

Higher-order networks

An introduction to simplicial complexes

Lesson I

LTCC Course
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Ginestra Bianconi

School of Mathematical Sciences, Queen Mary University of London
Alan Turing Institute



Queen Mary
University of London

**The
Alan Turing
Institute**

Outline of the course

- 1. Higher order networks structure and maximum entropy models**
- 2. Higher-order non-equilibrium network models and emergent geometry**
- 3. Simplicial topology an introduction**
- 4. Dynamics of higher-order topological signals**
- 5. The Dirac operator and its applications**

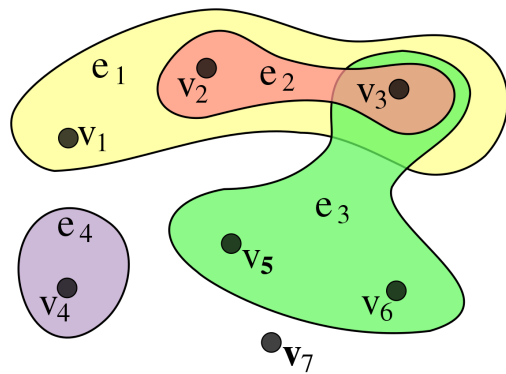
Lesson I:

Higher order networks structure

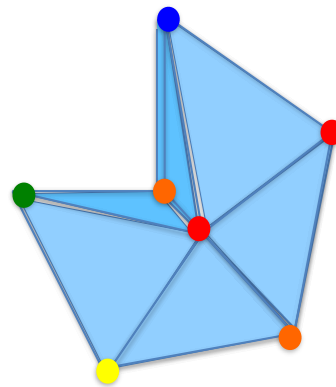
- **Higher-order networks**
 1. **Definitions**
 2. **Introduction to the higher-order combinatorial properties**
- **Background on networks and maximum entropy models**
- **Maximum Entropy models of simplicial complexes**

Higher-order networks

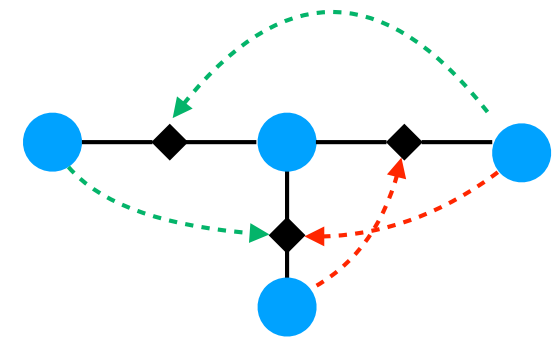
Higher-order networks are characterising the interactions between two or more nodes



Hypergraph



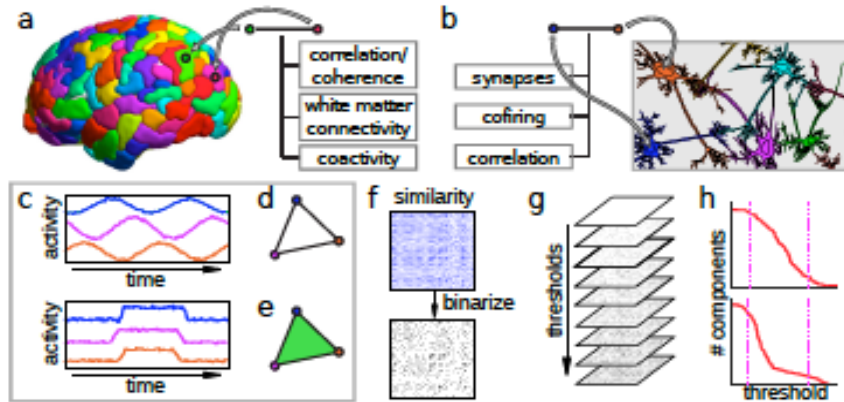
Simplicial complex



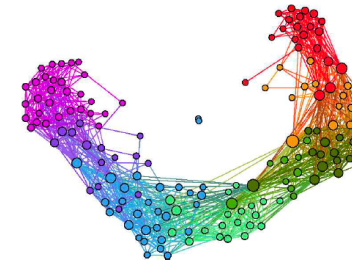
Network with triadic interactions

Higher-order network data

Brain data

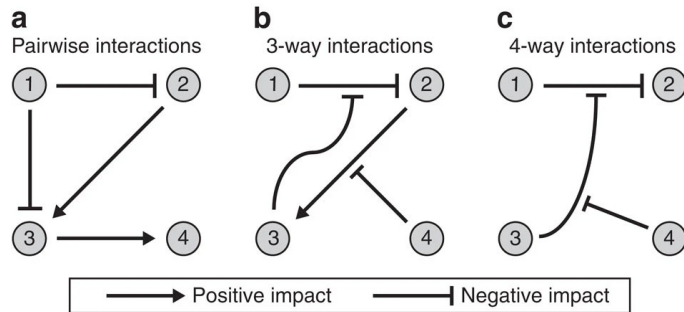


Face-to-face interactions

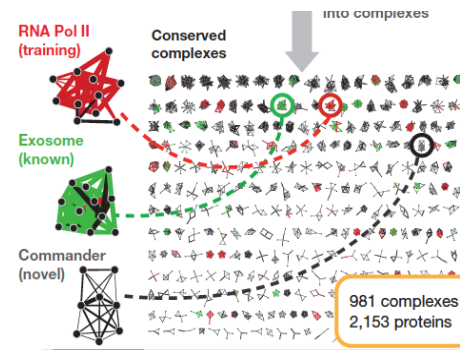


Collaboration networks

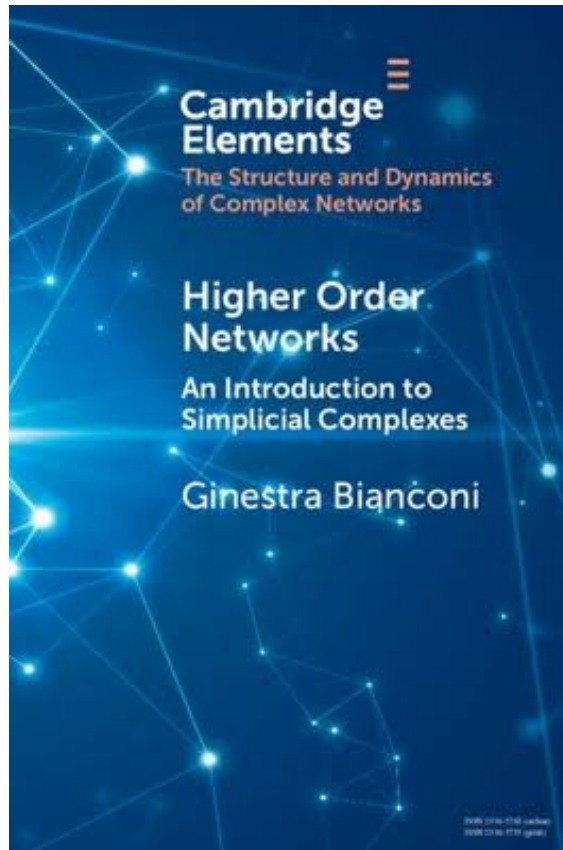
Ecosystems



Protein interactions



Higher-order networks



New book
by Cambridge University Press!!

