SIAM DS 2023 (arxiv ID: 2208.04848)

The low-rank hypothesis of complex systems:

From empirical and theoretical evidence to the emergence of higher-order interactions

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May 16, 2023

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Dynamica

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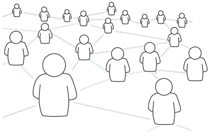
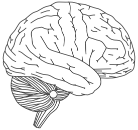
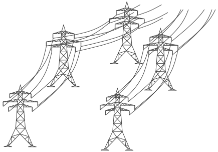
Sociological



Biological

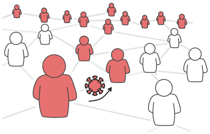


Technological



Complex systems : high dimension and emergent collective phenomena

Sociological



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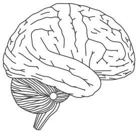

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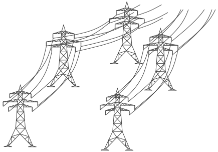

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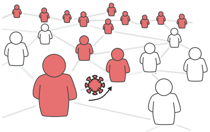

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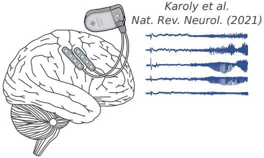

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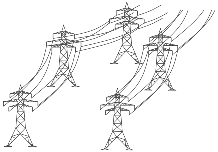

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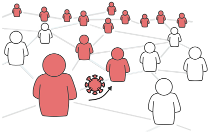

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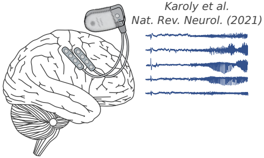

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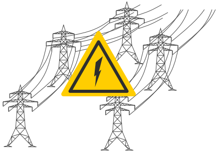

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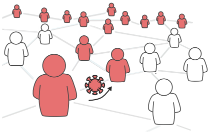

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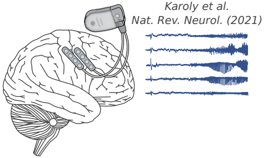

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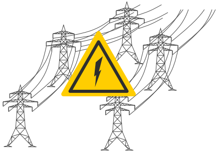
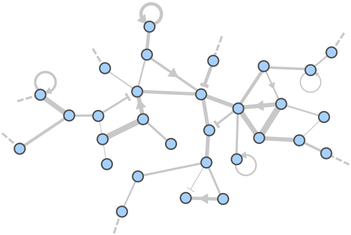


Complex network

W

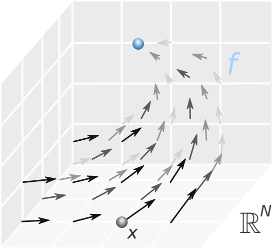


Vector field

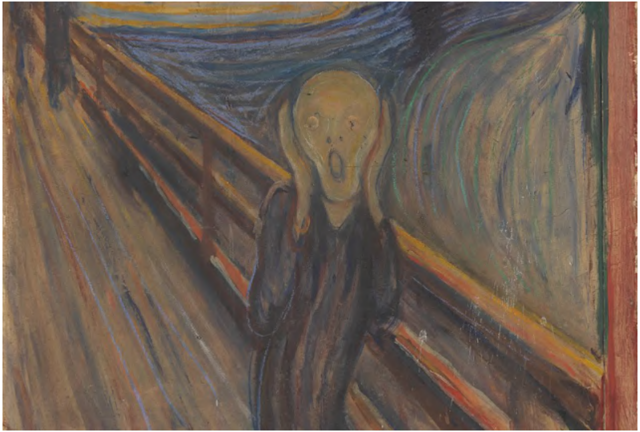
f

High-dimensional dynamics

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



A low-dimensional description of a high-dimensional complex system? Paradox?



"The Scream of Dimensionality"

Nature Vol. 261 June 10 1976 459

review article

Simple mathematical models with very complicated dynamics

Robert M. May*

E.g. : Logistic equations

First-order difference equations arise in many contexts in the biological, economic and social sciences. Such equations, even though simple and deterministic, can exhibit a surprising array of dynamical behaviour, from stable points, to a bifurcating hierarchy of stable cycles, to apparently random fluctuations. There are consequently many fascinating problems, some concerned with delicate mathematical aspects of the fine structure of the trajectories, and some concerned with the practical implications and applications. This is an interpretive review of them.

Statistical physics and biology

GIORGIO PARISI

The relationship between biology and physics has often been close and, at times, uneasy. During this century many physicists have moved to work in biology. Amongst the most famous are Francis

have a satisfactory formulation of the laws.

However, a knowledge of the laws that govern the behaviour of the constituent elements of the system does not necessarily imply an understanding of the

About spin-glasses:

enormous richness and complexity of such an apparently simple system. A more detailed description would take us

THE GENERAL AND LOGICAL THEORY OF AUTOMATA

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Neural Networks, Vol. 6, pp. 801–806, 1993
Printed in the USA.

0893-6080/93 $6.0(

Approximation of Dynamical Systems by Continuous Time Recurrent Neural Networks

KEN-ICHI FUNAHASHI AND YUICHI NAKAMURA

Toyohashi University of Technology

(*Received* 16 *March* 1992; *revised and accepted* 10 *November* 1992)

Abstract—*In this paper, we prove that any finite time trajectory of a given n-dimensional dynamical system can be approximately realized by the internal state of the output units of a continuous time recurrent neural network with n output units, some hidden units, and an appropriate initial condition. The essential idea of the proof is to embed*

What about the “dimensionality” of complex networks ?

