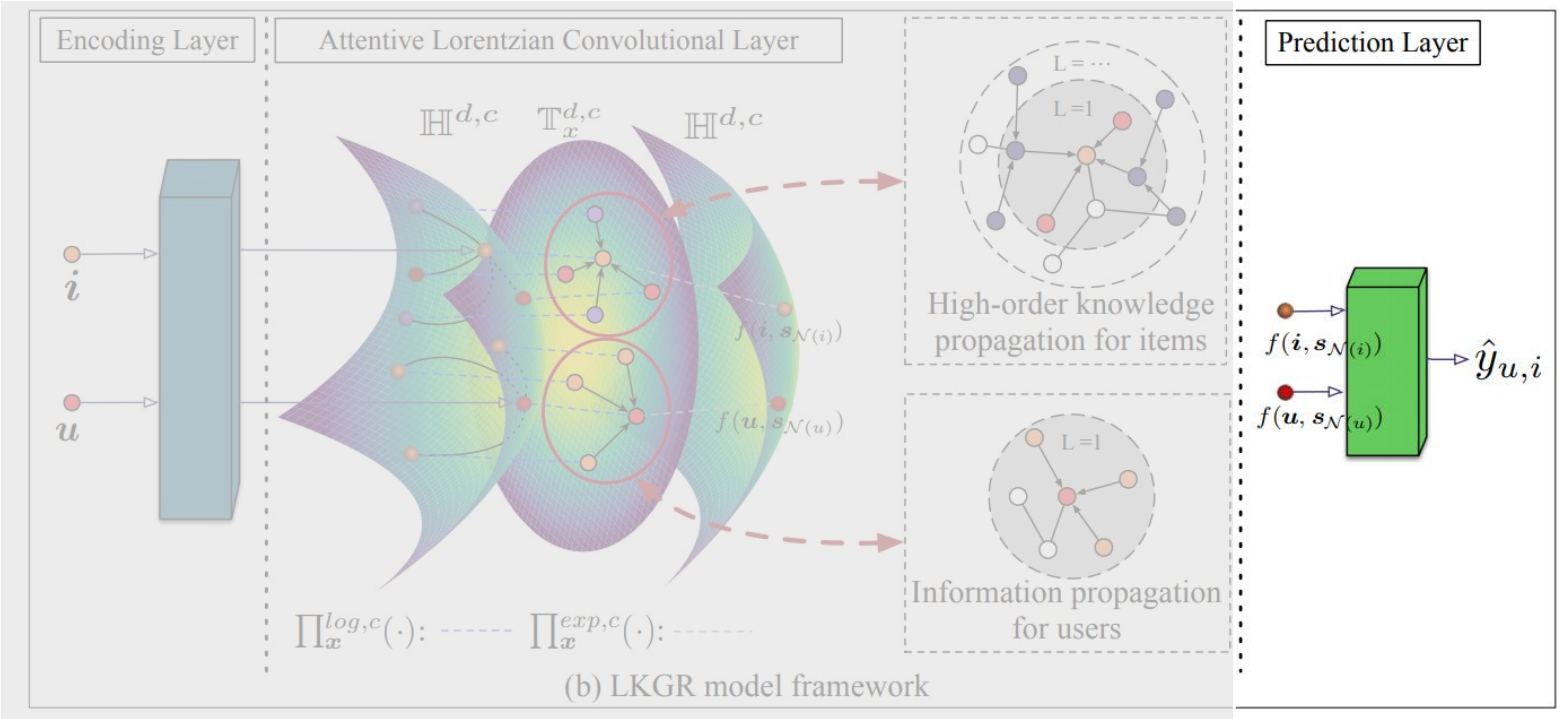
- **Attentive Lorentzian Convolutional Layer**



Chen, Yankai, et al. "Modeling Scale-free Graphs with Hyperbolic Geometry for Knowledge-aware Recommendation." WSDM '22.

3.1 HGRL for Recommendation Systems (WSDM '22)

- **Prediction Layer**



$$\hat{y}_{u,i} = g(\boldsymbol{u}, \boldsymbol{i}) = \left(\prod_o^{log,c}(\boldsymbol{u})\right)^T \prod_o^{log,c}(\boldsymbol{i}).$$

Chen, Yankai, et al. "Modeling Scale-free Graphs with Hyperbolic Geometry for Knowledge-aware Recommendation." WSDM '22.

3.1 HGRL for Recommendation Systems (WSDM '22)

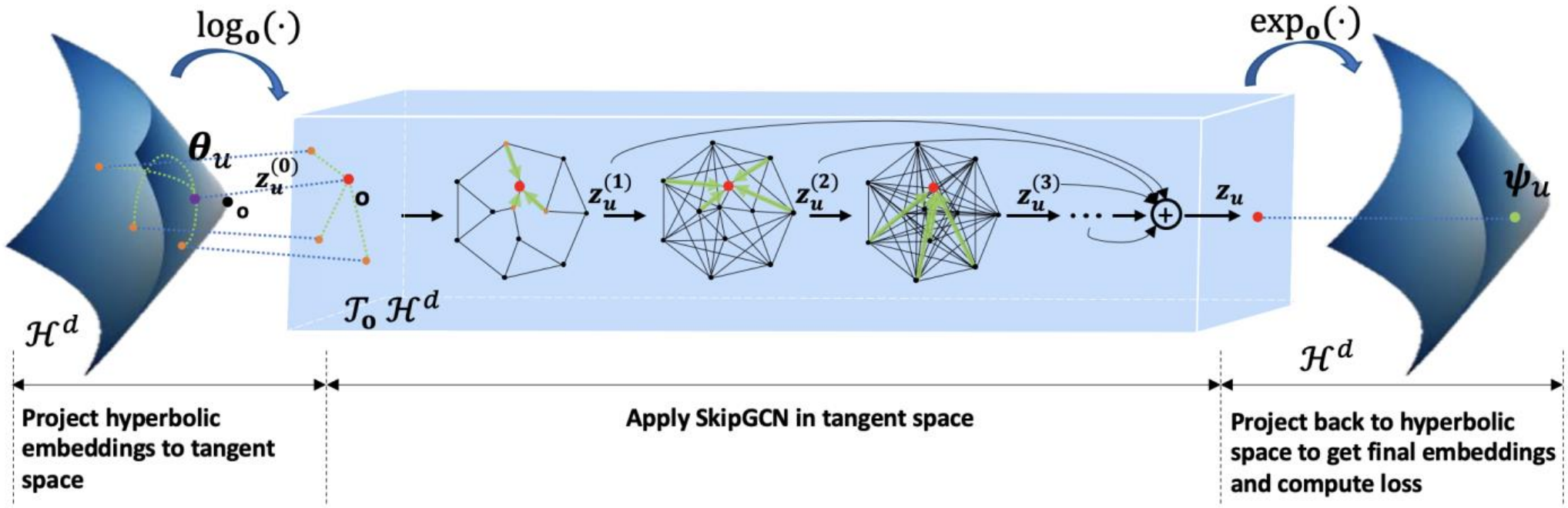
Table 2: Average results of Top@20 recommendation task. Underline indicates the second-best model performance. Bold denotes the empirical improvements against second-best models, and * denotes scenarios where a Wilcoxon signed-rank test indicates a statistically significant improvement under 95% confidence level between our model and second-best models.

Model	Book-Crossing		MovieLens-20M		Dianping-Food	
	Recall@20(%)	NDCG@20(%)	Recall@20(%)	NDCG@20(%)	Recall@20(%)	NDCG@20(%)
BPRMF	4.67 (8.7e-3)	2.80 (4.3e-3)	20.48 (1.6e-2)	15.77 (9.1e-3)	19.90 (3.0e-2)	10.79 (2.0e-2)
NFM	3.93 (2.2e-2)	2.17 (1.5e-2)	19.79 (3.3e-2)	14.28 (1.1e-2)	23.85 (3.9e-2)	<u>12.48</u> (3.0e-2)
CKE	4.38 (9.6e-3)	2.24 (4.2e-2)	21.52 (1.2e-2)	15.73 (1.3e-2)	22.24 (3.1e-2)	12.09 (1.5e-2)
RippleNet	7.12 (2.1e-2)	5.09 (1.7e-2)	13.74 (2.6e-2)	9.77 (1.7e-2)	21.20 (4.1e-2)	10.99 (2.0e-2)
KGNN-LS	<u>8.51</u> (2.2e-2)	<u>6.06</u> (1.7e-2)	20.20 (1.0e-2)	15.49 (1.3e-2)	15.52 (4.9e-2)	7.92 (2.9e-2)
KGCN	7.85 (2.9e-2)	5.93 (2.3e-2)	19.24 (3.2e-2)	13.87 (1.6e-2)	19.03 (3.0e-2)	9.34 (1.5e-2)
KGAT	5.34 (6.1e-3)	3.01 (7.9e-3)	<u>21.80</u> (7.7e-3)	<u>16.81</u> (1.1e-2)	15.57 (2.4e-2)	7.67 (1.7e-2)
CKAN	6.19 (1.1e-2)	3.47 (5.3e-3)	17.48 (1.7e-2)	12.48 (1.4e-2)	<u>24.10</u> (3.9e-2)	**13.33** (2.0e-2)
LKGR	**9.48*** (2.3e-2)	**6.50*** (1.6e-2)	**25.14*** (4.1e-2)	**18.34*** (4.7e-2)	**24.97*** (4.4e-2)	10.45 (1.9e-2)
% Improv.	11.40%	7.26%	15.32%	9.10%	3.61%	N/A

Chen, Yankai, et al. "Modeling Scale-free Graphs with Hyperbolic Geometry for Knowledge-aware Recommendation." WSDM '22.

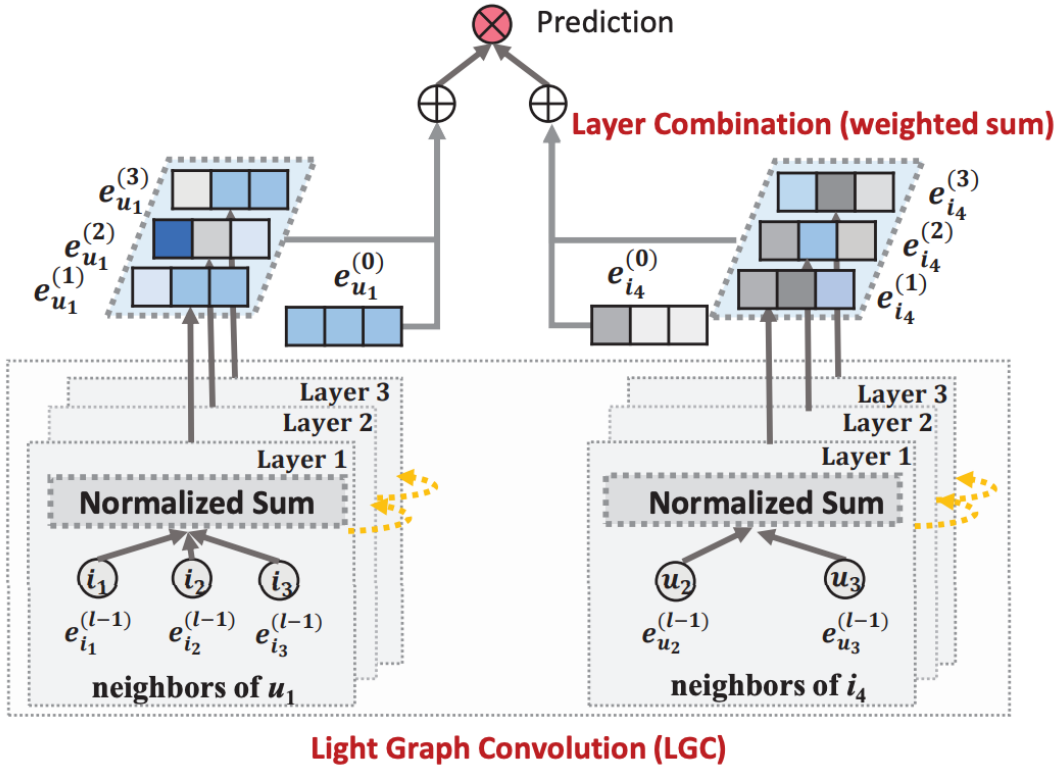
Revisit: HGCF (WWW '21)

- GNN for user-item network modeling in hyperbolic space



Sun, Jianing, et al. "Hgcf: Hyperbolic graph convolution networks for collaborative filtering." *The WebConf 2021*

Revisit: LightGCN (SIGIR '20)



$$\mathbf{e}_u^{(k+1)} = \sum_{i \in \mathcal{N}_u} \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_i|}} \mathbf{e}_i^{(k)},$$

$$\mathbf{e}_i^{(k+1)} = \sum_{u \in \mathcal{N}_i} \frac{1}{\sqrt{|\mathcal{N}_i|}\sqrt{|\mathcal{N}_u|}} \mathbf{e}_u^{(k)}.$$

Note: where $\mathbf{e}_u^k$ and $\mathbf{e}_i^k$ respectively denote the refined embedding of user u and item i after k layers propagation. N_u denotes the set of items that are interacted by user u, N_i denotes the set of users that interact with item i.

Xiangnan He, et al. "Lightgcn: Simplifying and powering graph convolution network for recommendation." SIGIR. 2020.

Revisit: Experimental Comparison

Table 2: Recall (top table) and NDCG (bottom table) results for all datasets. The best performing model on each dataset and metric is highlighted in bold, and second best model is underlined. Asterisks denote statistically significant Wilcoxon signed rank test for the difference in scores between the best and second best models.

Datasets		BPRMF	WRMF	VAE-CF	TransCF	CML	LRML	SML	NGCF	LightGCN	HAE	HVAE	Ours
Amazon-CD	R@10	0.0779	0.0863	0.0786	0.0518	0.0864	0.0502	0.0475	0.0758	0.0929	0.0666	0.0781	**0.0962***
	R@20	0.1200	0.1313	0.1155	0.0791	0.1341	0.0771	0.0734	0.1150	0.1404	0.0963	0.1147	**0.1455***
Amazon-Book	R@10	0.0611	0.0623	0.0740	0.0407	0.0665	0.0522	0.0479	0.0658	0.0799	0.0634	0.0774	**0.0867***
	R@20	0.0974	0.0919	0.1066	0.0632	0.1023	0.0834	0.0768	0.1050	0.1248	0.0912	0.1125	**0.1318***
Yelp2020	R@10	0.0325	0.0470	0.0429	0.0247	0.0363	0.0326	0.0319	0.0458	0.0522	0.0360	0.0421	**0.0543***
	R@20	0.0556	0.0793	0.0706	0.0424	0.0638	0.0562	0.0544	0.0764	0.0866	0.0588	0.0691	**0.0884***

Datasets		BPRMF	WRMF	VAE-CF	TransCF	CML	LRML	SML	NGCF	LightGCN	HAE	HVAE	Ours
Amazon-CD	N@10	0.0610	0.0651	0.0615	0.0396	0.0639	0.0405	0.0361	0.0591	0.0726	0.0565	0.0629	**0.0751***
	N@20	0.0974	0.0817	0.0752	0.0488	0.0813	0.0492	0.0456	0.0718	0.0881	0.0657	0.0749	**0.0909***
Amazon-Book	N@10	0.0594	0.0563	0.0716	0.0392	0.0624	0.0515	0.0422	0.0655	0.0780	0.0709	0.0778	**0.0869***
	N@20	0.0971	0.0730	0.0878	0.0474	0.0808	0.0626	0.0550	0.0791	0.0938	0.0789	0.0901	**0.1022***
Yelp2020	N@10	0.0283	0.0372	0.0353	0.0214	0.0310	0.0287	0.0255	0.0405	**0.0461**	0.0331	0.0371	0.0458
	N@20	0.0512	0.0506	0.0469	0.0277	0.0428	0.0369	0.0347	0.0513	0.0582	0.0409	0.0465	**0.0585***

Questions: In what aspect, hyperbolic model is superior to the Euclidean counterpart?

Sun, Jianing, et al. "Hgcf: Hyperbolic graph convolution networks for collaborative filtering." *The WebConf 2021*

3.1 HGRL for Recommendation Systems

Table 1: Statistics of the experimental data.

Dataset	#User	#Item			#Interactions	Density
		All	H20(%)	T80(%)		
Amazon-CD	22,947	18,395	46	54	422,301	0.10%
Amazon-Book	52,406	41,264	47	53	1,861,118	0.09%
Yelp2020	71,135	45,063	62	37	1,940,014	0.05%

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

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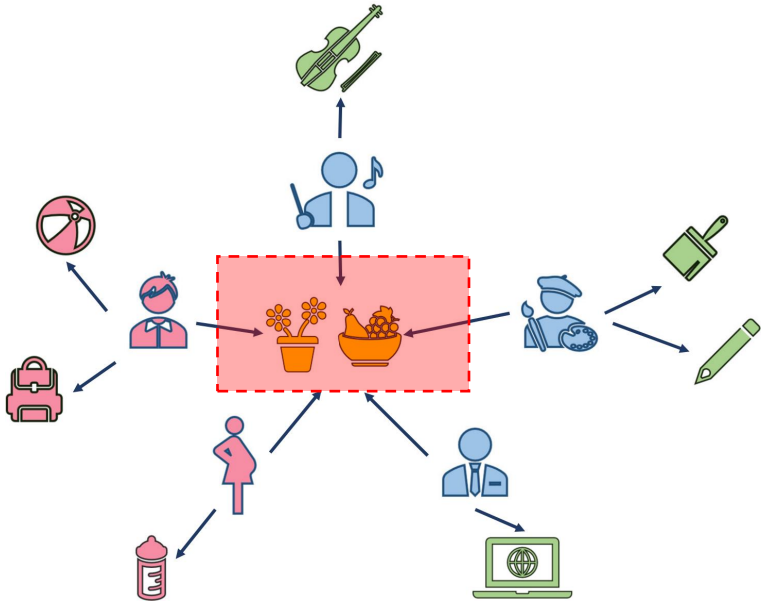

In general, the H20 items account for the minority.

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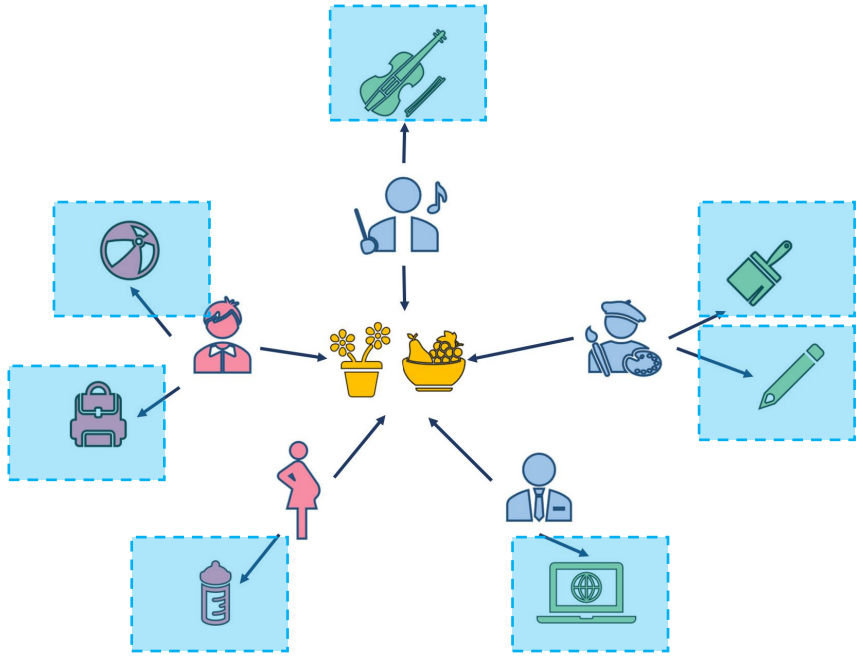

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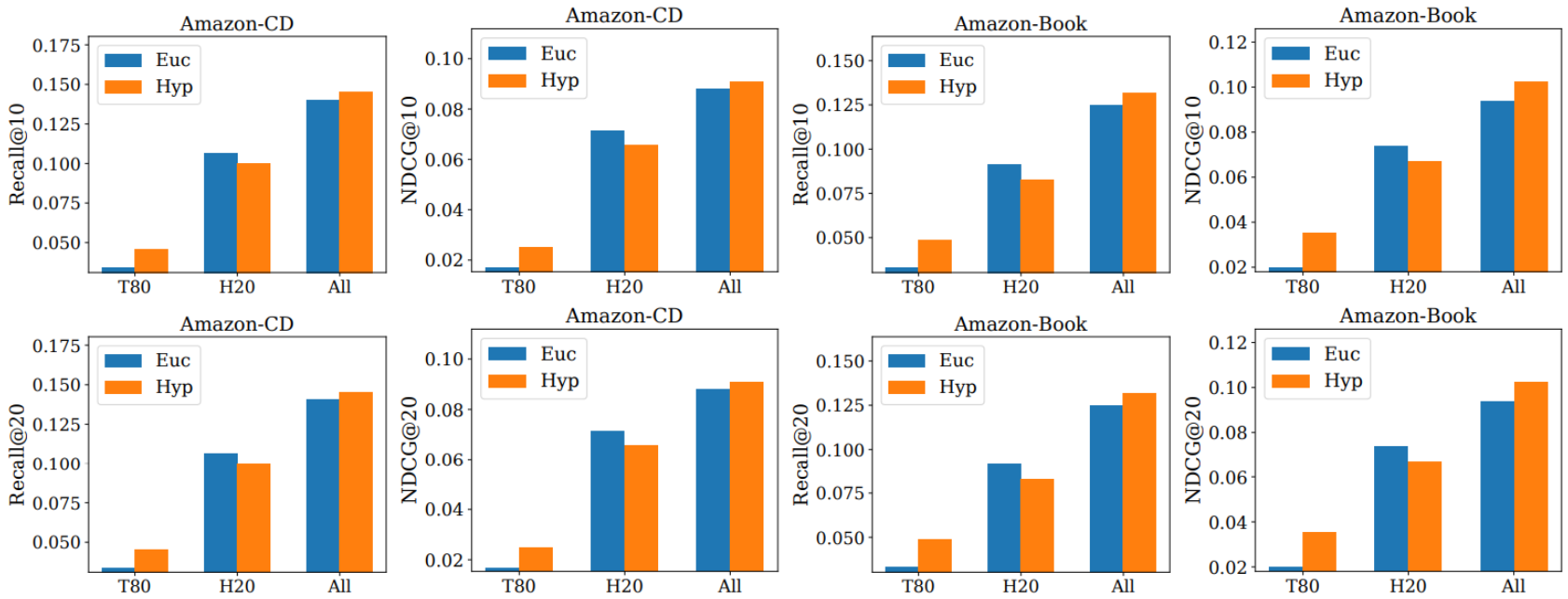
Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)



Observations

- The overall recommendation performance of the hyperbolic model is better than that of the Euclidean model.
- Tail items get greater emphasis in the hyperbolic model as the results on tail items are far beyond that of the Euclidean counterpart.
- Head items receive moderate attention in the hyperbolic model as the performance of HGCF is sightly lower than that of LightGCN.

