Inherent uncertainty of hyperbolic embeddings of complex networks

NESS 2023 — Exploiting Latent Structure in Relational Data

Simon Lizotte, Jean-Gabriel Young and Antoine Allard

June 6, 2023

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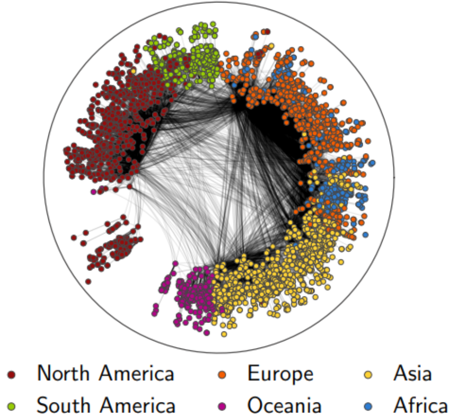
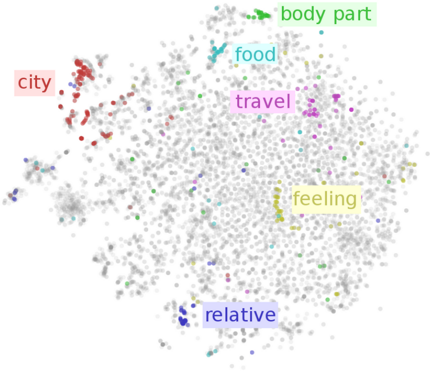
The power of embeddings



World airport network embedding.



Wikipedia word embedding.

Images obtained from Désy, B. (2022). *Effets de la dimension des réseaux hyperboliques sur la modélisation de la structure communautaire* [MSc thesis, Université Laval] and `https://medium.com/@marwane.baghou/named-entity-recognition-crf-neural-network-6e0a32cc5cd5`.

Hyperbolic space: a natural network geometry

Networks obtained from hyperbolic geometry have properties that *match empirical observations*:

- degree sequence;
- *small-worldness*;
- shortest paths;
- community structure.

ARTICLES
PUBLISHED ONLINE: 16 NOVEMBER 2008 | DOI: 10.1038/NPHYS1130

nature physics

Navigability of complex networks

Marián Boguñá[1]*, Dmitri Krioukov[2] and K. C. Claffy[2]

Routing information through networks is a universal phenomenon in both natural and man-made complex systems. When each node has full knowledge of the global network connectivity, finding short communication paths is merely a matter of distributed computation. However, in many real networks, nodes communicate efficiently even without such global intelligence. Here, we show that the peculiar structural characteristics of many complex networks support efficient communication without global

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OPEN **The inherent community structure of hyperbolic networks**

Bianka Kovács[1] & Gergely Palla[1,2,3]

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Network geometry

Marián Boguñá[1,2], Ivan Bonamassa[3], Manlio De Domenico[4], Shlomo Havlin[3], Dmitri Krioukov[5,6,7,8] and M. Ángeles Serrano[1,2,9]

PHYSICAL REVIEW RESEARCH **2**, 043113 (2020)

Link prediction with hyperbolic geometry

Maksim Kitsak,[1,2] Ivan Voitalov,[3,2] and Dmitri Krioukov[4,2]

[1]*Faculty of Electrical Engineering, Delft University of Technology, Mathematics and Computer Science, 2600 GA Delft, The Netherlands*
[2]*Network Science Institute, Northeastern University, 177 Huntington Avenue, Boston, Massachusetts 02115, USA*
[3]*Department of Physics, Northeastern University, 110 Forsyth Street, 111 Dana Research Center, Boston, Massachusetts 02115, USA*
[4]*Department of Physics, Department of Mathematics, Department of Electrical and Computer Engineering,*

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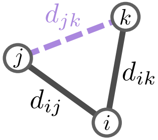
Networks obtained from hyperbolic geometry have properties that *match empirical observations*:

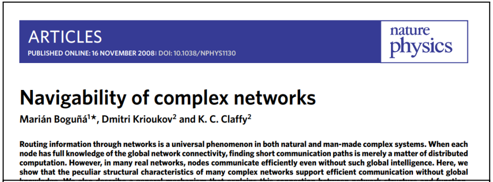
- degree sequence;
- *small-worldness*;
- shortest paths;
- community structure.

Chiefly, the triangle inequality

$$d_{jk} \leq d_{ij} + d_{jk}$$



naturally induces clustering.



