Rethinking interactions among the constituents of complex systems

THE CASE FOR LATENT HYPERBOLIC GEOMETRY

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Outline

1. Why models and the challenge of clustering
2. A geometric approach to clustering
3. Euclid and hyperbolic geometry
4. A hyperbolic solution to clustering
5. Rethinking interactions: the case of directed graphs
6. Rethinking interactions: the case of modular structure

Network models

Why ?

- Mathematical representation → analytical results and predictions.
- Identify the mechanisms behind a set of topological properties.
- Disentangle the effect of various topological properties (e.g. assortative mixing vs. clustering on the percolation threshold [1]).
- Identify significant patterns of connection in real networks (i.e. null models).
- Perform in silico controlled experiments (e.g. simulation of epidemic spreading).
- ...

[1] Phys. Rev. E 80, 020901 (2009)
[2] SIAM Rev. 60, 315 (2018)
[3] Phys. Rev. Lett. 89, 208701 (2002)
[4] Phys. Rev. X 9, 011023 (2019)
[5] Soc. Networks 5, 109 (1983)
[6] Appl. Netw. Sci. 4, 122 (2019)
[7] Nature 393, 440 (1998)
[8] SIAM Rev. 45, 167 (2003)

Network models

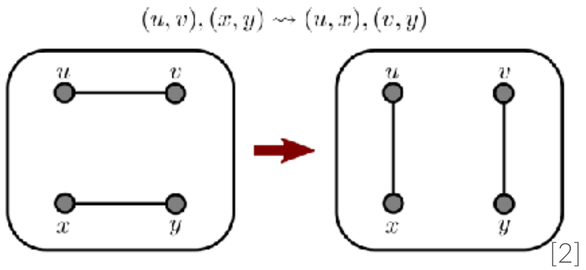
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Some examples of equilibrium (fixed size) network models

Configuration model (and variations)

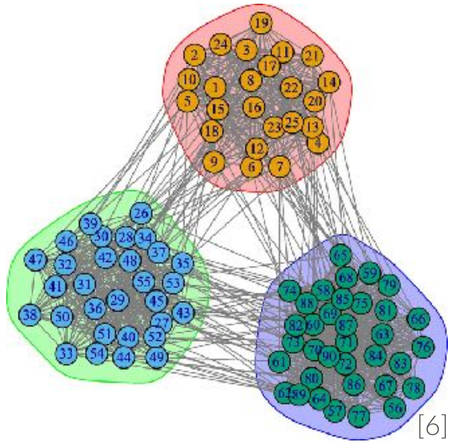
- ▷ degree sequence/distribution [2]
- ▷ degree-degree correlations [3]
- ▷ k-core/onion decomposition [4]



[2]

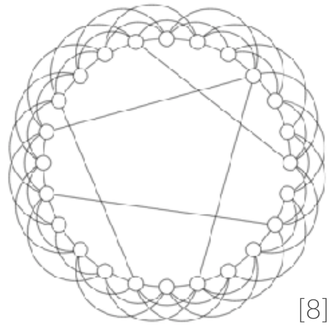
Stochastic block models

- ▷ community structure/detection [5]


[6]

Watts-Strogatz model

- ▷ small-world effect [7]


[8]

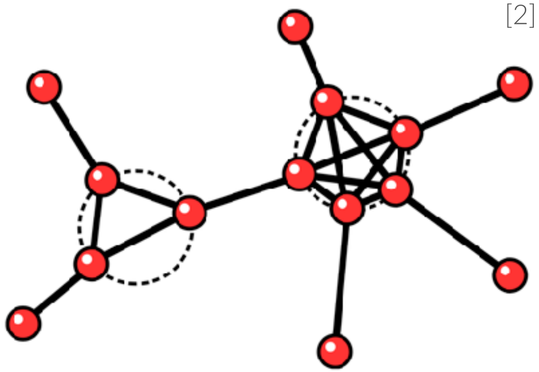
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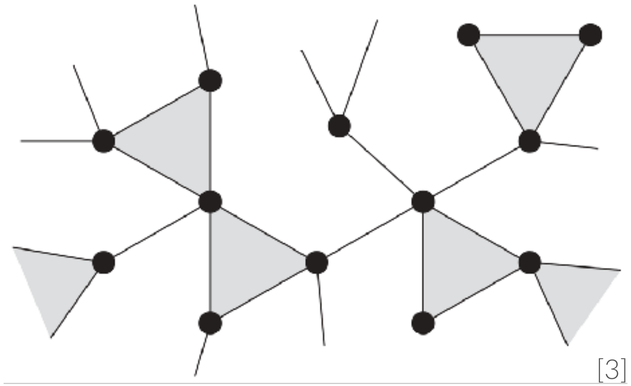
Modeling clustering

Trickier because clustering consists in three-node interactions while our mathematical tools rely on pairwise interactions either explicitly or implicitly.

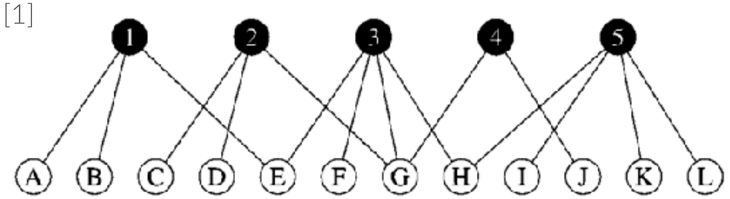
Most models therefore assume

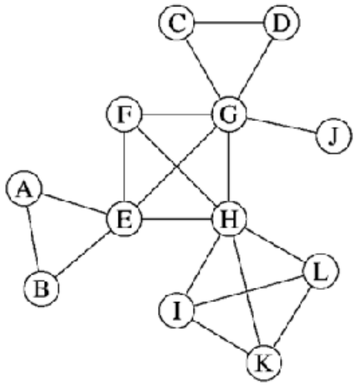
- an underlying tree-like structure
- that the networks are dense

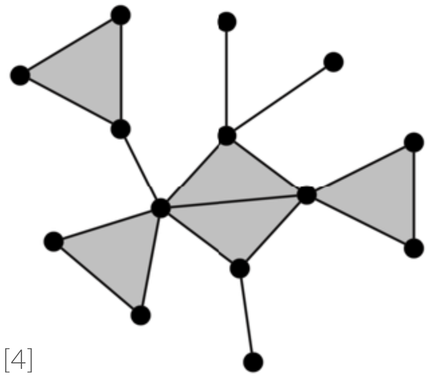

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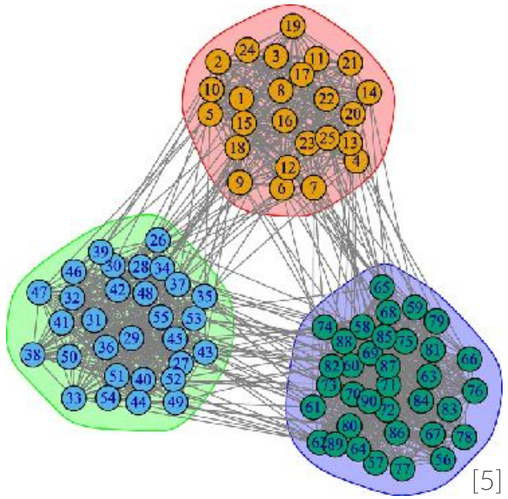

[3]

[1]






[4]


[5]

[1] Phys. Rev. E 68, 026121 (2003)
[2] Phys. Rev. E 80, 036107 (2009)
[3] Phys. Rev. Lett. 103, 058701 (2009)
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A geometric approach to clustering

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

For further info, see Phys. Rep. 499, 1–101 (2011)

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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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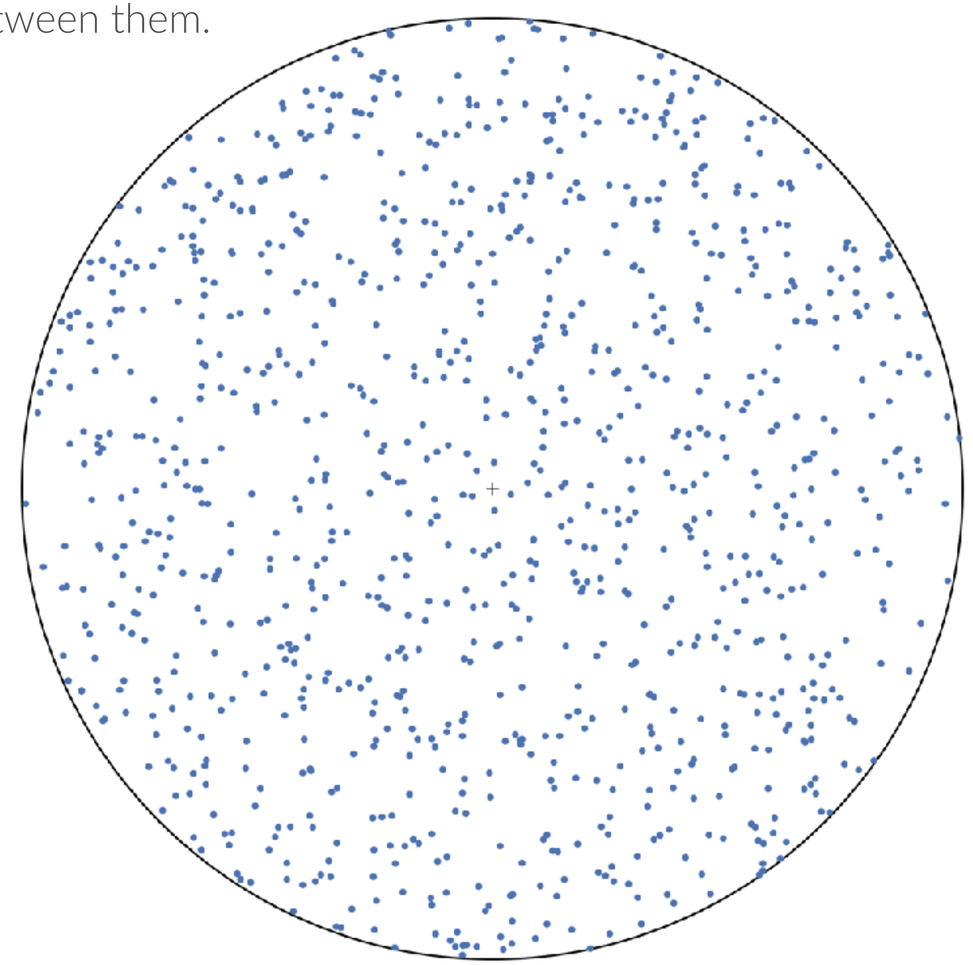
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Simple random geometric graph

1. Sprinkle N nodes uniformly on a disk of radius R.
2. Connect any nodes separated by a distance less than r.

✓ high clustering

✗ binomial/Poisson degree distribution



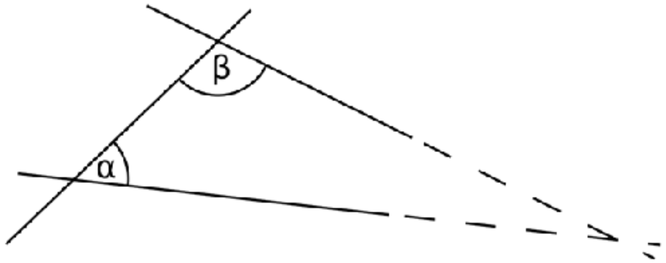
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Euclid’s postulates

1. A straight line segment can be drawn joining any two points.
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3. Given any straight line segment, a circle can be drawn having the segment as radius and one endpoint as center.
4. All right angles are congruent.

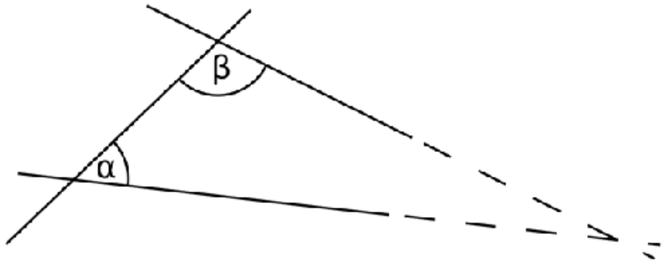
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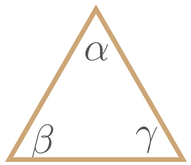


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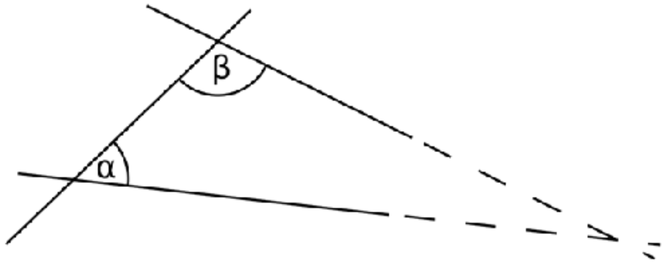
Trying to get rid of the fifth postulate motivated the discovery of non-Euclidean geometries.



