Network geometry: bringing data back into the fold

NetSci 2025 — Network Geometry: Theory and Applications

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Outline

1. Introducing network geometry (an incomplete and very biased primer)

2. Leveraging symmetries to go beyond pointwise estimates of coordinates/parameters

3. Embedding asymmetric (directed) networks unto a metric space (with symmetric distance function)

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2. Leveraging symmetries to go beyond pointwise estimates of coordinates/parameters
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Maximally random graph ensembles

The probability, $P(\mathbb{A})$, for a $N \times N$ adjacency matrix $\mathbb{A} = \{a_{ij}\} \in [0,1]^{\binom{N}{2}}$ that maximizes the entropy subjected to the L constraints ($l = 1, 2, \ldots, L$)

$$S(\{\mathbb{A}\}) = -\sum_{\mathbb{A}} P(\mathbb{A}) \ln P(\mathbb{A}) \qquad \bar{F}_l = \sum_{\mathbb{A}} F_l(\mathbb{A}) P(\mathbb{A})$$

is (α_l being the l-th Lagrange multiplier)

$$P(\mathbb{A}) \propto \exp\left(-\sum_{l=1}^{L} \alpha_l F_l(\mathbb{A})\right) .$$

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EPL 81, 28005 (2007)
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Example 1: fixing the expected number of edges

$$\bar{F}_1 = \sum_{i=1}^{N} \sum_{j=i+1}^{N} a_{ij} = M$$

yields the Bernouilli random graph ensemble

$$P(\mathbb{A}) = \prod_{i=1}^{N} \prod_{j=i+1}^{N} p^{a_{ij}} (1-p)^{1-a_{ij}} \quad \text{with} \quad p = \frac{1}{e^{\alpha_1} + 1} .$$

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Example 2: fixing the expected degree sequence

$$\bar{F}_l = \sum_{j=1}^{N} a_{lj} = k_l$$

for $l = 1, \ldots, N$ yields the soft configuration model

$$P(\mathbb{A}) = \prod_{i=1}^{N} \prod_{j=i+1}^{N} p_{ij}^{a_{ij}} (1-p_{ij})^{1-a_{ij}} \quad \text{with} \quad p_{ij} = \frac{1}{e^{-(\alpha_i+\alpha_j)} + 1} .$$

Redefining $\kappa_l = \sqrt{\langle\kappa\rangle N} e^{\alpha_l}$ for $l = 1, \ldots, N$ yields the Chung-Lu model

$$p_{ij} = \frac{1}{1 + \frac{\langle\kappa\rangle N}{\kappa_i \kappa_j}} \simeq \frac{\kappa_i \kappa_j}{\langle\kappa\rangle N} .$$

Studying the conditions for which p_{ij} can be factorized informs us on the degree-degree correlations observed in real networks.

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Modeling clustering

Idea: Assume that the vertices are embedded in a metric space and that any two vertices are connected with a probability that is a decreasing function of the distance between them.

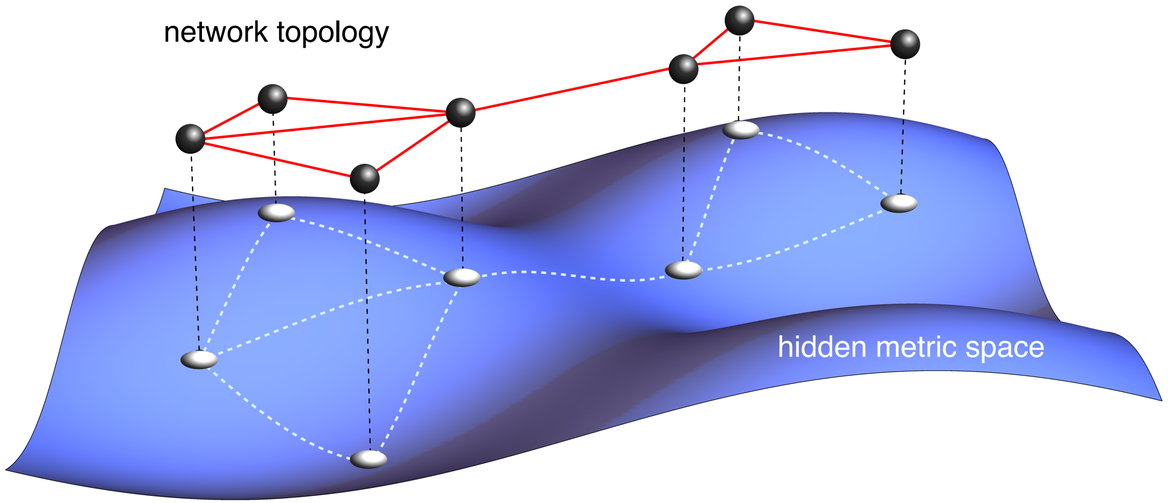
Courtesy of M. Boguñá

Modeling clustering

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Properties of any metric space:

Identity of indiscernibles	$d(x,y) = 0 \quad \Leftrightarrow \quad x = y$
Non-negativity	$d(x,y) \geq 0$
Symmetry	$d(x,y) = d(y,x)$
Triangle inequality	$d(x,y) \leq d(x,z) + d(z,y)$



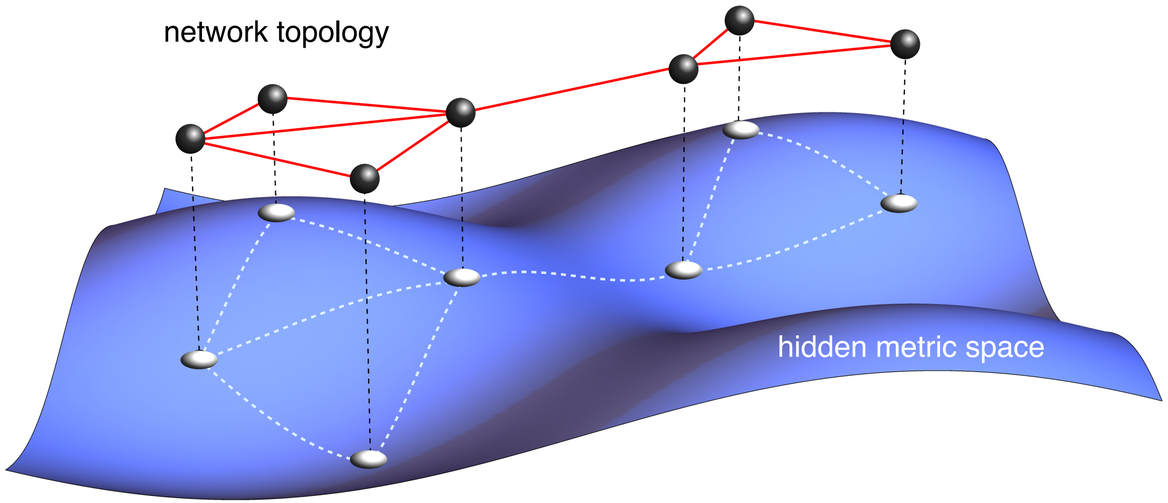
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Henceforth we consider that there is a distance matrix $\mathbb{X} = \{x_{ij}\}$ where x_{ij} is the distance between vertices i and j in the D-dimensional space.

Maximally random geometric graph ensembles

Example 3: fixing the expected number of edges and the expected total energy

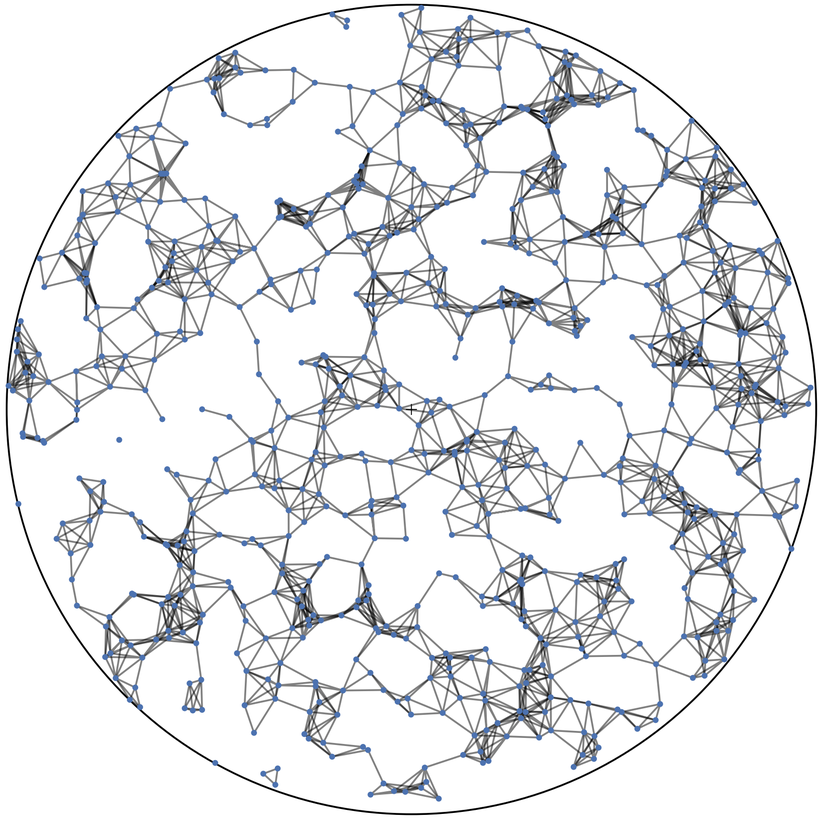
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$$\bar{F}_2 = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \varepsilon_{ij} a_{ij} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} f(x_{ij}) a_{ij} = E$$

yields the homogeneous random geometric graph ensemble

$$P(\mathbb{A}) = \prod_{i=1}^{N} \prod_{j=i+1}^{N} p_{ij}^{a_{ij}} (1 - p_{ij})^{1-a_{ij}} \quad \text{with} \quad p_{ij} = \frac{1}{e^{\beta(\varepsilon_{ij} - \mu)} + 1} \, .$$

The graphs will be sparse, highly clustered and small-world iif $f(x_{ij}) \sim \ln x_{ij}$ and $\beta \in [D, D+2]$.



Maximally random geometric graph ensembles

Example 4: fixing the expected degree sequence and the expected total energy

$$\bar{F}_l = \sum_{j=1}^{N} a_{lj} = k_l \quad (l = 1, \ldots, N)$$

$$\bar{F}_{N+1} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \varepsilon_{ij} a_{ij} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} f(x_{ij}) a_{ij} = E$$

yields the heterogeneous random geometric graph ensemble

$$P(\mathbb{A}) = \prod_{i=1}^{N} \prod_{j=i+1}^{N} p_{ij}^{a_{ij}} (1 - p_{ij})^{1 - a_{ij}} \quad \text{with} \quad p_{ij} = \frac{1}{e^{\beta \varepsilon_{ij} - \alpha_i - \alpha_j} + 1} \, .$$

The graphs will be sparse, highly clustered, small-world and devoid of non-structural degree-degree correlation iif $f(x_{ij}) = \ln x_{ij}$ and $\beta \in [D, D+2]$[a]. Redefining $\alpha_l = -(\beta/D) \ln(\sqrt{\mu} \kappa_l)$ yields

$$p_{ij} = \frac{1}{e^{\beta(\varepsilon_{ij} - \mu)} + 1} \quad \text{with} \quad \varepsilon_{ij} = \ln \left(\frac{x_{ij}}{(\kappa_i \kappa_j)^{\frac{1}{D}}} \right) \, .$$

[a] No upper bound if expected degree sequence is scale-free.

