Simplicity meets complexity

Challenges in reproducing complex connectivity patterns with simple models

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Outline

1. Are simple models enough to study complex systems/networks?

2. “Simple” ways to encode structural complexity

   (a) latent metric space

   (b) stub types

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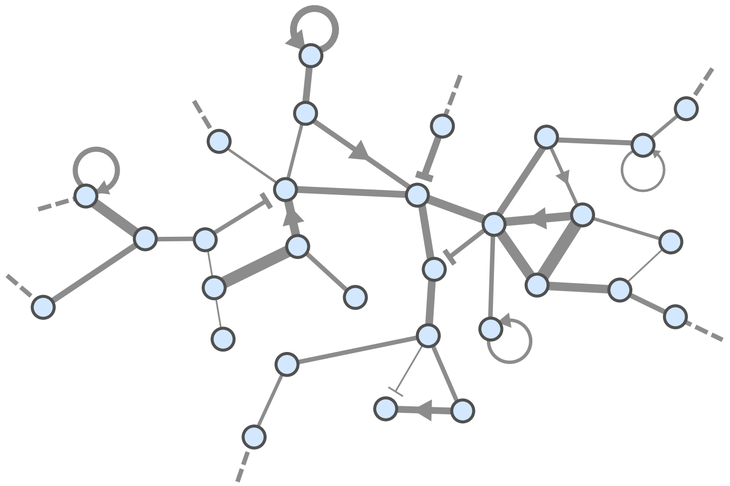
   (b) stub types



Modeling the dynamics of complex systems

Complex network

W

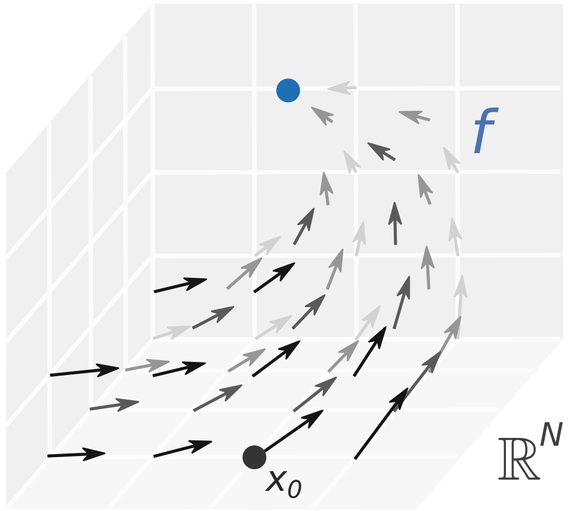


Vector field

f

High-dimensional dynamics

$\dot{x}=f(x;W)$



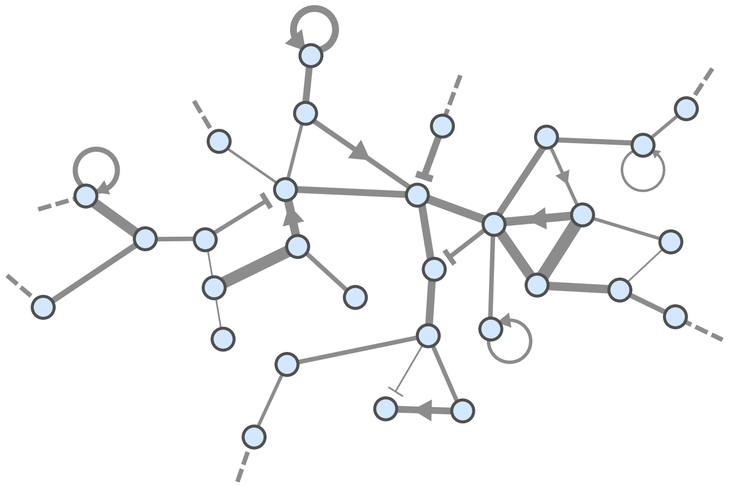
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Most mathematical models involve low-dimensional representations of the networks and/or dynamical observables.

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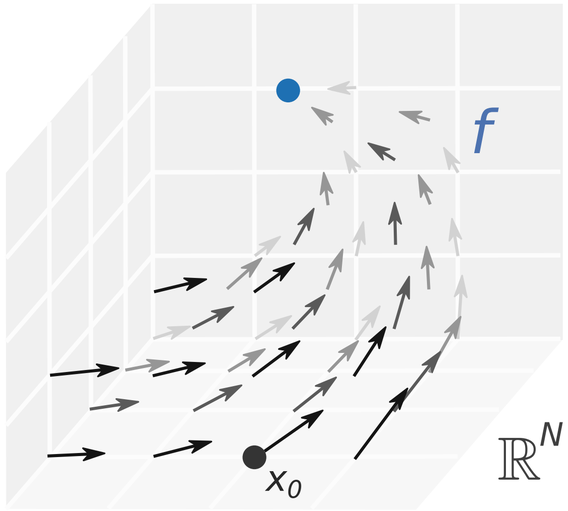


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Can we justify such a low-dimensional approach beyond mathematical and/or conceptual convenience?

The rank of adjacency matrices

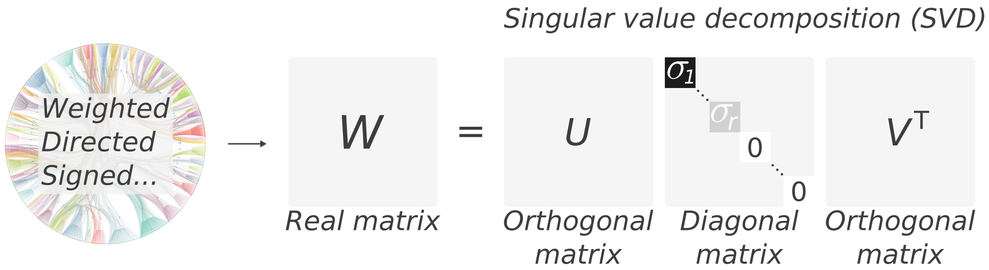
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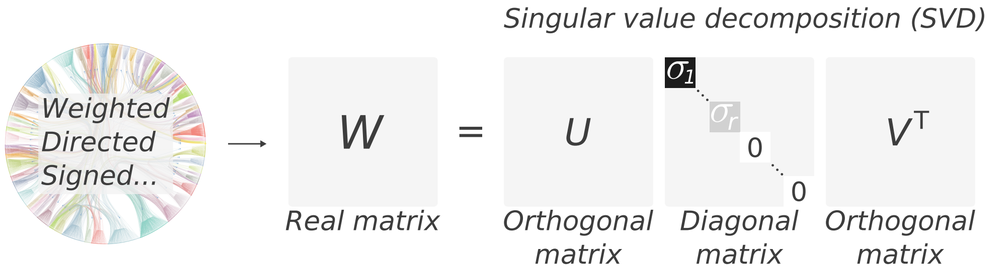


$$\mathbf{W} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\intercal = \sigma_1 \begin{bmatrix} | \\ \mathbf{u}_1 \\ | \end{bmatrix} \begin{bmatrix} — & \mathbf{v}_1^\intercal & — \end{bmatrix} + \sigma_2 \begin{bmatrix} | \\ \mathbf{u}_2 \\ | \end{bmatrix} \begin{bmatrix} — & \mathbf{v}_2^\intercal & — \end{bmatrix} + \sigma_3 \begin{bmatrix} | \\ \mathbf{u}_3 \\ | \end{bmatrix} \begin{bmatrix} — & \mathbf{v}_3^\intercal & — \end{bmatrix} + \dots$$

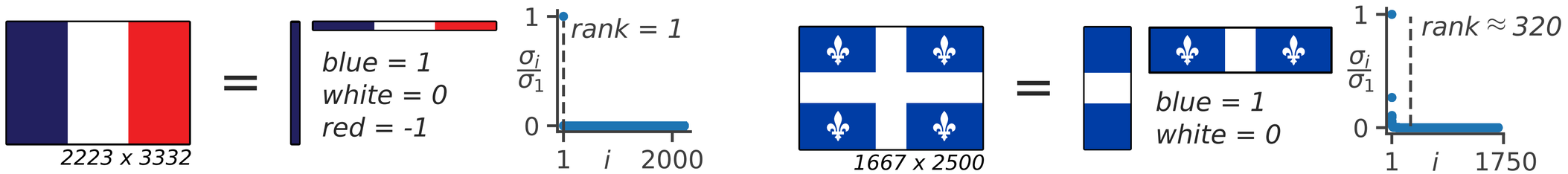
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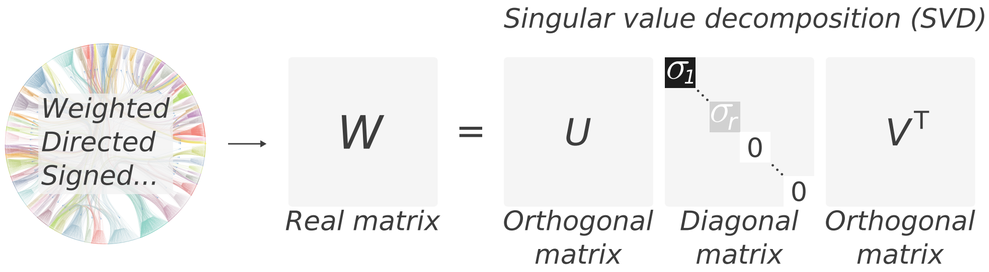
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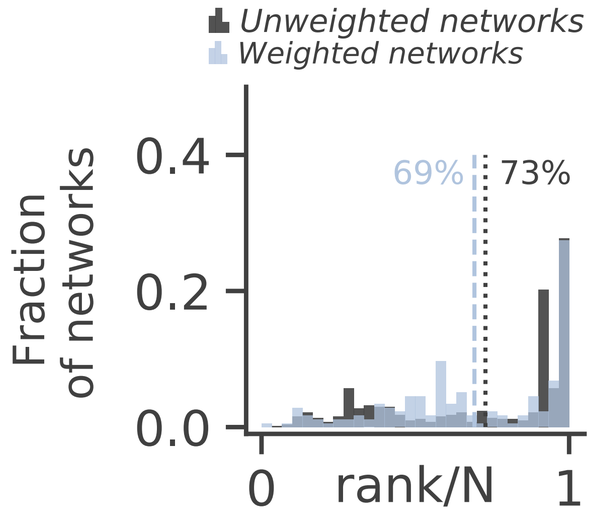
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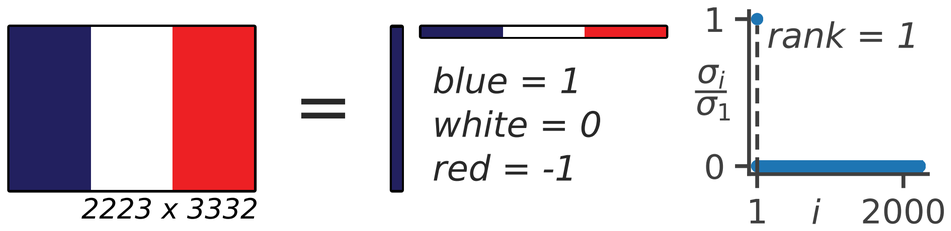


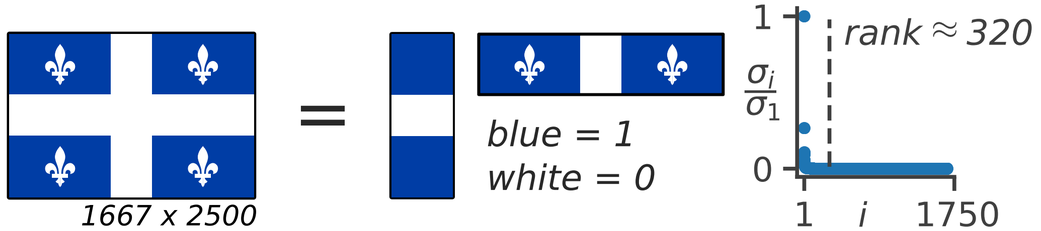
Full-rank (or almost full rank) adjacency matrices are very common!



Results for 679 empirical networks (502 unweighted networks and 177 weighted networks) downloaded from Netzschleuder.