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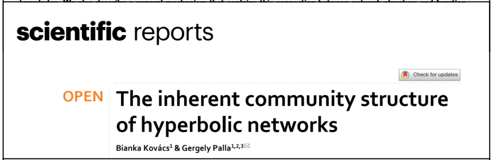

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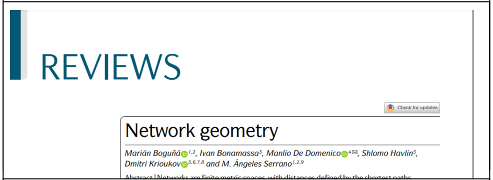

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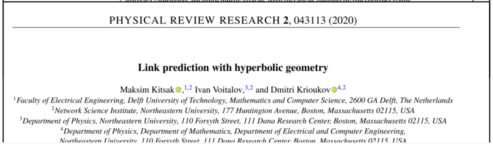

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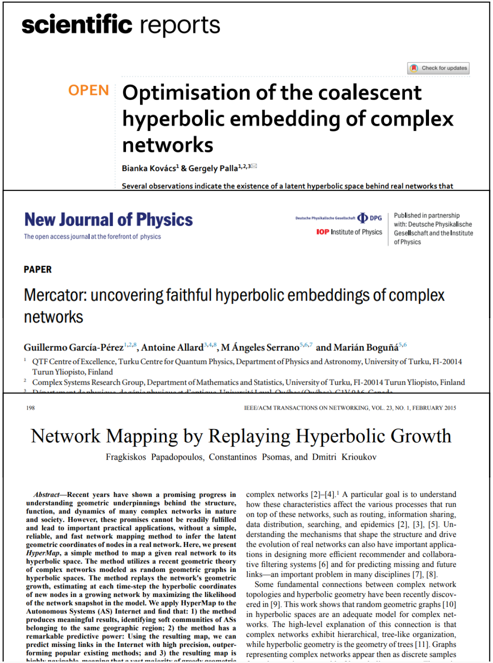
Current methods rely on *heuristics* and use *likelihood optimization*.

While these approaches allow for fast and good results, they cannot quantify the *embedding uncertainty*.



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Optimisation of the coalescent hyperbolic embedding of complex networks

Bianka Kovács[1] & Gergely Palla[1,2,3]

Several observations indicate the existence of a latent hyperbolic space behind real networks that

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PAPER

Mercator: uncovering faithful hyperbolic embeddings of complex networks

Guillermo García-Pérez[1,2,8], Antoine Allard[3,4,8], M Ángeles Serrano[5,6,7] and Marián Boguñá[5,6]

[1] QTF Centre of Excellence, Turku Centre for Quantum Physics, Department of Physics and Astronomy, University of Turku, FI-20014 Turun Yliopisto, Finland

[2] Complex Systems Research Group, Department of Mathematics and Statistics, University of Turku, FI-20014 Turun Yliopisto, Finland

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Network Mapping by Replaying Hyperbolic Growth

Fragkiskos Papadopoulos, Constantinos Psomas, and Dmitri Krioukov

Abstract—Recent years have shown a promising progress in understanding geometric underpinnings behind the structure, function, and dynamics of many complex networks in nature and society. However, these promises cannot be readily fulfilled and lead to important practical applications, without a simple, reliable, and fast network mapping method to infer the latent geometric coordinates of nodes in a real network. Here, we present *HyperMap*, a simple method to map a given real network to its hyperbolic space. The method utilizes a recent geometric theory of complex networks modeled as random geometric graphs in hyperbolic spaces. The method replays the network's geometric growth, estimating at each time-step the hyperbolic coordinates of new nodes in a growing network by maximizing the likelihood of the network snapshot in the model. We apply HyperMap to the Autonomous Systems (AS) Internet and find that: 1) the method produces meaningful results, identifying soft communities of ASs belonging to the same geographic region; 2) the method has a remarkable predictive power: Using the resulting map, we can predict missing links in the Internet with high precision, outperforming popular existing methods; and 3) the resulting map is

complex networks [2]–[4].[1] A particular goal is to understand how these characteristics affect the various processes that run on top of these networks, such as routing, information sharing, data distribution, searching, and epidemics [2], [3], [5]. Understanding the mechanisms that shape the structure and drive the evolution of real networks can also have important applications in designing more efficient recommender and collaborative filtering systems [6] and for predicting missing and future links—an important problem in many disciplines [7], [8].