→

W

Real matrix
rank $W = r$

What about the "dimensionality" of complex networks ?

Singular value decomposition (SVD)

$\longrightarrow$ $W = U \,\mathrm{diag}(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0)\, V^{\mathsf{T}}$

W	U	$\sigma_1 \ldots \sigma_r$, 0 … 0	V^{T}
Real matrix rank $W = r$	*Orthogonal matrix*	*Diagonal matrix*	*Orthogonal matrix*

Rank r : how many singular values are not zero

What about the “dimensionality” of complex networks ?

Singular value decomposition (SVD)

$$\longrightarrow \; W = U \begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & \ddots \; 0 \end{pmatrix} V^{\mathsf{T}} \simeq U_n \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} V_n^{\mathsf{T}}$$

Exact for n = r

W	U		V^{T}
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$\longrightarrow$

Singular value decomposition (SVD) *Optimal low-rank approximation*

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Real matrix rank $W = r$ — *Orthogonal matrix* — *Diagonal matrix* — *Orthogonal matrix*

Exact for $n = r$

Eckart-Young theorem (1936)

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Singular value decomposition (SVD) — *Optimal low-rank approximation*

$$W = U \begin{pmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & 0 \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} V^\top \simeq U_n \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} V_n^\top$$

Real matrix rank $W = r$ — *Orthogonal matrix* (U) — *Diagonal matrix* — *Orthogonal matrix* ($V^\top$)

Exact for $n = r$
Eckart-Young theorem (1936)

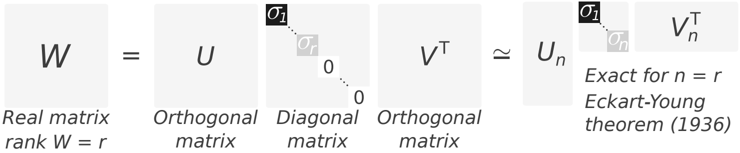
Rank r : how many singular values are not zero

Effective rank : how many singular values are significant

e.g., the stable rank is $\text{srank}(W) = \sum_{i=1}^{r} \sigma_i^2 / \sigma_1^2$

What about the “dimensionality” of complex networks ?

Singular value decomposition (SVD) *Optimal low-rank approximation*



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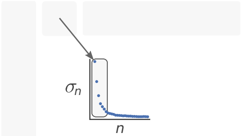
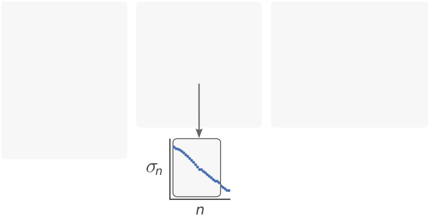


Low effective rank

or



High effective rank

?

First indicator of the low-rank hypothesis

We observe that many **random graphs** are described as

Random weight matrix | *Expected weight matrix* $\langle W \rangle$ | *Random noise matrix*

$$W = \Phi(L) + R$$

Low-rank matrix L

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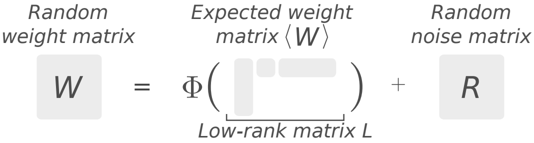

Model	**Low-rank matrix** L	$\mathrm{rank}(L)$	$\Phi(L)$
$\mathcal{G}(N,p)$	$Np\,\hat{\mathbf{1}}\hat{\mathbf{1}}^\top$	1	L
Chung-Lu	$\frac{\lVert\kappa\rVert^2}{2M}\hat{\boldsymbol{\kappa}}\hat{\boldsymbol{\kappa}}^\top$	1	L

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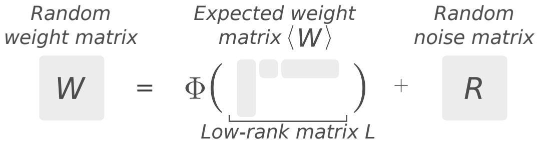

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Degree-corrected stochastic block	$\Lambda \circ (\hat{\boldsymbol{\kappa}}_{\mathrm{in}}\hat{\boldsymbol{\kappa}}_{\mathrm{out}}^\top)$	$\leq$ #blocks	L

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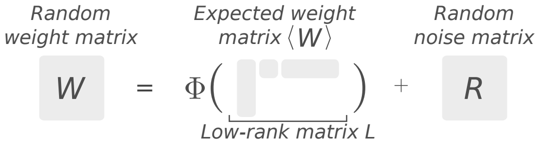

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Degree-corrected stochastic block	$\Lambda \circ (\hat{\boldsymbol{\kappa}}_{\text{in}}\hat{\boldsymbol{\kappa}}_{\text{out}}^\top)$	$\leq$ #blocks	L
Soft configuration*	$\boldsymbol{y}\bar{\boldsymbol{y}}^\top$	1	$\frac{L}{1-L}$
S^1 random geometric	$\frac{R^2}{\mu^2}\left(\bar{\boldsymbol{\kappa}}_{\text{in}}\,\bar{\boldsymbol{\kappa}}_{\text{out}}^\top\right)\circ\bar{\theta}$	≤ 3 **	$\frac{1}{1+L^{\beta/2}}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