**Providing a general view of the interplay
between topology and dynamics**



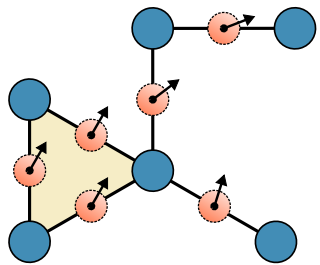


The physics of higher-order interactions in complex systems

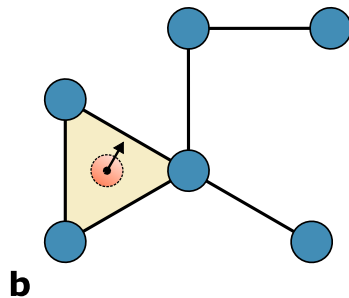
Federico Battiston¹✉, Enrico Amico^{2,3}, Alain Barrat^{4,5}, Ginestra Bianconi^{6,7},
Guilherme Ferraz de Arruda⁸, Benedetta Franceschiello^{9,10}, Iacopo Iacopini¹, Sonia Kéfi^{11,12},
Vito Latora^{6,13,14,15}, Yamir Moreno^{8,15,16,17}, Micah M. Murray^{9,10,18}, Tiago P. Peixoto^{1,19},
Francesco Vaccarino^{10,20} and Giovanni Petri^{8,21}✉

Complex networks have become the main paradigm for modelling the dynamics of interacting systems. However, networks are intrinsically limited to describing pairwise interactions, whereas real-world systems are often characterized by higher-order interactions involving groups of three or more units. Higher-order structures, such as hypergraphs and simplicial complexes, are therefore a better tool to map the real organization of many social, biological and man-made systems. Here, we highlight recent evidence of collective behaviours induced by higher-order interactions, and we outline three key challenges for the physics of higher-order systems.

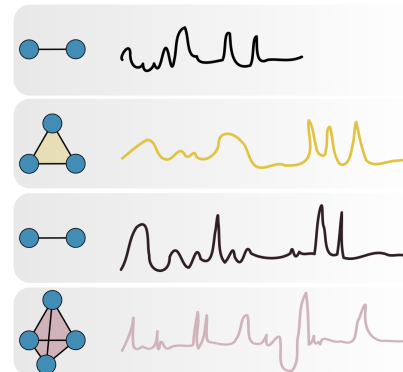
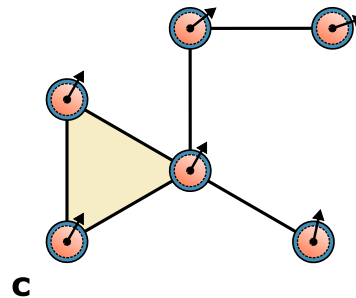
Edge dynamics



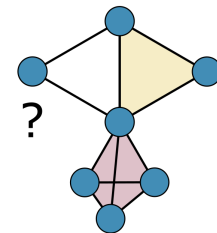
Upward projection



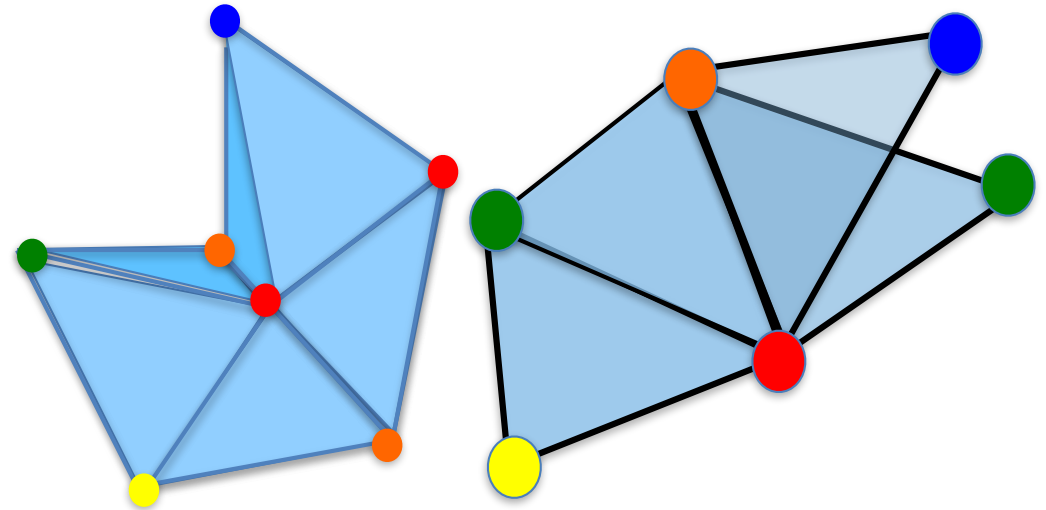
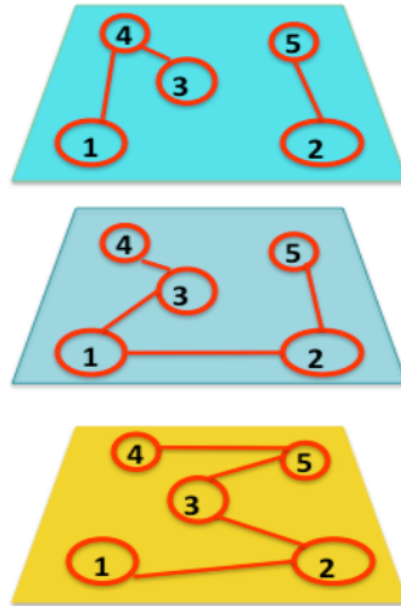
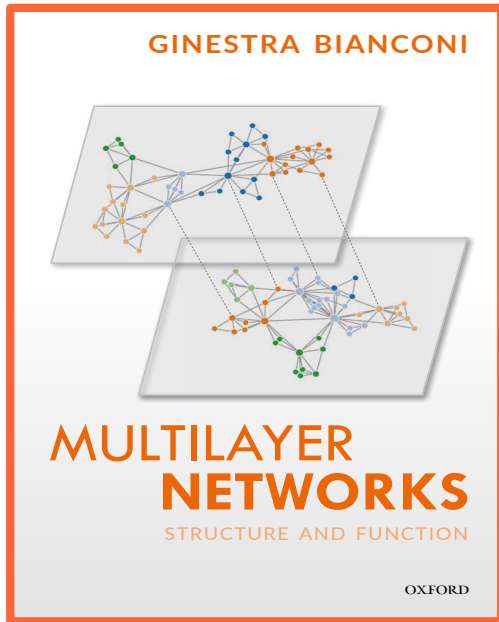
Downward projection