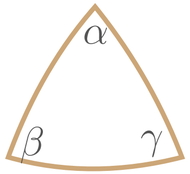
Euclidean geometry
no curvature
$\alpha + \beta + \gamma = \pi$

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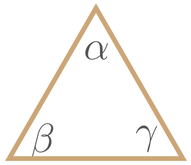
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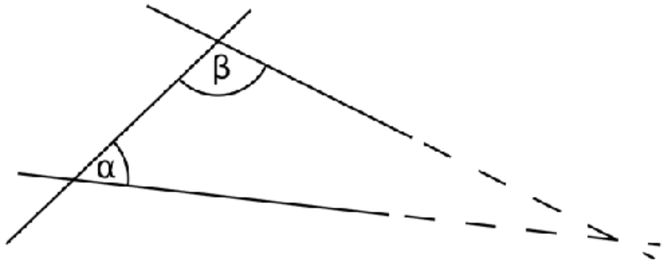
spherical geometry
positive curvature
$\alpha + \beta + \gamma > \pi$



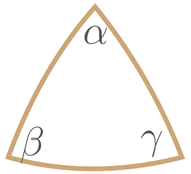
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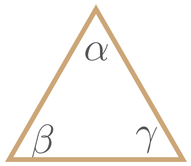
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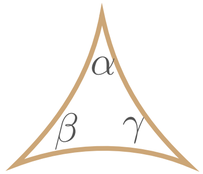
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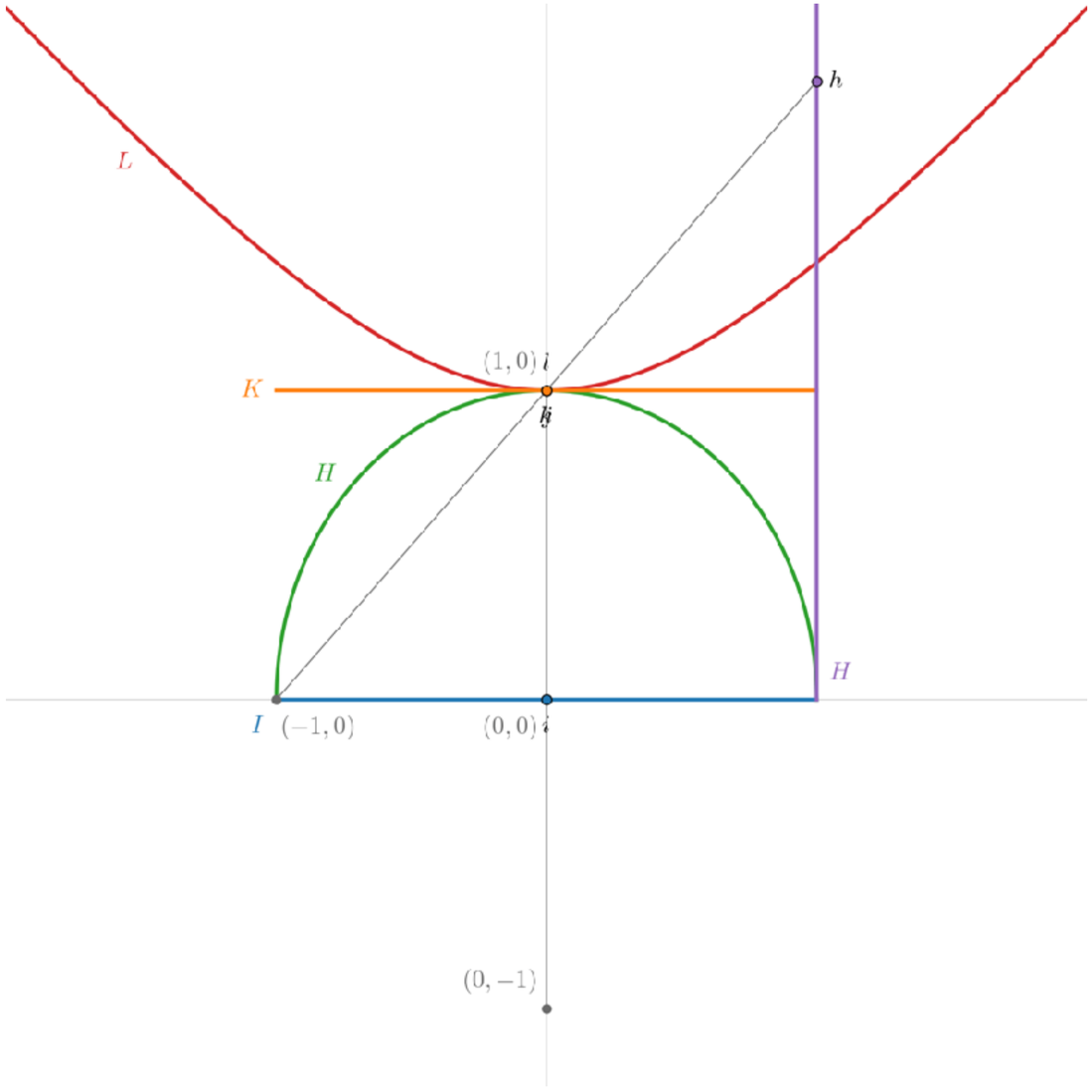


hyperbolic geometry
negative curvature
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Hyperbolic geometry

- There are 5 models of hyperbolic geometry in $\mathbb{R}^{D,1}$:
  - H: the half-space model;
  - I: the interior of the disk model;
  - J: the hemisphere model;
  - K: the Klein model;
  - L: the hyperboloid model.
- They are isometrically equivalent.
- They have their own metric, geodesics, isometries, and so on.
- Each model supplies its own natural intuitions.

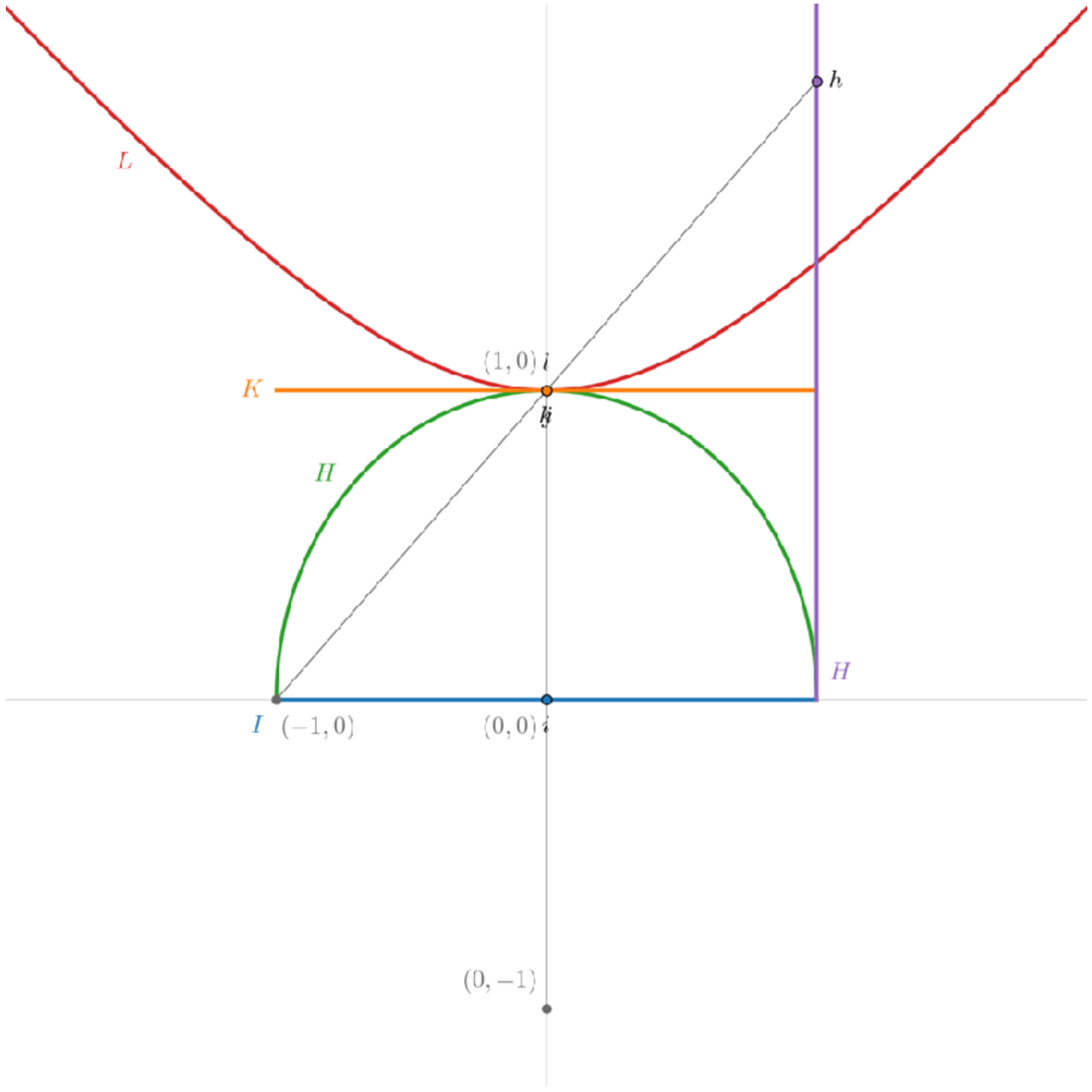
The five analytic models and their connecting isometries in $D = 1$.



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Hyperbolic geometry

- Space of constant negative curvature (as opposed to flat or Euclidean space, or spherical space)
- Model for the $D = 2$ hyperbolic space : positive sheet of the hyperboloid defined by

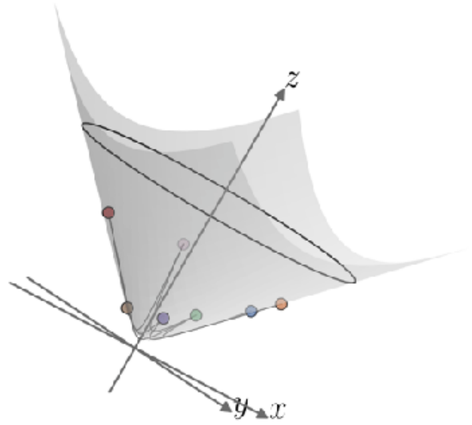
$$x^2 + y^2 - z^2 = -1$$

- Distance between points (x_1, y_1, z_1) and (x_2, y_2, z_2) is

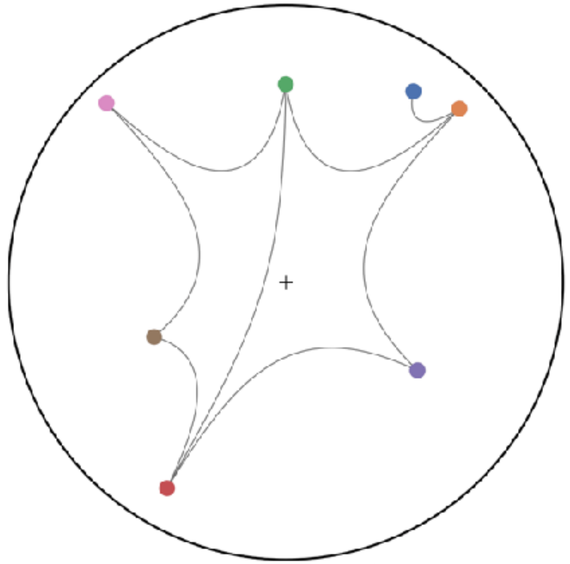
$$d(1,2) = \operatorname{arccosh}\big(z_1 z_2 - x_1 x_2 - y_1 y_2\big)$$

- Polar coordinates

$$\begin{aligned} x &= \sinh(r)\cos(\theta) \\ y &= \sinh(r)\sin(\theta) \\ z &= \cosh(r) \end{aligned}$$



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



hyperbolic disk (r, θ)

For further info, see Flavors of geometry (Cambridge University Press, 1997)
or Foundations of Hyperbolic Manifolds (Springer, 2019)

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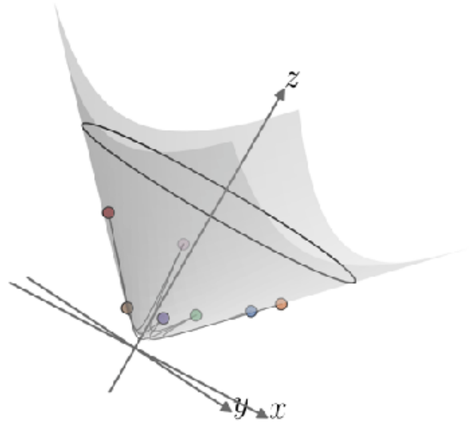
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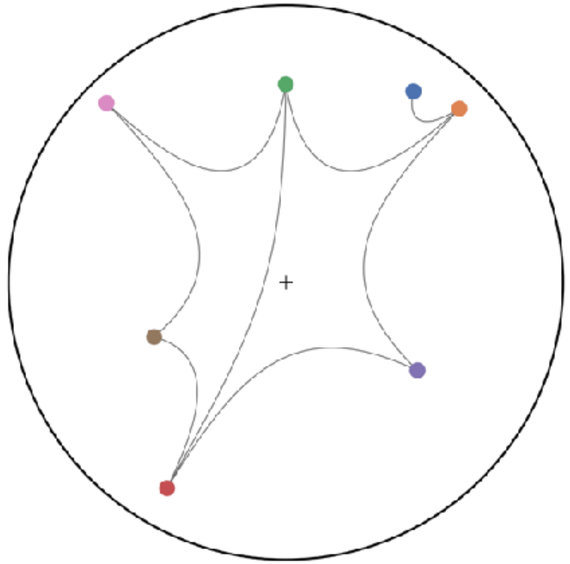
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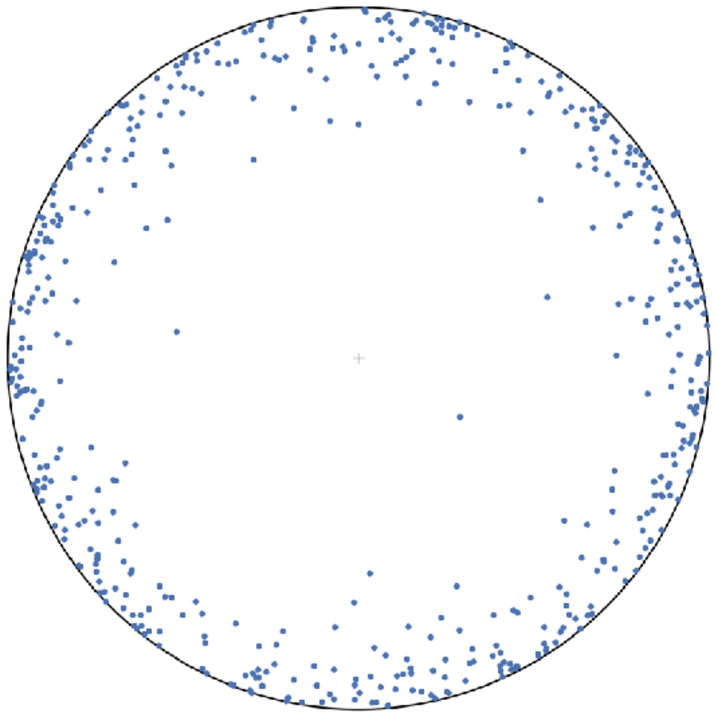
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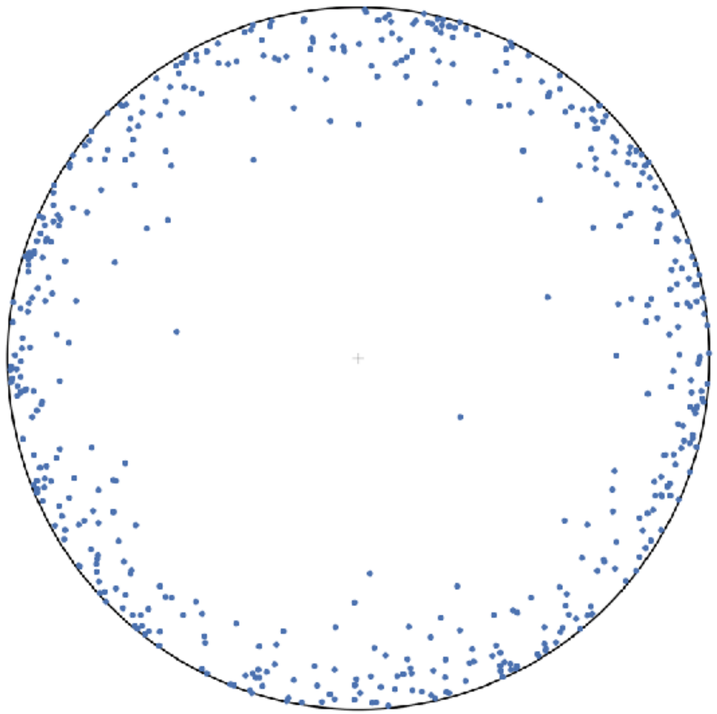
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Hyperbolic geometry

Simple random geometric graph

1. Sprinkle N nodes uniformly on the hyperbolic disk of radius R.
2. Connect any nodes separated by a distance less than $r = R$.