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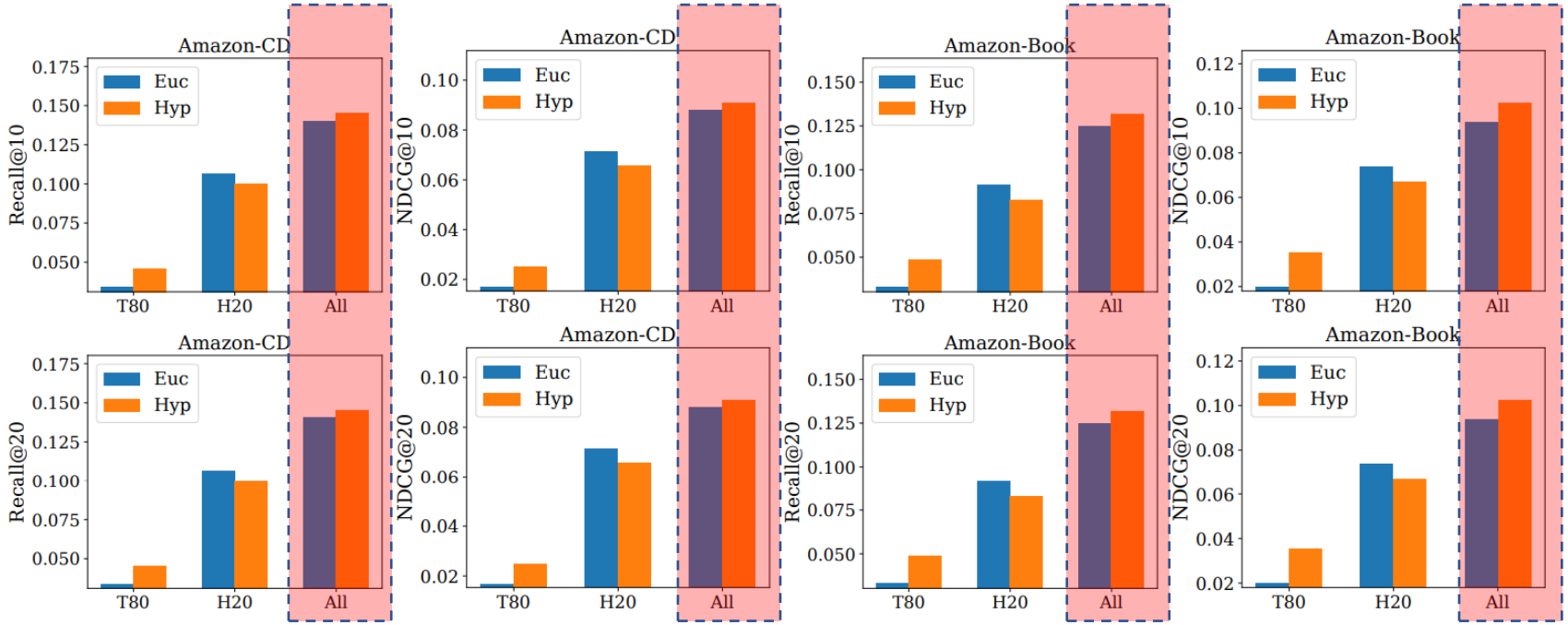

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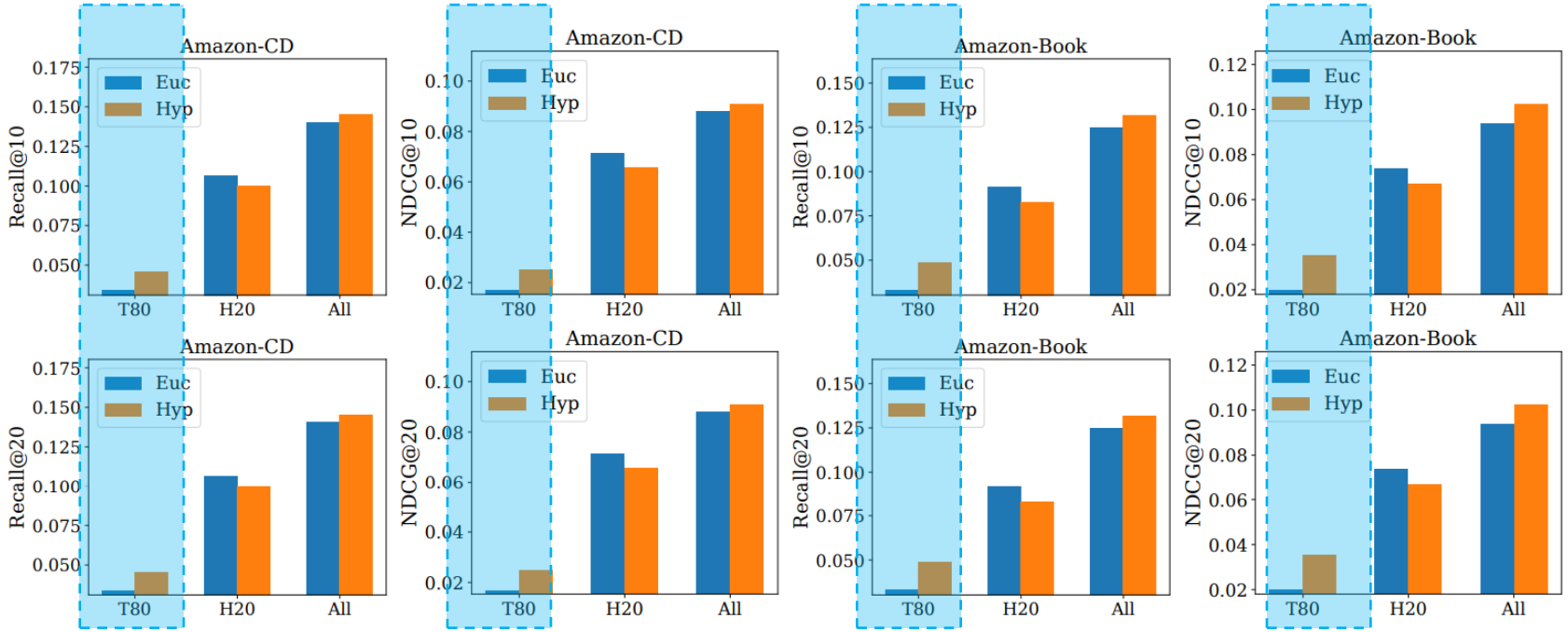

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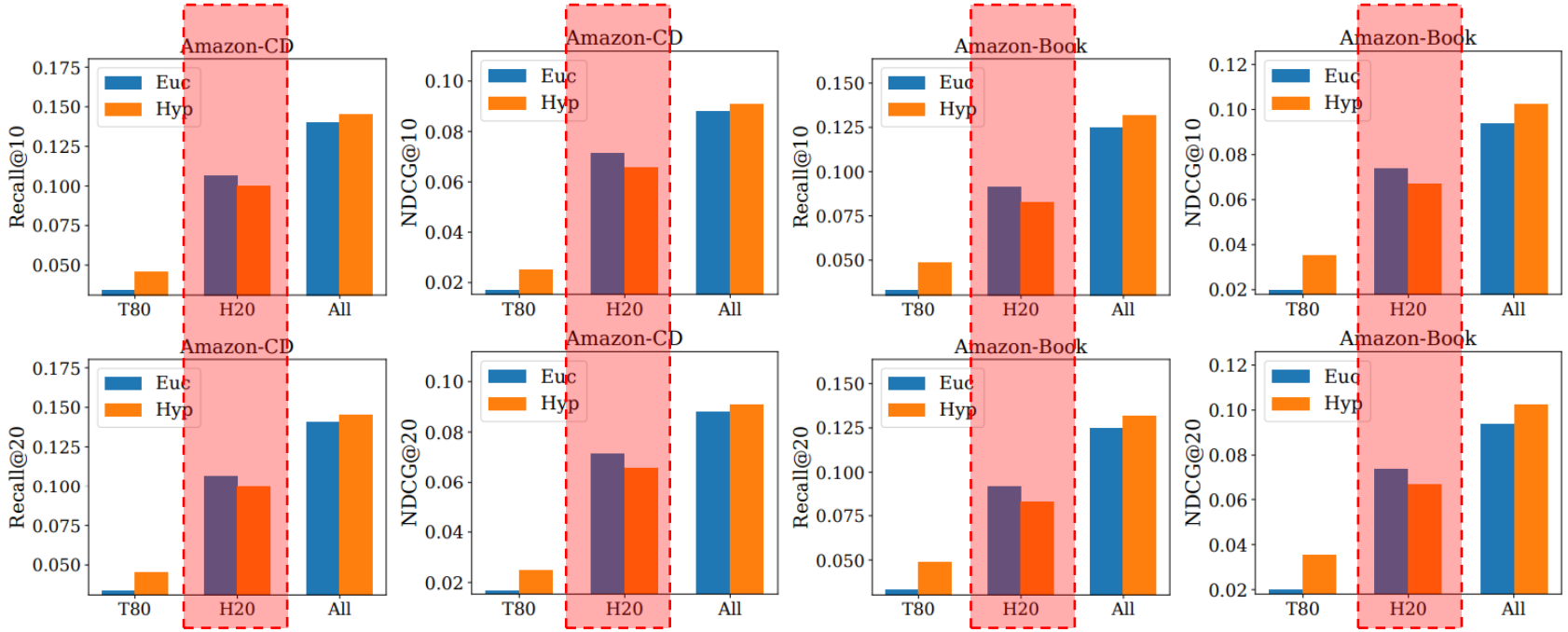

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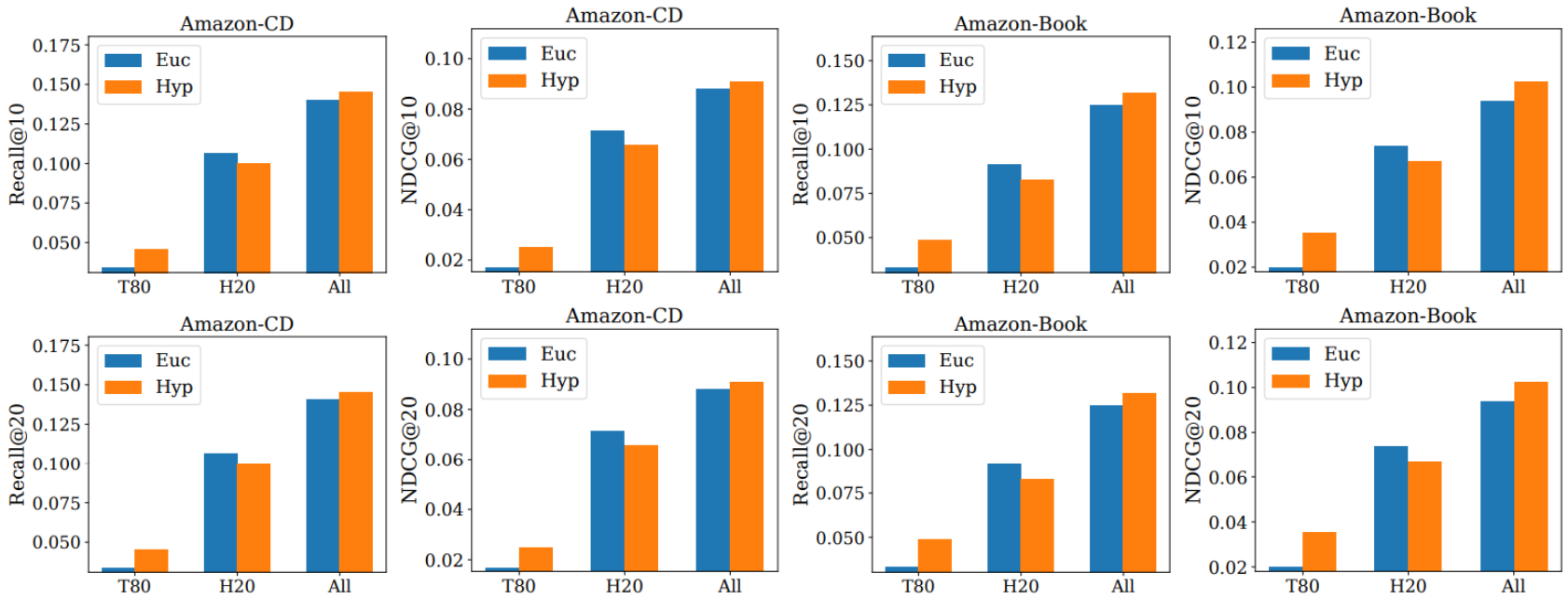
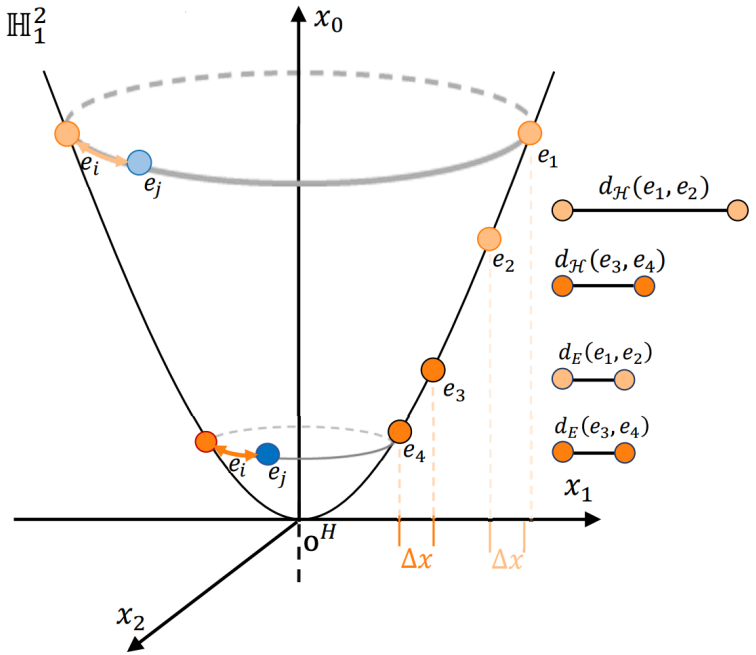


Problems

- There is still large room for improvement for tail items.
- There is an urgent need to improve the performance on head items.

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)



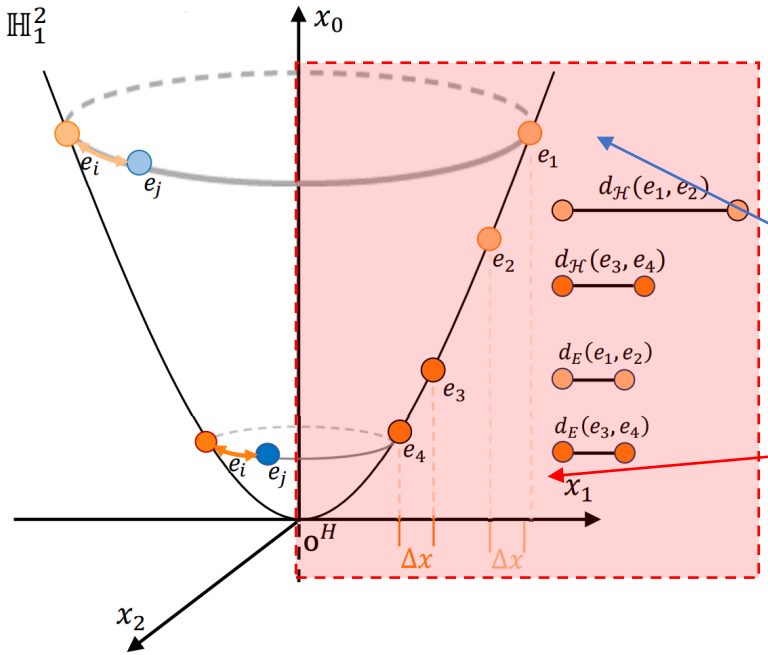
$$\ell(u, i, j) = \max(\underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_i)}_{\text{Pull}} - \underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_j)}_{\text{Push}} + m, 0),$$

Note: d_H is the hyperbolic distance and m determines the margin between the distance difference between positive pair (u, i) and negative pair (u,j).

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)

Hyperbolic-aware Margin Learning (HAML)



Large Margin

Small Margin

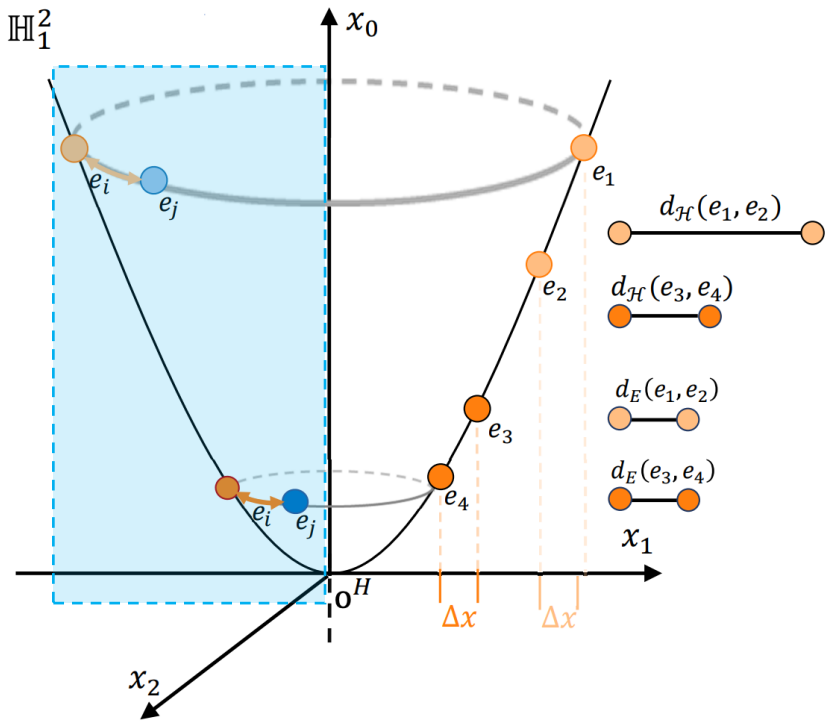
$$\ell(u,i,j) = \max(\underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_i)}_{\text{Pull}} - \underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_j)}_{\text{Push}} + m, 0),$$

$$m^{\mathcal{H}}_{ui} = \text{sigmoid}(\delta),$$

$$\delta = \frac{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{o}) + d^2_{\mathcal{H}}(\mathbf{e}_i, \mathbf{o}) - d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_i)}{\mathbf{e}_{u,0}\mathbf{e}_{i,0}},$$

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)



Informative Sampling

Hyperbolic Informative Negative Sampling

Algorithm 1: HINS algorithm

Input: Hyper parameters n_{neg}; Item set $\mathcal{I}$; the embedding matrix E; The index of the user u, its current positive item i and its other positive item $\mathcal{N}_u$ in the training set.

Output: The informative item index j.

Random sample n_{neg} items $\mathcal{I}_u^{[n]}$ from $\mathcal{I} \backslash \mathcal{N}_u$;

forall *item index* $\bar{j}$ *in* $\mathcal{I}_u^{[n]}$ **do**
- Get the embeddings of the $\bar{j}$ from E, i.e., $\mathbf{e}_{\bar{j}}$;
- Let $j = -1, d_{\min} = +\infty$;
- Compute the hyperbolic distance $d_{\mathcal{H}}(\mathbf{e}_{\bar{j}}, \mathbf{e}_i)$;
- **if** $d_{\mathcal{H}}(\mathbf{e}_{\bar{j}}, \mathbf{e}_i) < d_{\min}$ **then**
  - $d_{\min} = d_{\mathcal{H}}(\mathbf{e}_{\bar{j}}, \mathbf{e}_i)$;
  - $j = \bar{j}$;
- **end**

end

Return j;

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)

Datasets		WRMF	VAE-CF	TransCF	CML	LRML	SML	NGCF	LightGCN	HAE	HAVE	HGCF	Ours	Δ(%)
Amazon-CD	R@10	0.0863	0.0786	0.0518	0.0864	0.0502	0.0475	0.0758	0.0929	0.0666	0.0781	0.0962	**0.1079***	+12.16
	R@20	0.1313	0.1155	0.0791	0.1341	0.0771	0.0734	0.1150	0.1404	0.0963	0.1147	0.1455	**0.1586***	+9.00
Amazon-Book	R@10	0.0623	0.0740	0.0407	0.0665	0.0522	0.0479	0.0658	0.0799	0.0634	0.0774	0.0867	**0.0965***	+11.30
	R@20	0.0919	0.1066	0.0632	0.1023	0.0834	0.0768	0.1050	0.1248	0.0912	0.1125	0.1318	**0.1449***	+9.94
Yelp2020	R@10	0.0470	0.0429	0.0247	0.0363	0.0326	0.0319	0.0458	0.0522	0.0360	0.0421	0.0527	**0.0570***	+8.16
	R@20	0.0793	0.0706	0.0424	0.0638	0.0562	0.0544	0.0764	0.0866	0.0588	0.0691	0.0884	**0.0948***	+7.24

Datasets		WRMF	VAE-CF	TransCF	CML	LRML	SML	NGCF	LightGCN	HAE	HAVE	HGCF	Ours	Δ(%)
Amazon-CD	N@10	0.0651	0.0615	0.0396	0.0639	0.0405	0.0361	0.0591	0.0726	0.0565	0.0629	0.0751	**0.0848***	+12.92
	N@20	0.0817	0.0752	0.0488	0.0813	0.0492	0.0456	0.0718	0.0881	0.0657	0.0749	0.0909	**0.1010***	+11.11
Amazon-Book	N@10	0.0563	0.0716	0.0392	0.0624	0.0515	0.0422	0.0655	0.0780	0.0709	0.0778	0.0869	**0.0978***	+12.54
	N@20	0.0730	0.0878	0.0474	0.0808	0.0626	0.0550	0.0791	0.0938	0.0789	0.0901	0.1022	**0.1142***	+11.74
Yelp2020	N@10	0.0372	0.0353	0.0214	0.0310	0.0287	0.0255	0.0405	0.0461	0.0331	0.0371	0.0458	**0.0502***	+9.13
	N@20	0.0506	0.0469	0.0277	0.0428	0.0369	0.0347	0.0513	0.0582	0.0409	0.0465	0.0585	**0.0633***	+8.21

The proposed method outperforms all baselines in both Recall and NDCG metrics.

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

3.1 HGRL for Recommendation Systems (KDD '22)

Datasets	Models	R@20		R@10		R@5		N@20		N@10		N@5	
		H20	T80	H20	T80	H20	T80	H20	T80	H20	T80	H20	T80
Amazon-CD	LightGCN	0.1062	0.0342	0.0741	0.0188	0.0493	0.0104	0.0712	0.0169	0.0608	0.0118	0.0529	0.0084
	HGCF	0.0998	0.0457	0.0667	0.0295	0.0439	0.0179	0.0658	0.0251	0.0550	0.0201	0.0486	0.0157
	HICF(Ours)	**0.1027**	**0.0559**	**0.0717**	**0.0362**	**0.0476**	**0.0222**	**0.0692**	**0.0318**	**0.0596**	**0.0252**	**0.0527**	**0.0197**
	$\Delta_{\mathcal{H}}(\%)$	+2.91	+22.32	+7.50	+22.71	+8.43	+24.02	+5.17	+26.69	+8.36	+25.37	+8.44	+25.48
Amazon-Book	LightGCN	0.0915	0.0333	0.0624	0.0175	0.0390	0.0104	0.0740	0.0198	0.0635	0.0145	0.0589	0.0104
	HGCF	0.0829	0.0489	0.0550	0.0317	0.0344	0.0197	0.0670	0.0352	0.0578	0.0291	0.0539	0.0251
	HICF(Ours)	**0.0898**	**0.0551**	**0.0603**	**0.0362**	**0.0387**	**0.0227**	**0.0738**	**0.0404**	**0.0642**	**0.0336**	**0.0605**	**0.0293**
	$\Delta_{\mathcal{H}}(\%)$	+8.32	+12.68	+9.64	+14.20	+12.50	+15.23	+10.15	+14.77	+11.07	+15.46	+12.24	+16.73
Yelp2020	LightGCN	0.0836	0.0030	0.0512	0.0010	0.0298	0.0003	0.0567	0.0015	0.0448	0.0006	0.0380	0.0004
	HGCF	0.0788	**0.0096**	0.0473	**0.0054**	0.0270	0.0030	0.0526	**0.0059**	0.0417	0.0043	0.0354	**0.0033**
	HICF(Ours)	**0.0854**	0.0094	**0.0518**	0.0052	**0.0299**	0.0029	**0.0576**	0.0057	**0.0461**	0.0041	**0.0395**	0.0032
	$\Delta_{\mathcal{H}}(\%)$	+8.38	-2.08	+9.51	-3.70	+10.74	-3.33	+9.51	-3.39	+10.55	-4.65	+11.58	-3.03

For head items, the performances of HICF comprehensively outperform that of HGCF and the improvements are up to 8.43% on Amazon-CD, 12.50% on Amazon-Book, and 11.58% on Yelp.

In addition, HICF narrows the performance gap of the tail items with Euclidean LightGCN on Amazon-CD and Amazon-Book and impressively surpasses the performance of LightGCN on Yelp.