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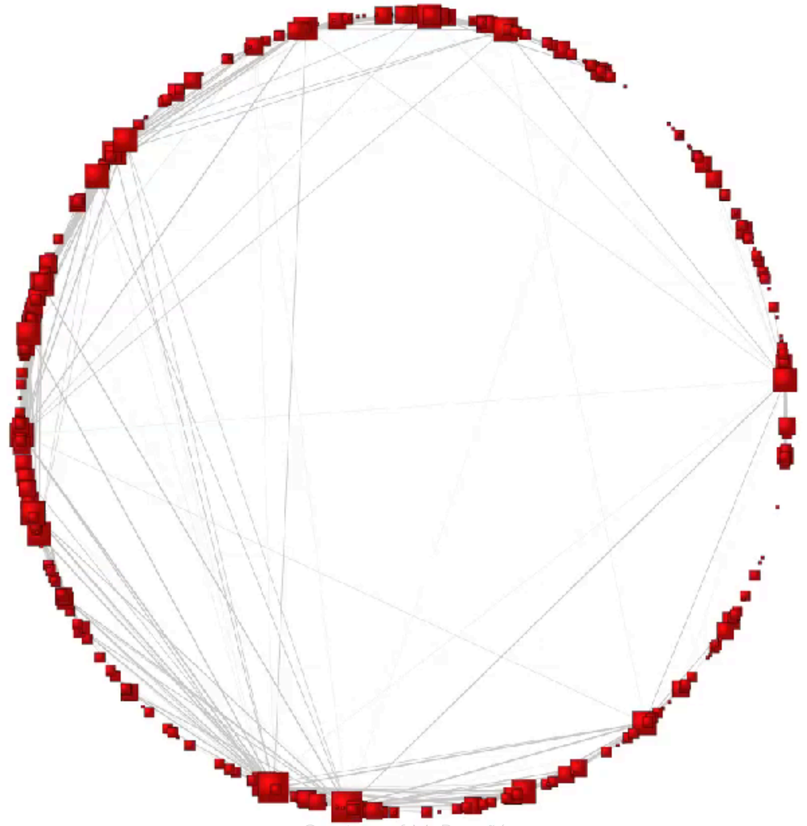
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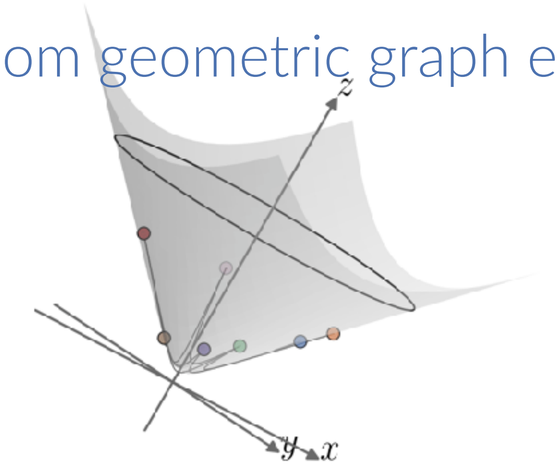
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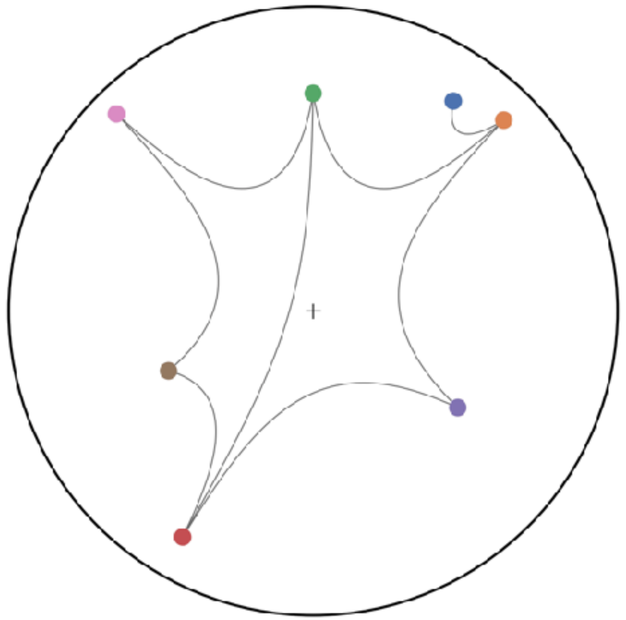
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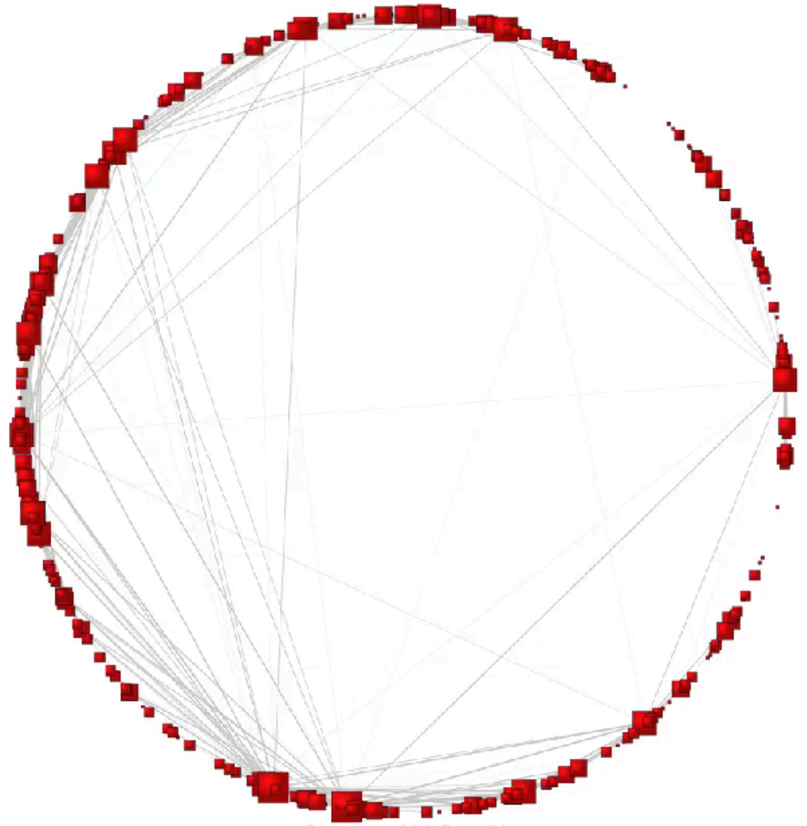


hyperboloid in $\mathbb{R}^{2,1}$



hyperbolic disk (r, θ)

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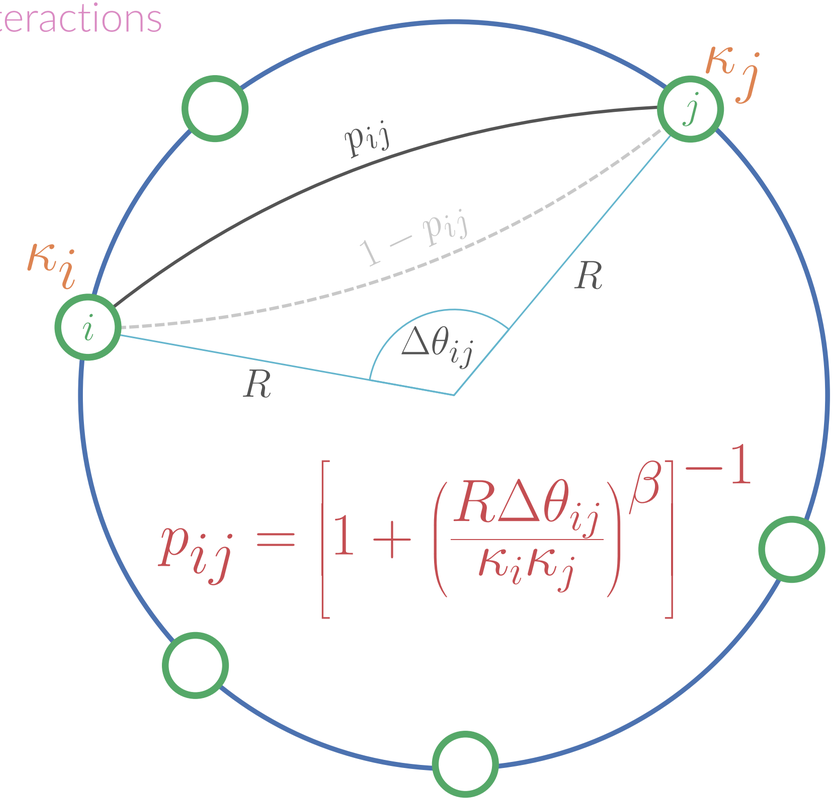
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A geometric approach to clustering : the $\mathbb{S}^1/\mathbb{H}^2$ model

The $\mathbb{S}^1$ model

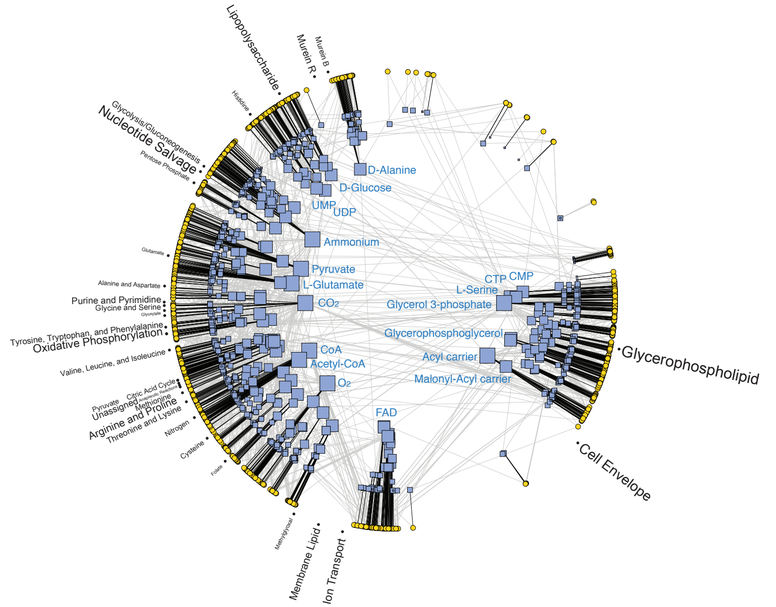
1. Sprinkle N nodes uniformly on a circle of radius R.
2. Assign an expected degree κ to each node according to some pdf $\rho(\kappa)$.
3. Draw a link between node i and node j with probability p_{ij}.

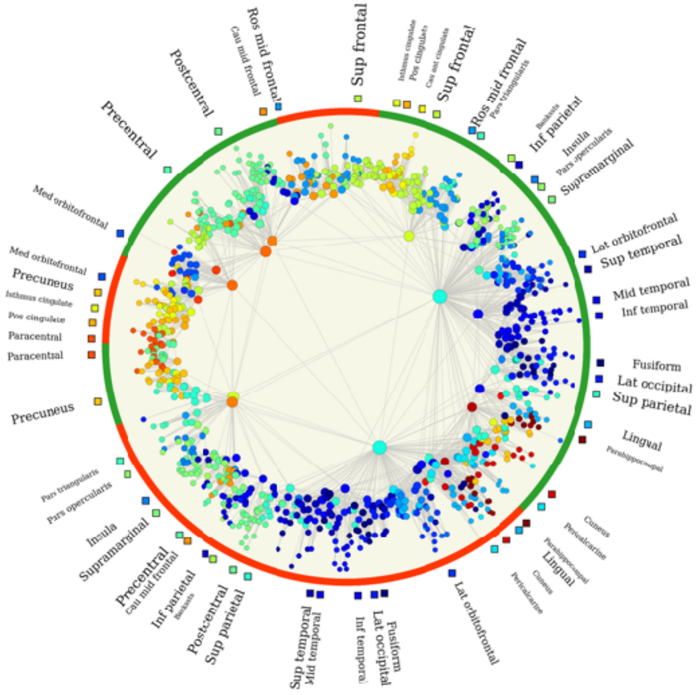
★ fixes the expected degree of nodes (κ) → soft configuration model (CM)
★ triangle inequality of the underlying metric space → triangles from pairwise interactions
★ level of clustering tuned with parameter β

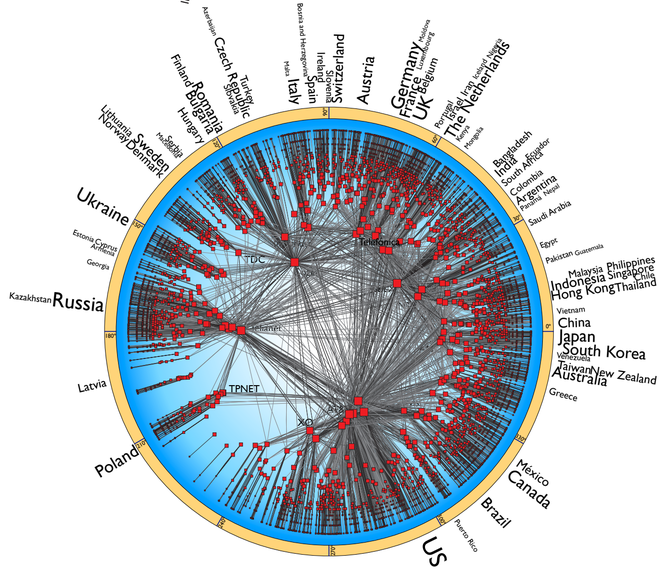


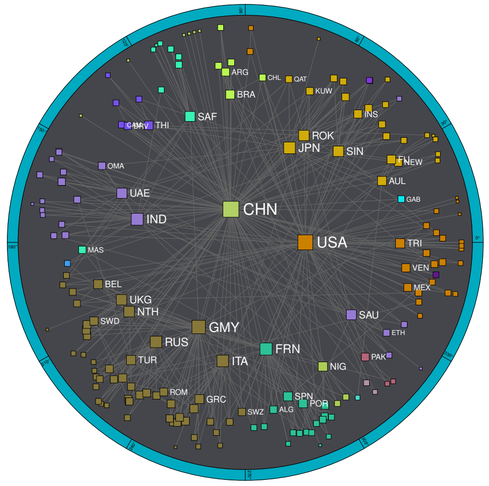
A powerful and versatile framework

- Amenable to many analytical calculations [1,2,3]
- Generalizable to weighted [5], bipartite [6,7,8], multiplex [9,10] and growing [11] networks
- Geometrical interpretation of preferential attachment [11]
- Parsimonious explanation of self-similarity [4]
- Generalizable to networks with community structure [12,13,14]
- Mapping of real complex networks unto hyperbolic space [15,16]
  - Reproduction of additional properties than the ones used to fit the parameters [15].
  - Identification of biochemical pathways in E. Coli [8]
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  - Organization of the human connectome [18,20]
  - Self-similar architecture [19]
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Review Article | Published: 29 January 2021

Network geometry

Marián Boguñá, Ivan Bonamassa, Manlio De Domenico ✉, Shlomo Havlin, Dmitri Krioukov & M. Ángeles Serrano

Nature Reviews Physics **3**, 114–135 (2021)