* Garlaschelli, *Phys. Rev. Lett.*, 2009

** Gower, *Linear Algebra Appl.*, 1985

Impact on the random weight matrix

Hermann Weyl, Math. Ann., 1912

Ky Fan, PNAS, 1951

$$\sigma_{i+j-1}(A+B) \leq \sigma_i(A) + \sigma_j(B) \qquad \forall\, 1 \leq i,\, j,\, i+j-1 \leq N,$$

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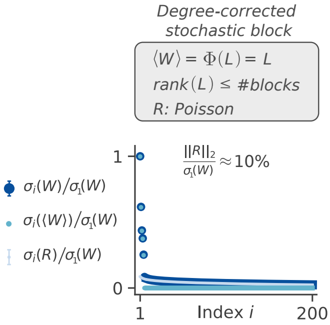
$$\Downarrow$$

$$|\sigma_i(W) - \sigma_i(\langle W \rangle)| \leq \underbrace{\|R\|_2}_{\text{"Noise strength"}}$$

"the singular values of W cannot deviate from those of $\langle W \rangle$ more than $\|R\|_2$"

Second indicator of the low-rank hypothesis : Rapid singular value decrease



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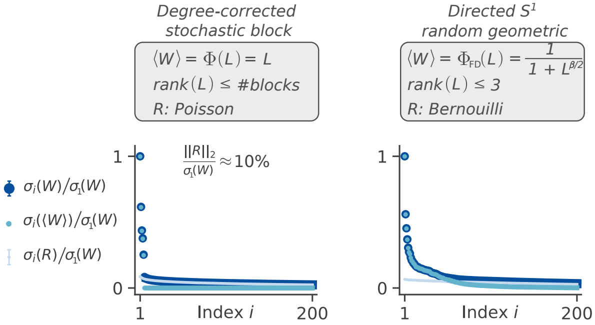

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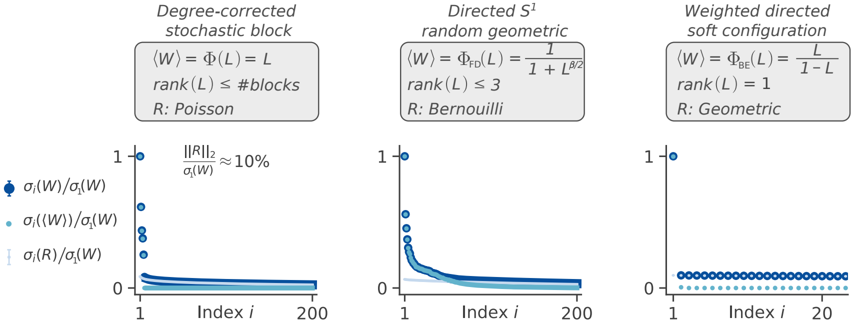

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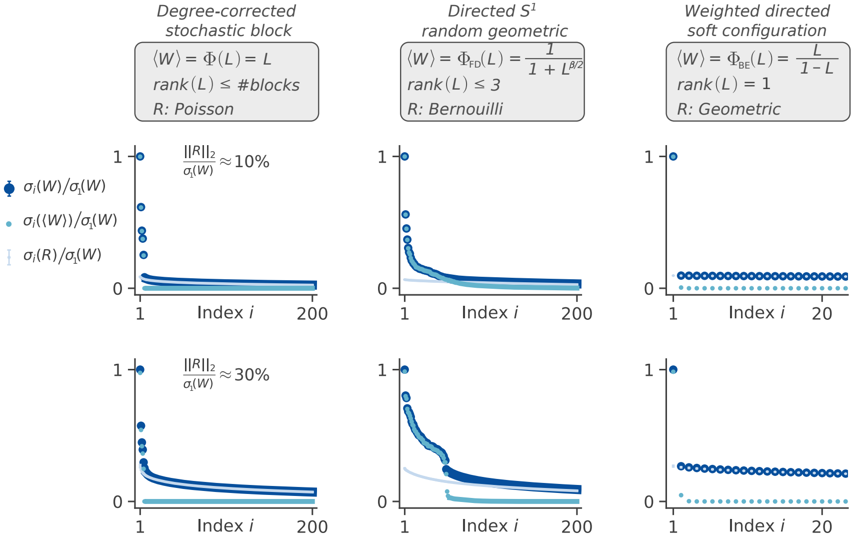


Third indicator of the low-rank hypothesis : low-effective ranks

Degree-corrected stochastic block

$\langle W \rangle = \Phi(L) = L$

$rank(L) \leq \#blocks$

R: Poisson

Directed S^1 random geometric

$\langle W \rangle = \Phi_{FD}(L) = \dfrac{1}{1 + L^{\beta/2}}$

$rank(L) \leq 3$

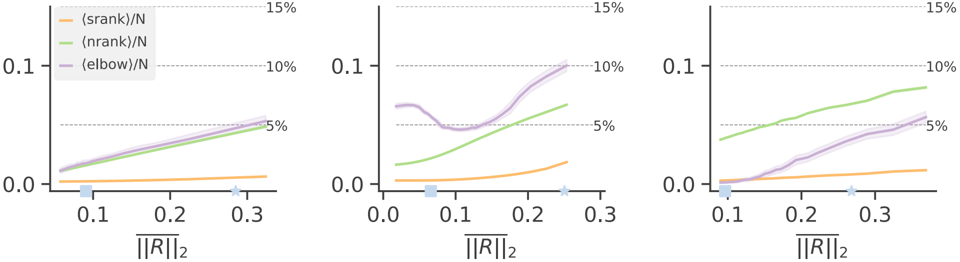
R: Bernouilli

Weighted directed soft configuration

$\langle W \rangle = \Phi_{BE}(L) = \dfrac{L}{1 - L}$

$rank(L) = 1$

R: Geometric



The low-rank hypothesis

It is the assumption that networks' weight matrices have rapidly decreasing singular values, implying low effective ranks.

