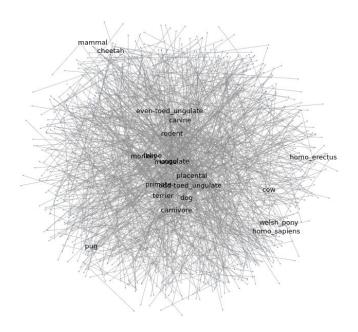
## Hyperbolic Machine Learning



Hyperbolic Geometry & Data Science Seminar, 21.01.21, Sebastian Damrich

#### Overview

Trees in Hyperbolic Space

Riemannian Gradient Descent

Shallow hyperbolic ML

Hyperbolic Deep ML

### Euclidean, spherical and hyperbolic geometry

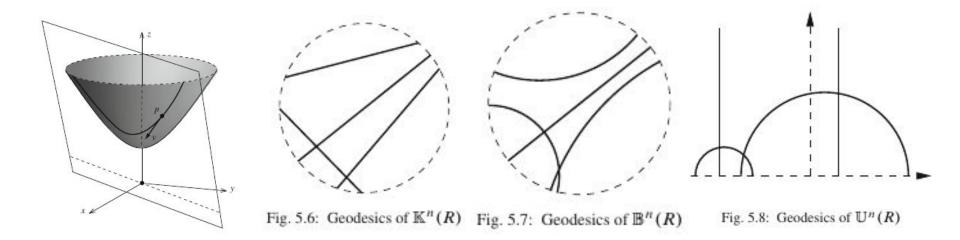
TABLE I: Characteristic properties of Euclidean, spherical, and hyperbolic geometries. *Parallel lines* is the number of lines that are parallel to a line and that go through a point not belonging to this line, and  $\zeta = \sqrt{|K|}$ .

Property	Euclidean	Spherical	Hyperbolic
Curvature $K$	0	> 0	< 0
Parallel lines	1	0	$\infty$
Triangles are	normal	thick	thin
Shape of triangles			
Sum of $\triangle$ angles	$\pi$	$> \pi$	$<\pi$
Circle length	$2\pi r$	$2\pi\sin\zeta r$	$2\pi \sinh \zeta r$
Disk area	$2\pi r^2/2$	$2\pi(1-\cos\zeta r)$	$2\pi(\cosh\zeta r - 1)$

Hyperbolic Geometry of Complex Networks, Krioukov, ..., Boguñá

## Equivalent models

Fig. 5.5: A great hyperbola

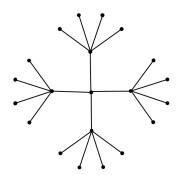


Introduction to Riemannian Manifolds, Lee, Springer

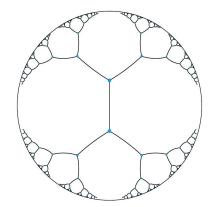
### Trees in hyperbolic space

"hyperbolic space is a continuous analogue of trees; trees are a discretised hyperbolic space"

hyperbolic space has "more space" than Euclidean space



not enough space for tree with constant branching factor in euclidean space http://bjlkeng.github.io/posts/hyperbolic-geometry-andpoincare-embeddings/



Area grows exponentially and can fit a tree with constant branching factor

Poincaré Embeddings for Learning Hierarchical Representations, Nickel, Kiela Neurips'17

#### Trees in hyperbolic space

#### Theorem:

Given  $\epsilon > 0$  and a positively weighted tree T = (V, E, w), then there is some  $\eta > 0$  such that V can be embedded into the Poincaré disk such that  $\eta T$  is the MST of the embedded points and the distortion (product of max distance contraction and elongation) is at most  $1 + \epsilon$ .

Low Distortion Delaunay Embedding of Trees in Hyperbolic Plane, Sarkar, 2012

### Hierarchical data is everywhere

Language: Hypernymys, Entailment of sentences, Translation...

