Hyperbolic Neural Networks

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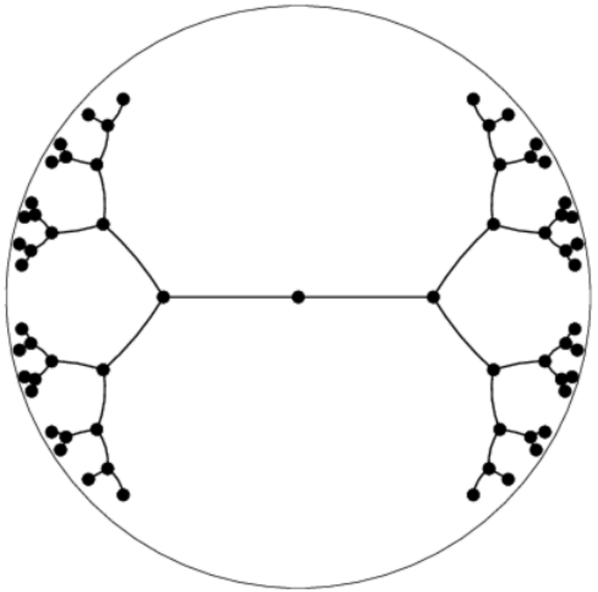
Why Non-Euclidean Spaces

Inherent properties of Euclidean space is **Flatness**

Any scientific fields study data with an **underlying structure** that is a **non-Euclidean**



- **Better representations ：** Euclidean space simply doesn't fit many types of data structures: **hierarchy**(its abstract network representation: the tree)
- **Unlocking the full potential of models :** The space the points live in can be the limit of performance of these models.
- **More flexible operations :** The flatness of Euclidean space means that certain operations require a large number of dimensions and complexity to perform

Limitations of a Flat World

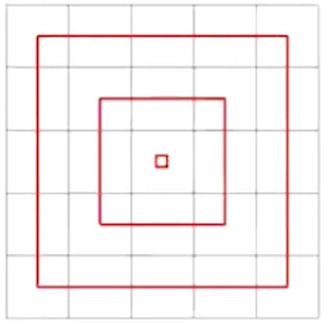
Hierarchical relationship dataset :

- Lexical databases:WordNet, Wikipedia categories, biological and chemical taxonomies such as phylogenetic relations
- Knowledge graphs : Freebase

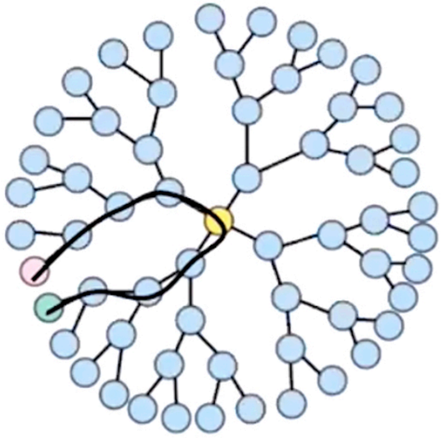
To get **continuous representations**, need to embed a tree into a **continuous space**

Properties :

- Distance
- Growth(expand) : **exponential**



$S \propto r^2$



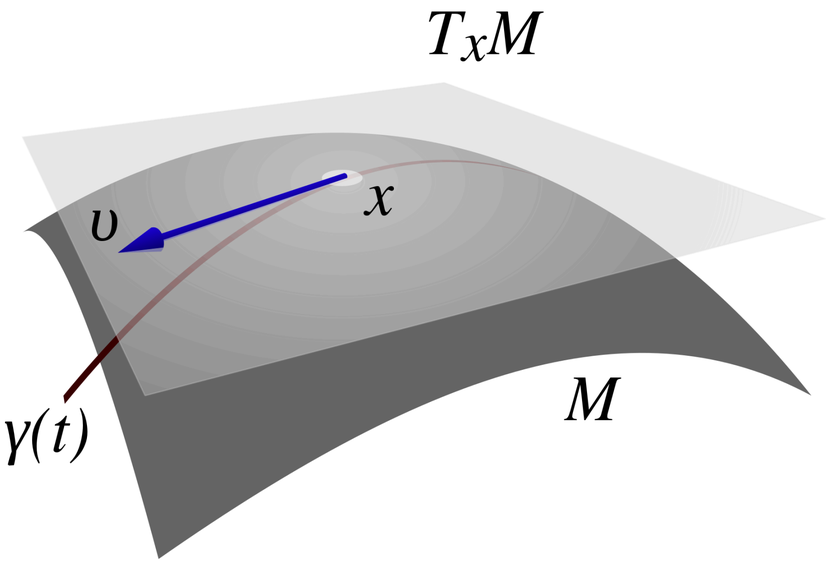
$S \propto a^r$

Euclidean space : polynomial $V = 4/3\pi r^3$

Differential Geometry

Replace $\mathbb{R}^n$ with n-dimensional manifold $\mathscr{M}$

- A model : $f : \mathscr{M} \to \mathscr{M}$, compute $f(p)$ for $p \in \mathscr{M}$
- Train the model : computing derivatives for f
- Embedding space : corresponds to the input data.