✓ high clustering

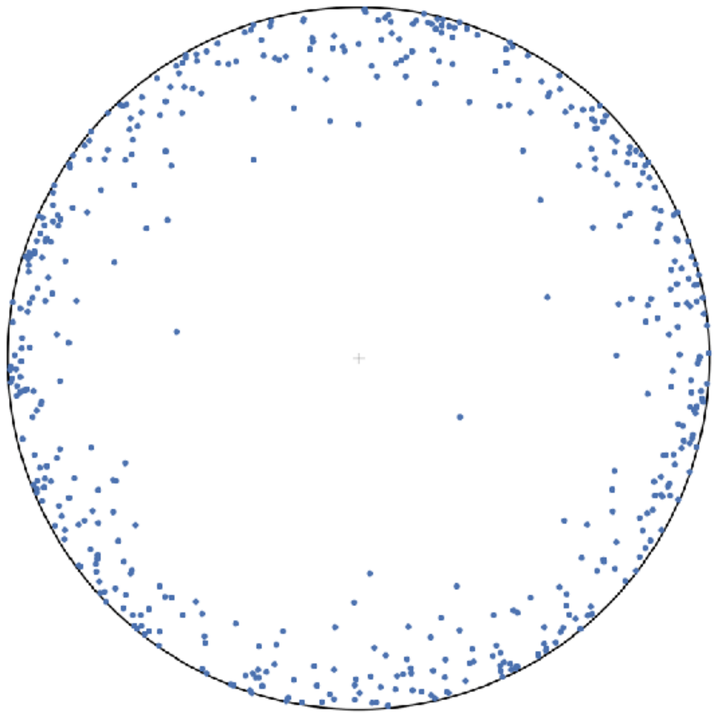
✓ power-law degree distribution with exponent -3

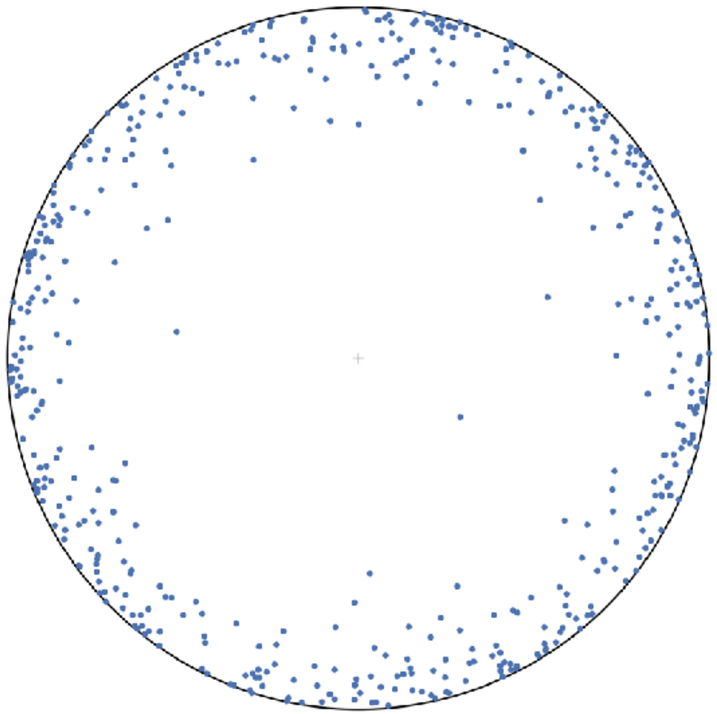
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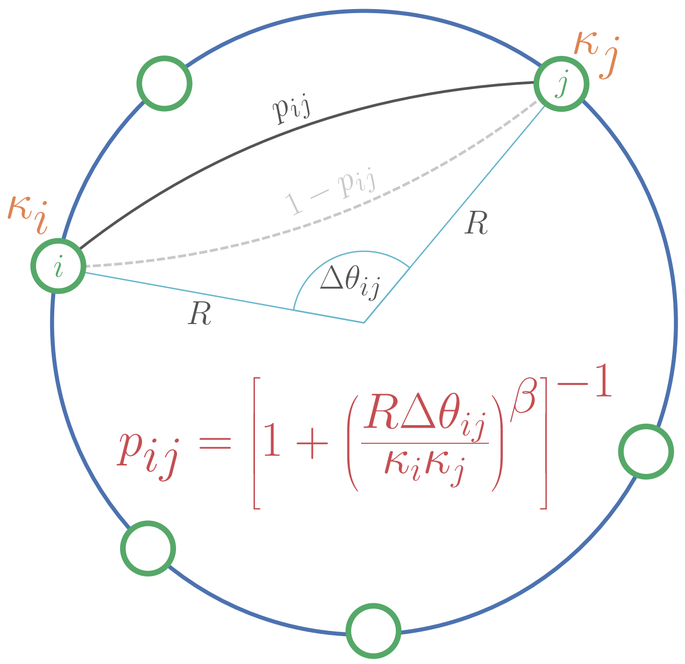


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A geometric approach to clustering : the $\mathbb{S}^1/\mathbb{H}^2$ model



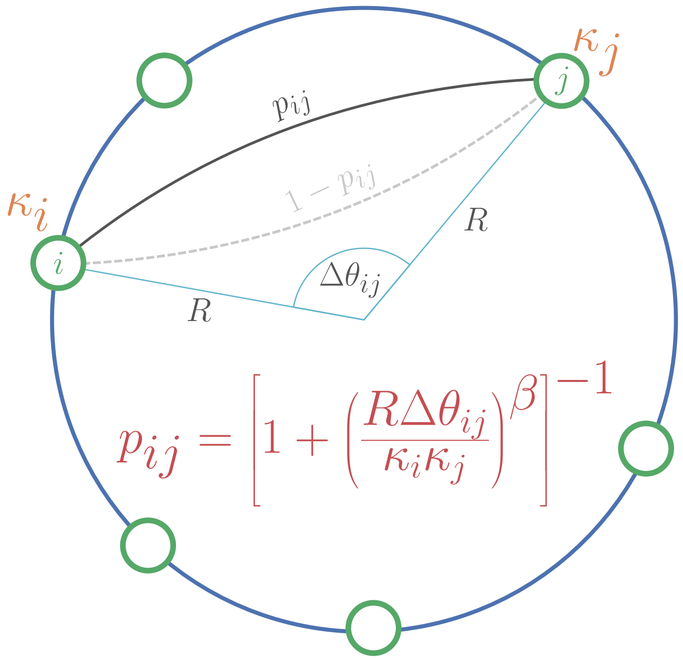
The $\mathbb{S}^1$ model

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

[1] Phys. Rev. E 80, 035101 (2009)
[2] Phys. Rev. E 82, 036106 (2010)
[3] Phys. Rev. Lett. 100, 078701 (2008)
[4] Nat. Rev. Phys. 3, 114 (2021)
[5] Nat. Commun. 8, 14103 (2017)
[6] Phys. Rev. E 84, 026114 (2011)
[7] Phys. Rev. E 95, 032309 (2017)
[8] Mol. Biosyst. 8, 843 (2012)
[9] Nat. Phys. 12, 1076 (2016)
[10] Phys. Rev. Lett. 118, 218301 (2017)
[11] Nature 489, 537 (2012)
[12] Sci. Rep. 5, 9421 (2015)
[13] J. Stat. Phys. 173, 775 (2018)
[14] New J. Phys. 20, 052002 (2018)
[15] New J. Phys. 21, 123033 (2019)
[16] Nat. Commun. 8, 1615 (2017)
[17] Nat. Commun. 1, 62 (2010)
[18] PNAS 117, 20244 (2020)

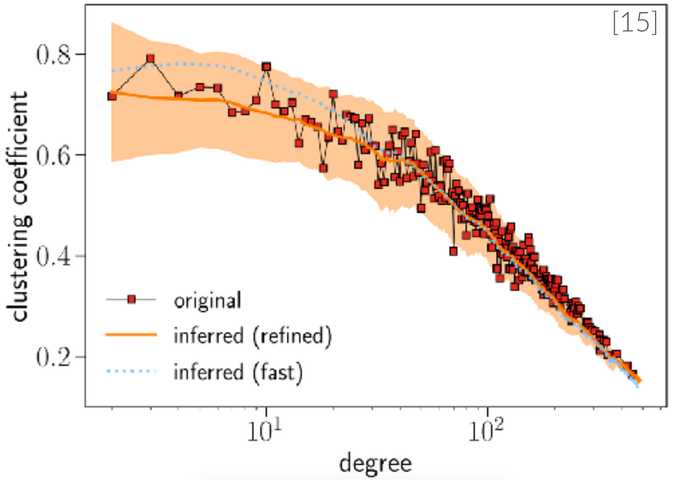
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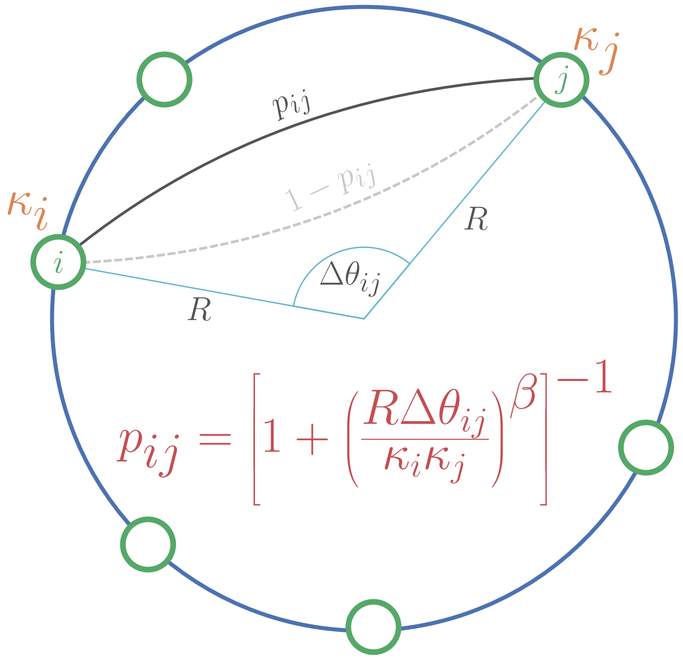
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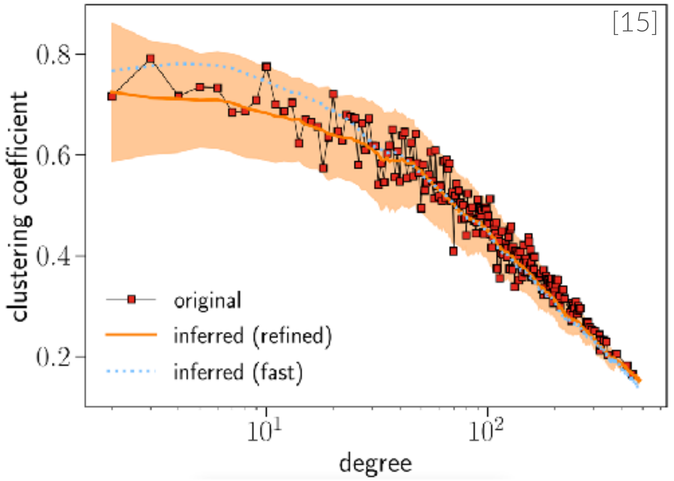
★ fixes the expected degree of nodes (κ) → soft configuration model (CM)
★ triangle inequality of the underlying metric space → triangles from pairwise interactions
★ level of clustering tuned with parameter β



[1] Phys. Rev. E 80, 035101 (2009)
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[3] Phys. Rev. Lett. 100, 078701 (2008)
[4] Nat. Rev. Phys. 3, 114 (2021)
[5] Nat. Commun. 8, 14103 (2017)
[6] Phys. Rev. E 84, 026114 (2011)
[7] Phys. Rev. E 95, 032309 (2017)
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[15] New J. Phys. 21, 123033 (2019)
[16] Nat. Commun. 8, 1615 (2017)
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[18] PNAS 117, 20244 (2020)

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.
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Other properties and generalizations

- ▷ Amenable to many analytical calculations
- ▷ Geometric interpretation in terms of hyperbolic geometry (the $\mathbb{H}^2$ model) [1,2]
- ▷ Parsimonious explanation of self-similarity [3,4]
- ▷ Generalizable to weighted [5], bipartite [6,7,8], multiplex [9,10] and growing [11] networks
- ▷ Generalizable to networks with community structure [12,13,14]
- ▷ Mapping of real complex networks unto hyperbolic space [15,16]
- ▷ Identification of biochemical pathways in E. Coli [8]
- ▷ Efficient Internet routing protocols [17]
- ▷ Multiscale organization of the human connectome [18]
- ▷ Geometrical interpretation of preferential attachment [11]
- ▷ ...

