Inherent uncertainty of hyperbolic embeddings of complex networks

NetSci 2023 — Network Geometry (13B)

Simon Lizotte, Jean-Gabriel Young and Antoine Allard

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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

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

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

REVIEWS

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Network geometry

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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*

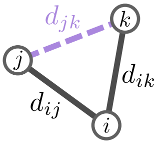
Hyperbolic space: a natural network geometry

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

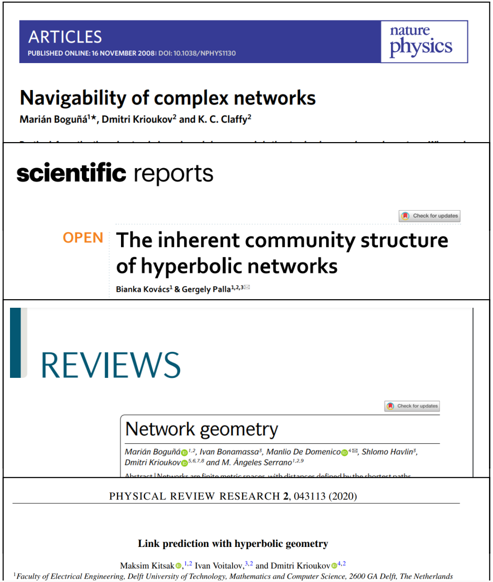
- degree sequence;
- *small-worldness*;
- shortest paths;
- community structure.

Chiefly, the triangle inequality

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



naturally induces clustering.



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Current embedding algorithms' main limitation

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

These approaches yield fast and good results, but they provide little insight on the *likelihood's landscape*.

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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

198 IEEE/ACM TRANSACTIONS ON NETWORKING, VOL. 23, NO. 1, FEBRUARY 2015

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

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

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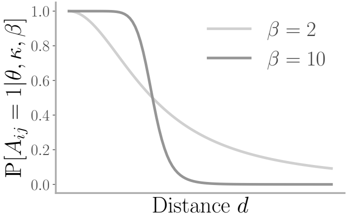
Goal: characterize the *embeddings' landscape*.

$\mathbb{S}^1$ model

The likelihood of the $\mathbb{S}^1$ model[1] is

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



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where

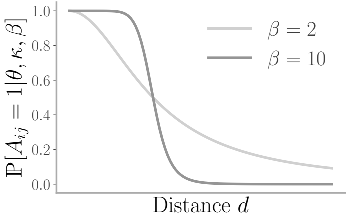
$$\mathbb{P}[A_{ij} = 1 \mid \theta, \kappa, \beta] = \frac{1}{1 + \left(\frac{R\Delta(\theta_i,\theta_j)}{\mu\kappa_i\kappa_j}\right)^{\beta}},$$

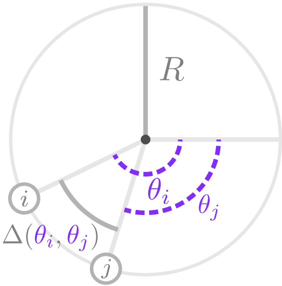
and

κ_i: expected degree of vertex i;

β: controls the sharpness of the sigmoid;

$\Delta(\cdot,\cdot)$: angular separation.





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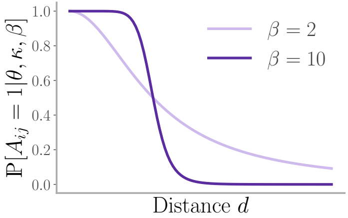

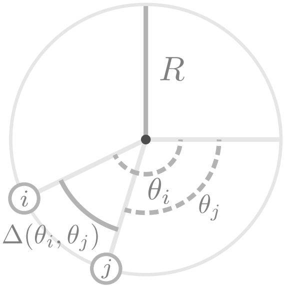

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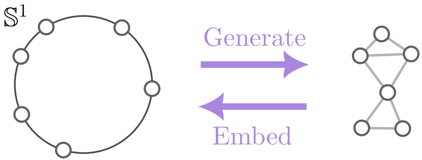
We infer the coordinates that generated a synthetic graph.

1. Choose the $\mathbb{S}^1$ model's parameters θ, κ and β.
2. Generate a synthetic graph with the likelihood $g \sim \mathbb{P}[G = g|\theta, \kappa, \beta]$.



Stan Development Team. 2022. `https://mc-stan.org`.