Calculus at each point of the manifold : **linear approximations —> tangent spaces(tangent vectors)**

exp map : tangent space to the manifold
log map : the manifold to tangent space

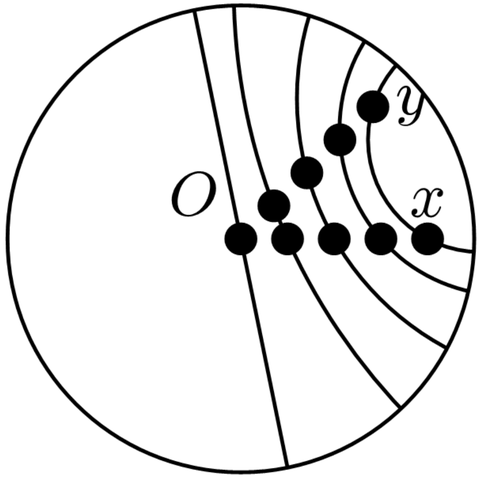
Riemannian metric : vary at each point, enables us to measure inner products between tangent vectors so, express geometric quantities (e.g., angles, lengths, and distances)

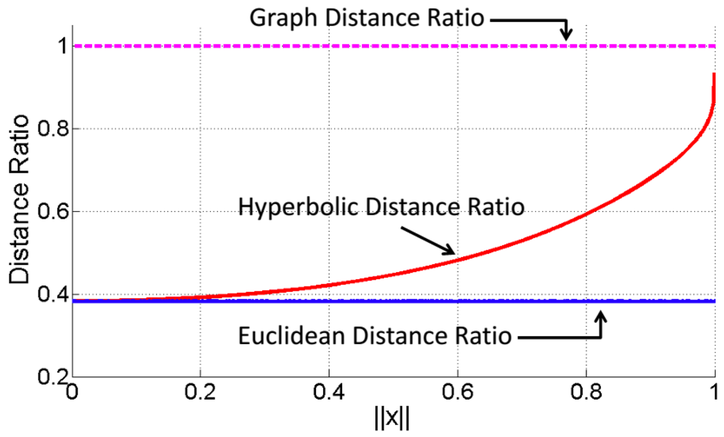
Hyperbolic Embeddings

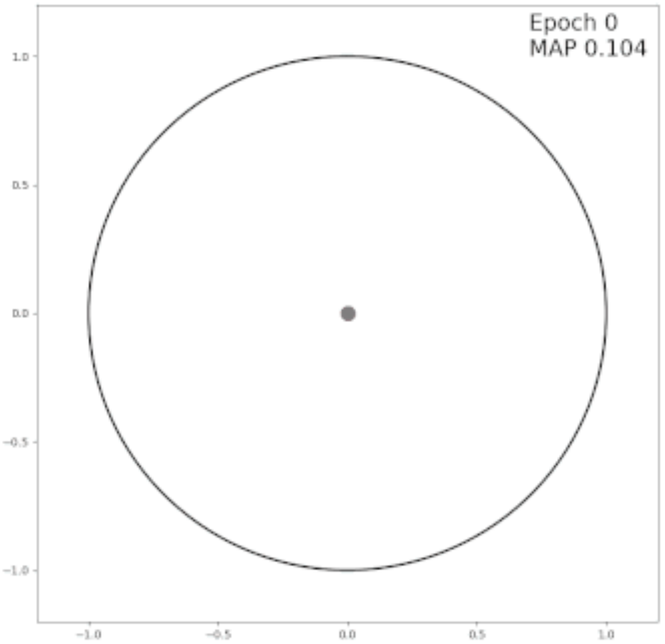
Reproduce an arbitrarily good approximation to tree distance
Embed trees with arbitrarily **low distortion**, with just two dimensions

Tree : $d(x, y) = d(x, O) + d(O, y)$

$$\frac{d_H(x, y)}{d_H(x, O) + d_H(O, y)} \qquad \frac{dE(x, y)}{dE(x, O) + d_E(O, y)}$$







