Dynamics on networks through the lens of spectral and information theories

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Outline

Dimension reduction of dynamics on modular and heterogeneous directed networks

Marina Vegué, Vincent Thibeault, Patrick Desrosiers, Antoine Allard

Dimension reduction is a common strategy to study non-linear dynamical systems composed by a large number of variables. The goal is to find a smaller version of the system whose time evolution is easier to predict while preserving some of the key dynamical features of the original system. Finding such a reduced representation for complex systems is, however, a difficult task. We address this problem for dynamics on weighted directed networks, with special emphasis on modular and heterogeneous networks. We propose a two-step dimension-reduction method that takes into account the properties of the adjacency matrix. First, units are partitioned into groups of similar connectivity profiles. Each group is associated to an observable that is a weighted average of the nodes' activities within the group. Second, we derive a set of conditions that must be fulfilled for these observables to properly represent the original system's behavior, together with a method for approximately solving them. The result is a reduced adjacency matrix and an approximate system of ODEs for the observables' evolution. We show that the reduced system can be used to predict some characteristic features of the complete dynamics for different types of connectivity structures, both synthetic and derived from real data, including neuronal, ecological, and social networks. Our formalism opens a way to a systematic comparison of the effect of various structural properties on the overall network dynamics. It can thus help to identify the main structural driving forces guiding the evolution of dynamical processes on networks.

arXiv:2206.11230

Duality between predictability and reconstructability in complex systems

Charles Murphy, Vincent Thibeault, Antoine Allard, Patrick Desrosiers

Predicting the evolution of a large system of units using its structure of interaction is a fundamental problem in complex system theory. And so is the problem of reconstructing the structure of interaction from temporal observations. Here, we find an intricate relationship between predictability and reconstructability using an information-theoretical point of view. We use the mutual information between a random graph and a stochastic process evolving on this random graph to quantify their codependence. Then, we show how the uncertainty coefficients, which are intimately related to that mutual information, quantify our ability to reconstruct a graph from an observed time series, and our ability to predict the evolution of a process from the structure of its interactions. Interestingly, we find that predictability and reconstructability, even though closely connected by the mutual information, can behave differently, even in a dual manner. We prove how such duality universally emerges when changing the number of steps in the process, and provide numerical evidence of other dualities occurring near the criticality of multiple different processes evolving on different types of structures.

arXiv:2206.04000

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Dimension reduction: general idea

For a non-linear dynamical system composed of a large number of variables ($\{x_i\}_{i=1,\ldots,N}$), find a system

- composed of a smaller number of variables ($\{\chi_i\}_{i=1,\ldots,n}$) where $n \ll N$;
- that is easier to analyze;
- preserves (some) key dynamical features of the original system.

$$
\begin{aligned}
\dot{x}_1 &= f_1(x_1, \ldots, x_N) \\
\dot{x}_2 &= f_2(x_1, \ldots, x_N) \\
&\vdots \\
\dot{x}_N &= f_N(x_1, \ldots, x_N)
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\dot{\chi}_1 &= g_1(\chi_1, \ldots, \chi_n) \\
\dot{\chi}_2 &= g_2(\chi_1, \ldots, \chi_n) \\
&\vdots \\
\dot{\chi}_n &= g_n(\chi_1, \ldots, \chi_n)
\end{aligned}
$$

The idea of dimension reduction has been around for a while and is present in various scientific disciplines.

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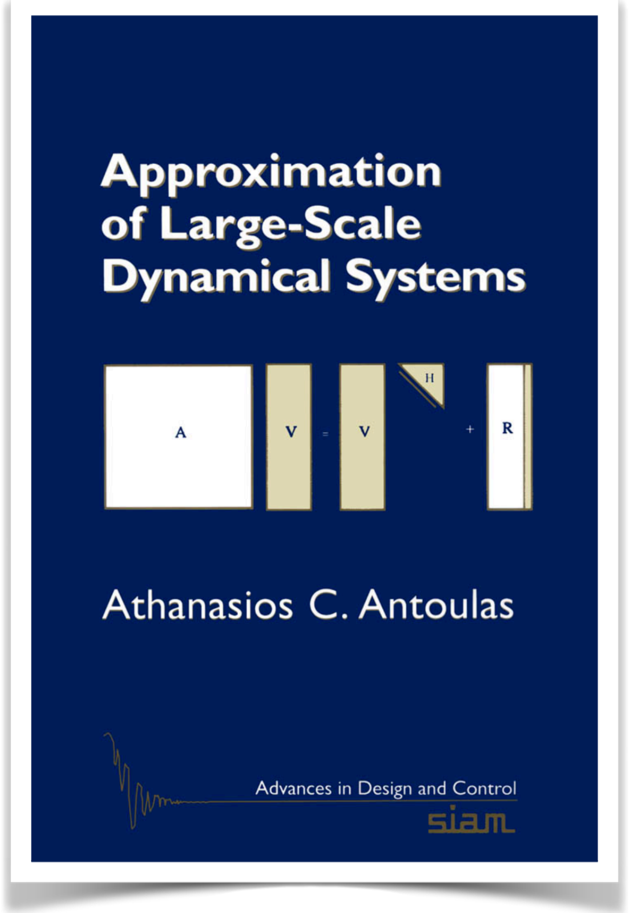
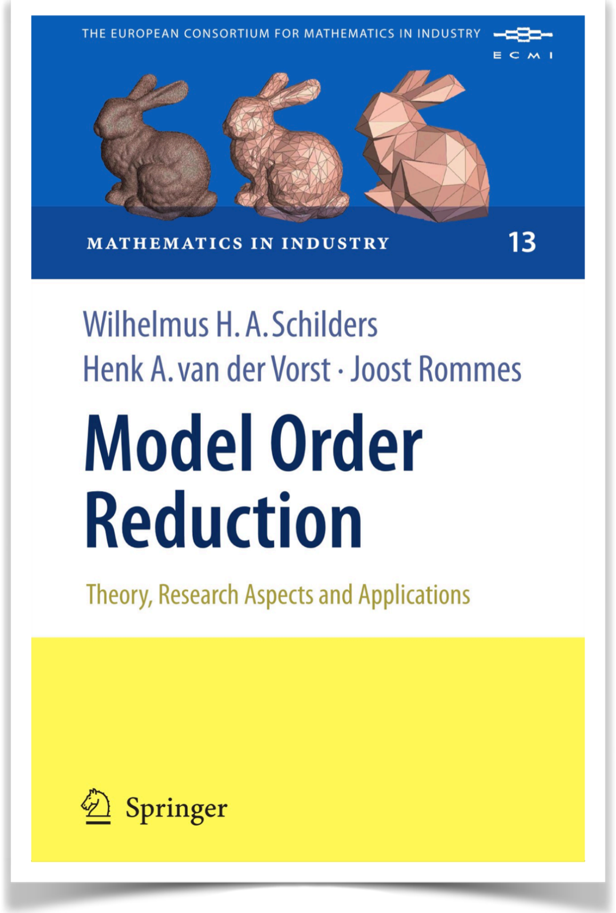
A GENERAL ANALYSIS OF APPROXIMATE LUMPING IN CHEMICAL KINETICS

GENYUAN LI and HERSCHEL RABITZ†
Department of Chemistry, Princeton University, Princeton, NJ 08540, U.S.A.





Yet, many complex network systems still elude the best dimension reduction techniques.

ANNUAL REVIEWS

Annual Review of Control, Robotics, and Autonomous Systems

Model Reduction Methods for Complex Network Systems

X. Cheng[1] and J.M.A. Scherpen[2]

FUTURE ISSUES

1. The approximation of complex network systems with nonlinear couplings and nonlinear subsystems is still challenging and requires further investigation.
2. How to reduce the topological complexity of dynamic networks composed of heterogeneous subsystems is not yet clear.
3. The application of reduced-order network models for designing controllers and observers for large-scale networks is appealing, and obtaining provable guarantees on the functionality of the controllers or observers based on reduced-order models should be further explored.

Although successful, dimension reduction of dynamics on networks has thus far been limited to

- undirected networks;
- "homogenous" networks (e.g., uniform communities, homogeneous degree distribution);
- very low values of n $(= 1, 2)$.

PHYSICAL REVIEW E **95**, 062307 (2017)

Collapse of resilience patterns in generalized Lotka-Volterra dynamics and beyond

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PNAS

Predicting tipping points in mutualistic networks through dimension reduction

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LETTER

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Universal resilience patterns in complex networks

Jianxi Gao[1]*, Baruch Barzel[2]* & Albert-László Barabási[1,3,4,5]

PHYSICAL REVIEW RESEARCH **2**, 043215 (2020)

Threefold way to the dimension reduction of dynamics on networks: An application to synchronization

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Article

Dimensionality reduction of complex dynamical systems

Chengyi Tu, Paolo D'Odorico, Samir Suweis

PHYSICAL REVIEW X **9**, 011042 (2019)

Spectral Dimension Reduction of Complex Dynamical Networks

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PHYSICAL REVIEW RESEARCH **4**, 023257 (2022)

Dimension reduction of dynamical systems on networks with leading and non-leading eigenvectors of adjacency matrices

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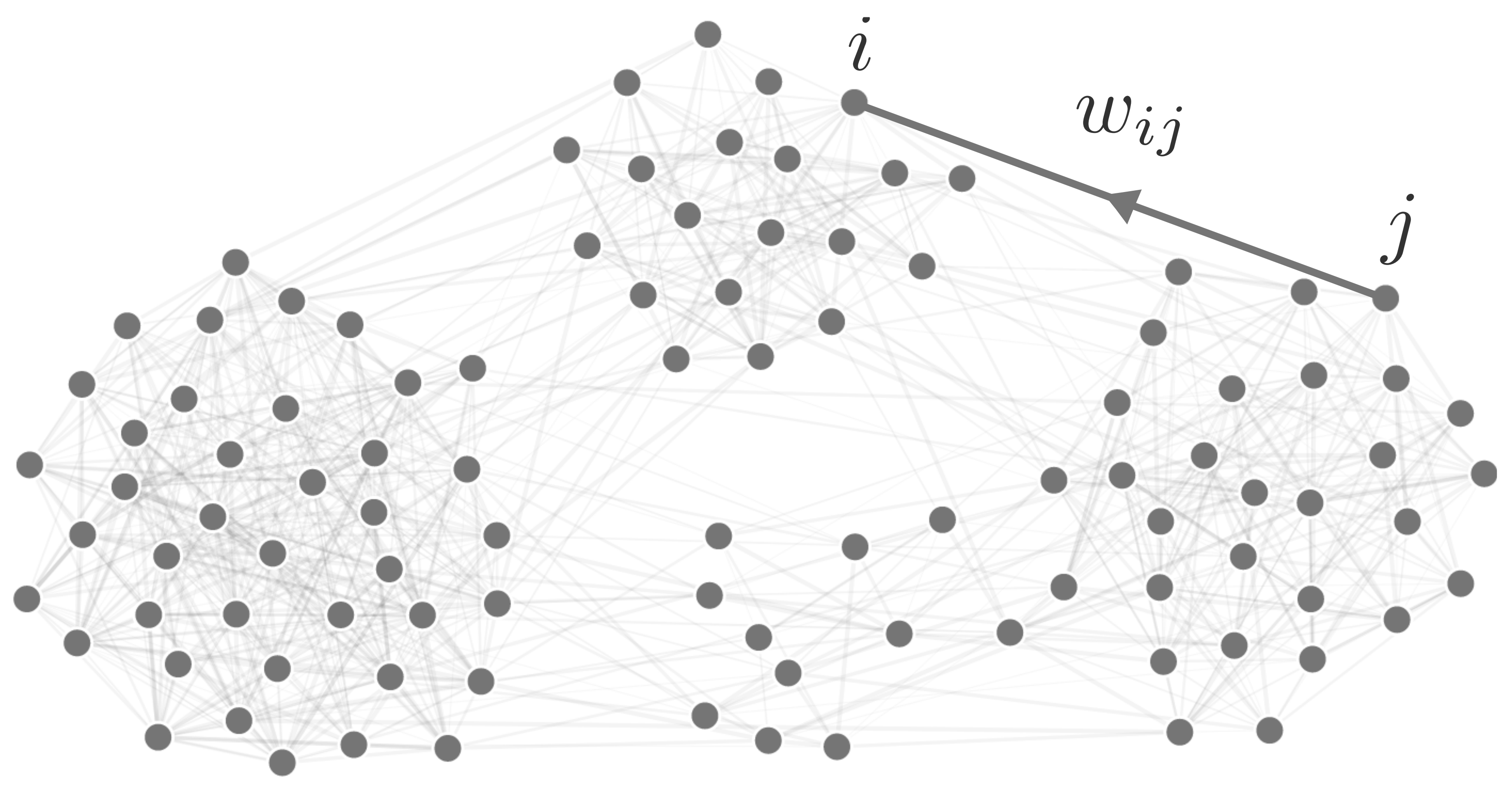
Our approach to dimension reduction

Original system:

- N nodes
- magnitude of interaction from node j to node i is w_{ij};
- self-dynamics $f(x_i)$ is the same for every nodes;
- interaction dynamics $g(x_i, x_j)$ is the same for every interactions;
- dynamics has the generic form

$$\dot{x}_i = f(x_i) + \sum_{j=1}^{N} w_{ij} g(x_i, x_j) \qquad \text{for } i = 1, \ldots, N$$