Reconstruction



Generalized network structures



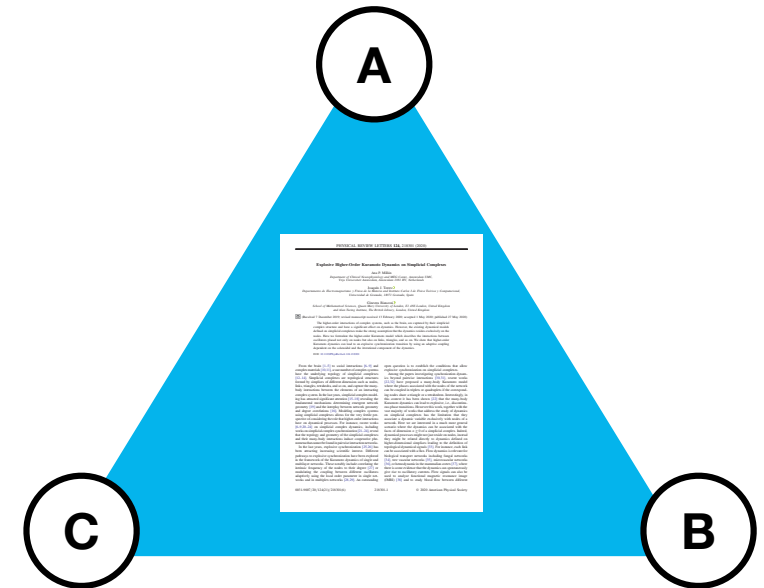
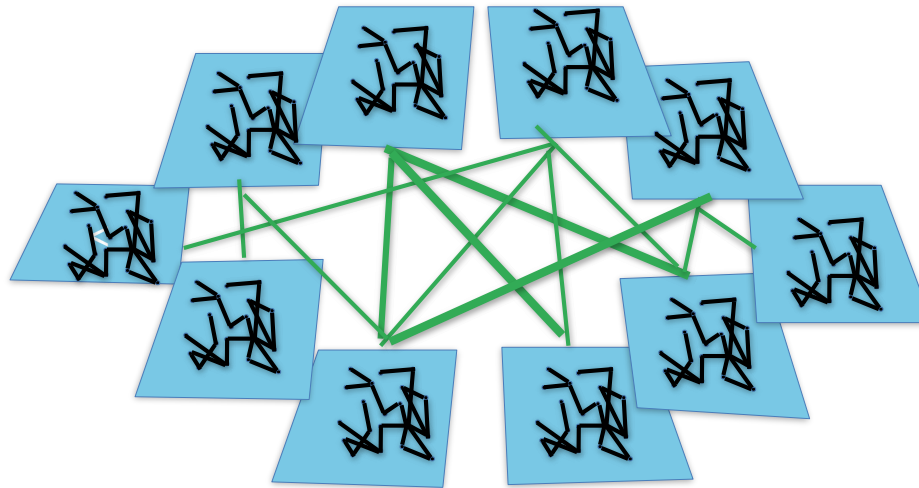
Going beyond the framework of simple networks

is of fundamental importance

for understanding the relation between structure and

dynamics in complex systems

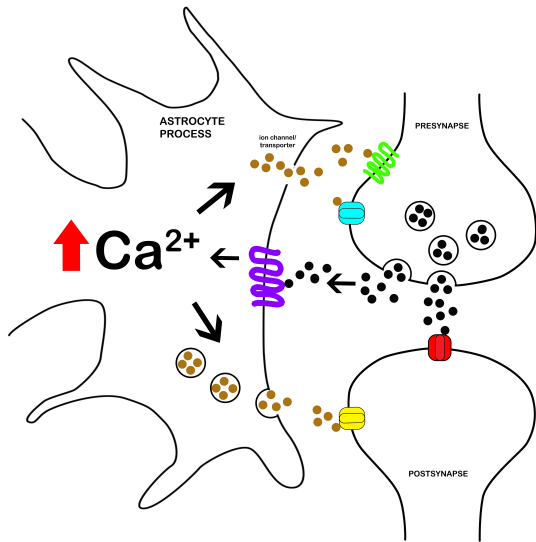
Collaboration Networks



Jacovacci, Wu, Bianconi (2015)

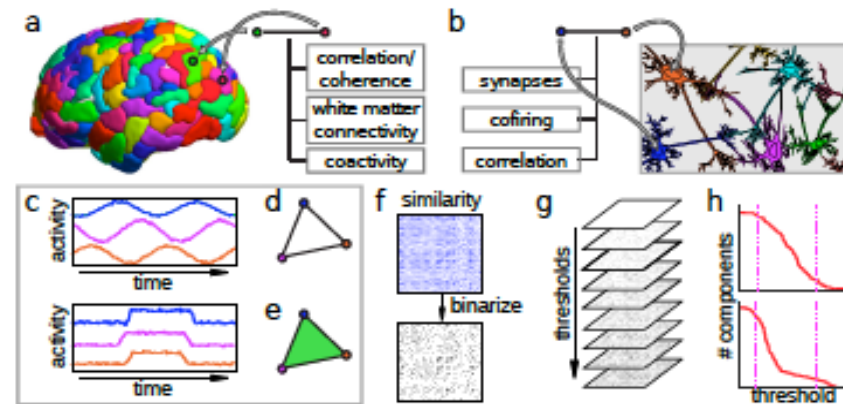
Each paper includes higher-order interactions among the corresponding team

Higher-order interactions in the brain



- POSTSYNAPTIC IONOTROPIC RECEPTOR
- EXTRASYNAPTIC IONOTROPIC RECEPTOR
- PRESYNAPTIC IONOTROPIC RECEPTOR
- NEUROTRANSMITTERS
- GLIOTRANSMITTERS
- Gq GPCR OF ASTROCYTE
- PRESYNAPTIC METABOTROPIC RECEPTOR

Cho, Barcelon and Lee (2016)

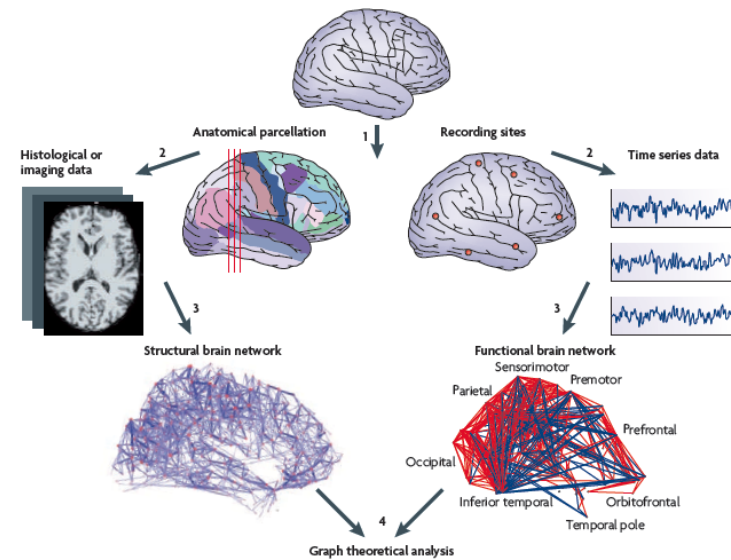
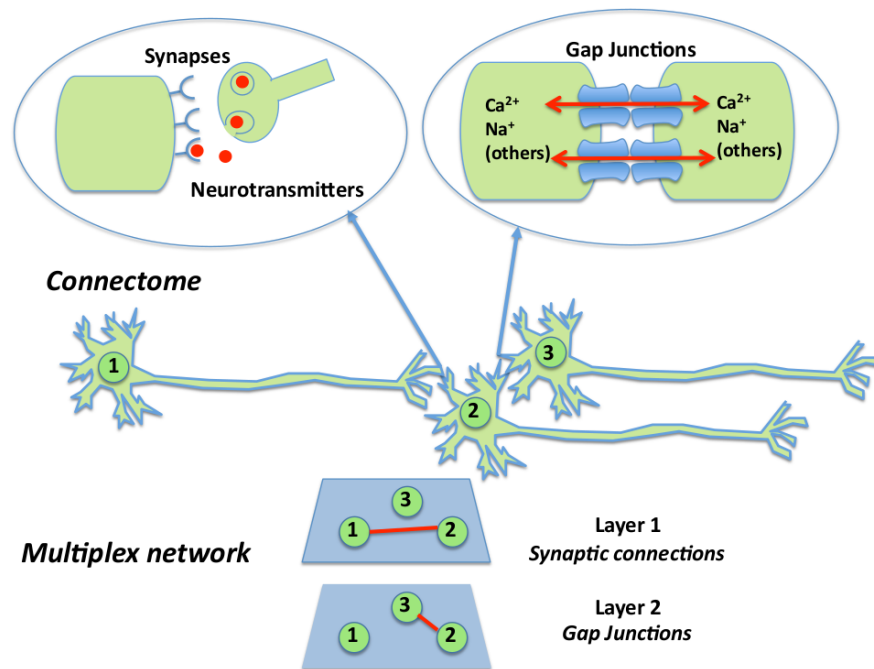