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3.1 HGRL for Recommendation Systems (KDD '22)

Datasets	Models	R@20		R@10		R@5		N@20		N@10		N@5	
		H20	T80	H20	T80	H20	T80	H20	T80	H20	T80	H20	T80
Amazon-CD	LightGCN	0.1062	0.0342	0.0741	0.0188	0.0493	0.0104	0.0712	0.0169	0.0608	0.0118	0.0529	0.0084
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	$\Delta_{\mathcal{H}}(\%)$	+2.91	+22.32	+7.50	+22.71	+8.43	+24.02	+5.17	+26.69	+8.36	+25.37	+8.44	+25.48
Amazon-Book	LightGCN	0.0915	0.0333	0.0624	0.0175	0.0390	0.0104	0.0740	0.0198	0.0635	0.0145	0.0589	0.0104
	HGCF	0.0829	0.0489	0.0550	0.0317	0.0344	0.0197	0.0670	0.0352	0.0578	0.0291	0.0539	0.0251
	HICF(Ours)	**0.0898**	**0.0551**	**0.0603**	**0.0362**	**0.0387**	**0.0227**	**0.0738**	**0.0404**	**0.0642**	**0.0336**	**0.0605**	**0.0293**
	$\Delta_{\mathcal{H}}(\%)$	+8.32	+12.68	+9.64	+14.20	+12.50	+15.23	+10.15	+14.77	+11.07	+15.46	+12.24	+16.73
Yelp2020	LightGCN	0.0836	0.0030	0.0512	0.0010	0.0298	0.0003	0.0567	0.0015	0.0448	0.0006	0.0380	0.0004
	HGCF	0.0788	**0.0096**	0.0473	**0.0054**	0.0270	0.0030	0.0526	**0.0059**	0.0417	0.0043	0.0354	**0.0033**
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	$\Delta_{\mathcal{H}}(\%)$	+8.38	-2.08	+9.51	-3.70	+10.74	-3.33	+9.51	-3.39	+10.55	-4.65	+11.58	-3.03

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In addition, HICF narrows the performance gap of the tail items with Euclidean LightGCN on Amazon-CD and Amazon-Book and impressively surpasses the performance of LightGCN on Yelp.

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3.1 HGRL for Recommendation Systems (KDD '22)

Datasets	Models	R@20		R@10		R@5		N@20		N@10		N@5	
		H20	T80	H20	T80	H20	T80	H20	T80	H20	T80	H20	T80
Amazon-CD	LightGCN	0.1062	0.0342	0.0741	0.0188	0.0493	0.0104	0.0712	0.0169	0.0608	0.0118	0.0529	0.0084
	HGCF	0.0998	0.0457	0.0667	0.0295	0.0439	0.0179	0.0658	0.0251	0.0550	0.0201	0.0486	0.0157
	HICF(Ours)	**0.1027**	**0.0559**	**0.0717**	**0.0362**	**0.0476**	**0.0222**	**0.0692**	**0.0318**	**0.0596**	**0.0252**	**0.0527**	**0.0197**
	$\Delta_{\mathcal{H}}(\%)$	+2.91	+22.32	+7.50	+22.71	+8.43	+24.02	+5.17	+26.69	+8.36	+25.37	+8.44	+25.48
Amazon-Book	LightGCN	0.0915	0.0333	0.0624	0.0175	0.0390	0.0104	0.0740	0.0198	0.0635	0.0145	0.0589	0.0104
	HGCF	0.0829	0.0489	0.0550	0.0317	0.0344	0.0197	0.0670	0.0352	0.0578	0.0291	0.0539	0.0251
	HICF(Ours)	**0.0898**	**0.0551**	**0.0603**	**0.0362**	**0.0387**	**0.0227**	**0.0738**	**0.0404**	**0.0642**	**0.0336**	**0.0605**	**0.0293**
	$\Delta_{\mathcal{H}}(\%)$	+8.32	+12.68	+9.64	+14.20	+12.50	+15.23	+10.15	+14.77	+11.07	+15.46	+12.24	+16.73
Yelp2020	LightGCN	0.0836	0.0030	0.0512	0.0010	0.0298	0.0003	0.0567	0.0015	0.0448	0.0006	0.0380	0.0004
	HGCF	0.0788	**0.0096**	0.0473	**0.0054**	0.0270	0.0030	0.0526	**0.0059**	0.0417	0.0043	0.0354	**0.0033**
	HICF(Ours)	**0.0854**	0.0094	**0.0518**	0.0052	**0.0299**	0.0029	**0.0576**	0.0057	**0.0461**	0.0041	**0.0395**	0.0032
	$\Delta_{\mathcal{H}}(\%)$	+8.38	-2.08	+9.51	-3.70	+10.74	-3.33	+9.51	-3.39	+10.55	-4.65	+11.58	-3.03

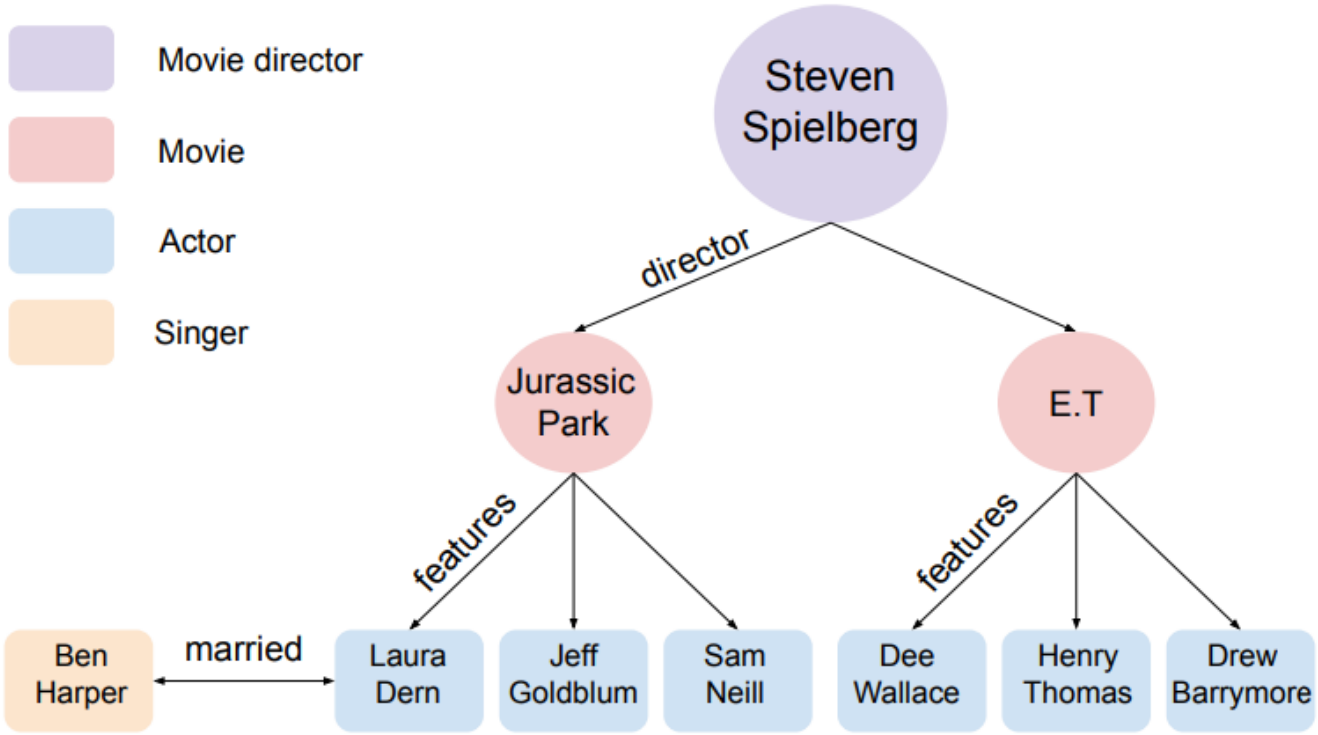
For head items, the performances of HICF comprehensively outperform that of HGCF and the improvements are up to 8.43% on Amazon-CD, 12.50% on Amazon-Book, and 11.58% on Yelp.

In addition, HICF narrows the performance gap of the tail items with Euclidean LightGCN on Amazon-CD and Amazon-Book and impressively surpasses the performance of LightGCN on Yelp.

Yang, Menglin, Zhihao Li, Min Zhou, Jiahong Liu, and Irwin King. "HICF: Hyperbolic Informative Collaborative Filtering." KDD 2022.

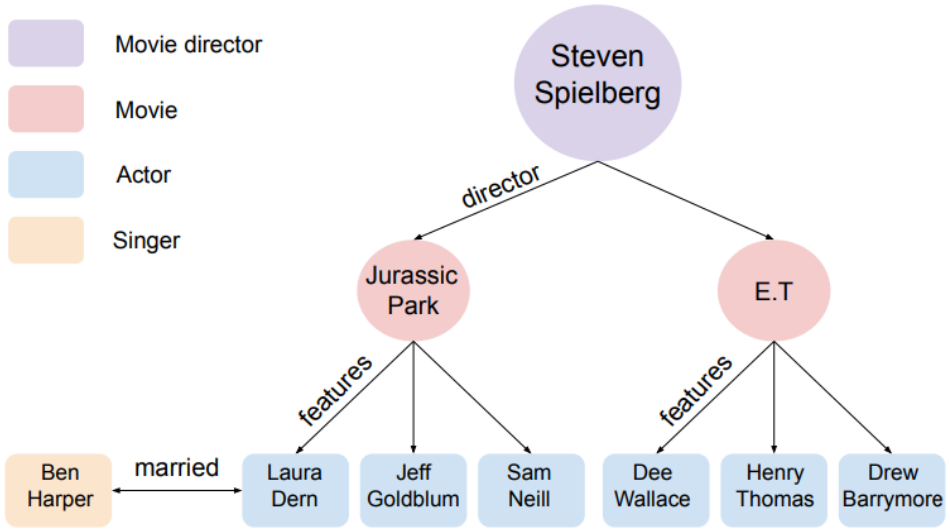
Contents

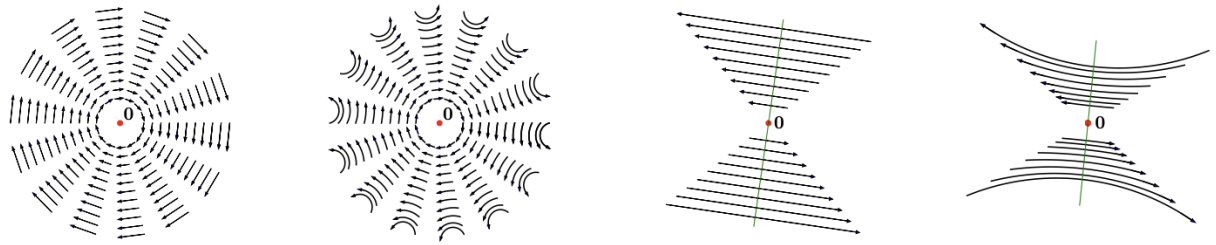
3.2 HGRL for Knowledge Graph (ACL '19)



Chami, Ines, et al. "Low-dimensional hyperbolic knowledge graph embeddings." *ACL 2019*

3.2 HGRL for Knowledge Graph (ACL '19)

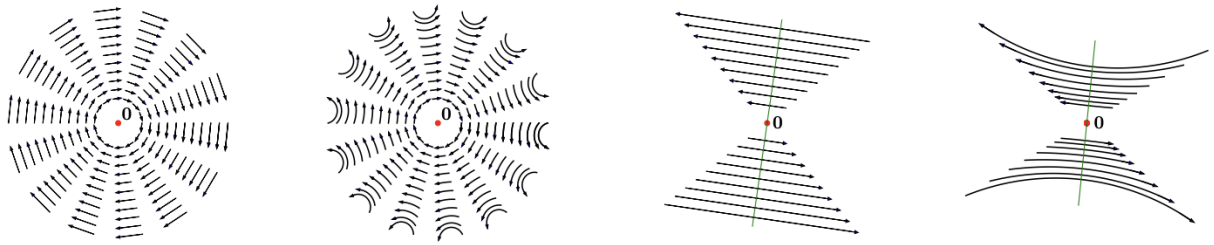




(a) Rotations (b) Reflections

Chami, Ines, et al. "Low-dimensional hyperbolic knowledge graph embeddings." *ACL 2019*

3.2 HGRL for Knowledge Graph (ACL '19)



(a) Rotations (b) Reflections

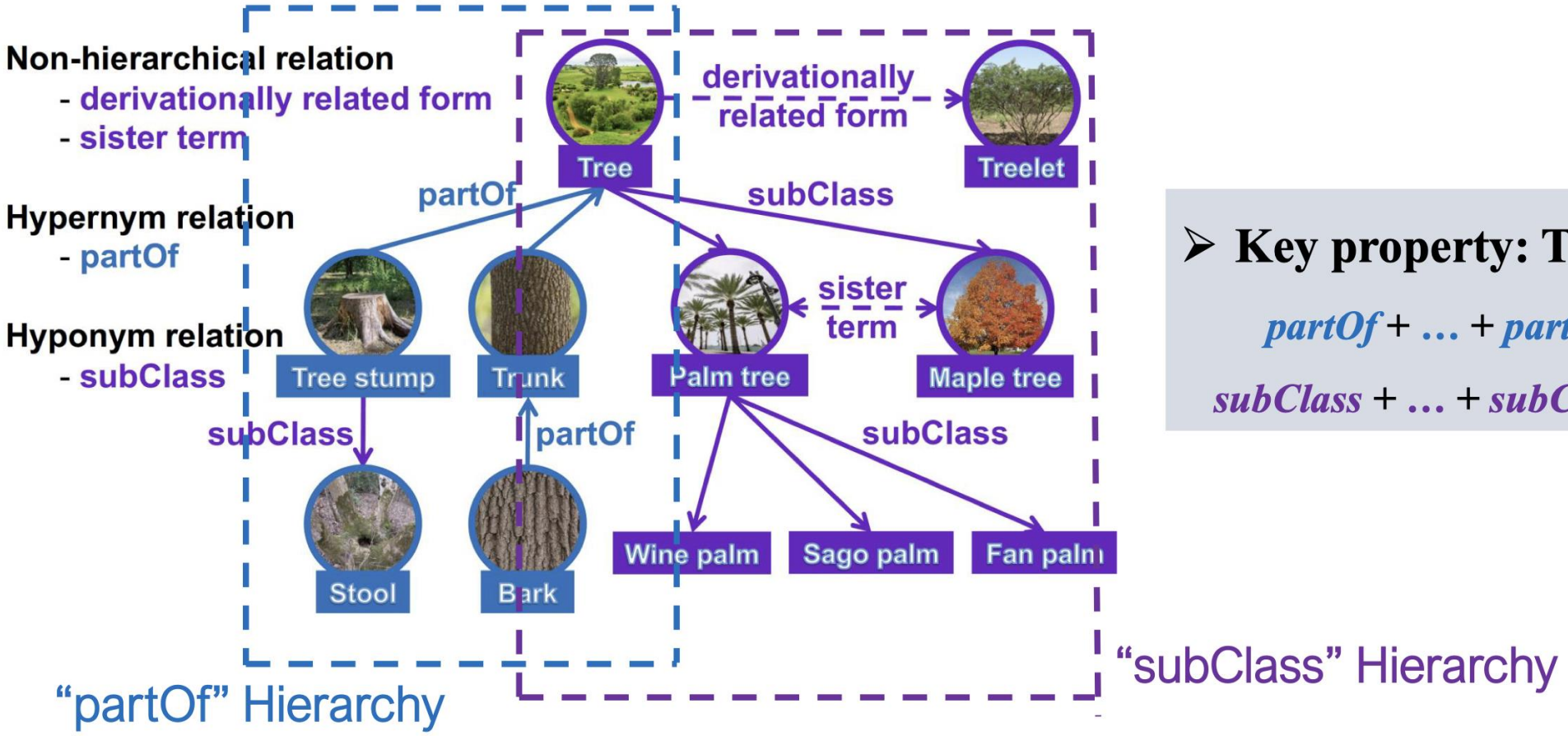
$$\mathrm{Rot}(\Theta_r) = \mathrm{diag}(G^+(\theta_{r,1}), \ldots, G^+(\theta_{r,\frac{d}{2}})), \quad (4)$$

$$\mathrm{Ref}(\Phi_r) = \mathrm{diag}(G^-(\phi_{r,1}), \ldots, G^-(\phi_{r,\frac{n}{2}})), \quad (5)$$

$$\text{where } G^{\pm}(\theta) := \begin{bmatrix} \cos(\theta) & \mp\sin(\theta) \\ \sin(\theta) & \pm\cos(\theta) \end{bmatrix}. \quad (6)$$

Chami, Ines, et al. "Low-dimensional hyperbolic knowledge graph embeddings." *ACL 2019*

3.2 HGRL for Knowledge Graph (NeurIPS '21)



- **Key property: Transitivity**

$$partOf + \ldots + partOf = partOf$$

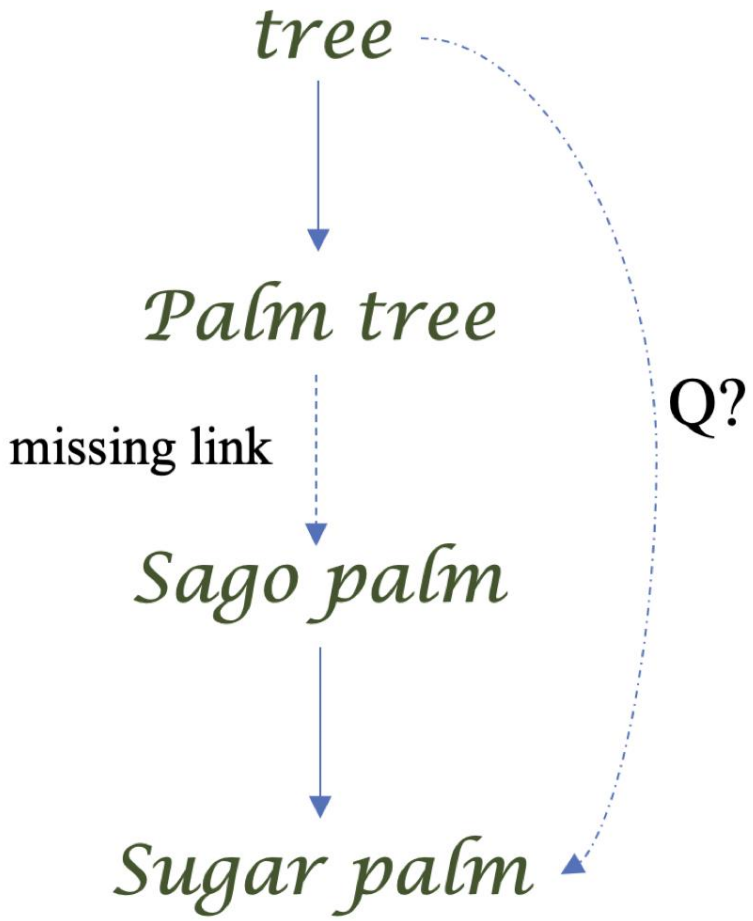
$$subClass + \ldots + subClass = subclass$$

Bai, Yushi, et al. "Modeling heterogeneous hierarchies with relation-specific hyperbolic cones." *NeurIPS* 2021.

3.2 HGRL for Knowledge Graph (NeurIPS '21)

- To do hierarchical reasoning that involves cross-layer connection
  - Ancestor-Descendant Prediction

- Such task requires:
  - Model Transitivity
  - Model non-hierarchical Properties



Bai, Yushi, et al. "Modeling heterogeneous hierarchies with relation-specific hyperbolic cones." *NeurIPS* 2021

3.2 HGRL for Knowledge Graph (NeurIPS '21)

Entity ➡ Hyperbolic Cone

Relation

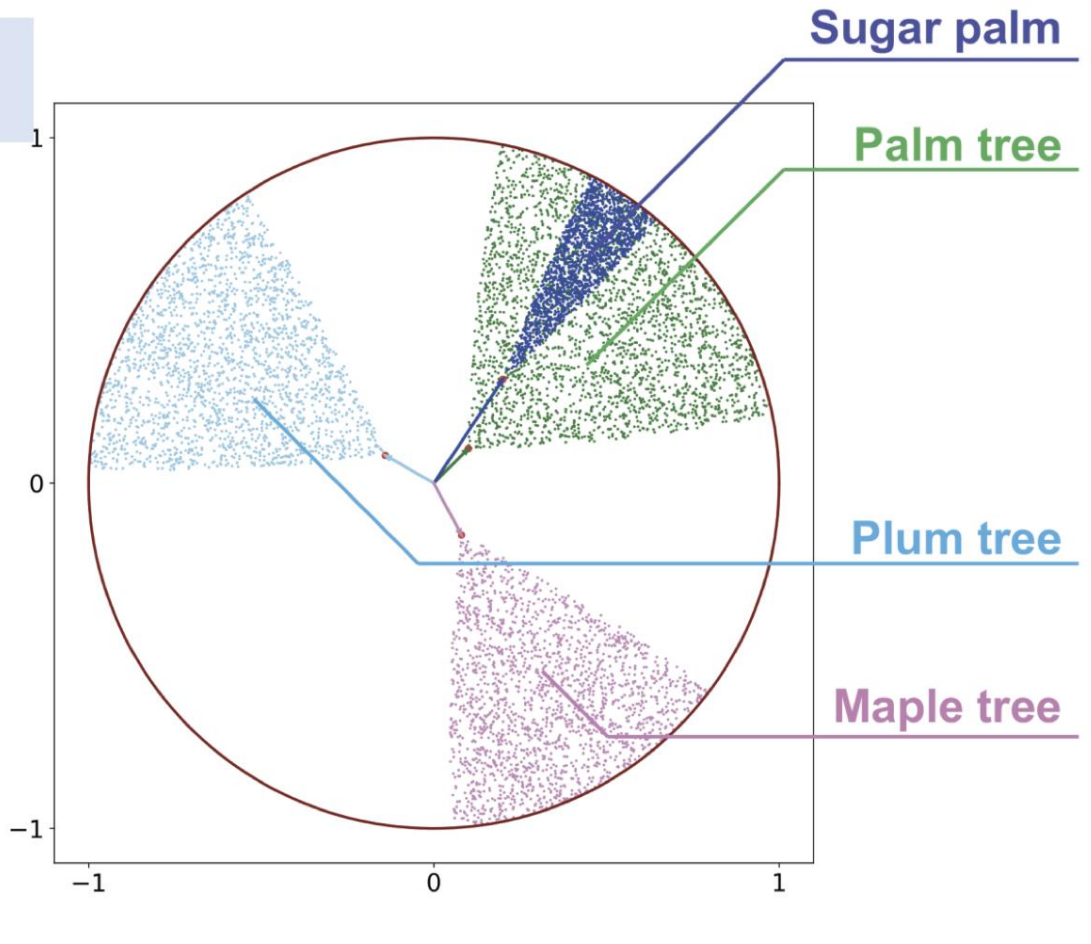
⬇

Cone Transformation

Partial ordering

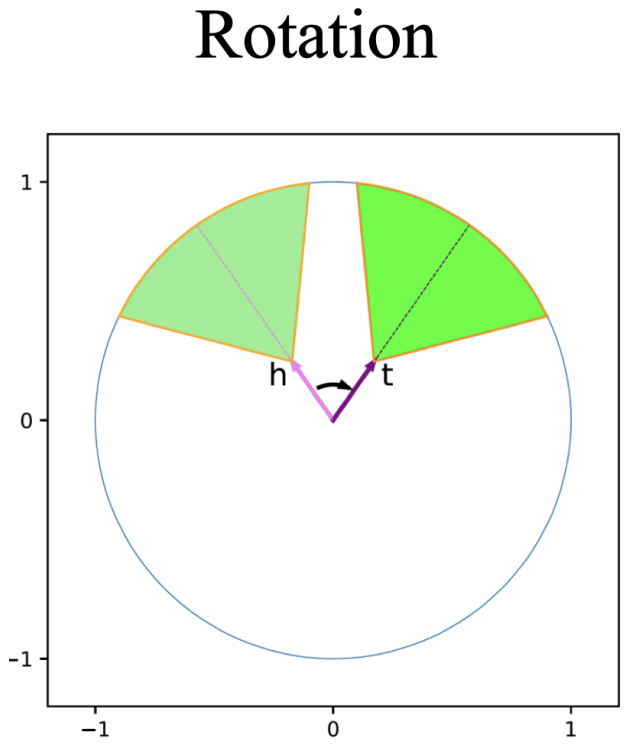
⬇

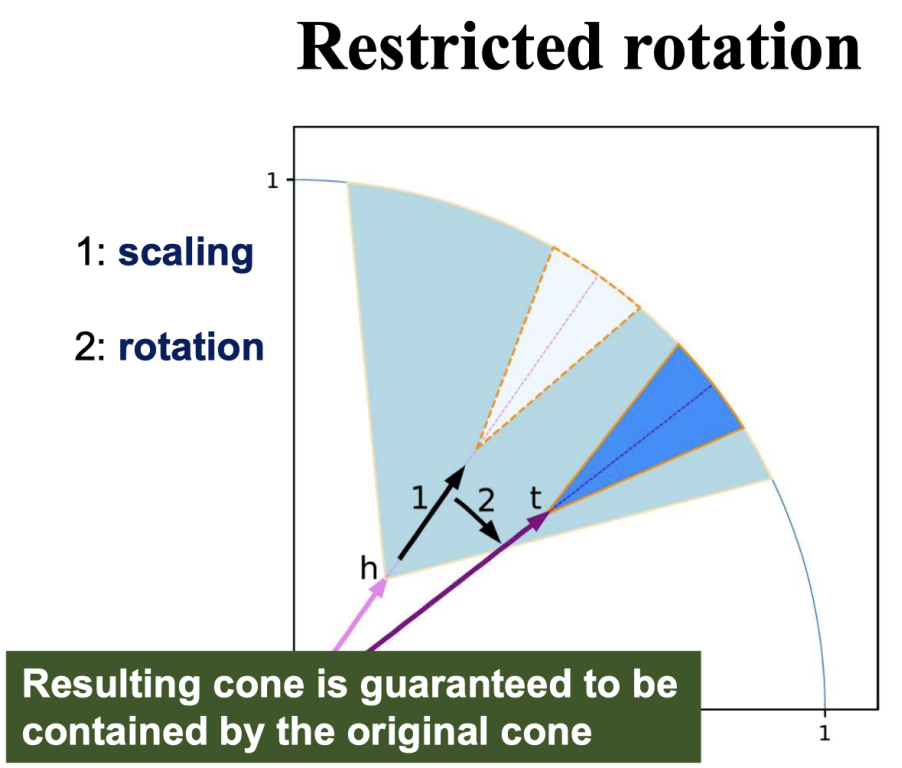
Cone containment



Bai, Yushi, et al. "Modeling heterogeneous hierarchies with relation-specific hyperbolic cones." *NeurIPS* 2021.