Some fundamental connections between complex network topologies and hyperbolic geometry have been recently discovered in [9]. This work shows that random geometric graphs [10] in hyperbolic spaces are an adequate model for complex networks. The high-level explanation of this connection is that complex networks exhibit hierarchical, tree-like organization, while hyperbolic geometry is the geometry of trees [11]. Graphs representing complex networks appear then as discrete samples

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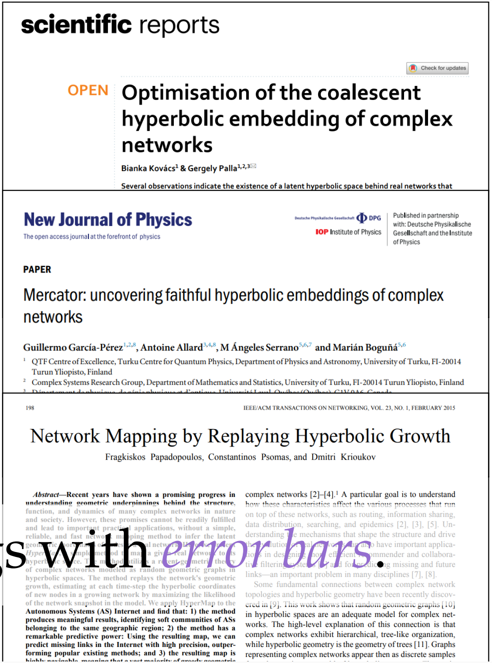
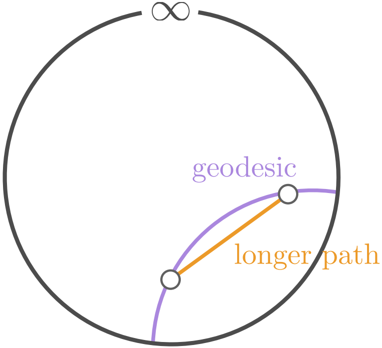


Goal: *robust* embeddings with *error bars*.

The n-dimensional hyperbolic space $\mathbb{H}^n$ is a smooth manifold of *constant negative curvature*.

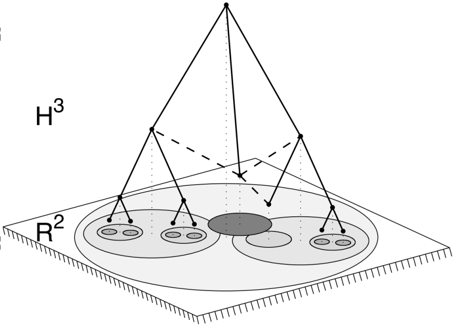


Geodesic in the Poincaré disk model (representation of $\mathbb{H}^2$).

Why hyperbolic geometry?

Hyperbolic geometry has two important features

- its inherent tree-like structure models *hierarchical communities*;
- its negative curvature gives *more space* for vertices; a disk area scales differently with its radius r



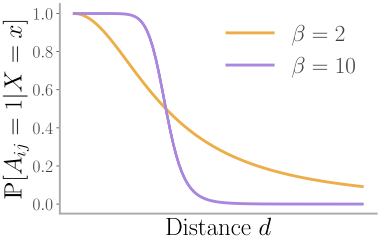
$$\underset{(\mathbb{R}^2)}{r^2} < \underset{(\mathbb{H}^2)}{e^r}$$

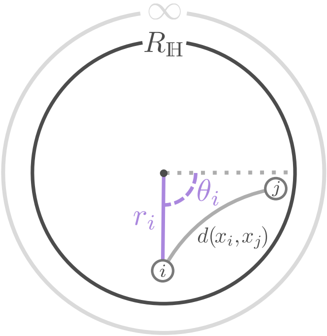
Image from Krioukov, D. et al. (2010). *Hyperbolic geometry of complex networks*. Physical Review E, 82.