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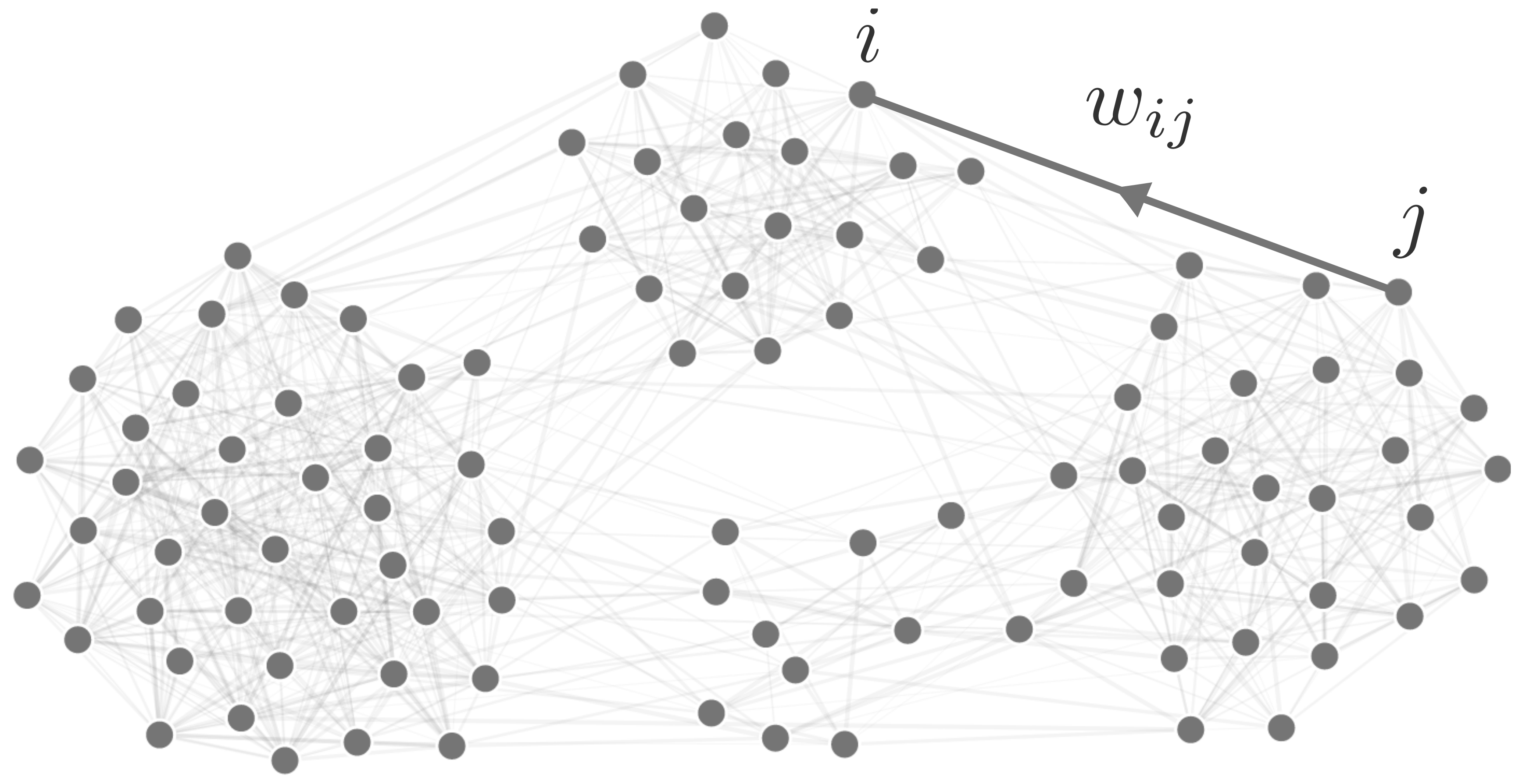


Examples:

1. Neuronal dynamics (Hopfield's continuous model)

$$\dot{x}_i = -x_i + \sum_{j=1}^{N} w_{ij} \frac{1}{1 + \mathrm{e}^{-\tau(x_j - \mu)}}$$

with parameters τ and μ. Proc. Natl. Acad. Sci. U.S.A. 80:3088 (1984)

2. Epidemiological dynamics (SIS)

$$\dot{x}_i = -x_i + \gamma(1 - x_i) \sum_{j=1}^{N} w_{ij} x_j$$

with parameter γ. Rev. Mod. Phys. 87:925 (2015)

3. Ecological mutualistic dynamics

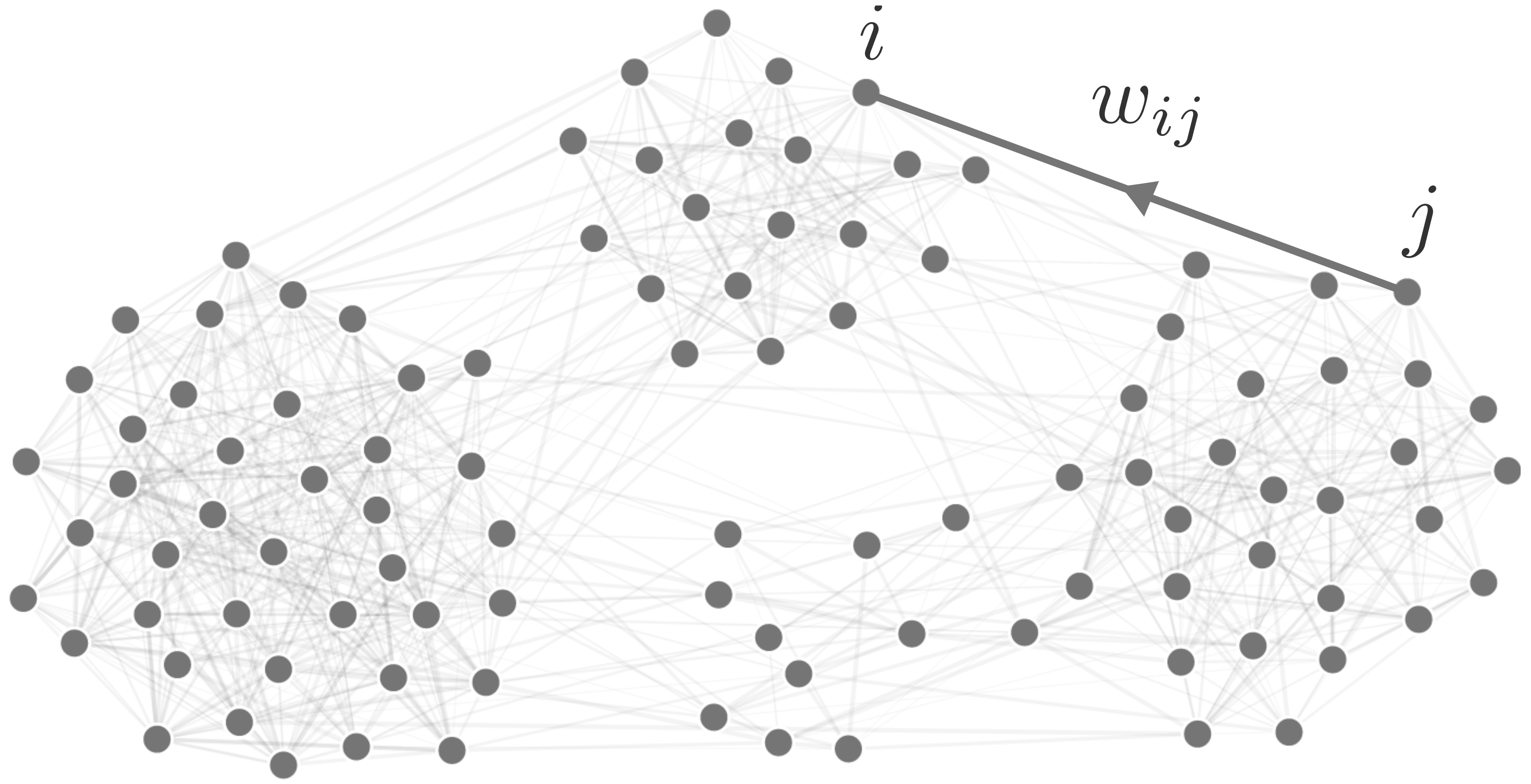
$$\dot{x}_i = B + x_i \left(1 - \frac{x_i}{K}\right)\left(\frac{x_i}{C} - 1\right) + \sum_{j=1}^{N} w_{ij} \frac{x_i x_j}{D + E x_i + H x_j}$$

with parameters B, C, D, E, H and K. Am. Nat. 159:231 (2002)

Our approach to dimension reduction

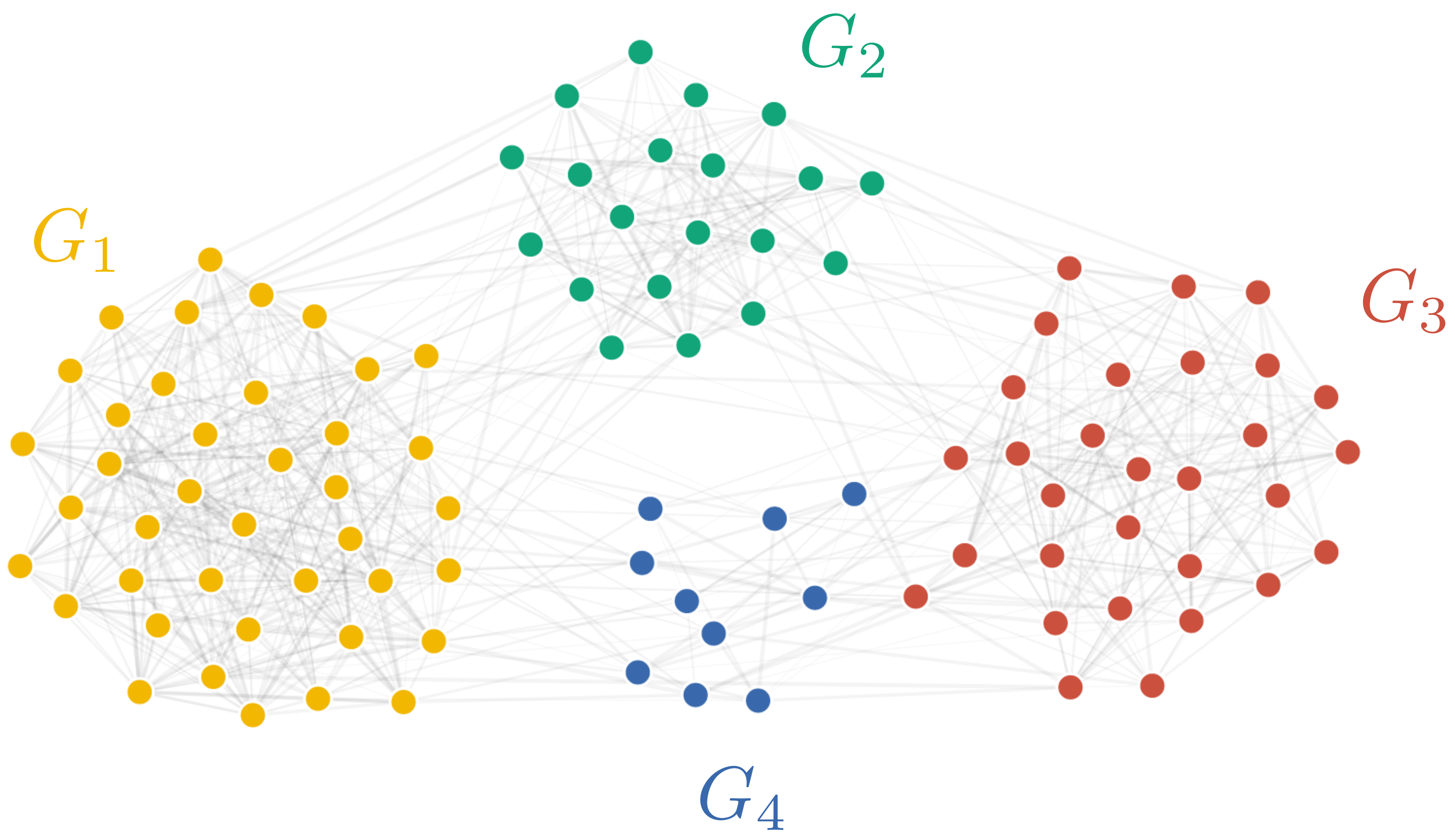
Original system:

$$\dot{x}_i = f(x_i) + \sum_{j=1}^{N} w_{ij} g(x_i, x_j) \qquad \text{for } i = 1, \dots, N$$