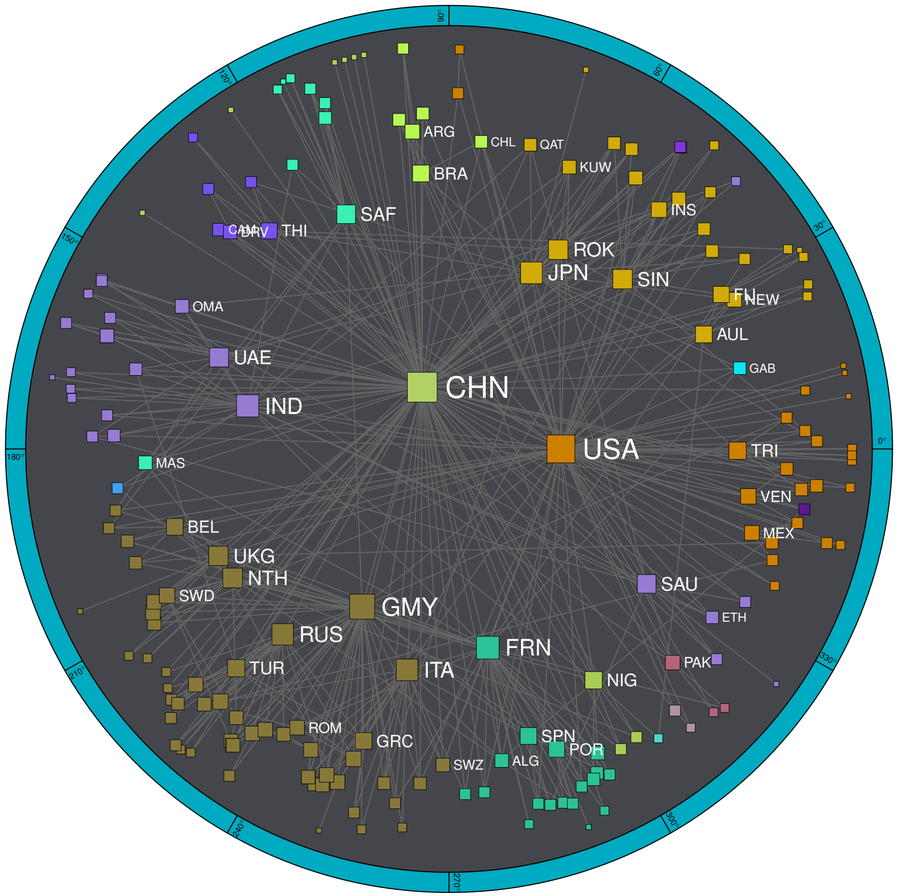
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Most embedding algorithms rely on maximum likelihood and/or machine learning heuristics to obtain pointwise estimates for the coordinates (and other parameters).



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Sustaining the Internet with hyperbolic mapping

Marián Boguñá, Fragkiskos Papadopoulos & Dmitri Krioukov

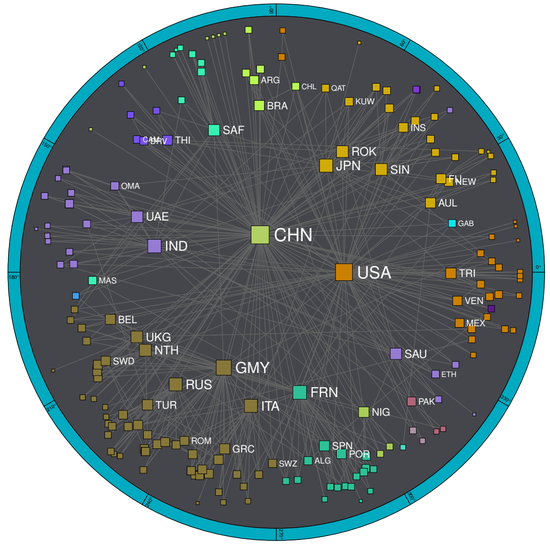
Nature Communications **1**, Article number: 62 (2010)

Mercator: uncovering faithful hyperbolic embeddings of complex networks

Guillermo García-Pérez, Antoine Allard, M Ángeles Serrano and Marián Boguñá

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New Journal of Physics, Volume 21, December 2019



$$\mathbb{P}\Big(\overbrace{\mathbb{A}}^{\text{adj. mat.}} \;\Big|\; \underbrace{\{\kappa_i\},\{\theta_i\}}_{\text{coordinates}}, \overbrace{\beta}^{\text{param.}} \Big) = \underbrace{\prod_{i=1}^{N}\prod_{j=i+1}^{N} \Big(\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta)\Big)^{a_{ij}} \Big(1-\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta)\Big)^{1-a_{ij}}}_{\text{likelihood}}$$

Probability of connection in the $\mathbb{S}^1$ model:

$$\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta) = \left[1+\left(\frac{M}{\beta\sin(\pi/\beta)}\frac{\Delta\theta_{ij}}{\kappa_i\kappa_j}\right)^{\beta}\right]^{-1}$$

Angular distance:

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

Number of edges (known from data):

$$M = \sum_{i=1}^{N}\sum_{j=i+1}^{N} a_{ij}$$

$N\times N$ adjacency matrix (known from data):

$$\mathbb{A} = \{a_{ij}\}$$

"Radial" coordinates (related to degree/popularity):

$$\{\kappa_i\} = \{\kappa_1,\kappa_2,\kappa_3,\ldots,\kappa_{N-1},\kappa_N\}$$

Angular coordinates (related to similarity/community):

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Coupling with geometry (related to clustering): β

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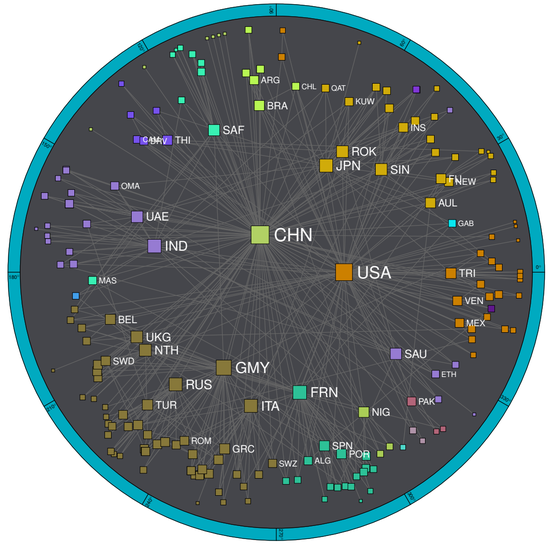
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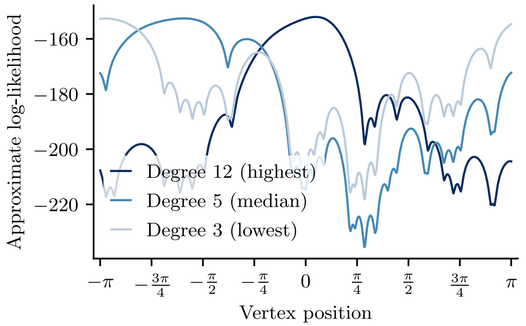
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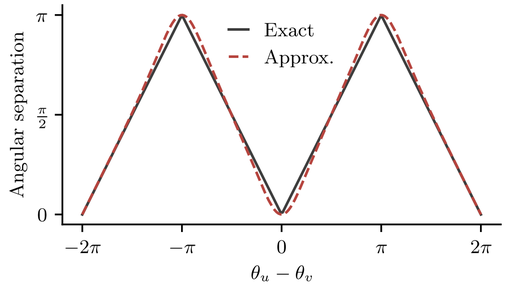
▷ Difficult optimization problem

- rugged landscape
- gradient not always well defined

▷ Open questions:

- are there more than one plausible embeddings?
- how precise are the estimates for the coordinates/parameters?





Distribution of embeddings: Bayesian inference

$$\underbrace{\mathbb{P}\left(\{\kappa_i\}, \{\theta_i\}, \beta \,\middle|\, \mathbb{A}\right)}_{\text{posterior}} \propto \underbrace{\mathbb{P}\left(\mathbb{A} \,\middle|\, \{\kappa_i\}, \{\theta_i\}, \beta\right)}_{\text{likelihood}} \underbrace{\mathbb{P}\left(\{\kappa_i\}, \{\theta_i\}, \beta\right)}_{\text{prior}}$$

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$$\kappa_i \propto \frac{2}{\pi\gamma(1+(\kappa_i/\gamma)^2)}\,\mathbb{1}[\kappa_i > \varepsilon], \quad \varepsilon = 10^{-10},\ \gamma = 4$$

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$$\propto \underbrace{\prod_{i=1}^{N}\prod_{j=i+1}^{N}\Big(\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta)\Big)^{a_{ij}}\Big(1-\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta)\Big)^{1-a_{ij}}}_{\text{likelihood}}\ \underbrace{\mathbb{P}(\beta)\prod_{i=1}^{N}\mathbb{P}(\kappa_i)\mathbb{P}(\theta_i)}_{\text{prior}}$$

Probability of connection in the $\mathbb{S}^1$ model:

$$\mathbb{P}(a_{ij}=1|\kappa_i,\kappa_j,\theta_i,\theta_j,\beta) = \left[1+\left(\frac{M}{\beta\sin(\pi/\beta)}\frac{\Delta\theta_{ij}}{\kappa_i\kappa_j}\right)^{\beta}\right]^{-1}$$

Angular distance:

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

Number of edges (known from data):

$$M = \sum_{i=1}^{N}\sum_{j=i+1}^{N} a_{ij}$$

$N\times N$ adjacency matrix (known from data):

$$\mathbb{A} = \{a_{ij}\}$$

"Radial" coordinates (related to degree/popularity):

$$\{\kappa_i\} = \{\kappa_1,\kappa_2,\kappa_3,\ldots,\kappa_{N-1},\kappa_N\}$$

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- With the posterior, we can characterize the coordinates/parameters
  - expected values

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  - variances, covariances, standard deviations
  - most likely values
  - …

- Difficulties: posterior is hard to work with (no convenient closed form) and these integrals cannot be solved analytically

- Solution: sampling approximations using Markov Chain Monte Carlo

Distribution of embeddings: Bayesian inference

Priors:

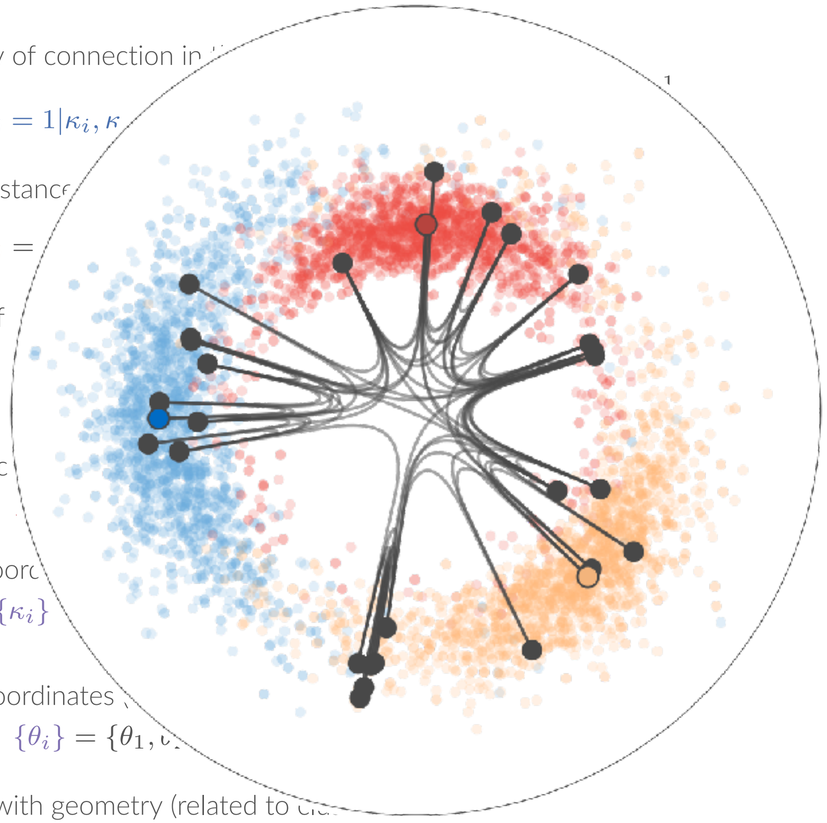
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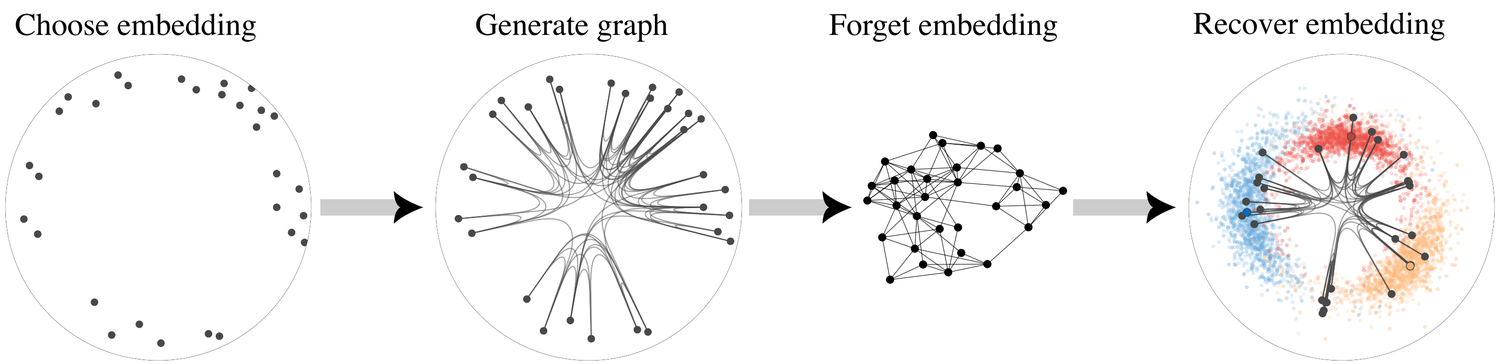
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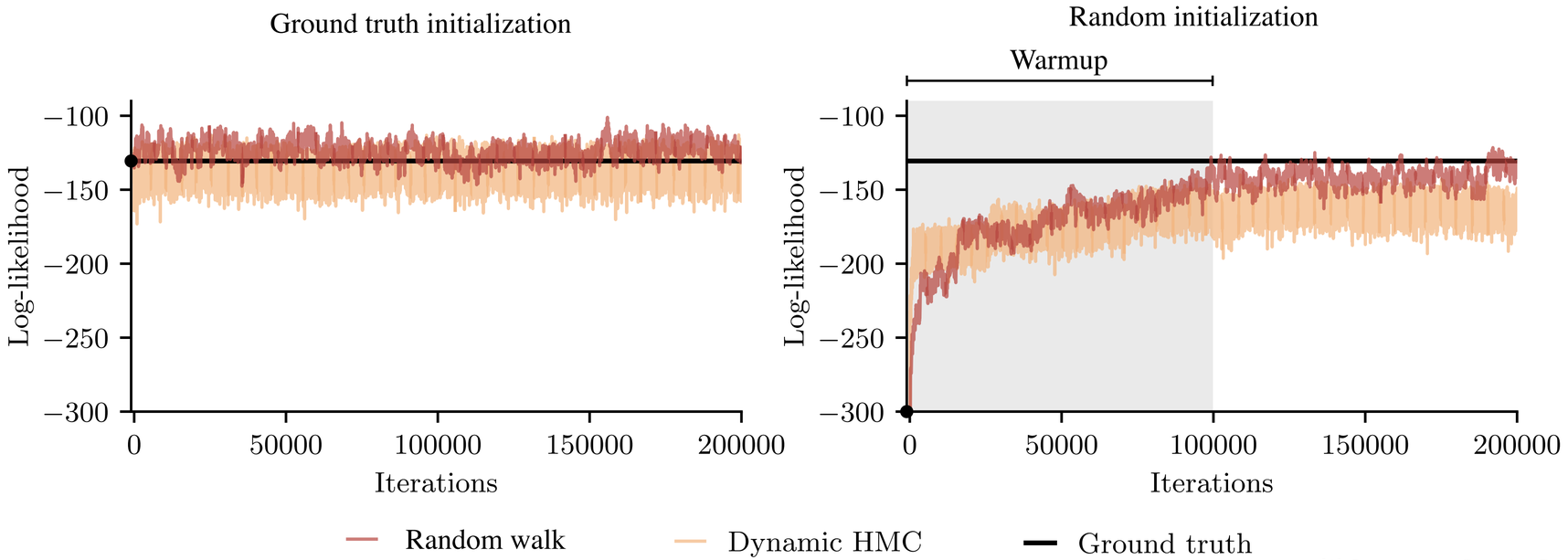
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Testing standard sampling methods