The likelihood of the $\mathbb{H}^2$ model is

$$\mathbb{P}[G = g \mid X = x] = \prod_{i<j} \mathbb{P}[A_{ij} = a_{ij} | X = x],$$

where X are the vertices coordinate,





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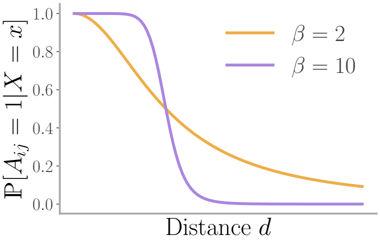
$$\mathbb{P}[G = g \mid X = x] = \prod_{i<j} \mathbb{P}[A_{ij} = a_{ij} | X = x],$$

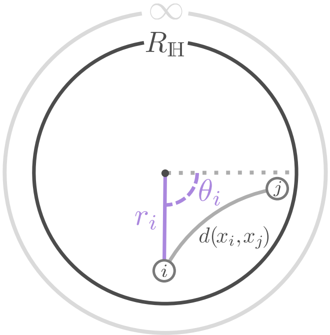
where X are the vertices coordinate, and

$$\mathbb{P}[A_{ij} = 1 \mid X = x] = \frac{1}{1 + e^{\beta[R_{\mathbb{H}} - d(x_i, x_j)]/2}},$$

where

$d(\cdot, \cdot)$: hyperbolic distance function;
x_i: coordinates (r_i, θ_i) of vertex i;
β: controls the sharpness of the sigmoid;
$R_{\mathbb{H}}$: hyperbolic disk radius.





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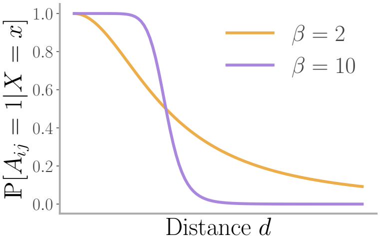

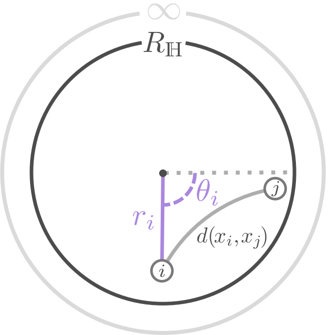

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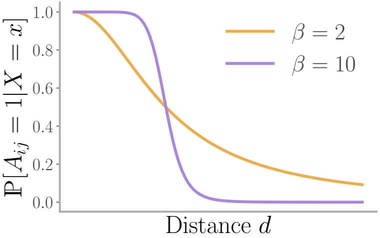

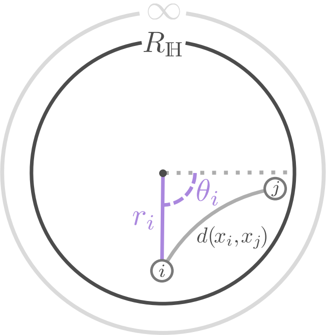

$\mathbb{H}^2 \to \mathbb{S}^1$: decoupling r and θ

Using the transformation

$$\kappa_i = \frac{\mu \pi \kappa_0}{n} e^{-r_i/2},$$

where κ_i is the *expected degree* of vertex i

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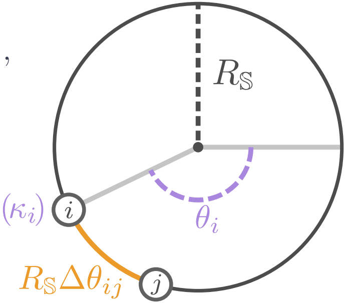
we obtain the $\mathbb{S}^1$ model

$$\mathbb{P}[A_{ij} = 1 \mid X = x] = \frac{1}{1 + \left(\frac{R_{\mathbb{S}} \Delta\theta_{ij}}{\mu \kappa_i \kappa_j}\right)^{\beta}},$$



where

$\Delta\theta_{ij}$: angular separation between θ_i and θ_j;
μ: controls the average degree;
$R_{\mathbb{S}}$: circle radius.

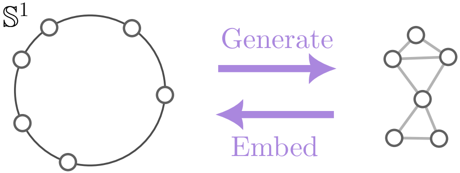
Embedding as Bayesian inference

$$
\begin{aligned}
f_{\Theta|G=g,\kappa,\beta}(\theta) &= \frac{\mathbb{P}[G=g|\theta,\kappa,\beta]\pi(\theta)}{\mathbb{P}[G=g]} \\
&= \frac{1}{\mathbb{P}[G=g]}\left(\frac{1}{2\pi}\right)^n \prod_{i<j}\left(1+\left(\frac{R_{\mathbb{S}}\Delta\theta_{ij}}{\mu\kappa_i\kappa_j}\right)^{\beta(2a_{ij}-1)}\right)^{-1} \\
\theta &\sim \mathrm{Uniform}(-\pi,\pi)
\end{aligned}
$$

We *sample* the posterior density f using Hamiltonian Monte Carlo (HMC).