Images: Tracking of dividing cells, different resolutions, crops

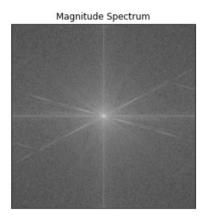
Biology: Developmental processes

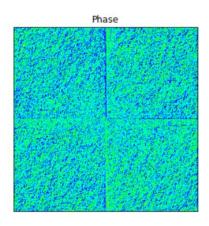
Many graphs are rather tree-like than flat

## Representation learning

Representing data in a way that makes downstream tasks easy, e.g.







### Representation learning

Representing data in a way that makes downstream tasks easy, e.g.

Embedding data points in a metric space

Use distance for clustering, retrieving similar data points, ...

More compact than relational information

Deep Neural Networks sequence of transformed representation

Often representation as point in Euclidean space, but not well suited for hierarchies.

→ Learn representations in hyperbolic space instead

#### Riemannian Stochastic Gradient Descent

Gradient descent is ubiquitous in Machine Learning

$$\min_{\theta} f(\theta)$$

$$\theta = \theta_t - \eta_t \text{ grad } \theta_t$$

#### Riemannian Stochastic Gradient Descent

Gradient descent is ubiquitous in Machine Learning

$$\begin{aligned}
& \underset{\theta}{\text{min}} \quad f(\theta) \\
& \theta_{t+n} = \theta_t - \eta_t \text{ grad } f|_{\theta_t} \\
&= \exp_{\theta_t} \left( -\eta_t \cdot \text{grad } f|_{\theta_t} \right)
\end{aligned}$$

#### Riemannian Gradient Descent

$$\begin{aligned} \min_{\theta \in \mathcal{M}} & & & & & \\ \theta \in \mathcal{M} & & \\ \theta$$

#### Riemannian Stochastic Gradient Descent

Theorem (Bonnabel):

Given a cost function  $f: M \to R$  on a Riemannian Manifold, (an approximation of) Riemannian Stochastic Gradient Descent converges almost surely to a critical point of f and grad f to 0 under mild conditions.

Stochastic gradient descent on Riemannian manifolds, Bonnabel 2013

## Shallow hyperbolic ML

Embed a graph G=(V, E) (representing a hierarchy) into hyperbolic space.

Let v<sub>i</sub> is embedded as p<sub>i</sub> in hyperbolic space.

Perform Riemannian gradient descent on loss function L(p, E).

Data: Undirected version of transitive closure of directed WordNet dataset

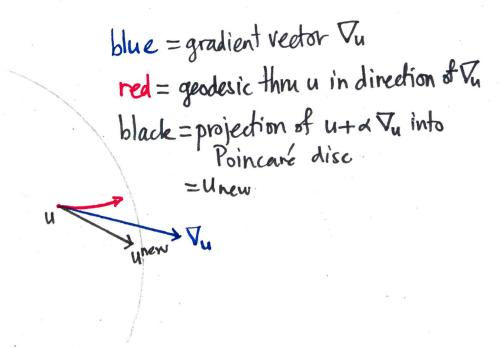
Loss: 
$$\mathcal{L}(\Theta) = \sum_{(u,v)\in\mathcal{D}} \log \frac{e^{-d(\boldsymbol{u},\boldsymbol{v})}}{\sum_{\boldsymbol{v}'\in\mathcal{N}(u)} e^{-d(\boldsymbol{u},\boldsymbol{v}')}}$$