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Outline

1. Why models and the challenge of clustering
2. A geometric approach to clustering
3. Euclid and hyperbolic geometry
4. A hyperbolic solution to clustering
5. **Rethinking interactions: the case of directed graphs**
6. Rethinking interactions: the case of modular structure

Three challenges in modeling directed networks

Properties of any metric space

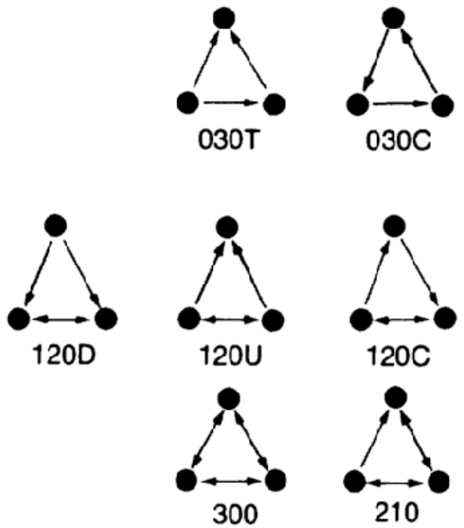
Identity of indiscernibles	$d(x, y) = 0 \quad \Leftrightarrow \quad x = y$
Non-negativity	$d(x, y) \geq 0$
Symmetry	$d(x, y) = d(y, x)$
Triangle inequality	$d(x, y) \leq d(x, z) + d(z, y)$

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Clustering : 7 cycles of length 3



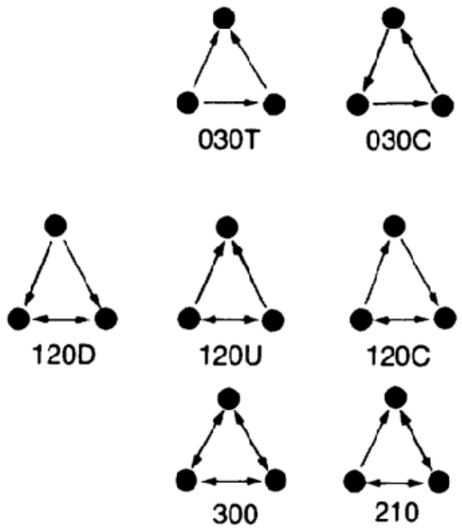
Adapted from Holland & Leinhardt. Local Structure in Social Networks. Sociol. Methodol., 7, 1–45 (1976)

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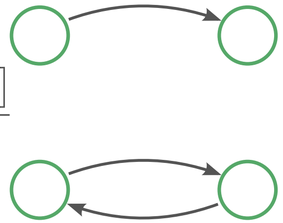
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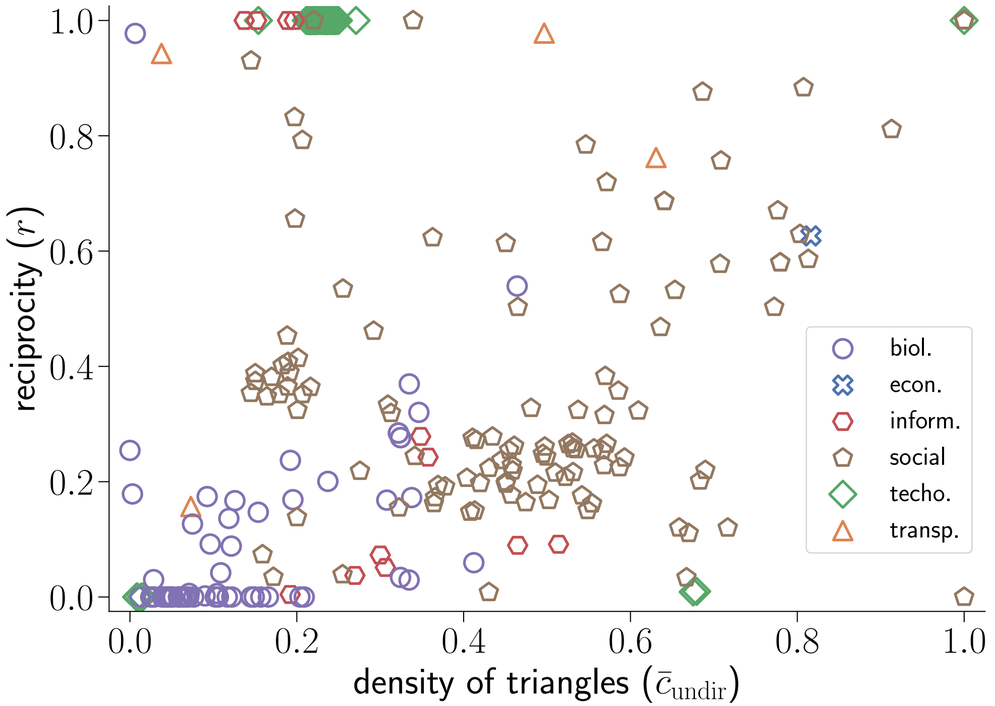


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Reciprocity : cycles of length 2

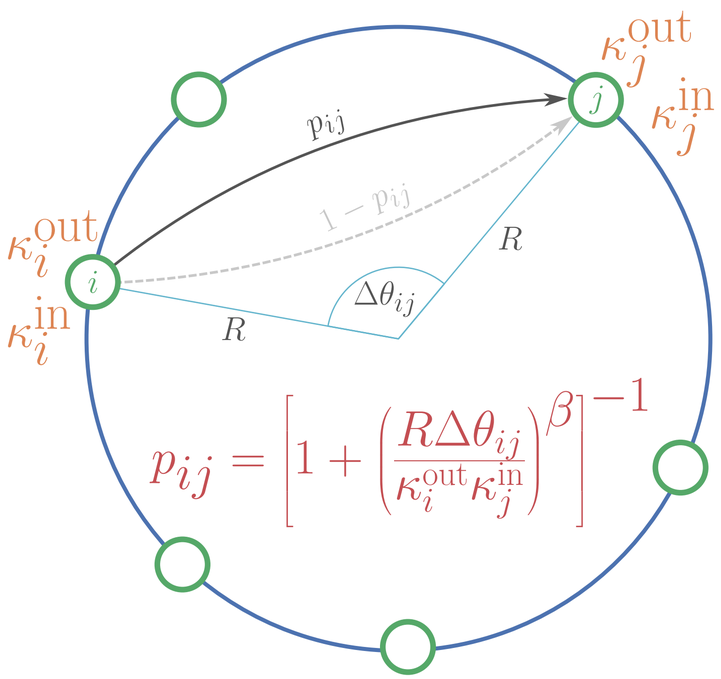
$$r = \frac{L^{\leftrightarrow}}{L} = \frac{[\text{number of reciprocal links}]}{[\text{number of links}]}$$





292 network datasets downloaded from Netzschleuder (networks.skewed.de).

The directed $\mathbb{S}^1$ model



The directed $\mathbb{S}^1$ model

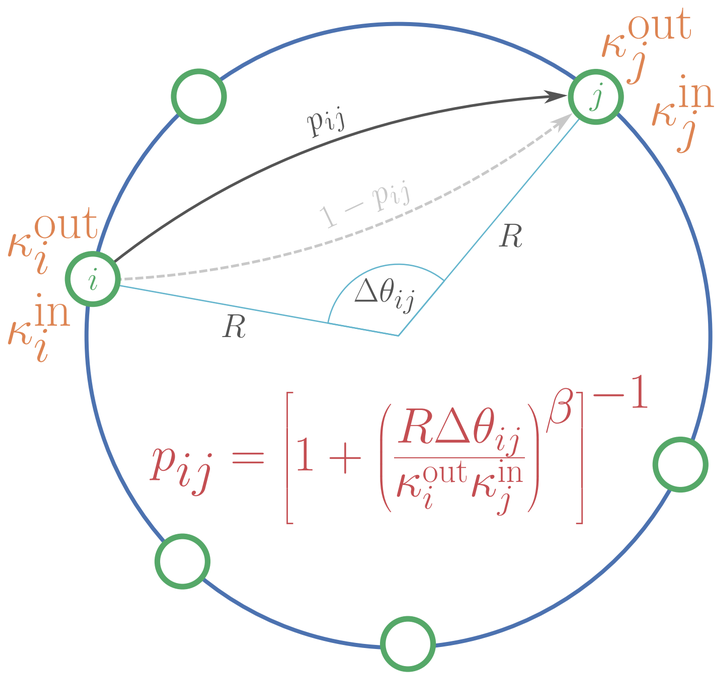
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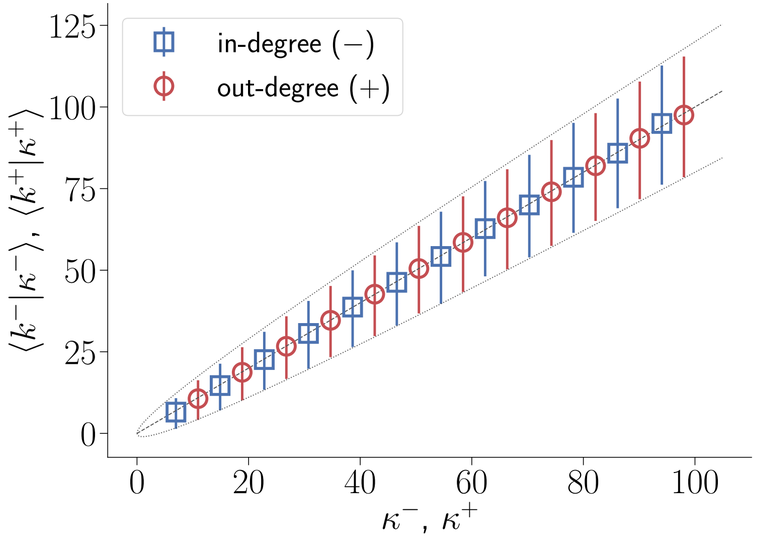


$$\mathbb{E}\left[k^{\text{in}}\middle|\kappa^{\text{in}}\right] \simeq \kappa^{\text{in}}$$
$$\mathbb{E}\left[k^{\text{out}}\middle|\kappa^{\text{out}}\right] \simeq \kappa^{\text{out}}$$
$$P(k^{\text{in}}, k^{\text{out}}) \simeq \iint \frac{[\kappa^{\text{in}}]^{k^{\text{in}}} \mathrm{e}^{-\kappa^{\text{in}}}}{k^{\text{in}}!} \frac{[\kappa^{\text{out}}]^{k^{\text{out}}} \mathrm{e}^{-\kappa^{\text{out}}}}{k^{\text{out}}!} \times \rho(\kappa^{\text{in}}, \kappa^{\text{out}}) d\kappa^{\text{in}} d\kappa^{\text{out}}$$

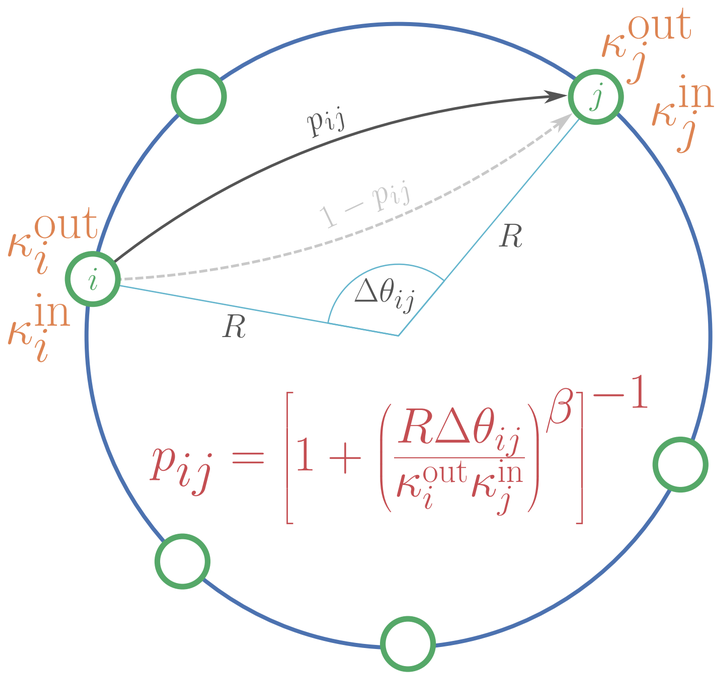
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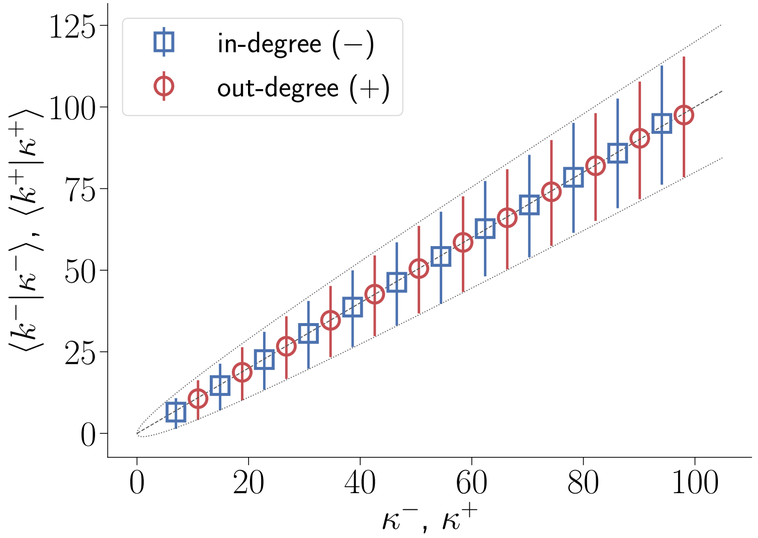


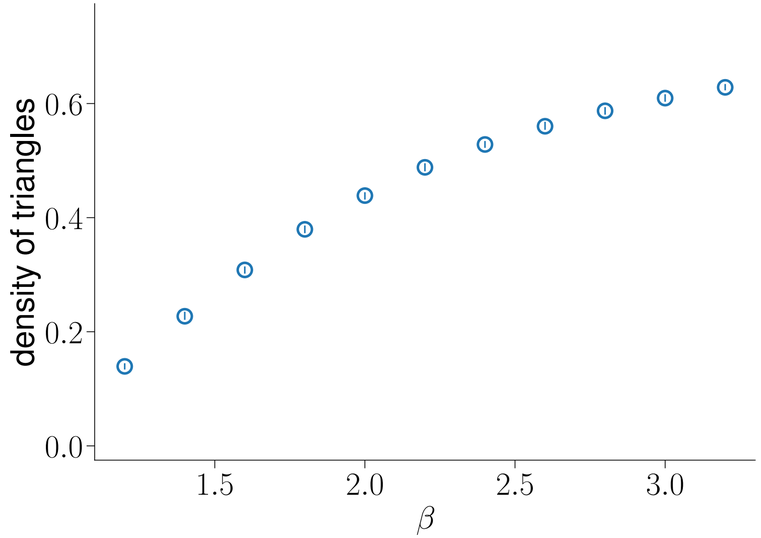
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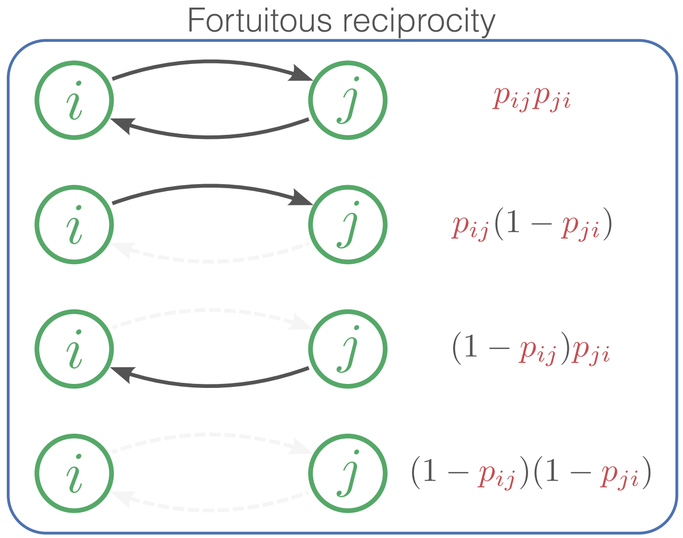
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Reciprocity in the directed $\mathbb{S}^1$ model