Validation: infer the coordinates that generated a synthetic graph.

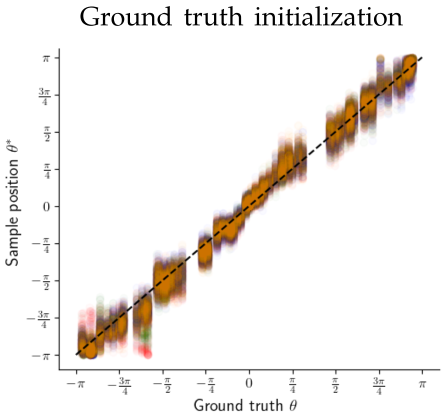
1. Choose the $\mathbb{S}^1$ model's parameters θ, κ and β.
2. Generate a synthetic graph with the likelihood $g \sim \mathbb{P}[G = g|\theta, \kappa, \beta]$.
3. Use HMC[1] to sample θ^* from the posterior f.
4. Compare the sample θ^* to the ground truth θ.



Stan Development Team. 2022. *Stan Modeling Language Users Guide and Reference Manual*, 2.32. `https://mc-stan.org`.

Sample of the posterior

Superposition of the samples obtained from 4 chains. Each chain has a different color.



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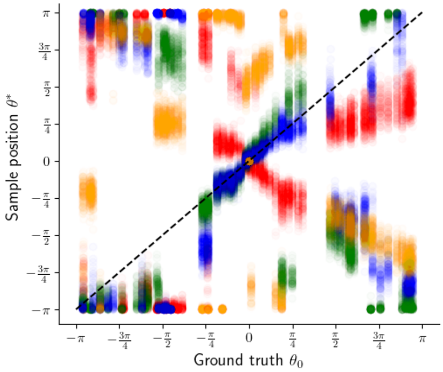
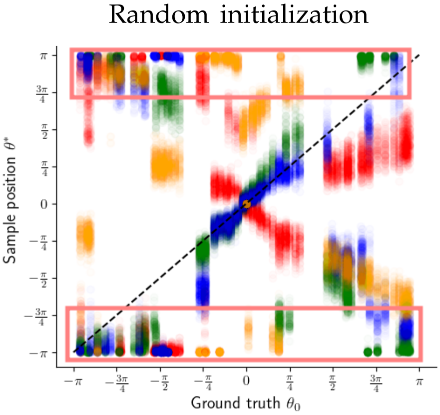
Random initialization



Superposition of the samples obtained from 4 chains. Each chain has a different color.

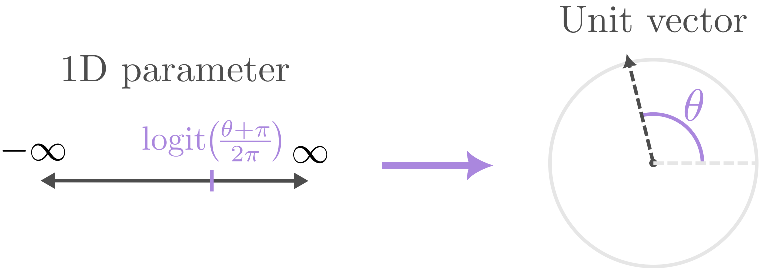
Issue #1: boundaries are *not periodic*.



HMC works with random variables defined on the real numbers $\mathbb{R}$. Using $\theta \in [-\pi, \pi]$ requires a bijective and differentiable function $g : [-\pi, \pi] \to \mathbb{R}$

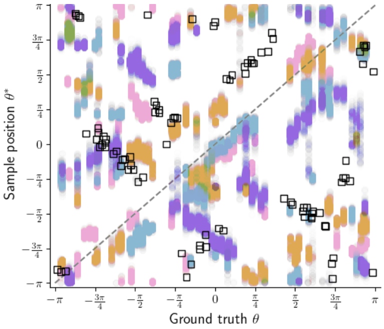
$$\theta \mapsto \operatorname{logit}\left(\frac{\theta + \pi}{2\pi}\right) = -\log\left(\exp\left\{-\frac{\theta + \pi}{2\pi}\right\} - 1\right). \tag{1}$$

The angle of a unit vector is inherently periodic.