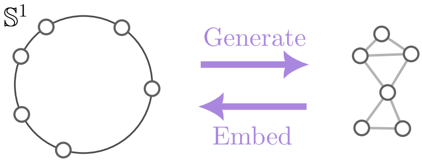
Embedding inference scheme

We 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. Sample[1] the posterior obtained using Bayes' rule

$$f(\theta|G=g) = \frac{\pi(\theta)}{\mathbb{P}[G=g]} \prod_{i<j} \left(1 + \left(\frac{R\Delta(\theta_i, \theta_j)}{\mu\kappa_i\kappa_j}\right)^{\beta(2a_{ij}-1)}\right)^{-1},$$

$$\pi(\theta) = \left(\frac{1}{2\pi}\right)^n.$$



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Hamiltonian Monte Carlo (HMC) has poor mixing because of the *multimodality of the posterior*.

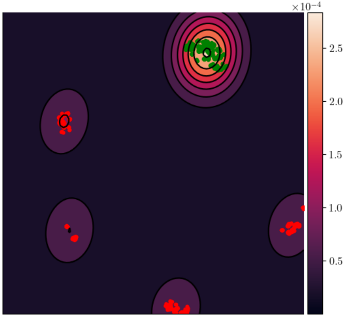
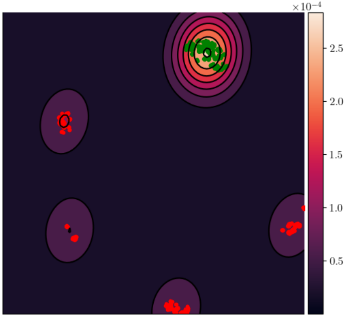


Figure: Multidimensional scaling (MDS) of the posterior sample obtained from 4 chains initialized randomly (red) and initialized at the ground truth (green).

Hamiltonian Monte Carlo (HMC) has poor mixing because of the *multimodality of the posterior*.

Solved issues:

1. incorrect boundary periodicity;
2. symmetry-equivalent embeddings;
3. incoherent cluster alignments.



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Issues with out-of-the-box HMC

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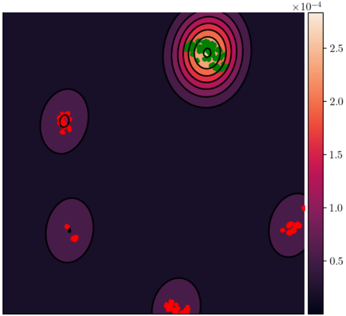

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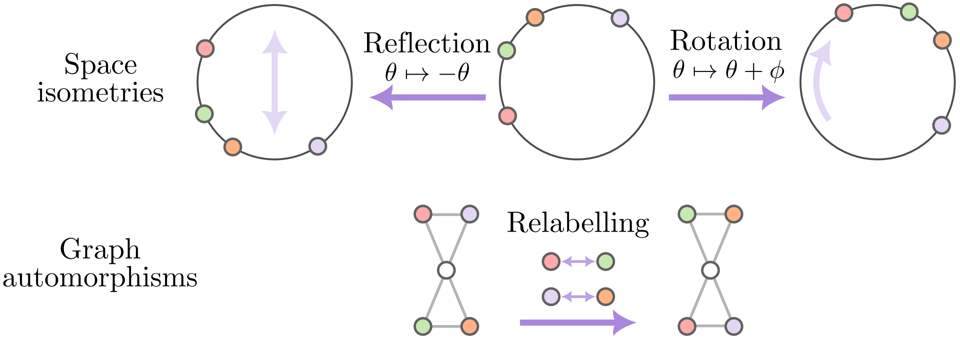
Issue #2: Symmetries cause equivalent embeddings



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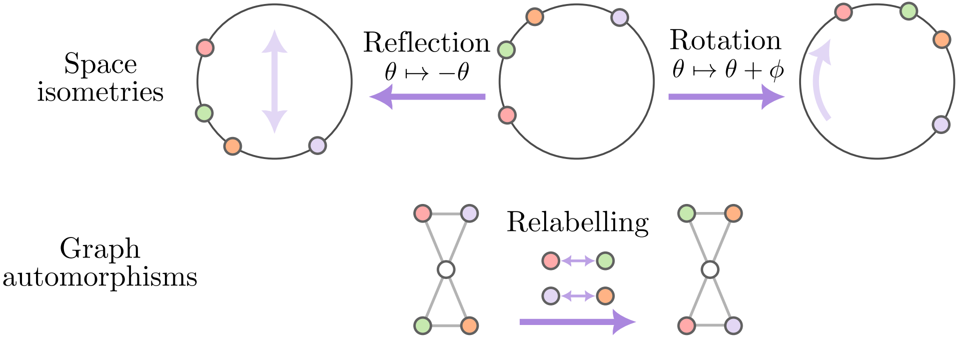


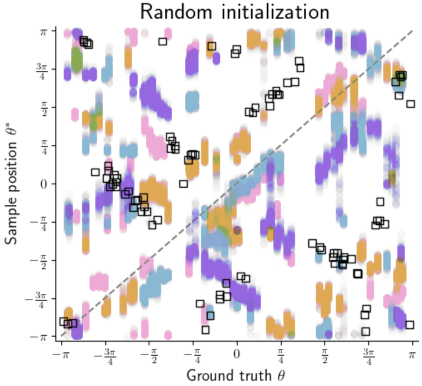
We *fix the vertex* of the largest degree at $\theta = 0$ to limit rotations. Samples are aligned[2] after running HMC.