3.2 HGRL for Knowledge Graph (NeurIPS '21)



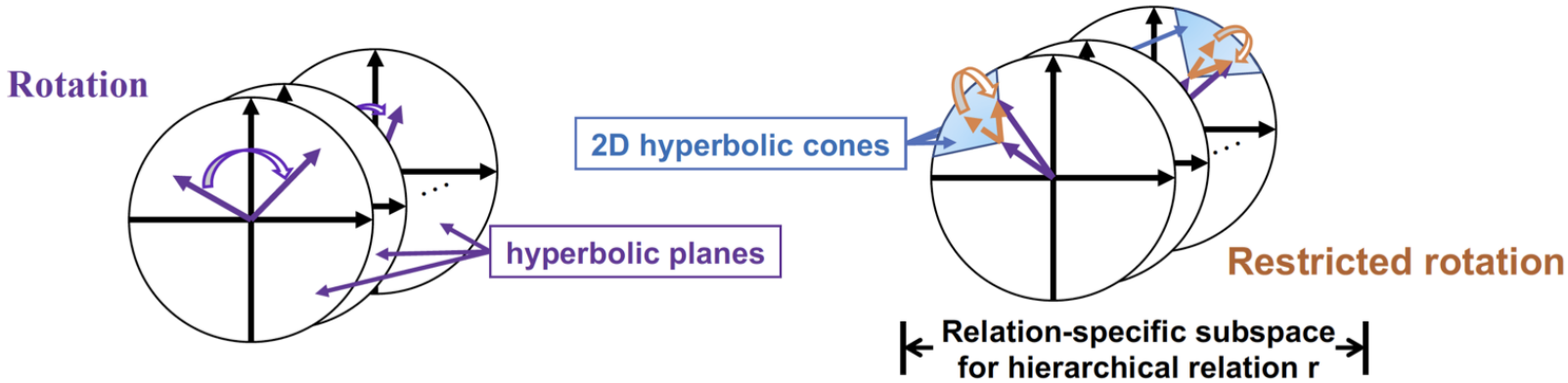


Bai, Yushi, et al. "Modeling heterogeneous hierarchies with relation-specific hyperbolic cones." *NeurIPS* 2021.

3.2 HGRL for Knowledge Graph (NeurIPS '21)

- Motivation behind two kinds of transformations?
  - Restricted rotation: Capture hierarchical property (transitivity)
  - Rotation: Capture other non-hierarchical properties (composition)

- Why allocating subspace for each hierarchical relation?
  - Partial ordering of different hierarchical relations are preserved in different subspaces



Bai, Yushi, et al. "Modeling heterogeneous hierarchies with relation-specific hyperbolic cones." *NeurIPS* 2021.

Contents

Hyperbolic Space for Image Embedding

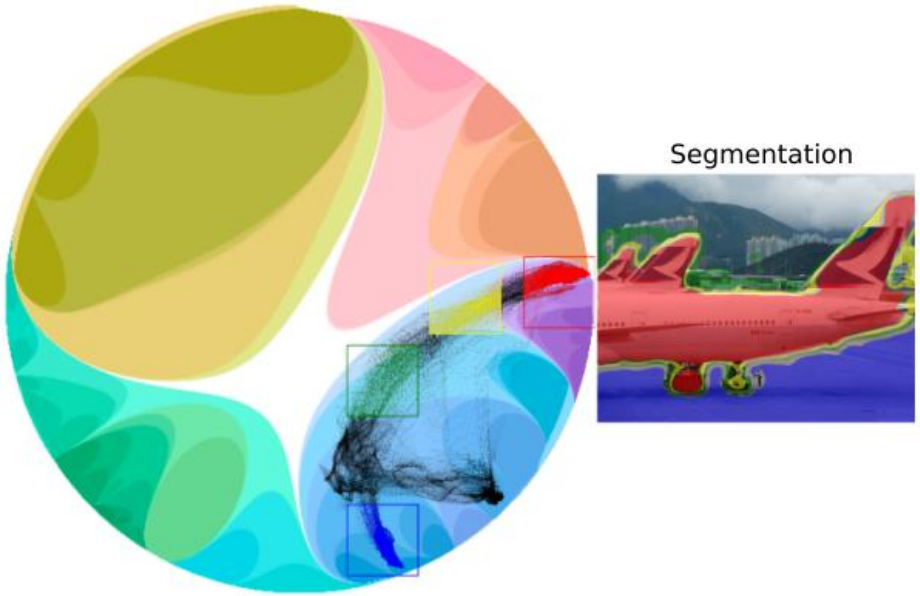


Image segmentation

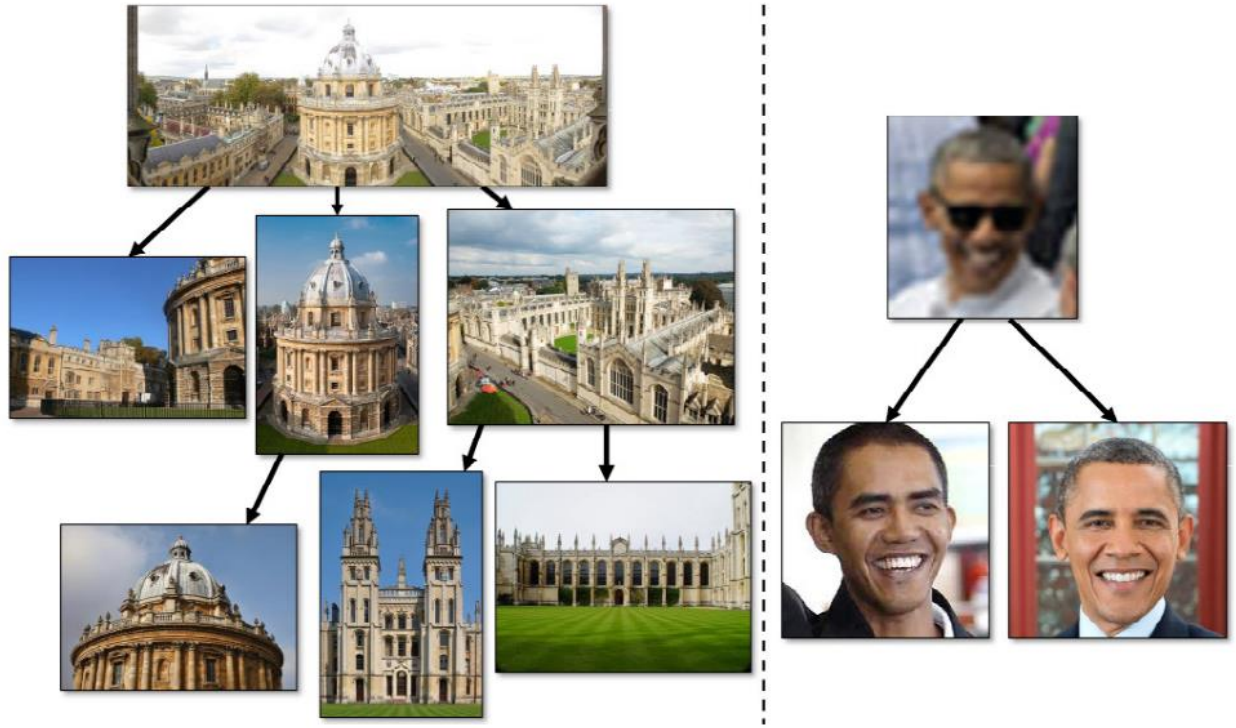
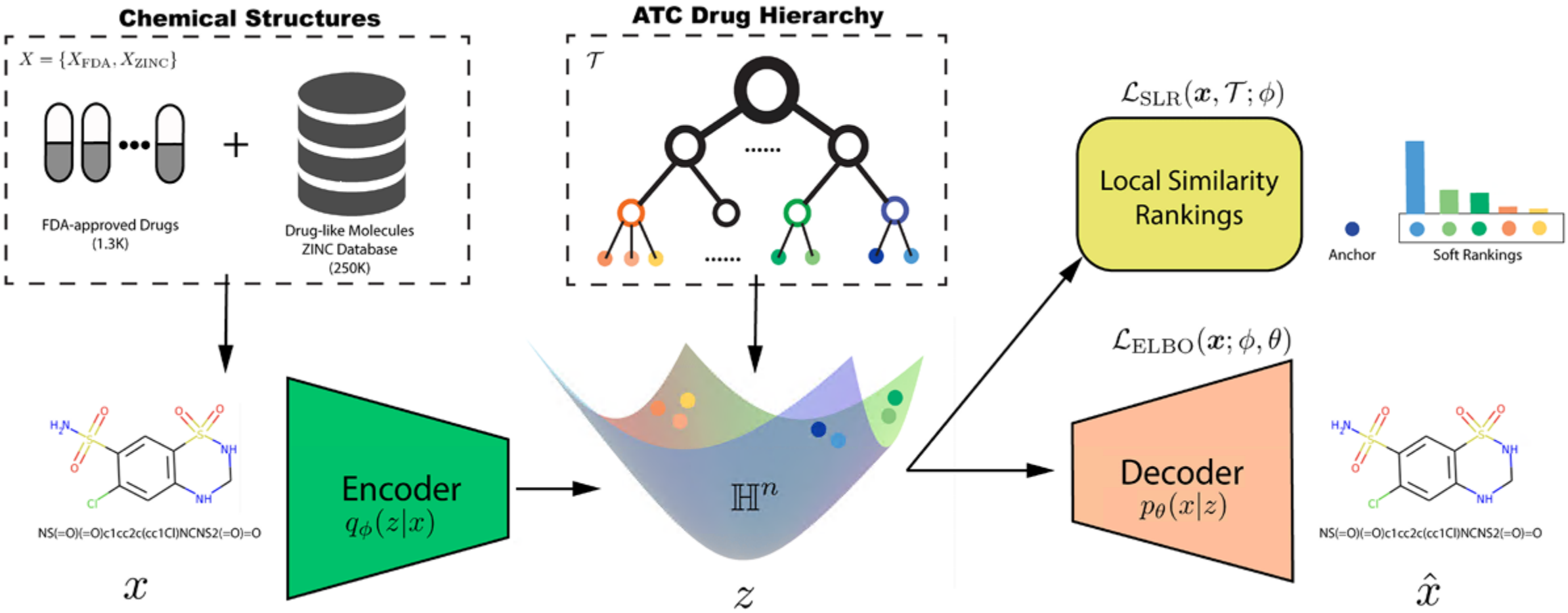


Image classification

Hyperbolic space provides spacious room and additionally present uncertainty information.

Left: GhadimiAtigh, Mina, et al. "Hyperbolic Image Segmentation." CVPR (2022). Right: Khrulkov, Valentin, et al. "Hyperbolic image embeddings." CVPR (2020).

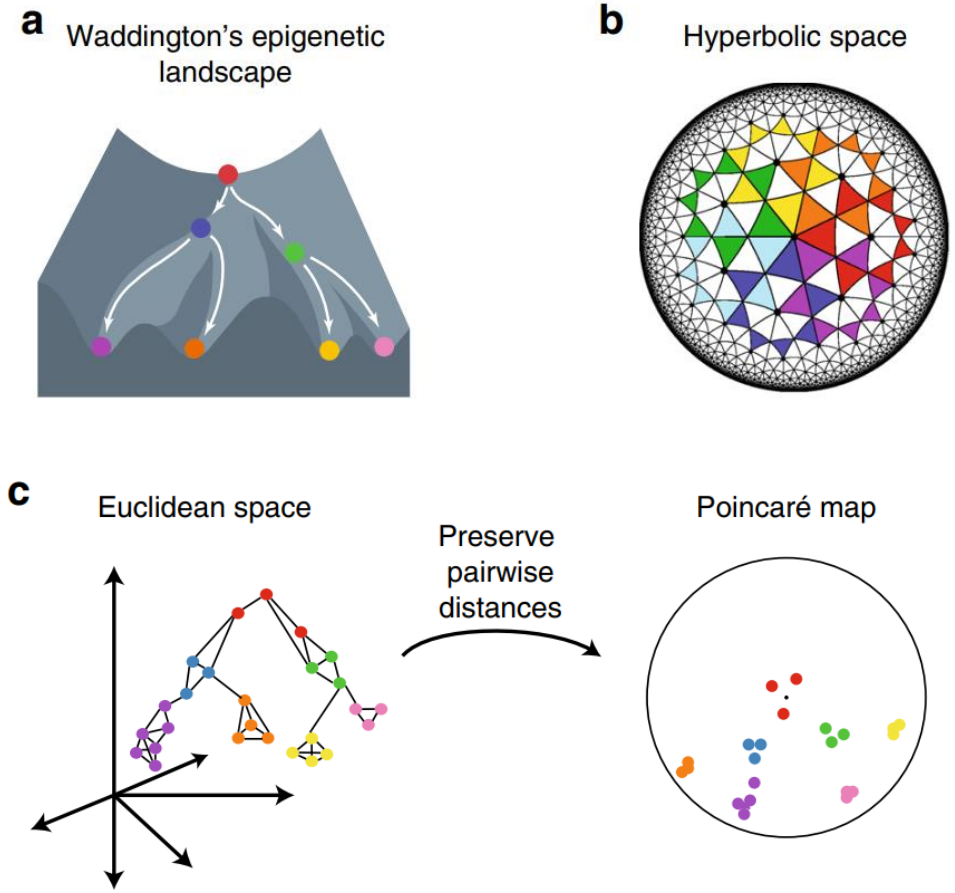
Hyperbolic Space for Drug Generation

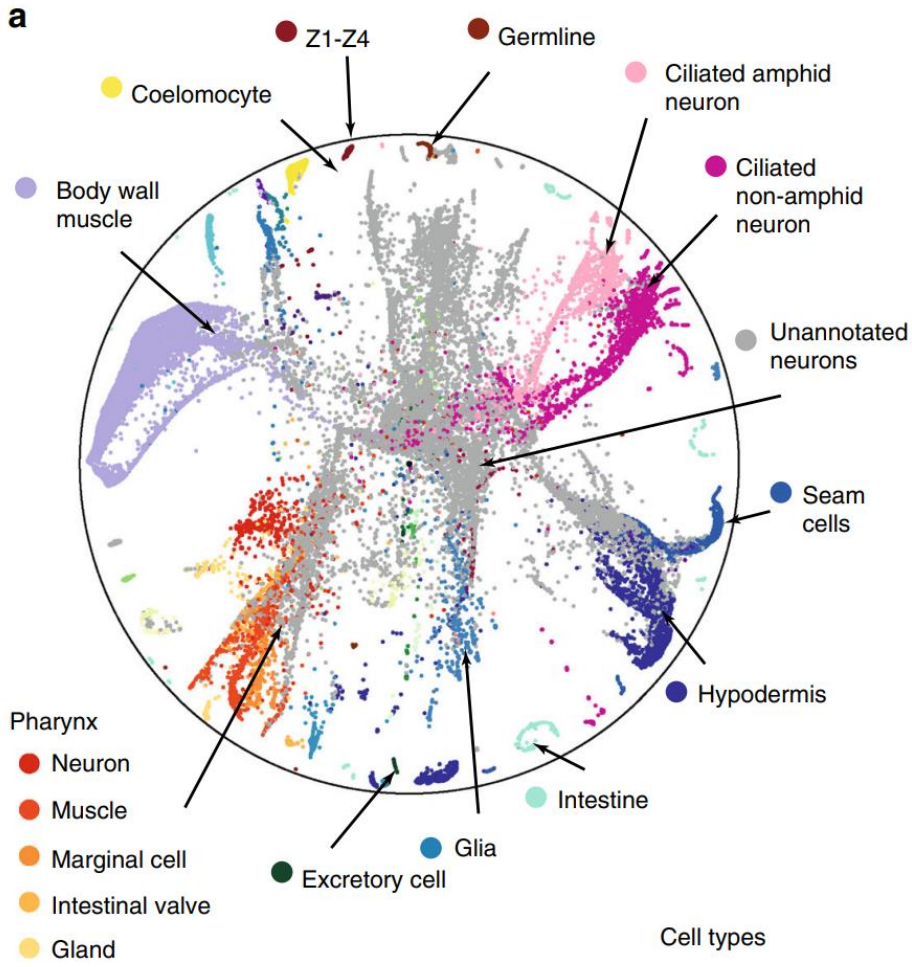


Hyperbolic spaces help inject hierarchies knowledge for drug generation.

Yu, Ke, Shyam Visweswaran, and Kayhan Batmanghelich. "Semi-supervised hierarchical drug embedding in hyperbolic space." Journal of chemical information and modeling 60.12 (2020): 5647-5657.

Hyperbolic Space for Cell Analyzing

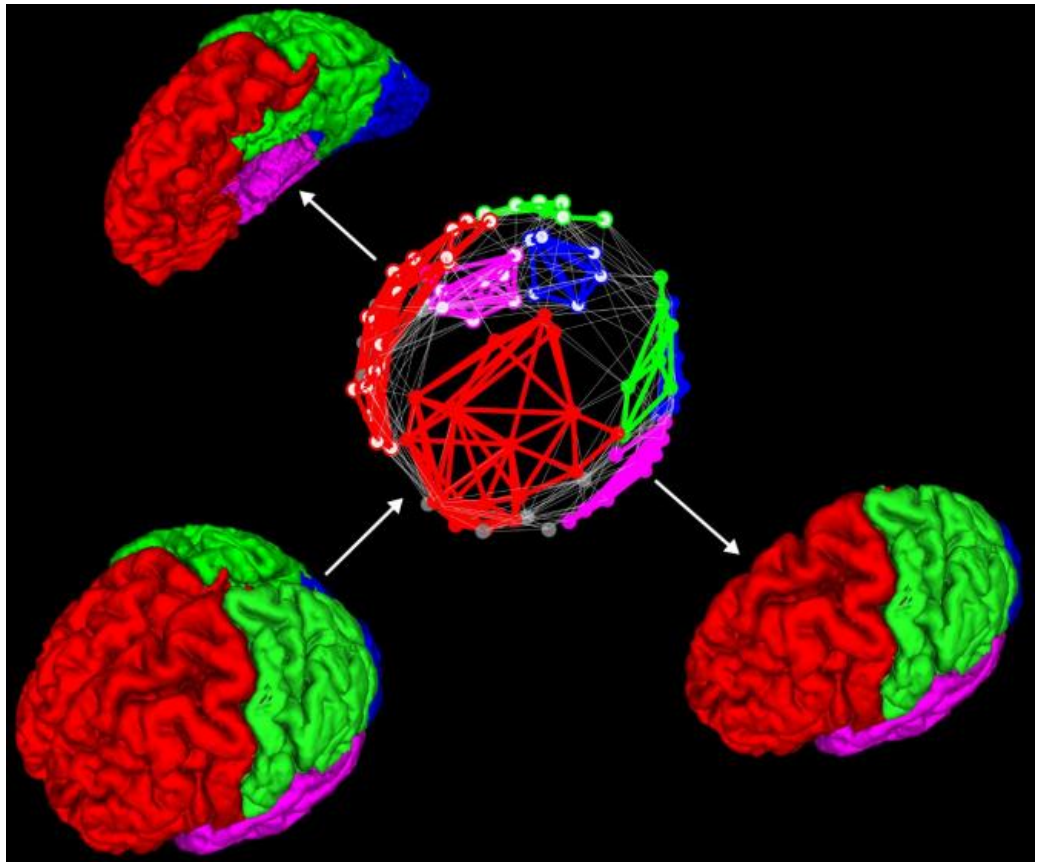




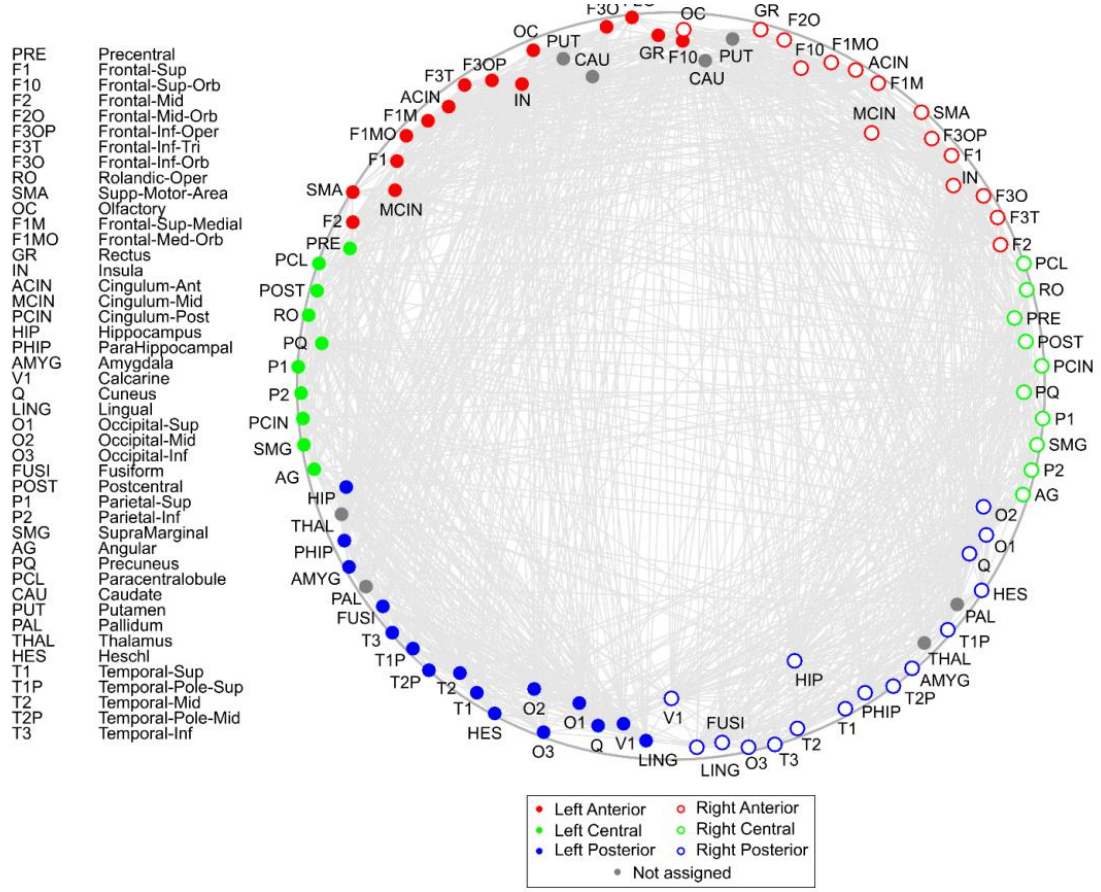
Hyperbolic maps discover hierarchies and branching processes.