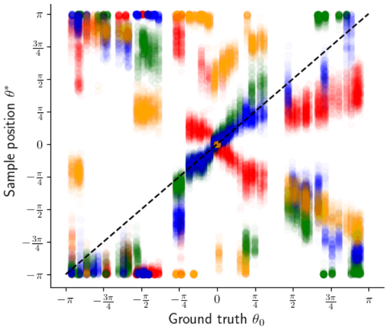


Maximum *a posterori* (MAP) shown with $\square$.

θ as angle of unit vector



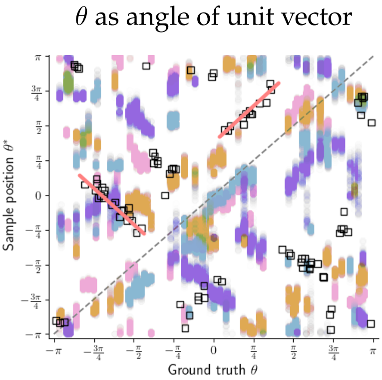
θ as 1D parameter

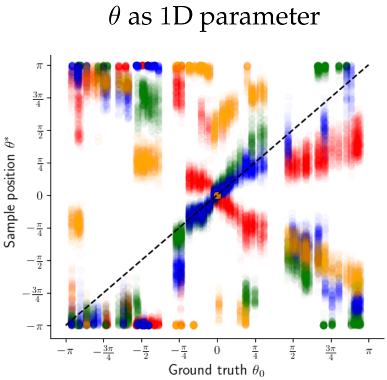


Sampling attempt 2

Maximum *a posterori* (MAP) shown with □.

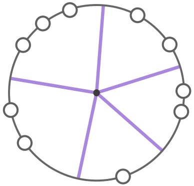
Issue #2: Clusters with *different alignments*.





Cluster angle swap move to help the HMC sampler exit local maxima.

1. Cluster identification



The move is "self-reversible" and unbiased, meaning that the acceptance probability is determined only by the posterior distribution.

Fixing cluster alignments with new MCMC move

Cluster angle swap move to help the HMC sampler exit local maxima.

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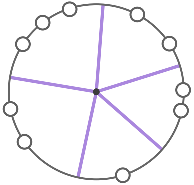
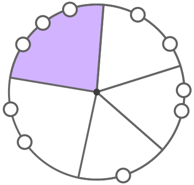


2. Select cluster



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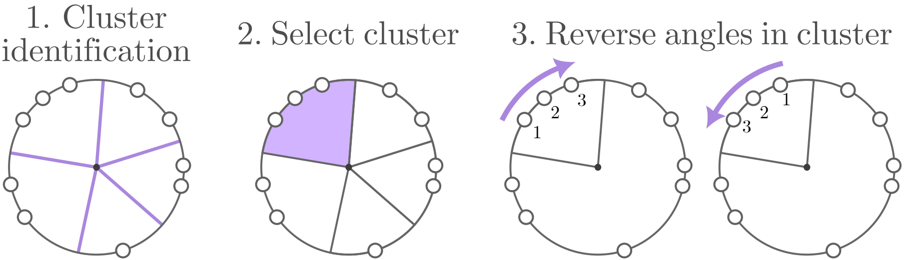

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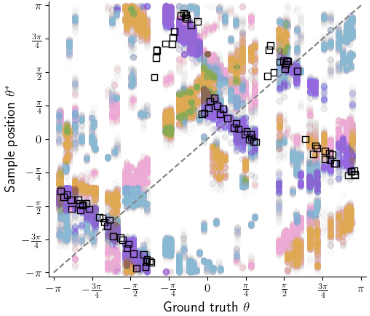
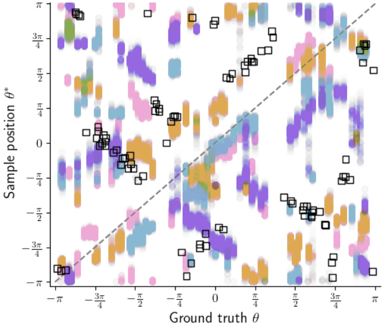
Sampling attempt 3