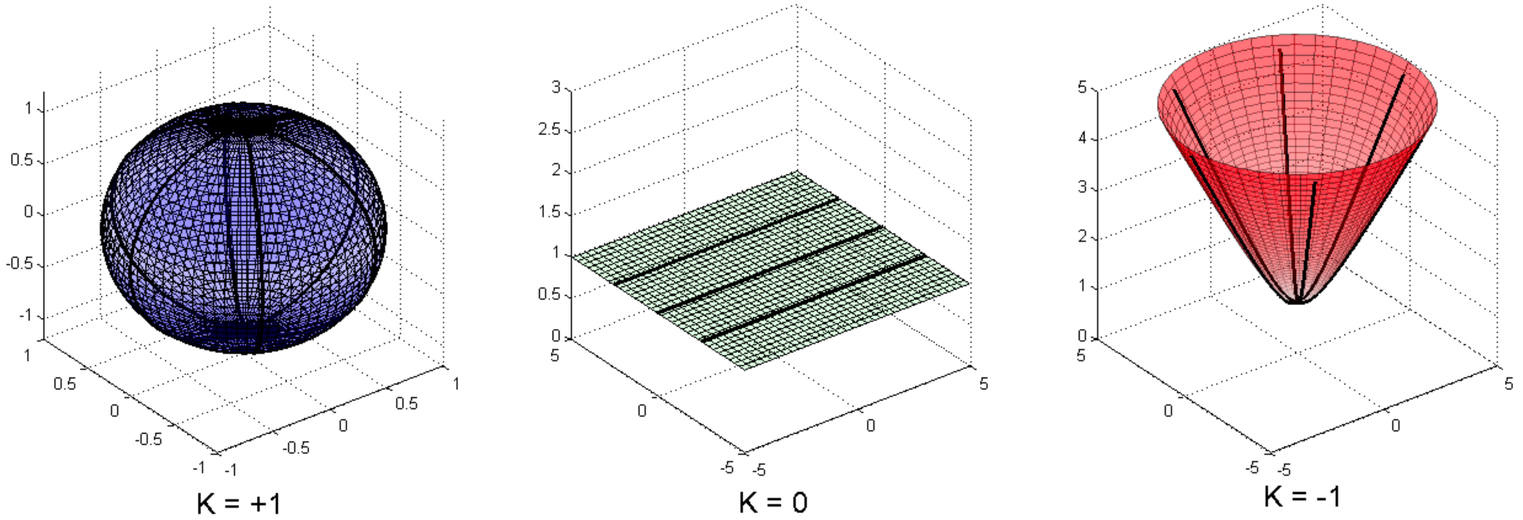
Right Space

Often data doesn't have such a nicely regimented structure(tree)

Match the structure of our data

- Trees fit hyperbolic space
- Cycles fit spherical space

Three model spaces: hyperbolic, Euclidean, and spherical



combination:
product manifold

These well-studied spaces offer simple and explicit **closed-form** expressions for many functions of interest: distances, *exp* and *log* maps, parametrizations for geodesics

Reference

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2. Hyperbolic Graph Neural Networks, Facebook AI, 2019 NIPS , Maximilian Nickel and Douwe Kiela

3. Hyperbolic Graph Convolutional Neural Networks, Stanford snap , NIPS 2019 , Jure Leskovec

4. Hyperbolic Attention Networks, DeepMind, 2019 ICLR , Caglar Gulcehre

5. Hyperbolic Graph Attention Network, BUPT, 2020 AAAI, Chuan Shi

HNN

Hyperbolic Neural Networks

Generalize deep neural models to non-Euclidean domain

1. 双曲空间的表征能力在很多方面不如欧氏空间， 主要是缺少相应的神经网络层数。

2. 本文通过将莫比乌斯陀螺向量空间的形式性与双曲空间的庞加莱模型的黎曼几何相结合，将深度学习推广到双曲空间。

Gyrovector spaces

Möbius addition. The *Möbius addition* of x and y in $\mathbb{D}_c^n$ is defined as

$$x \oplus_c y := \frac{(1 + 2c\langle x, y\rangle + c\|y\|^2)x + (1 - c\|x\|^2)y}{1 + 2c\langle x, y\rangle + c^2\|x\|^2\|y\|^2}. \tag{4}$$

In particular, when $c = 0$, one recovers the Euclidean addition of two vectors in $\mathbb{R}^n$. Note that without loss of generality, the case $c > 0$ can be reduced to $c = 1$. Unless stated otherwise, we will use $\oplus$ as $\oplus_1$ to simplify notations. For general $c > 0$, this operation is not commutative nor associative. However, it satisfies $x \oplus_c \mathbf{0} = \mathbf{0} \oplus_c x = x$. Moreover, for any $x, y \in \mathbb{D}_c^n$, we have $(-x) \oplus_c x = x \oplus_c (-x) = \mathbf{0}$ and $(-x) \oplus_c (x \oplus_c y) = y$ (left-cancellation law). The *Möbius substraction* is then defined by the use of the following notation: $x \ominus_c y := x \oplus_c (-y)$. See [29, section 2.1] for a geometric interpretation of the Möbius addition.

C = 0 退化到欧氏空间

Möbius scalar multiplication. For $c > 0$, the *Möbius scalar multiplication* of $x \in \mathbb{D}_c^n \setminus \{\mathbf{0}\}$ by $r \in \mathbb{R}$ is defined as

$$r \otimes_c x := (1/\sqrt{c}) \tanh(r \tanh^{-1}(\sqrt{c}\|x\|)) \frac{x}{\|x\|}, \tag{5}$$

and $r \otimes_c \mathbf{0} := \mathbf{0}$. Note that similarly as for the Möbius addition, one recovers the Euclidean scalar multiplication when c goes to zero: $\lim_{c\to 0} r \otimes_c x = rx$. This operation satisfies desirable properties such as $n \otimes_c x = x \oplus_c \cdots \oplus_c x$ (n additions), $(r + r') \otimes_c x = r \otimes_c x \oplus_c r' \otimes_c x$ (scalar distributivity[3]), $(rr') \otimes_c x = r \otimes_c (r' \otimes_c x)$ (scalar associativity) and $|r| \otimes_c x / \|r \otimes_c x\| = x/\|x\|$ (scaling property).