Giusti et al (2016)



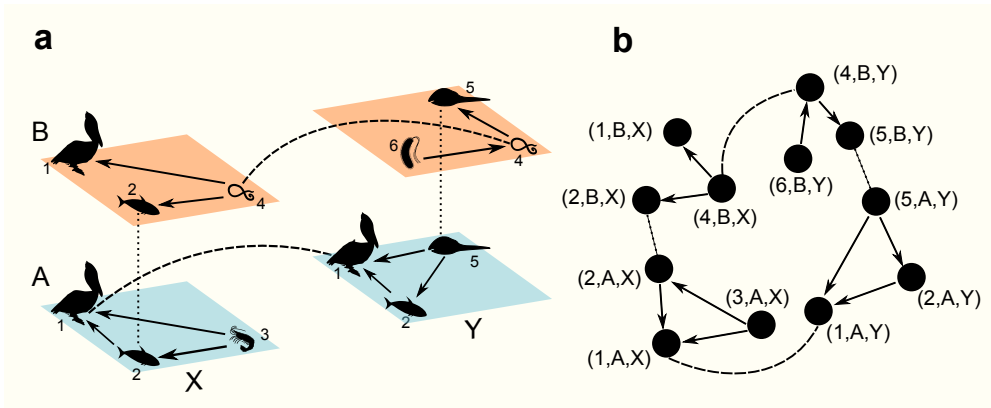
Petri et al. (2014)

Multilayer brain networks

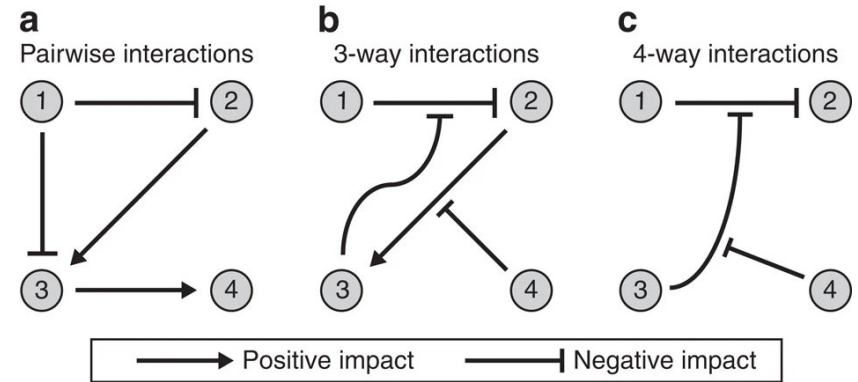


Bullmore and Sporns (2009)

Ecosystems

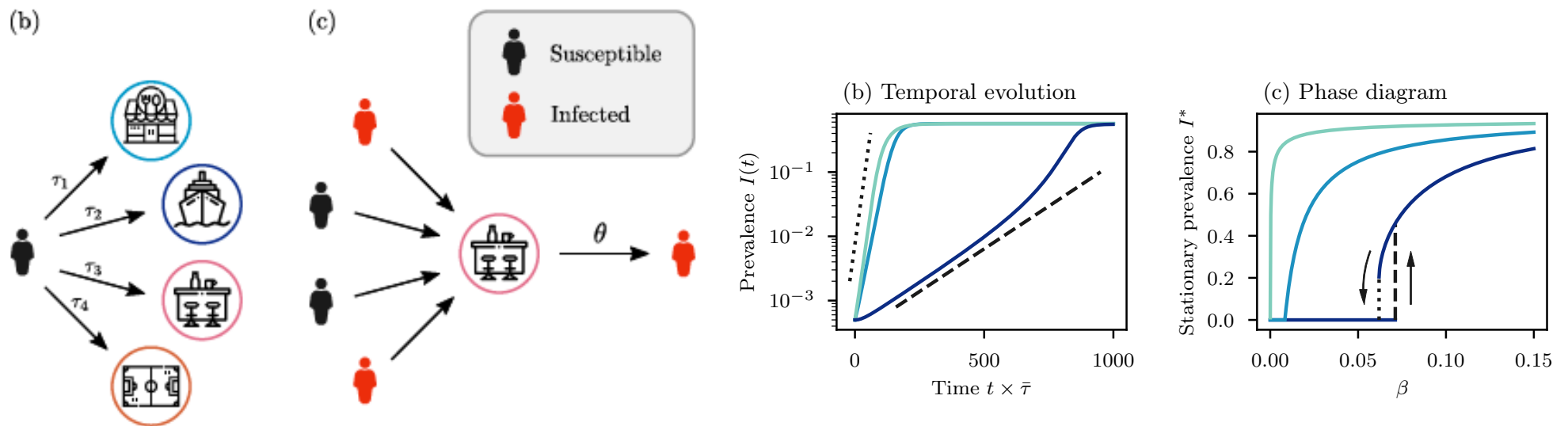


Pilosof et al. (2016)



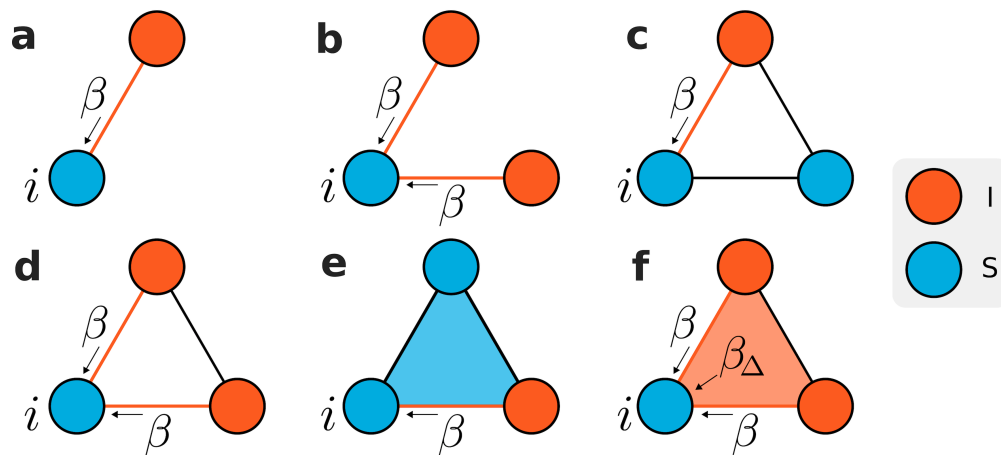
Bairey et al. (2017)

Explosive Epidemic Spreading on co-location hypergraphs

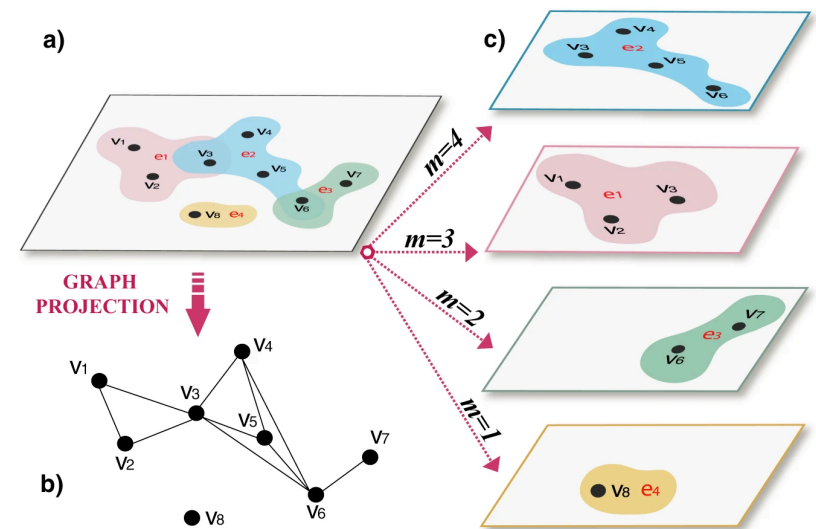


St-Onge, et. al PRL (2021)