Step 1: Define the variables of the reduced system

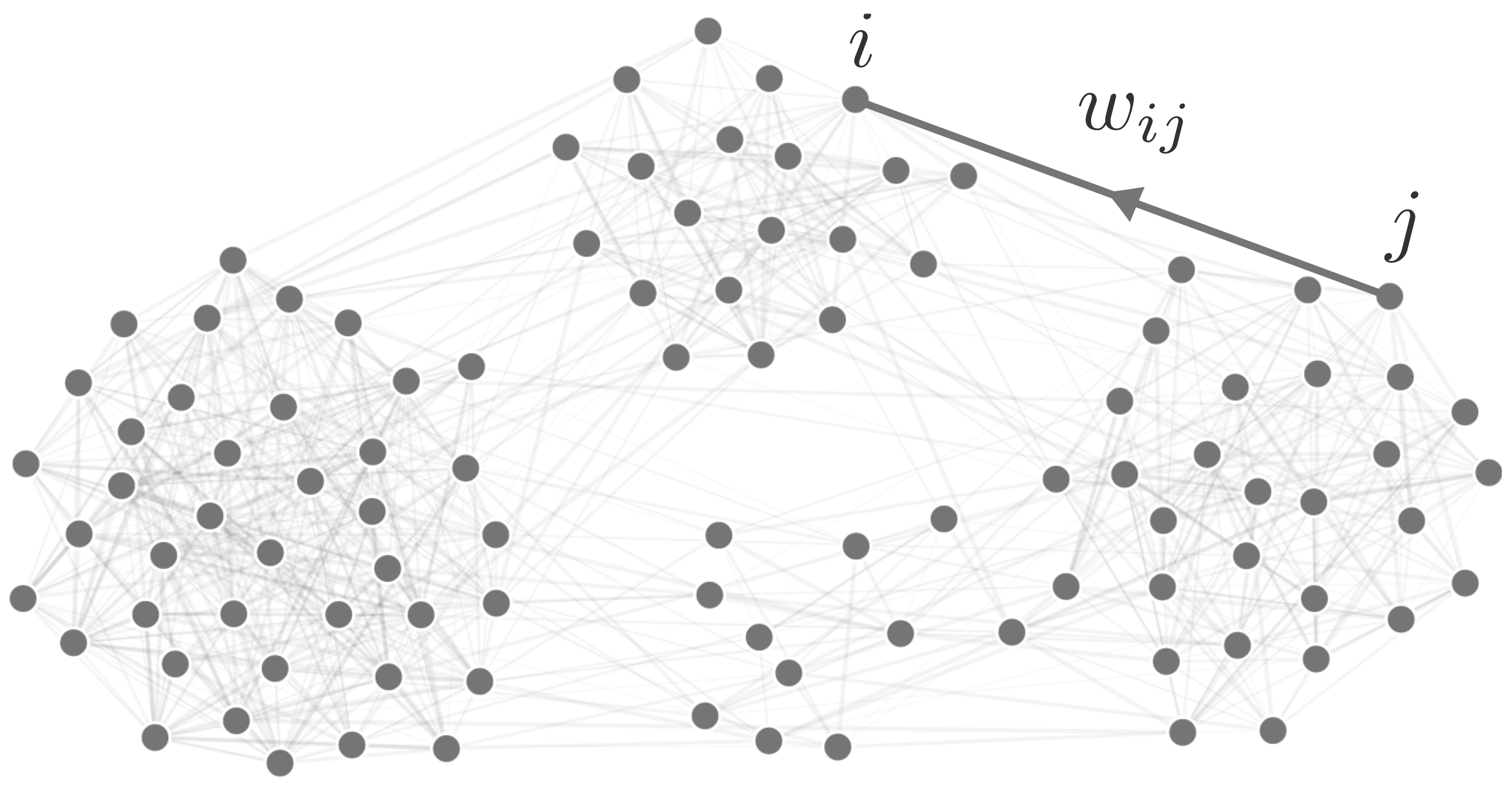
- node heterogeneity is solely encoded in the adjacency matrix (by construction);
- nodes can be classified into n groups that share similar connectivity properties (e.g. assortative communities, bipartite networks; by assumption);
- nodes with similar connectivity profiles have similar activities (by assumption);
- build one *linear* observable for each group $\nu = 1, \dots, n$:



$$\chi_\nu = \sum_{i=1}^{N} a_{\nu i} x_i \quad \text{with} \quad \sum_{i=1}^{N} a_{\nu i} = 1 \quad \text{and} \quad a_{\nu i} = 0 \text{ if } i \notin G_\nu$$

Our approach to dimension reduction

Original system:

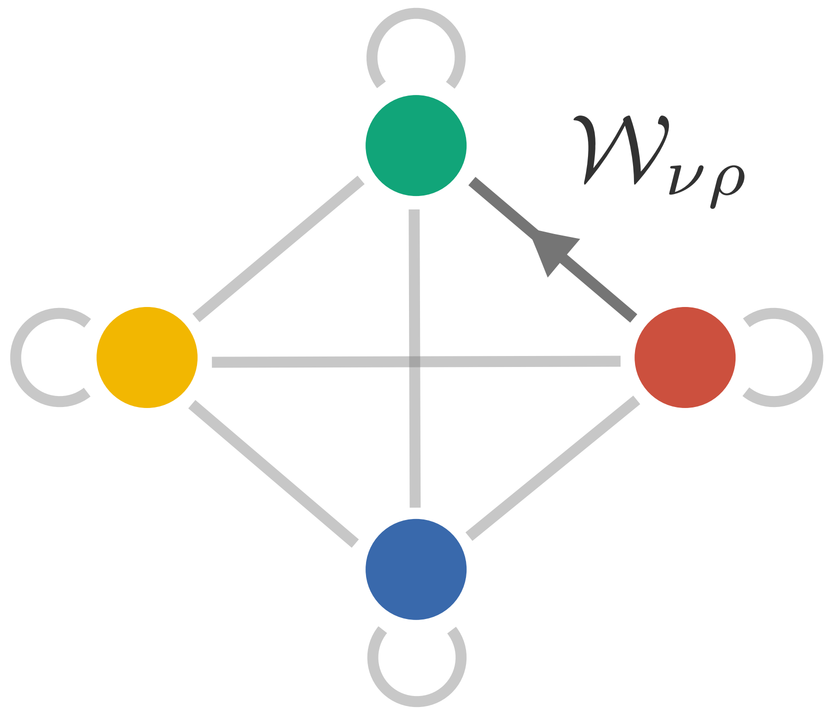


$$\dot{x}_i = f(x_i) + \sum_{j=1}^{N} w_{ij} g(x_i, x_j) \qquad \text{for } i = 1, \ldots, N$$

Step 2: Derive the equations of the reduced system

- nodes with similar connectivity profiles have similar activities (by assumption);
- first-order Taylor expansion around the value of the appropriate observable (where $i \in G_\nu$ and $j \in G_\rho$)

$$\begin{aligned}
\dot{\chi}_\nu &= \sum_{i=1}^{N} a_{\nu i} \dot{x}_i = \sum_{i=1}^{N} a_{\nu i} f(x_i) + \sum_{i,j=1}^{N} a_{\nu i} w_{ij} g(x_i, x_j) \\
&\approx \sum_{i=1}^{N} a_{\nu i} \Big[f(\chi_\nu) + f'(\chi_\nu)(x_i - \chi_\nu) \Big] + \sum_{i,j=1}^{N} a_{\nu i} w_{ij} \Big[g(\chi_\nu, \chi_\rho) + g^{(1)}(\chi_\nu, \chi_\rho)(x_i - \chi_\nu) + g^{(2)}(\chi_\nu, \chi_\rho)(x_j - \chi_\rho) \Big] \\
&\approx f(\chi_\nu) + \sum_{\rho=1}^{n} \mathcal{W}_{\nu\rho} g(\chi_\nu, \chi_\rho)
\end{aligned}$$



where $\mathcal{W}_{\nu\rho} = \sum_{\substack{i \in G_\nu \\ j \in G_\rho}} a_{\nu i} w_{ij}$ are the weights of the *reduced adjacency matrix*.

Our approach to dimension reduction

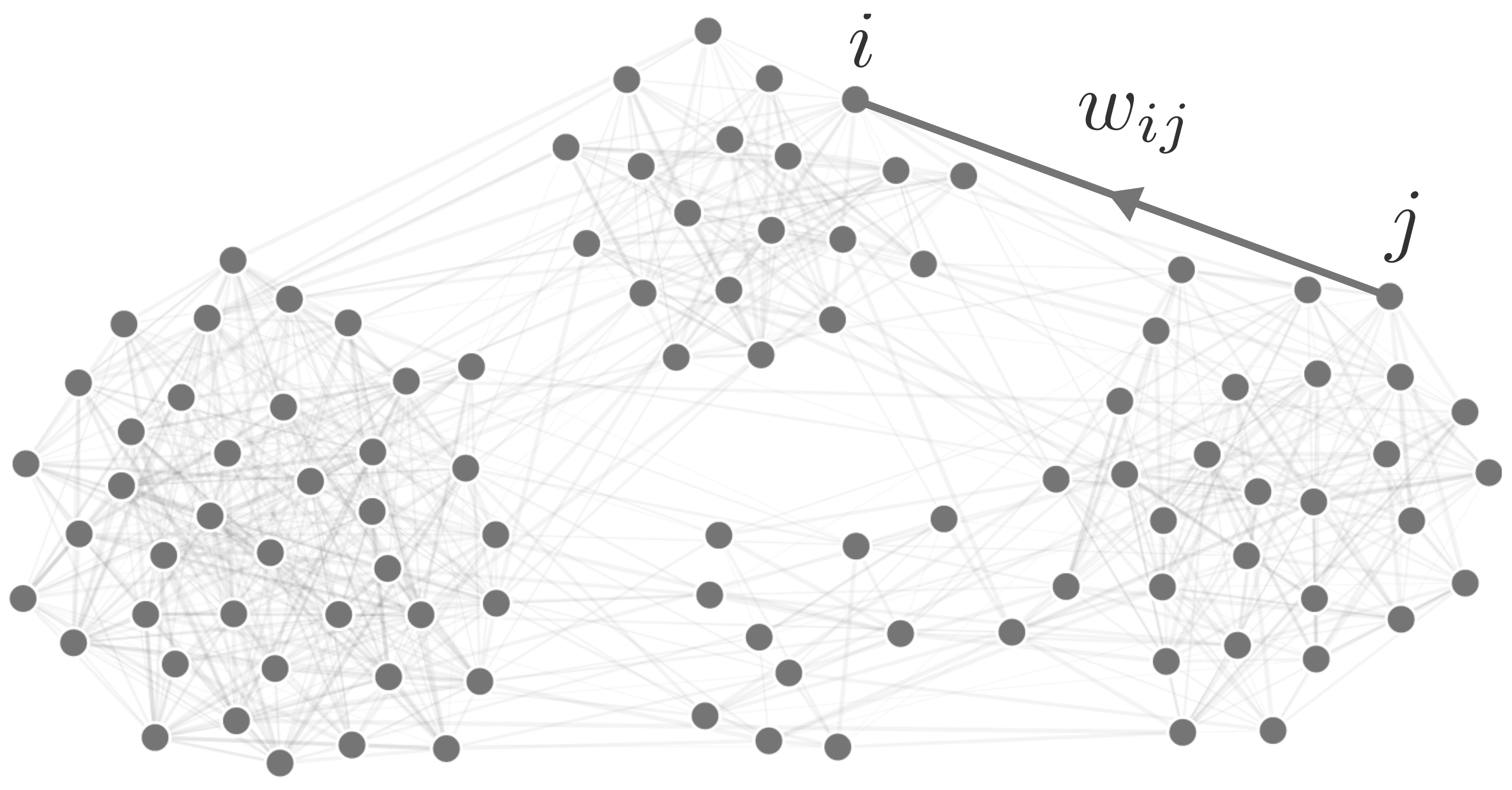
Step 3: Solve the compatibility equations

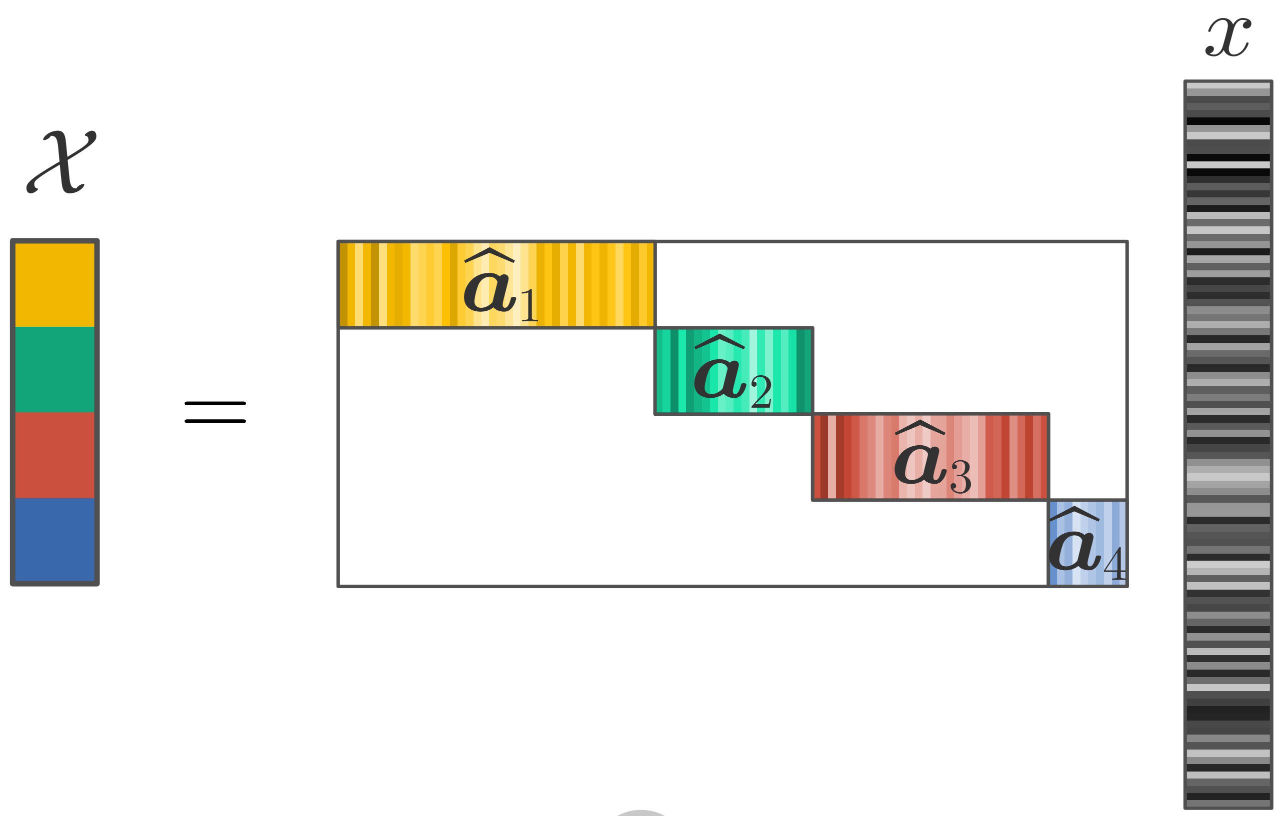
- the *closed* reduced system is obtained when using the weights $\{a_{\nu i}\}$ satisfying the compatibility equations