欧氏空间中存在着很多的向量运算操作： 向量加减，数乘，

Gyrovector spaces 类似于欧氏中的向量空间为双曲空间提供一种代数形式规范

Distance. If one defines the generalized hyperbolic metric tensor g^c as the metric conformal to the Euclidean one, with conformal factor $\lambda_x^c := 2/(1 - c\|x\|^2)$, then the induced distance function on $(\mathbb{D}_c^n, g^c)$ is given by[4]

$$d_c(x, y) = (2/\sqrt{c}) \tanh^{-1}\left(\sqrt{c}\| - x \oplus_c y\|\right). \tag{6}$$

Again, observe that $\lim_{c\to 0} d_c(x, y) = 2\|x - y\|$, *i.e.* we recover Euclidean geometry in the limit[5]. Moreover, for $c = 1$ we recover $d_{\mathbb{D}}$ of Eq. (2).

Hyperbolic Neural Networks

神经网络是由一系列基本操作组合而成

Lemma 2. *For any point $x \in \mathbb{D}_c^n$, the exponential map $\exp_x^c : T_x\mathbb{D}_c^n \to \mathbb{D}_c^n$ and the logarithmic map $\log_x^c : \mathbb{D}_c^n \to T_x\mathbb{D}_c^n$ are given for $v \neq \mathbf{0}$ and $y \neq x$ by:*

$$\exp_x^c(v) = x \oplus_c \left(\tanh\left(\sqrt{c} \frac{\lambda_x^c \|v\|}{2} \right) \frac{v}{\sqrt{c}\|v\|} \right), \quad \log_x^c(y) = \frac{2}{\sqrt{c}\lambda_x^c} \tanh^{-1}(\sqrt{c}\| -x \oplus_c y\|) \frac{-x \oplus_c y}{\| -x \oplus_c y\|}. \tag{10}$$

Exponential map : $T_x\mathbb{D}_c^n \to \mathbb{D}_c^n$ 切平面—> 双曲面

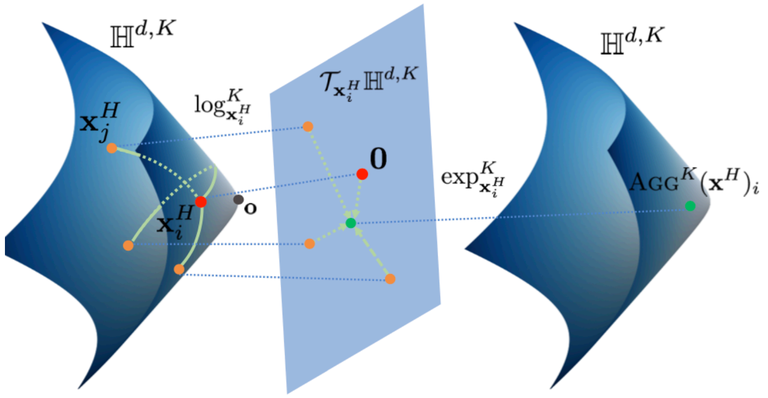
Logarithmic map : $\mathbb{D}_c^n \to T_x\mathbb{D}_c^n$

前馈神经网络

Definition 3.2 (Möbius version)**.** For $f : \mathbb{R}^n \to \mathbb{R}^m$, we define the *Möbius version of* f as the map from $\mathbb{D}_c^n$ to $\mathbb{D}_c^m$ by:

$$f^{\otimes_c}(x) := \exp_{\mathbf{0}}^c(f(\log_{\mathbf{0}}^c(x))), \tag{24}$$

where $\exp_{\mathbf{0}}^c : T_{\mathbf{0}_m}\mathbb{D}_c^m \to \mathbb{D}_c^m$ and $\log_{\mathbf{0}}^c : \mathbb{D}_c^n \to T_{\mathbf{0}_n}\mathbb{D}_c^n$.



切平面是一个线性空间

先映射到切平面，执行 FNN，再映射回双

HGCN

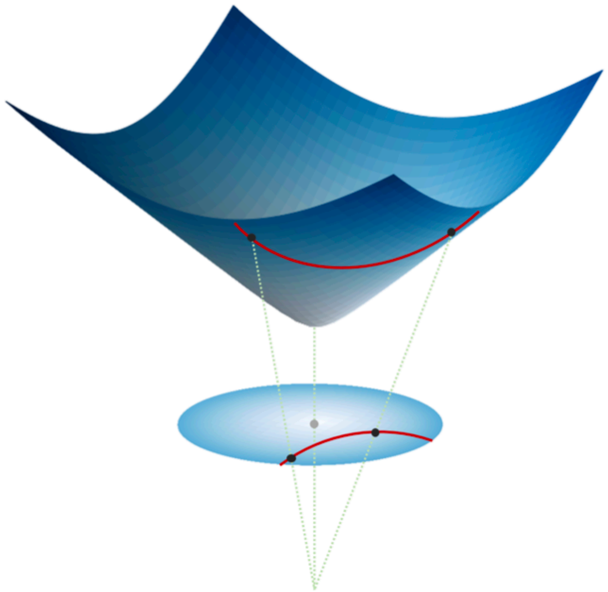
Hyperbolic Graph Convolutional Neural Networks