Simplicial social contagions and social contagion on hypergraphs

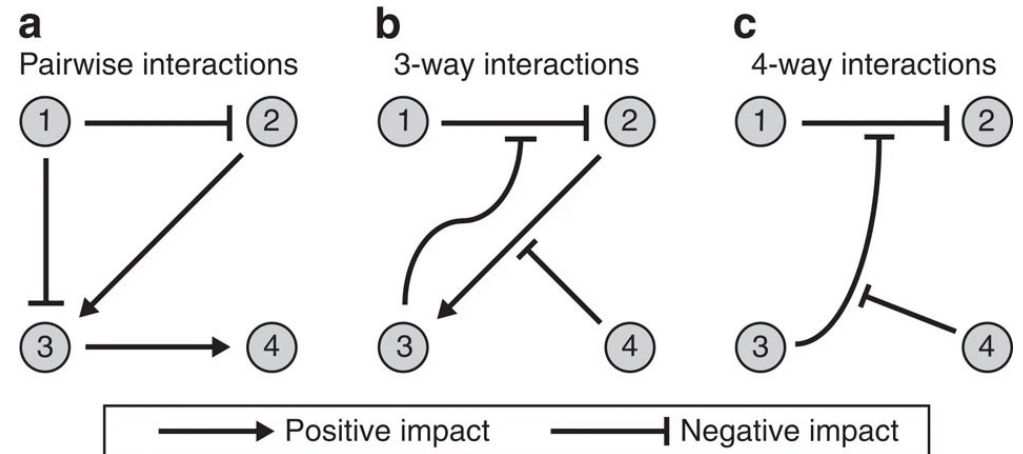
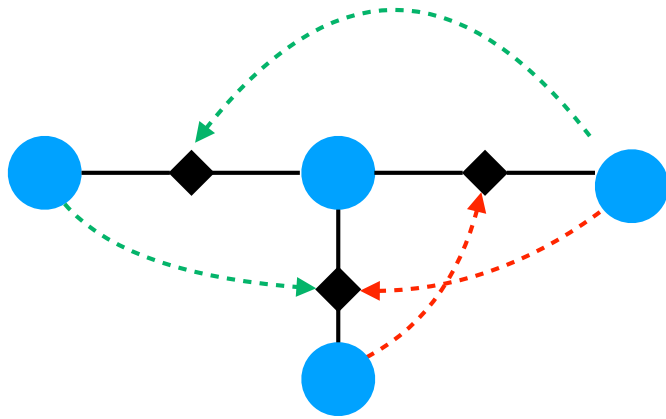


Iacopini et al. (2019)



De arruda et al. (2021)

Triadic interactions

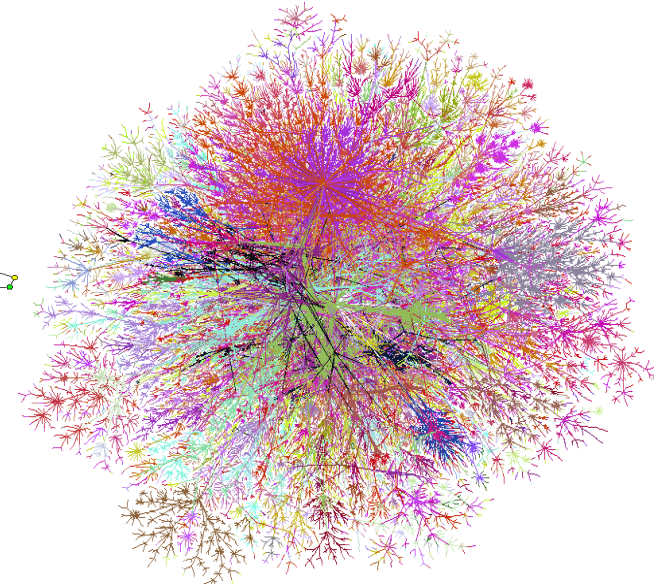
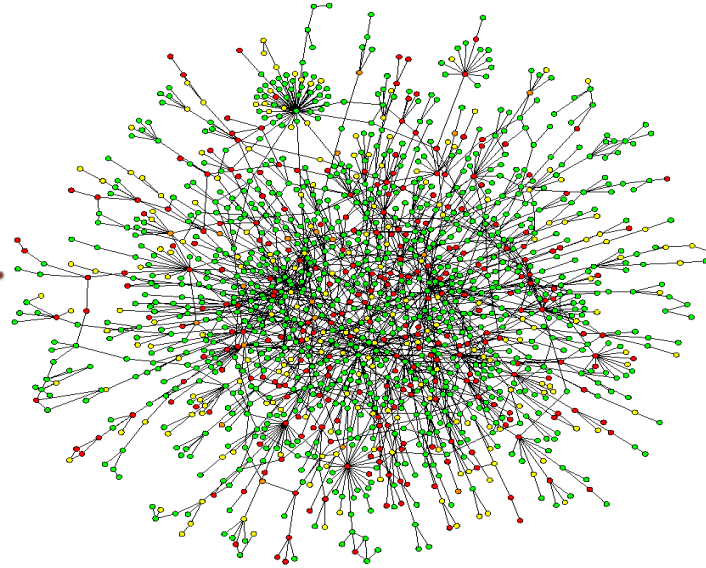
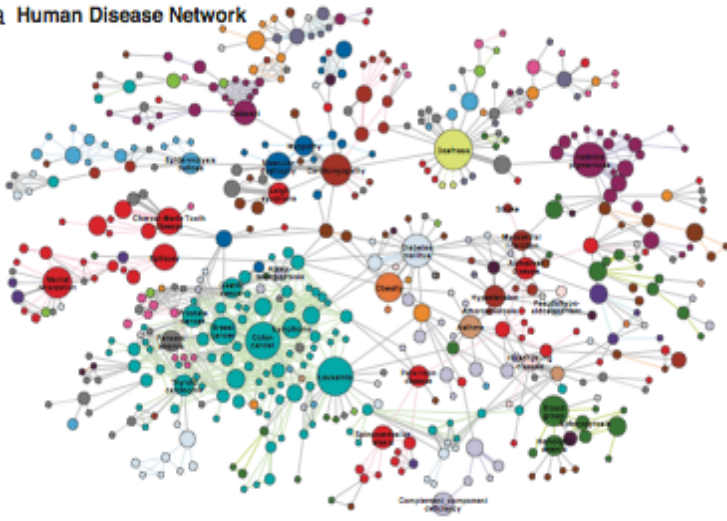


Sun, Radicchi, Kurths GB (2022)

Background on network science

Networks

a Human Disease Network



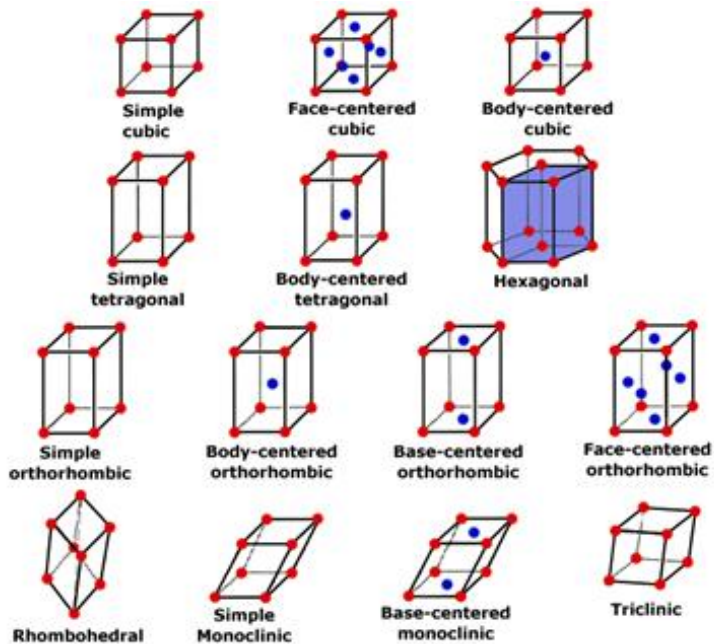
describe

the interactions between the elements
of large complex systems.