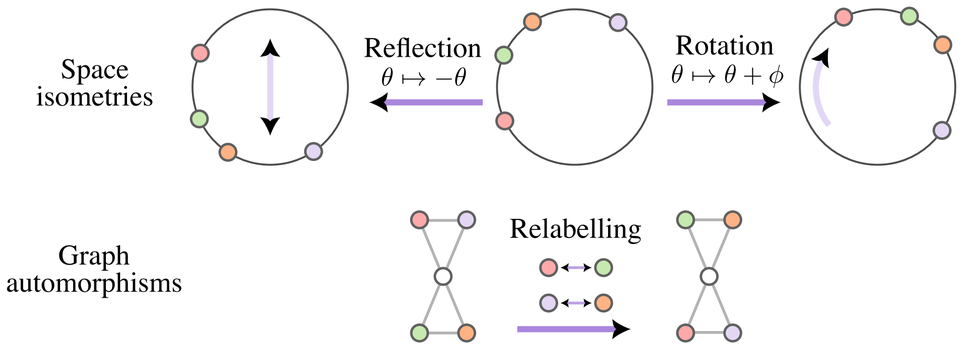
Hamiltonian Monte-Carlo [1, 2] (“state-of-the-art”) and random walk (“naive”) do not explore the space efficiently.



[1] Gelman et al., Bayesian Data Analysis (Chapman & Hall / CRC Press, 2013
[2] arXiv:1701.02434 (2017)

Model symmetries and quasi-symmetries

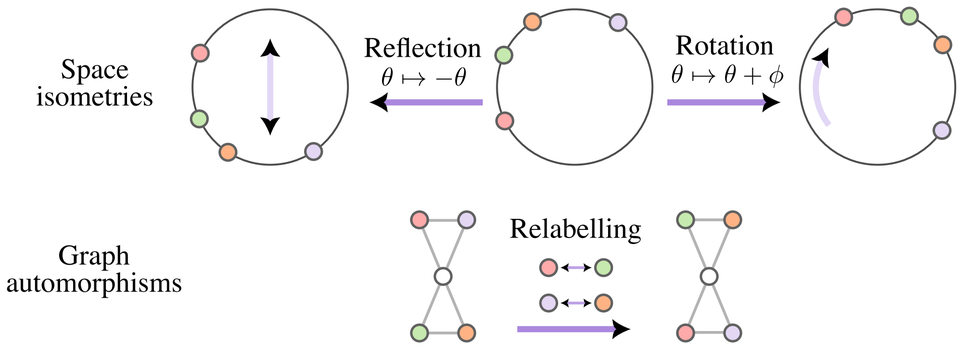
The $\mathbb{S}^1$ model is non-identifiable because of graph and space symmetries.



Embeddings require a post-processing alignment.

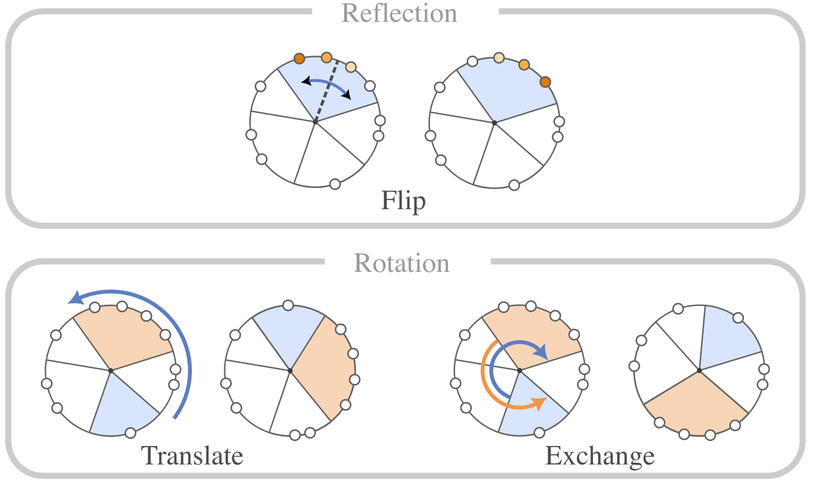
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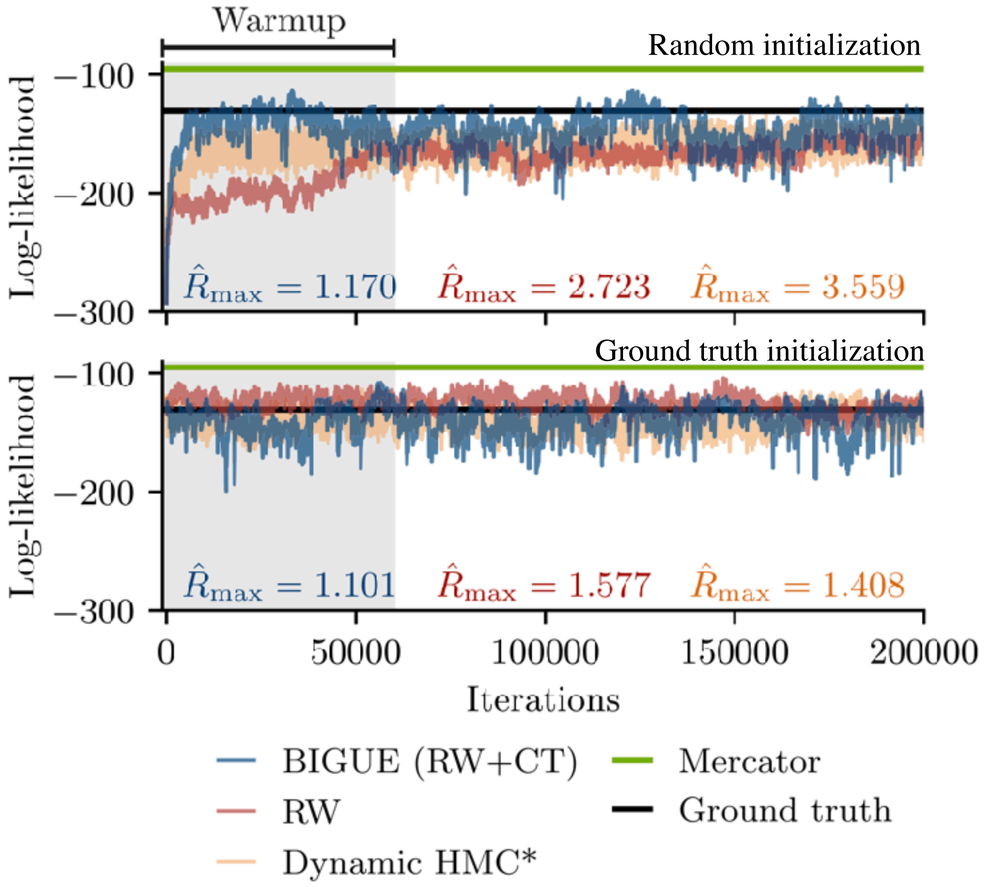


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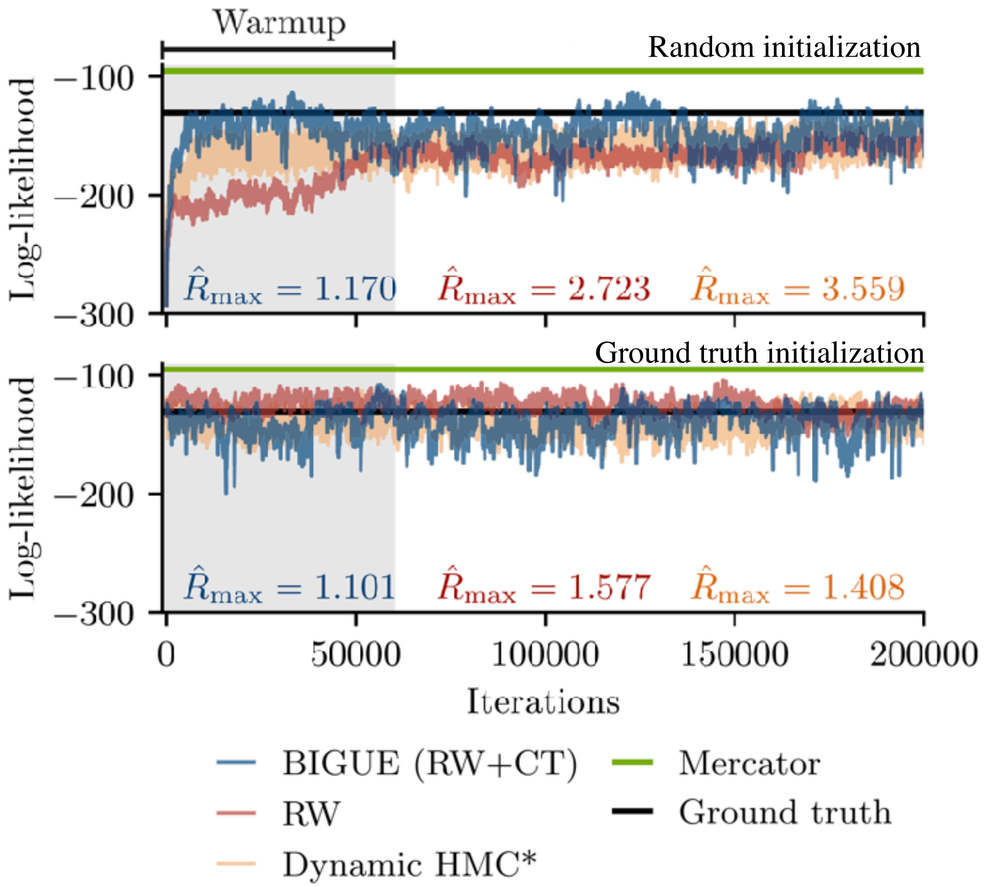
Weakly connected clusters are almost independent. They can be moved in bulk to boost space exploration, without significantly affecting the likelihood.