图卷积和双曲神经网络结合

1. 应用双曲面模型

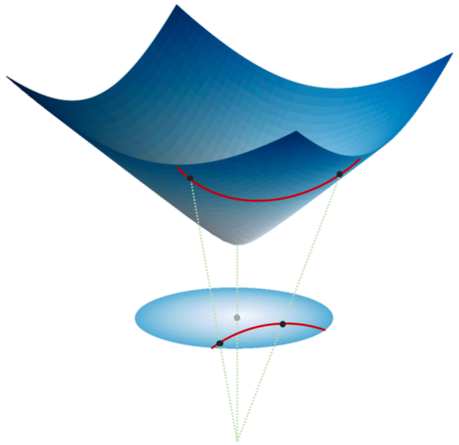
2.在双曲面上进行 GCN(GAT)

3.Trainable curvature



Hyperboloid manifold

双曲面是双曲线的推广　　simplicity and numerical stability



$$y_1^2 + y_2^2 + y_3^2 - y_4^2 = -1$$

$$\mathbb{H}^{d,K} := \left\{ \mathbf{x} \in \mathbb{R}^{d+1} : \langle \mathbf{x}, \mathbf{x} \rangle_{\mathscr{L}} = -K, x_0 > 0 \right\} \quad \mathscr{T}_{\mathbf{x}}\mathbb{H}^{d,K} := \left\{ \mathbf{v} \in \mathbb{R}^{d+1} : \langle \mathbf{v}, \mathbf{x} \rangle_{\mathscr{L}} = \right.$$

双曲空间内积：Minkowski inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_{\mathscr{L}} := -x_0 y_0 + x_1 y_1 + \ldots + x_d y_d$$

较为接近欧氏内积，较为稳定

距离和指对映射

Proposition 3.1. *Let* $\mathbf{x} \in \mathbb{H}^{d,K}$, $\mathbf{u} \in \mathcal{T}_{\mathbf{x}}\mathbb{H}^{d,K}$ *be unit-speed. The unique unit-speed geodesic* $\gamma_{\mathbf{x}\to\mathbf{u}}(\cdot)$ *such that* $\gamma_{\mathbf{x}\to\mathbf{u}}(0) = \mathbf{x}$, $\dot{\gamma}_{\mathbf{x}\to\mathbf{u}}(0) = \mathbf{u}$ *is* $\gamma^K_{\mathbf{x}\to\mathbf{u}}(t) = \cosh\left(\frac{t}{\sqrt{K}}\right)\mathbf{x} + \sqrt{K}\sinh\left(\frac{t}{\sqrt{K}}\right)\mathbf{u}$, *and the intrinsic distance function between two points* $\mathbf{x}, \mathbf{y}$ *in* $\mathbb{H}^{d,K}$ *is then:*

$$d^K_{\mathcal{L}}(\mathbf{x}, \mathbf{y}) = \sqrt{K}\operatorname{arcosh}(-\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}/K). \tag{4}$$

Proposition 3.2. *For* $\mathbf{x} \in \mathbb{H}^{d,K}$, $\mathbf{v} \in \mathcal{T}_{\mathbf{x}}\mathbb{H}^{d,K}$ *and* $\mathbf{y} \in \mathbb{H}^{d,K}$ *such that* $\mathbf{v} \neq \mathbf{0}$ *and* $\mathbf{y} \neq \mathbf{x}$, *the exponential and logarithmic maps of the hyperboloid model are given by:*

$$\exp^K_{\mathbf{x}}(\mathbf{v}) = \cosh\left(\frac{||\mathbf{v}||_{\mathcal{L}}}{\sqrt{K}}\right)\mathbf{x} + \sqrt{K}\sinh\left(\frac{||\mathbf{v}||_{\mathcal{L}}}{\sqrt{K}}\right)\frac{\mathbf{v}}{||\mathbf{v}||_{\mathcal{L}}}, \quad \log^K_{\mathbf{x}}(\mathbf{y}) = d^K_{\mathcal{L}}(\mathbf{x}, \mathbf{y})\frac{\mathbf{y} + \frac{1}{K}\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}\mathbf{x}}{||\mathbf{y} + \frac{1}{K}\langle \mathbf{x}, \mathbf{y} \rangle_{\mathcal{L}}\mathbf{x}||_{\mathcal{L}}}.$$

HGCN

1. 将欧氏空间特征 map 双曲空间

$$\mathbf{x}^{0,H} = \exp_{\mathbf{o}}^{K}\left((0,\mathbf{x}^{0,E})\right) = \left(\sqrt{K}\cosh\left(\frac{\left\|\mathbf{x}^{0,E}\right\|_2}{\sqrt{K}}\right), \sqrt{K}\sinh\left(\frac{\left\|\mathbf{x}^{0,E}\right\|_2}{\sqrt{K}}\right)\frac{\mathbf{x}^{0,E}}{\left\|\mathbf{x}^{0,E}\right\|_2}\right)$$

将$(0,\mathbf{x}^{0,E})$ 看作切平面的一个点

2. 在双曲空间进行特征变换

leverage the exp and log maps

$$\mathbf{h}_i^{\ell,E} = W^{\ell}\mathbf{x}_i^{\ell-1,E} + \mathbf{b}^{\ell}$$

平移

$$W \otimes^{K} \mathbf{x}^{H} := \exp_{\mathbf{o}}^{K}\left(W\log_{\mathbf{o}}^{K}\left(\mathbf{x}^{H}\right)\right) \qquad \mathbf{x}^{H} \oplus^{K} \mathbf{b} := \exp_{\mathbf{x}^{\mathrm{H}}}^{K}\left(P_{\mathbf{o}\to\mathbf{x}^{H}}^{K}(\mathbf{b})\right)$$