No exponential, but approximation

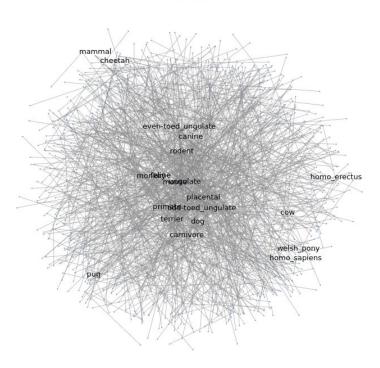
$$oldsymbol{ heta}_{t+1} \leftarrow \operatorname{proj}\left(oldsymbol{ heta}_t - \eta_t rac{(1 - \|oldsymbol{ heta}_t\|^2)^2}{4} 
abla_E
ight)$$

$$\operatorname{proj}(\boldsymbol{\theta}) = \begin{cases} \boldsymbol{\theta} / \|\boldsymbol{\theta}\| - \varepsilon & \text{if } \|\boldsymbol{\theta}\| \ge 1 \\ \boldsymbol{\theta} & \text{otherwise,} \end{cases}$$

"Buzz lightyear update"



loss:3.93

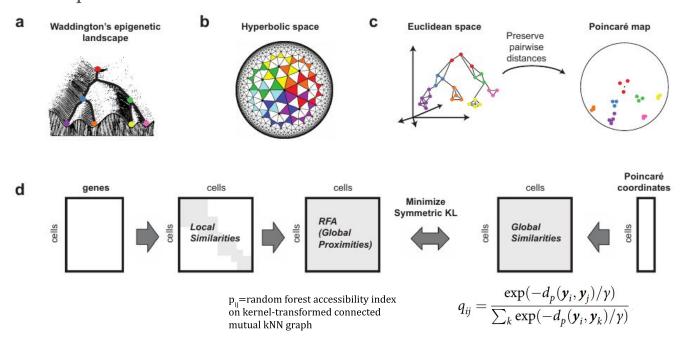


			Dimensionality						
			5	10	20	50	100	200	
ET tion	Euclidean	Rank MAP	3542.3 0.024	2286.9 0.059	1685.9 0.087	1281.7 0.140	1187.3 0.162	1157.3 0.168	
WORDNET Reconstruction									
W	Poincaré	Rank MAP	4.9 0.823	4.02 0.851	3.84 0.855	3.98 0.86	3.9 0.857	3.83 0.87	
d.	Euclidean	Rank MAP	3311.1 0.024	2199.5 0.059	952.3 0.176	351.4 0.286	190.7 0.428	81.5 0.490	
WORDNET Link Pred.									
r «	Poincaré	Rank MAP	5.7 0.825	<b>4.3</b> 0.852	4.9 0.861	4.6 <b>0.863</b>	4.6 0.856	4.6 0.855	

Clemens Fruböse improved this with a clever initialisation.

# Poincaré Maps for Analyzing Complex Hierarchies in Single-Cell Data Klimovskaia, ..., Bottou, Nickel, 2020

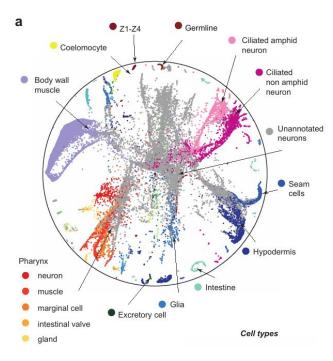
Application to scRNA data of developing cell population Gene expression measurements for cells



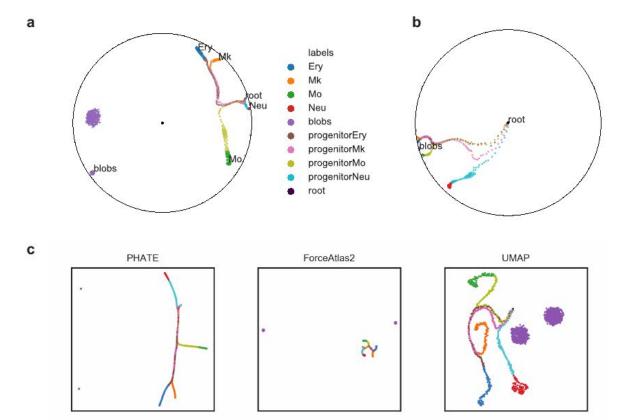
# Poincaré Maps for Analyzing Complex Hierarchies in Single-Cell Data Klimovskaia, ..., Bottou, Nickel, 2020