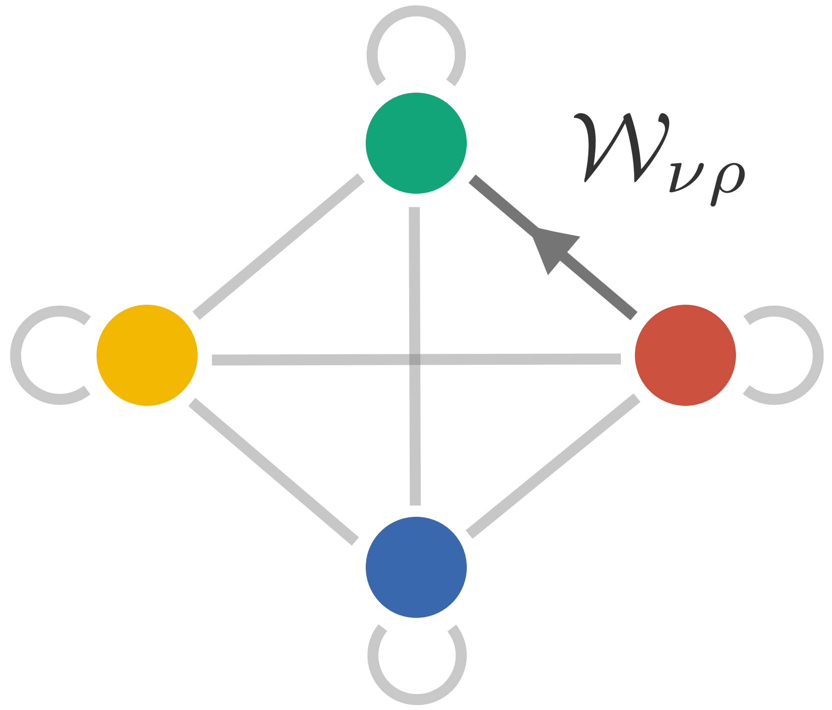
$$\boldsymbol{W}_{\nu\rho}^T \widehat{\boldsymbol{a}}_\nu = \mathcal{W}_{\nu\rho} \widehat{\boldsymbol{a}}_\rho$$
$$\boldsymbol{K}_{\nu\rho} \widehat{\boldsymbol{a}}_\nu = \mathcal{W}_{\nu\rho} \widehat{\boldsymbol{a}}_\nu$$

with $\boldsymbol{W} = \begin{pmatrix} \boldsymbol{W}_{11} & \cdots & \boldsymbol{W}_{1n} \\ \vdots & \ddots & \vdots \\ \boldsymbol{W}_{n1} & \cdots & \boldsymbol{W}_{nn} \end{pmatrix}$ and $\boldsymbol{K}_{\nu\rho} = \begin{pmatrix} k^\rho_{i_1} & & & \\ & k^\rho_{i_2} & & \\ & & \ddots & \\ & & & k^\rho_{i_{m_\nu}} \end{pmatrix}$

where $\{i_1, i_2, \ldots, i_{m_\nu}\} = G_\nu$ and $k_i^\rho = \sum_{j \in G_\rho} w_{ij}$.







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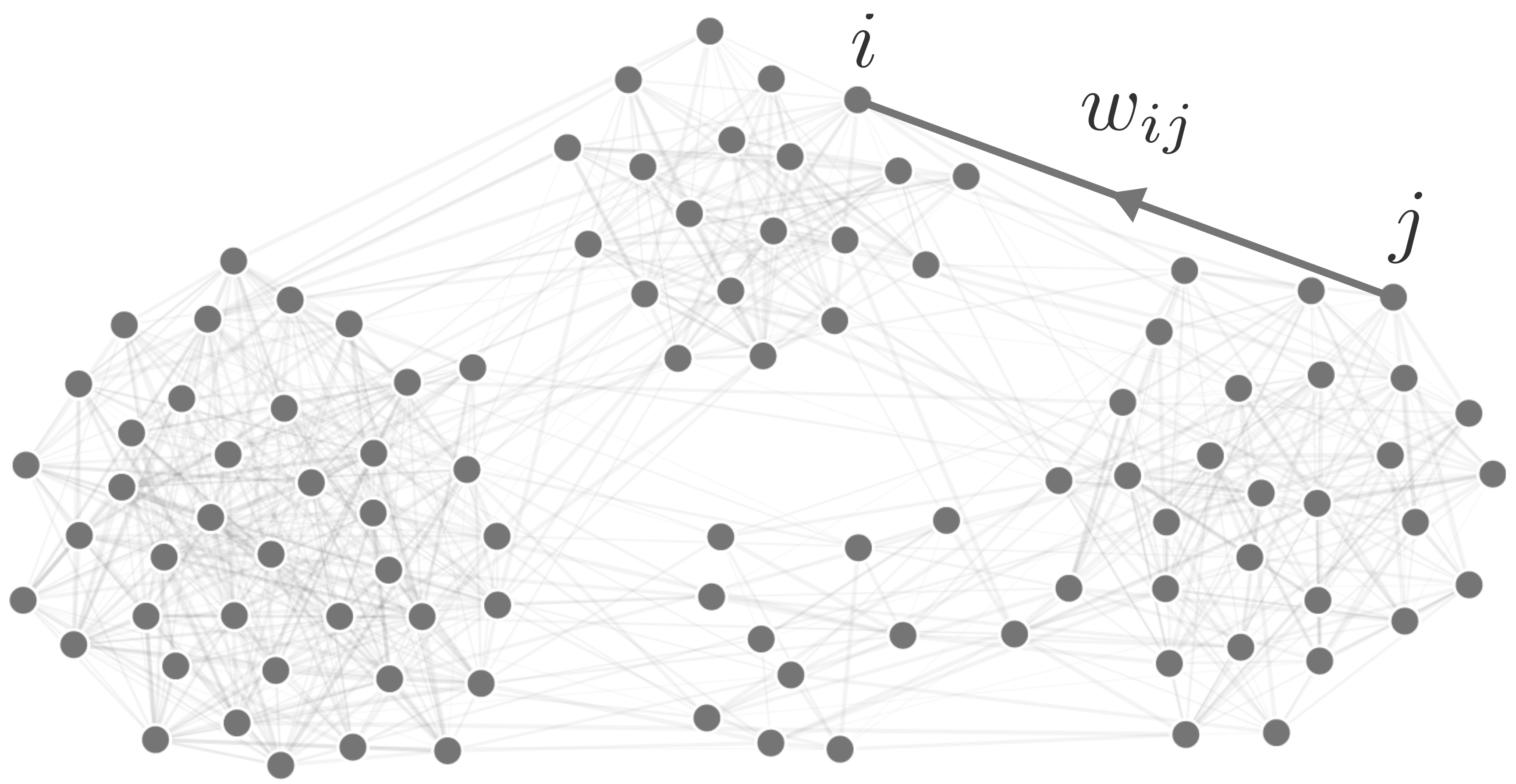
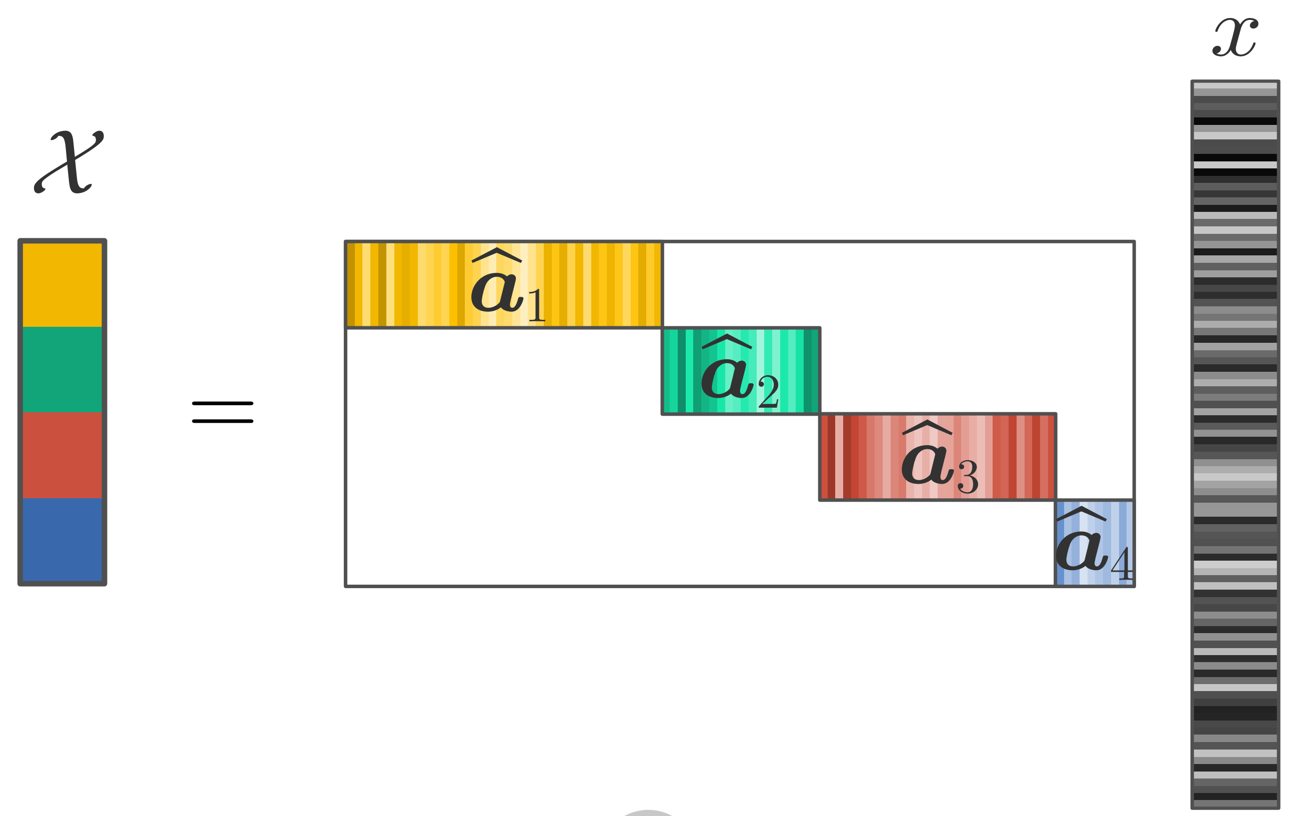
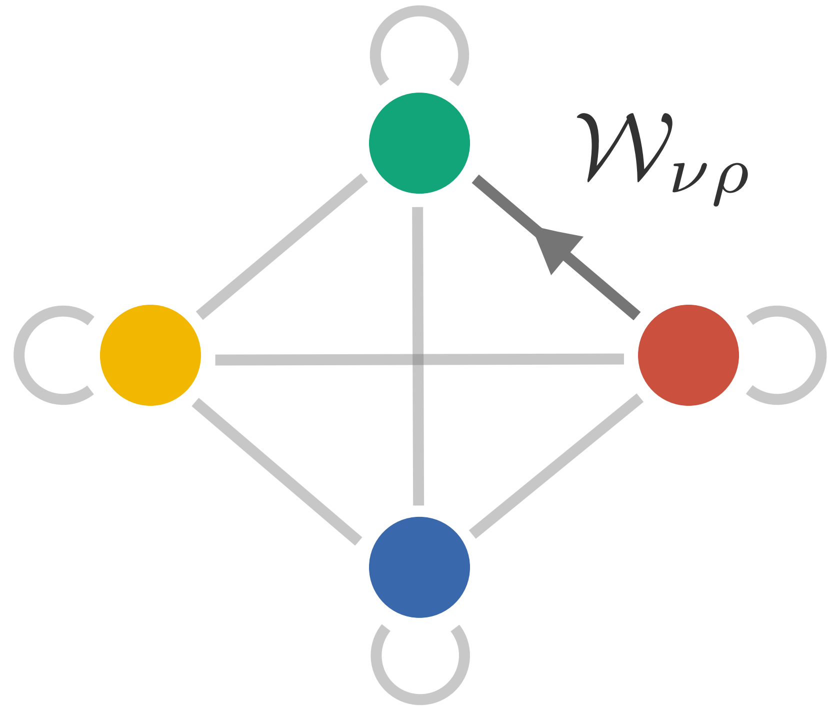
where $\{i_1, i_2, \ldots, i_{m_\nu}\} = G_\nu$ and $k_i^\rho = \sum_{j \in G_\rho} w_{ij}$.

1. Challenge: the compatibility equations *cannot* be fullfilled simultaneously in general.
2. Observation: if the connectivity properties in each groups are very similar, then $\boldsymbol{K}_{\nu\rho} \propto \boldsymbol{I}$.
3. Heuristic: find the $\widehat{\boldsymbol{a}}_\nu$ by solving the equations involving $\boldsymbol{W}_{\nu\rho}^T$.