3. Attention based aggregation

$$w_{ij} = \mathrm{SOFTMAX}_{j\in\mathcal{N}(i)}\left(\mathrm{MLP}\left(\log_{\mathbf{o}}^{K}\left(\mathbf{x}_i^{H}\right)\|\log_{\mathbf{o}}^{K}\left(\mathbf{x}_j^{H}\right)\right)\right)$$

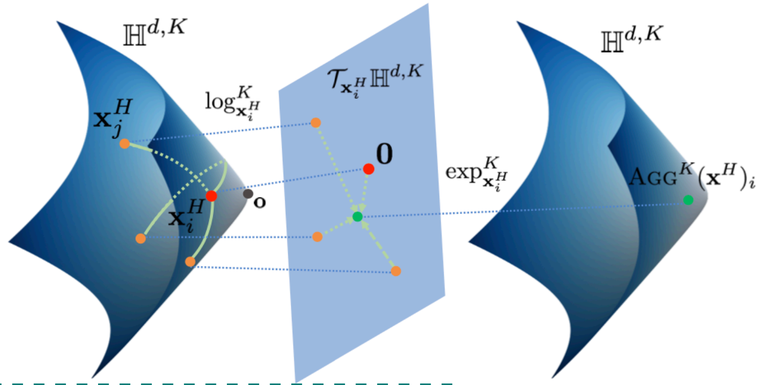
切平面计算权值

$$\mathrm{AGG}^{K}\left(\mathbf{x}^{H}\right)_i = \exp_{\mathbf{x}_i^{H}}^{K}\left(\sum_{j\in\mathcal{N}(i)} w_{ij}\log_{\mathbf{x}_i^{H}}^{K}\left(\mathbf{x}_j^{H}\right)\right)$$

$$\sigma^{\otimes^{K_{\ell-1},K_{\ell}}}\left(\mathbf{x}^{H}\right) = \exp_{\mathbf{o}}^{K_{\ell}}\left(\sigma\left(\log_{\mathbf{o}}^{K_{\ell-1}}\left(\mathbf{x}^{H}\right)\right)\right)$$

不同曲率非线性激活

HGCN Architecture



给定一个网络$\mathcal{G}=(\mathcal{V},\mathcal{E})$， 以及相应的欧氏空间特征 $\left(\mathbf{x}^{0,E}\right)_{i\in\mathcal{V}}$

1. HGCN 第一层将特征映射到双曲空间
2. HGCN 之后堆叠多个图卷积层：

$$\mathbf{h}_i^{\ell,H} = \left(W^\ell \otimes^{K_{\ell-1}} \mathbf{x}_i^{\ell-1,H}\right) \oplus^{K_{\ell-1}} \mathbf{b}^\ell \qquad \text{(hyperbolic feature transform)}$$

$$\mathbf{y}_i^{\ell,H} = \text{AGG}^{K_{\ell-1}}(\mathbf{h}^{\ell,H})_i \qquad \text{(attention-based neighborhood aggregation)}$$

$$\mathbf{x}_i^{\ell,H} = \sigma^{\otimes^{K_{\ell-1},K_\ell}}(\mathbf{y}_i^{\ell,H}) \qquad \text{(non-linear activation with different curvatures)}$$

1. link prediction

使用 费米-狄拉克分布计算

$$p\left((i,j)\in\mathcal{E}\,|\,\mathbf{x}_i^{L,H},\mathbf{x}_j^{L,H}\right) = \left[e^{\left(d_{\mathcal{L}}^{K_L}\left(\mathbf{x}_i^{L,H},\mathbf{x}_j^{L,H}\right)^2 - r\right)/t} + 1\right]^{-1}$$