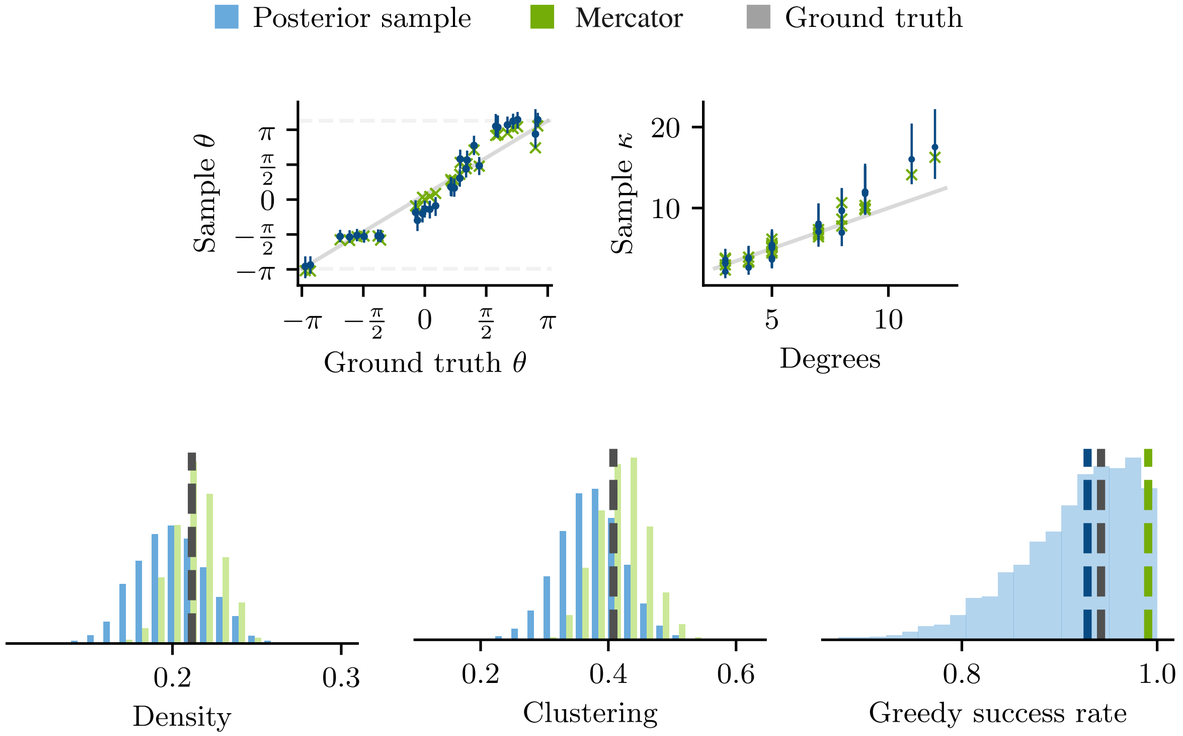


A better suited sampling method

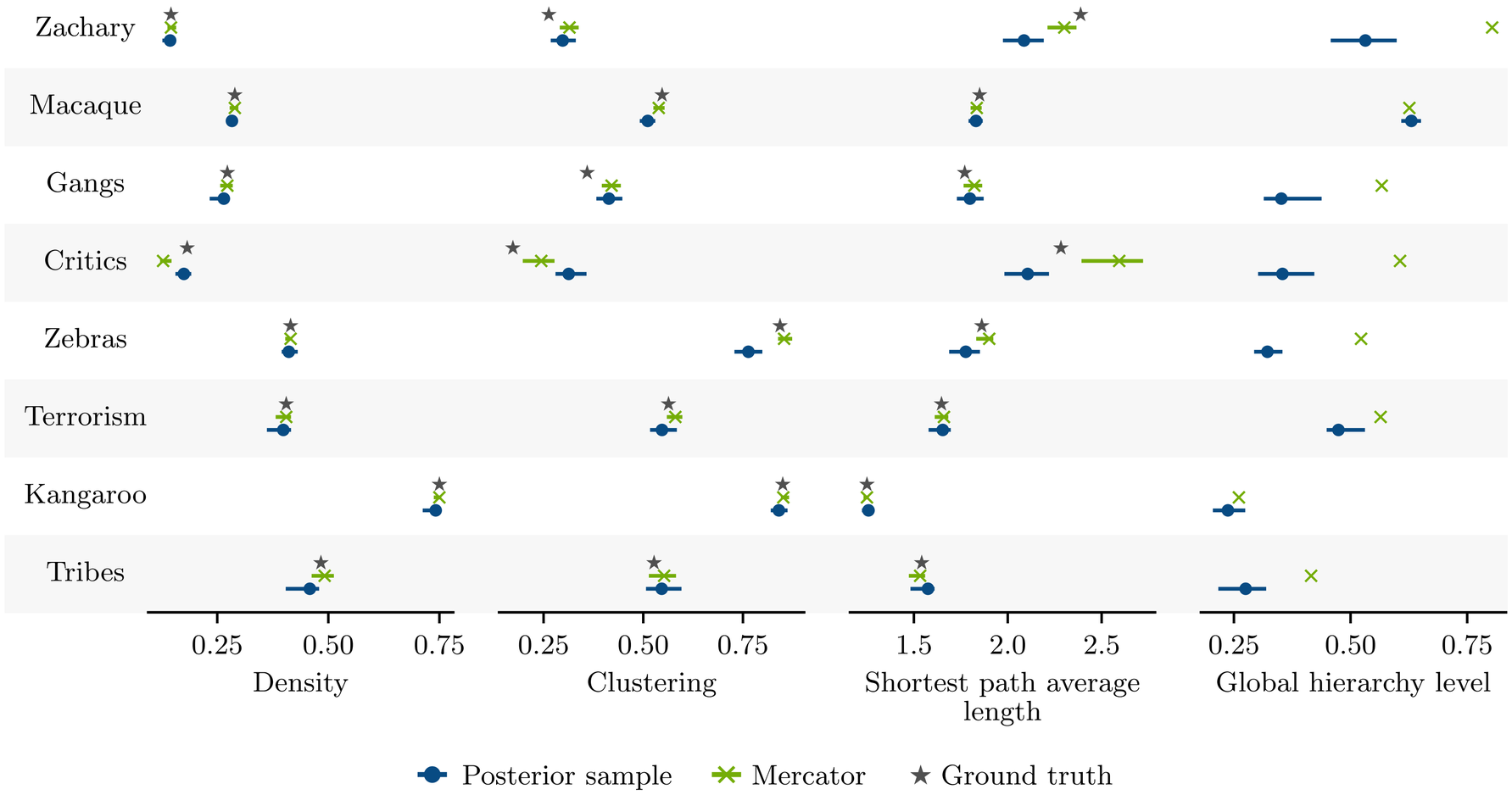


A better suited sampling method





Difference with pointwise embeddings



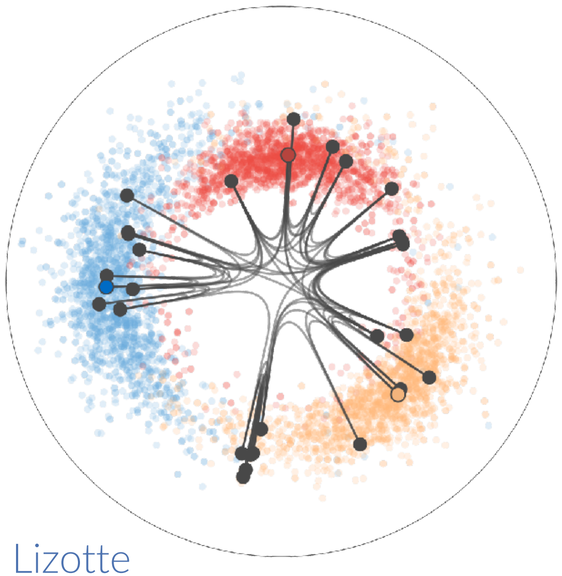
Main takeaways

- Symmetries of the embedding space can be leveraged to design efficient embedding algorithms.
- Around the most likely coordinates, there is a cloud of plausible alternatives (the typical set) whose properties may be quite different from that of pointwise embeddings.

Symmetry-driven embedding of networks in hyperbolic space

Simon Lizotte, Jean-Gabriel Young & Antoine Allard

Communications Physics **8**, Article number: 199 (2025)

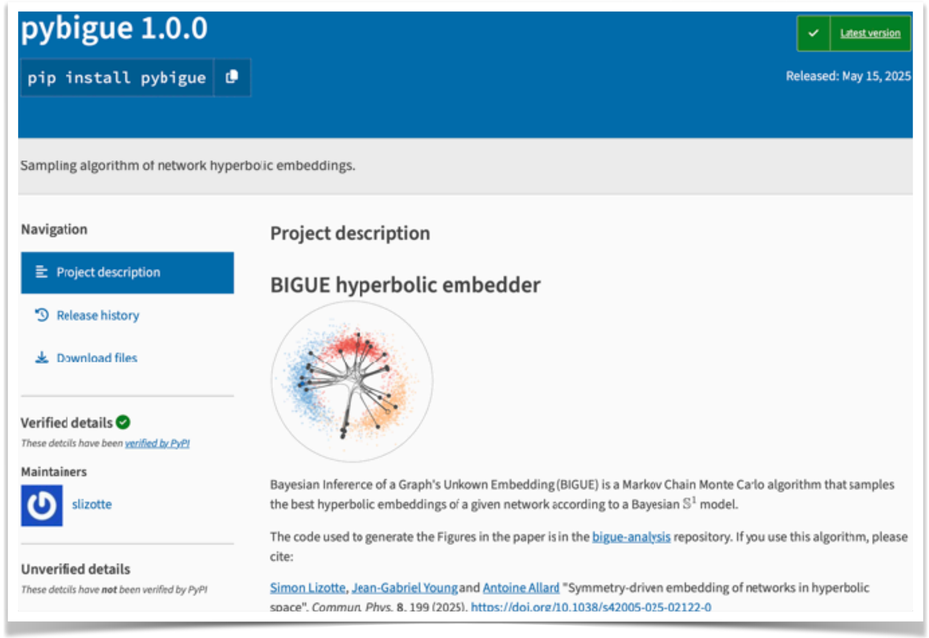




Simon Lizotte
Université Laval

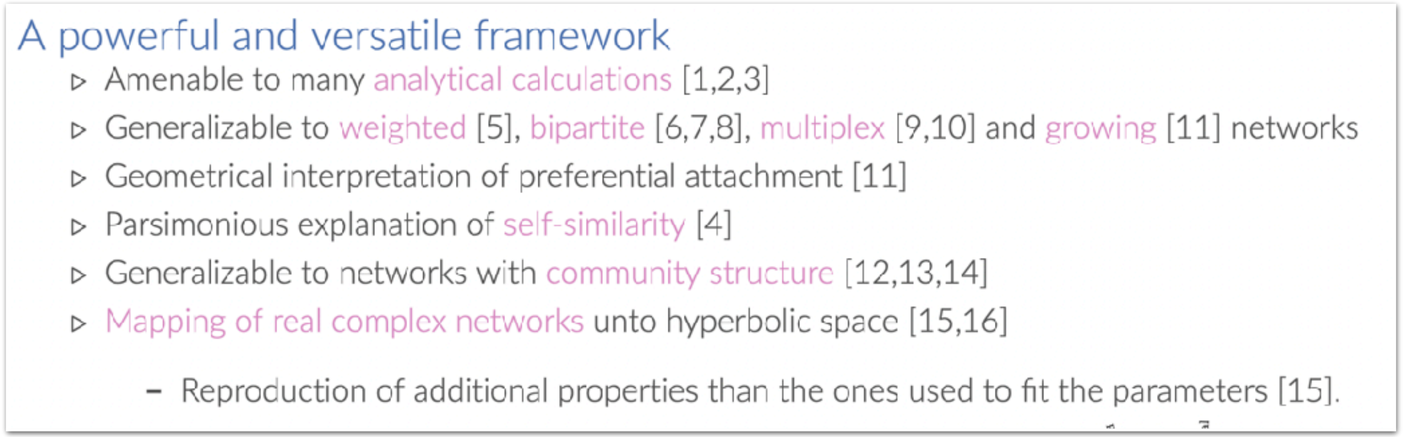
Jean-Gabriel Young
University of Vermont





Outline

1. Introducing network geometry (an incomplete and very biased primer)
2. Leveraging symmetries to go beyond pointwise estimates of coordinates/parameters
3. **Embedding asymmetric (directed) networks unto a metric space (with symmetric distance function)**



Three challenges in modeling directed networks

Properties of any metric space

Identity of indiscernibles	$d(x,y) = 0 \quad \Leftrightarrow \quad x = y$
Non-negativity	$d(x,y) \geq 0$
Symmetry	$d(x,y) = d(y,x)$
Triangle inequality	$d(x,y) \leq d(x,z) + d(z,y)$

with community structure[29,32,115]. The model has yet to be extended to directed networks, because it is not clear how to reconcile the intrinsic symmetry of metric distances with asymmetric interactions among nodes.