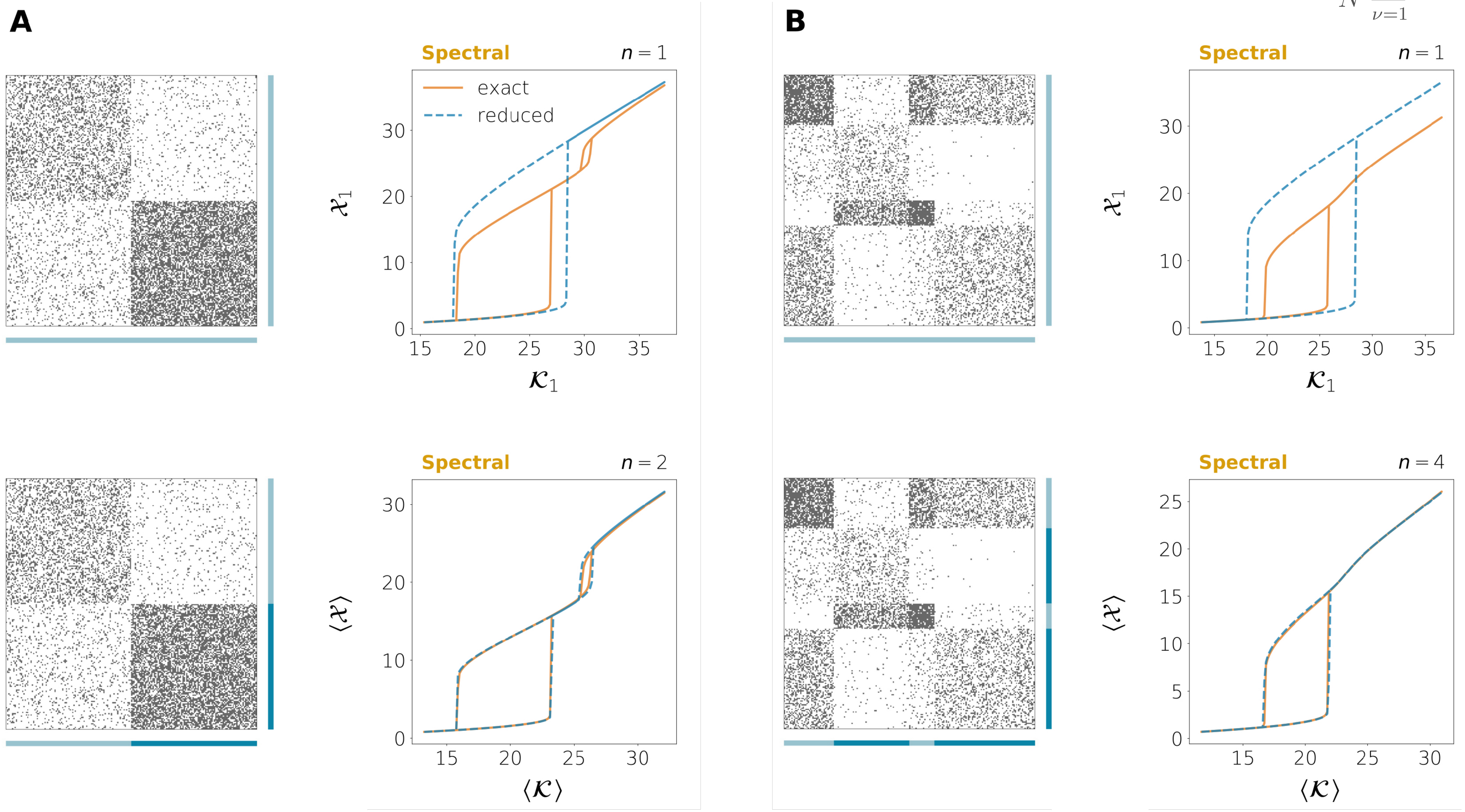




$$\langle \mathcal{K} \rangle = \frac{1}{N} \sum_{\nu=1}^{n} |G_\nu| \sum_{\rho=1}^{n} \mathcal{W}_{\nu\rho}$$

$$\langle \chi \rangle = \frac{1}{N} \sum_{\nu=1}^{n} |G_\nu| \chi_\nu$$

Validation on homogeneous networks with community structure



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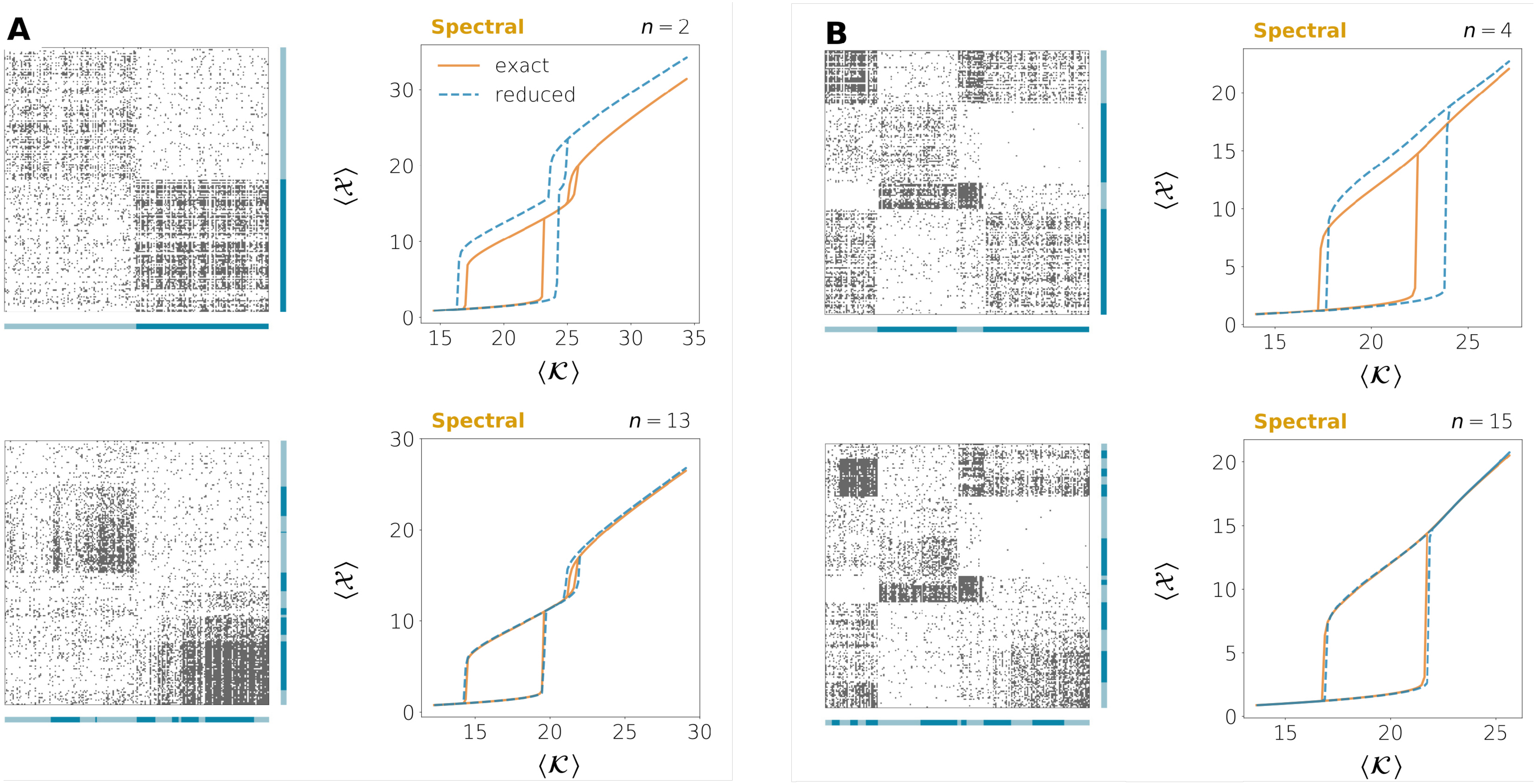
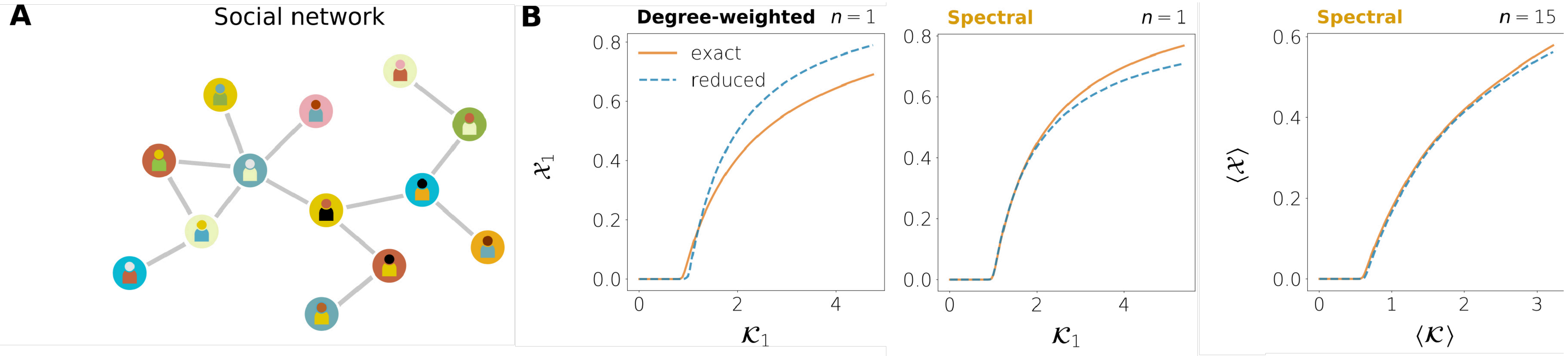
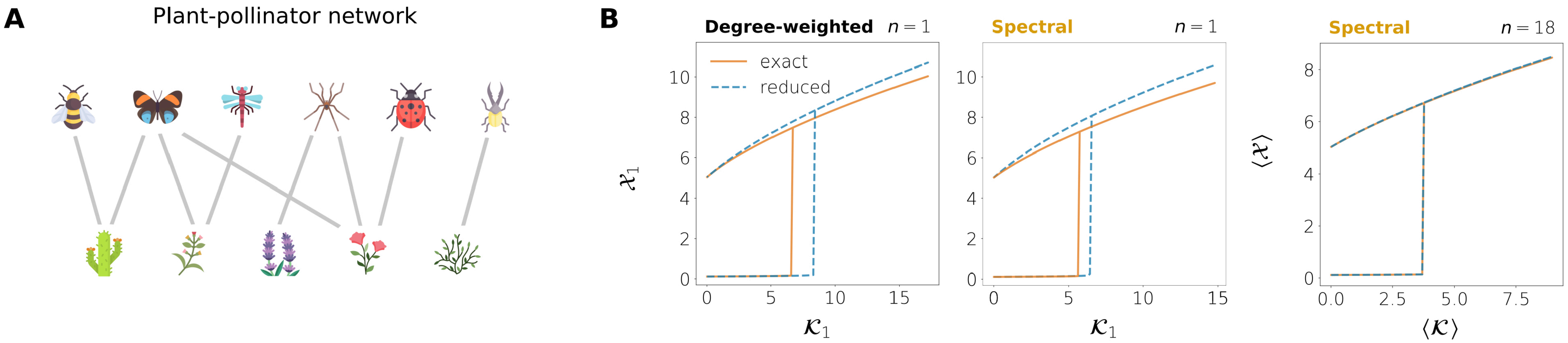
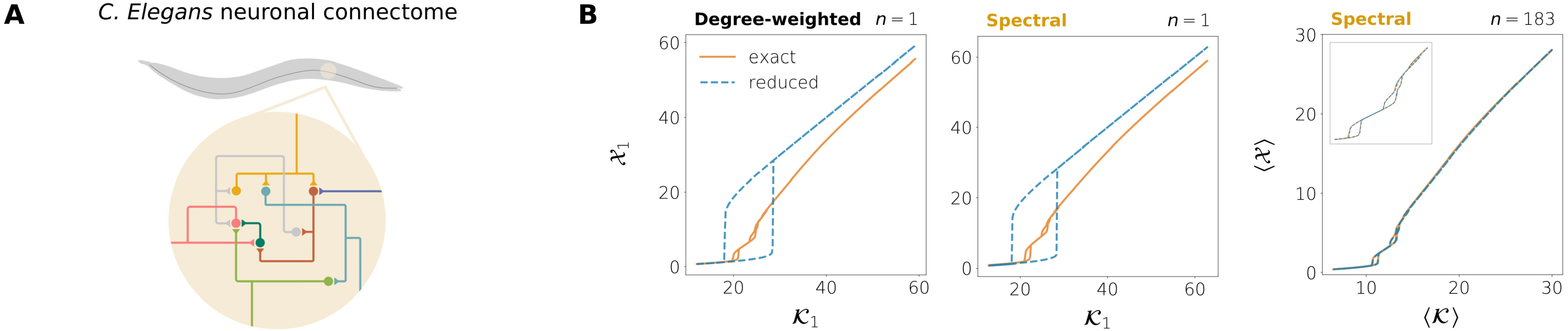


Real networks







Take-home message:

- extension of the dimension reduction formalism to heterogeneous and directed networks;
- observables have a clear interpretation (i.e. weighted average);
- n provides an idea of the *effective* dimension of a dynamics.