2. node classification

将最后一层的输出使用 log 映射映射到切平面空间，用欧氏逻辑回归

HGCN:Trainable curvature

不同曲率会影响实验结果

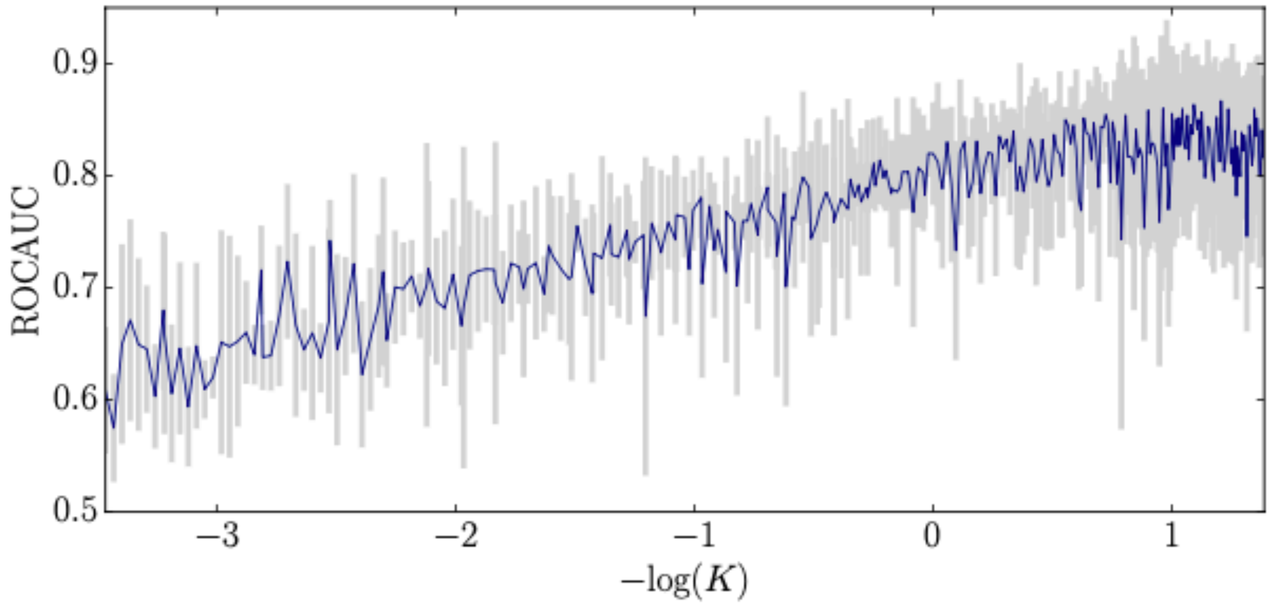


Figure 4: Decreasing curvature $(-1/K)$ improves link prediction performance on DISEASE.

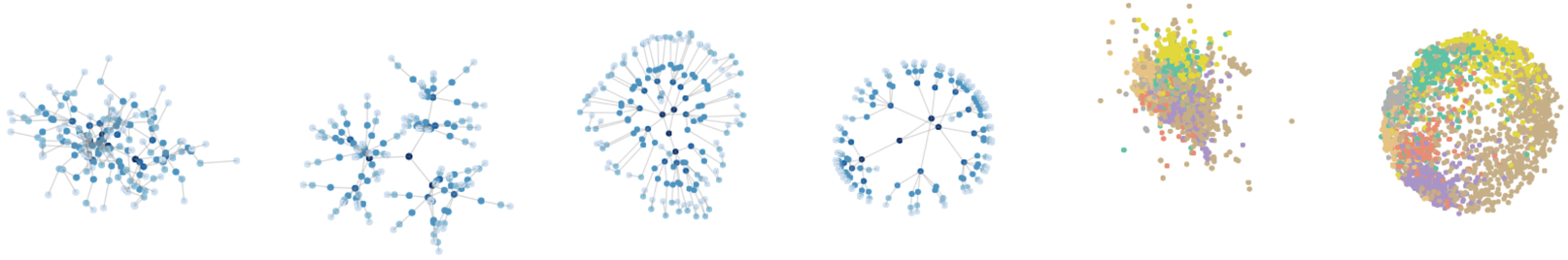
Results Analyze

	Dataset	Disease		Disease-M		Human PPI		Airport		PubMed		Cora	
	Hyperbolicity δ	$\delta = 0$		$\delta = 0$		$\delta = 1$		$\delta = 1$		$\delta = 3.5$		$\delta = 11$	
	Method	LP	NC	LP	NC	LP	NC	LP	NC	LP	NC	LP	NC
Shallow	Euc	59.8 ± 2.0	32.5 ± 1.1	-	-	-	-	92.0 ± 0.0	60.9 ± 3.4	83.3 ± 0.1	48.2 ± 0.7	82.5 ± 0.3	23.8 ± 0.7
Shallow	Hyp [29]	63.5 ± 0.6	45.5 ± 3.3	-	-	-	-	94.5 ± 0.0	70.2 ± 0.1	87.5 ± 0.1	68.5 ± 0.3	87.6 ± 0.2	22.0 ± 1.5
Shallow	Euc-Mixed	49.6 ± 1.1	35.2 ± 3.4	-	-	-	-	91.5 ± 0.1	68.3 ± 2.3	86.0 ± 1.3	63.0 ± 0.3	84.4 ± 0.2	46.1 ± 0.4
Shallow	Hyp-Mixed	55.1 ± 1.3	56.9 ± 1.5	-	-	-	-	93.3 ± 0.0	69.6 ± 0.1	83.8 ± 0.3	73.9 ± 0.2	85.6 ± 0.5	45.9 ± 0.3
NN	MLP	72.6 ± 0.6	28.8 ± 2.5	55.3 ± 0.5	55.9 ± 0.3	67.8 ± 0.2	55.3±0.4	89.8 ± 0.5	68.6 ± 0.6	84.1 ± 0.9	72.4 ± 0.2	83.1 ± 0.5	51.5 ± 1.0
NN	HNN[10]	75.1 ± 0.3	41.0 ± 1.8	60.9 ± 0.4	56.2 ± 0.3	72.9 ± 0.3	59.3 ± 0.4	90.8 ± 0.2	80.5 ± 0.5	94.9 ± 0.1	69.8 ± 0.4	89.0 ± 0.1	54.6 ± 0.4
GNN	GCN[21]	64.7 ±0.5	69.7 ± 0.4	66.0 ± 0.8	59.4 ± 3.4	77.0 ± 0.5	69.7 ± 0.3	89.3 ± 0.4	81.4 ± 0.6	91.1 ± 0.5	78.1 ± 0.2	90.4 ± 0.2	81.3 ± 0.3
GNN	GAT [41]	69.8 ±0.3	70.4 ± 0.4	69.5 ± 0.4	62.5 ± 0.7	76.8 ± 0.4	70.5 ± 0.4	90.5 ± 0.3	81.5 ± 0.3	91.2 ± 0.1	79.0 ± 0.3	**93.7** ± 0.1	**83.0** ± 0.7
GNN	SAGE [15]	65.9 ± 0.3	69.1 ± 0.6	67.4 ± 0.5	61.3 ± 0.4	78.1 ± 0.6	69.1 ± 0.3	90.4 ± 0.5	82.1 ± 0.5	86.2 ± 1.0	77.4 ± 2.2	85.5 ± 0.6	77.9 ± 2.4
GNN	SGC [44]	65.1 ± 0.2	69.5 ± 0.2	66.2 ± 0.2	60.5 ± 0.3	76.1 ± 0.2	71.3 ± 0.1	89.8 ± 0.3	80.6 ± 0.1	94.1 ± 0.0	78.9 ± 0.0	91.5 ± 0.1	81.0 ± 0.1
Ours	HGCN	**90.8** ± 0.3	**74.5** ± 0.9	**78.1** ± 0.4	**72.2** ± 0.5	**84.5** ± 0.4	**74.6** ± 0.3	**96.4** ± 0.1	**90.6** ± 0.2	**96.3** ± 0.0	**80.3** ± 0.3	92.9 ± 0.1	79.9 ± 0.2
Ours	(%) Err Red	-63.1%	-13.8%	-28.2%	-25.9%	-29.2%	-11.5%	-60.9%	-47.5%	-27.5%	-6.2%	+12.7%	+18.2%