Nat. Rev. Phys. 3, 114 (2021)

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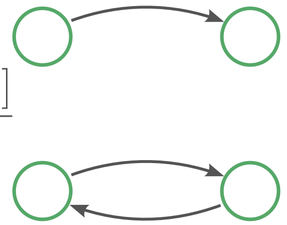
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Reciprocity : cycles of length 2

$$r = \frac{L^{\leftrightarrow}}{L} = \frac{\text{[number of reciprocal links]}}{\text{[number of links]}}$$



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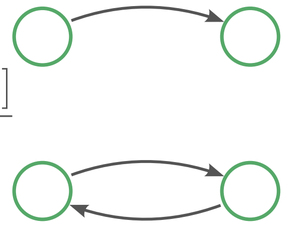
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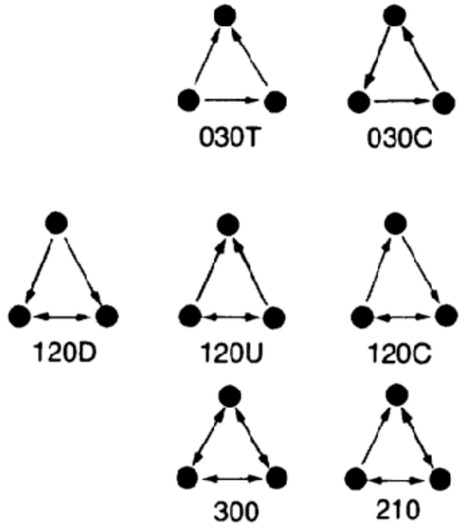
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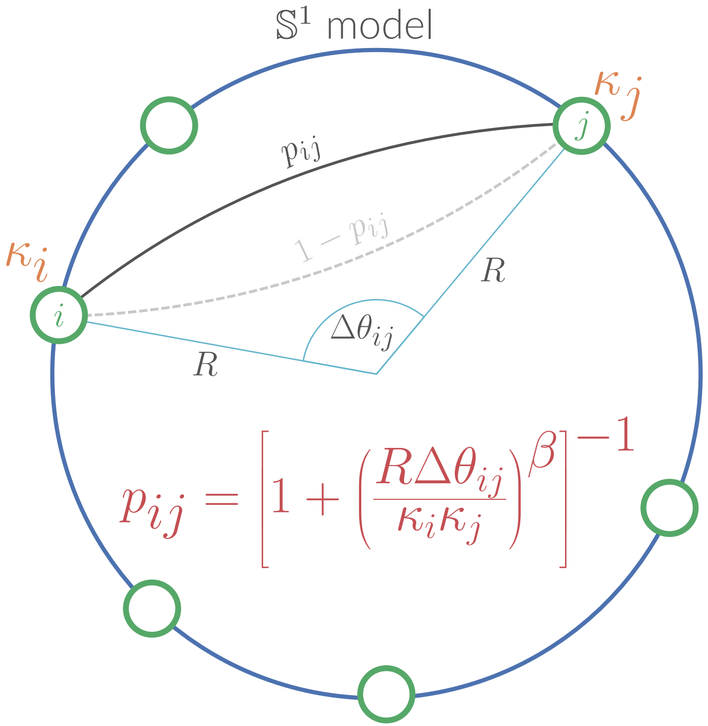


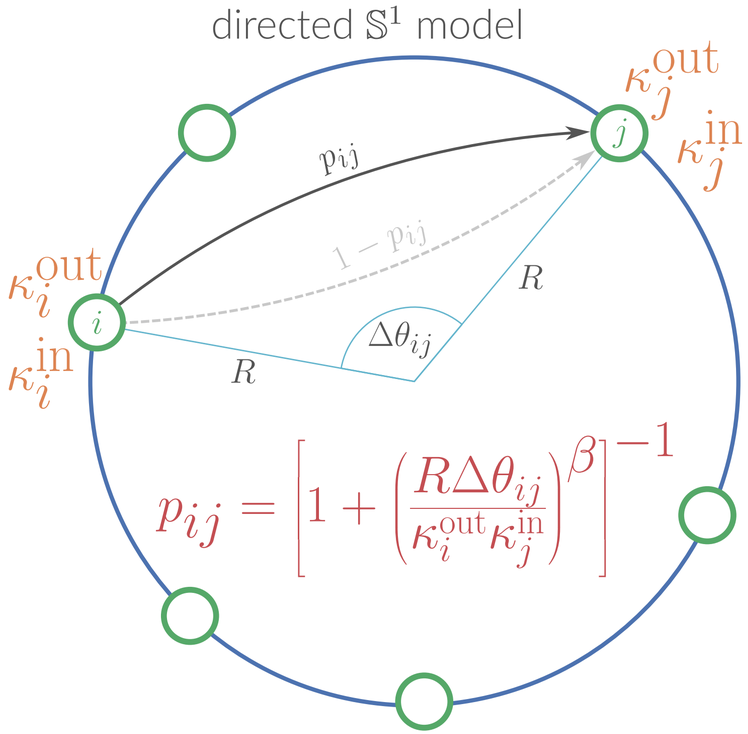
Clustering : 7 cycles of length 3



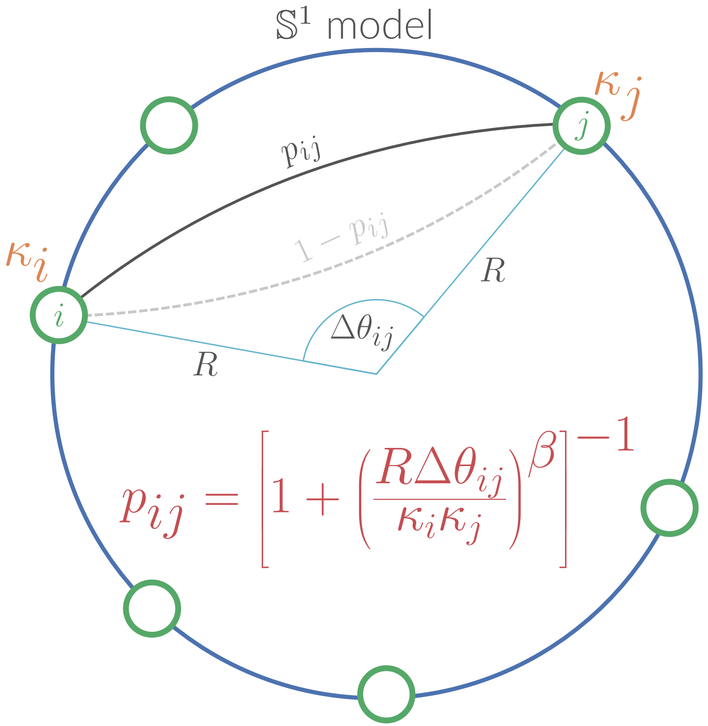
Adapted from Holland & Leinhardt. Local Structure in Social Networks. Sociol. Methodol., 7, 1–45 (1976)

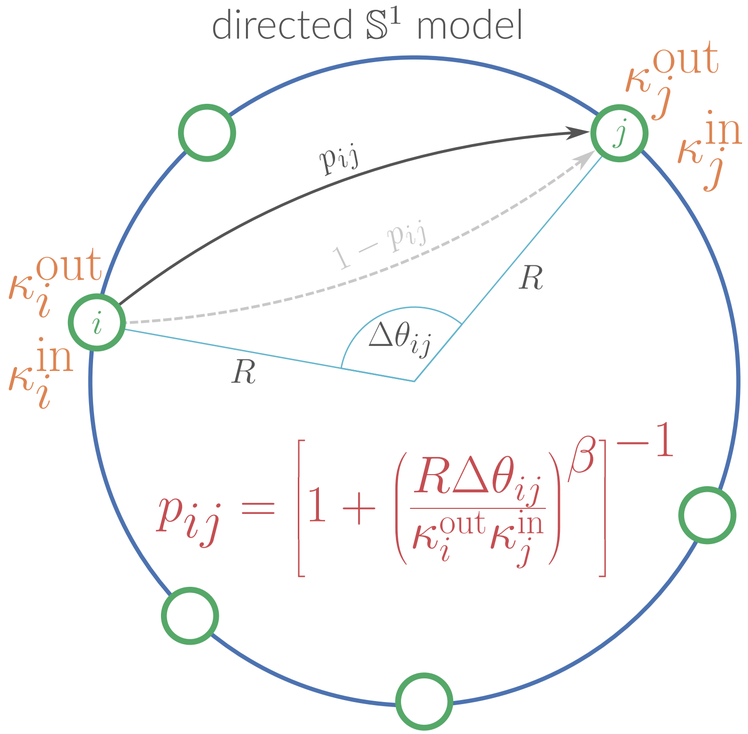
The directed $\mathbb{S}^1$ model: A straightforward generalization



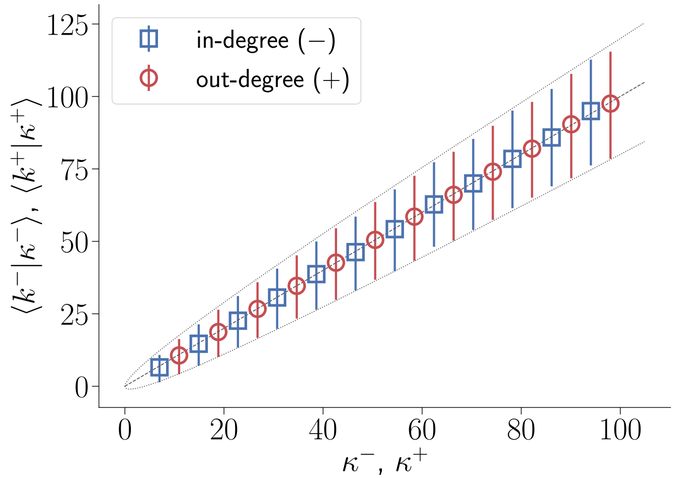


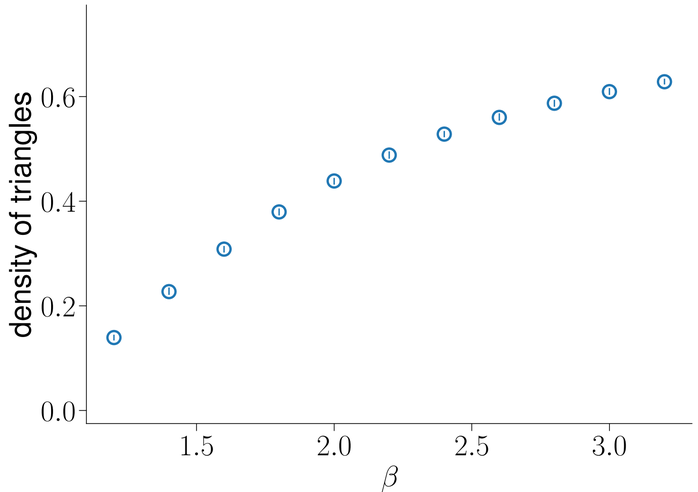
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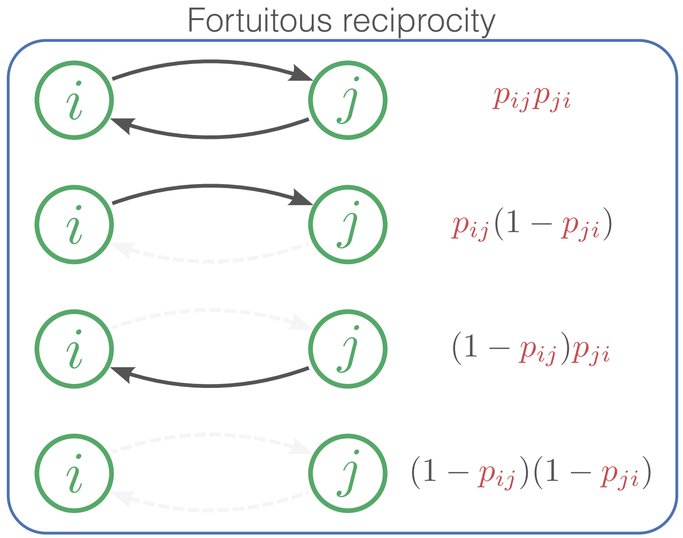
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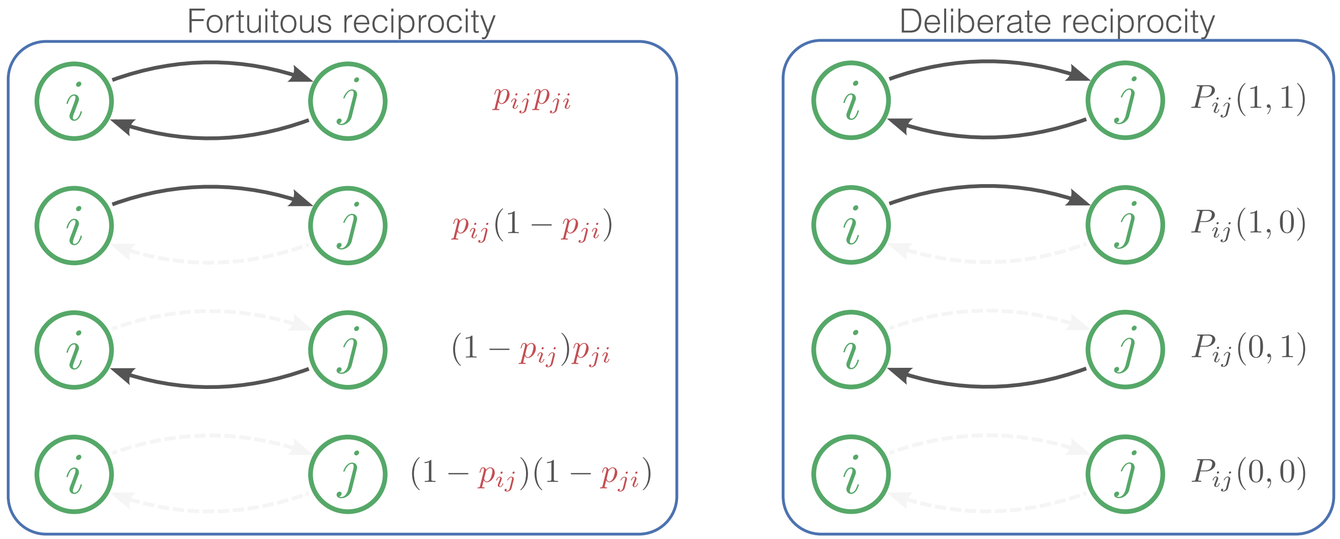
The directed-reciprocal $\mathbb{S}^1$ model: A new link between connections and distances

A random network model defines the probability p_{ij} for a directed link to exist from node i to node j.