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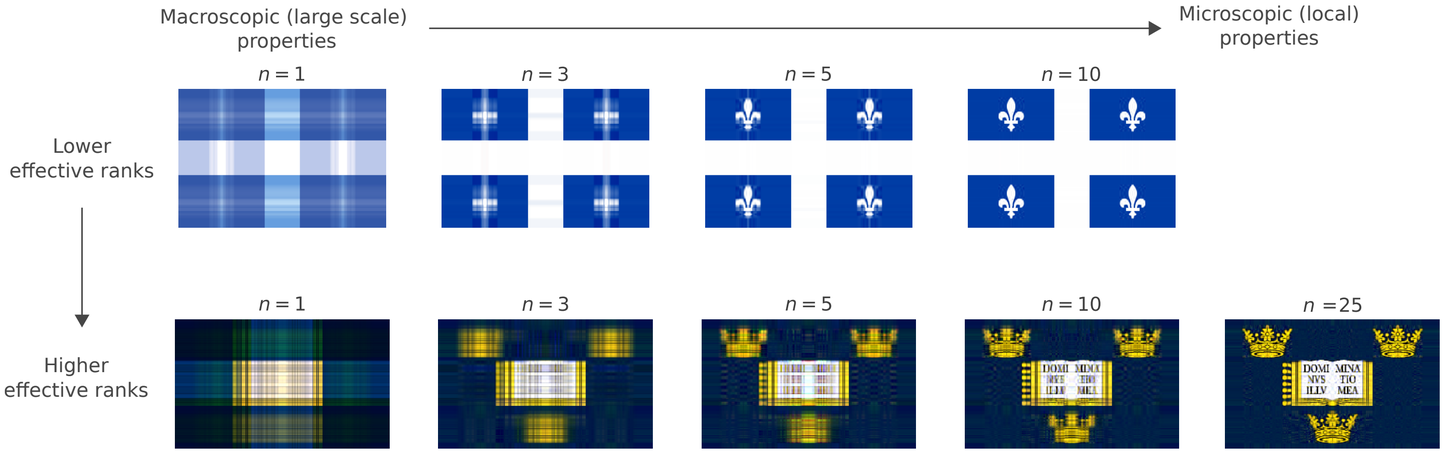


The effective ranks of adjacency matrices

$$\mathbf{W} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top \simeq \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$$

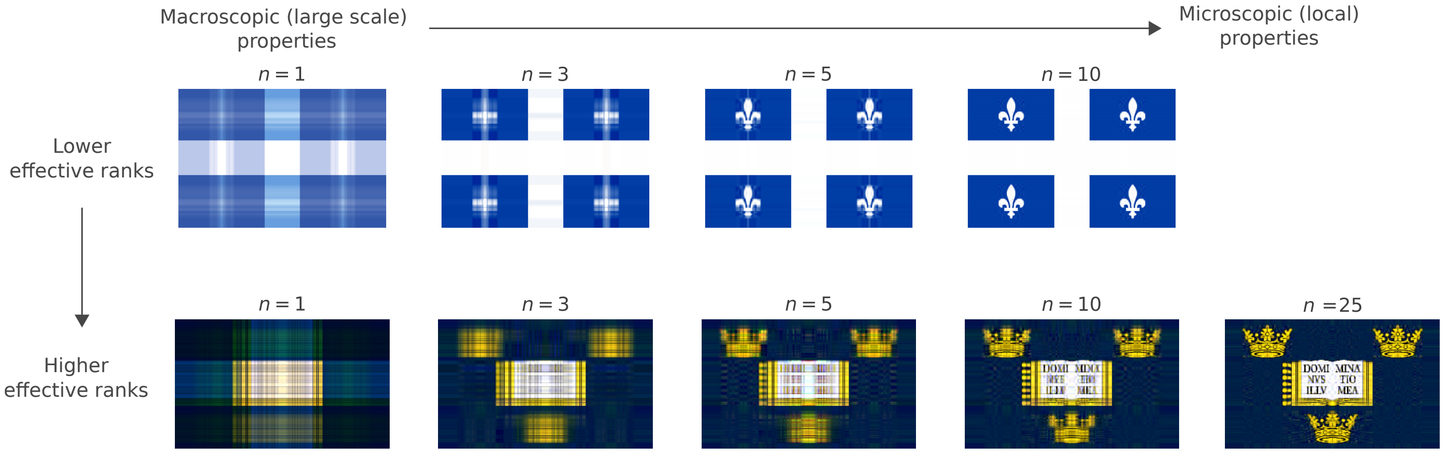
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Effective rank n of a matrix

- number of "significant" nonzero singular values
- term after which it is "reasonable" to truncate the sum

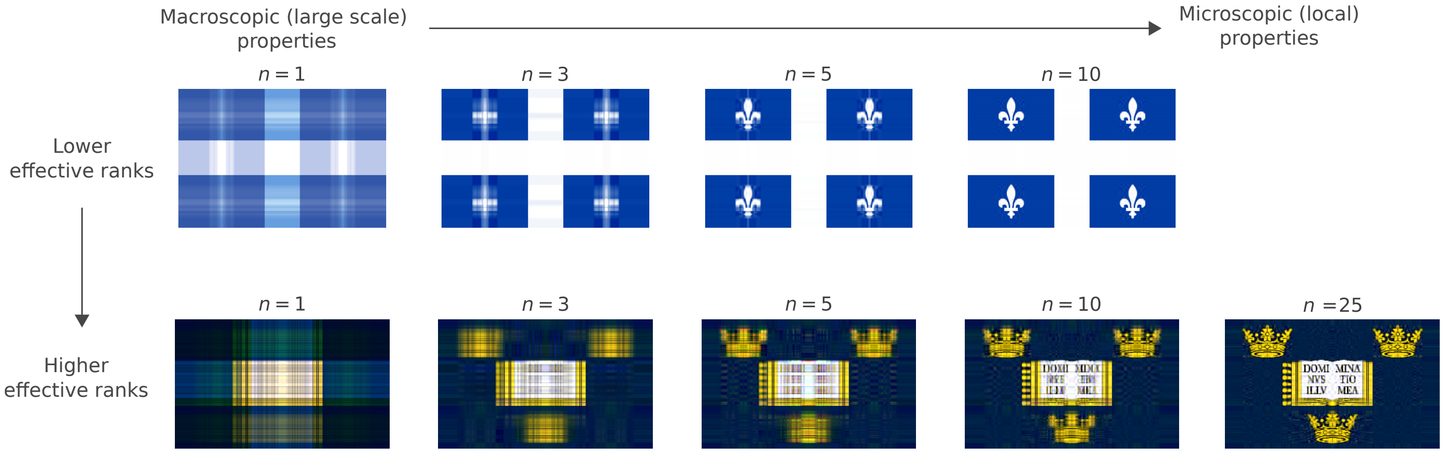
Abbreviation	Expression
srank	$\sum_{i=1}^{r} \sigma_i^2 / \sigma_1^2$
nrank	$\sum_{i=1}^{r} \sigma_i / \sigma_1$
energy	$\min\left[\arg\max_{\ell \in \{1,\ldots,N\}} \left(\sum_{i=1}^{\ell} \sigma_i^2 / \sum_{j=1}^{r} \sigma_j^2 > \tau\right)\right]$
elbow	$\frac{1}{\sqrt{2}} \arg\max_{i \in \{1,\ldots,N\}} \left\lvert \frac{i-1}{N-1} + \frac{\sigma_i - \sigma_N}{\sigma_1 - \sigma_N} - 1 \right\rvert - 1$
erank	$\exp\left\lvert -\sum_{i=1}^{r} \frac{\sigma_i}{\sum_{j=1}^{r} \sigma_j} \log \frac{\sigma_i}{\sum_{j=1}^{r} \sigma_j} \right\rvert$
thrank	$\#\left\{\sigma_i \mid i \in \{1, \ldots, N\} \text{ and } \sigma_i > \frac{4\sigma_{\text{med}}}{\sqrt{3}\mu_{\text{med}}}\right\}$
shrank	$\#\{s^*(\sigma_i) \mid i \in \{1, \ldots, N\} \text{ and } s^*(\sigma_i) > 0\}$

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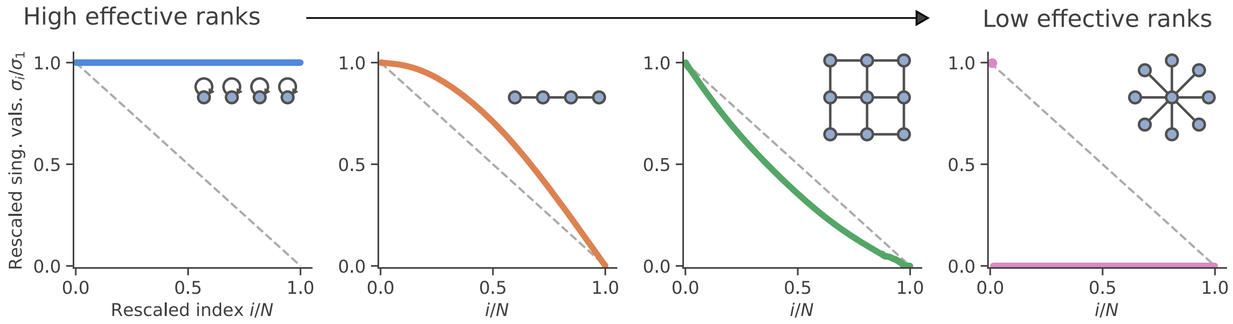
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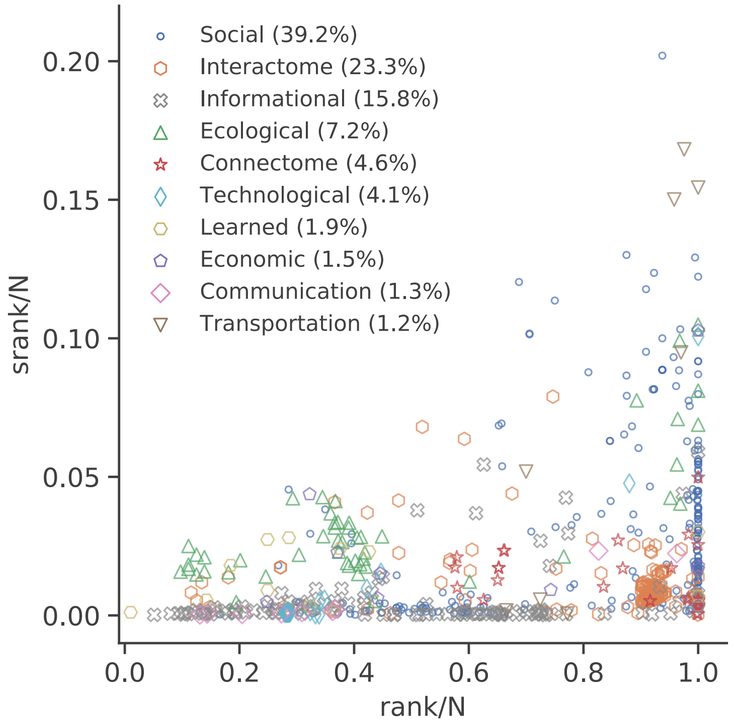
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The singular values (and the effective rank) encode information about the network's topology.



The effective ranks of adjacency matrices

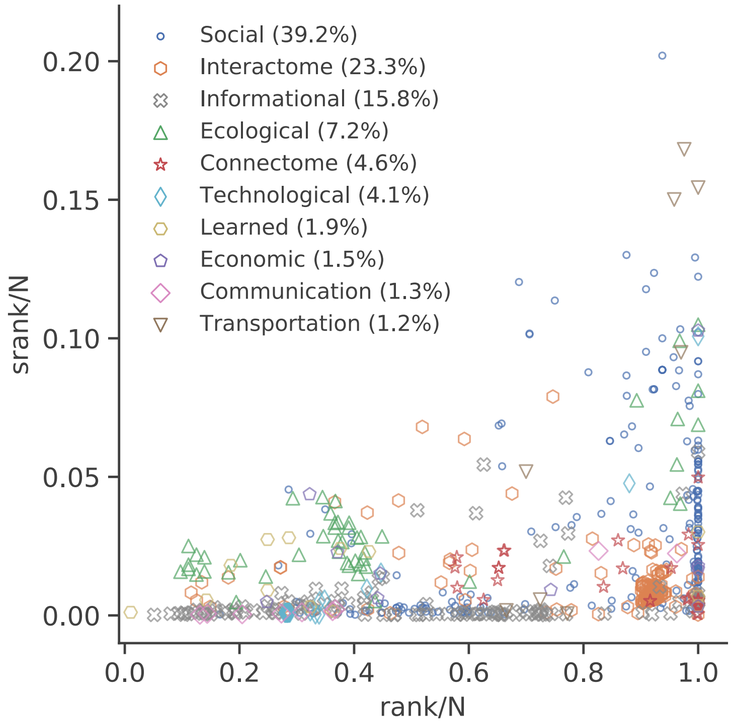
Many empirical networks appear to have a low effective rank!



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But what does “low” mean?

A *workable* definition of “low” effective rank

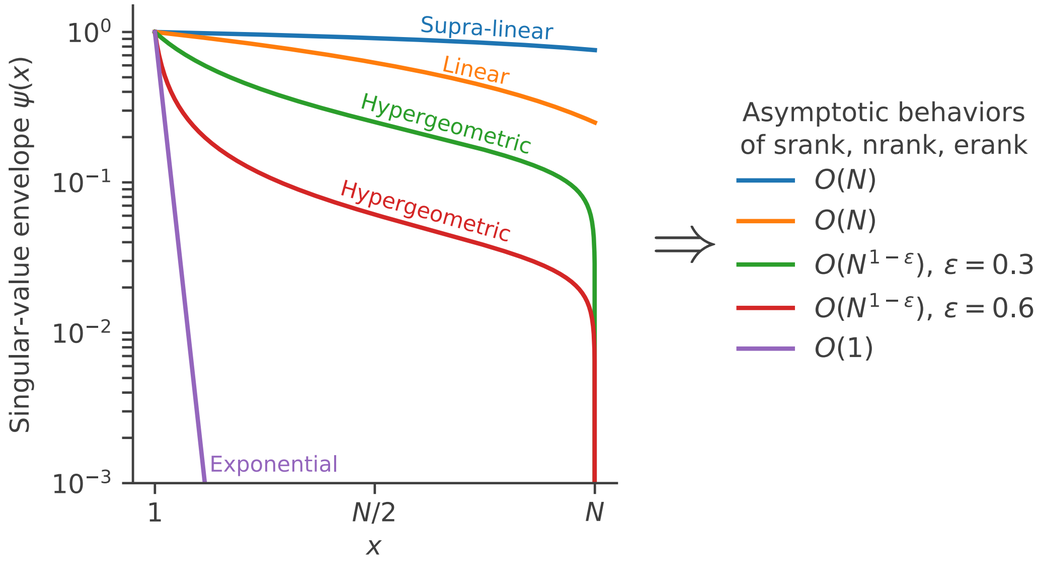
Hint: the rapid decrease of the dominant singular values of the adjacency matrix implies a low effective rank

- low effective rank? $\Rightarrow$ effective rank scales at most sublinearly as the number of nodes, N, goes to infitnity ($N^{1-\varepsilon}$ with $\varepsilon \in (0, 1]$)