Klimovskaia, Anna, et al. "Poincaré maps for analyzing complex hierarchies in single-cell data." Nature communications 11.1 (2020): 1-9.

Hyperbolic Space for Brain Structure



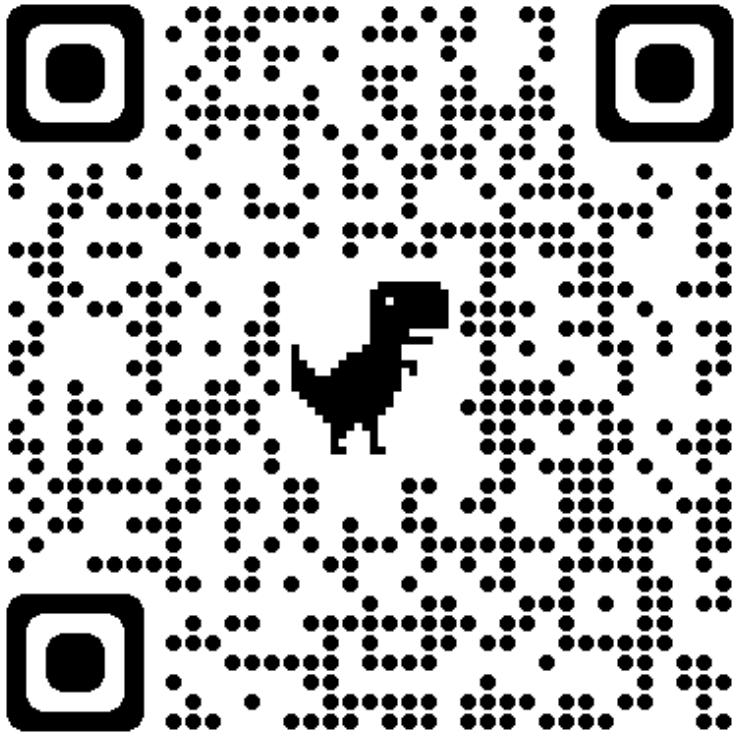
PRE	Precentral
F1	Frontal-Sup
F10	Frontal-Sup-Orb
F2	Frontal-Mid
F2O	Frontal-Mid-Orb
F3OP	Frontal-Inf-Oper
F3T	Frontal-Inf-Tri
F3O	Frontal-Inf-Orb
RO	Rolandic-Oper
SMA	Supp-Motor-Area
OC	Olfactory
F1M	Frontal-Sup-Medial
F1MO	Frontal-Med-Orb
GR	Rectus
IN	Insula
ACIN	Cingulum-Ant
MCIN	Cingulum-Mid
PCIN	Cingulum-Post
HIP	Hippocampus
PHIP	ParaHippocampal
AMYG	Amygdala
V1	Calcarine
Q	Cuneus
LING	Lingual
O1	Occipital-Sup
O2	Occipital-Mid
O3	Occipital-Inf
FUSI	Fusiform
POST	Postcentral
P1	Parietal-Sup
P2	Parietal-Inf
SMG	SupraMarginal
AG	Angular
PQ	Precuneus
PCL	Paracentralobule
CAU	Caudate
PUT	Putamen
PAL	Pallidum
THAL	Thalamus
HES	Heschl
T1	Temporal-Sup
T1P	Temporal-Pole-Sup
T2	Temporal-Mid
T2P	Temporal-Pole-Mid
T3	Temporal-Inf



Hyperbolic space provides separatable room for different sub-structures.

Cacciola, Alberto, et al. "Coalescent embedding in the hyperbolic space unsupervisedly discloses the hidden geometry of the brain." BOOK OF ABSTRACTS. 2017.

Break

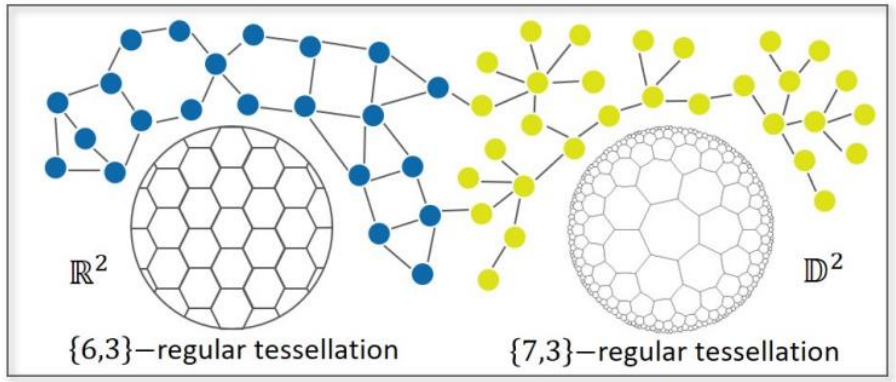


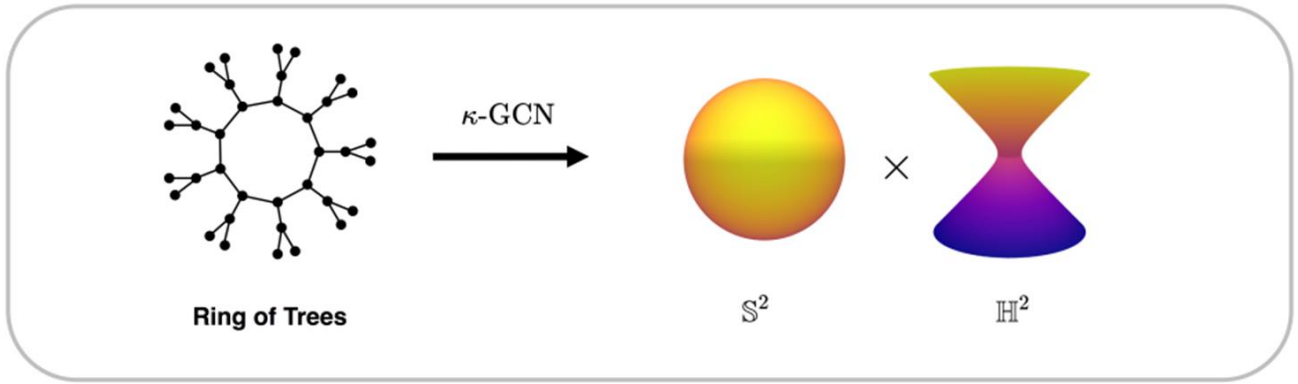
4. Advanced Topics

Contents

4.1 Complex Structures

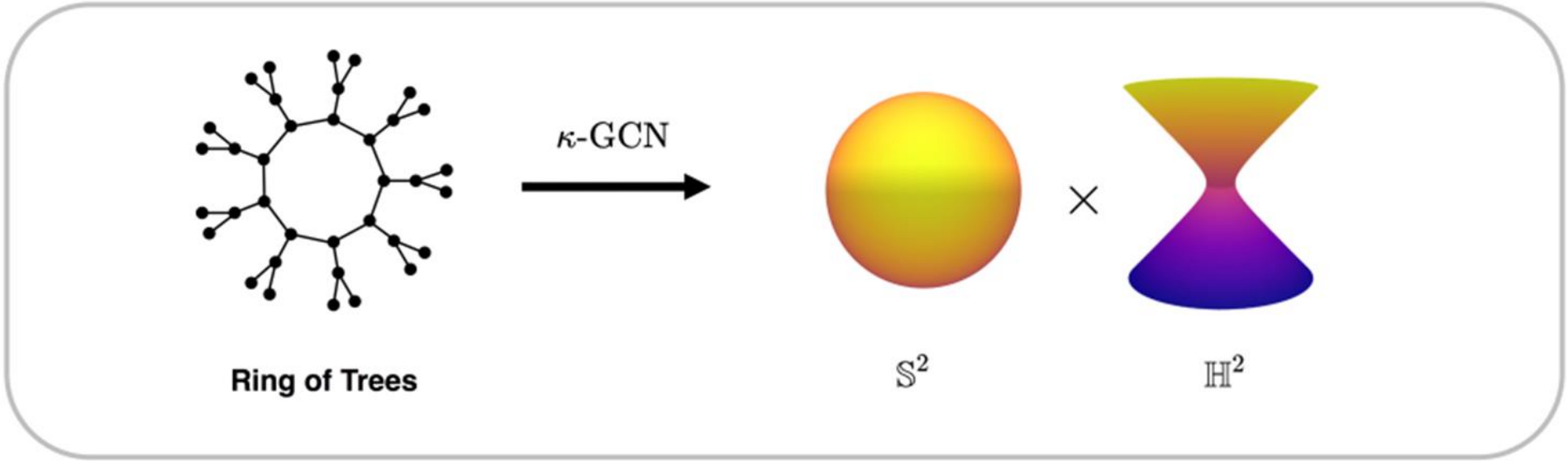
- Interaction learning of mix spaces
  - Constant Curvature Graph Convolutional Networks. ICML 2020
  - Graph Geometry Interaction learning. NeurIPS 2020
  - Mixed-curvature multi-relational graph neural network for knowledge graph completion. WebConf 2021
  - A self-supervised mixed-curvature graph neural network. AAAI2022
  - Dual-Geometric Space Embedding Model for Two-View Knowledge Graphs. KDD2022
  - …
- Encapsulate network curvature into embedding space
  - Heterogeneous manifolds for curvature-aware graph embedding. *ICLR 2022 Workshop*
  - *Hyperbolic Curvature Graph Neural Network. arXiv 2022*
  - …





Constant Curvature Graph Convolution Networks

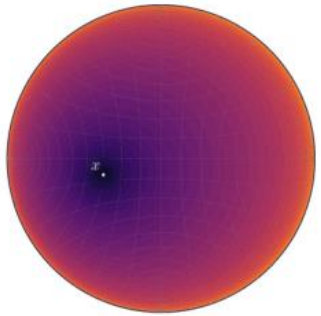
- Embed graphs into hyperbolic and spherical space



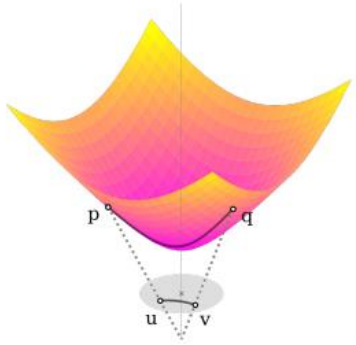
Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Constant Curvature Graph Convolution Networks

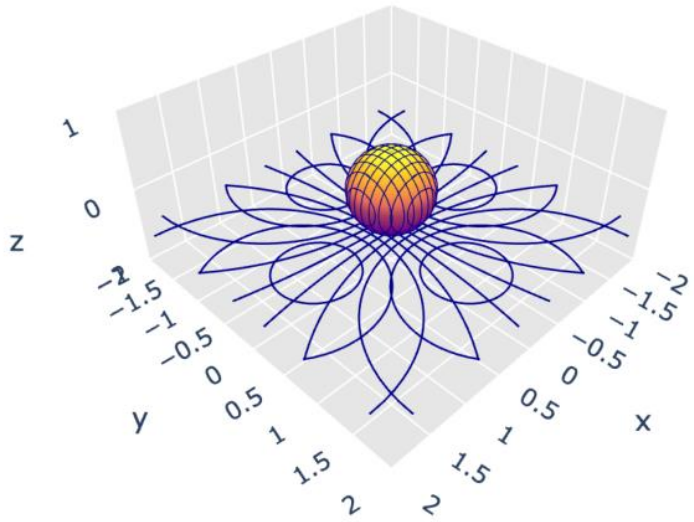
- Unified formalism of the κ − sterogrpah model for any $\kappa \in \mathbb{R}$



Heatmap of $d_{\mathbb{H}}^{\kappa}$



Projection of hyperboloid



Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Constant Curvature Graph Convolution Networks

- Unified formalism of the $\kappa-$ sterogrpah model for any $\kappa \in \mathbb{R}$:

$$\mathfrak{st}_\kappa^d = \{\boldsymbol{x} \in \mathbb{R}^d \mid -\kappa\|\boldsymbol{x}\|_2^2 < 1\}$$

	$\mathbb{R}^d$	$\mathfrak{st}_\kappa^d$
$\boldsymbol{x} \oplus_\kappa \boldsymbol{y}$	$\boldsymbol{x} + \boldsymbol{y}$	$\frac{(1-2\kappa \boldsymbol{x}^T \boldsymbol{y} - \kappa\|\|\boldsymbol{y}\|\|^2)\boldsymbol{x} + (1+\kappa\|\|\boldsymbol{x}\|\|^2)\boldsymbol{y}}{1-2\kappa \boldsymbol{x}^T \boldsymbol{y} + \kappa^2\|\|\boldsymbol{x}\|\|^2\|\|\boldsymbol{y}\|\|^2}$
$r \otimes_\kappa \boldsymbol{x}$	$r\boldsymbol{x}$	$\tan_\kappa\left(r \cdot \tan_\kappa^{-1}\|\|\boldsymbol{x}\|\|\right)\frac{\boldsymbol{x}}{\|\|\boldsymbol{x}\|\|}$
$\gamma_{\boldsymbol{x}\to\boldsymbol{y}}(t)$	$\boldsymbol{x} + t(\boldsymbol{y} - \boldsymbol{x})$	$\boldsymbol{x} \oplus_\kappa \left(t \otimes_\kappa \left(-\boldsymbol{x} \oplus_\kappa \boldsymbol{y}\right)\right)$

Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Constant Curvature Graph Convolution Networks

- Extend the vanilla GCN to the constant curvature GCN

$$\boldsymbol{H}^{(t+1)} = \sigma\left(\hat{\boldsymbol{A}}\boldsymbol{H}^{(t)}\boldsymbol{W}^{(t)}\right) \quad \Rightarrow \quad \boldsymbol{H}^{(l+1)} = \sigma^{\otimes_\kappa}\left(\hat{\boldsymbol{A}} \boxtimes_\kappa \left(\boldsymbol{H}^{(l)} \otimes_\kappa \boldsymbol{W}^{(l)}\right)\right)$$

where $\sigma^{\otimes_\kappa}$ is the κ-stereographic version of σ

- Learn the curvature to adapt to the geometry of the data

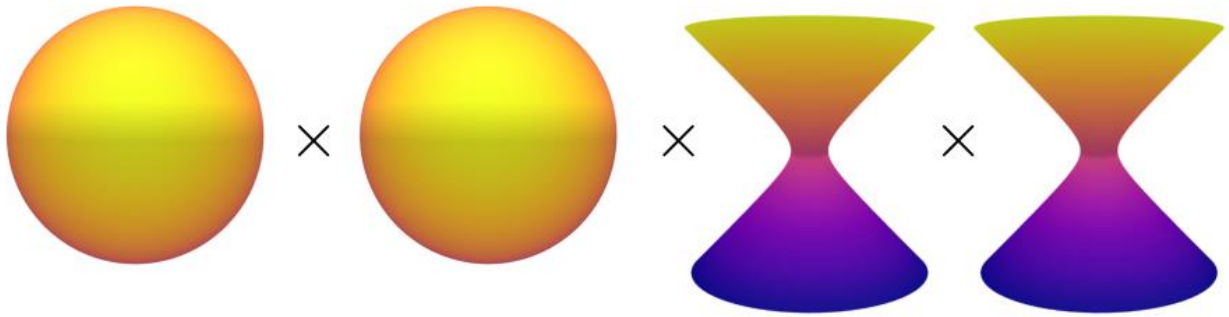
$$\kappa\text{-GCN} \xrightarrow{\kappa \to 0} \text{GCN}.$$

Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Constant Curvature Graph Convolution Networks

- Embed in product space via gyrovector space structure

$$\mathfrak{st}_{\kappa_1}^d \times \cdots \times \mathfrak{st}_{\kappa_m}^d$$



Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Constant Curvature Graph Convolution Networks

- Experiments on distortion task
  - Minimize the discrepancy between embedding distances and graph distances

$$L(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \frac{1}{n^2} \sum_{i,j} \left(\left(\frac{d_\kappa(\boldsymbol{x}_i, \boldsymbol{x}_j)}{d_{\boldsymbol{G}}(i,j)} \right)^2 - 1 \right)^2$$

  - Results on tree (negative curvature), spherical graph (positive curvature) and toroidal graph (product of positive curvature)
    - The best performing architecture is the one that matches the underlying geometry of the graph.

Model	Tree	Toroidal	Spherical
$\mathbb{E}^{10}$ (GCN)	0.0502	0.0603	0.0409
$\mathbb{H}^{10}$ (κ-GCN)	**0.0029**	0.272	0.267
$\mathbb{S}^{10}$ (κ-GCN)	0.473	0.0485	**0.0337**
$\mathbb{H}^5 \times \mathbb{H}^5$ (κ-GCN)	0.0048	0.112	0.152
$\mathbb{S}^5 \times \mathbb{S}^5$ (κ-GCN)	0.51	**0.0464**	0.0359

Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICLM 2020

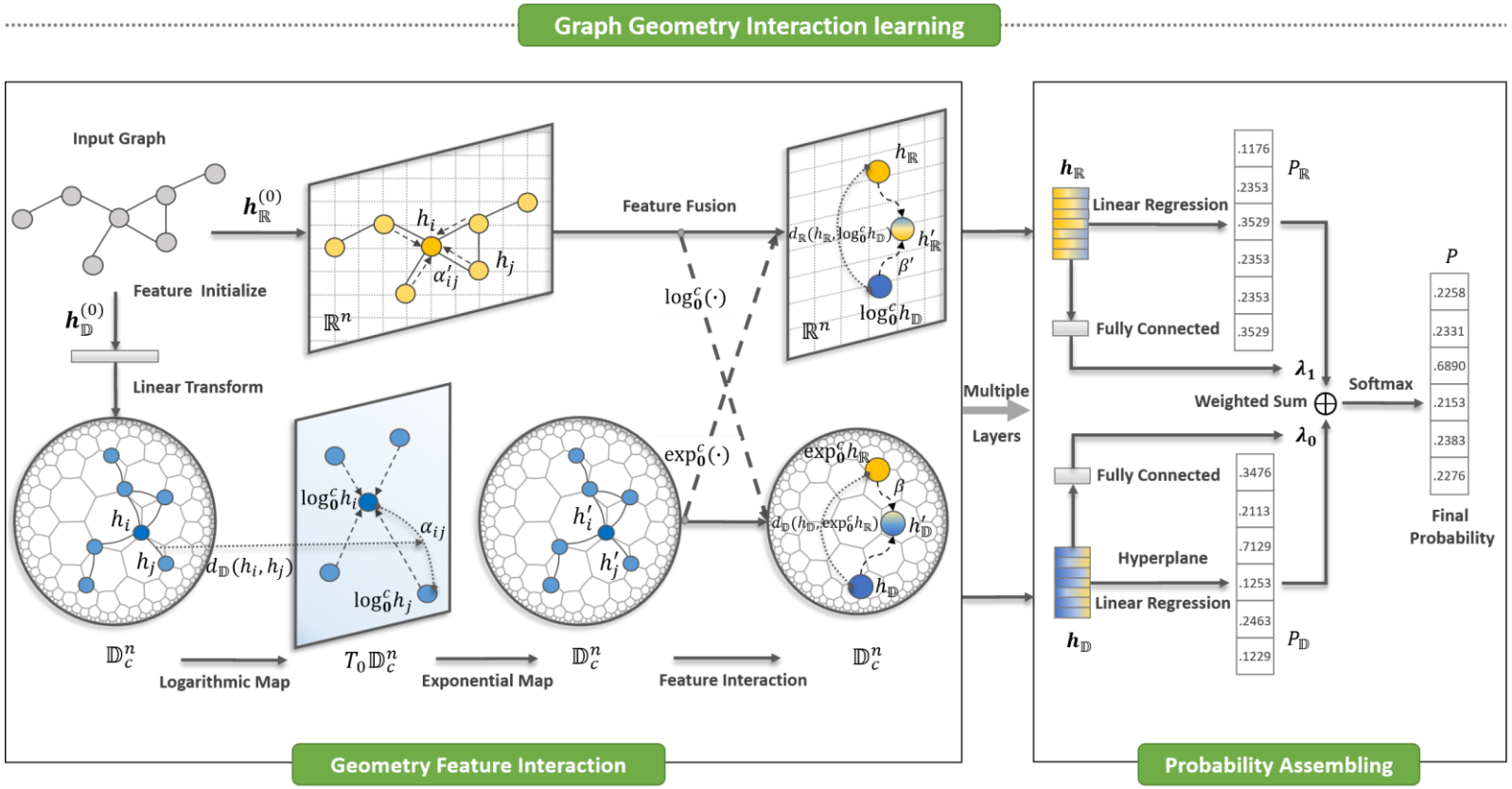
Constant Curvature Graph Convolution Networks

- Experiments on Node Classification

Model	Citeseer	Cora	Pubmed	Airport
$\mathbb{E}^{16}$ [3]	72.9 ± 0.54	81.4 ± 0.4	79.2 ± 0.39	81.4 ± 0.29
$\mathbb{H}^{16}$ [1]	71 ± 0.49	80.3 ± 0.46	$\mathbf{79.8 \pm 0.43}$	$\mathbf{84.4 \pm 0.41}$
$\mathbb{H}^{16}$ (κ-GCN)	$\mathbf{73.2 \pm 0.51}$	81.2 ± 0.5	78.5 ± 0.36	81.9 ± 0.33
$\mathbb{S}^{16}$ (κ-GCN)	72.1 ± 0.45	$\mathbf{81.9 \pm 0.45}$	78.8 ± 0.49	80.9 ± 0.58
Prod-GCN	71.1 ± 0.59	80.8 ± 0.41	78.1 ± 0.6	81.7 ± 0.44

Bachmann , G. et.al. Constant Curvature Graph Convolution Networks. ICML 2020

Graph Geometry Interaction Learning(GIL)