#### Versatile embedding:

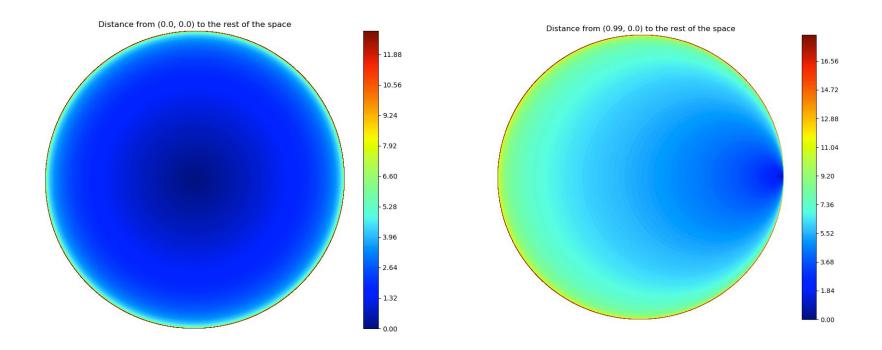
agglomerative clustering for lineage detection pseudotime inference visualisation



# Poincaré Maps for Analyzing Complex Hierarchies in Single-Cell Data Klimovskaia, ..., Bottou, Nickel, 2020



#### Distance distortion in Poincaré disk



#### Gyrovectors

Hyperbolic space is not a vector space.

But carries more complicated structure of "gyrovector space".

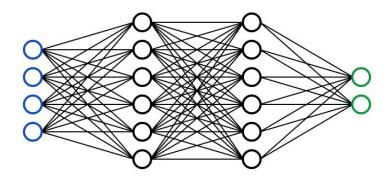
Addition  $x \oplus_c y$  , scalar multiplication  $\ r \otimes_c x$ 

Geodesics, translation, exponential, logarithm can be expressed in terms of gyrovector operations.

Parameter c is negative curvature  $c \rightarrow 0$  give normal real vector space.

## Hyperbolic Deep Learning

Remember: Simple fully connected neural network is sequence of affine maps and non-linear maps:



https://victorzhou.com/series/neural-networks-from-scratch/

$$f(x) = \varphi_{N}(W_{N}(... \varphi_{2}(W_{2}(\varphi_{1}(W_{1}x+b_{1}))+b_{2})...)+b_{N})$$

With Euclidean input x, Euclidean parameter matrices W<sub>i</sub> and biases b<sub>i</sub>, learnt by Gradient descent.

Hyperbolic Neural Network:

Neural network with hidden representation and / or parameters in hyperbolic space.

Define

multinomial logistic regression linear layer

for hyperbolic activations.

Map between Euclidean space input and hyperbolic activations via exponential at origin.

Linear layer:

For 
$$f: \mathbb{R}^n \to \mathbb{R}^m$$
, we define  $f^{\otimes_c}(x) := \exp^c_{\mathbf{0}}(f(\log^c_{\mathbf{0}}(x)))$ 

 $\rightarrow$  do map in tangent space of the origin, which is isomorphic to R<sup>n</sup>.

Bias b in D<sup>n</sup> 
$$x \leftarrow x \oplus_c b = \exp_x^c(P_{\mathbf{0} \to x}^c(\log_{\mathbf{0}}^c(b)))$$

Non-linearity also in tangent space of origin

- → defines fully connected feed-forward hyperbolic network
- → Euclidean gradient descent wrt Euclidean weight matrix, Riemannian GD wrt hyperbolic bias parameter