A reciprocal connection between node i and node j occurs with probability $p_{ij}p_{ji}$.



$$r = \mathbb{E}\left[\frac{L^{\leftrightarrow}}{L}\right] = \mathbb{E}\left[\frac{k^{\leftrightarrow}}{k^{\text{out}}}\right] \approx \frac{\mathbb{E}\left[k^{\leftrightarrow}\right]}{\mathbb{E}\left[k^{\text{out}}\right]}$$

$$\simeq \iiiint \frac{\kappa_i^{\text{out}}\kappa_j^{\text{in}}}{\langle\kappa\rangle^2} \frac{1-\left(\frac{\kappa_i^{\text{out}}}{\kappa_i^{\text{in}}}\frac{\kappa_j^{\text{in}}}{\kappa_j^{\text{out}}}\right)^{\beta-1}}{1-\left(\frac{\kappa_i^{\text{out}}}{\kappa_i^{\text{in}}}\frac{\kappa_j^{\text{in}}}{\kappa_j^{\text{out}}}\right)^{\beta}}$$

$$\times\, \rho(\kappa_i^{\text{in}}, \kappa_i^{\text{out}})\rho(\kappa_j^{\text{in}}, \kappa_j^{\text{out}}) d\kappa_i^{\text{in}}\kappa_i^{\text{out}} d\kappa_j^{\text{in}}\kappa_j^{\text{out}}$$

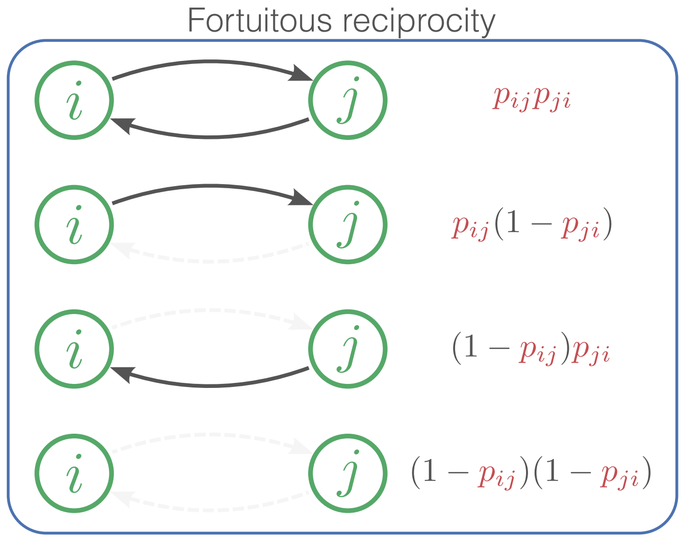
κ^{in} : in-degree

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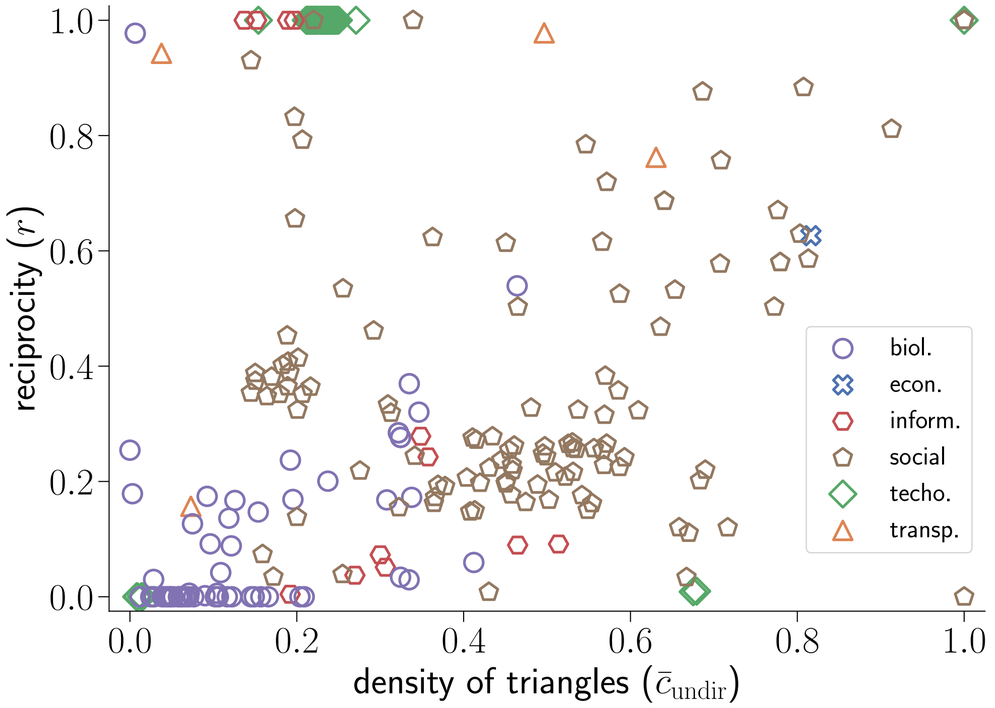
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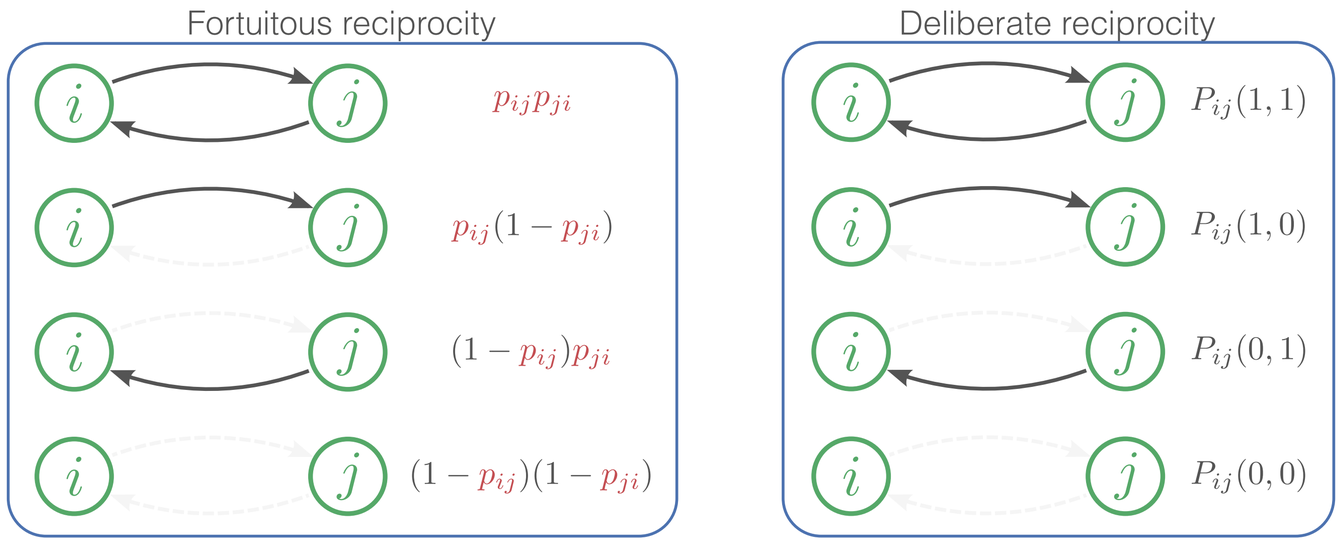


292 network datasets downloaded from Netzschleuder (networks.skewed.de).

A realistic model will need to go beyond fortuitous reciprocity.

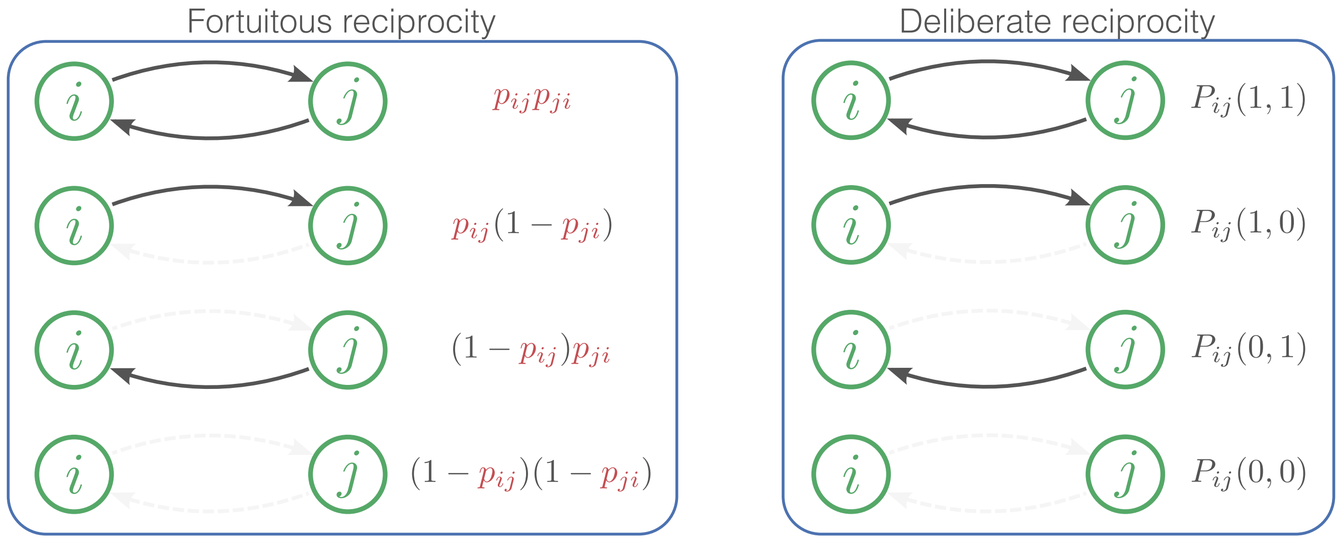
Deliberate reciprocity in random directed networks

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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Condition 1: Preserves marginal probabilities

$$P_{ij}(1,0) + P_{ij}(1,1) = p_{ij}$$
$$P_{ij}(0,1) + P_{ij}(1,1) = p_{ji}$$

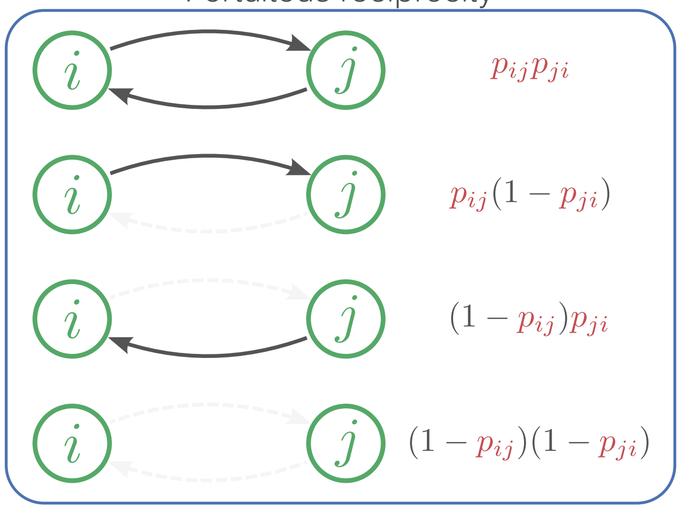
Condition 2: Normalized

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

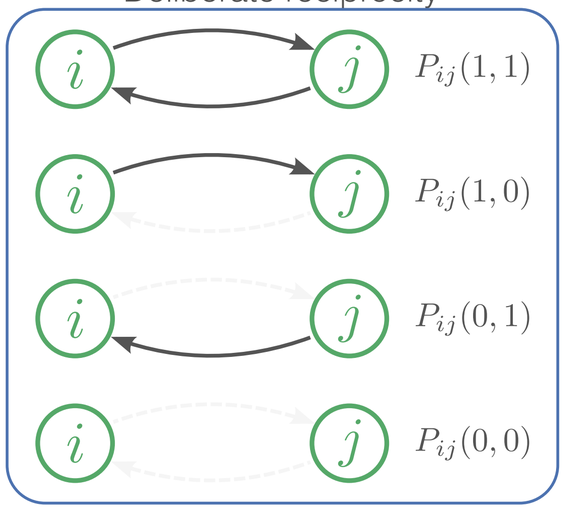
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Fortuitous reciprocity



Deliberate reciprocity



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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

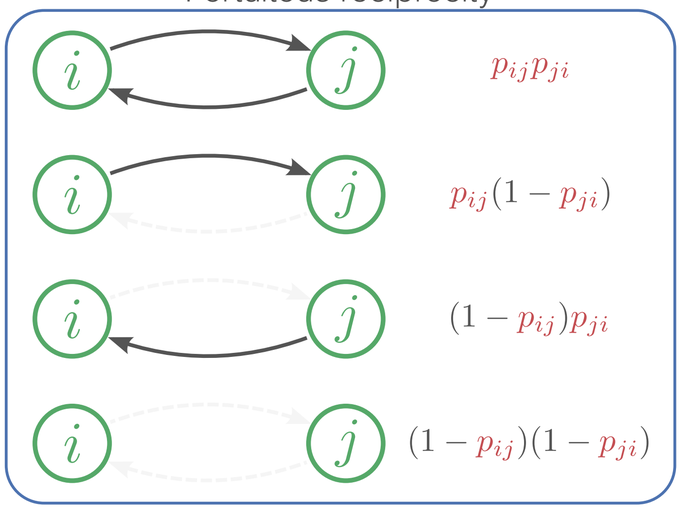
$\nu = 0$: fortuitous reciprocity

$\nu = -1$: minimal reciprocity

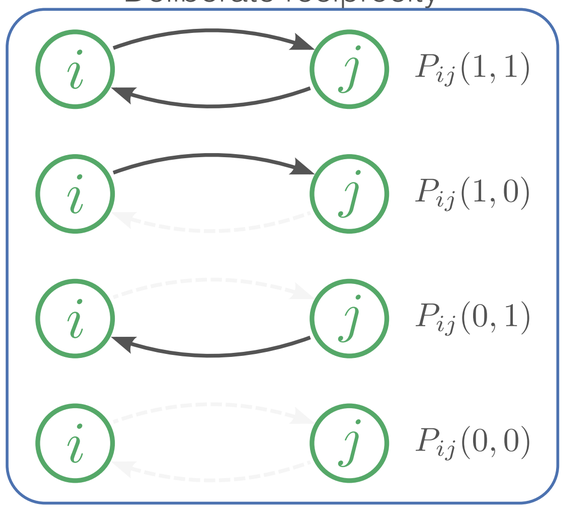
Deliberate reciprocity in random directed networks