What else can be found in the manuscript?

- formal derivation of the reduced system as well as an extension including correction terms;
- systematic method to approximate the compatibility equations;
- sensibility analysis about the choice for the node partition;
- algorithm to refine the partitions;
- detailled case studies.

Open questions:

- How can we take into account signed interactions (e.g. inhibitory/exitatory synapses)?
- Is there a way to know the value fo n beforehand?

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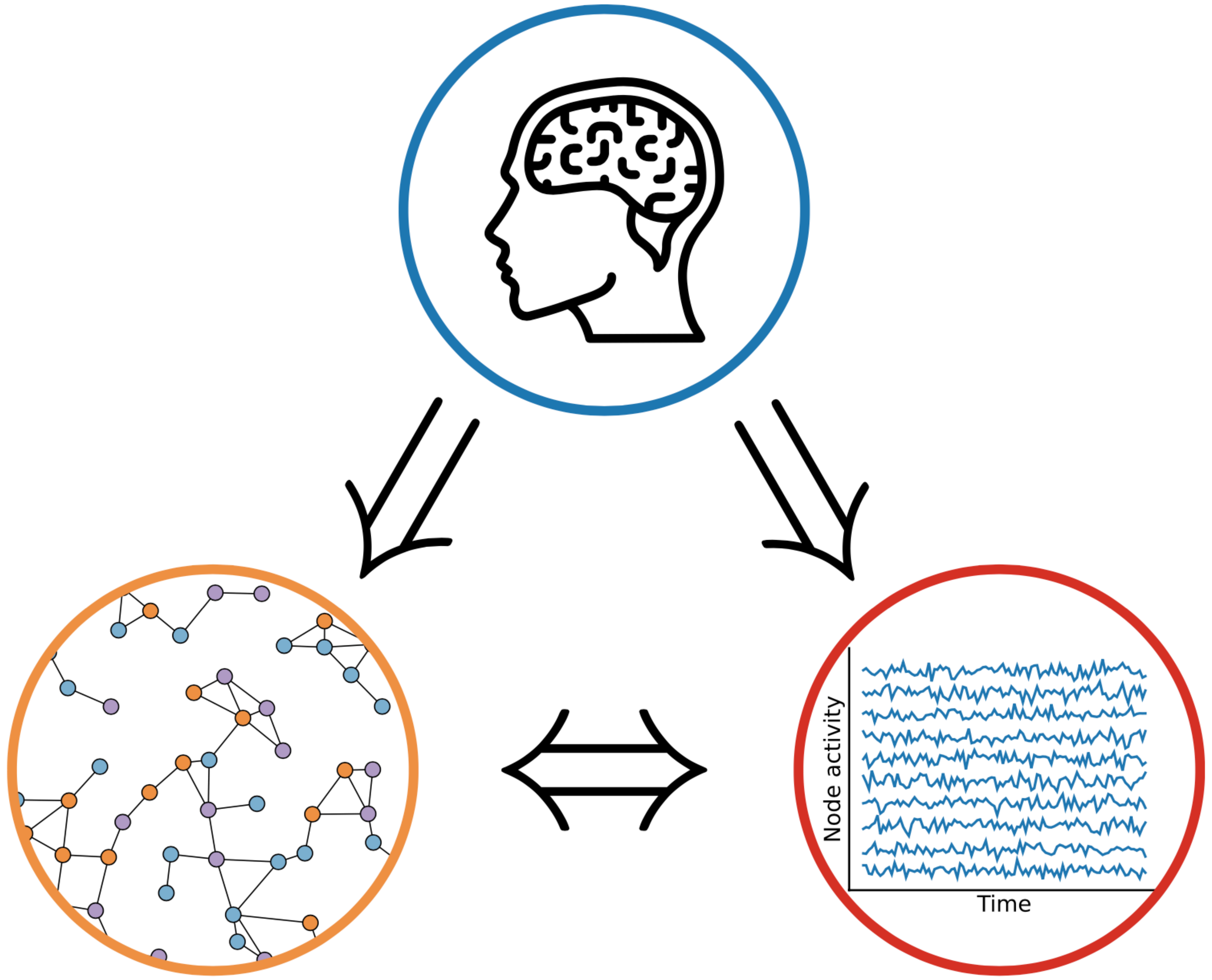
Duality between predictability and reconstructability in complex systems

Charles Murphy, Vincent Thibeault, Antoine Allard, Patrick Desrosiers

Predicting the evolution of a large system of units using its structure of interaction is a fundamental problem in complex system theory. And so is the problem of reconstructing the structure of interaction from temporal observations. Here, we find an intricate relationship between predictability and reconstructability using an information-theoretical point of view. We use the mutual information between a random graph and a stochastic process evolving on this random graph to quantify their codependence. Then, we show how the uncertainty coefficients, which are intimately related to that mutual information, quantify our ability to reconstruct a graph from an observed time series, and our ability to predict the evolution of a process from the structure of its interactions. Interestingly, we find that predictability and reconstructability, even though closely connected by the mutual information, can behave differently, even in a dual manner. We prove how such duality universally emerges when changing the number of steps in the process, and provide numerical evidence of other dualities occurring near the criticality of multiple different processes evolving on different types of structures.

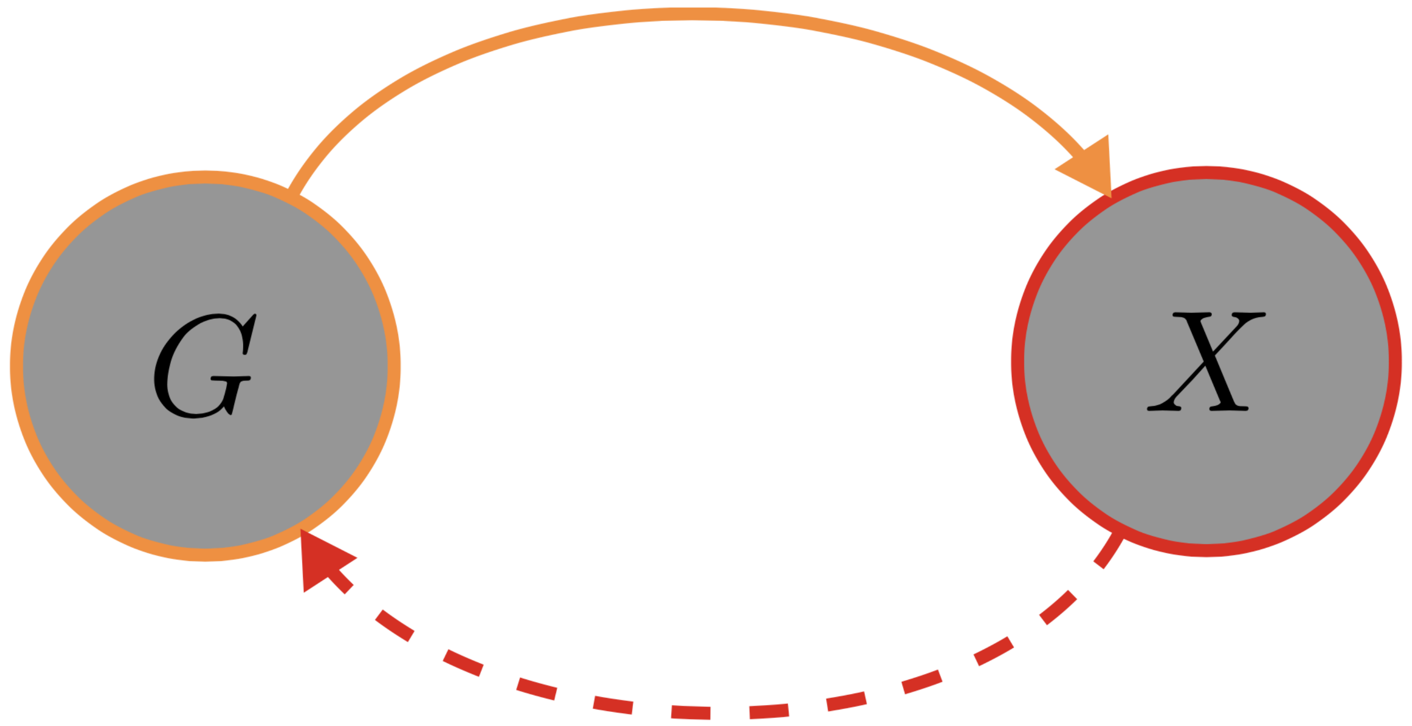
arXiv:2206.04000

Structure-function relationship (SFR) in complex systems



Structure-function relationship: the interplay between a process $X = (X_{i,t})$ and a graph G.

- $X_{i,t}$ is the state of node i at time t;
- G determines how the nodes interact within X.



Why should we care?

Prediction: Function from structure

To what extent does knowing the structure allow us to predict the behavior of the system?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ARTICLE

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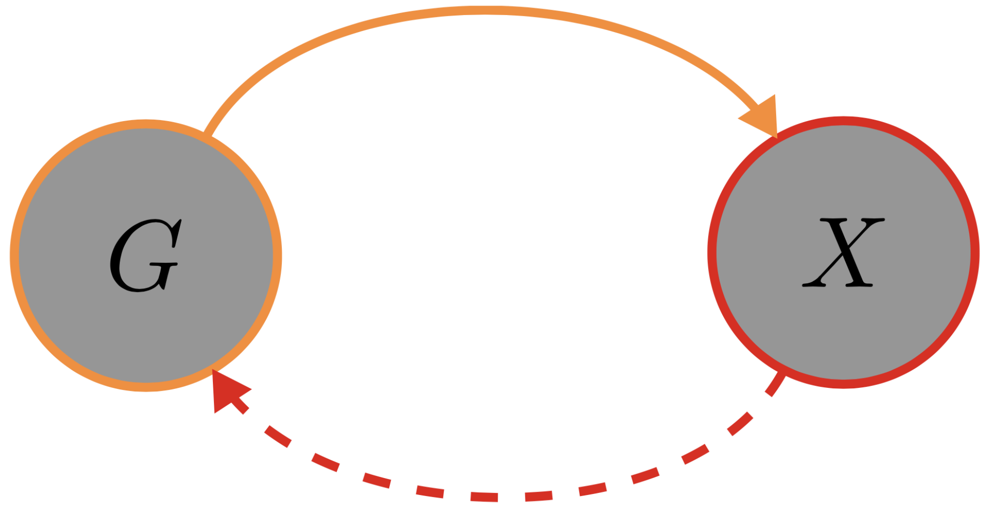
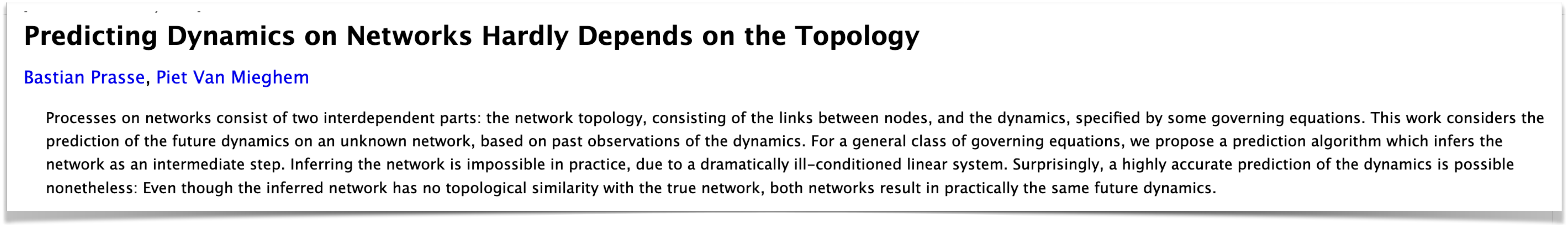
On the predictability of infectious disease outbreaks

Samuel V. Scarpino[1,2,3,4,5,6] & Giovanni Petri[6,7]