Euclidean multinomial logistic regression Simple classifier method, for each input x, probability distribution over K outputs

$$p(y = k|x) \propto \exp\left(\left(\langle a_k, x \rangle - b_k\right)\right), \text{ where } b_k \in \mathbb{R}, \ x, a_k \in \mathbb{R}^n$$

i.e. single layer neural network with output dimension K and softmax non-linearity:

$$p(Y|x) = softmax((a_1, ..., a_K)^Tx - b)$$

but hyperbolic modelling is different than hyperbolic feed-forward layer

Define hyperplane and rewrite linear map as signed distance to hyperplane:

$$H_{a,b} = \{ x \in \mathbb{R}^n : \langle a, x \rangle - b = 0 \},$$

$$p(y = k|x) \propto \exp(\operatorname{sign}(\langle a_k, x \rangle - b_k) ||a_k|| d(x, H_{a_k, b_k})), b_k \in \mathbb{R}, x, a_k \in \mathbb{R}^n.$$

Choose point p<sub>k</sub> on hyperplane and rewrite again:

$$p(y=k|x) \propto \exp(\operatorname{sign}(\langle -p_k+x, a_k \rangle) ||a_k|| d(x, \tilde{H}_{a_k, p_k})), \text{ with } p_k, x, a_k \in \mathbb{R}^n$$

This definition carries over to hyperbolic space

$$\tilde{H}_{a,p}^c := \{ x \in \mathbb{D}_c^n : \langle \log_p^c(x), a \rangle_p = 0 \} = \exp_p^c(\{a\}^\perp)$$

$$p(y=k|x) \propto \exp(\operatorname{sign}(\langle \log_p^c(x), a_k \rangle_p) \sqrt{g_{p_k}^c(a_k, a_k)} d_c(x, \tilde{H}_{a_k, p_k}^c)), \quad \forall x \in \mathbb{D}_c^n,$$

Input x and parameter  $p_k$  in  $D^n$  but parameters  $a_k$  in  $T_pD^n = R^n$  and output in R.

 $\rightarrow$  Gradients wrt  $a_k$  are Euclidean, Gradients wrt x,  $p_k$  are Riemannian.

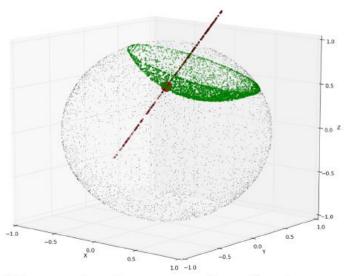


Figure 1: An example of a hyperbolic hyperplane in  $\mathbb{D}_1^3$  plotted using sampling. The red point is p. The shown normal axis to the hyperplane through p is parallel to a.

Reformulate several parts of the Hyperbolic Neural Network, in particular unify fully connected layer with multinomial logistic regression

Old MLR (Ganea et al):

$$p(y=k|x) \propto \exp(\operatorname{sign}(\langle \log_p^c(x), a \rangle_p) \sqrt{g_{p_k}^c(a_k, a_k)} d_c(x, \tilde{H}_{a_k, p_k}^c)), \quad \forall x \in \mathbb{D}_c^n,$$

is overparametrized

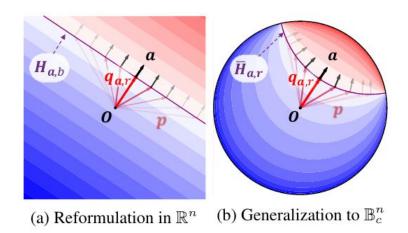
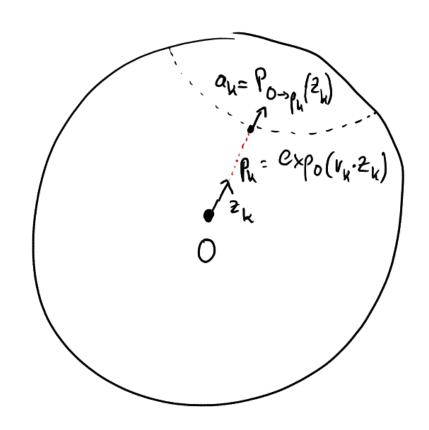


Figure 2: Whichever pair of a and p is chosen, a determined discriminative hyperplane is the same. Considering one bias point  $q_{a,r}$  per one discriminative hyperplane solves this over-parameterization.