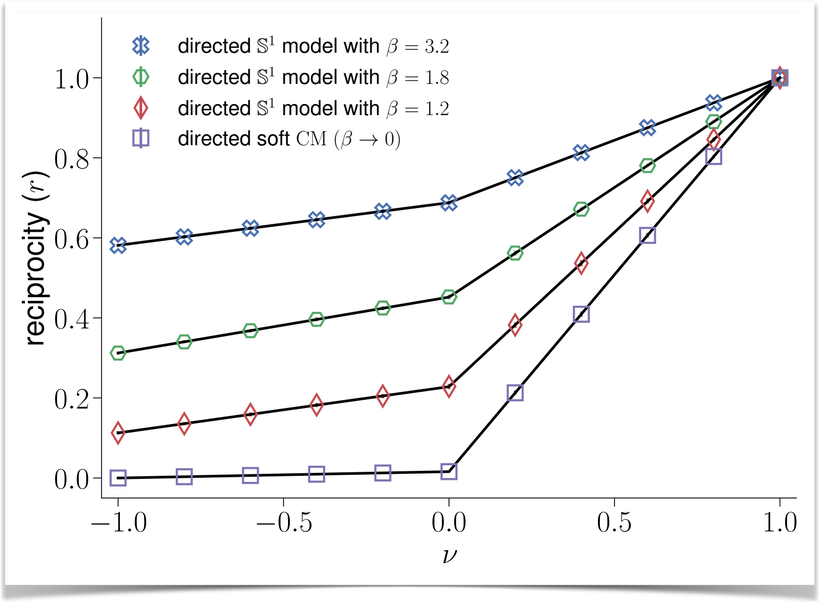
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Fitting the directed $\mathbb{S}^1$ model to real networks

Inputs from a real network :

1. joint degree distribution $P(k^{\text{in}}, k^{\text{out}})$
2. reciprocity r
3. density of triangles

Assuming uniform angular positions for nodes,

1. infer $(\kappa^{\text{in}}, \kappa^{\text{out}})$ to replicate $P(k^{\text{in}}, k^{\text{out}})$ on average (analytical)
2. set ν to reproduce r (analytical)
3. adjust β to recreate the density of triangles (semi-analytical)

Generate a sample of random directed networks :

1. assign angular positions randomly
2. draw directed links using the probabilities defined by the framework for deliberate reciprocity

Inference algorithm adapted from New J. Phys. 21, 123033 (2019).

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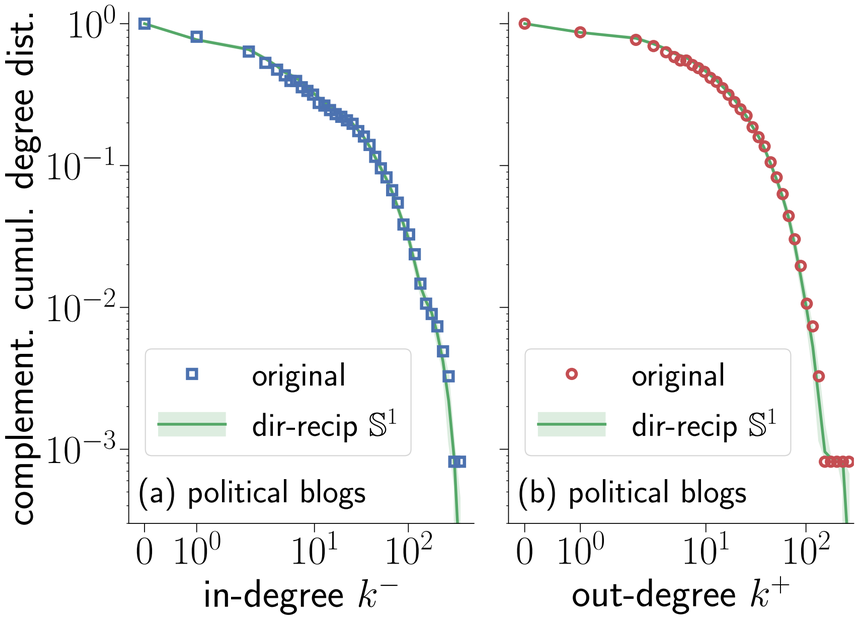
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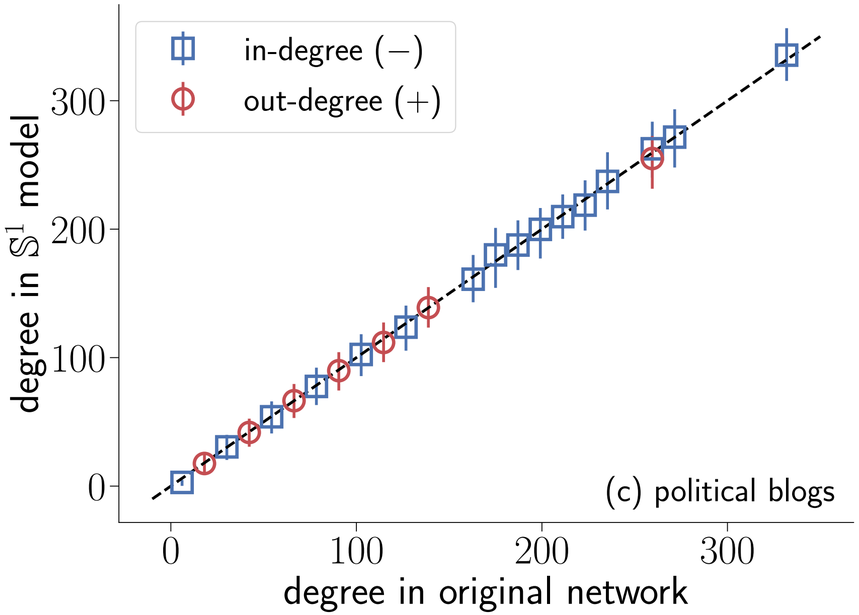
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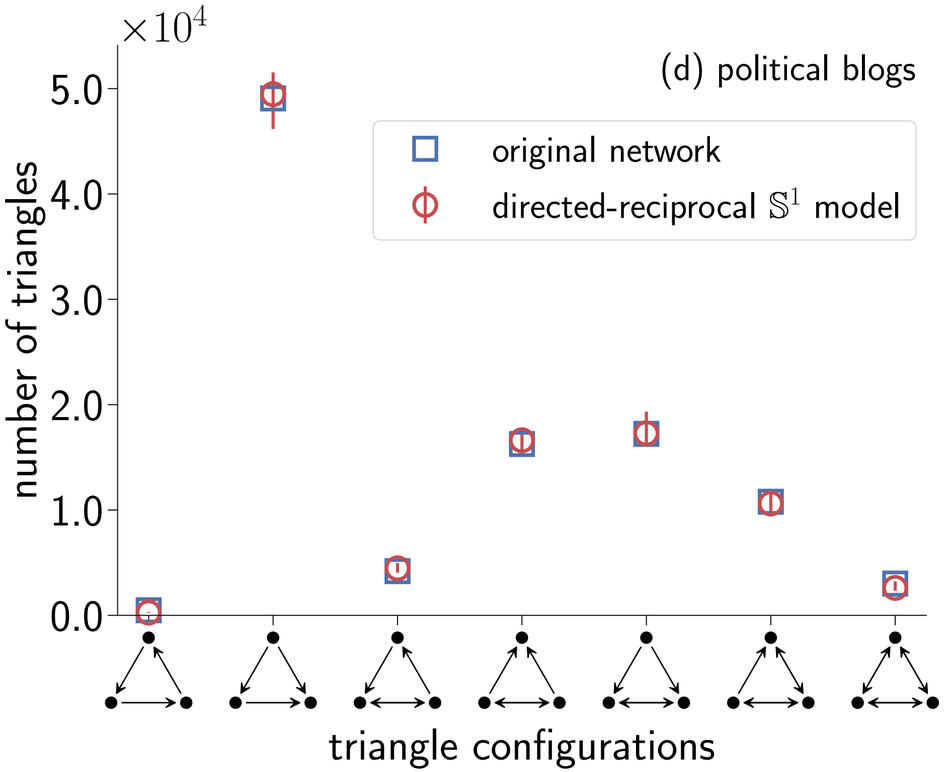
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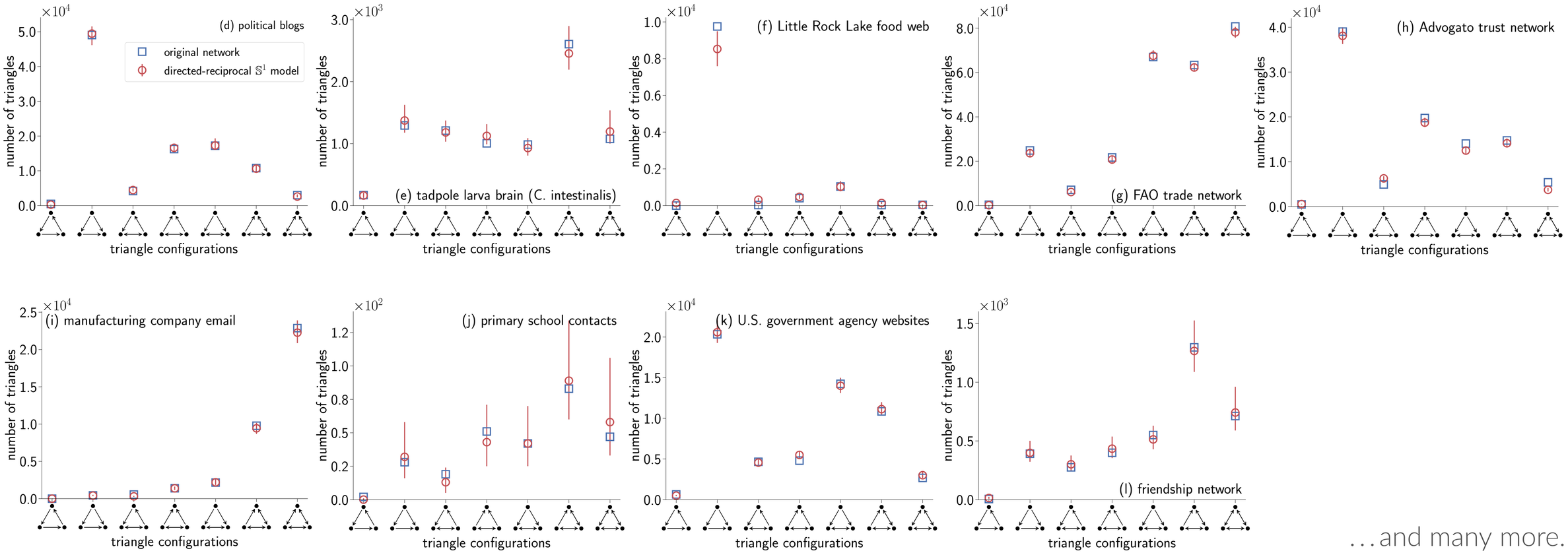


Inference algorithm adapted from New J. Phys. 21, 123033 (2019).

Realistic clustering patterns in directed geometric networks



Realistic clustering patterns in directed geometric networks



. . . and many more.

Coupled with an underlying geometry, the joint degree distribution, the reciprocity, and the density of triangles fix the clustering patterns in the network.

Summary

1. Presented a generalization of the $\mathbb{S}^1$ model to directed networks.
2. Proposed a general approach to control reciprocity in any random network model.
3. Showed that the interplay between in/out-degree, reciprocity and clustering in directed networks can be accurately captured by a geometric approach.

Further details

- ▷ Allard, Serrano & Boguñá, *Geometric description of clustering in directed networks*, Nat. Phys. (in press), arXiv:2302.09055
- https://github.com/networkgeometry/directed-geometric-networks

Ongoing work / open questions

- ▷ How to infer the angular positions as well. Does this information improve the accuracy of the model?
- ▷ Can we disentangle the effect of ν, β and the correlation between in- and out-degrees on the accuracy of the model?
- ▷ Why are some real networks not fitted well by the model?
- ▷ What about vertex-wise reciprocity? Is it uniform/heterogeneous? Is the model accurate?

Outline

1. Why models and the challenge of clustering
2. A geometric approach to clustering
3. Euclid and hyperbolic geometry
4. A hyperbolic solution to clustering
5. Rethinking interactions: the case of directed graphs
6. **Rethinking interactions: the case of modular structure**

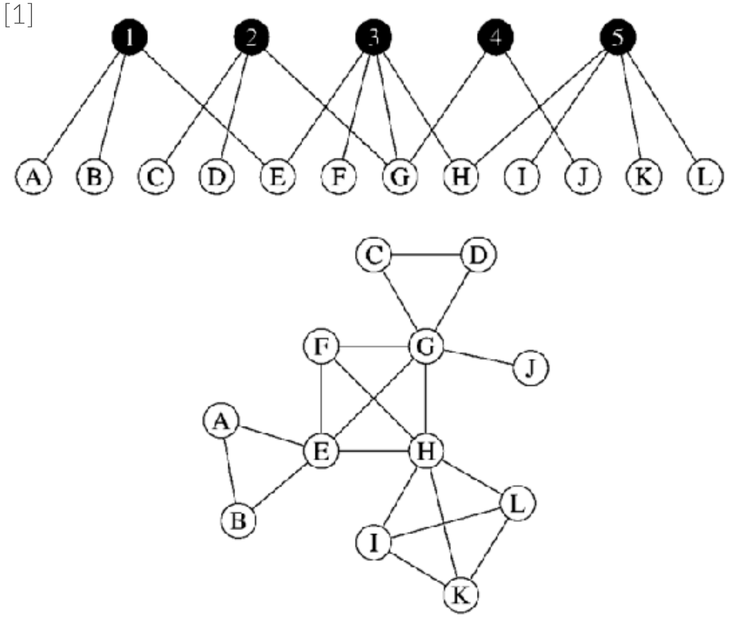
Modeling clustering

Trickier because clustering consists in three-node interactions while our mathematical tools rely on pairwise interactions either explicitly or implicitly.