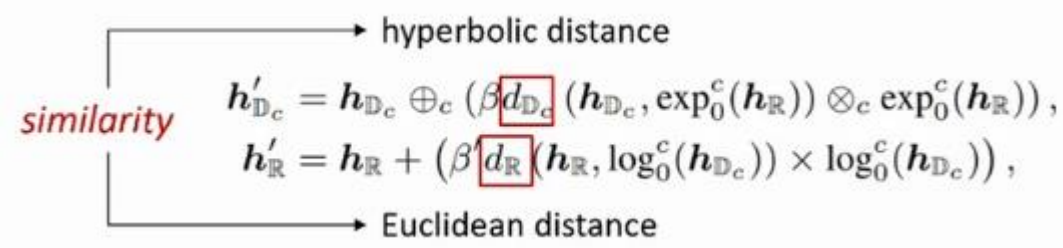
Geometry Interaction Learning

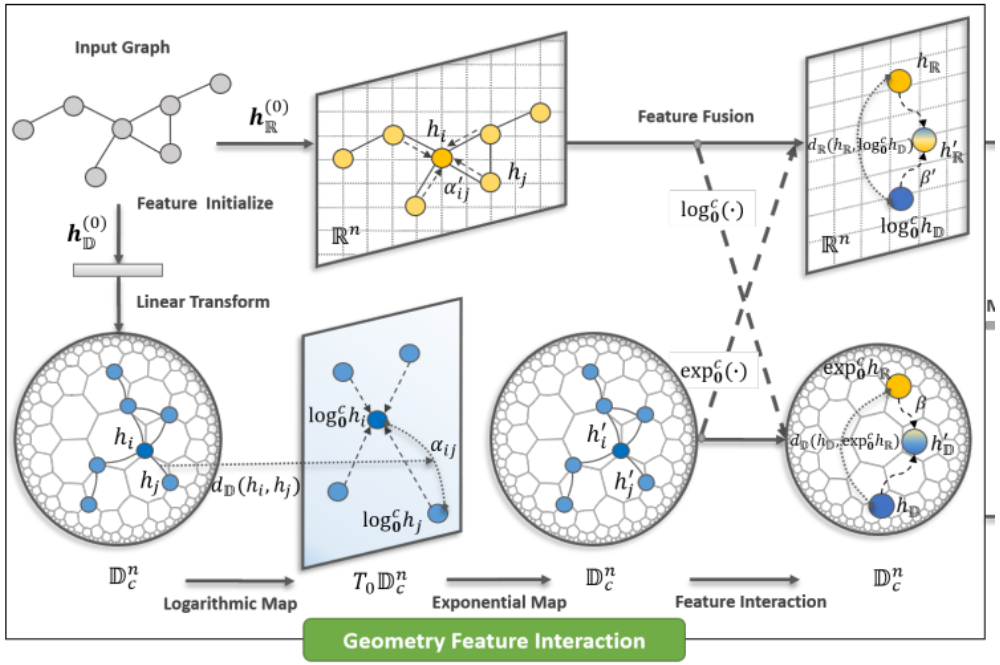
- Euclidean space: powerful simplicity and efficiency
- Hyperbolic space: ability for hierarchical structure

Zhu S, et al. "Graph geometry interaction learning.“ NeuRIPS 2020

Graph Geometry Interaction Learning(GIL)

- Geometry Message Propagation
  - Dual Feature propagation： propagates neighbor information simultaneously in a Euclidean space and a hyperbolic space via a distance-aware attention mechanism
  - Dual Feature Interaction: node features undergo an adaptive adjustment from the dual feature space based on distance similarity





Zhu S, et al. "Graph geometry interaction learning.“ NeuRIPS 2020

Graph Geometry Interaction Learning(GIL)

- Probability Assembling
  - One classifier

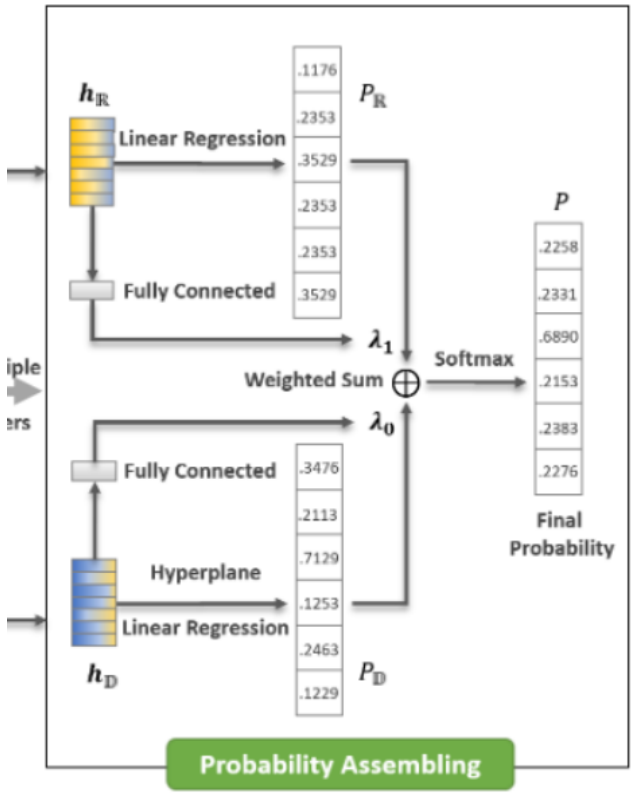
$$P = \text{Euc-Softmax}\left(f\left(\log_0^c(\boldsymbol{X}_{\mathbb{D}_c})||\boldsymbol{X}_{\mathbb{R}}\right)\right),$$
$$P = \text{Hyp-Softmax}\left(g\left(\boldsymbol{X}_{\mathbb{D}_c}||\exp_0^c(\boldsymbol{X}_{\mathbb{R}})\right)\right),$$

  - Two classifier

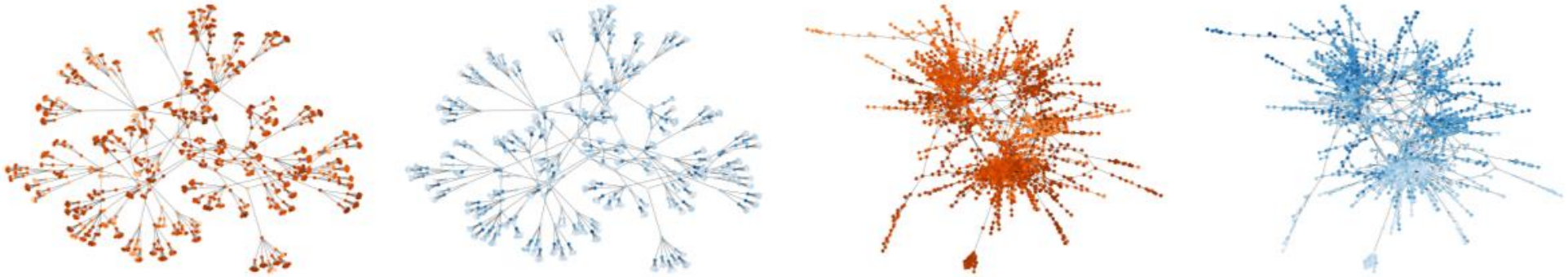
$$P = \boldsymbol{\lambda}_0 P_{\mathbb{D}_c} + \boldsymbol{\lambda}_1 P_{\mathbb{R}},$$
$$s.t.\ \boldsymbol{\lambda}_0 + \boldsymbol{\lambda}_1 = \mathbf{1},$$

Final probability of two parts are determined by the *node features*

$$\boldsymbol{\lambda}_0 = \text{sigmoid}\left(FC_0\left(\log_0^c(\boldsymbol{X}_{\mathbb{D}_c}^\top)\right)\right),\ \boldsymbol{\lambda}_1 = \text{sigmoid}\left(FC_1\left(\boldsymbol{X}_{\mathbb{R}}^\top\right)\right),$$
$$[\boldsymbol{\lambda}_0, \boldsymbol{\lambda}_1] = \frac{[\boldsymbol{\lambda}_0, \boldsymbol{\lambda}_1]}{\max\left(\|[\boldsymbol{\lambda}_0, \boldsymbol{\lambda}_1]\|_2, \epsilon\right)},$$



Zhu S, et al. "Graph geometry interaction learning.“ NeuRIPS 2020



(a) Disease: Hyperbolic (b) Disease: Euclidean (c) Citeseer: Hyperbolic (d) Citeseer: Euclidean

Encapsulate continuous and discrete curvature

- Curvature on network: measures the changes of local connectivity

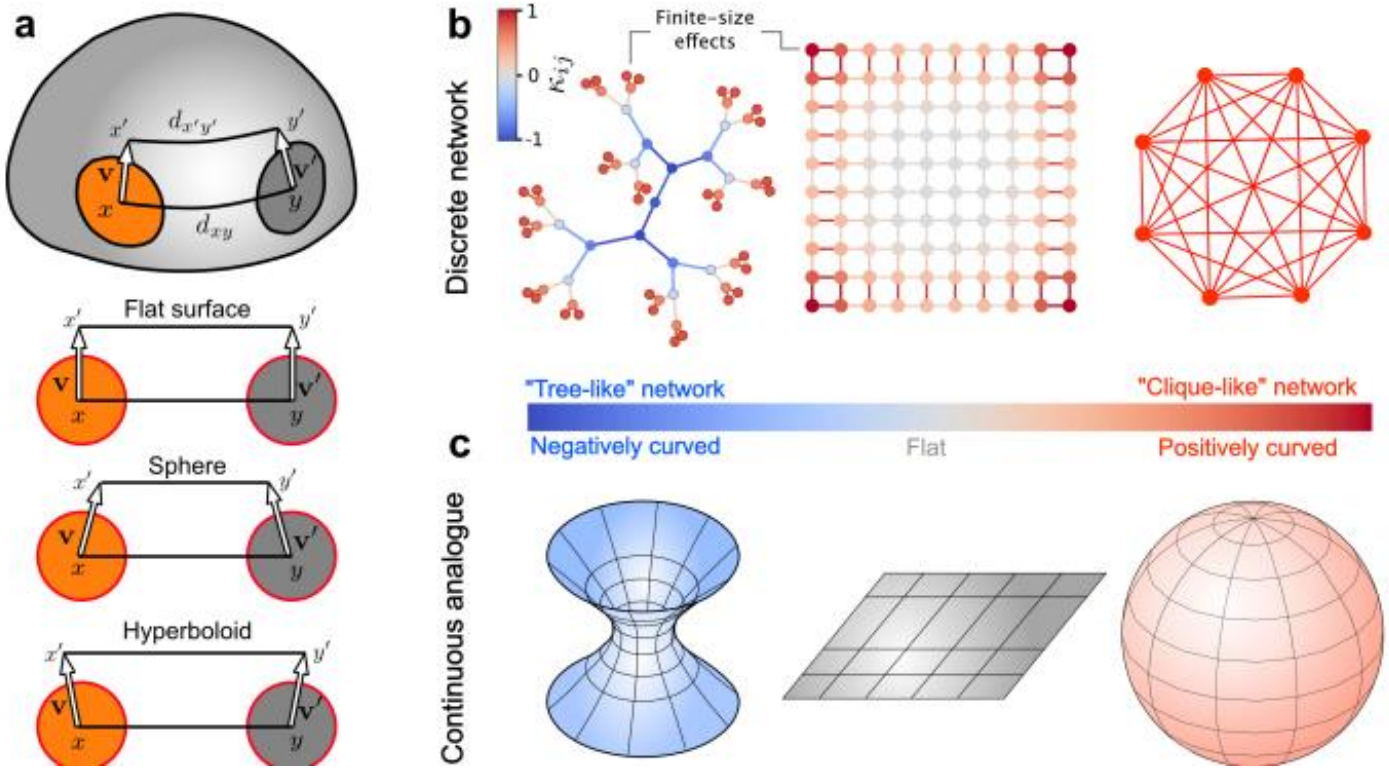


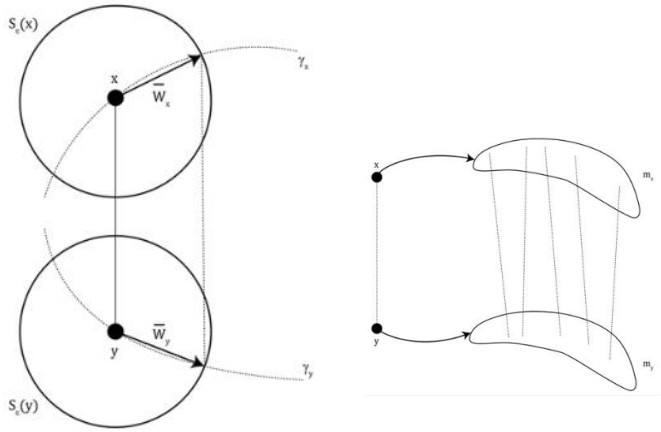
Fig. Ricci and dynamical Ollivier Ricci curvature on canonical surfaces and graph structures

Gosztolai., A. et. al. Unfolding the multiscale structure of networks with dynamical Ollivier-Ricci curvature. Nature Communications. 2021

Discrete Ricci Curvature

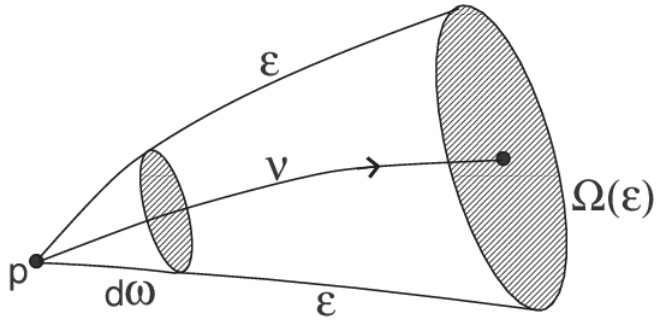
Ollivier-Ricci curvature

- ✓ Basic idea: Optimal transport
- ✓ Emphasizes clustering



Forman-Ricci curvature

- ✓ Basic idea: Dispersion
- ✓ Emphasize network dynamic



Source: Comparative analysis of two discretizations of Ricci curvature for complex networks

Froman-Ricci Curvature

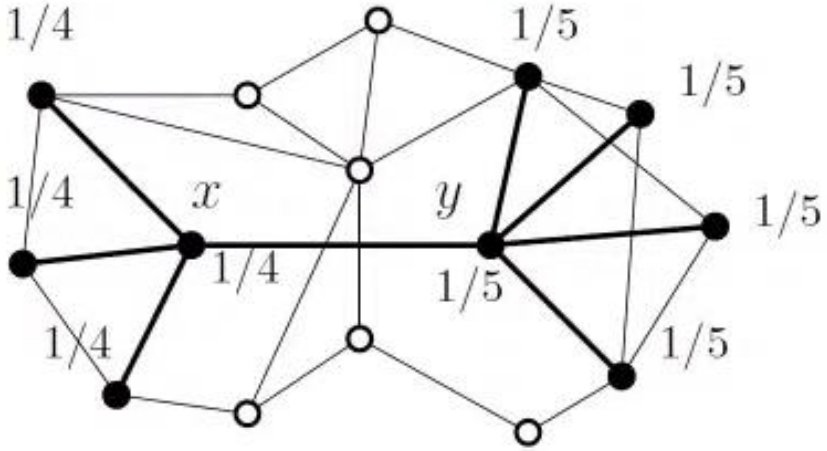
- Quantifies the degree of spread of the vertices
- Consider **triangles** as faces, and Δ_{uv} is the number of triangles that contain u, v. All edges have weight

$$F(u,v) = 4 - \deg(u) - \deg(v) + 3\Delta_{uv}$$

Ollivier-Ricci Curvature

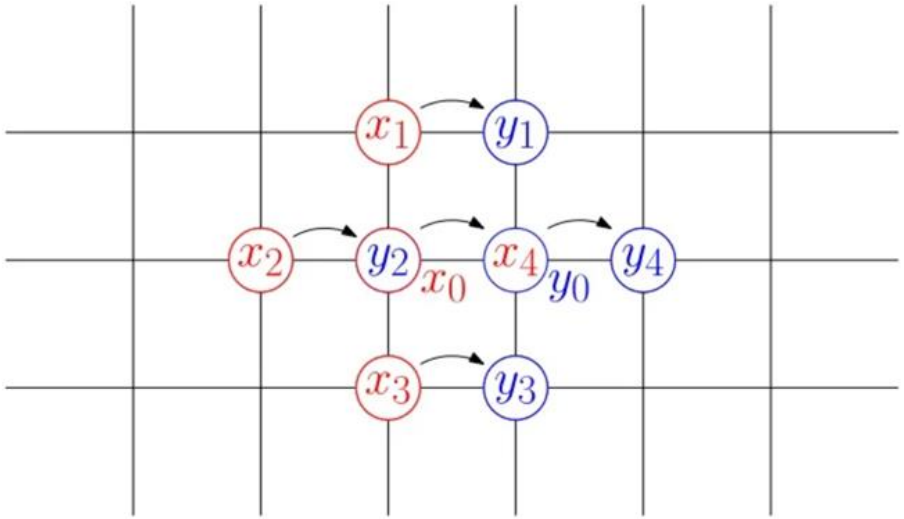
- For an edge xy, consider **the distance** from x's neighbors to y's neighbors and compare it with the length of xy
- How to compute the **distance** of x's neighbors to y's neighbors?
    - Optimal transport distance

$$\kappa_{xy} = 1 - \frac{W(m_x, m_y)}{d(x, y)},$$



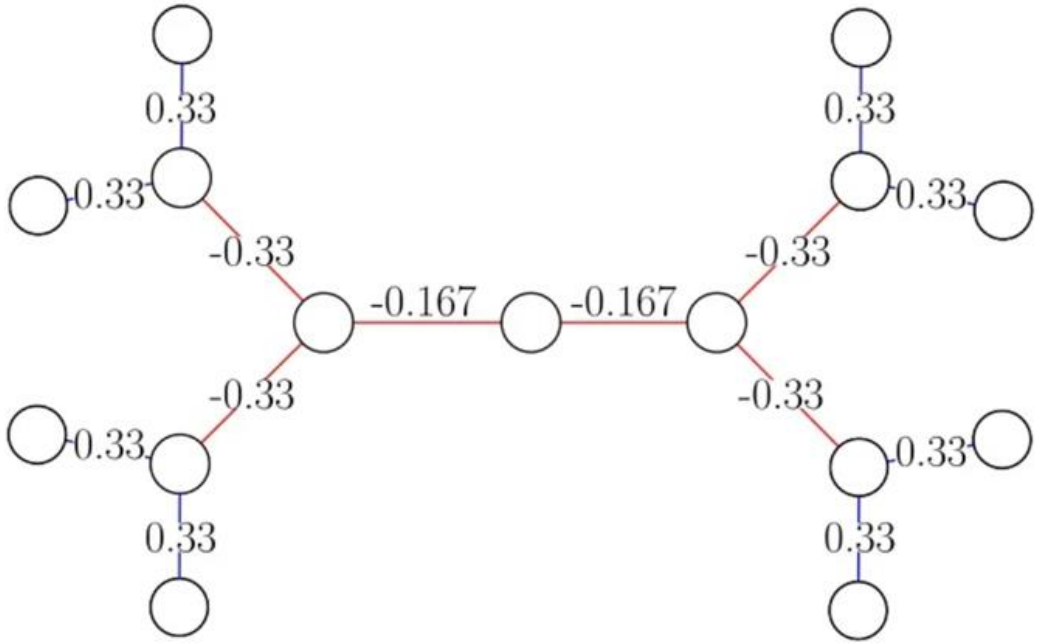
Curvature on Network

- Zero Curvature: 2D grid



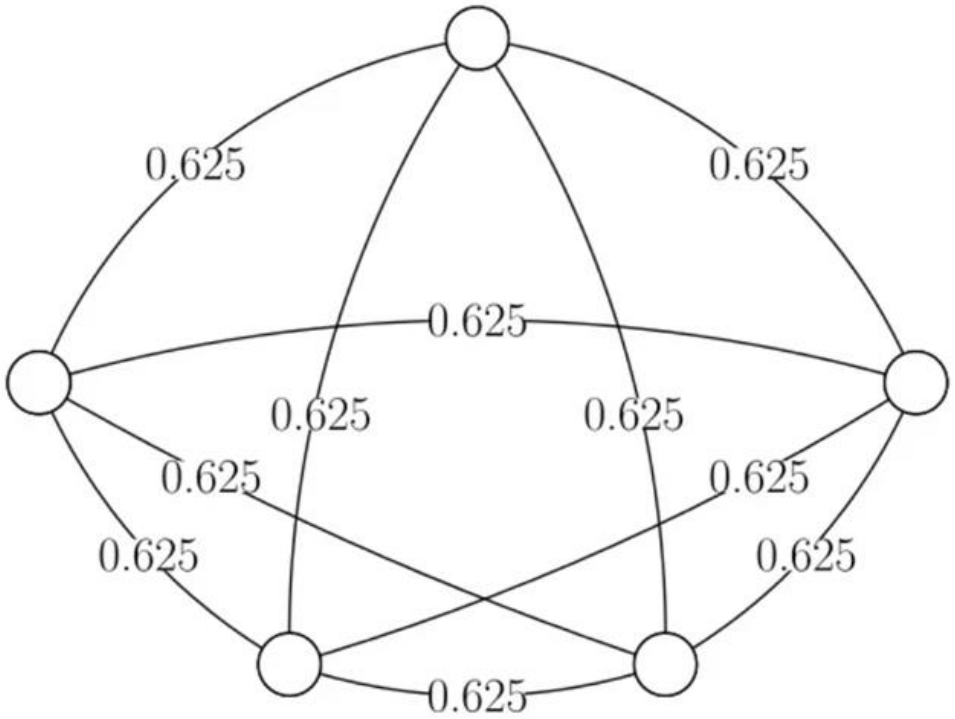
Curvature on Network

- Negative curvature: $k(x,y) = \frac{1}{d_x} + \frac{1}{d_y} - 1, d_x$ is degree of x.



Curvature on Network

- Positive Curvature: Complete graph



Curvature-aware graph embedding

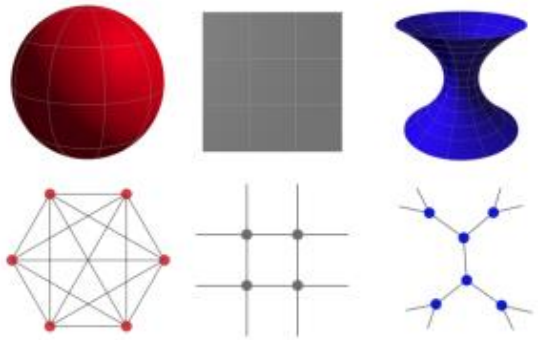
- Adapt an augmented Forman curvature:

$$\mathrm{F}(i,j) = 4 - d_i - d_j + 3\gamma \sharp_\Delta(i,j), \quad \gamma > 0,$$

$$\mathrm{F}(i) = \frac{1}{d_i} \sum_{j:j\sim i} \mathrm{F}(i,j)$$

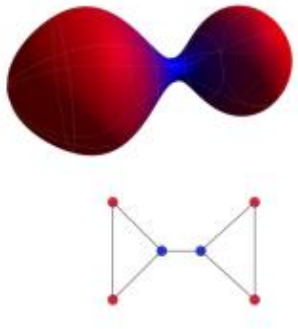
Degree of node i

The number of triangles at the edge(i,j)



(a) Space forms (sphere, plane, hyperboloid)

(b) Product manifold



(c) Heterogeneous manifold

Heterogeneous manifolds for curvature-aware graph embedding. ICLR workshop 2022

Curvature-aware graph embedding

- Loss function: Minimize distance and curvature depending loss

$$\mathcal{L}(\{y_i\}) = \mathcal{L}_{\mathrm{d}}(\{y_i\}) + \tau \mathcal{L}_{\mathrm{c}}(\{y_i\}),$$

$$\mathcal{L}_d(\{y_i\}) = \sum_{i,j} \left| \frac{d^2_{g_h}(z_i, z_j) + (r_i - r_j)^2}{d^2_G(x_i, x_j)} - 1 \right|$$

Measures the relative squared distance Distortion.

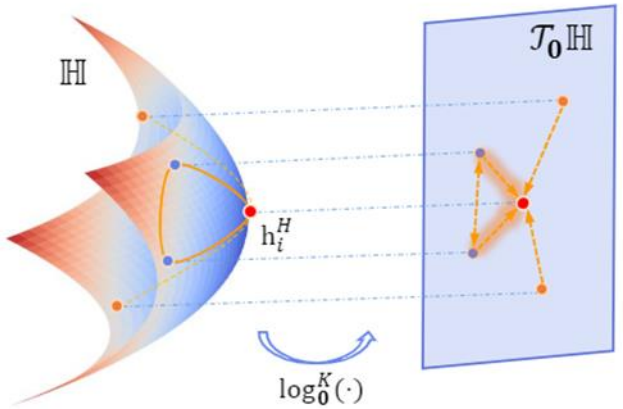
$$\mathcal{L}_c(\{y_i\}) = \sum_i \frac{\left(\mathrm{F}(x_i) - \mathrm{R}_h - \mathrm{R}_\alpha(r_i)\right)^2}{\left(|\mathrm{F}(x_i)| + \epsilon\right)^2},$$

Measures how close the local geometry of the manifold around the embedded nodes resembles that of the graph.