New MLR:

Geodesic from origin to hyperplane is orthogonal.

- → use direction of this geodesic and scalar to define the point
- → parallel transport direction from origin to tangent space of point on hyperplane

Instead of  $p_k$  in  $D^n$  and  $a_k$  in  $T_{pk}D^n = R^n$ , only  $z_k$  in  $T_0D^n = R^n$  and  $r_k$  in R

Fully connected layer in Euclidean space is stack of translated scalar products

$$y = Ax - b$$
  
 $y_k = \langle a_k, x \rangle - b_k$ 

In MLR, we would do  $v_k(\boldsymbol{x}) = \operatorname{sign}(\langle \boldsymbol{a}_k, \ominus_c \boldsymbol{q}_{\boldsymbol{a}_k, r_k} \oplus_c \boldsymbol{x} \rangle) d_c\left(\boldsymbol{x}, \bar{H}^c_{\boldsymbol{a}_k, r_k}\right) \|\boldsymbol{a}_k\|^c_{\boldsymbol{q}_{\boldsymbol{a}_k, r_k}}$ 

But in FC layer Ganea et al do  $y = \exp_{\mathbf{0}}^{c}(A \log_{\mathbf{0}}^{c}(x)) \oplus_{c} b$  $\rightarrow$  use hyperplane method everywhere to get scores and map back to hyperbolic

space by using them as distance to axis orthogonal hyperplanes at the origin.

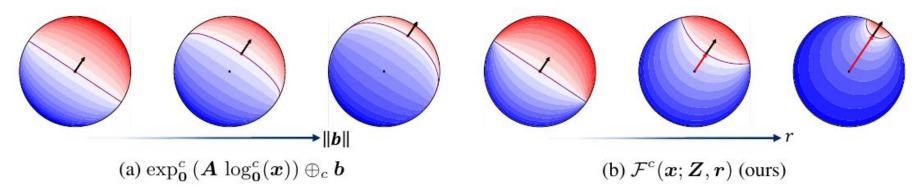


Figure 3: Comparison of FC layers in input spaces  $\mathbb{B}_c^n$ . The values at a certain dimension of output spaces are illustrated as contour plots. Black arrows depict the orientation parameters, and they are fixed for the comparison. Their orthogonal curves show discriminative hyperplanes where the values are zeros. As a bias parameter b or  $r_k$  changes, the outline of the contour landscape in (a) remains unchanged, whereas in (b) the focused regions are dynamically squeezed according to the geodesics.

Chami, ..., Leskovec NeurIPS'19

HNN + Graph Convolution Network + Attention + trainable curvature link prediction and node classification in various transductive / inductive graph settings