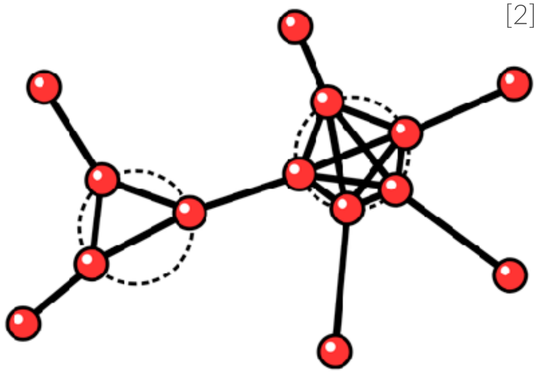
Most models therefore assume

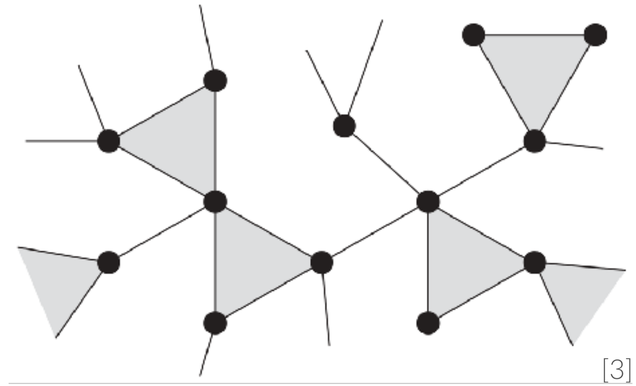
- an underlying tree-like structure
- that the networks are dense

[1]



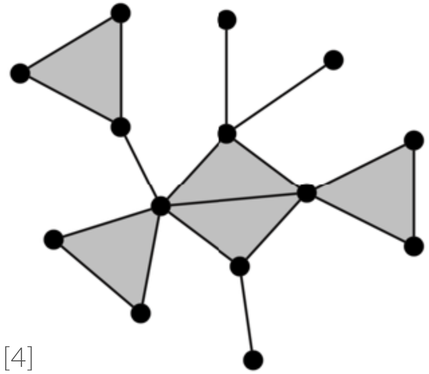
[2]

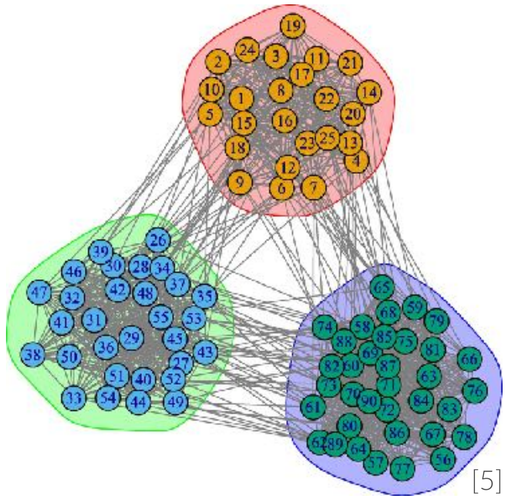




[3]

[4]





[5]

[1] Phys. Rev. E 68, 026121 (2003)
[2] Phys. Rev. E 80, 036107 (2009)
[3] Phys. Rev. Lett. 103, 058701 (2009)
[4] Phys. Rev. E 82, 066118 (2010)
[5] Appl. Netw. Sci. 4, 122 (2019)

The importance of modular architecture

The modular architecture has a major influence of several dynamical processes.

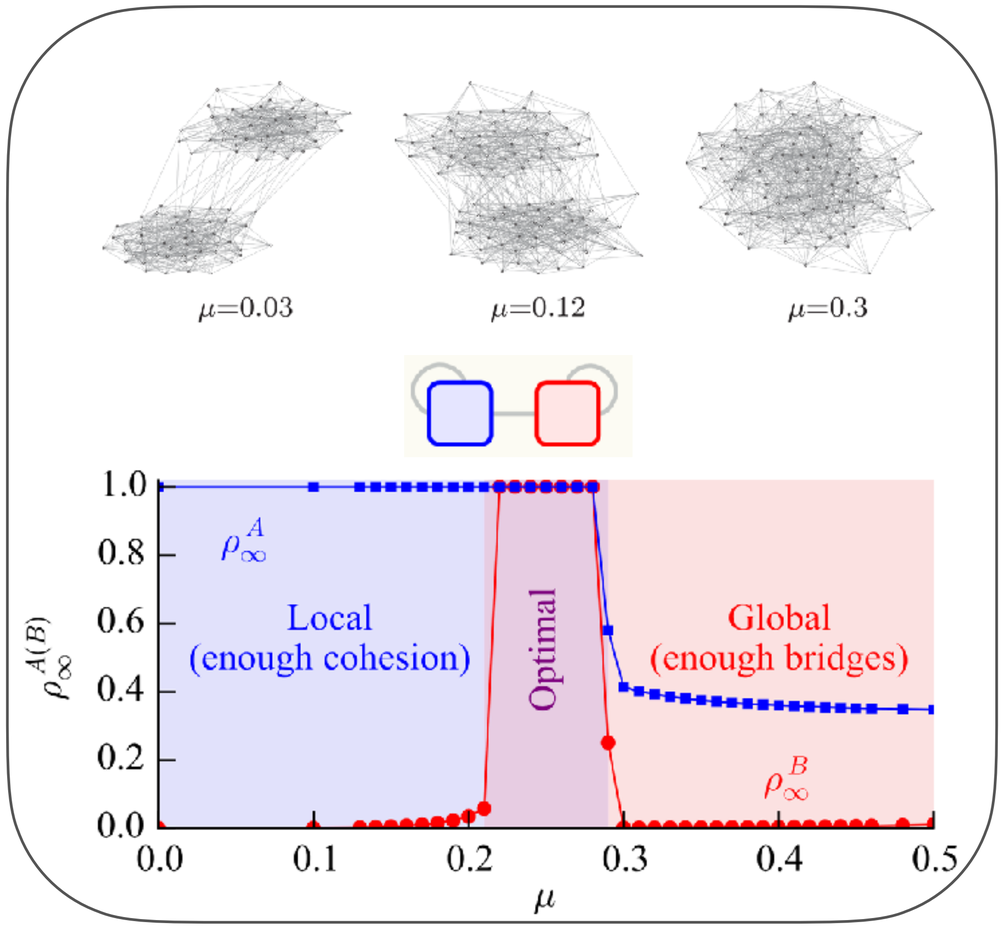
- information diffusion [1]
- neural dynamics and memory performance [2]
- ...

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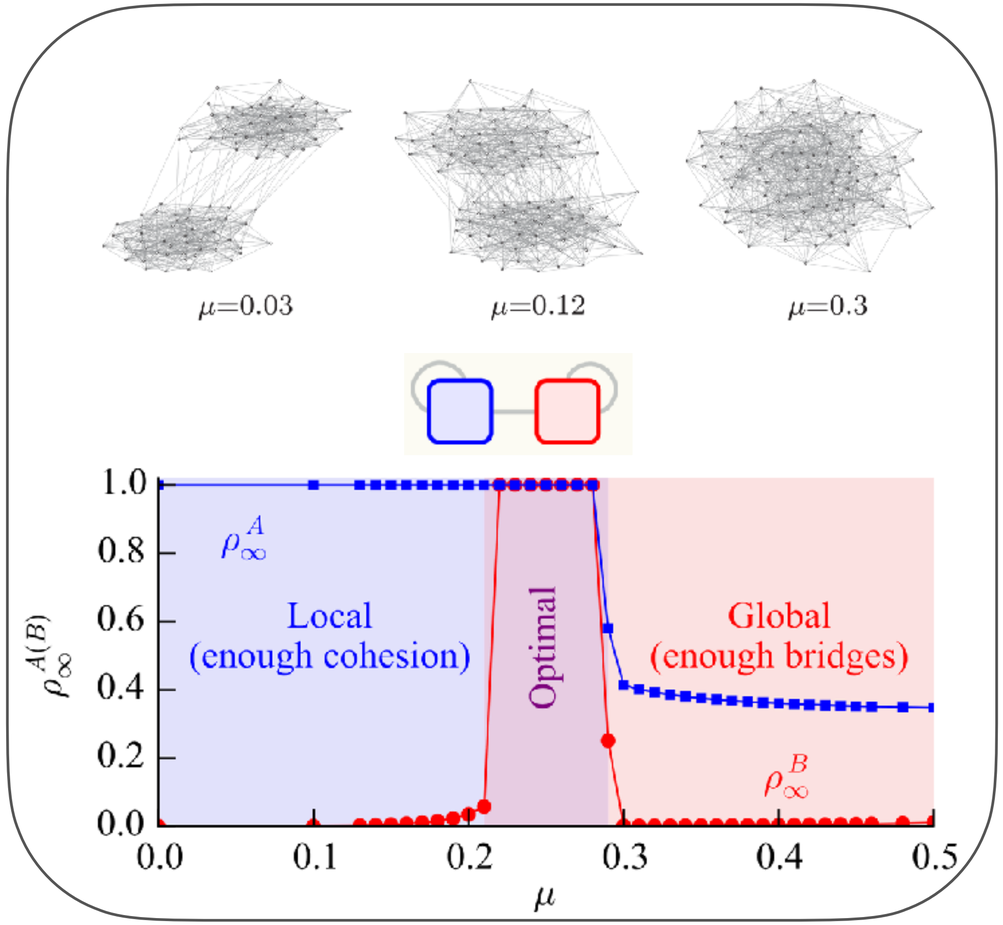


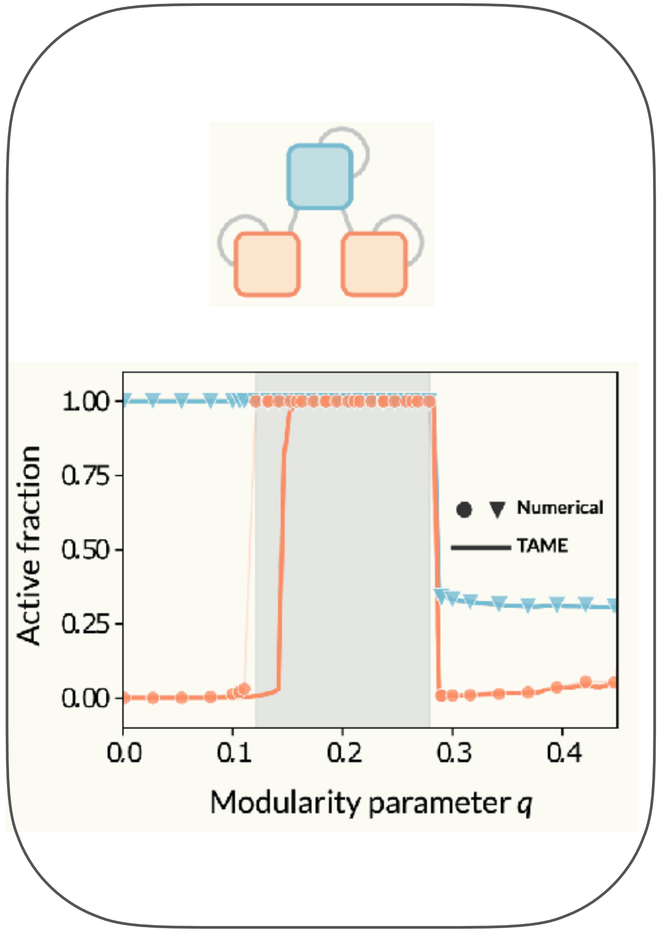
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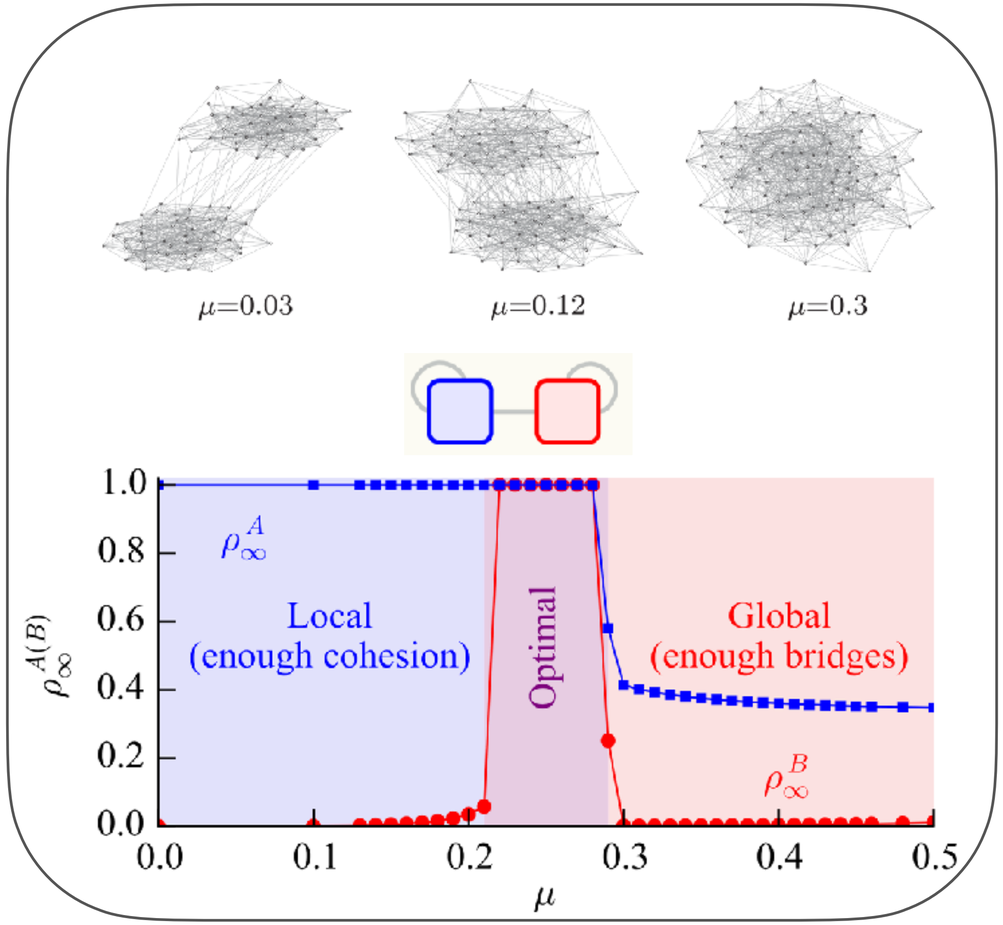