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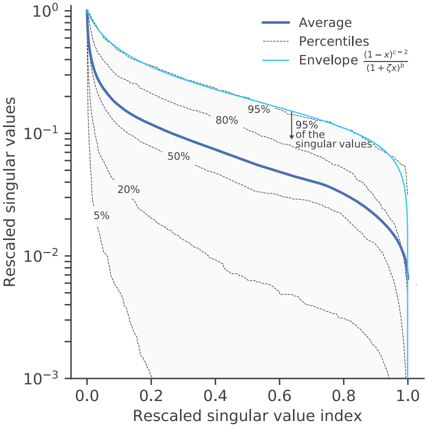
Let's verify it for real complex networks!

Experimental verification for real networks



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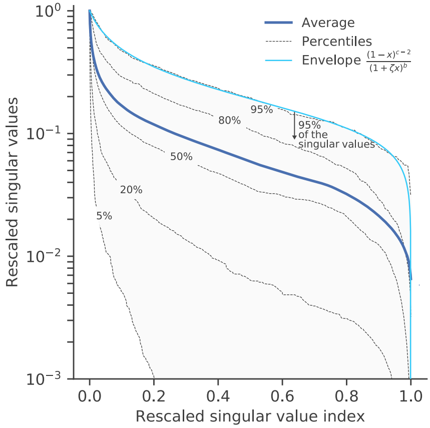

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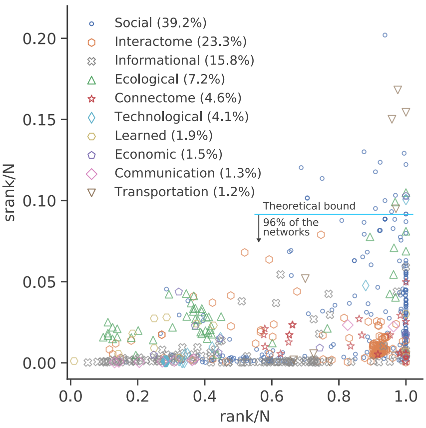
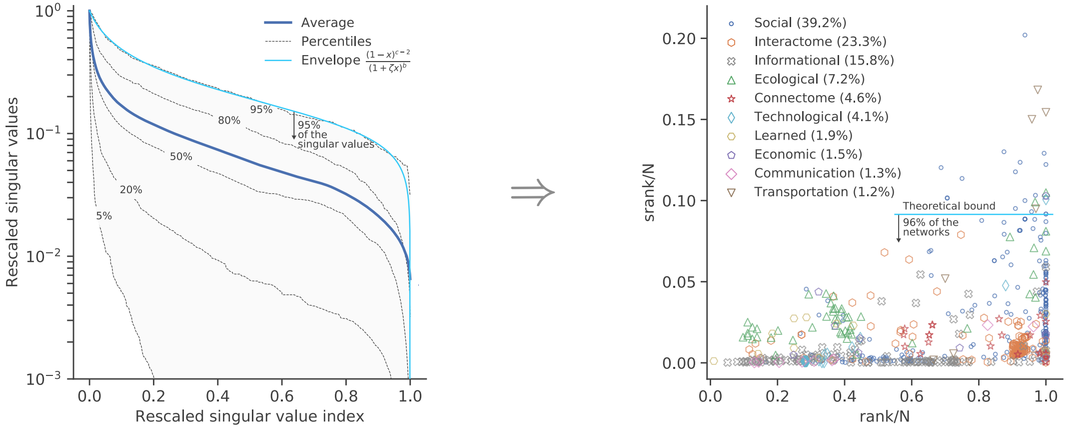


Many real complex networks have low effective ranks !*

* Udell, Townsend, "Why Are Big Data Matrices Approximately Low Rank ?", *SIAM J. Math. Data Sci.*, 2019

Experimental verification for real networks



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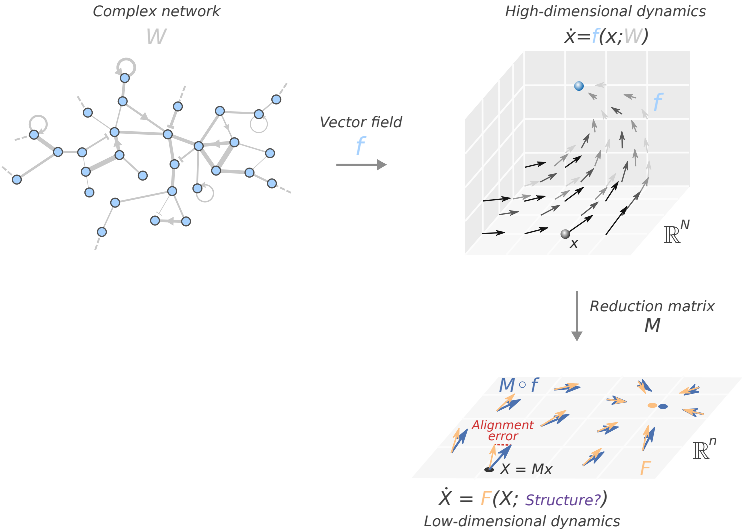
What's the consequence for *dynamics* on these networks ?