	Dataset Hyperbolicity $\delta$	$\begin{array}{cc} \text{DISEASE} \\ \delta & \delta = 0 \end{array}$		DISEASE-M $\delta = 0$		Human PPI $\delta = 1$		AIRPORT $\delta = 1$		РивМер $\delta = 3.5$		Cora $\delta = 11$	
	Method	LP	NC	LP	NC	LP	NC	LP	NC	LP	NC	LP	NC
W(	Euc Hyp 291	$59.8 \pm 2.0$ $63.5 \pm 0.6$	$32.5 \pm 1.1$ $45.5 \pm 3.3$	-	(5)	-	91	$92.0 \pm 0.0$ $94.5 \pm 0.0$	$60.9 \pm 3.4$ $70.2 \pm 0.1$	$83.3 \pm 0.1$ $87.5 \pm 0.1$	$48.2 \pm 0.7$ $68.5 \pm 0.3$	$82.5 \pm 0.3$ $87.6 \pm 0.2$	$23.8 \pm 0.7$ $22.0 \pm 1.5$
Shall	EUC-MIXED HYP-MIXED	$49.6 \pm 1.1$ $55.1 \pm 1.3$	$35.2 \pm 3.4$ $56.9 \pm 1.5$	-	-	-	-	$91.5 \pm 0.1$ $93.3 \pm 0.0$	$68.3 \pm 2.3$ $69.6 \pm 0.1$	$86.0 \pm 1.3$ $83.8 \pm 0.3$	$63.0 \pm 0.3$ $73.9 \pm 0.2$	$84.4 \pm 0.2$ $85.6 \pm 0.5$	$46.1 \pm 0.4$ $45.9 \pm 0.3$
Z	MLP HNN 10	$72.6 \pm 0.6$ $75.1 \pm 0.3$	$28.8 \pm 2.5$ $41.0 \pm 1.8$	$55.3 \pm 0.5$ $60.9 \pm 0.4$	$55.9 \pm 0.3$ $56.2 \pm 0.3$	$67.8 \pm 0.2$ $72.9 \pm 0.3$	$55.3\pm0.4$ $59.3\pm0.4$	$89.8 \pm 0.5$ $90.8 \pm 0.2$	$68.6 \pm 0.6 \\ 80.5 \pm 0.5$	$84.1 \pm 0.9$ $94.9 \pm 0.1$	$72.4 \pm 0.2$ $69.8 \pm 0.4$	$83.1 \pm 0.5$ $89.0 \pm 0.1$	$51.5 \pm 1.0$ $54.6 \pm 0.4$
GNN	GCN 21 GAT 41 SAGE 15 SGC 44	$64.7 \pm 0.5$ $69.8 \pm 0.3$ $65.9 \pm 0.3$ $65.1 \pm 0.2$	$69.7 \pm 0.4$ $70.4 \pm 0.4$ $69.1 \pm 0.6$ $69.5 \pm 0.2$	$66.0 \pm 0.8$ $69.5 \pm 0.4$ $67.4 \pm 0.5$ $66.2 \pm 0.2$	$59.4 \pm 3.4$ $62.5 \pm 0.7$ $61.3 \pm 0.4$ $60.5 \pm 0.3$	$77.0 \pm 0.5$ $76.8 \pm 0.4$ $78.1 \pm 0.6$ $76.1 \pm 0.2$	$69.7 \pm 0.3$ $70.5 \pm 0.4$ $69.1 \pm 0.3$ $71.3 \pm 0.1$	$89.3 \pm 0.4$ $90.5 \pm 0.3$ $90.4 \pm 0.5$ $89.8 \pm 0.3$	$81.4 \pm 0.6$ $81.5 \pm 0.3$ $82.1 \pm 0.5$ $80.6 \pm 0.1$	$91.1 \pm 0.5$ $91.2 \pm 0.1$ $86.2 \pm 1.0$ $94.1 \pm 0.0$	$78.1 \pm 0.2$ $79.0 \pm 0.3$ $77.4 \pm 2.2$ $78.9 \pm 0.0$	$90.4 \pm 0.2$ $93.7 \pm 0.1$ $85.5 \pm 0.6$ $91.5 \pm 0.1$	$81.3 \pm 0.3$ $83.0 \pm 0.7$ $77.9 \pm 2.4$ $81.0 \pm 0.1$
ILS	HGCN	$90.8 \pm 0.3$	$74.5 \pm 0.9$	$78.1 \pm 0.4$	$72.2 \pm 0.5$	$84.5 \pm 0.4$	<b>74.6</b> $\pm$ 0.3	$96.4 \pm 0.1$	$90.6 \pm 0.2$	$96.3 \pm 0.0$	$80.3 \pm 0.0$	$92.9 \pm 0.1$	$79.9 \pm 0.2$
On	(%) 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  $\delta$  (lower is more hyperbolic).

