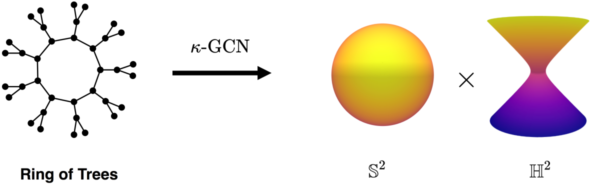
Constant Curvature Graph Convolutional Networks



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Overview

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- Introduce graph neural networks producing embeddings in product spaces
- Differentiable **transitions** in geometry during training in each component

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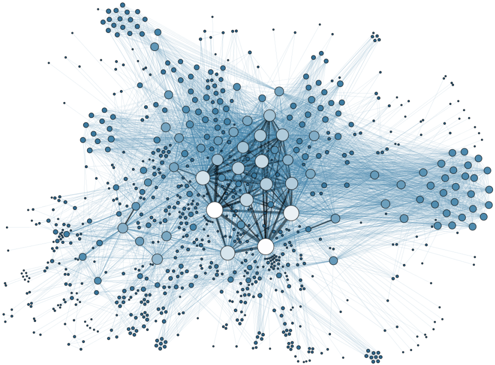

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- Lots of data available in the form of **graphs** (social networks, railway tracks, phylogenetic trees etc.)

- Node set $\boldsymbol{V} = \{1, \ldots, n\}$ and adjacency matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$

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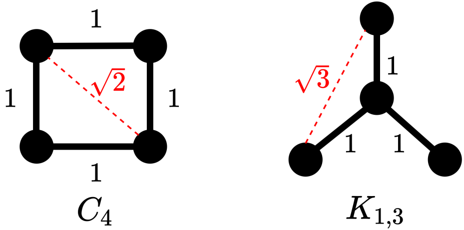

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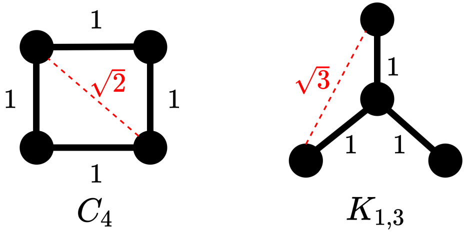

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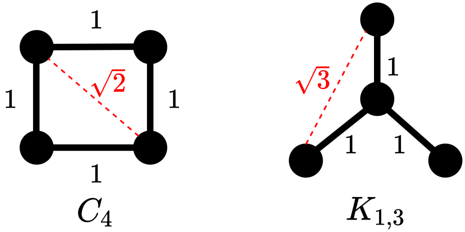

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- Arbitrary low distortion in **spherical** and **hyperbolic** space

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- **Computationally attractive** expressions for distance, exponential map etc.

Hyperbolic Space as Poincaré Ball

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- $\mathbb{H}^n = \{\boldsymbol{x} : ||\boldsymbol{x}||_2 \leq \frac{1}{\sqrt{c}}\}$ with curvature $-c$ equipped with **Riemannian tensor** $g^c_{\boldsymbol{x}} = \frac{4}{(1-c||\boldsymbol{x}||^2)^2}\mathbb{1}$

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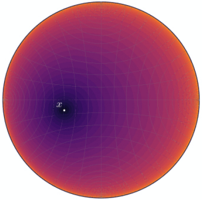
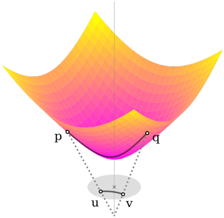
- $d_{\mathbb{H}}^c(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{\sqrt{c}} \cosh^{-1}\left(1 + \frac{\frac{2}{c}||\boldsymbol{x}-\boldsymbol{y}||_2^2}{\left(\frac{1}{c}-||\boldsymbol{x}||_2^2\right)\left(\frac{1}{c}-||\boldsymbol{y}||_2^2\right)}\right)$



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



Projection of hyperboloid [4]

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- Geodesic $\gamma_{\boldsymbol{x}\to\boldsymbol{y}}(t) = \boldsymbol{x} \oplus_c (t \otimes_c (-\boldsymbol{x} \oplus_c \boldsymbol{y}))$

Spherical Space as Stereographic Projection

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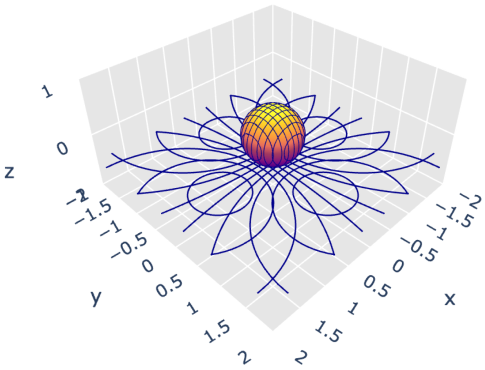

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$r \otimes_\kappa \boldsymbol{x}$	$r\boldsymbol{x}$	$\tan_\kappa\left(r \cdot \tan_\kappa^{-1} \|\|\boldsymbol{x}\|\|\right)\frac{\boldsymbol{x}}{\|\|\boldsymbol{x}\|\|}$
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- More unifying expressions for **distance**, **exponential map** etc. in our paper!