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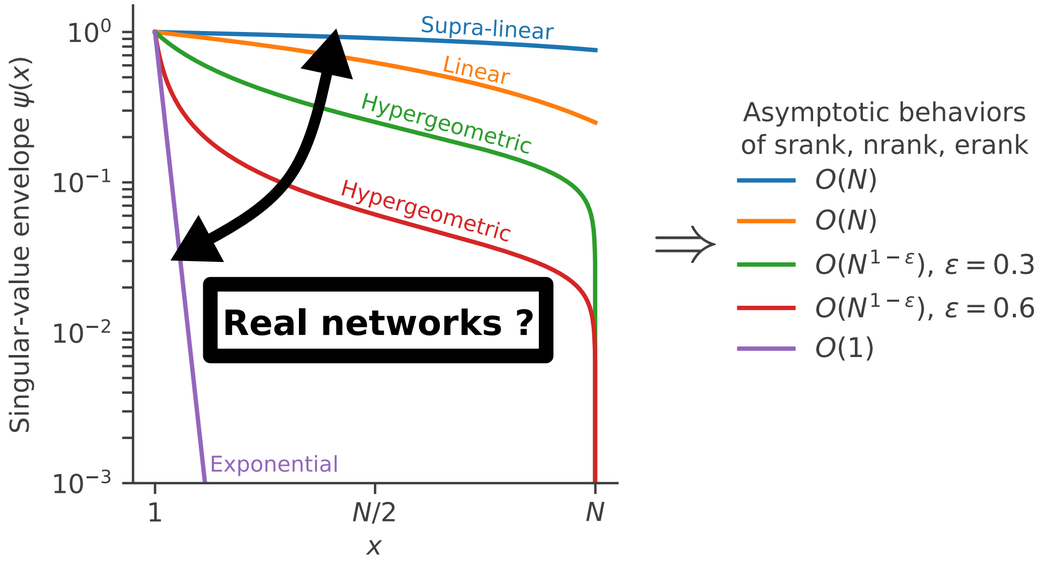
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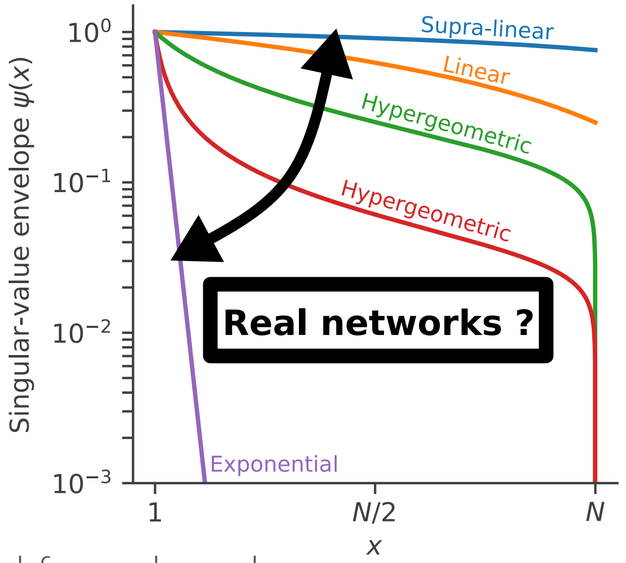
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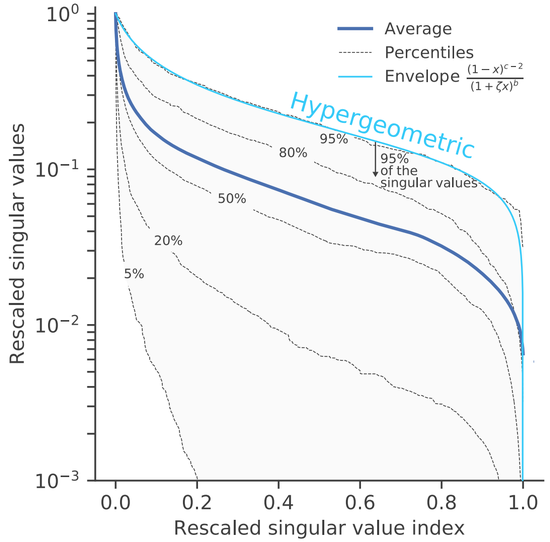


⇒

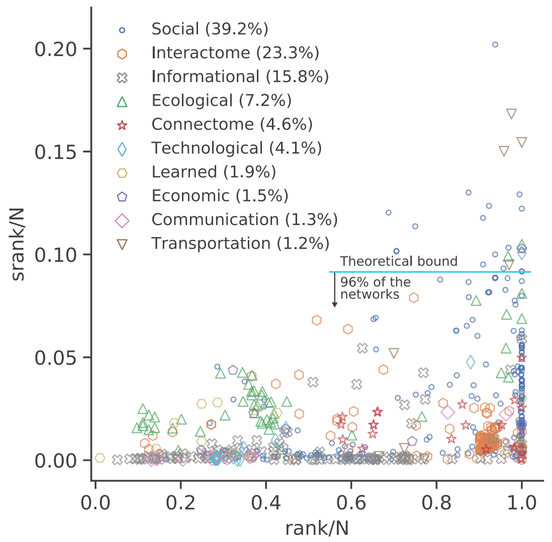
Asymptotic behaviors of srank, nrank, erank

- $O(N)$
- $O(N)$
- $O(N^{1-\varepsilon})$, $\varepsilon = 0.3$
- $O(N^{1-\varepsilon})$, $\varepsilon = 0.6$
- $O(1)$

The singular values of approx. 96% of considered networks are bounded from above by an hypergeometric envelope ⇒ sublinear effective ranks!



⇒



Workable definition of low effective rank: ∼10% of the number of nodes N

Approx. 96% of the 679 networks qualify for having a low effective rank!

The impact of effective low rank on the dynamics

Many dynamics on networks have the form

$$\dot{\boldsymbol{x}} = \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \mathbf{g}(\boldsymbol{x}, \mathbf{W}\boldsymbol{x}) = \mathbf{g}(\boldsymbol{x}, \boldsymbol{y})$$

with $\boldsymbol{x} \in \mathbb{R}^N$.

Examples:

- SIS (mean-field) : $\dot{x}_i = -d_i x_i + \gamma(1 - x_i)\, y_i$
- Wilson-Cowan: $\dot{x}_i = -d_i x_i + (1 - a x_i) \frac{1}{1+e^{-b(\gamma\, y_i - c)}}$
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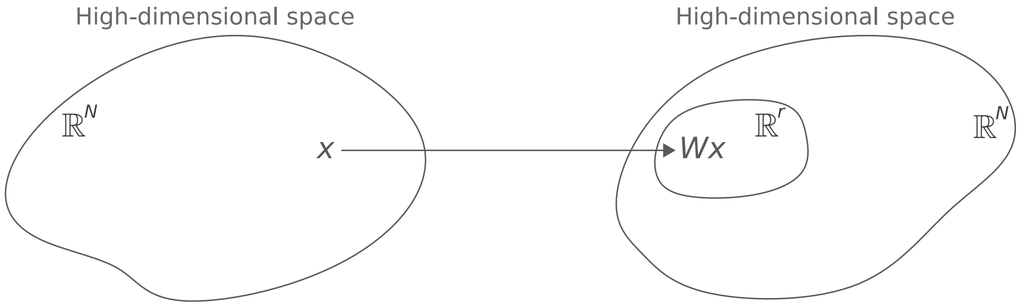
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Low rank $\mathbf{W} \Rightarrow \mathbf{W}\boldsymbol{x}$ belongs to a low-dimensional subspace



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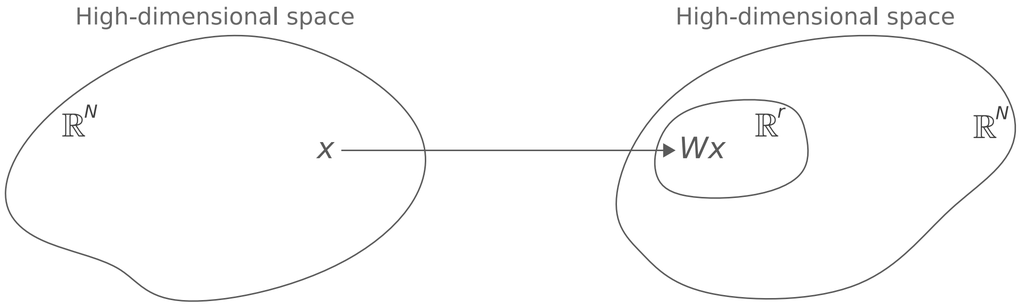
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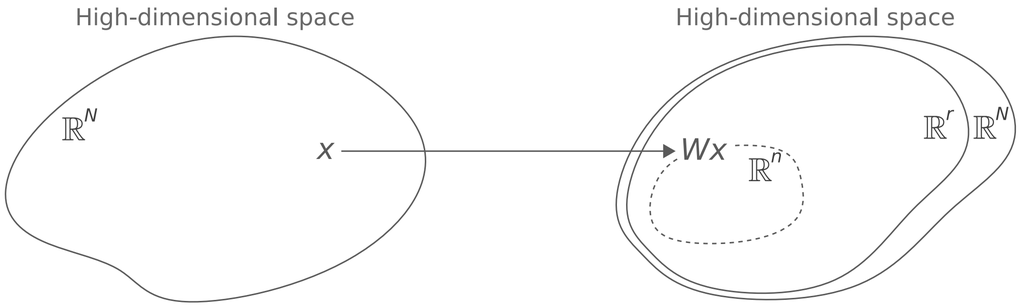
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Low *effective* rank $\mathbf{W} \Rightarrow \mathbf{W}\boldsymbol{x}$ belongs to an *effectively* low-dimensional subspace



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Original dynamics

$$\dot{\boldsymbol{x}} = \mathbf{g}(\boldsymbol{x}, \mathbf{W}\boldsymbol{x})$$

Reduced dynamics (with $\boldsymbol{X} = \mathbf{M}\boldsymbol{x}$)

$$\dot{\boldsymbol{X}} = \mathbf{M}\mathbf{g}(\mathbf{M}^{+}\mathbf{X}, \mathbf{W}\mathbf{M}^{+}\mathbf{X})$$

where n is the dimension of the reduced system
$\mathbf{M}^{+}$ denotes the pseudoinverse of $\mathbf{M}$
$\mathbf{M} = \mathbf{V}_n^{\top}$ is n-truncated right singular vector matrix

The alignment error is

$$\mathcal{E}(x) \leq \frac{1}{\sqrt{n}} \left[\|\mathbf{V}_n^{\top} \mathbf{J}'_x (\mathbf{I} - \mathbf{V}_n \mathbf{V}_n^{\top}) x\| + \sigma_{n+1} \|\mathbf{V}_n^{\top} \mathbf{J}'_y\|_2 \|x\| \right]$$

where $\mathbf{J}'_x, \mathbf{J}'_y$ are Jacobian matrices

The impact of effective low rank on the dynamics

Many dynamics on networks have the form

$$\dot{\boldsymbol{x}} = \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \mathbf{g}(\boldsymbol{x}, \mathbf{W}\boldsymbol{x}) = \mathbf{g}(\boldsymbol{x}, \boldsymbol{y})$$

with $\boldsymbol{x} \in \mathbb{R}^N$.

Examples:

- SIS (mean-field) : $\dot{x}_i = -d_i x_i + \gamma(1 - x_i)\, y_i$
- Wilson-Cowan: $\dot{x}_i = -d_i x_i + (1 - a x_i)\frac{1}{1+e^{-b(\gamma\, y_i - c)}}$
- Recurrent Neural Networks (RNN): $\dot{x}_i = -d_i x_i + \tanh(\gamma y_i + c_i)$
- Kuramoto-Sakaguchi: $\dot{z}_j = \mathrm{i}\omega_j z_j + \gamma\, e^{-\mathrm{i}\alpha}\, y_j - \gamma\, e^{\mathrm{i}\alpha}\, z_j^2\, \bar{y}_j$ with $z_j = e^{\mathrm{i}\theta_j}$
- Population dynamics: $\dot{x}_i = -d x_i + \gamma x_i y_i$ (Lotka-Volterra)
  $\dot{x}_i = -d x_i - s x_i^2 + \gamma \frac{x_i y_i}{\alpha + y_i}$
  $\dot{x}_i = a - d\, x_i + b x_i^2 - c x_i^3 + \gamma\, x_i\, y_i$

for $i, j \in \{1, ..., N\}$ and $y_i = \sum_{j=1}^{N} W_{ij} x_j$.