Dimension reduction of dynamical systems is about aligning vector fields.



High-dimensional dynamics : $\dot{x} = f(x)$

Low-dimensional dynamics : $\dot{X} = F(X)$ where $X = Mx$

Theorem (simplified)

The vector field F^* that minimizes the quadratic error between the projected dynamics $\dot{p} = f(p)$ with $p = M^+Mx$ and the reduced dynamics in $\mathbb{R}^N$ [$M^+F(X)$] is

$$F^*(X) = Mf(M^+X).$$

Proof : Just use least-squares.

Theorem (simplified)

The alignment error $\mathcal{E}(x)$ *for some* $x \in \mathbb{R}^N$ *is upper-bounded by*

$$\mathcal{E}(x) \leq \frac{1}{\sqrt{n}}\left[\|V_n^\top J_x(x',y')(I - V_n V_n^\top)x\| + \sigma_{n+1}\|V_n^\top J_y(x',y')\|_2\|x\|\right].$$

σ_i : *i-th singular values of* W

$M = V_n^\top$: *n-truncated right singular vector matrix (justification, Eckart-Young)*

J_x, J_y : *Jacobian matrices evaluated at some point* x', y'

n : *dimension of the reduced system*

Choice of M and upper bound on the alignment error $\mathcal{E}_f(x)$

Theorem (simplified)

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First intuitive consequence : $\frac{\mathcal{E}(x)}{\|x\|} \leq \frac{\sigma_{n+1}}{\sqrt{n}}$

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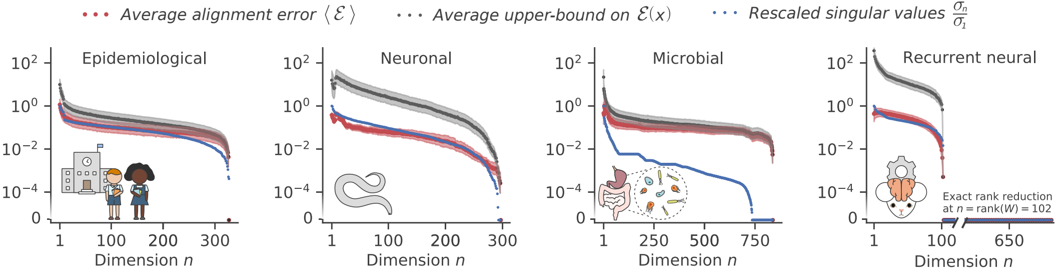
First intuitive consequence : $\frac{\mathcal{E}(x)}{\|x\|} \leq \frac{\sigma_{n+1}}{\sqrt{n}}$

Second consequence : $J_x(x', y') = aI$ and $n \geq \text{rank}(W) \quad \Rightarrow \quad$ *Exact* dim. red.

Alignment error for dynamics on real complex networks

Third consequence :

Rapid singular value decreases can induce rapid alignment error decrease.