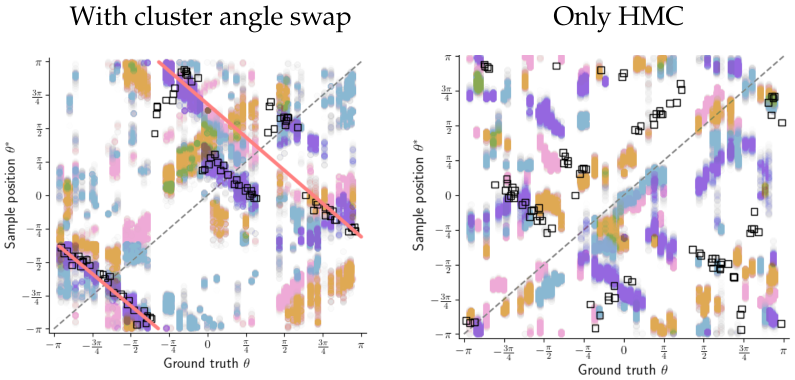
With cluster angle swap



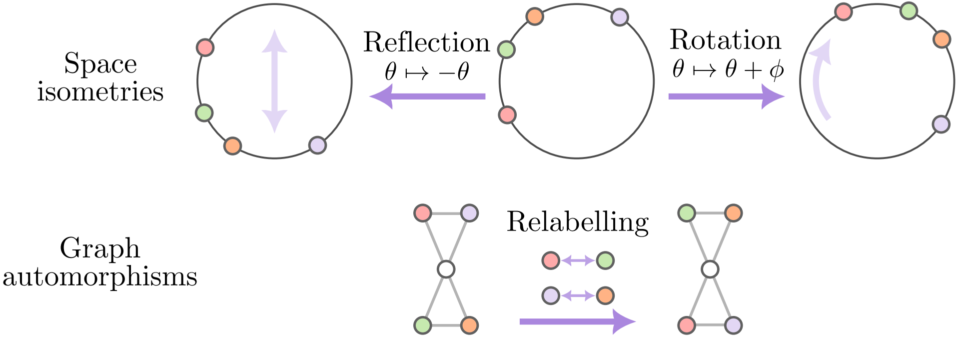
Only HMC



Issue #3: Straight line is *misaligned*.



Natural symmetries: isometries and graph automorphisms



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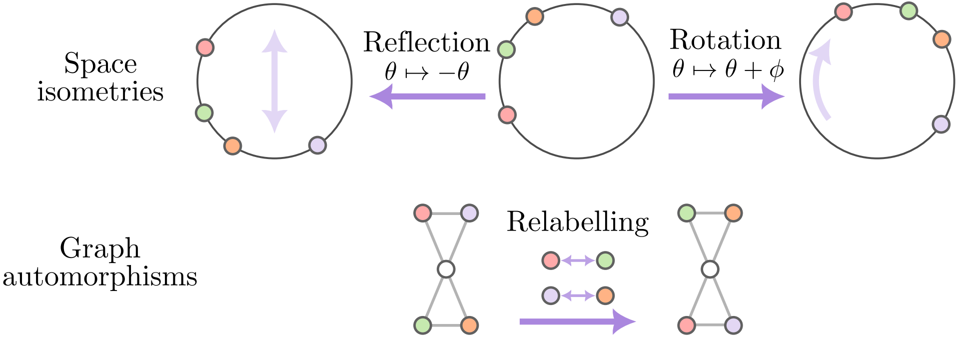
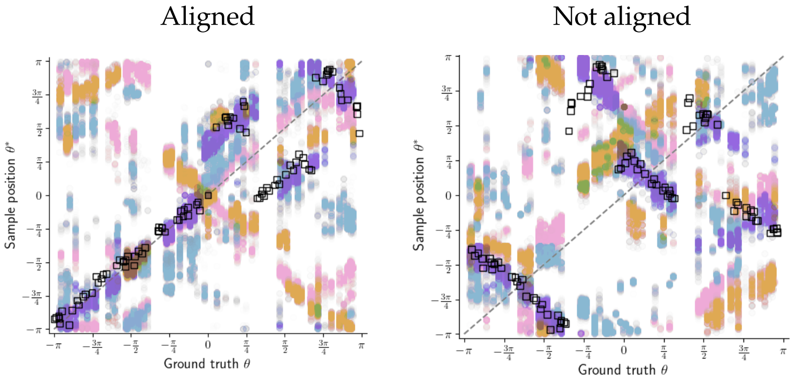