Original dynamics

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$$\dot{\boldsymbol{X}} = \mathbf{M}\mathbf{g}(\mathbf{M}^{+}\mathbf{X}, \mathbf{W}\mathbf{M}^{+}\mathbf{X})$$

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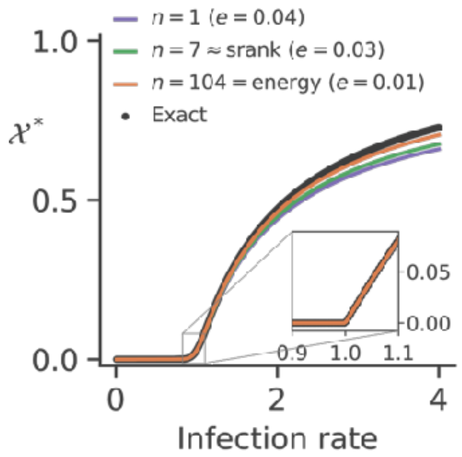
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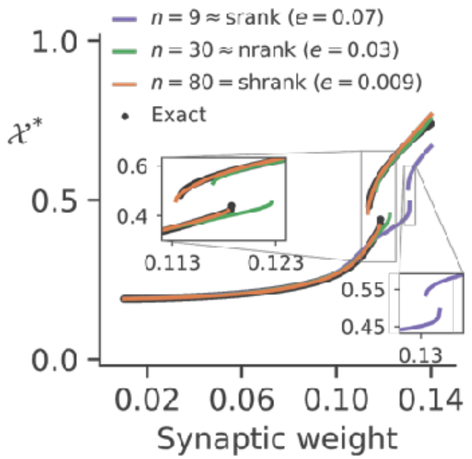
$$\mathcal{E}(x) \leq \frac{1}{\sqrt{n}} \left[\|\mathbf{V}_n^{\top} \mathbf{J}'_x (\mathbf{I} - \mathbf{V}_n \mathbf{V}_n^{\top}) x\| + \sigma_{n+1} \|\mathbf{V}_n^{\top} \mathbf{J}'_y\|_2 \|x\| \right]$$

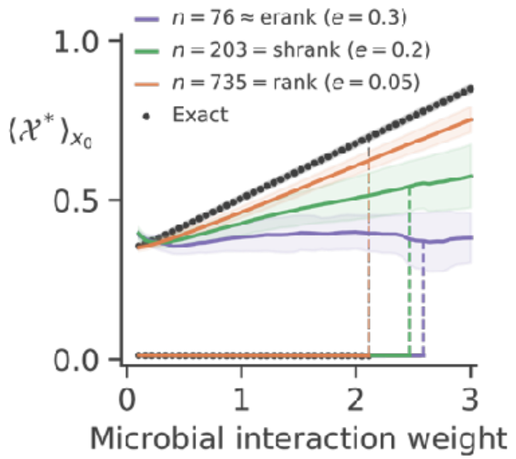
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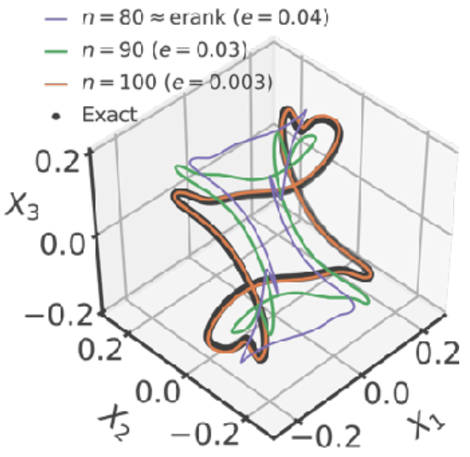
Rapid singular value decrease can induce
rapid alignment error decrease!

Reproduction of the dynamics with increasing accuracy

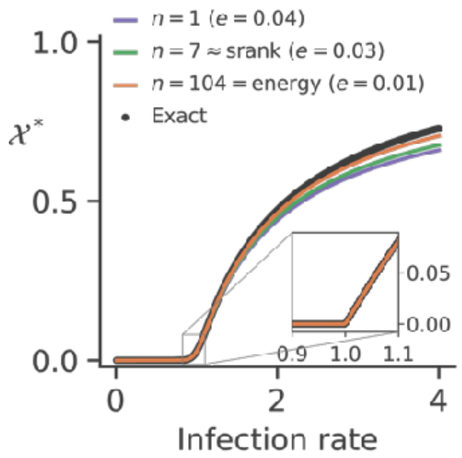


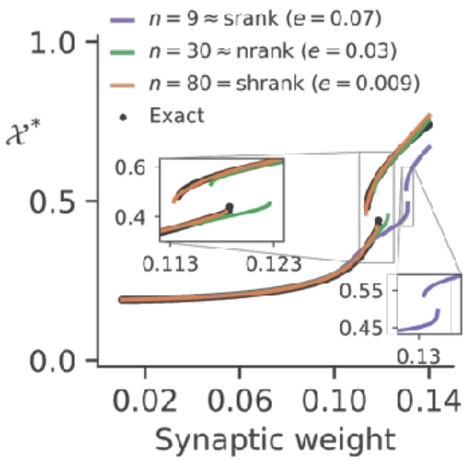


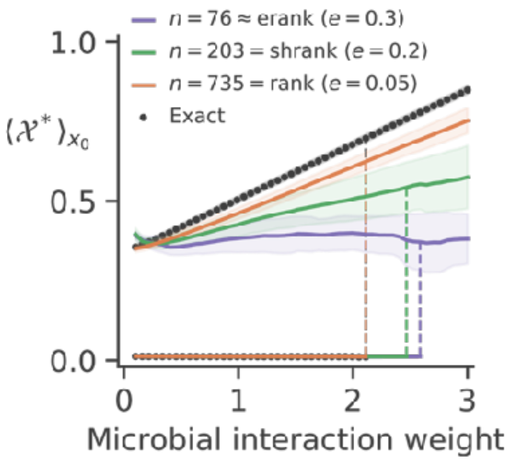


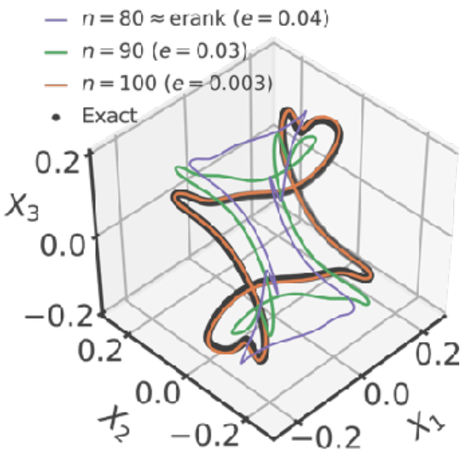


Reproduction of the dynamics with increasing accuracy









Emergence of higher-order interactions

Original Quenched mean-field SIS dynamics

$$\dot{x}_i = -\alpha x_i + \beta(1-x_i)\sum_{j=1}^{N} W_{ij}x_j, \quad i \in \{1,...,N\}$$

Reduced dynamics

$$\dot{X}_\mu = -\alpha X_\mu + \beta\sum_{\nu=1}^{n}\mathcal{W}_{\mu\nu}X_\nu - \beta\sum_{\nu,\tau=1}^{n}\mathcal{W}^{(3)}_{\mu\nu\tau}X_\nu X_\tau, \quad \mu \in \{1,...,n\}$$

Original Kuramoto-Sakaguchi dynamics

$$\dot{z}_j = i\omega_j z_j + \sum_{k=1}^{N} W_{jk}[z_k e^{-i\alpha} - z_j^2 \bar{z}_k e^{i\alpha}], \quad j \in \{1,...,N\}$$

Reduced dynamics

$$\dot{Z}_\mu = i\sum_{\nu=1}^{n}\Omega_{\mu\nu}Z_\nu + \sum_{\nu=1}^{n}\mathcal{W}^{(2)}_{\mu\nu}Z_\nu e^{-i\alpha} - \sum_{\alpha,\beta,\gamma=1}^{n}\mathcal{W}^{(4)}_{\mu\alpha\beta\gamma}Z_\alpha Z_\beta \bar{Z}_\gamma e^{i\alpha}$$

Main takeaways

- The rapid decrease of the singular values of adjacency matrices (i.e. low effective rank) offers a *justification* for low-dimensional mathematical models beyond mathematical and/or conceptual convenience.
- A large proportion of real networks can be considered as having a low effective rank.
- The higher-order interactions observed in some systems could be a byproduct of a low-dimensional representation used to analyze them.


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Article

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The low-rank hypothesis of complex systems

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Vincent Thibeault[1,2], Antoine Allard[1,2] & Patrick Desrosiers[1,2,3]

Challenges and open questions

- Could we measure the effective dimension independently?
- Could we design a random graph model based on observed singular values (singular vectors)?
- Are some of the higher-order interactions inferred from time series artifacts of coarse-grained observations?
- Could we designed more interpretable observables, perhaps nonlinear ones?



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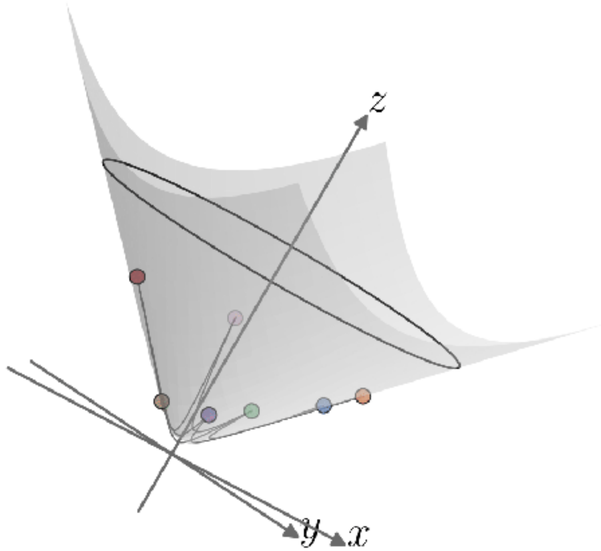
Outline

1. Are simple models enough to study complex systems/networks?

2. **“Simple” ways to encode structural complexity**

   (a) latent metric space

   (b) stub types



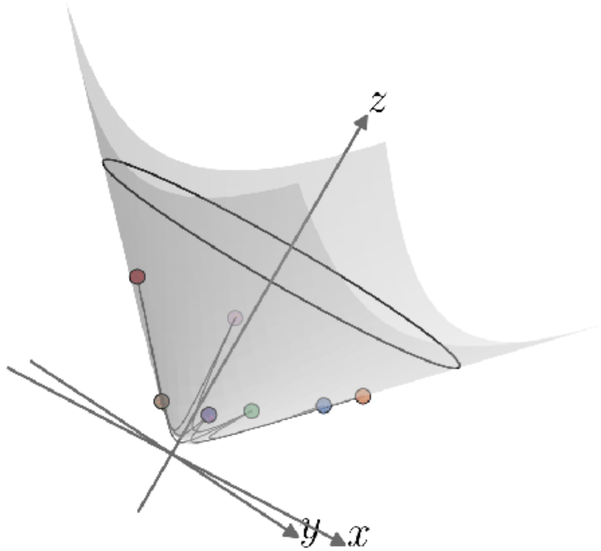
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Maximally random graph ensembles

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)

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

Phys. Rev. E 70, 066117 (2004)
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 factorised informs us on the degree-degree correlations observed in real networks.

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Modeling clustering

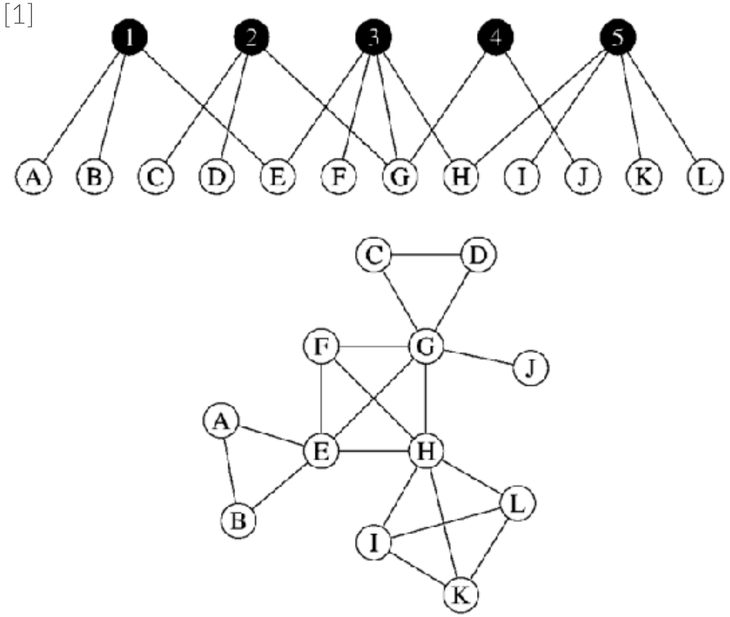
Tricky because clustering consists in three-node interactions while our mathematical tools rely on pairwise interactions either explicitly or implicitly.

Straightforward inclusion of triangles to the maximally random graph ensemble formalism yields unwanted behavior (ex.: triangle agglutination in the Strauss model [6]).