Randomness and order

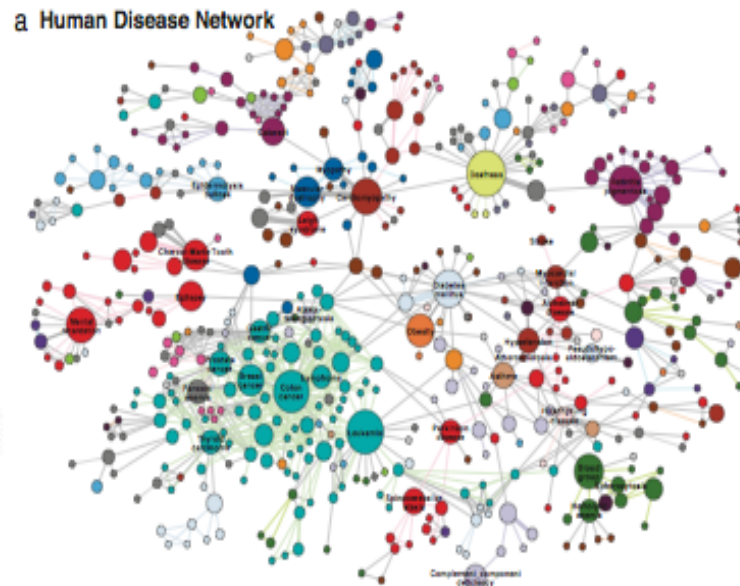
Complex networks

LATTICES



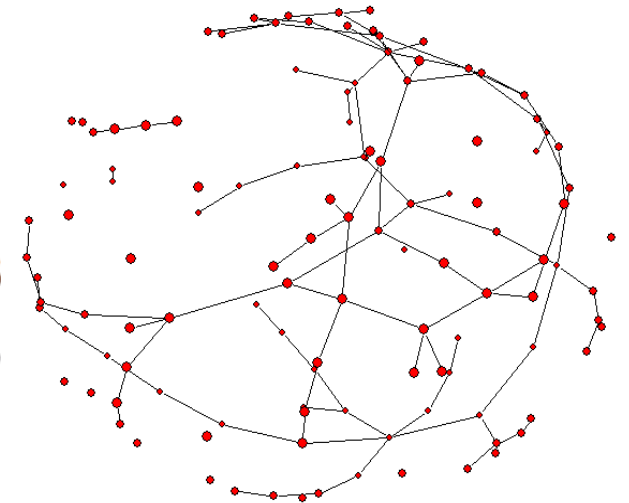
Regular networks
Symmetric

COMPLEX NETWORKS



Scale free networks
Small world
With communities
**ENCODING INFORMATION IN
THEIR STRUCTURE**

RANDOM GRAPHS



Totally random
Binomial degree
distribution

Universalities

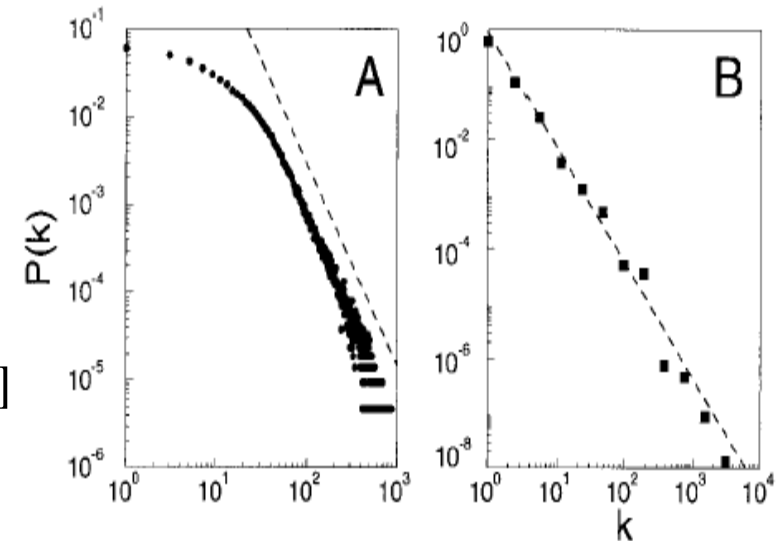
- **Small-world:** $d_H = \infty$

[Watts & Strogatz 1998]

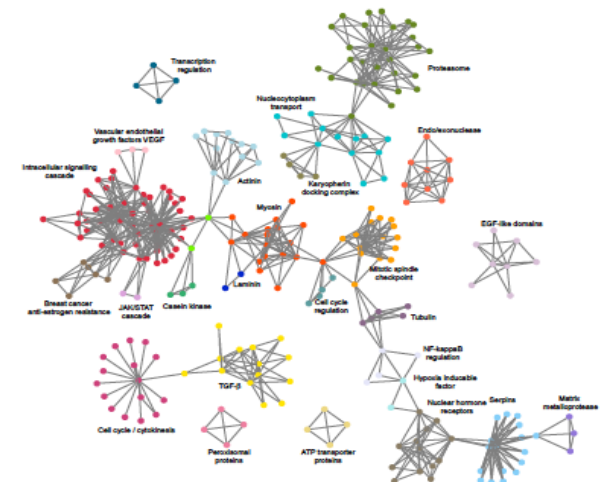
- **Scale-free:** $P(k) \sim k^{-\gamma}$ **for** $k \gg 1$
[Barabasi & Albert 1999]
with $\gamma \in (2,3)$

$$\langle k \rangle \rightarrow \text{const} \quad \langle k^2 \rangle \rightarrow \infty$$

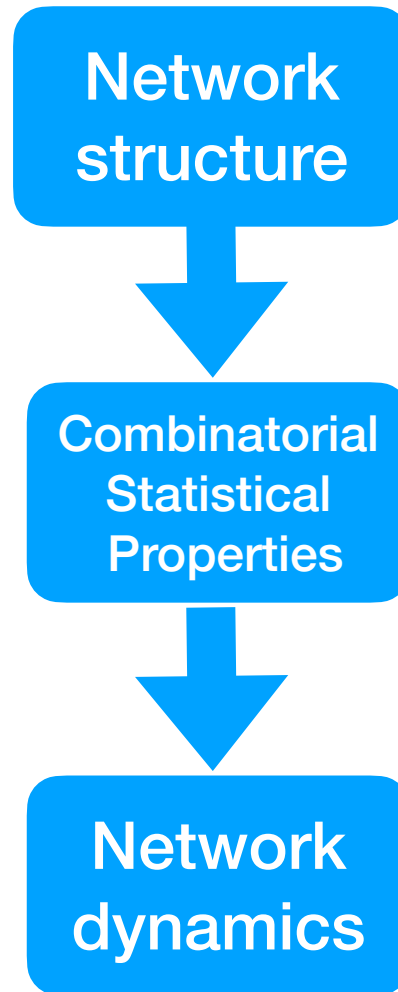
for $N \rightarrow \infty$



- **Modularity:** Local communities of nodes
[Fortunato 2010]