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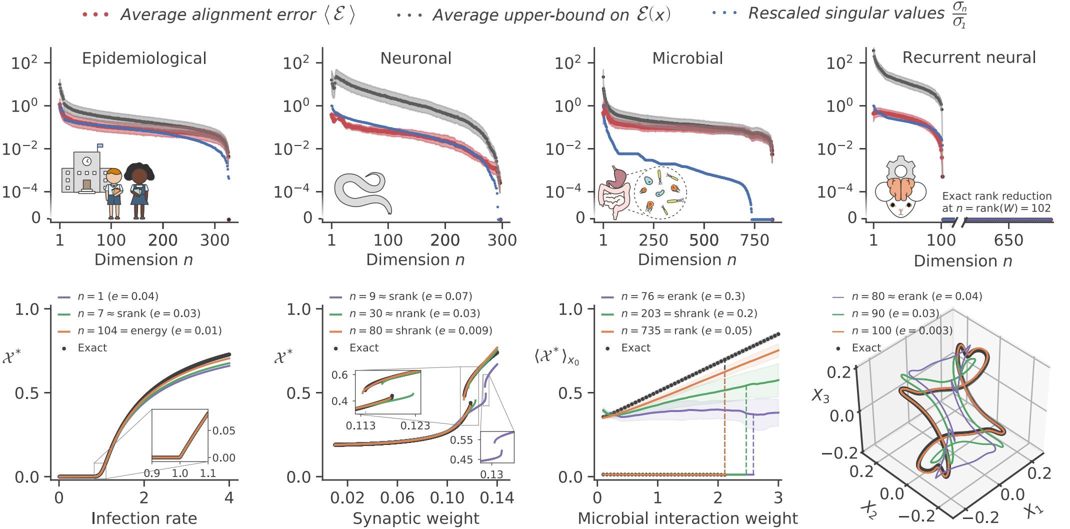
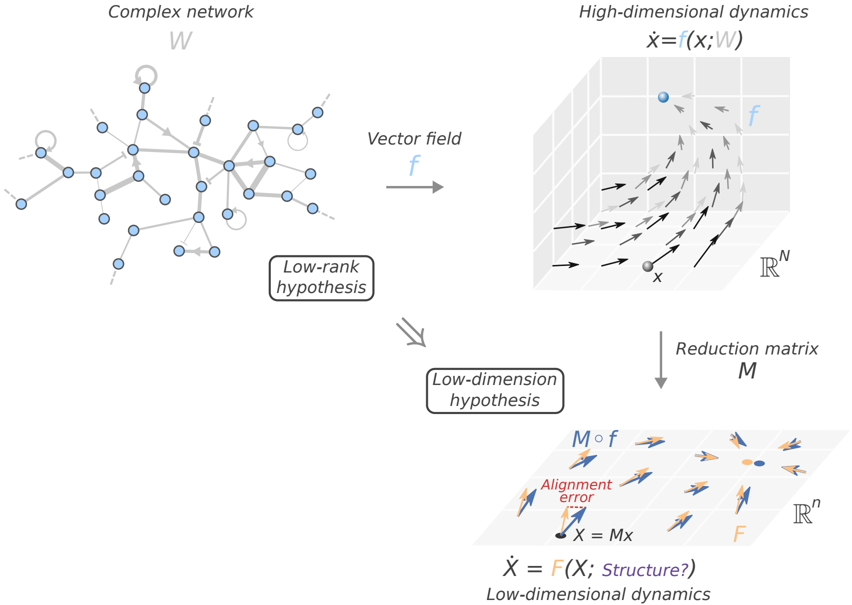
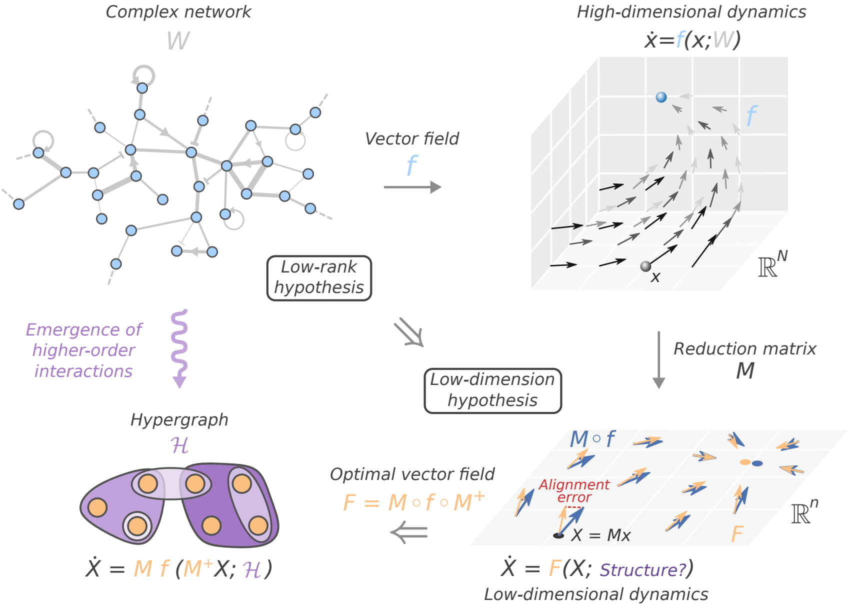


Induced low-dimension hypothesis



A surprise : Higher-order interactions



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

Examples

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

Reduced QMF SIS :

$$\dot{X}_\mu = -\alpha X_\mu + \beta \sum_{\nu=1}^{n} \mathcal{W}_{\mu\nu}^{(2)} X_\nu - \beta \sum_{\nu,\tau=1}^{n} \mathcal{W}_{\mu\nu\tau}^{(3)} X_\nu X_\tau, \quad \mu \in \{1, ..., n\}$$

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

Reduced QMF SIS :

$\dot{X}_\mu = -\alpha X_\mu + \beta \sum_{\nu=1}^{n} \mathcal{W}^{(2)}_{\mu\nu} X_\nu - \beta \sum_{\nu,\tau=1}^{n} \mathcal{W}^{(3)}_{\mu\nu\tau} X_\nu X_\tau, \quad \mu \in \{1, ..., n\}$

Kuramoto-Sakaguchi : $\dot{z}_j = i\omega_j z_j + \sum_{k=1}^{N} W_{jk}[z_k e^{-i\alpha} - z_j^2 \bar{z}_k e^{i\alpha}]$

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

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Reduced Kuramoto-Sakaguchi :

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

$$\mathcal{W}_{\mu\alpha\beta\gamma}^{(4)} = \sum_{j,k=1}^{N} M_{\mu j} M_{j\alpha}^{+} M_{j\beta}^{+} W_{jk} M_{k\gamma}^{+}.$$

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

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Reduced Kuramoto-Sakaguchi :

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

$$\mathcal{W}_{\mu\alpha\beta\gamma}^{(4)} = \sum_{j,k=1}^{N} M_{\mu j} M_{j\alpha}^{+} M_{j\beta}^{+} W_{jk} M_{k\gamma}^{+}.$$

The HOIs depend on the *reduction matrix* and the *nonlinearity* of the dynamics.

Conclusion

1. The low-rank hypothesis has been defined with three indicators along with its impacts.
2. Many real networks have rapidly decreasing singular values, leading to low *effective* ranks.
3. Alignment errors can rapidly decrease following the networks' singular values.
4. Dimension reduction can lead to the emergence of *higher-order interactions* that depends on the chosen *observables* and the *nonlinearity* of the system.

Acknowledgments

All details are in the manuscript : `https://arxiv.org/abs/2208.04848`

Some references : Valdano and Arenas, *Phys. Rev. X*, 2019
Udell and Townsend, *SIAM J. Math. Data Sci.*, 2019
Thibeault et al., *Phys. Rev. Res.*, 2020

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Questions ?