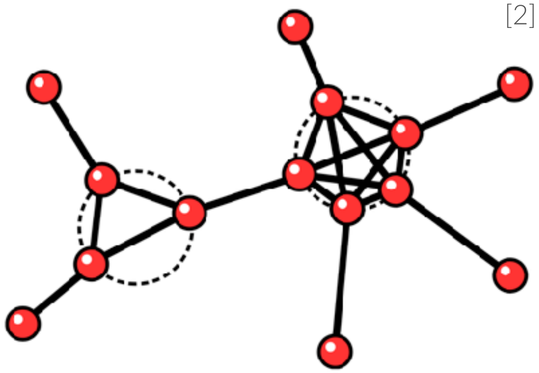
Most models therefore assume

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

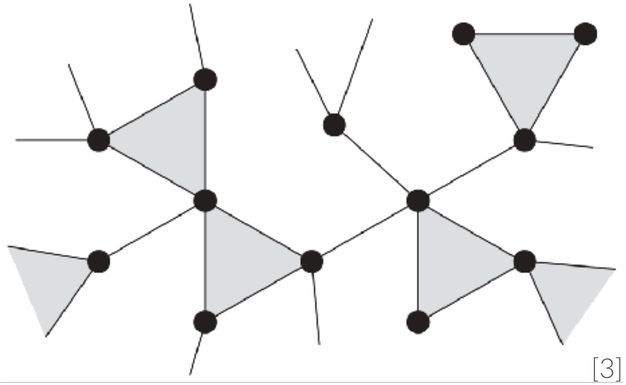
[1]



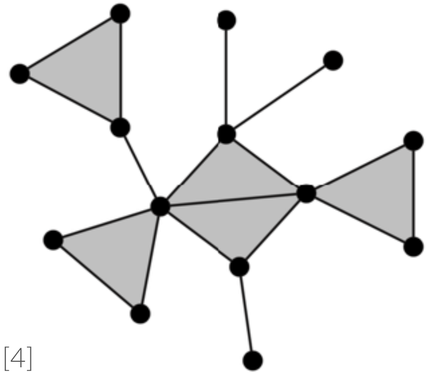
[2]



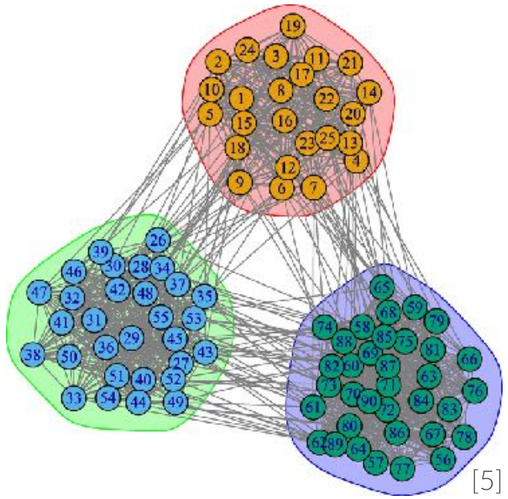
[3]



[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)
[6] Phys. Rev. E 72, 026136 (2005)

Modeling clustering

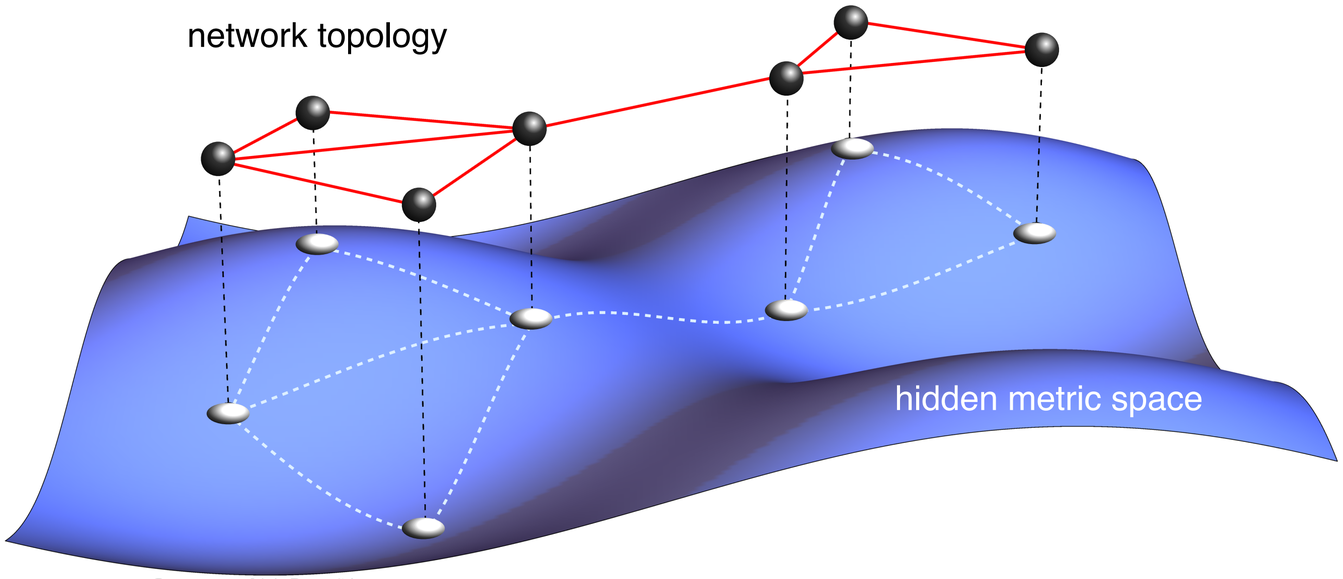
Assume that the nodes are embedded in a metric space and that any two nodes are connected with a probability that is a decreasing function of the distance between them.

Modeling 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.

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	$d(x,y) \leq d(x,z) + d(z,y)$



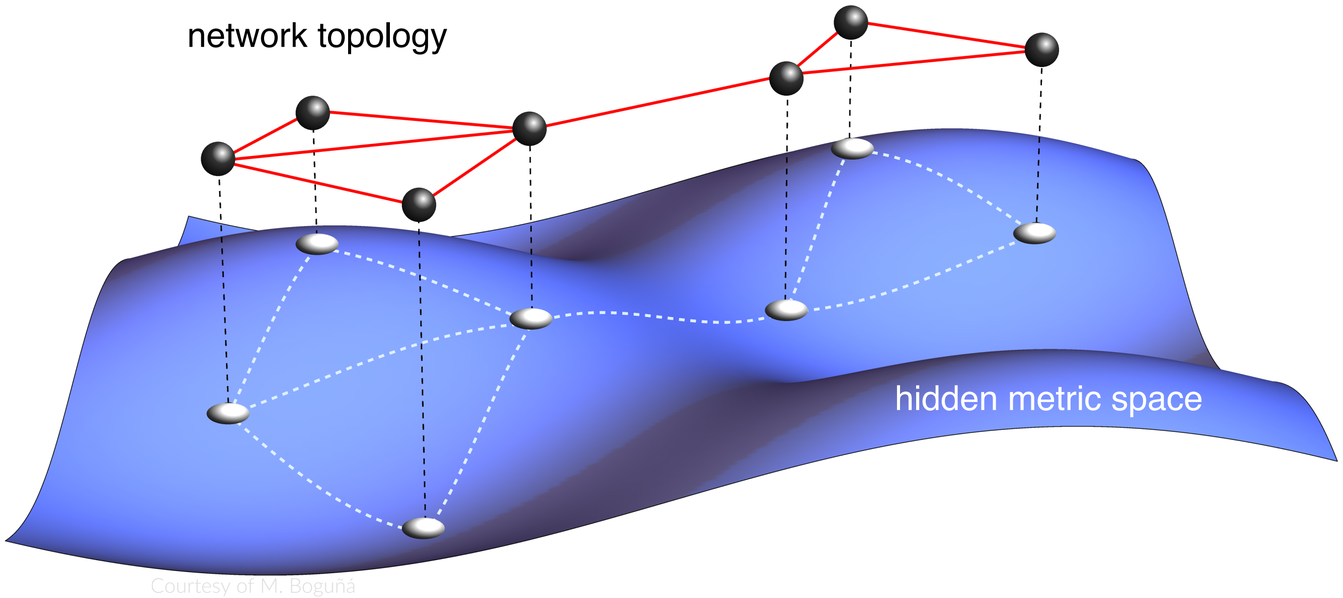
Courtesy of M. Boguñá

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Courtesy of M. Boguñá

Henceforth we assume that there is a distance matrix

$$\mathbb{X} = \{x_{ij}\}$$

where x_{ij} is the distance between vertices i and j.

Maximally random geometric graph ensembles

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

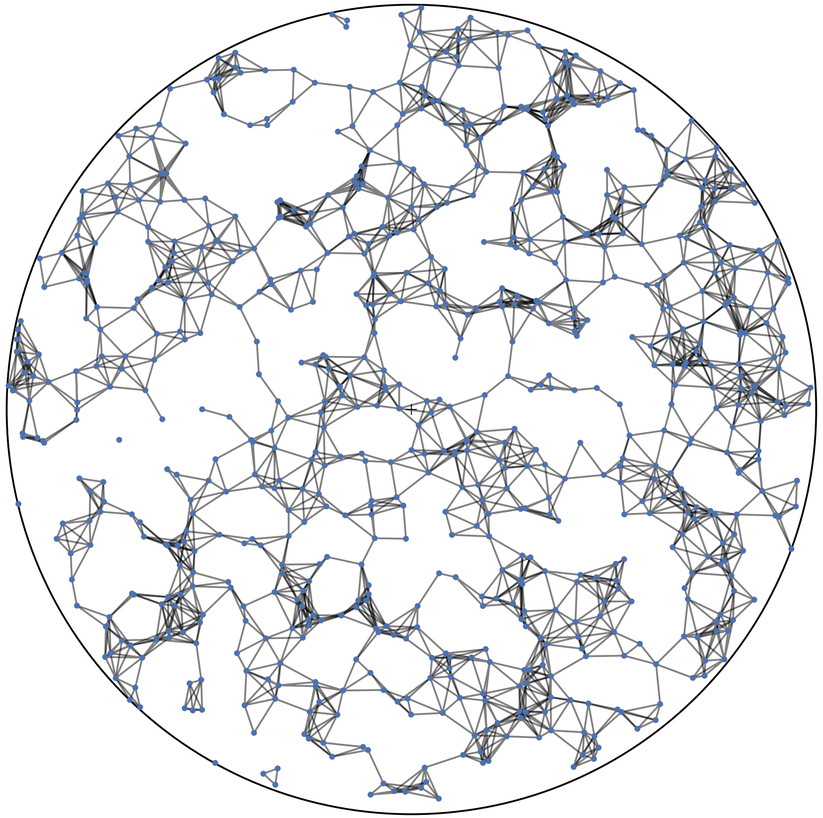
$$\bar{F}_1 = \sum_{i=1}^{N} \sum_{j=i+1}^{N} a_{ij} = M$$

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

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.

Phys. Rev. E 80, 035101 (2009)
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Maximally random geometric graph ensembles

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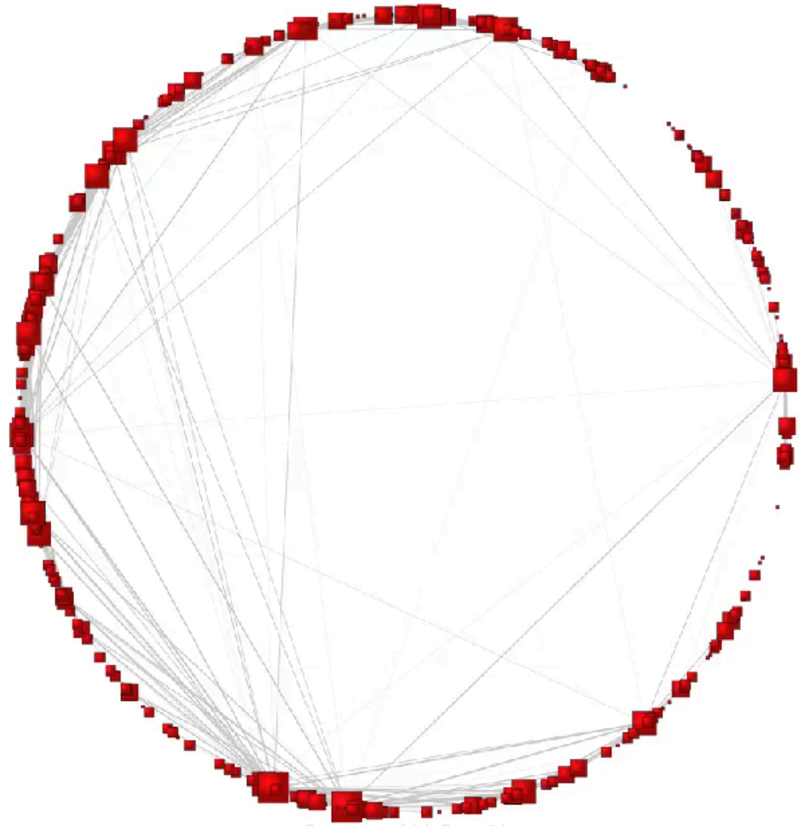
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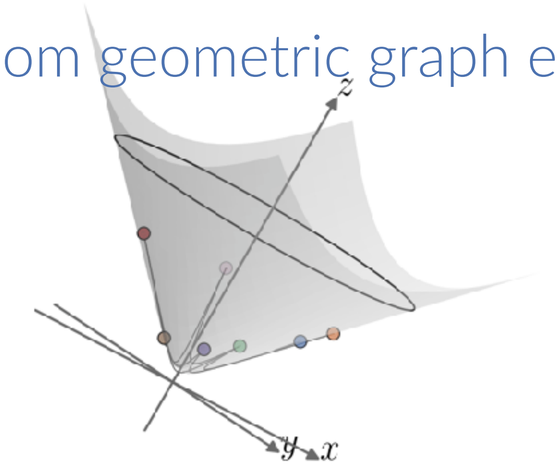
When the geometry is a D-dimensional sphere, $\mathbb{S}^D$ the model can be mapped to a purely geometric model in hyperbolic space $\mathbb{H}^{D+1}$.