Reconstruction: Structure from function

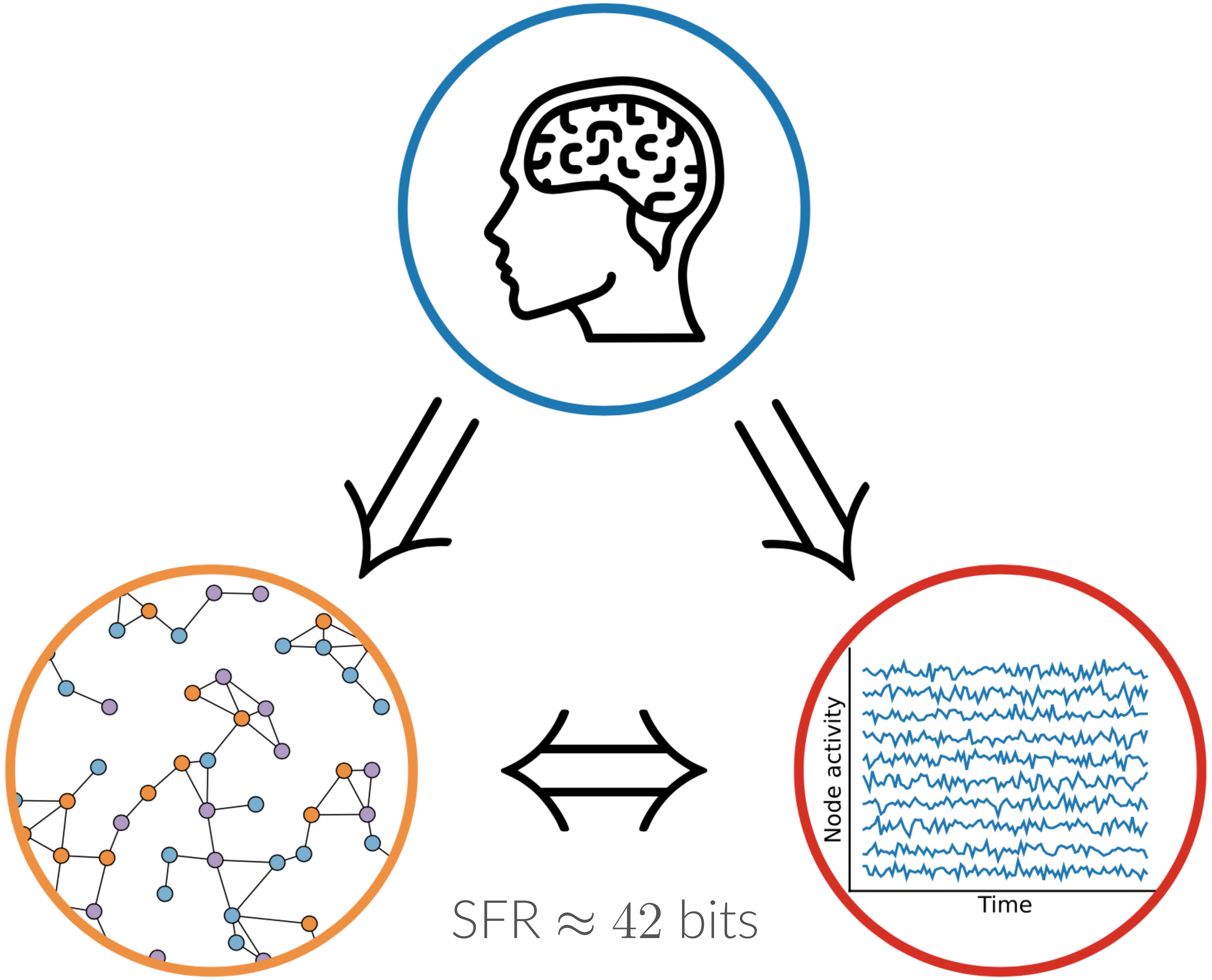
To what extent can we hope to reconstruct the underlying network from detailled time series?


Predicting Dynamics on Networks Hardly Depends on the Topology

Bastian Prasse, Piet Van Mieghem

Processes on networks consist of two interdependent parts: the network topology, consisting of the links between nodes, and the dynamics, specified by some governing equations. This work considers the prediction of the future dynamics on an unknown network, based on past observations of the dynamics. For a general class of governing equations, we propose a prediction algorithm which infers the network as an intermediate step. Inferring the network is impossible in practice, due to a dramatically ill-conditioned linear system. Surprisingly, a highly accurate prediction of the dynamics is possible nonetheless: Even though the inferred network has no topological similarity with the true network, both networks result in practically the same future dynamics.

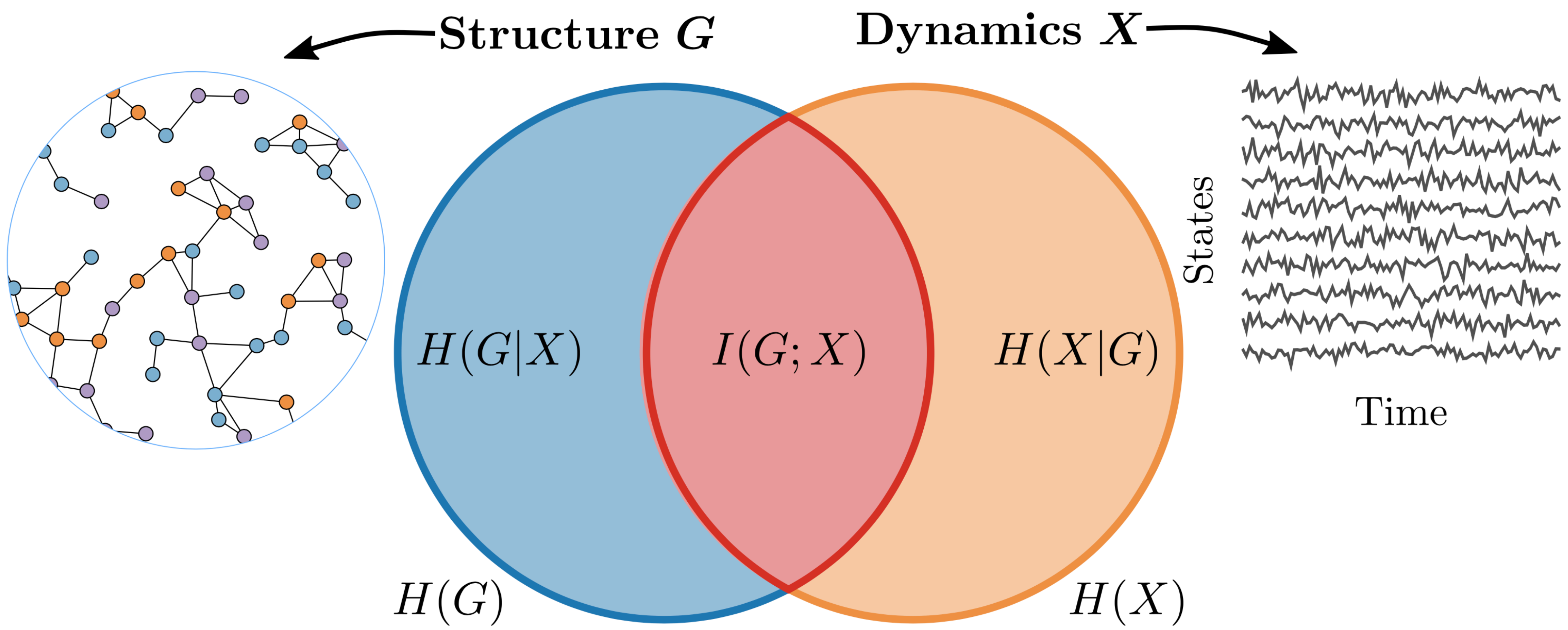
Our objective: to measure the SFR using information theory



Our objective: to measure the SFR using information theory

For the framework of information theory to be meaningful in this context, we assume that

- G is a random graph ensemble, i.e. $G \sim P(G)$;
- X is a stochastic process conditioned on G, i.e. $X \sim P(X|G)$.



All other quantities can be computed from $P(G)$ and $P(X|G)$

$$
\begin{aligned}
H(G) &= \langle -\log P(G) \rangle \\
H(X) &= \langle -\log P(X) \rangle \\
H(G|X) &= \langle -\log P(G|X) \rangle \\
H(X|G) &= \langle -\log P(X|G) \rangle
\end{aligned}
$$

where

$$
P(X) = \sum_{G^*} P(G^*) P(X|G^*)
$$

$$
P(G|X) = \frac{P(X|G)P(G)}{P(X)}
$$

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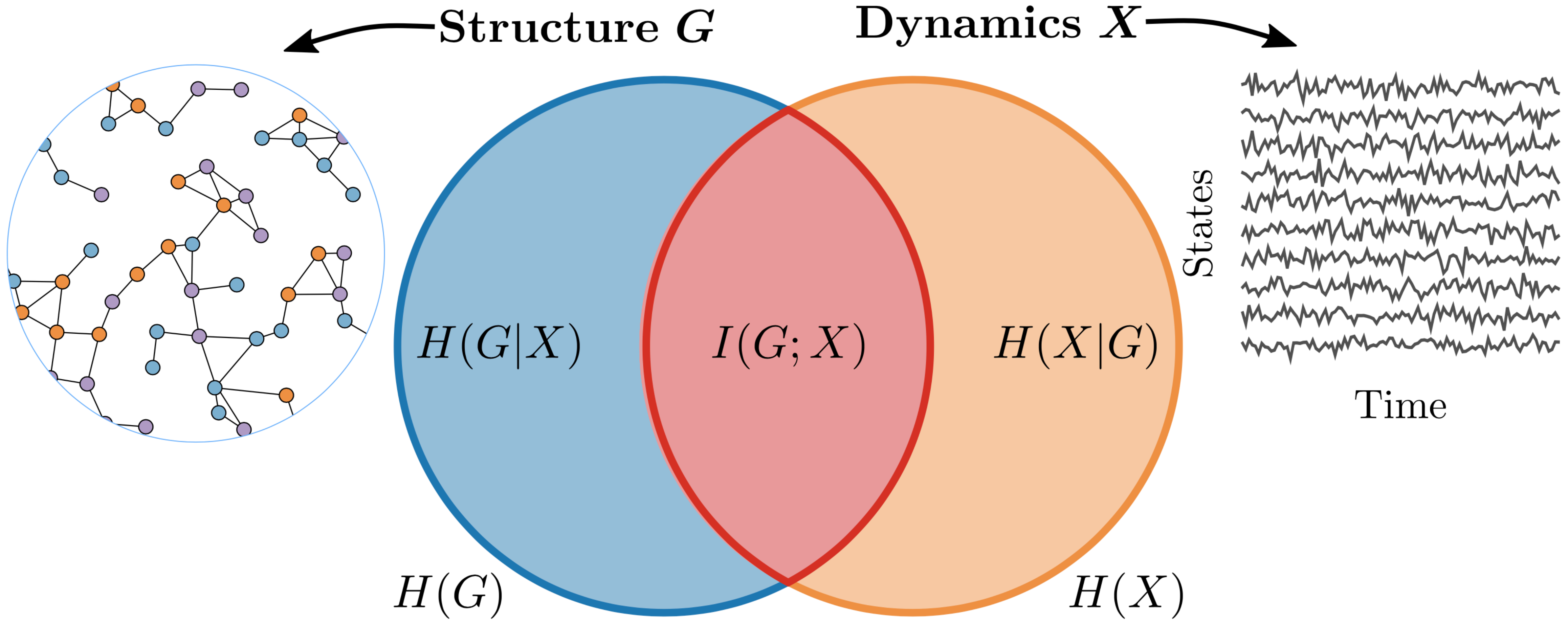

The mutual information $I(X;G)$ quantifies the *strength* of the relationship between X and G.

- it is the knowledge gained about X when G is known;
- it is the knowledge gained about G when X is known.

All other quantities can be computed from $P(G)$ and $P(X|G)$

$$
\begin{aligned}
H(G) &= \langle -\log P(G) \rangle \\
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P(X) = \sum_{G^*} P(G^*) P(X|G^*)
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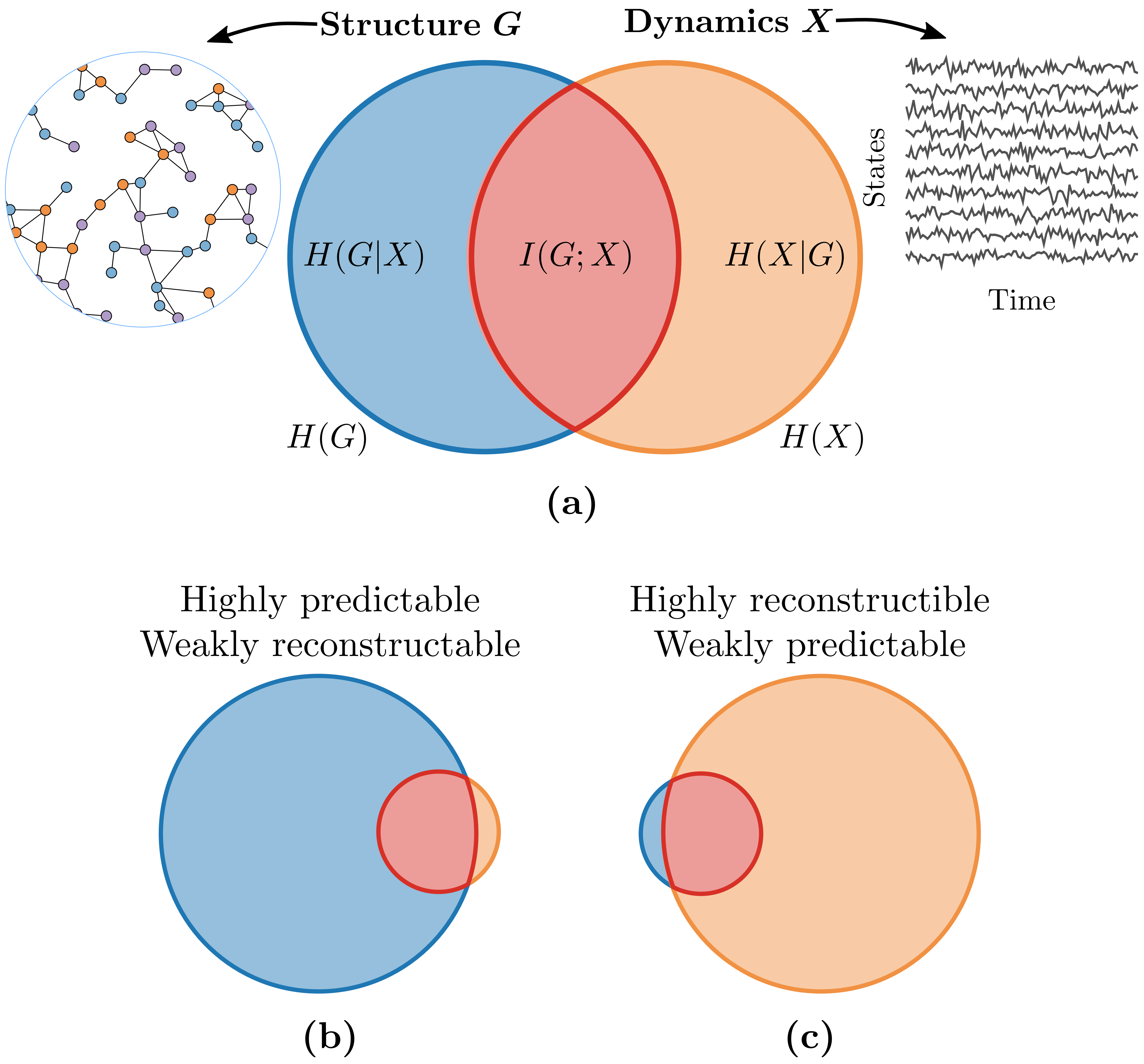
P(G|X) = \frac{P(X|G)P(G)}{P(X)}
$$