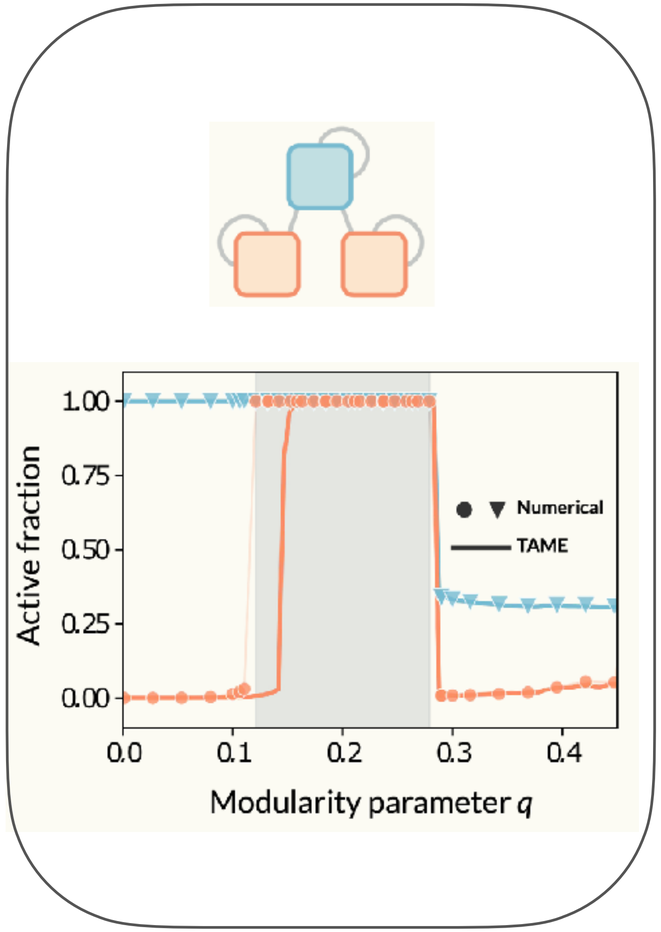
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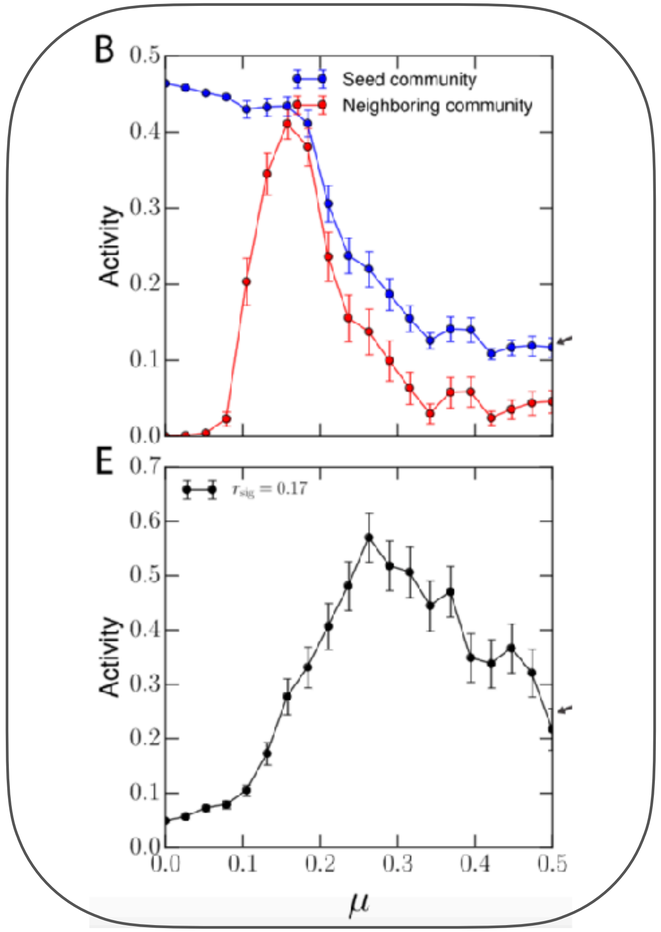
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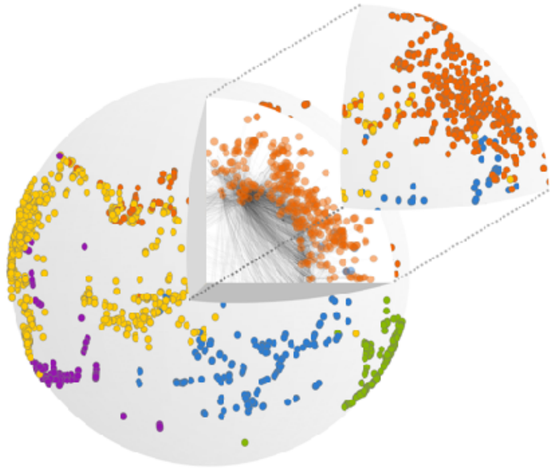




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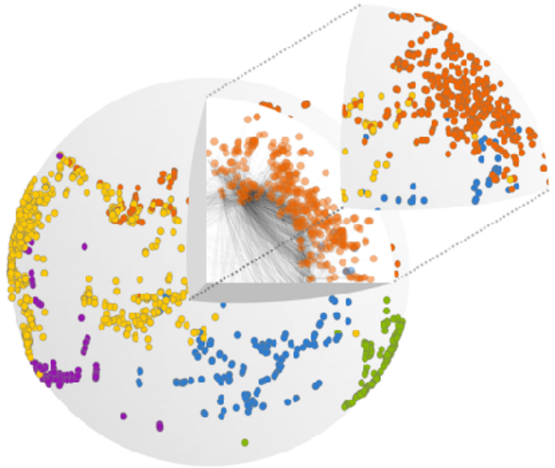
A hyperbolic solution to modular architecture?

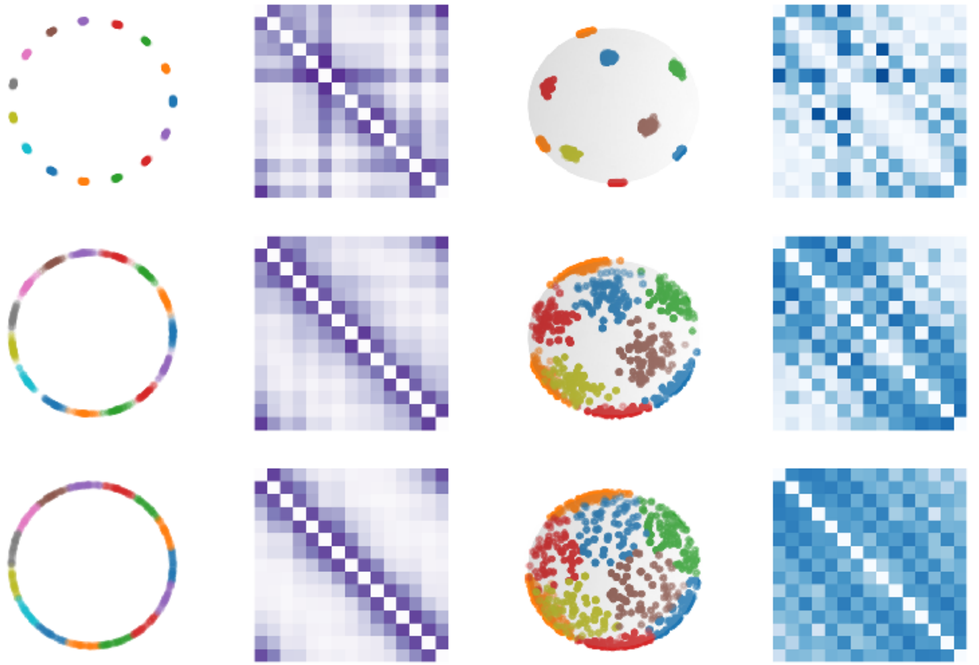
The $\mathbb{S}^1/\mathbb{H}^2$ models are easily generalizable to arbitrary dimensions.
This *extra space* allows for a rich modular architecture.



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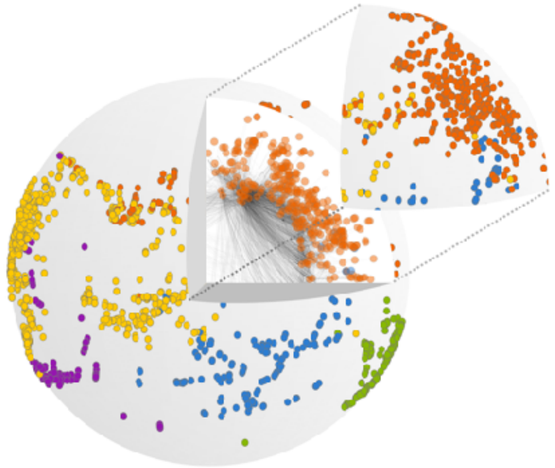
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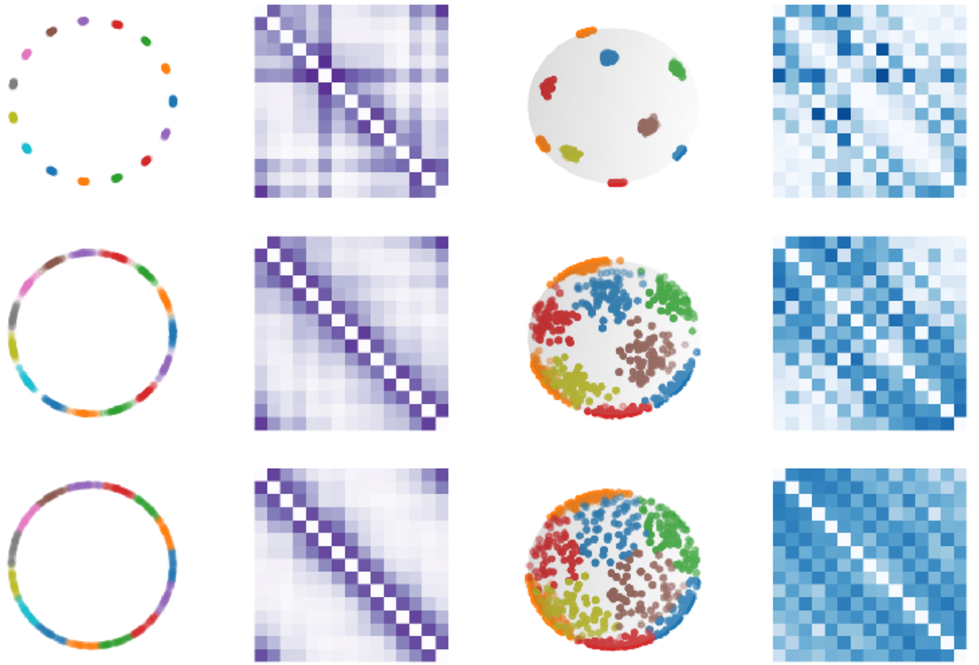




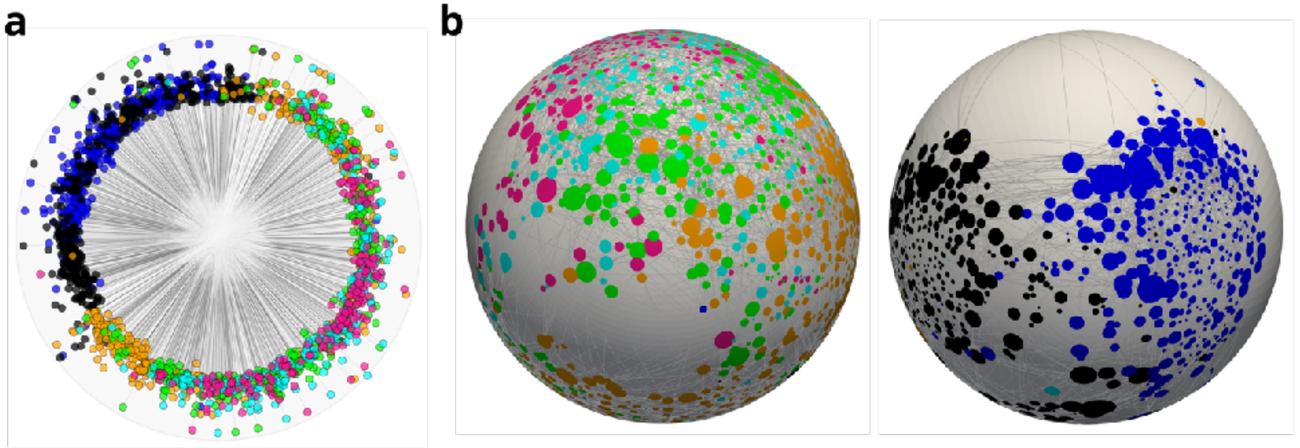
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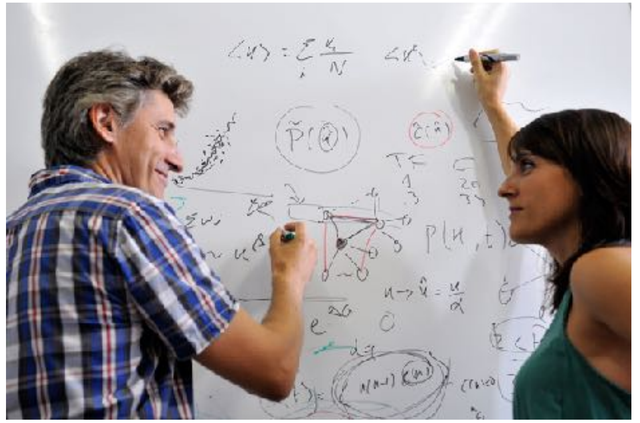


The modular architecture of several real complex networks are more naturally represented in more dimension.



Work done in collaboration with

- Robert Jankowski (U. Barcelona)
- M. Ángeles Serrano (U. Barcelona)
- Marián Boguñá (U. Barcelona)
- Patrick Desrosiers (CERVO Brain Research Centre)
- Béatrice Désy (Victoria University of Wellington)





Further details

- Allard, Serrano & Boguñá, *Geometric description of clustering in directed networks*, Nat. Phys. (in press), arXiv:2302.09055
- Jankowski, Allard, Boguñá & Serrano, *D-Mercator: multidimensional hyperbolic embedding of real networks*, arXiv:2304.06580
- Désy, Desrosiers & Allard, *Dimension matters when modeling network communities in hyperbolic spaces*, PNAS Nexus 2, pgad136 (2023)

- https://github.com/networkgeometry/directed-geometric-networks
- https://github.com/networkgeometry/d-mercator
- https://github.com/bdesy/communities_modelSd





Sentinelle Nord

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