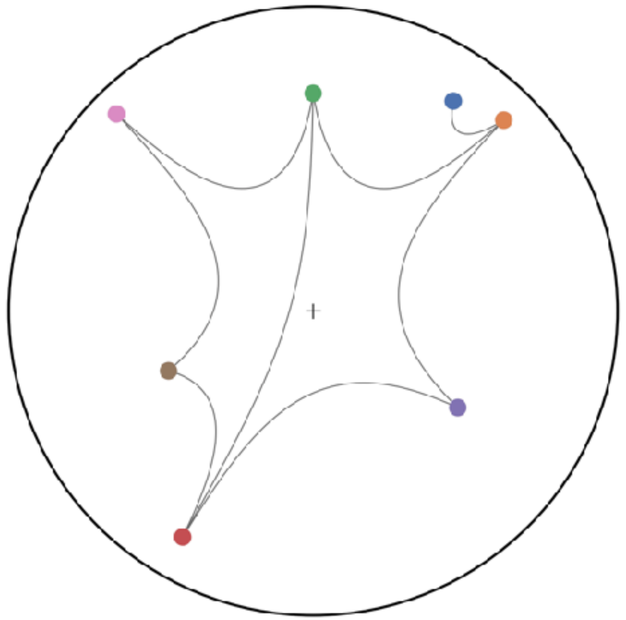
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Maximally random geometric graph ensembles

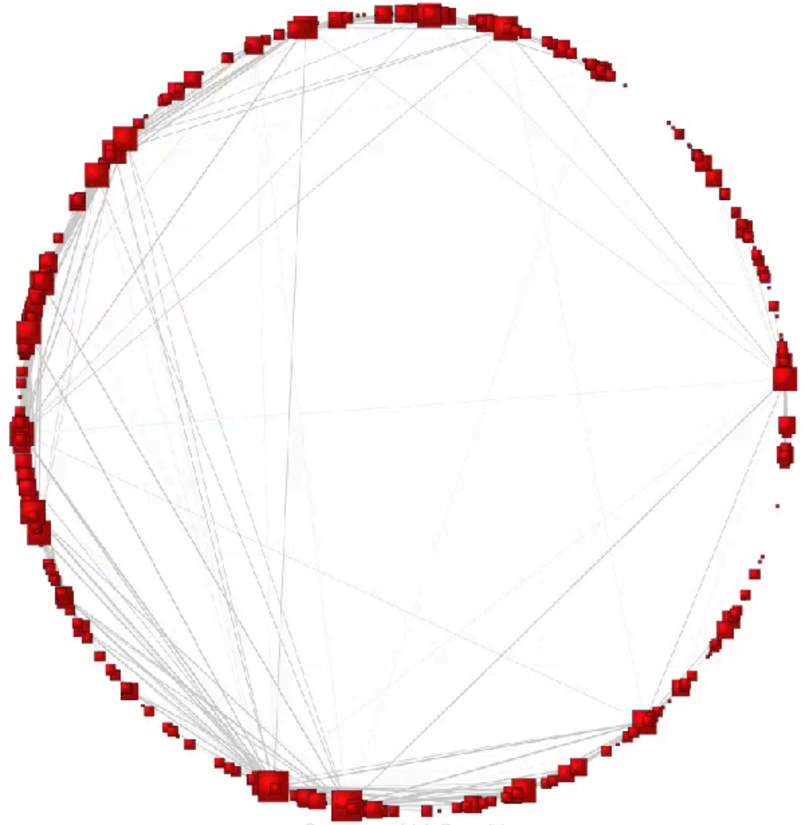


hyperboloid in $\mathbb{R}^{2,1}$



hyperbolic disk (r, θ)

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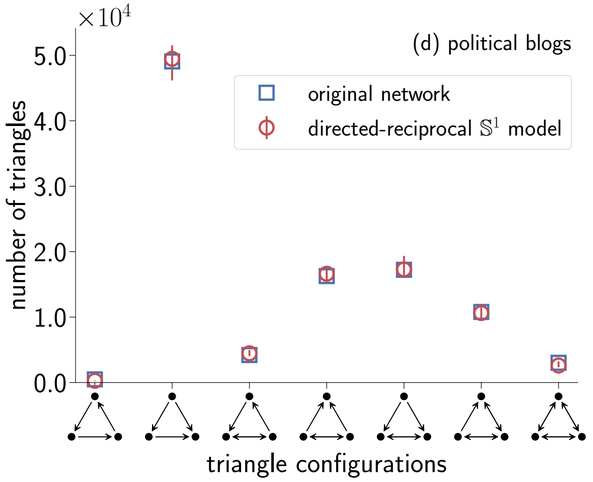
A powerful and versatile framework

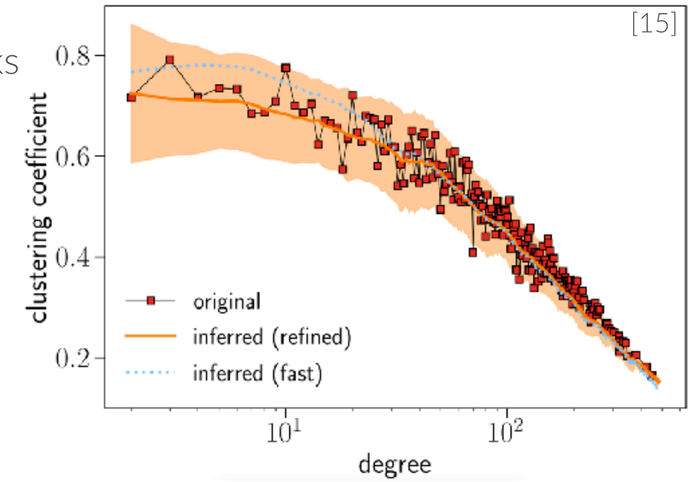
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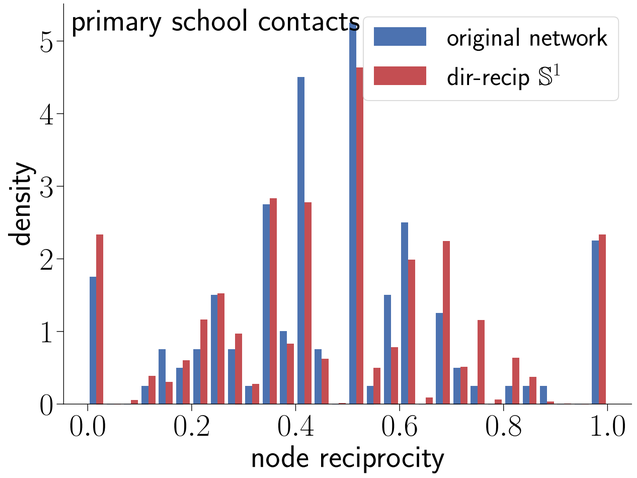
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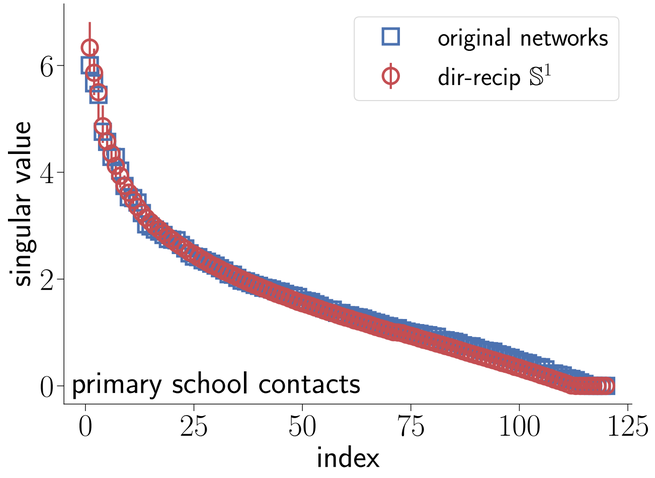
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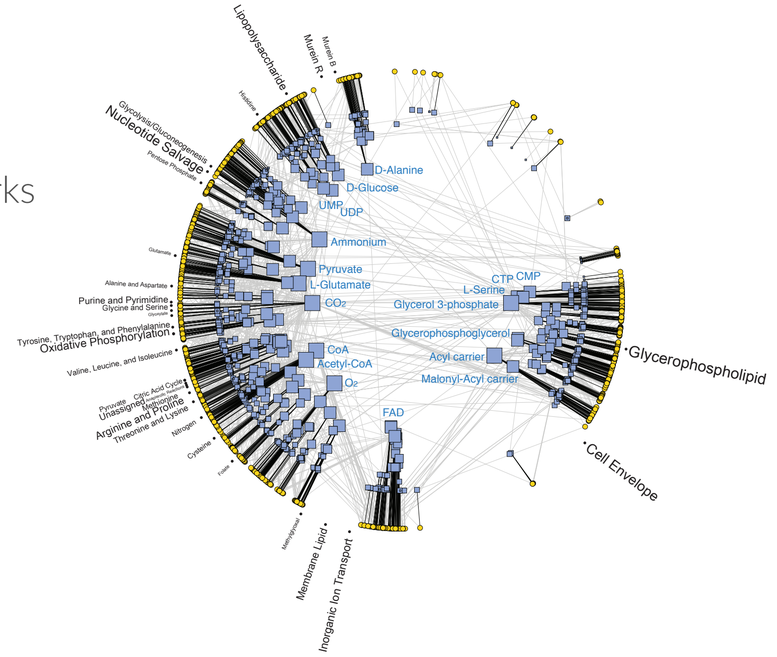




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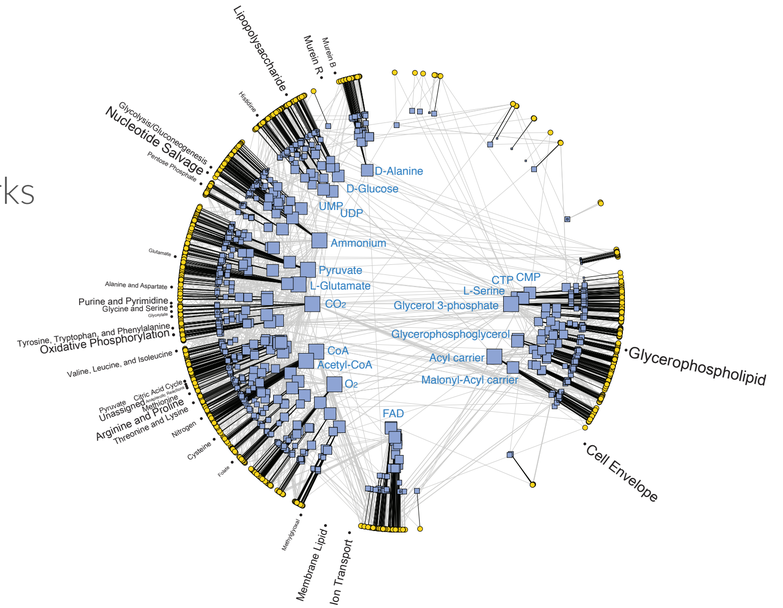
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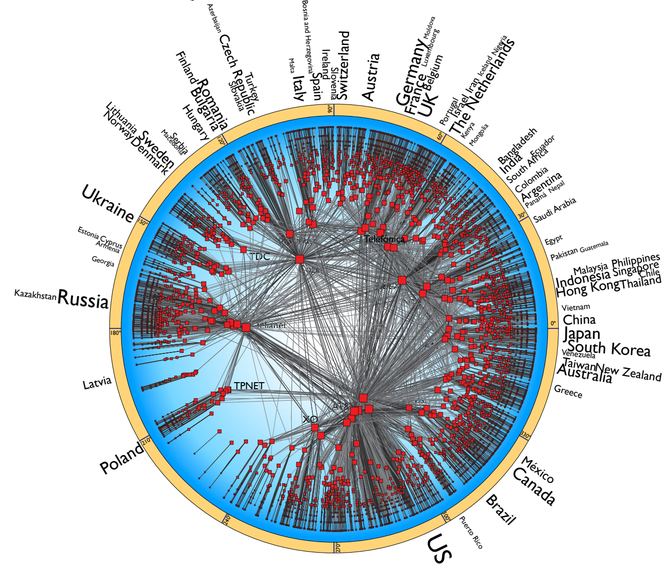


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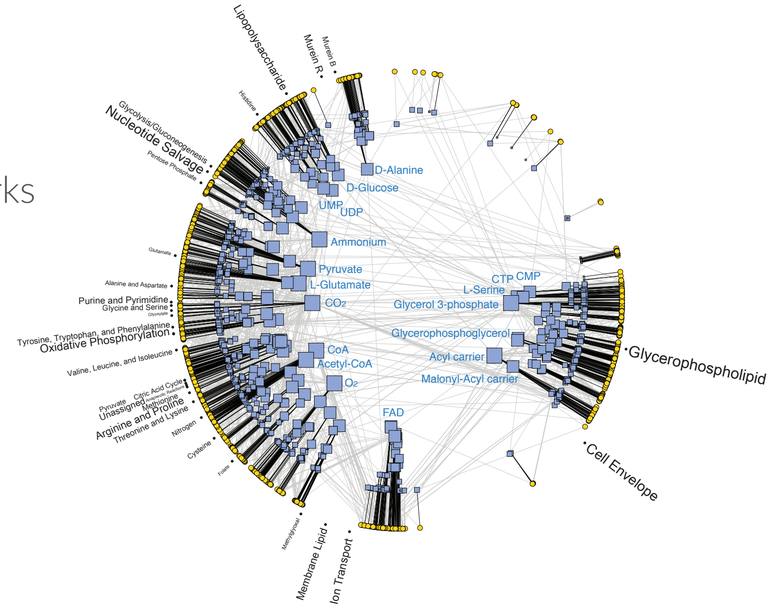