Thank you for your attention !

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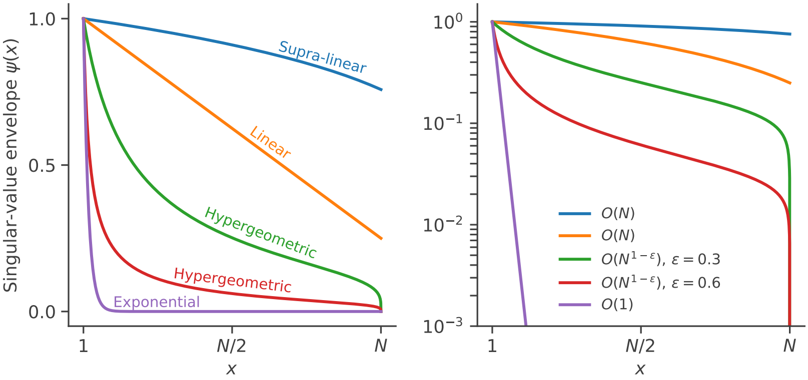
CRSNG NSERC
Sentinelle Nord
Calcul Québec

Low ?

How low ? The values of the effective ranks give a graded measure for that.

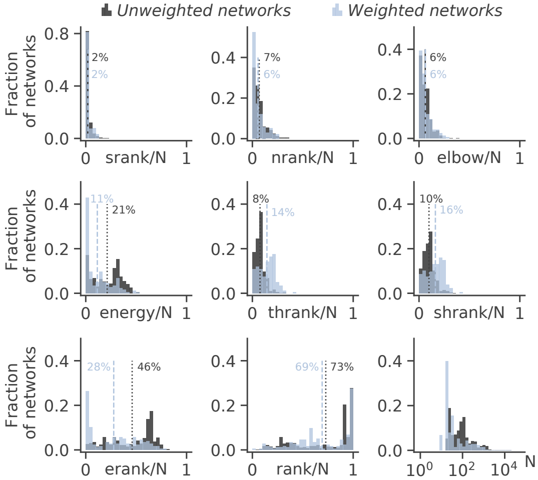
Low or high ? at most a sublinear growth $O(N^{1-\epsilon})$, with $\epsilon \in (0, 1]$, as $N \to \infty$

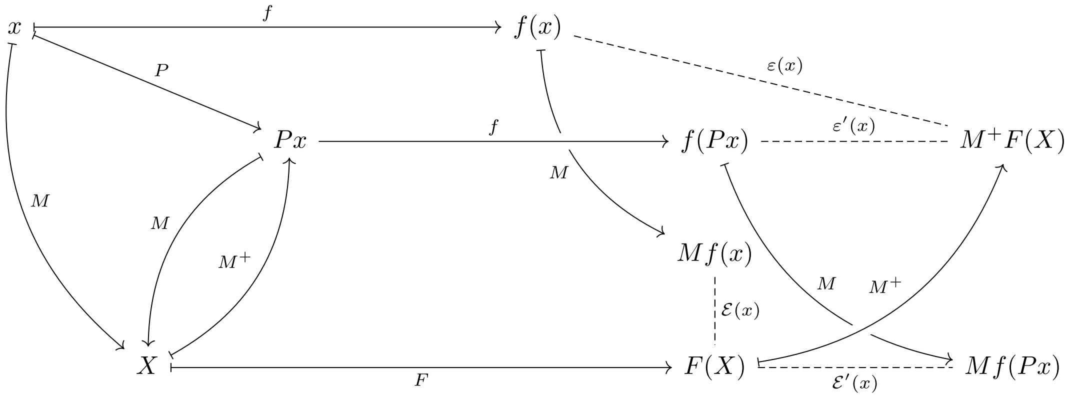
(valid only for growing graph models)

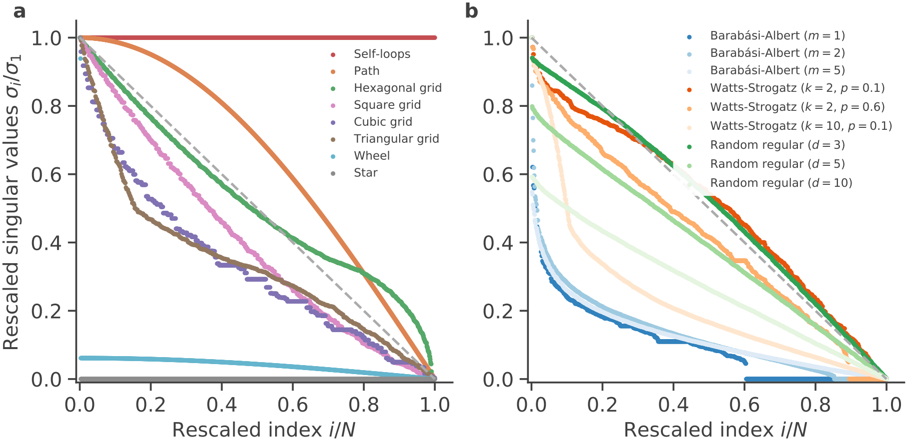


*Summarizes SI IIC in Thibeault et al., `https://arxiv.org/abs/2208.04848` (e.g., Theorem 3)