Chami, ..., Leskovec NeurIPS'19

- 1. **Citation networks**. CORA [36] and PUBMED [27] are standard benchmarks describing citation networks where nodes represent scientific papers, edges are citations between them, and node labels are academic (sub)areas. CORA contains 2,708 machine learning papers divided into 7 classes while PUBMED has 19,717 publications in the area of medicine grouped in 3 classes.
- 2. **Disease propagation tree**. We simulate the SIR disease spreading model [2], where the label of a node is whether the node was infected or not. Based on the model, we build tree networks, where node features indicate the susceptibility to the disease. We build transductive and inductive variants of this dataset, namely DISEASE and DISEASE-M (which contains multiple tree components).
- 3. **Protein-protein interactions (PPI) networks**. PPI is a dataset of human PPI networks [37]. Each human tissue has a PPI network, and the dataset is a union of PPI networks for human tissues. Each protein has a label indicating the stem cell growth rate after 19 days [40], which we use for the node classification task. The 16-dimensional feature for each node represents the RNA expression levels of the corresponding proteins, and we perform log transform on the features.
- 4. **Flight networks**. AIRPORT is a transductive dataset where nodes represent airports and edges represent the airline routes as from OpenFlights.org Compared to previous compilations [49], our dataset has larger size (2,236 nodes). We also augment the graph with geographic information (longitude, latitude and altitude), and GDP of the country where the airport belongs to. We use the population of the country where the airport belongs to as the label for node classification.

Chami, ..., Leskovec NeurIPS'19

Name	Nodes	Edges	Classes	Node features
Cora	2708	5429	7	1433
PUBMED	19717	88651	3	500
HUMAN PPI	17598	5429	4	17
<b>AIRPORT</b>	3188	18631	4	4
DISEASE	1044	1043	2	1000
DISEASE-M	43193	43102	2	1000

Table 3: Benchmarks' statistics

Citation network features: Word frequencies Airport

Chami, ..., Leskovec NeurIPS'19

HNN + Graph Convolution Network (Chami, ..., Leskovec NeurIPS'19)

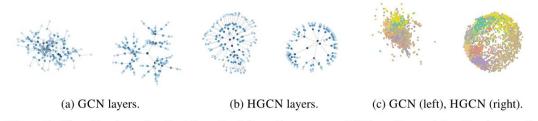


Figure 3: Visualization of embeddings for LP on DISEASE and NC on CORA (visualization on the Poincaré disk for HGCN). (a) GCN embeddings in first and last layers for DISEASE LP hardly capture hierarchy (depth indicated by color). (b) In contrast, HGCN preserves node hierarchies. (c) On CORA NC, HGCN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

#### Not enough time ...

#### More hyperbolic neural networks

Hyperbolic Graph Neural Networks; Liu, Nickel, Kiela NeurIPS'19 Hyperbolic Graph Convolutional Neural Networks; Chami, ..., Leskovec NeurIPS'19 Hyperbolic Attention Networks; Gulcehre, ..., Pascanu, de Freitas ICLR'19

#### Hyperbolic Autoencoder

Mixed-Curvature Variational Autoencoders; Skopek, Ganea, Bécigneul ICLR'20
Adversarial Autoencoders with Constant-Curvature Latent Manifolds; Grattarola, Livi, Alippi '20
A Wrapped Normal Distribution on Hyperbolic Space for Gradient-Based Learning; Nagano, ..., Koyama ICML'19
Continuous Hierarchical Representations with Poincaré Variational Auto-Encoders; Mathieu, ..., Teh NeurIPS'19

#### Learning Hierarchies

Hyperbolic Entailment Cones for Learning Hierarchical Embeddings; Ganea, ..., Hofmann ICML'18 Hyperbolic Disk Embeddings for Directed Acyclic Graphs; Suzuki, ..., Onoda ICML'18 Hierarchical Image Classification Using Entailment Cone Embeddings; Dhall, ..., Krause CVPR'20 Learning Continuous Hierarchies in the Lorentz Model of Hyperbolic Geometry; Nickel, Kiela ICML'18