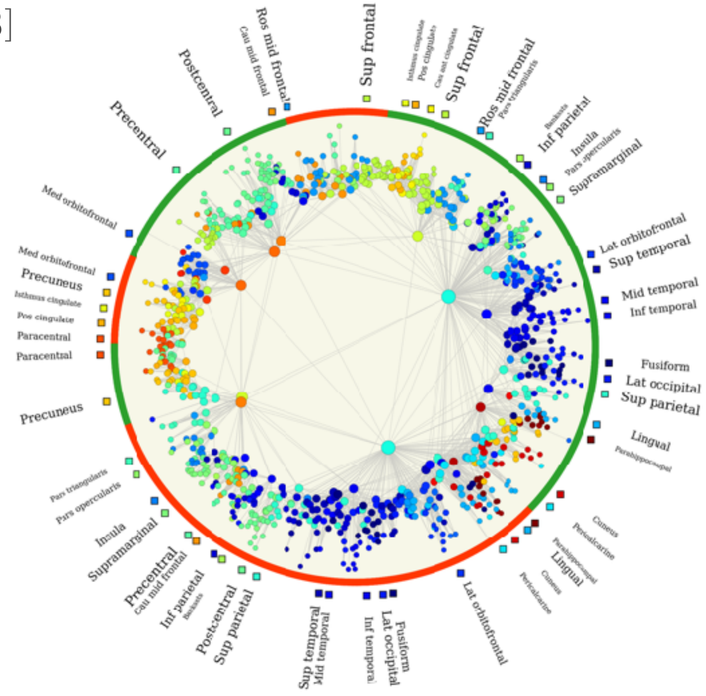


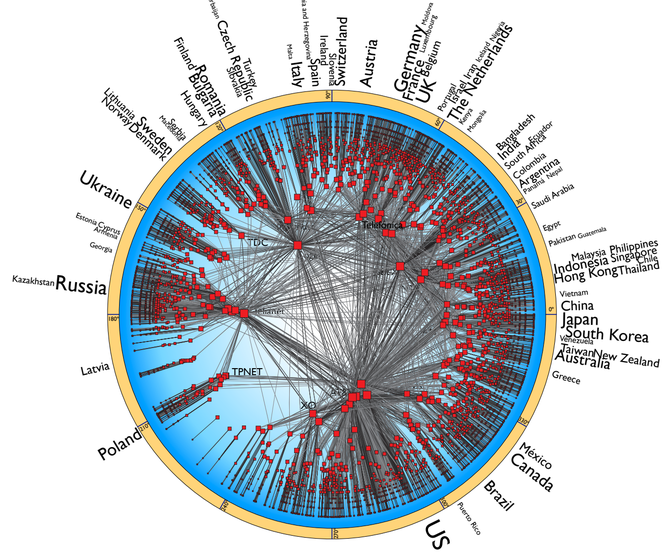
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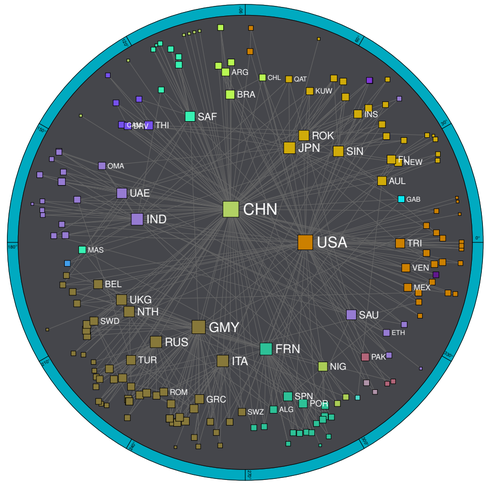


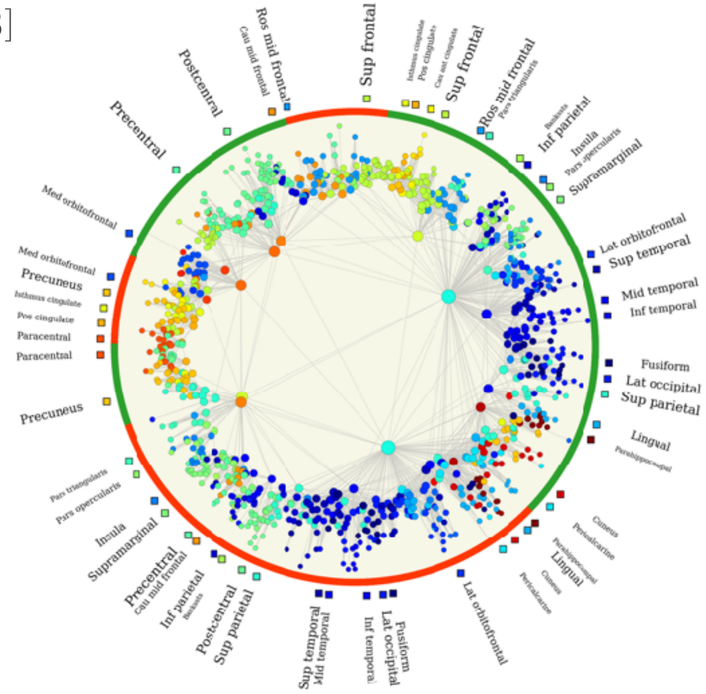


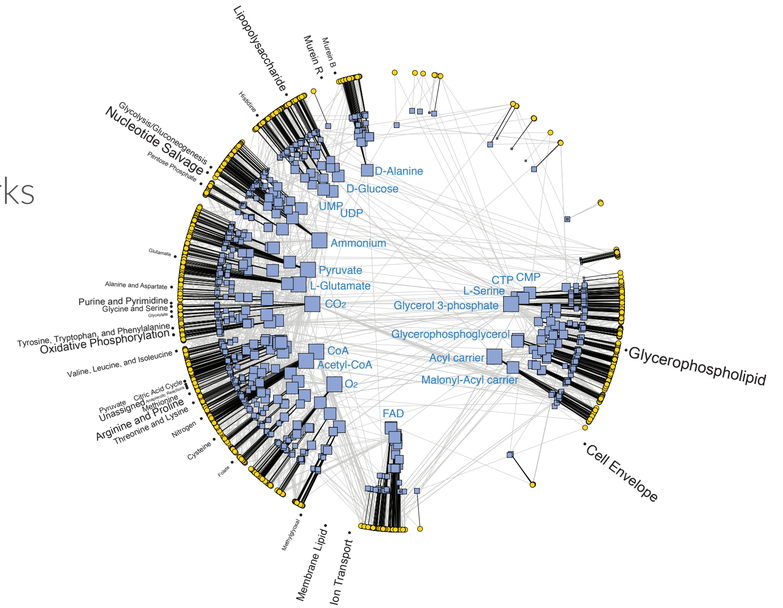
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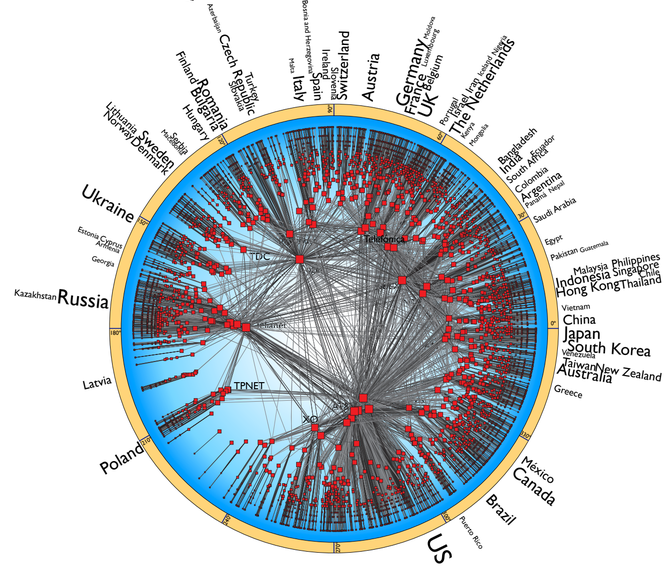
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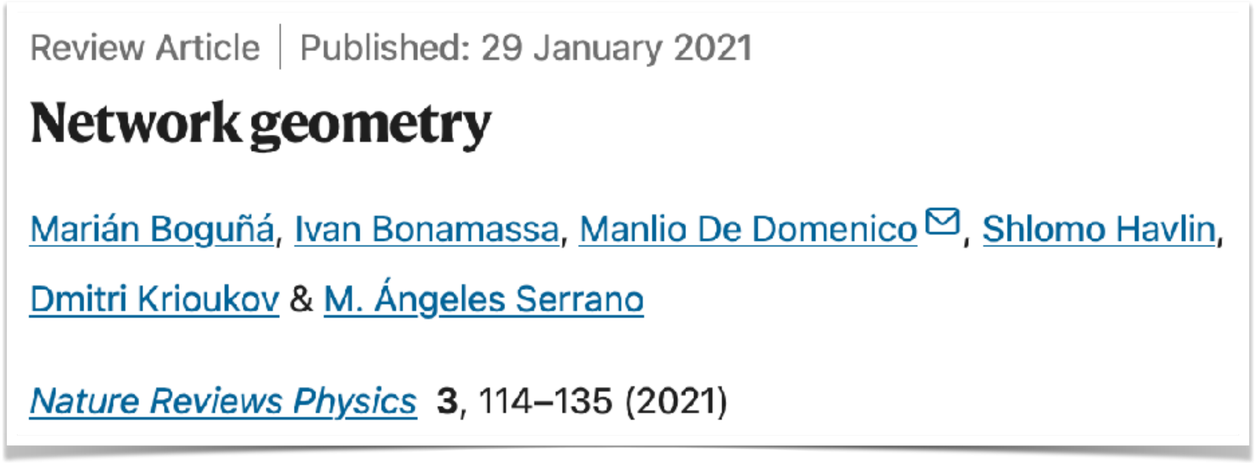




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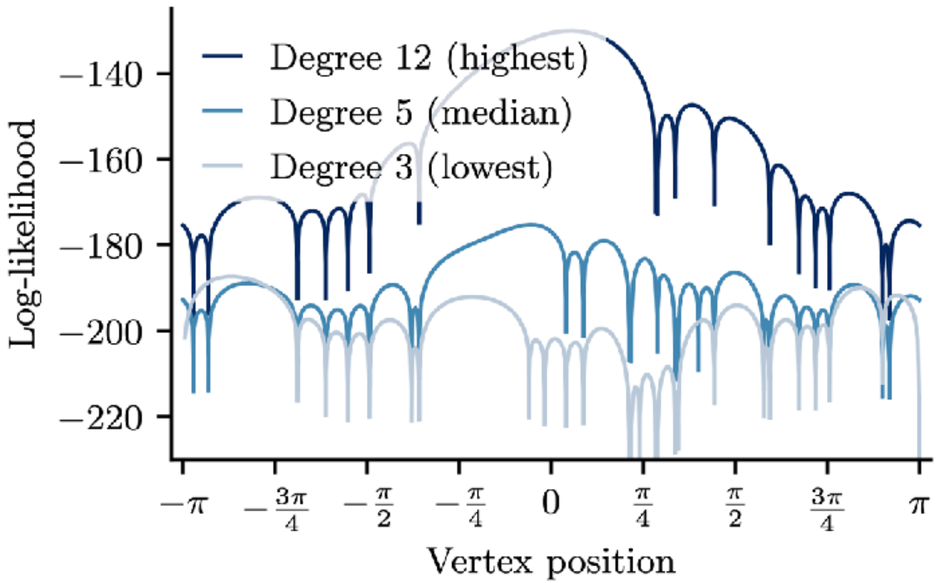
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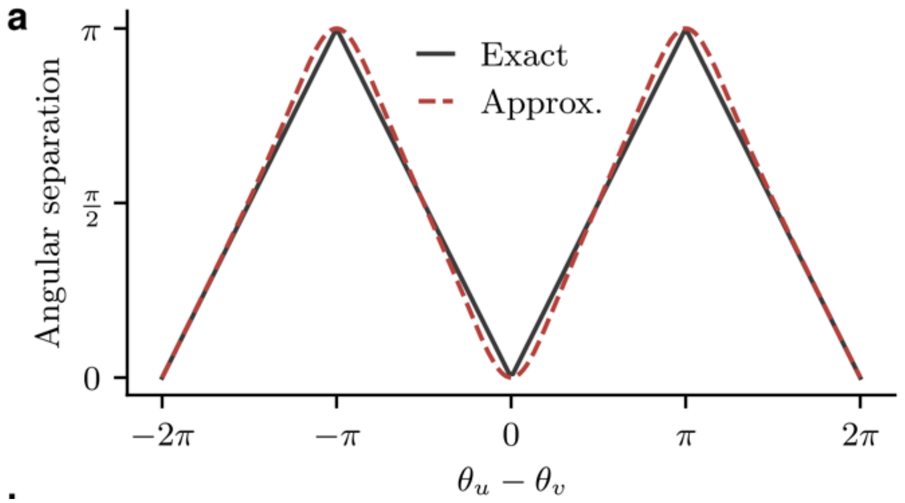
Challenges

Heterogeneous random geometric graph models are prime candidates to model real networked complex systems.

But they rely heavily on our capacity to find high-quality embeddings of the original datasets.

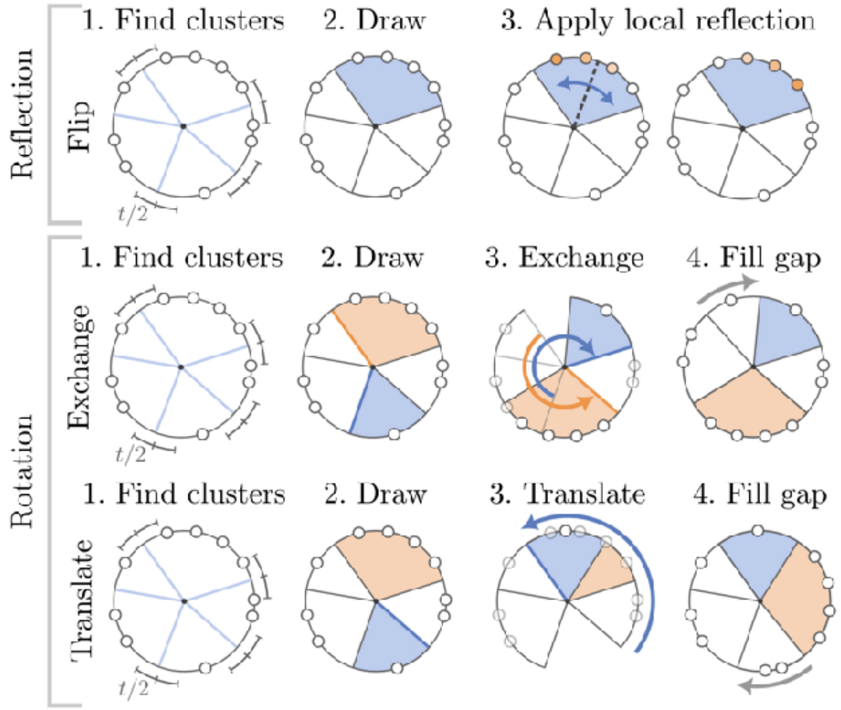
- ▷ Difficult optimization problem
  - rugged landscape
  - numerous symmetries (rotation, reflection, graph automorphisms)
  - gradient not always well defined
- ▷ Out-of-the-box solutions do not work well
  - Hamiltonian Monte Carlo
  - gradient descent
- ▷ Current state-of-the-art embedding methods
  - rely on heuristics
  - do not provide uncertainties (loglikelihood maximization)