Interplay between network structure and dynamics



Critical phenomena on scale-free networks

Scale free networks:

- **Percolation:**

Percolation threshold

$$p_c \frac{\langle k(k-1) \rangle}{\langle k \rangle} = 1$$

Scale free networks are robust to random damage

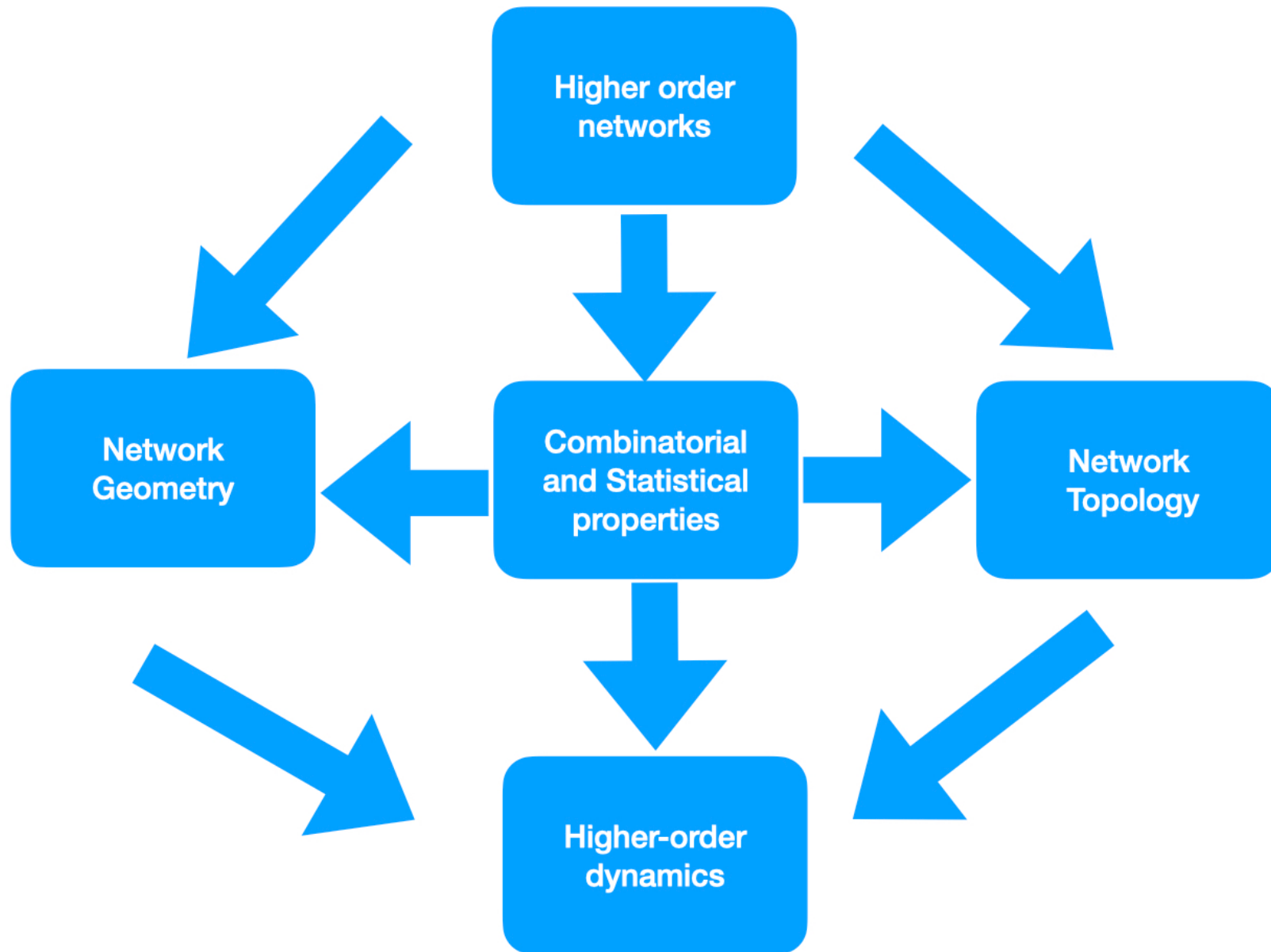
- **Epidemic spreading:**

Epidemic threshold

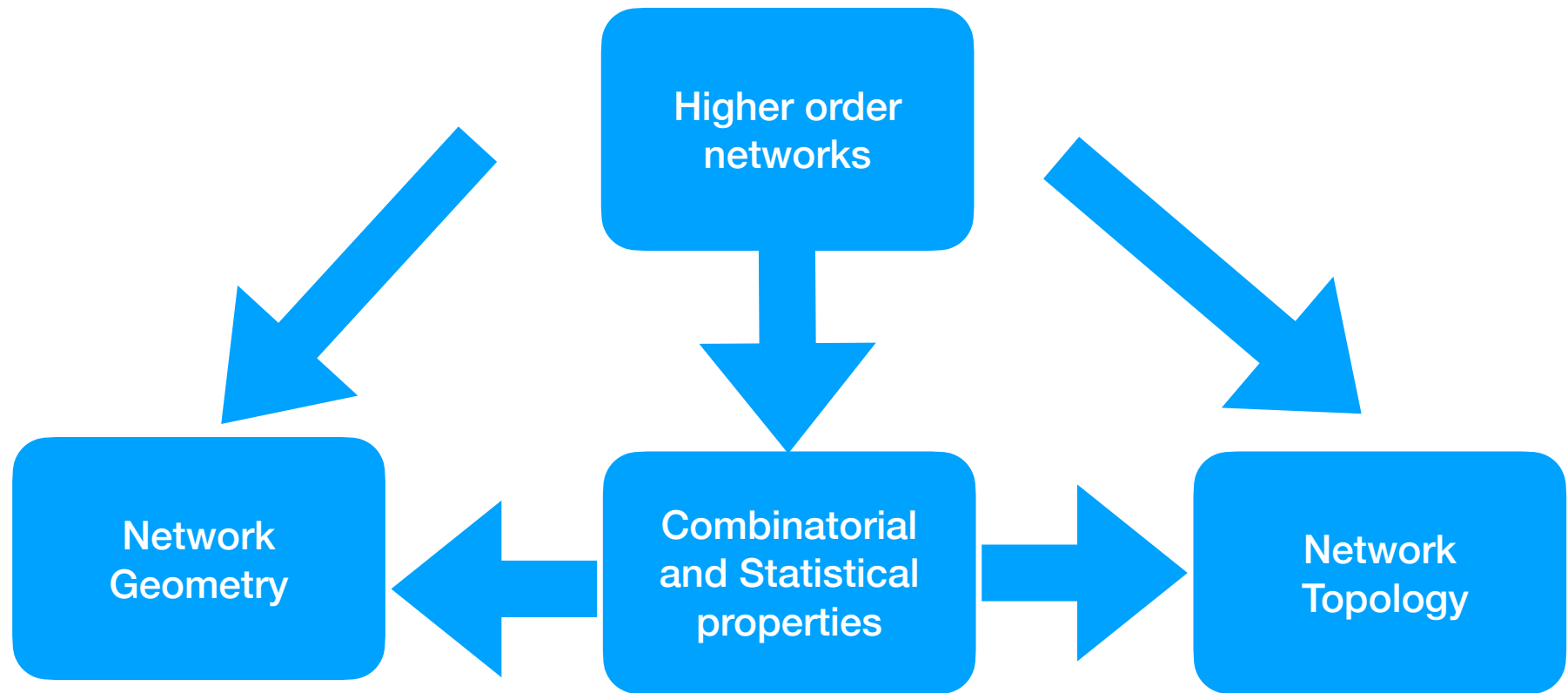
$$\lambda_c \frac{\langle k(k-1) \rangle}{\langle k \rangle} = 1$$