Di Giovanni, F. et.al Heterogeneous manifolds for curvature-aware graph embedding. ICLR workshop 2022

Curvature-aware graph embedding

- Curvature-guided message aggregation



$$\tilde{\mathbf{h}}_i^{\ell,H} = \exp_{\mathbf{0}}^{K_{l-1}}\left(\sum_{j\in N(i)} \tilde{\kappa}_{i,j} \cdot \log_{\mathbf{0}}^{K_{l-1}}(\mathbf{h}_j^{\ell,H})\right)$$

$$\tilde{\kappa}_{i,j} = \mathrm{softmax}_{j\in\mathcal{N}(i)}\left(\mathrm{MLP}(\kappa_{i,j} - |L_i - L_j|)\right)$$

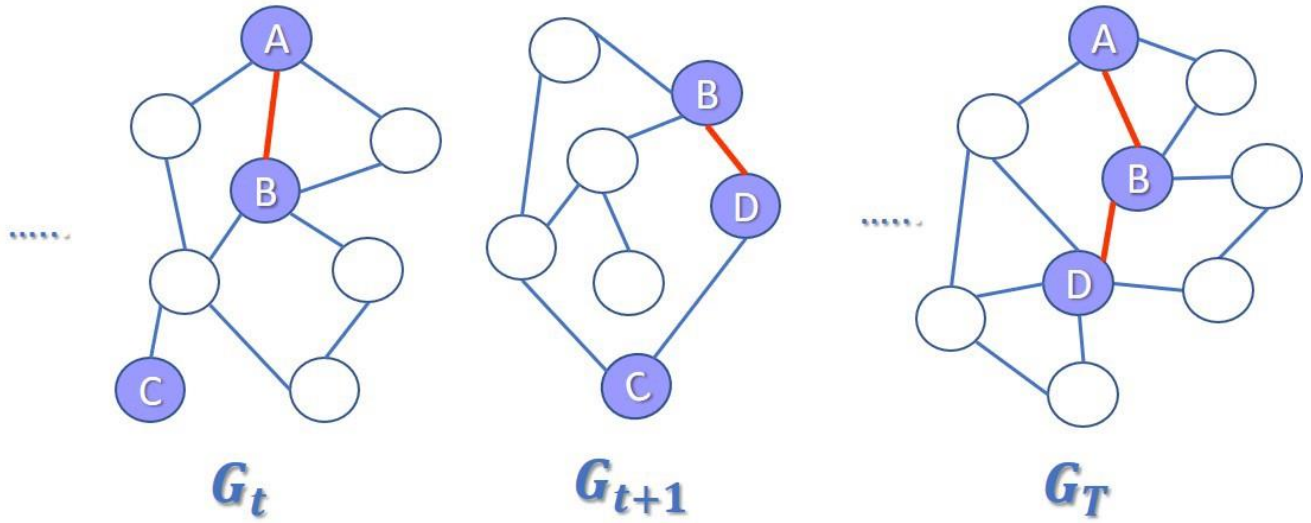
- Curvature-enhanced message exchange

$$l_{hc+} = \frac{1}{|E_\kappa|}\sum_{(i,j)\in E_\kappa} -\log\, p(\mathbf{x}_i^{\ell,\mathcal{H}}, \mathbf{x}_j^{\ell,\mathcal{H}}),$$

Yang, M. et.al. Hyperbolic Curvature Graph Neural Network. arXiv. 2022

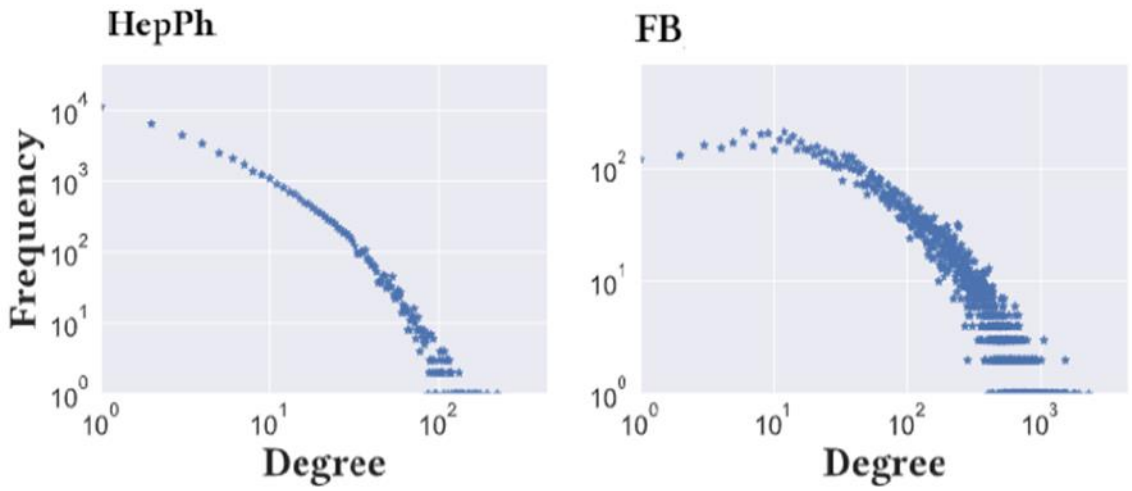
4.2 Evolving Interactions

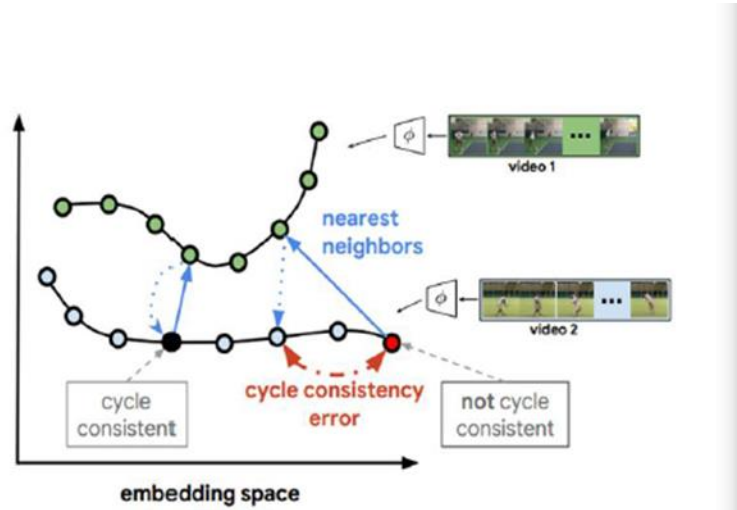
- Hyperbolic Variational Graph Neural Network for Modeling Dynamic Graphs AAAI2021
- Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021
- A Self-supervised Riemannian GNN with Time Varying Curvature for Temporal Graph Learning CIKM 2022
- …



https://towardsdatascience.com/tdgraphembed-temporal-dynamic-graph-level-embedding-1cc611bc7db0

Hyperbolic Temporal Network Embeddings





From: Temporal Cycle-Consistency Learning(CVPR 2019)

Yang. M. et.al. Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021

Hyperbolic Temporal Network Embeddings

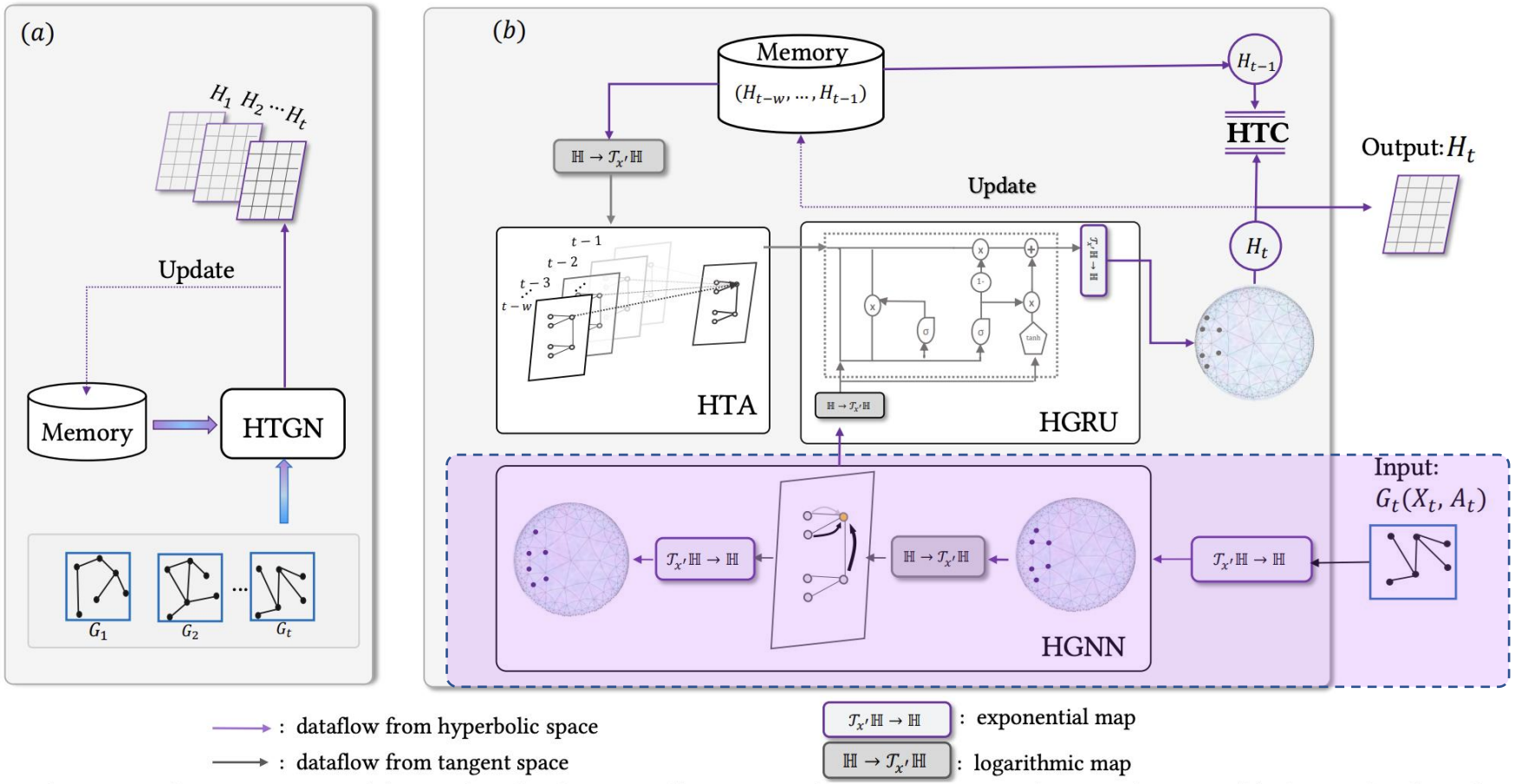
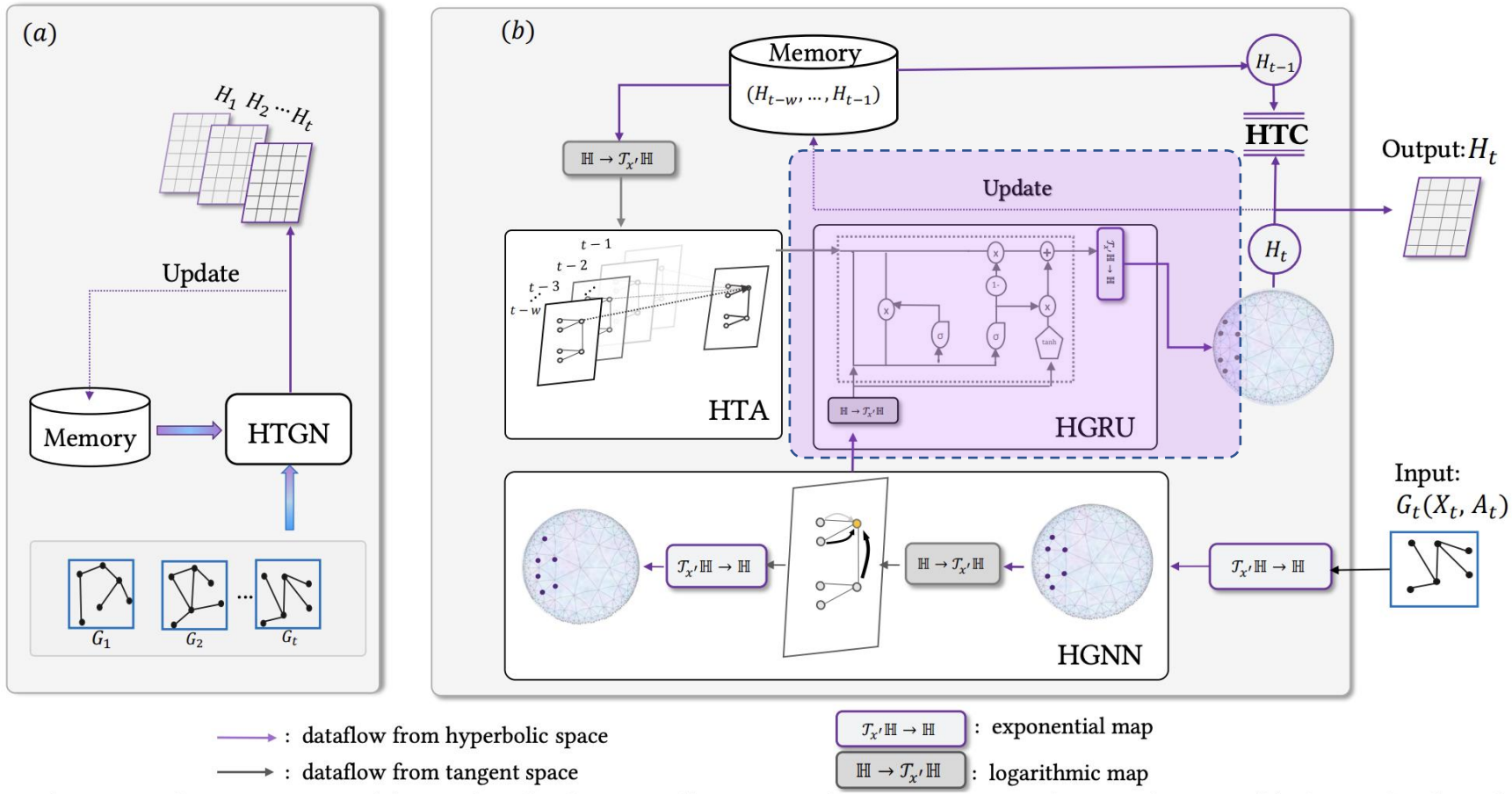


Figure 3: Schematic of HTGN. Figure (a) is a sketch of HTGN illustrating the recurrent paradigm and Figure (b) shows the data flow of an HTGN unit.

Yang. M. et.al. Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021

Hyperbolic Temporal Network Embeddings



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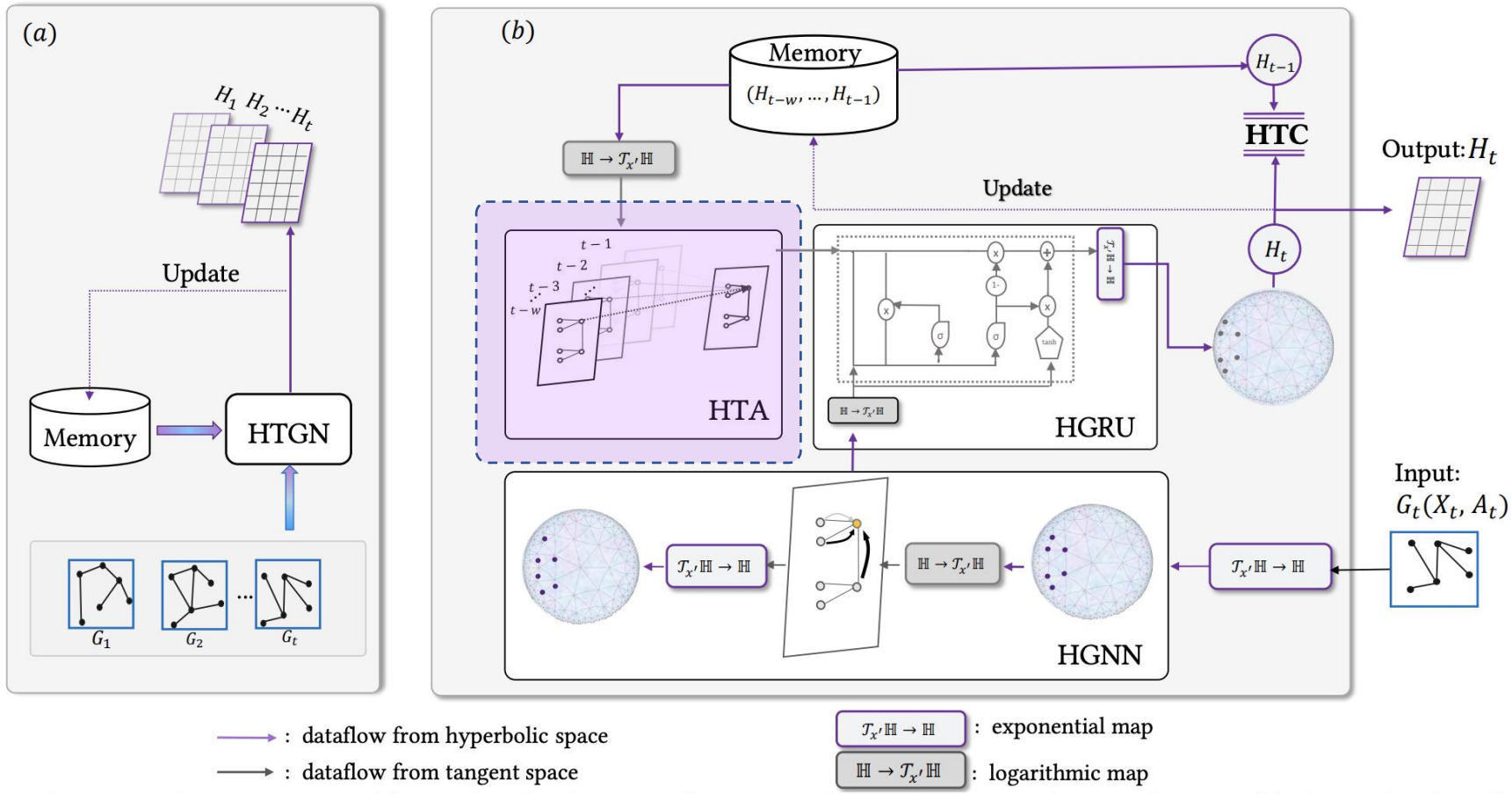
Yang. M. et.al. Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021

Hyperbolic Temporal Network Embeddings



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Yang. M. et.al. Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021

Hyperbolic Temporal Network Embeddings

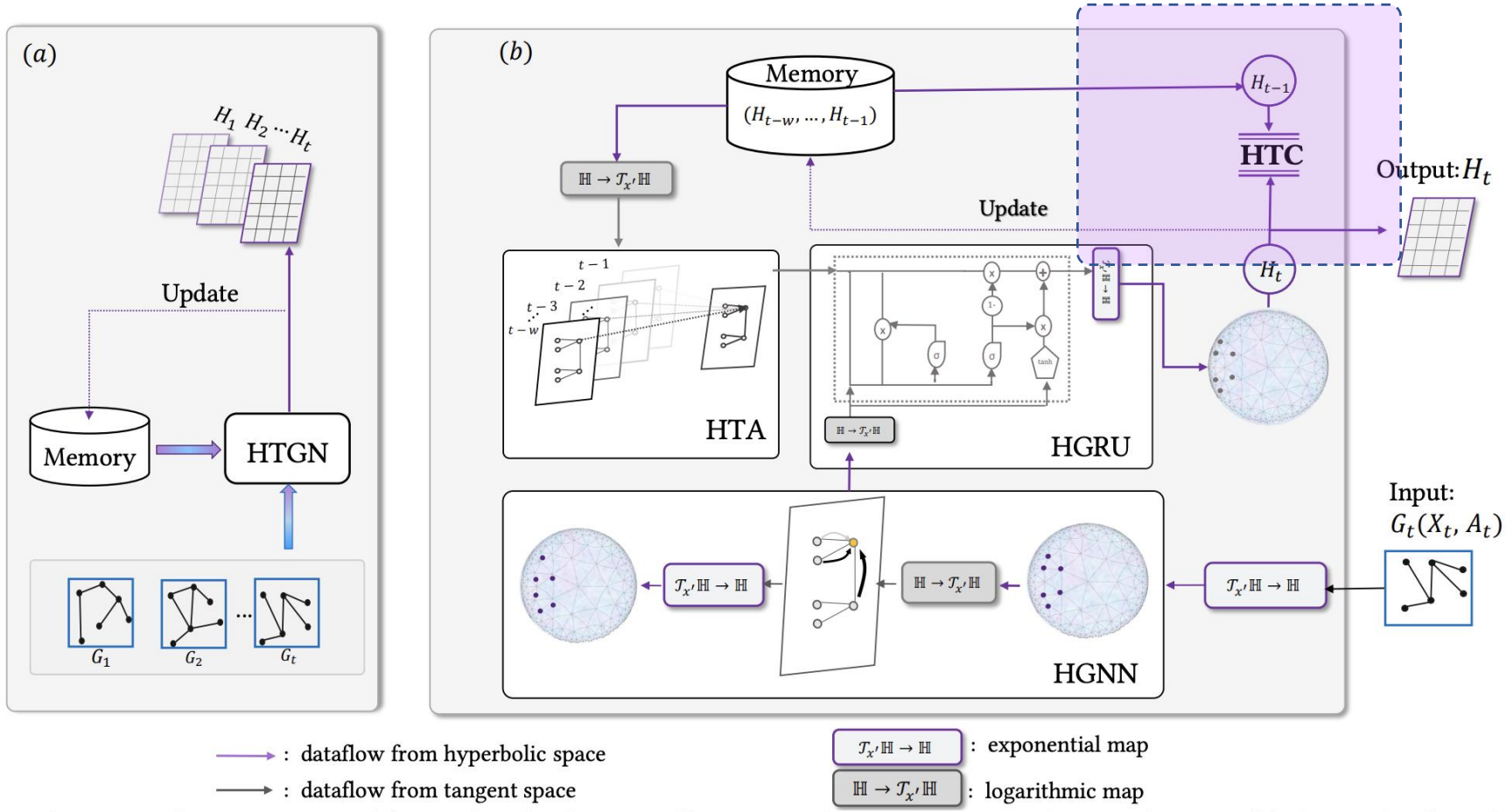


Figure 3: Schematic of HTGN. Figure (a) is a sketch of HTGN illustrating the recurrent paradigm and Figure (b) shows the data flow of an HTGN unit.

Yang. M. et.al. Discrete-time temporal network embedding via implicit hierarchical learning in hyperbolic space KDD2021

Table 2: Dataset statistics.

Datasets	DISEASE	HepPH	FB	AS733	Enron	COLAB
#Snapshots	7	36	36	30	11	10
#Test k	3	6	3	10	3	3
#Nodes	2665	15,330	45,435	6,628	184	315
#Total Edges	2664	976,097	180,011	13,512	790	943
Density ρ (0.01)*	0.41	1.37	0.04	0.2	3.37	0.94
Hyperbolicity $\delta^{\star}$	0.0	1.0	2.0	1.5	1.5	2.0

* 0.01 denotes the value is in units of 0.01.

$\star$ The smaller δ indicates the dataset has a more evident hierarchical structure.

Table 3: AUC (left) and AP (right) scores of dynamic link prediction on real-world dynamic graphs.