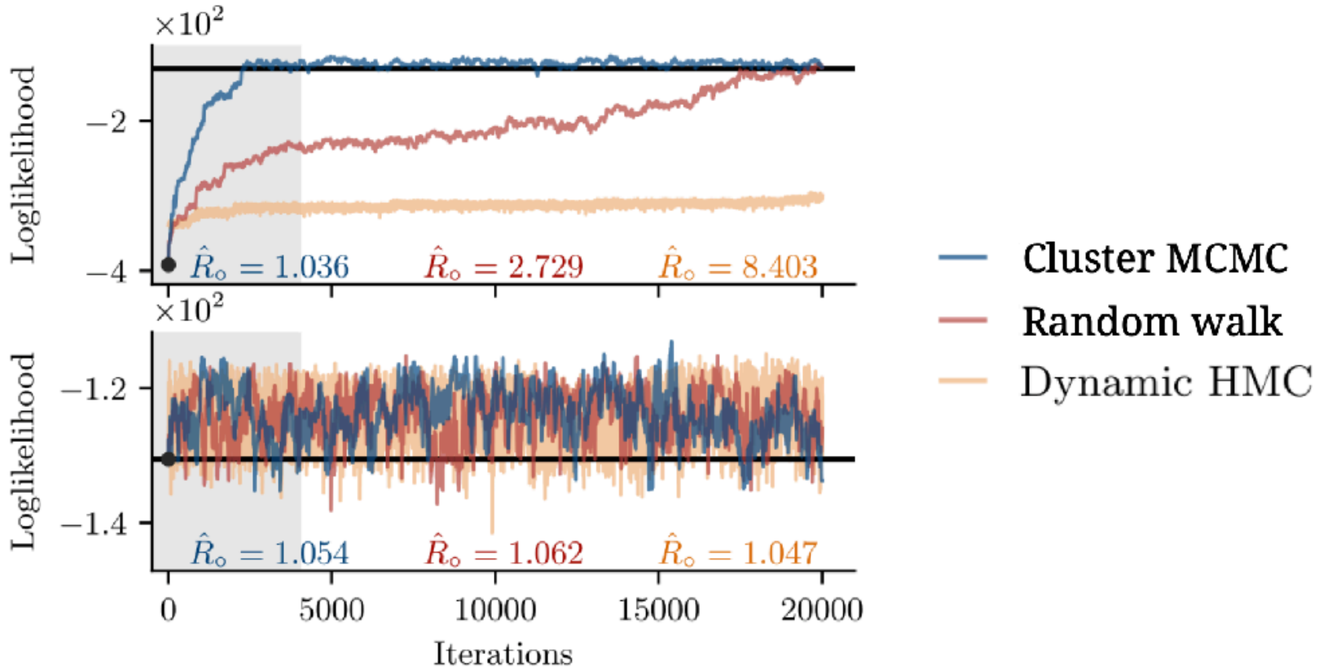


Challenges: some solutions

Leverage the specificities of the model to design better sampling algorithm.

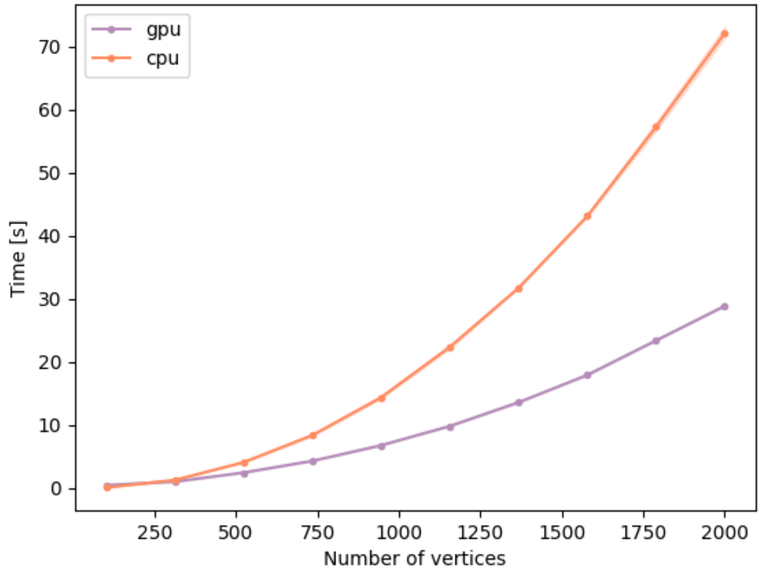


Better mixing and exploration than standard sampling algorithms.

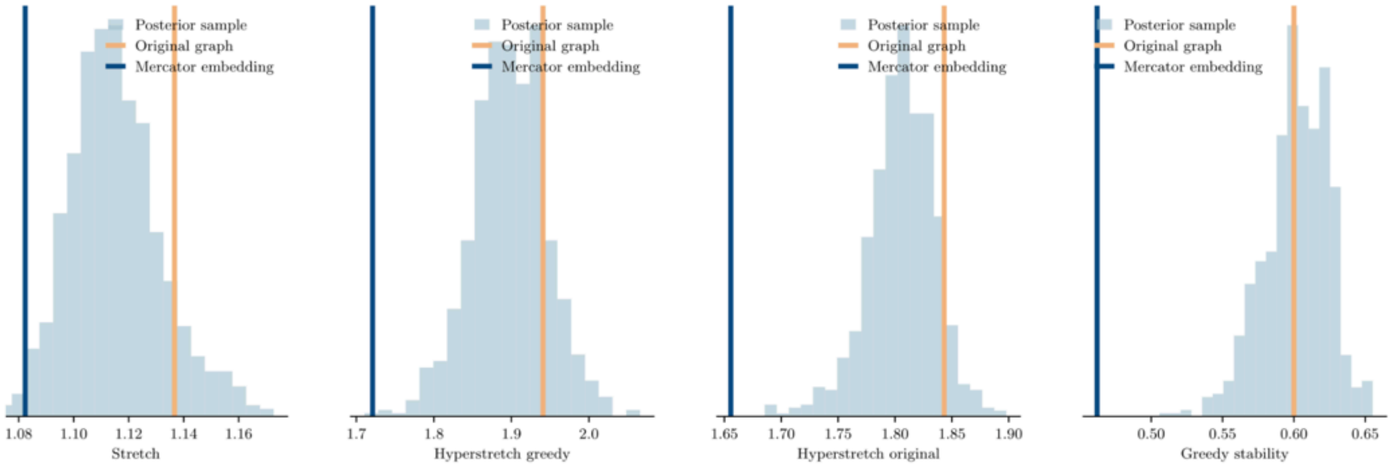


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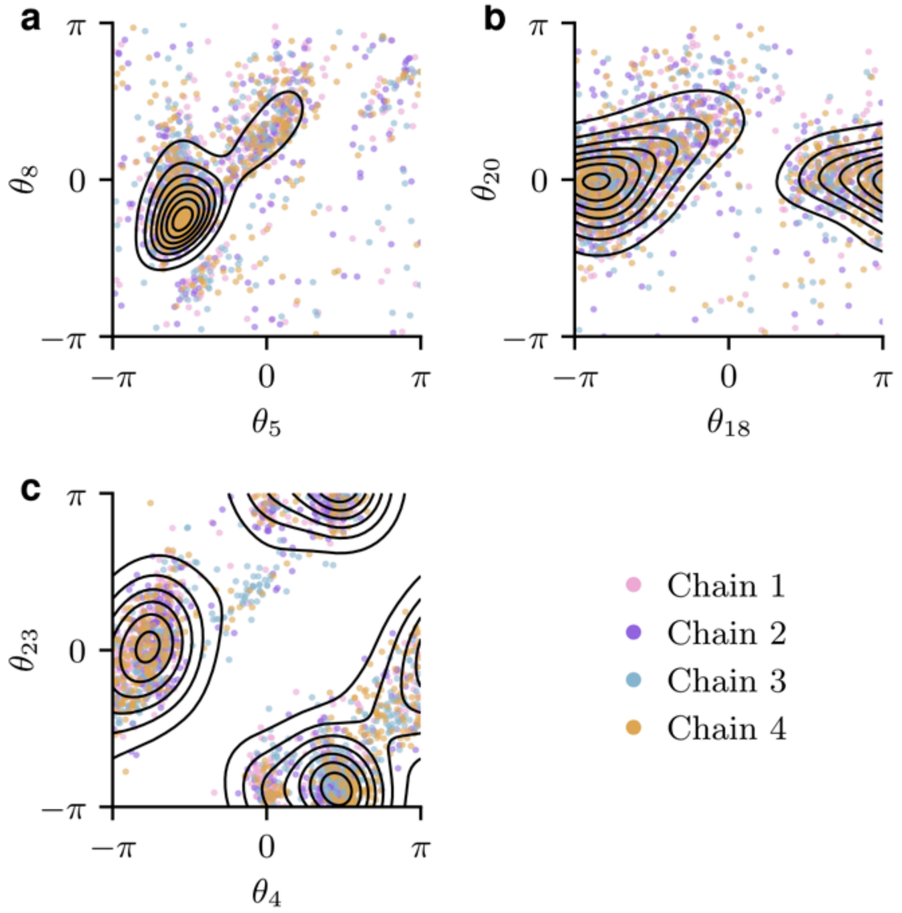
Still slow…



…but we now have uncertainties on graph metrics!



…and these uncertainties are not “trivial” (non-normal).



Challenges

- Network geometry is a promising framework, but its applicability relies heavily on our capacity to find high- bquality embeddings of the original datasets, which is hard.
- We cannot power our way through this challenge using GPUs or supercomputers: we need to design smarter algorithms.



M. Ángeles Serrano
Universitat de Barcelona & ICREA



Jérémi Lesage
Université Laval

Marián Boguñá
Universitat de Barcelona

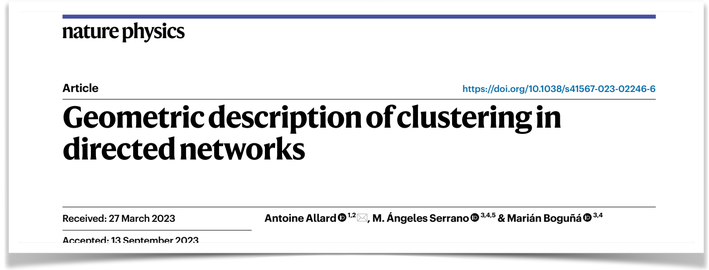


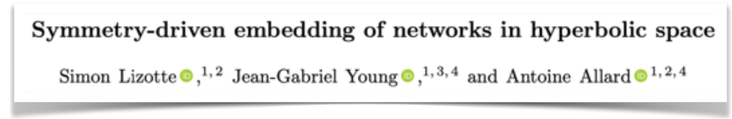


Jean-Gabriel Young
University of Vermont

Simon Lizotte
Université Laval







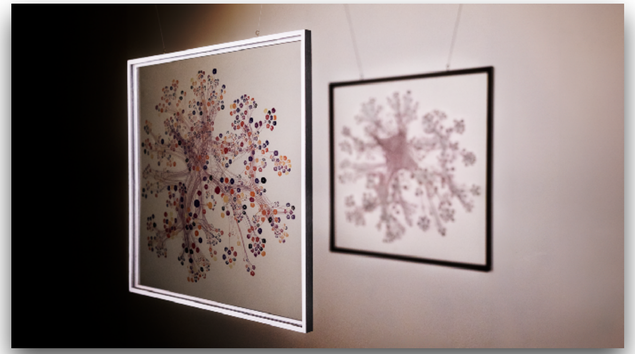
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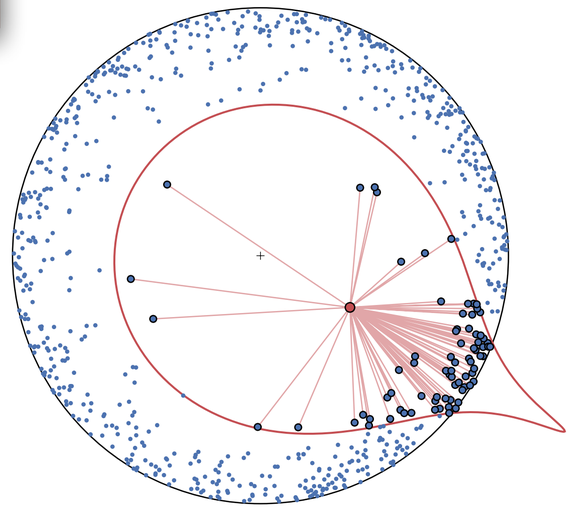


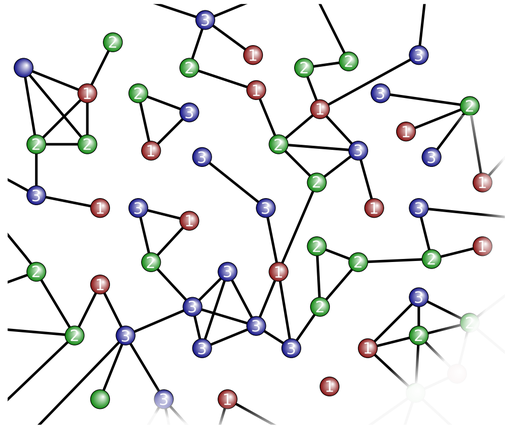
Preprint on arXiv expected early 2025

Theoretical justifications exist for the use of "simple" models of complex networks and of the dynamics they support.

Simple models can reproduce nontrivial complex connections patterns observed in real networks, but there are still several challenges ahead to bridge the gap between our models and real networks.







Slides

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