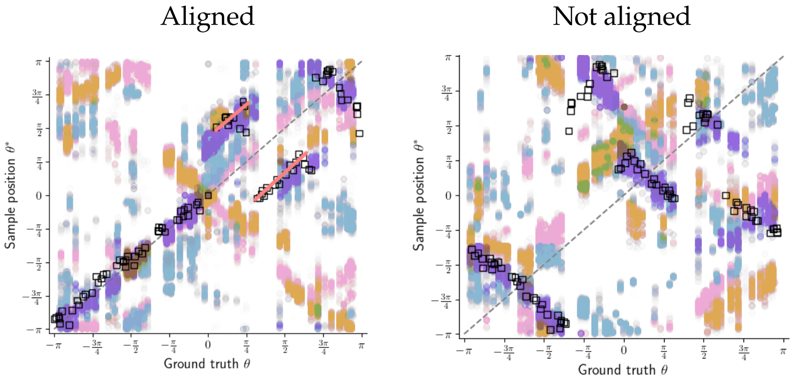
For each automorphism and reflection, we minimize the least squares $\sum_i (\hat{\theta}_i + \phi - \theta_i)^2$ for ϕ.

Aligned results



Issue #4: clusters have incorrect relative positions.

To be continued. . .



This project going forward

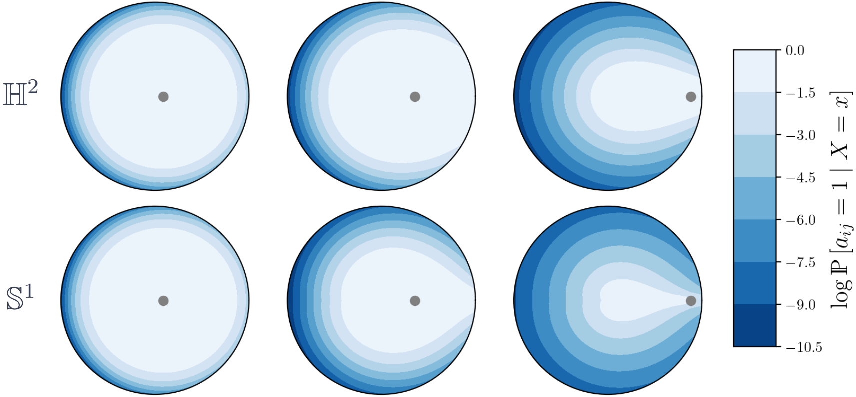
Next we want to

- improve the MCMC mixing such that the ground truth is accessible from any initialization;
- evaluate confidence intervals;
- infer the expected degrees κ;
- embed and compare our method to existing embeddings on a large number of graphs.

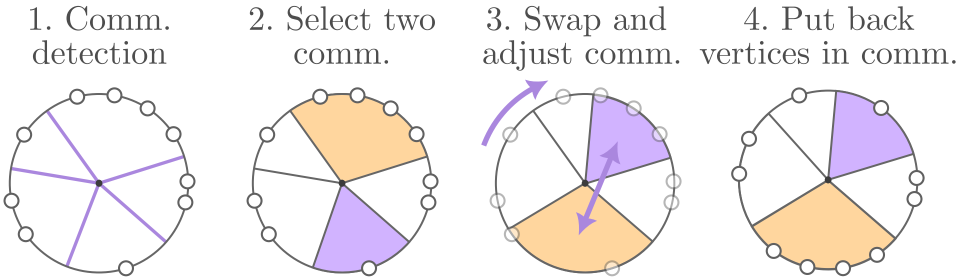
Key takeaways:

- The hyperbolic model is *simple*, yet it *reproduces simultaneously* many observed network properties.
- Our Bayesian approach will *yield error bars*, an information unavailable with current embedding algorithms.

$\mathbb{H}^2$ model vs $\mathbb{S}^1$ model: connection probability



New move considered: cluster swapping



The angular separation $\Delta\theta_{ij}$ is not differentiable

$$\Delta\theta_{ij} = \pi - |\pi - |\theta_i - \theta_j||.$$

The absolute value can be expressed with the Heaviside step function H

$$|x| = x(2H(x) - 1).$$

The step function is approximated with the sigmoid function σ_b

$$H(x) = \lim_{b\to\infty} \sigma_b(x)$$
$$\sigma_b(x) = \frac{1}{1 + e^{-bx}}.$$