The mutual information can be written from the *perspective* of X as well as from the *perspective* of G

$$
\begin{aligned}
I(X;G) &= H(G) - H(G|X) \\
&= H(X) - H(X|G)
\end{aligned}
$$

Two faces of the same coin



The mutual information can be written from the *perspective* of X as well as from the *perspective* of G

$$I(X;G) = H(G) - H(G|X)$$
$$= H(X) - H(X|G)$$

These two perspectives allow us to introduce

$$U(X|G) = \frac{I(X;G)}{H(X)} = 1 - \frac{H(X|G)}{H(X)} \quad \text{(predictability)}$$
$$U(G|X) = \frac{I(X;G)}{H(G)} = 1 - \frac{H(G|X)}{H(G)} \quad \text{(reconstructability)}$$

The evidence probability estimation problem

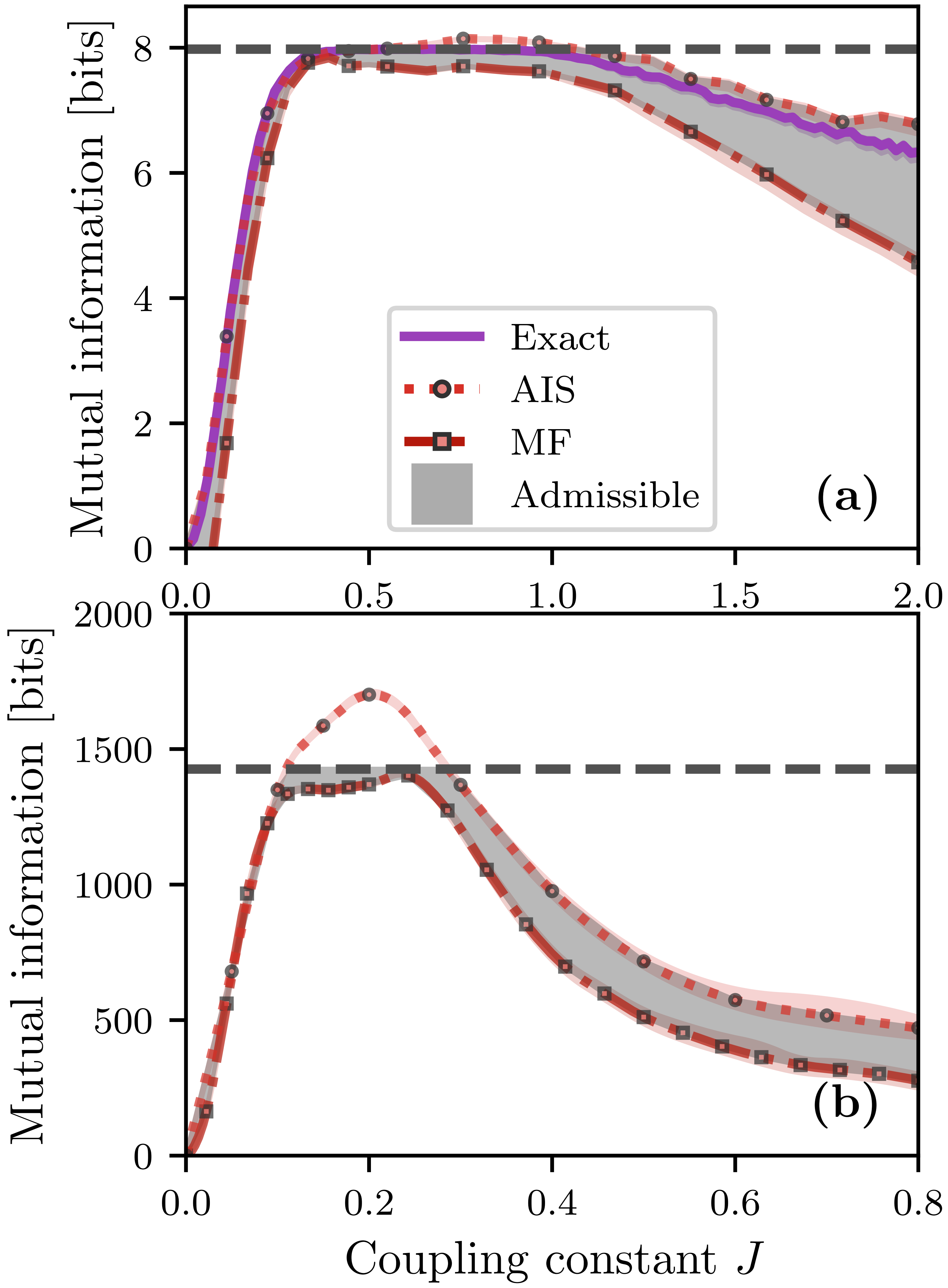
The computation of $H(X)$ and $H(G|X)$ requires the evaluation of the *log-evidence*

$$\log P(X) = \log \left[\sum_{G^* \in \mathcal{G}_N} P(G^*) P(X \mid G^*) \right]$$

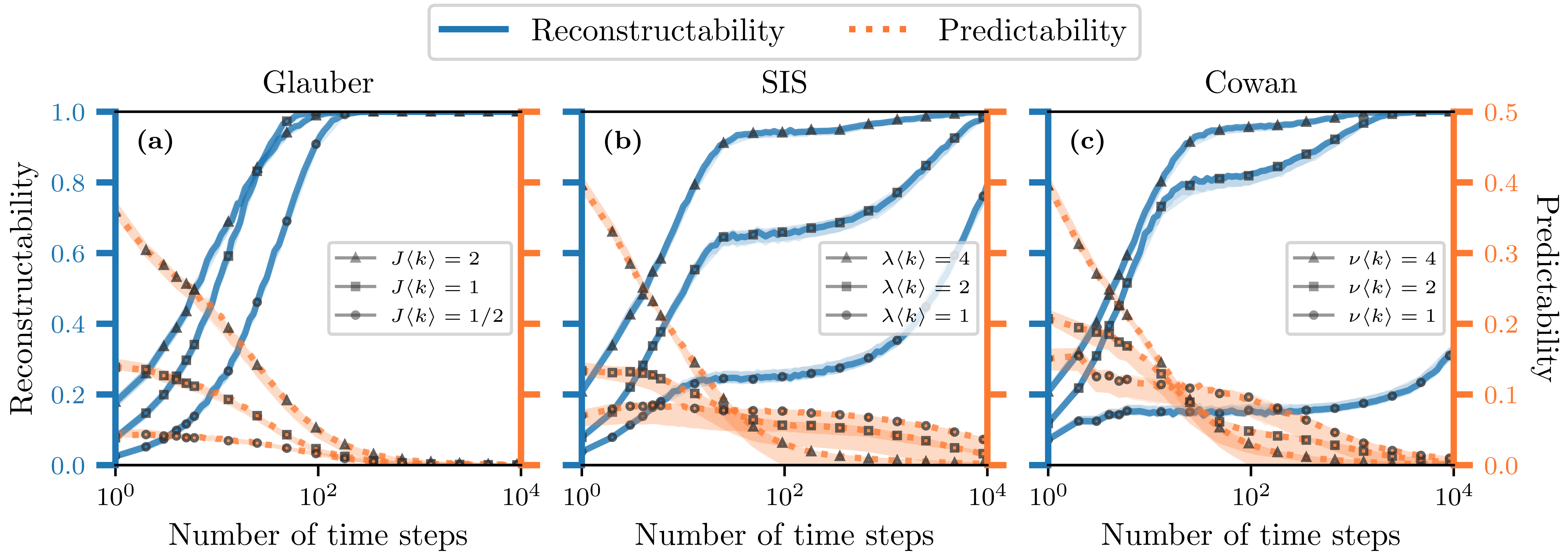
which involves the enumeration of *all* graphs and therefore becomes intractable with N.

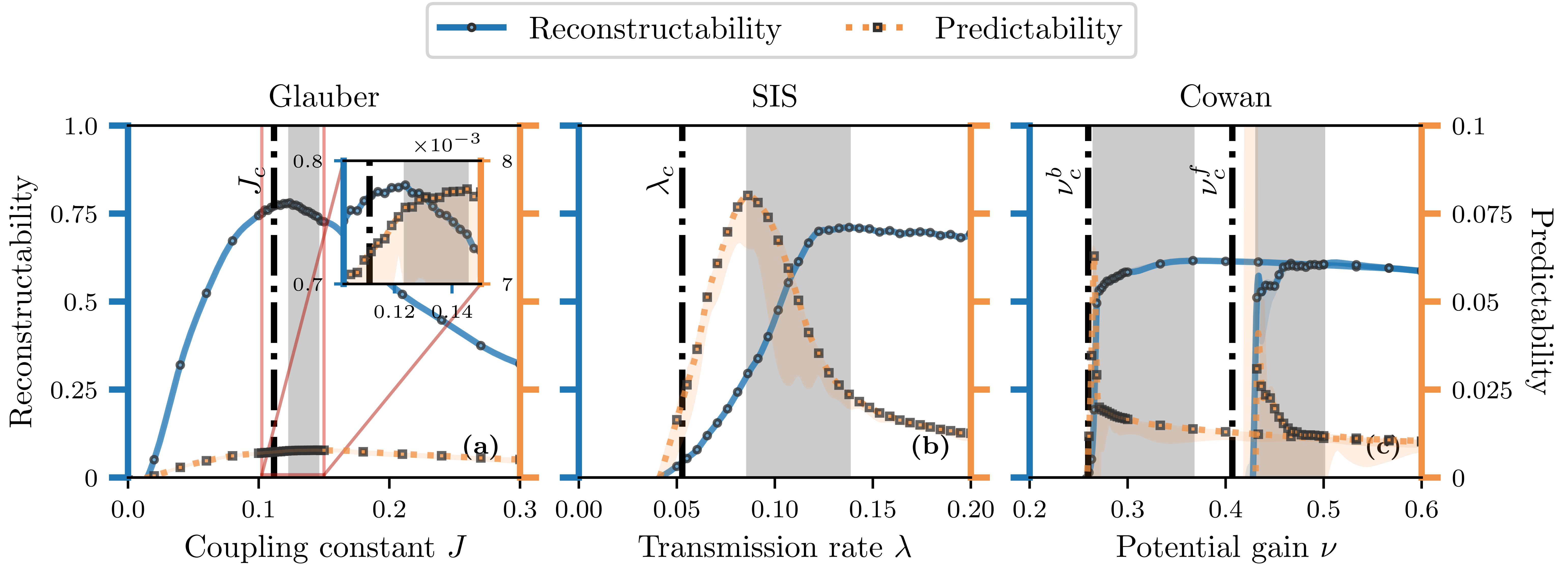
Two convenient approximations:

1. mean-field (MF) approximation: lower bound for $I(X;G)$
2. annealed importance sampling (AIS): upper bound for $I(X;G)$



Dual behavior of reconstructability and predictability





Take-home message:

- the SFR can be quantified using information theory (mutual information)
- mutual information provides information on both the reconstructability and the predictability
- reconstructability and predictability can behave in a dual manner
- limitations due to enumeration can be bypassed using biased estimators that provide upper and lower bounds

What else can be found in the manuscript?

- formal definition of duality
- formal proof of the T-duality
- description of the biased estimators and characterization of their bias (i.e. lower/upper bound)

Open questions:

- Is there a deep connection between duality and criticality?
- To what extent can we apply this framework to gain better insight about specific problems?

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Marina Vegué Llorente

Charles Murphy

Vincent Thibeault

Patrick Desrosiers

Dimension reduction of dynamics on modular and heterogeneous directed networks

Marina Vegué, Vincent Thibeault, Patrick Desrosiers, Antoine Allard

Dimension reduction is a common strategy to study non-linear dynamical systems composed by a large number of variables. The goal is to find a smaller version of the system whose time evolution is easier to predict while preserving some of the key dynamical features of the original system. Finding such a reduced representation for complex systems is, however, a difficult task. We address this problem for dynamics on weighted directed networks, with special emphasis on modular and heterogeneous networks. We propose a two-step dimension-reduction method that takes into account the properties of the adjacency matrix. First, units are partitioned into groups of similar connectivity profiles. Each group is associated to an observable that is a weighted average of the nodes' activities within the group. Second, we derive a set of conditions that must be fulfilled for these observables to properly represent the original system's behavior, together with a method for approximately solving them. The result is a reduced adjacency matrix and an approximate system of ODEs for the observables' evolution. We show that the reduced system can be used to predict some characteristic features of the complete dynamics for different types of connectivity structures, both synthetic and derived from real data, including neuronal, ecological, and social networks. Our formalism opens a way to a systematic comparison of the effect of various structural properties on the overall network dynamics. It can thus help to identify the main structural driving forces guiding the evolution of dynamical processes on networks.

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