2. Rotation ϕ which minimizes $\sum_i \Delta(\theta_i^* + \phi, \theta_i)^2$ across all combinations of automorphisms and reflections.

Issue #3: Clusters have different alignments

Superposition of the samples obtained from 4 chains. Each chain has a different color. Maximum *a posterori* (MAP) shown with □.

A *straight line* signals a perfect inference.



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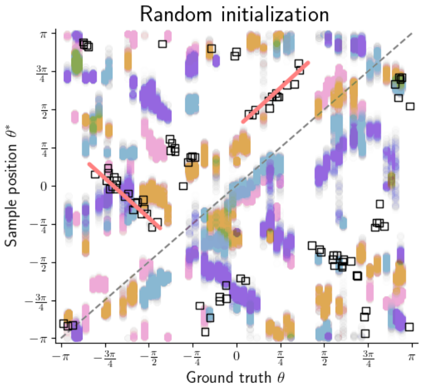
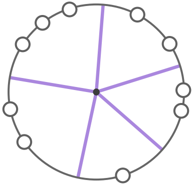


A *cluster angle swap* move helps the HMC sampler exit some local maxima.

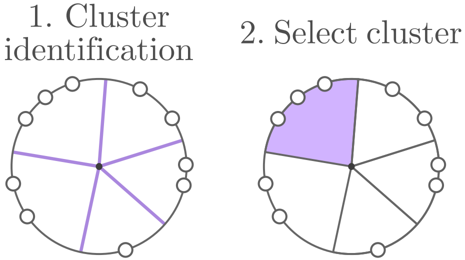
1. Cluster identification



This move is its own inverse. Its acceptance probability depends only on the posterior ratio.

Fixing cluster alignments with a new MCMC move

A *cluster angle swap* move helps the HMC sampler exit some local maxima.



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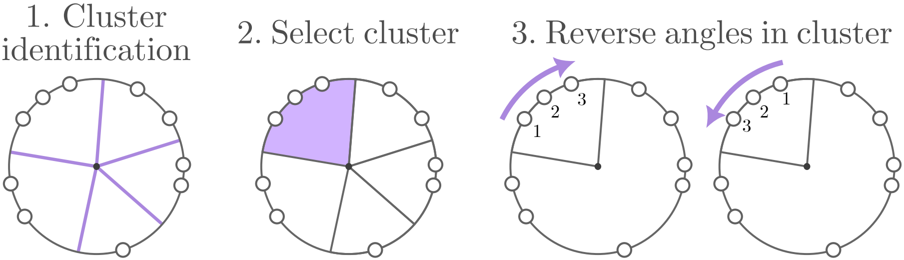

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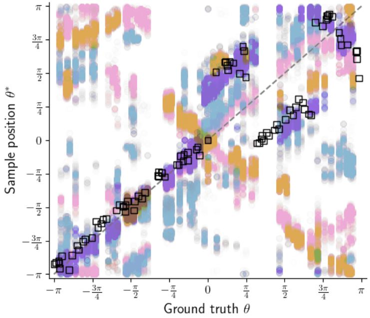
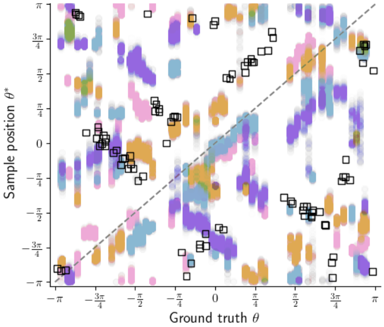
Sampling with HMC and cluster angle swap

With cluster angle swaps

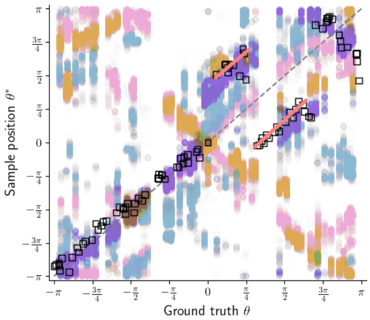


Only HMC



Issue #4: clusters have incorrect relative positions.