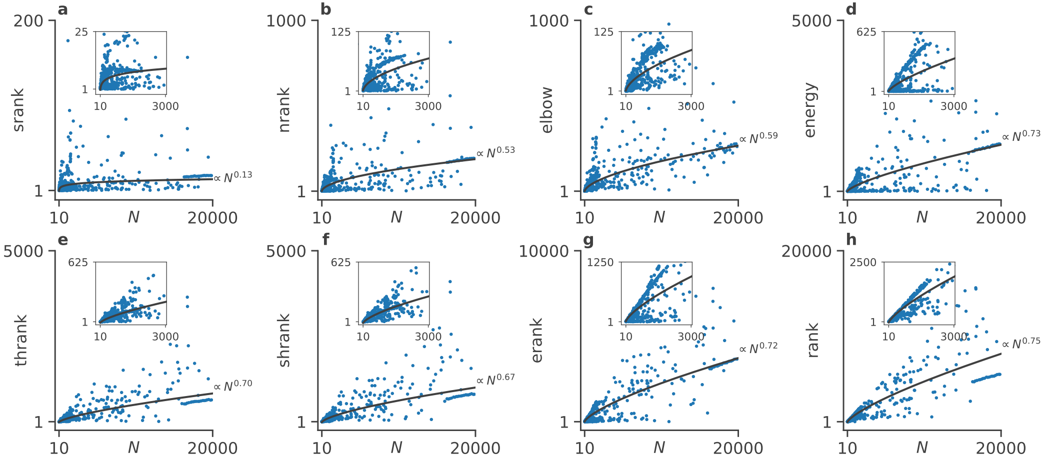
Other effective ranks



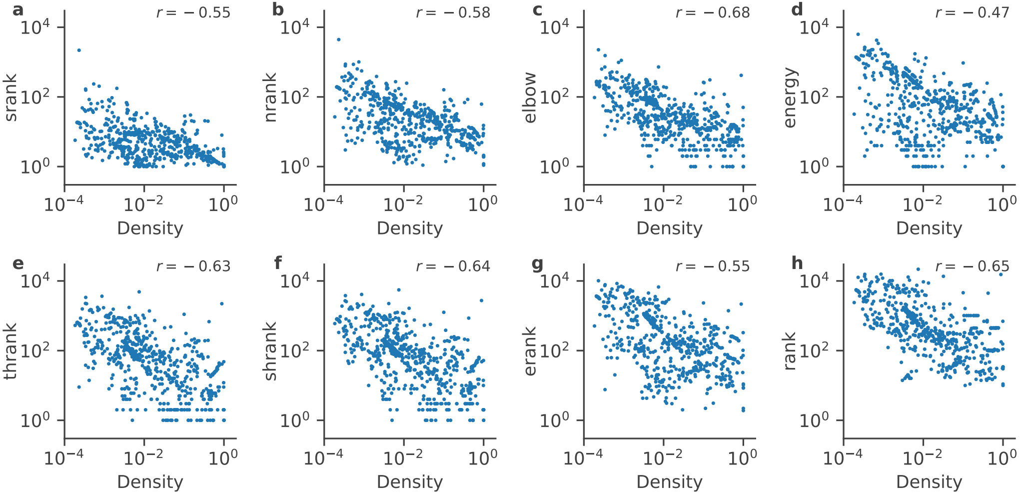

x
f
$f(x)$
P
$\varepsilon(x)$
Px
f
$f(Px)$
$\varepsilon'(x)$
$M^+F(X)$
M
M
M
M^+
$Mf(x)$
$\mathcal{E}(x)$
M
M^+
X
F
$F(X)$
$\mathcal{E}'(x)$
$Mf(Px)$


a
b
Rescaled singular values σ_i/σ_1
Rescaled index i/N
0.0
0.2
0.4
0.6
0.8
1.0
Self-loops
Path
Hexagonal grid
Square grid
Cubic grid
Triangular grid
Wheel
Star
Barabási-Albert ($m = 1$)
Barabási-Albert ($m = 2$)
Barabási-Albert ($m = 5$)
Watts-Strogatz ($k = 2$, $p = 0.1$)
Watts-Strogatz ($k = 2$, $p = 0.6$)
Watts-Strogatz ($k = 10$, $p = 0.1$)
Random regular ($d = 3$)
Random regular ($d = 5$)
Random regular ($d = 10$)

Effective ranks vs. number of vertices



Effective ranks vs. density



Theorem (Hypergeometric decrease (simplified))

Suppose that the singular values of matrix W satisfy the inequality

$$\frac{(1-x_i)^{c^*-2}}{(1+\zeta^* x_i)^{b^*}} \leq \frac{\sigma_i}{\sigma_1} \leq \frac{(1-x_i)^{c_*-2}}{(1+\zeta_* x_i)^{b_*}}, \qquad \forall i \in \{1, \ldots, N\},$$

where $x_i = (i-1)/(N-1)$ *and for some* $0 \leq b_* \leq b^*$, $2 \leq c_* \leq c^*$, $0 < \zeta_* \leq \zeta^*$. *Then,*

$$\frac{N-1}{2c^*-3} H(b^*, c^*, \zeta^*) \leq \operatorname{srank}(W) \leq 1 + \frac{N-1}{2c_*-3} H(b_*, c_*, \zeta_*),$$

where $H(b, c, \zeta) := {}_2F_1(1, 2b; 2(c-1); -\zeta)$, *the Gaussian hypergeometric function.*