	AUC						AP					
Dataset	**DISEASE**	**HepPh**	**FB**	**AS733**	**Enron**	**COLAB**	**DISEASE**	**HepPh**	**FB**	**AS733**	**Enron**	**COLAB**
GAE	72.55 ± 1.20	69.44 ± 0.56	63.07 ± 0.93	93.21 ± 1.53	92.50 ± 0.68	84.57 ± 0.64	60.55 ± 1.01	73.61 ± 0.58	65.35 ± 0.90	94.75 ± 0.90	*93.48 ± 0.64*	87.69 ± 0.44
VGAE	83.08 ± 1.27	72.39 ± 0.11	67.16 ± 0.53	*95.76 ± 0.91*	91.93 ± 0.34	85.16 ± 0.74	78.34 ± 1.25	75.78 ± 0.06	69.73 ± 0.17	96.42 ± 0.55	93.45 ± 0.49	88.70 ± 0.35
EvolveGCN	73.55 ± 4.23	76.82 ± 1.46	76.85 ± 0.85	92.47 ± 0.04	90.12 ± 0.69	83.88 ± 0.53	73.25 ± 3.44	81.18 ± 0.89	80.87 ± 0.64	95.28 ± 0.01	92.71 ± 0.34	87.53 ± 0.22
GRUGCN	79.25 ± 1.69	*82.86 ± 0.53*	*79.38 ± 1.02*	94.96 ± 0.35	92.47 ± 0.36	84.60 ± 0.92	65.26 ± 1.94	*85.87 ± 0.23*	*82.77 ± 0.75*	96.64 ± 0.22	93.38 ± 0.24	87.87 ± 0.58
DySAT	73.74 ± 2.28	81.02 ± 0.25	76.88 ± 0.08	95.06 ± 0.21	93.06 ± 0.97	*87.25 ± 1.70*	63.81 ± 1.86	84.47 ± 0.23	80.39 ± 0.14	*96.72 ± 0.12*	93.06 ± 1.05	*90.40 ± 1.47*
VGRNN	*86.44 ± 3.12*	77.65 ± 0.99	78.11 ± 1.11	95.17 ± 0.62	*93.10 ± 0.57*	85.95 ± 0.49	*82.00 ± 3.83*	80.95 ± 0.94	80.40 ± 0.74	96.69 ± 0.31	93.29 ± 0.69	87.77 ± 0.79
HTGN (Ours)	89.65 ± 0.70	91.13 ± 0.14	83.70 ± 0.33	98.75 ± 0.03	94.17 ± 0.17	89.26 ± 0.17	84.63 ± 0.65	89.52 ± 0.28	83.80 ± 0.43	98.41 ± 0.03	94.31 ± 0.26	91.91 ± 0.07
Gain (%)	+3.71	+9.98	+5.44	+3.12	+1.15	+2.30	+3.21	+4.25	+1.24	+1.75	+0.89	+1.67

Figure 4: AUC scores of different embedding dimensions on FB.

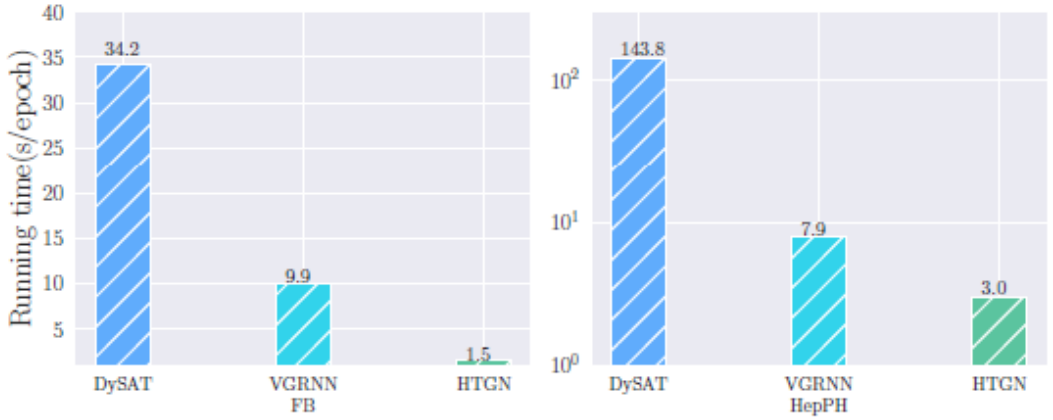


Figure 5: Running time on FB and HepPh.

Geometry-Aware Learning

- Enhancing hyperbolic graph embeddings via contrastive learning. NeurIPS 2021 Workshop
- HRCF: Enhancing collaborative filtering via hyperbolic geometric regularization. WebConf2022
- HICF: Hyperbolic Informative Collaborative Filtering. KDD2022
- …

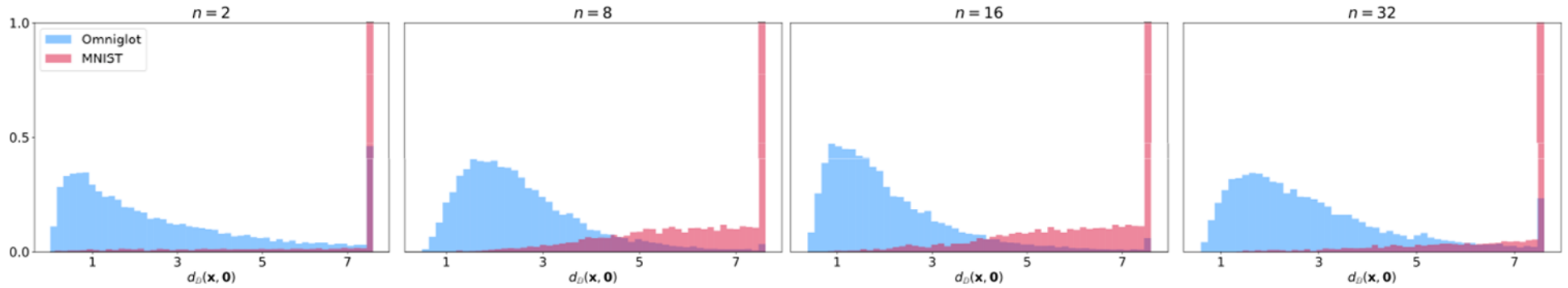


Figure source: Hyperbolic Image Embedding. CVPR 2020

Geometry-Aware Learning

- Hyperbolic space is more spacious in the area of hyperbolic space
  - Maintain the hierarchy but push the embeddings to the boundary

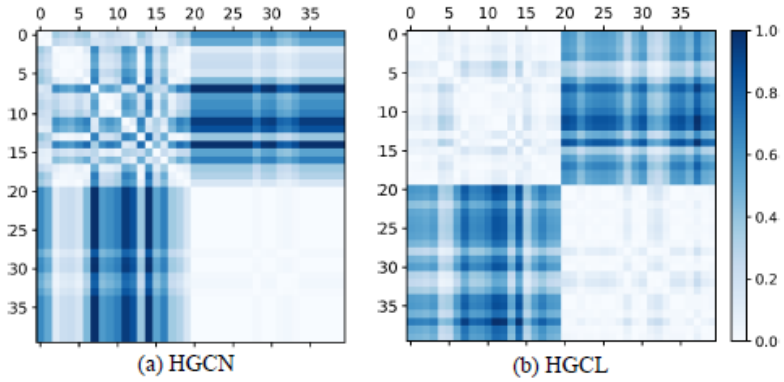


Figure 5: The distance heatmap among inter-class and intra-class embeddings on DISEASE

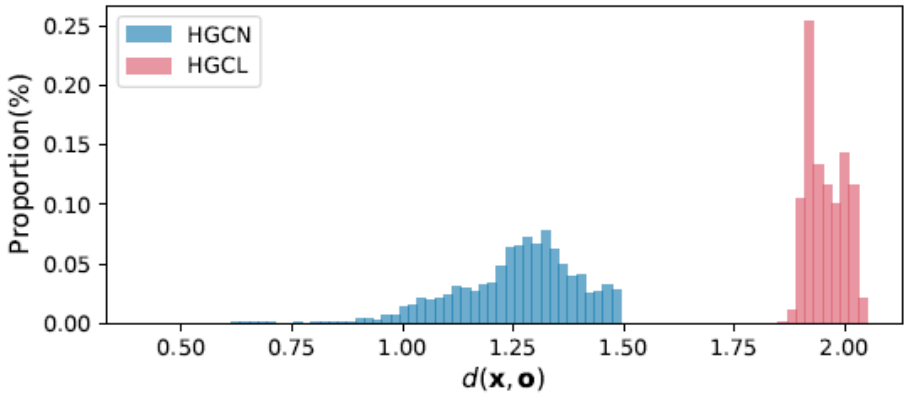
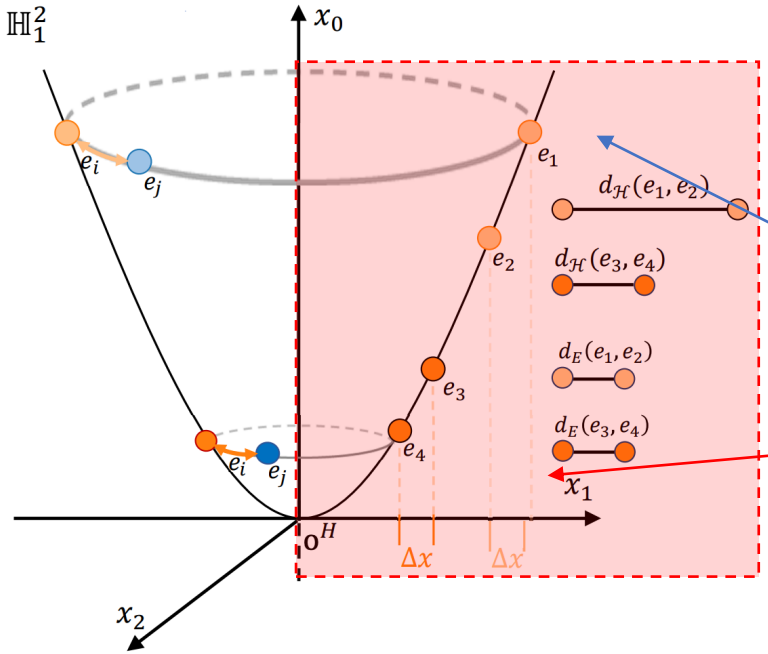


Figure 6: Distribution of the hyperbolic distance to the origin (HDO) embedded into the Poincaré ball on AIRPORT dataset

Enhancing hyperbolic graph embeddings via contrastive learning. NeurIPS 2021 Workshop

Geometry-Aware Learning

Hyperbolic-Aware Margin Learning (HAML)



Large Margin

Small Margin

$$\ell(u,i,j) = \max(\underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_i)}_{\text{Pull}} - \underbrace{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_j)}_{\text{Push}} + m, 0),$$

$$m^{\mathcal{H}}_{ui} = \text{sigmoid}(\delta),$$

$$\delta = \frac{d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{o}) + d^2_{\mathcal{H}}(\mathbf{e}_i, \mathbf{o}) - d^2_{\mathcal{H}}(\mathbf{e}_u, \mathbf{e}_i)}{\mathbf{e}_{u,0}\mathbf{e}_{i,0}},$$

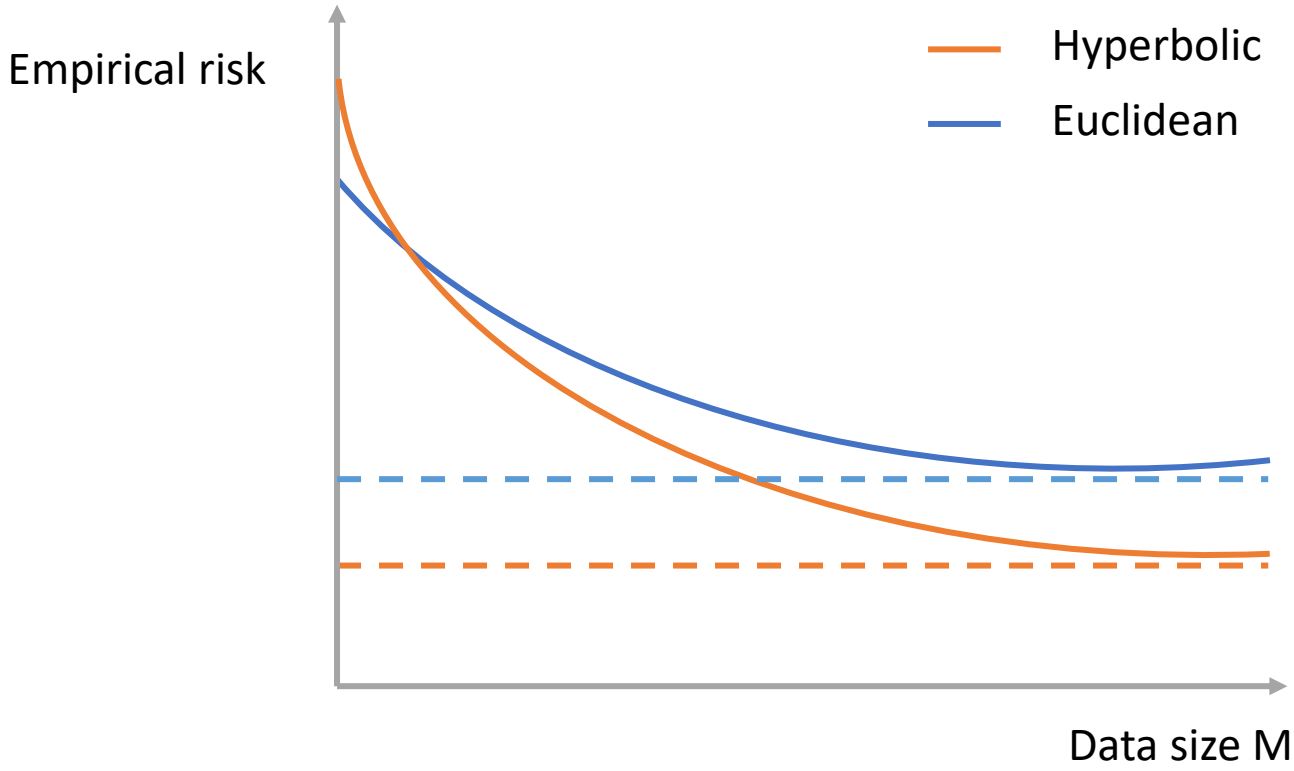
Yang,et.al. HICF: Hyperbolic Informative Collaborative Filtering KDD 2022.

4.4 Trustworthy and Scalability

- Trustworthy
  - Where are we in embedding spaces? A Comprehensive Analysis on Network Embedding Approaches for Recommender Systems. KDD 2021
  - Generalization Error Bounds for Graph Embedding Using Negative Sampling: Linear vs Hyperbolic. NeurIPS 2021
  - …
- Scalability
  - Fully connected hyperbolic neural network. ACL2022
  - Towards Scalable Hyperbolic Neural Networks using Taylor Series Approximations. arXiv 2022
  - Laplacian Features for Learning with Hyperbolic Space. arXiv 2022
  - …

Generalization Error Bounds

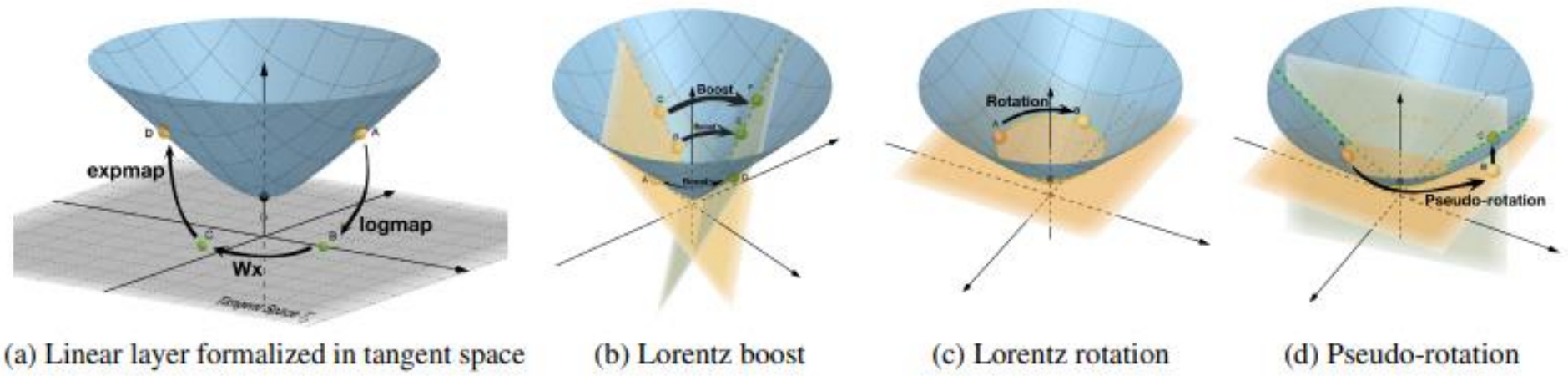
- Error is polynomial and exponential with respect to the embedding space's radius in linear and hyperbolic spaces
- An imbalanced distribution causes large generalization error
- Hyperbolic models give smaller empirical risk to tree-like dataset
- Hyperbolic space shows advantage for the case with large data size



Suzuki A, et.al. Generalization Error Bounds for Graph Embedding Using Negative Sampling: Linear vs Hyperbolic. NeurIPS 2021

HGNN Accelerating

- A fully hyperbolic framework to build hyperbolic networks based on the Lorentz model
  - Adapting the Lorentz transformations to formalize essential operations of neural network

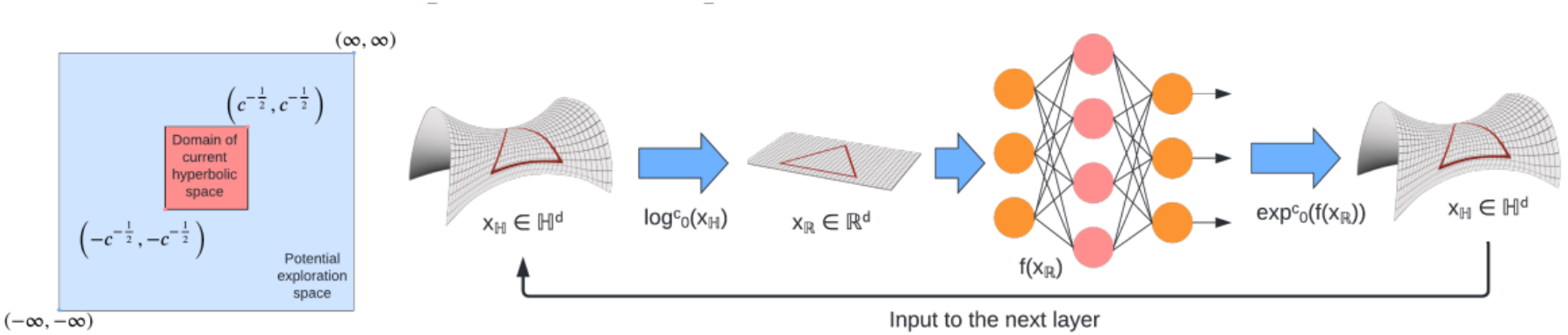


(a) Linear layer formalized in tangent space (b) Lorentz boost (c) Lorentz rotation (d) Pseudo-rotation

Chen. W. et.al. Fully Hyperbolic Neural Networks. ACL 2022

HGNN Accelerating

- Propose the approximation of hyperbolic operators using Taylor series expansions



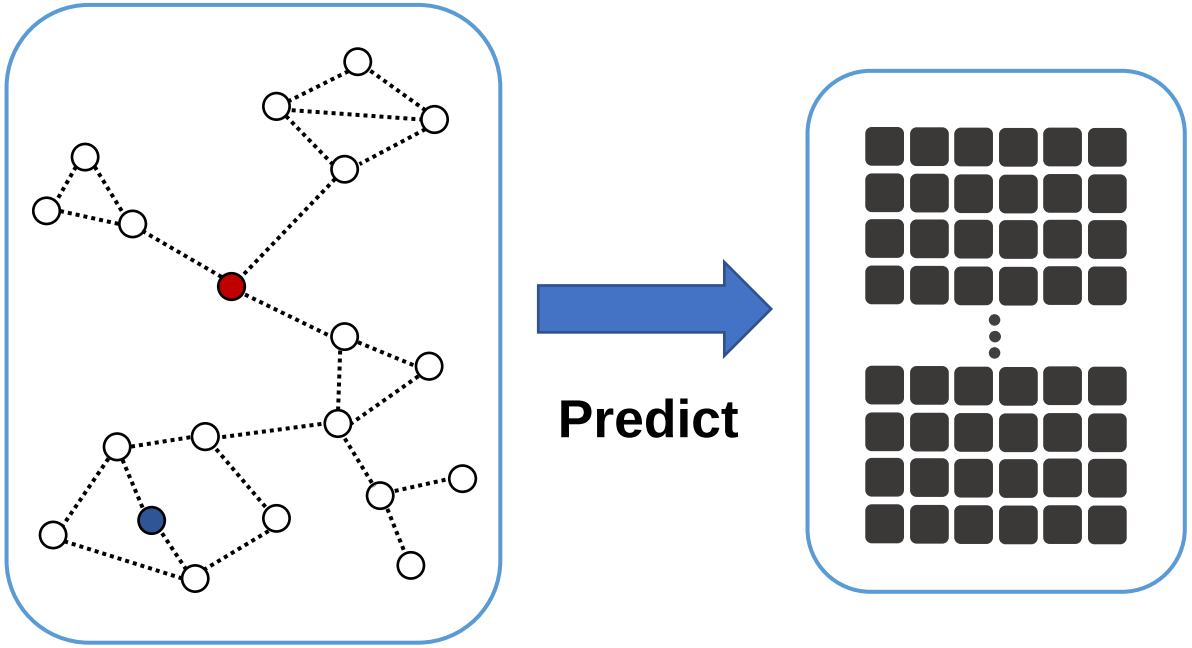
(a) Restricted $\mathbb{H}_c$ in the exploration space of $\mathbb{R}$.

(b) Information loss due to frequent $\log_0^c$ and $\exp_0^c$ mapping to operate in the Euclidean space and represent in the hyperbolic space, respectively.

Choudhary. N. et.al . Towards Scalable Hyperbolic Neural Networks using Taylor Series Approximations. arXiv 2022.

Scalable GNN

How to scaling up GNNs to large graphs?



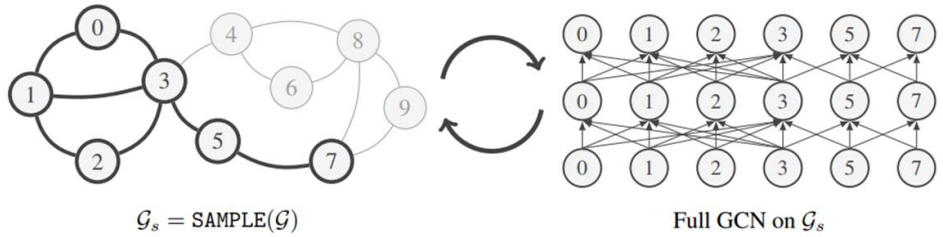
- Sampling-based Methods
- Decoupling-based Methods

High GPU costs and performance reduction

Scalable GNN

- Sampling-based Methods
  - Node-wise Sampling
    GraphSAGE
  - Layer-wise Sampling
    FastGCN, LADIES
  - Subgraph Sampling
    Cluster-GCN, Graphsaint
- Decoupling-based Methods

  SGC, SIGN, SAGN



Reduce the size of the graph on GPU

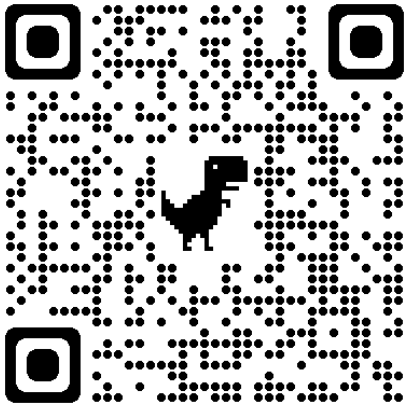
Scalable HGNN?

Summary

- HGRL is a still nascent but promising
  - Compatible、Light, and Fast
- Challenges& Opportunities
  - Domain Applications
  - Complex Structure
  - Evolving Interactions
  - Geometry-aware Learning
  - Trustworthy
  - Scalability
  - …

Resource

- Survey
  - Hyperbolic Graph Neural Networks: A Review of Methods and Application
  - Hyperbolic Deep Neural Networks: A Survey
- Tools
  - Geoopt: https://github.com/geoopt/geoopt
  - PyG: https://github.com/pyg-team/pytorch_geometric
  - https://github.com/alibaba/Curvature-Learning-Framework
- Related Tutorial
  - https://www.youtube.com/watch?v=MdPk3qD4Wig&ab_channel=HazyResearch
  - https://nurendra.me/hyperbolic-networks-tutorial/www-2022/



Acknowledgement

Thanks !