Table 1: ROC AUC for Link Prediction (LP) and F1 score for Node Classification (NC) tasks. For inductive datasets, we only evaluate inductive methods since shallow methods cannot generalize to unseen nodes/graphs. We report graph hyperbolicity values δ (lower is more hyperbolic).

Smaller the hyperbolicity values， underlying graph is more hyperbolic

Results Analyze



(a) GCN layers. (b) HGCN layers. (c) GCN (left), HGCN (right).

HGCN 学习到层级结构

Figure 3: Visualization of embeddings for LP on DISEASE and NC on CORA (visualization on the Poincaré disk for HGCN). (a) GCN embeddings in first and last layers for DISEASE LP hardly capture hierarchy (depth indicated by color). (b) In contrast, HGCN preserves node hierarchies. (c) On CORA NC, HGCN leads to better class separation (indicated by different colors).

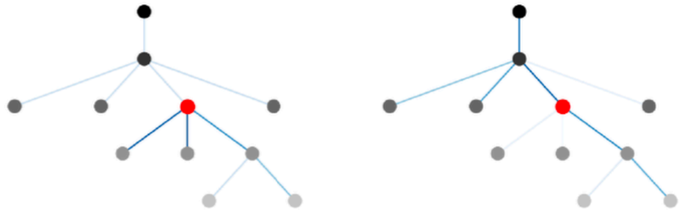


Figure 5: Attention: Euclidean GAT (left), HGCN (right). Each graph represents a 2-hop neighborhood of the DISEASE-M dataset.

更关注父节点， sick parents will propagate the disease to their children.

HGNN

Hyperbolic Graph Neural Networks

$$\mathbf{h}_u^{k+1} = \sigma\left(\sum_{v \in \mathcal{I}(u)} \tilde{\mathbf{A}}_{uv} \mathbf{W}^k \mathbf{h}_v^k \right)$$

$$\mathbf{h}_u^{k+1} = \sigma\left(\exp_{\mathbf{x}'}\left(\sum_{v \in \mathcal{I}(u)} \tilde{\mathbf{A}}_{uv} \mathbf{W}^k \log_{\mathbf{x}'}\left(\mathbf{h}_v^k\right) \right) \right)$$

NeurIPS 2019 announced accepted papers, we also became aware of the concurrently developed HGNN model [26] for learning GNNs in hyperbolic space. The main difference with our work is how our HGCN defines the architecture for neighborhood aggregation and uses a learnable curvature. Additionally, while [26] demonstrates strong performance on graph classification tasks and provides an elegant extension to dynamic graph embeddings, we focus on link prediction and node classification.

Challenges and Opportunities

The first phase of papers focused on : faithful representations

A clear **downstream use** awaited the development of non-Euclidean models

Challenges

- Is there a principled choice of analog for any particular Euclidean operation?
- Can we reliably and smoothly transform between spaces of varying curvature, including switching the sign
- Understand how geometry encodes relationships

Reference

1. *Hyperbolic Embeddings with a Hopefully Right Amount of Hyperbole: https://dawn.cs.stanford.edu/2018/03/19/hyperbolics/*
2. *Into the Wild: Machine Learning In Non-Euclidean Space: https://dawn.cs.stanford.edu/2019/10/10/noneuclidean/*