With cluster angle swaps



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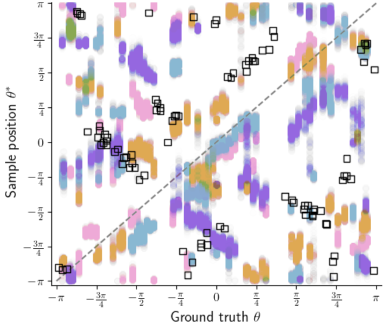

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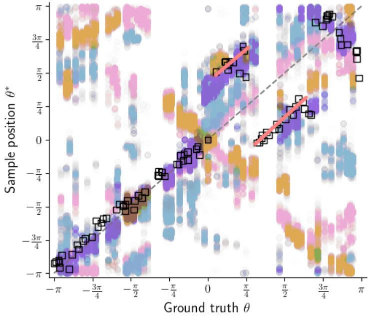
However, we believe these *clusters translations* could be, for certain graphs, nearly *equally probable*.

To be continued. . .

With cluster angle swaps



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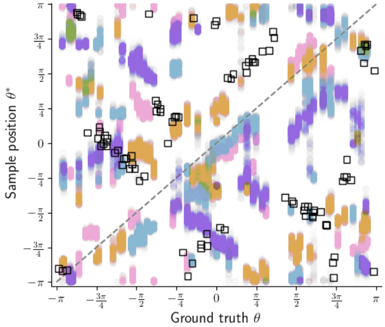


Next we want to

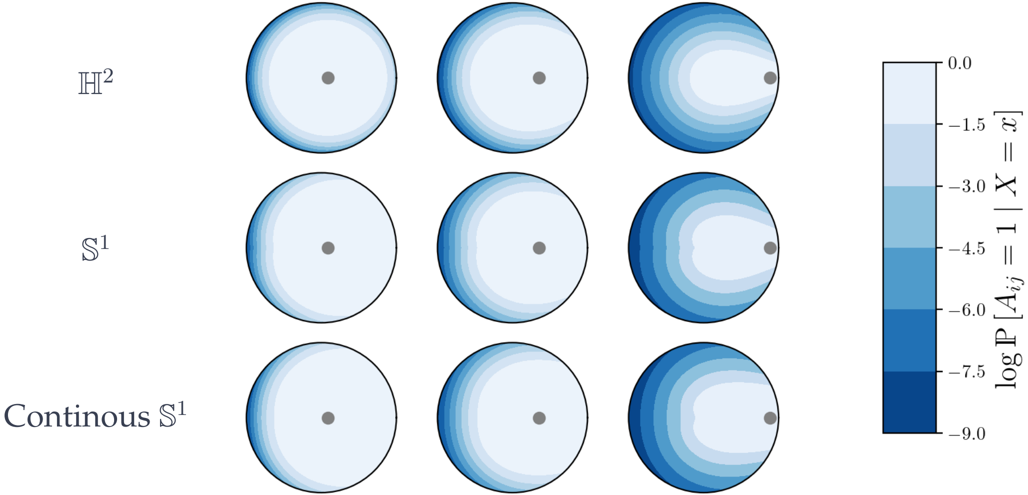
- improve the MCMC mixing such that the ground truth is accessible from any initialization;
- evaluate confidence intervals;
- infer the expected degrees κ;
- compare our method to other algorithms on a large variety of graphs.

Takeaways:

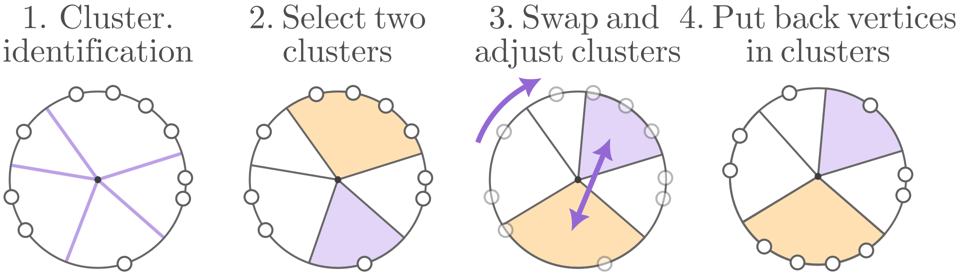
- Our Bayesian approach can *characterize the embeddings' landscape*.
- The posterior is *multimodal* and thus difficult to explore with MCMC.
- There could be *multiple good embeddings*.

Feel free to contact me at `simon.lizotte.1@ulaval.ca`.

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



New move considered: cluster swapping



Sigmoid approximation of the absolute value

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

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

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

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