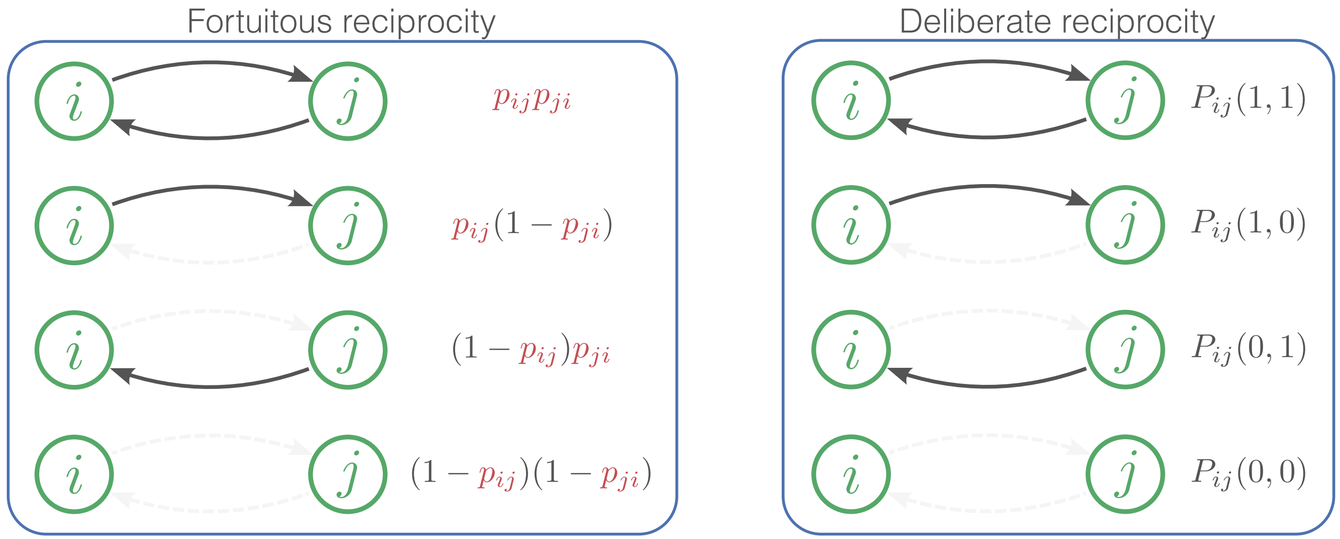
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Level of reciprocity controlled with parameter $-1 \leq \nu \leq 1$

$$P_{ij}(1,1) = \begin{cases} (1-\nu)p_{ij}p_{ji} + \nu \min\{p_{ij}, p_{ji}\} & 0 \leq \nu \leq 1 \\ (1+\nu)p_{ij}p_{ji} + \nu(1-p_{ij}-p_{ji})H(p_{ij}+p_{ji}-1) & -1 \leq \nu \leq 0 \end{cases}$$

$\nu = 1$: maximal reciprocity

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Condition 1: Preserves marginal probabilities

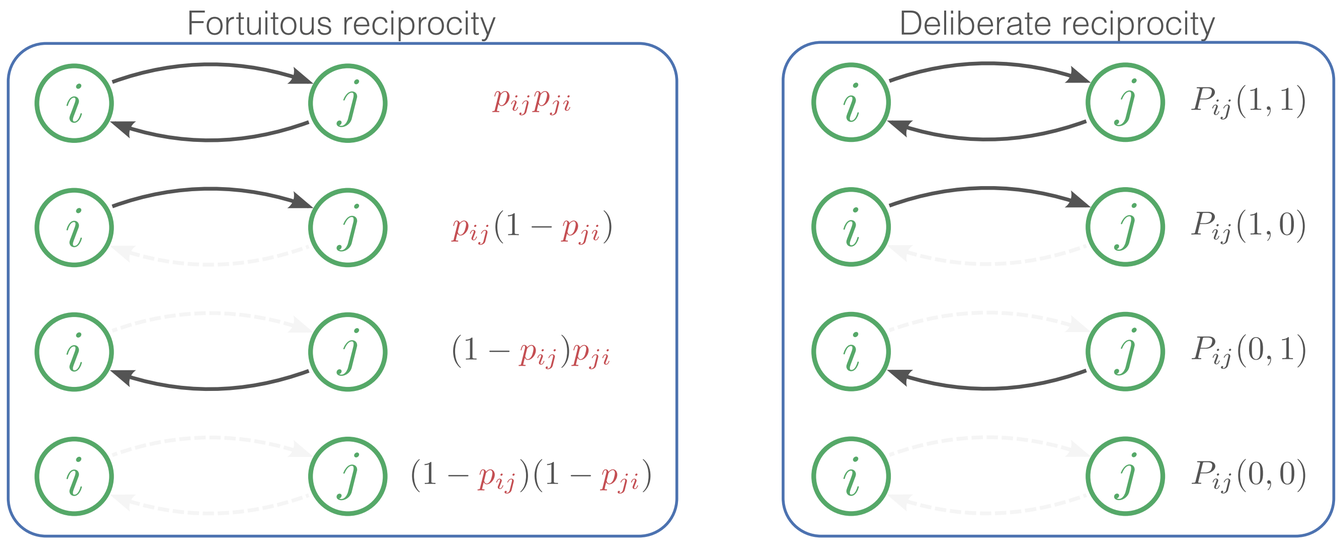
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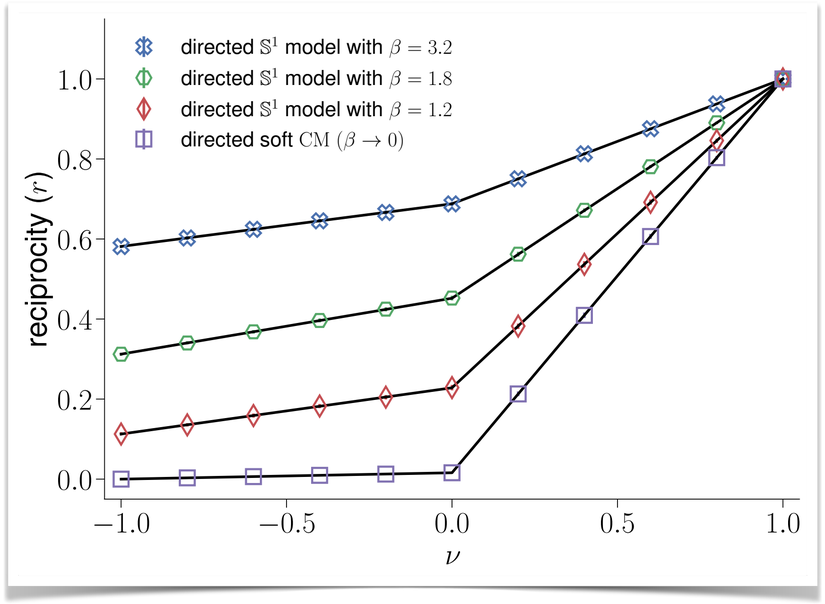
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$$\sum_{a_{ij}=0}^{1} \sum_{a_{ji}=0}^{1} P_{ij}(a_{ij}, a_{ji}) = 1$$

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$$\sum_{a_{ij}=0}^{1} \sum_{a_{ji}=0}^{1} P_{ij}(a_{ij}, a_{ji}) = 1$$

Fitting the directed-reciprocal $\mathbb{S}^1$ model to real networks

The likelihood of a network in the directed-reciprocal S^1 model is

$$\mathbb{P}\Big(\overbrace{\mathbb{A}}^{\text{adj. mat.}} \;\Big|\; \underbrace{\{\kappa_i^{\text{in}}\}, \{\kappa_i^{\text{out}}\}, \{\theta_i\}}_{\text{coordinates}}, \overbrace{\beta, \nu}^{\text{param.}} \Big) = \underbrace{\prod_{i=1}^{N} \prod_{j=i+1}^{N} P_{ij}(a_{ij}, a_{ji})}_{\text{likelihood}}$$

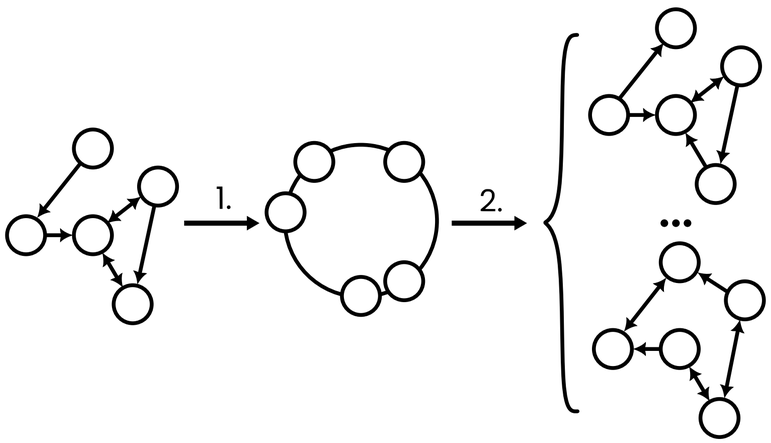
which we maximize using a combination of analytical results and numerical heuristics.

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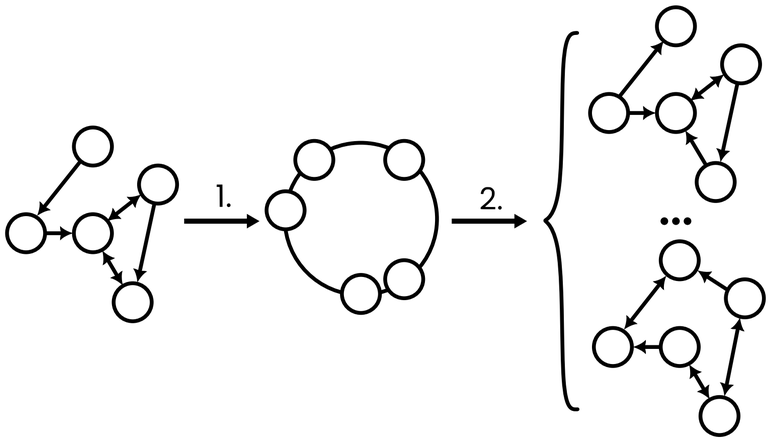


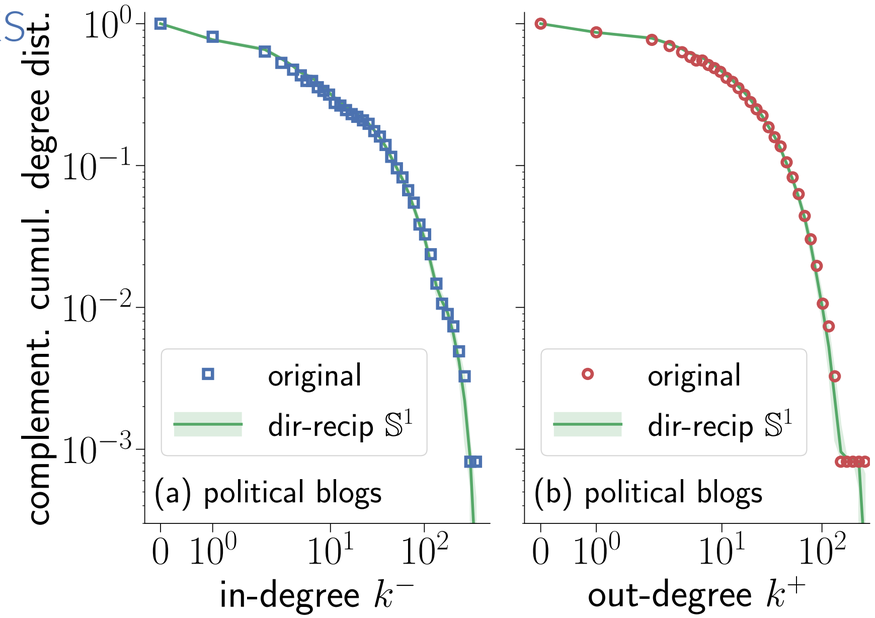
Fitting the directed-reciprocal $\mathbb{S}^1$ model to real networks