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- Embeddings $\boldsymbol{X}$ where $\boldsymbol{X}_{i\bullet} \in \mathfrak{st}_{\kappa}^{d}$, $\boldsymbol{W} \in \mathbb{R}^{d \times k}$ and $\boldsymbol{A} \in \mathbb{R}^{n \times n}$

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- Introduced in [2], we extended it to spherical spaces

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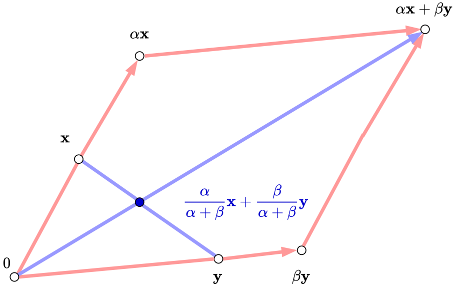

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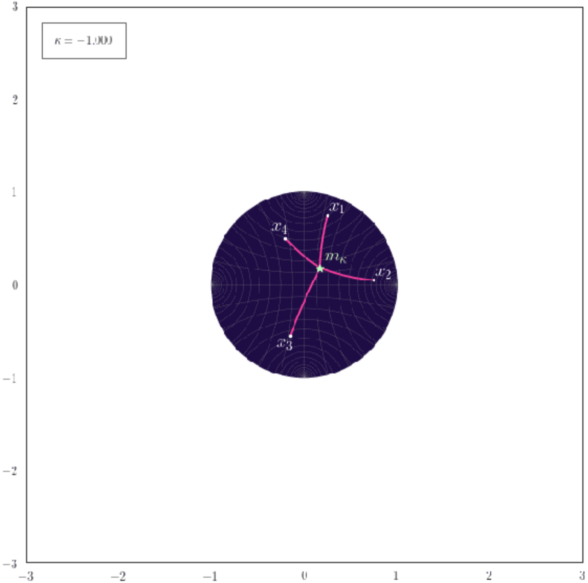
- Same scaling behaviour: $d_\kappa(\boldsymbol{0}, r \otimes_\kappa \boldsymbol{x}) = r \cdot d_\kappa(\boldsymbol{0}, \boldsymbol{x})$

Gyromidpoint for Varying Curvature



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- Enables **learning the curvature** κ with gradient descent with a differentiable change of sign

Our Contributions: 4) Constant Curvature GCN

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- Given graph $\boldsymbol{G} = (\boldsymbol{V}, \boldsymbol{A}, \boldsymbol{X})$ where $\boldsymbol{V} = \{1, \ldots, n\}$, adjacency $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ and node-level features $\boldsymbol{X} \in \mathbb{R}^{n \times d}$

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- We extend the vanilla **GCN** [3]:

$$\boldsymbol{H}^{(t+1)} = \sigma\left(\hat{\boldsymbol{A}}\boldsymbol{H}^{(t)}\boldsymbol{W}^{(t)}\right)$$

  for some non-linearity σ, $\hat{\boldsymbol{A}} = \tilde{\boldsymbol{D}}^{-\frac{1}{2}}\left(\boldsymbol{A} + \mathbb{1}\right)\tilde{\boldsymbol{D}}^{-\frac{1}{2}}$, $\tilde{\boldsymbol{D}}_{ii} = \sum_k \tilde{\boldsymbol{A}}_{ik}$ and trainable parameters $\boldsymbol{W}^{(l)}$

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- Allows for **differentiable transitions** in the geometry during training

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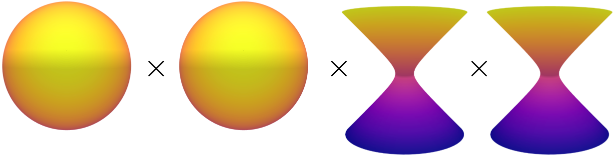

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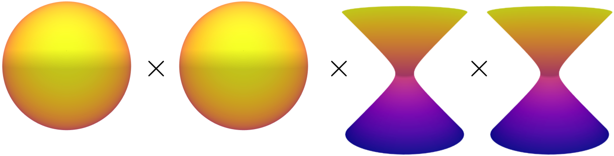

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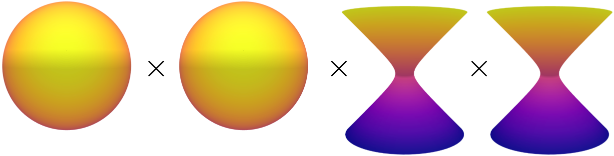

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- The **operations** extend component-wise while still preserving the desired properties

Experiments: Distortion Task

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- **Minimize** the discrepancy between embedding distances and graph distances

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

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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

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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

THANK YOU!

Check out our website **hyperbolicdeeplearning.com**

$\mathbb{H}\mathcal{D}\mathcal{L}$

HYPERBOLIC DEEP LEARNING

References

[1] Chami, I., Ying, R., Ré, C., and Leskovec, J. (2019). Hyperbolic graph convolutional neural networks. *Advances in Neural Information processing systems*.

[2] Ganea, O., Bécigneul, G., and Hofmann, T. (2018). Hyperbolic neural networks. In *Advances in Neural Information Processing Systems*, pages 5345–5355.

[3] Kipf, T. N. and Welling, M. (2017). Semi-supervised classification with graph convolutional networks. *International Conference on Learning Representations*.

[4] Nickel, M. and Kiela, D. (2018). Learning continuous hierarchies in the lorentz model of hyperbolic geometry. In *International Conference on Machine Learning*.