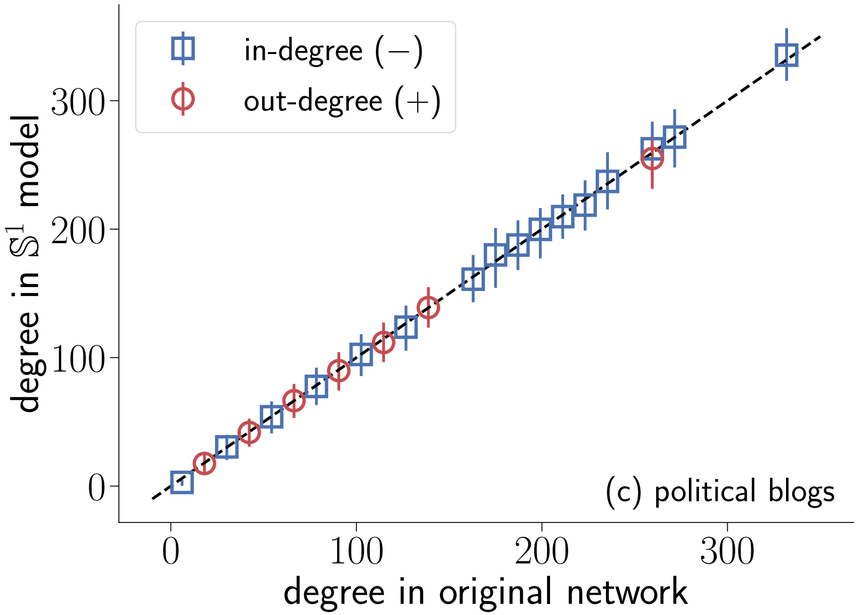
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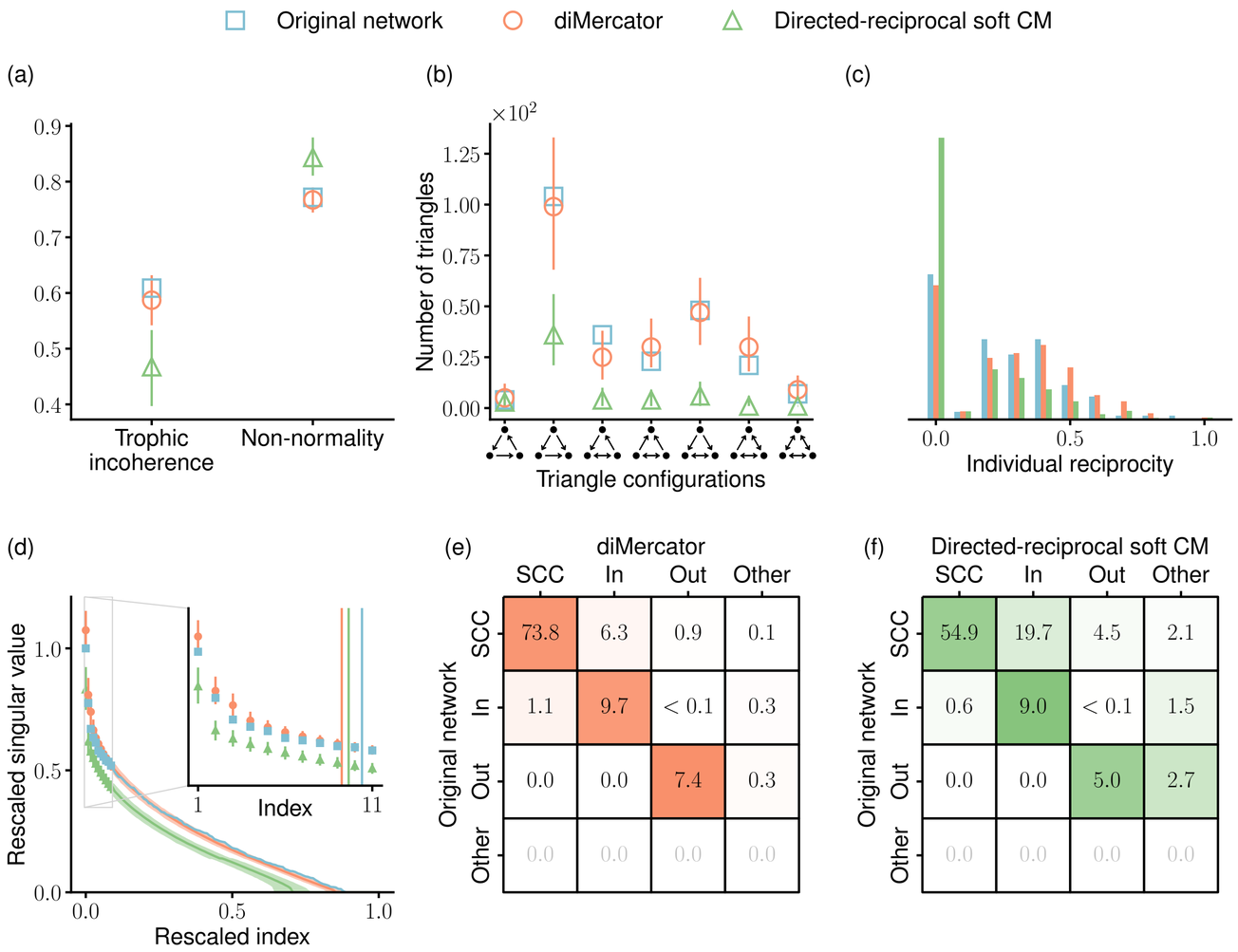
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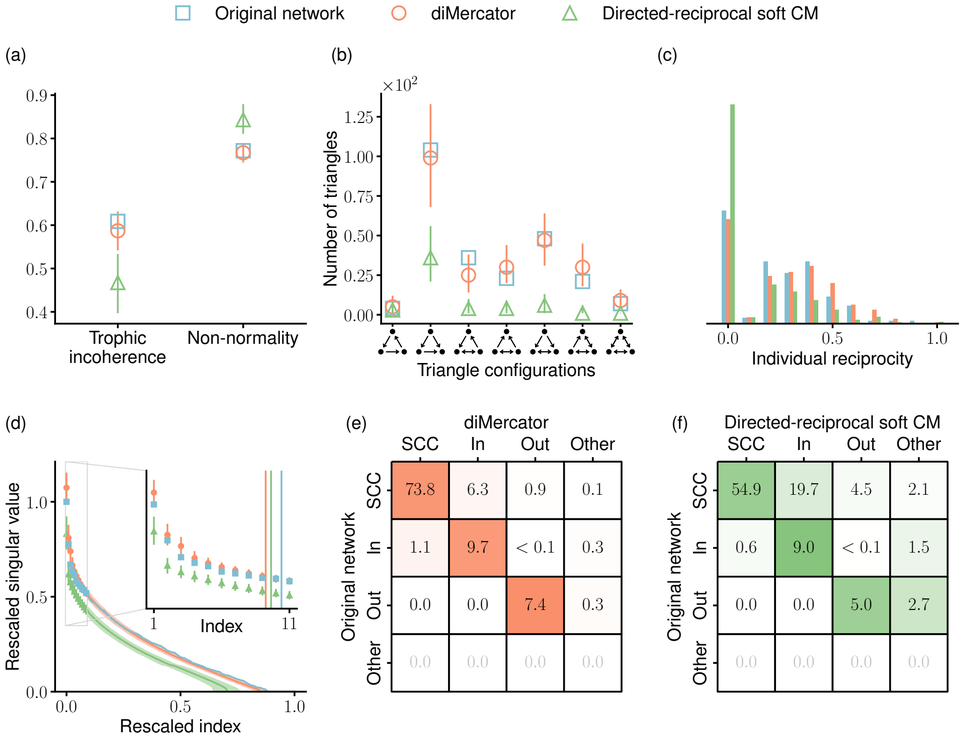




Fitting the directed-reciprocal $\mathbb{S}^1$ model to real networks



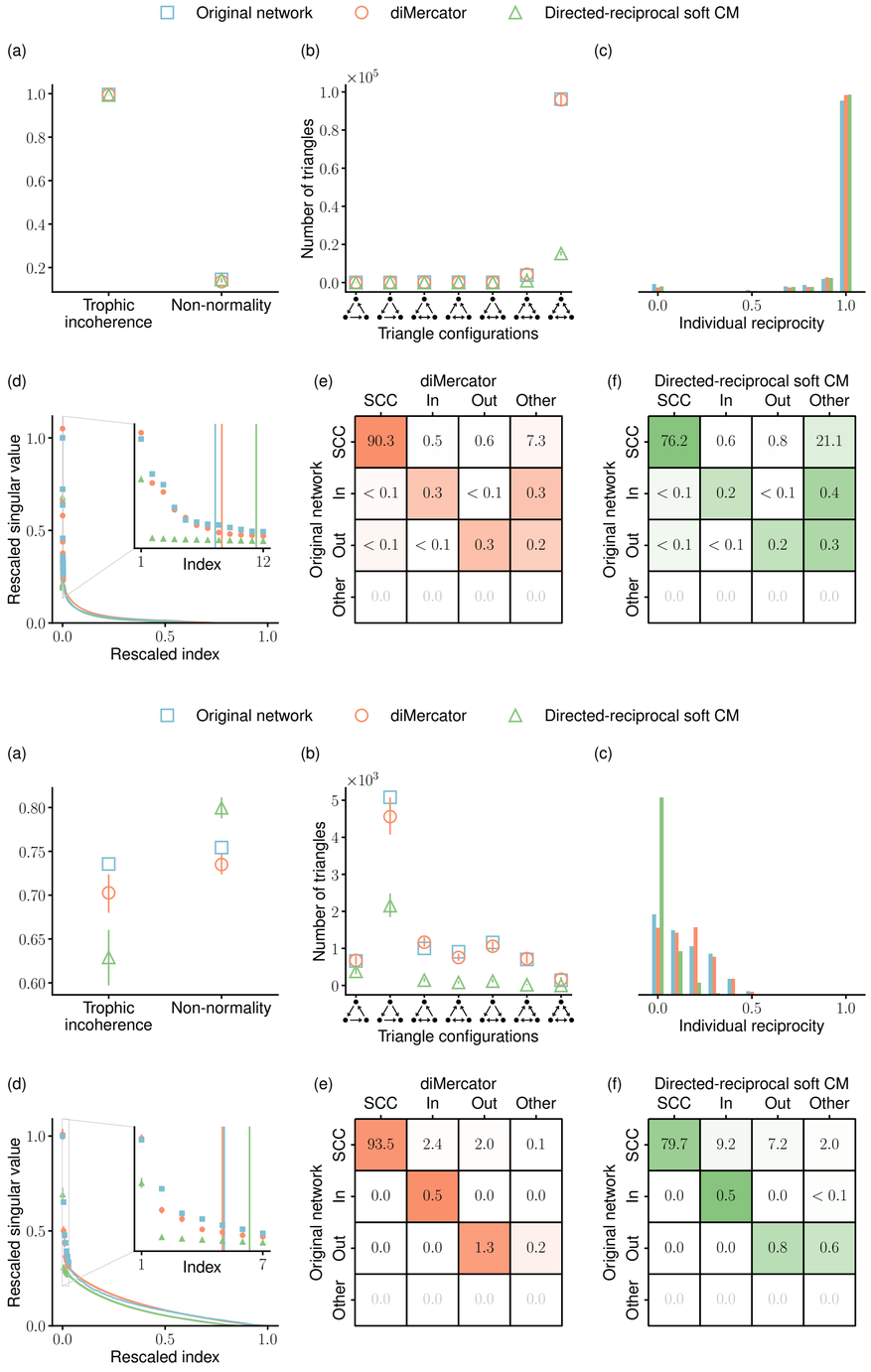
Fitting the directed-reciprocal $\mathbb{S}^1$ model to real networks



Fixing the degree sequence (on average), the global density of triangles and global reciprocity strongly constrains

- the non-normality [1]
- the trophic coherence [2]
- the clustering patterns
- the individual reciprocities
- the singular values
- the bow-tie organization

[1] Sci. Adv. 4, eaau9403 (2018)
[2] PNAS 111, 17923 (2014)



Main takeaways

- ▷ Rethinking the link between connections and distances allows the extension of the network geometry framework to directed networks.
- ▷ Assuming an underlying geometry is a simple modeling approach that can reproduce several complex topological properties observed in real networks.

Geometric description of clustering in directed networks

Antoine Allard ✉, M. Ángeles Serrano & Marián Boguñá

Nature Physics **20**, 150–156 (2024)



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Local topological patterns and geometry parsimoniously explains the mesoscale organization of empirical complex networks

Jérémi Lesage,[1,2] M. Ángeles Serrano,[3,4,5] Marián Boguñá,[3,4] and Antoine Allard[1,2]

Preprint on arXiv and code in GitHub are expected this summer.

Main takeaways

- Symmetries of the embedding space can be leveraged to design efficient embedding algorithms.
- Around the most likely coordinates, there is a cloud of plausible alternatives (the typical set) whose properties may be quite different from that of pointwise embeddings.
- Rethinking the link between connections and distances allows the extension of the network geometry framework to directed networks.
- Assuming an underlying geometry is a simple modeling approach that can reproduce several complex topological properties observed in real networks.

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The path of complexity

Laurent Hébert-Dufresne ✉, Antoine Allard, Joshua Garland, Elizabeth A. Hobson & Luis Zaman

npj Complexity **1**, Article number: 4 (2024)

npj | complexity

Aims & Scopes

npj Complexity considers research that explores all aspects of complex systems at the interface of multiple fields.

The journal covers a broad range of topics including but not limited to:

- Network science, including the analysis of complex networks such as social networks, biological networks, infrastructure and information networks
- Emergent phenomena, self-organization, and scaling in complex systems
- Nonlinear dynamics, chaos theory, and dynamical systems theory
- Agent-based modeling and simulation techniques for studying complex systems
- Complex adaptive systems, such as adaptive behavior in biological, ecological, and social systems
- Multi-scale analysis techniques across different levels of organization, from micro to macro scales
- Robustness and resilience of complex systems
- Evolutionary dynamics and game theory
- Digital humanities, dynamics of information, and science of science
- Information processing and computation in complex systems and artificial intelligence
- Interdisciplinary approaches to complex problems such as epidemics, climate change, misinformation, governance, and sustainability


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