The epidemic threshold is zero on scale-free networks

Higher-order network structure and dynamics



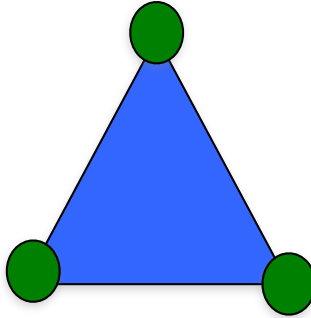
Higher order networks Structure



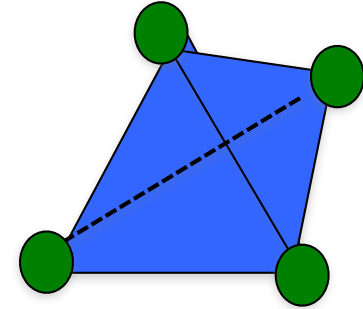
Hyperedges



2-hyperedge



3-hyperedge



4-hyperedge

An m -hyperedge is set nodes

$$\alpha = [i_1, i_2, i_3, \dots, i_m]$$

-it indicates the interactions between the m -nodes

Hypergraphs

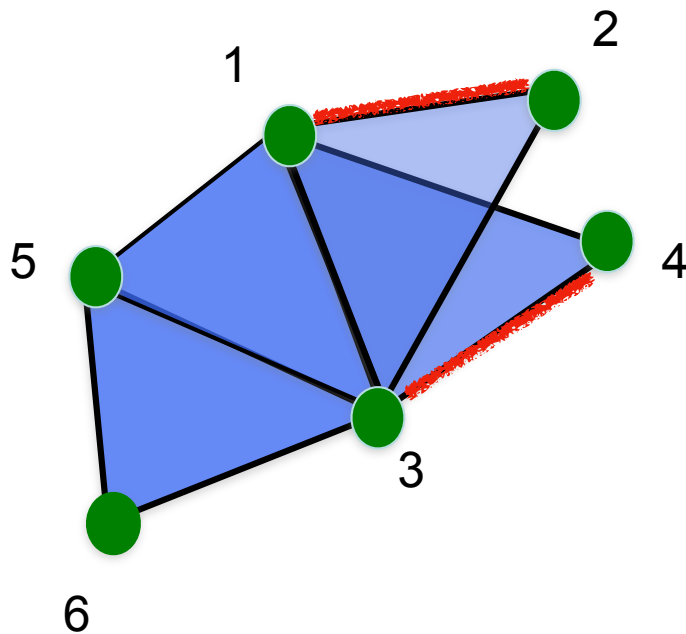
HYPERGRAPH

A hypergraph $\mathcal{G} = (V, E_H)$ is defined by a set V of N nodes and a set E_H of hyperedges, where a $(m + 1)$ -hyperedge indicates a set of $m + 1$ nodes

$$e = [v_0, v_1, v_2, \dots, v_m],$$

with generic value of $1 \leq m < N$.

An hyperedge describes the many-body interaction between the nodes.



Every hyperedge α formed by a subset of the nodes can belong or not to the hypergraph \mathcal{H}

$$\mathcal{H} = \{[1,2], [3,4], [1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

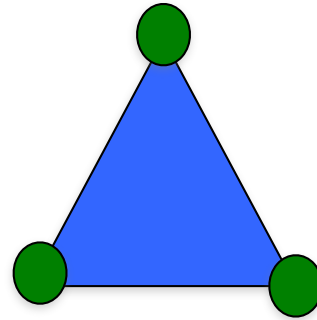
Simplices



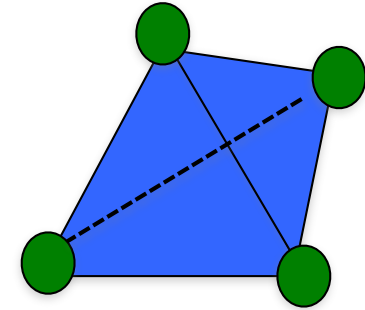
0-simplex



1-simplex



2-simplex



3-simplex

SIMPLICES

A d -dimensional simplex α (also indicated as a d -simplex α) is formed by a set of $(d + 1)$ interacting nodes

$$\alpha = [v_0, v_1, v_2, \dots, v_d].$$

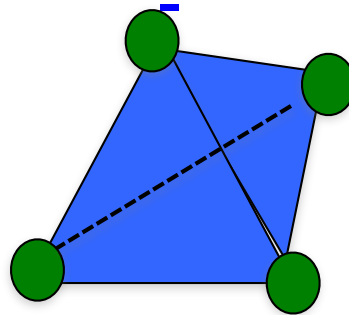
It describes a many body interaction between the nodes.

It allows for a topological and a geometrical interpretation of the simplex.

Faces of a simplex

FACES

A face of a d -dimensional simplex α is a simplex α' formed by a proper subset of nodes of the simplex, i.e. $\alpha' \subset \alpha$.



3-simplex

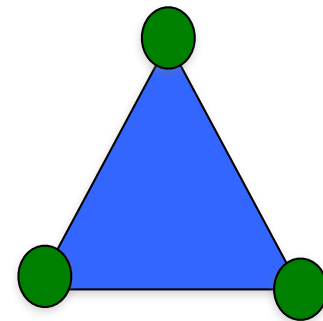
Faces



4 0-simplices



6 1-simplices



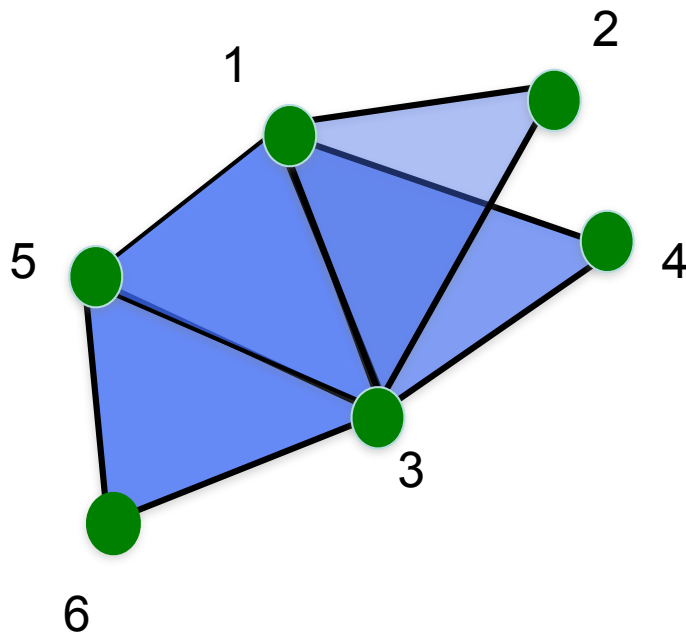
4 2-simplices

Simplicial complex

SIMPLICIAL COMPLEX

A simplicial complex \mathcal{K} is formed by a set of simplices that is closed under the inclusion of the faces of each simplex.

The dimension d of a simplicial complex is the largest dimension of its simplices.

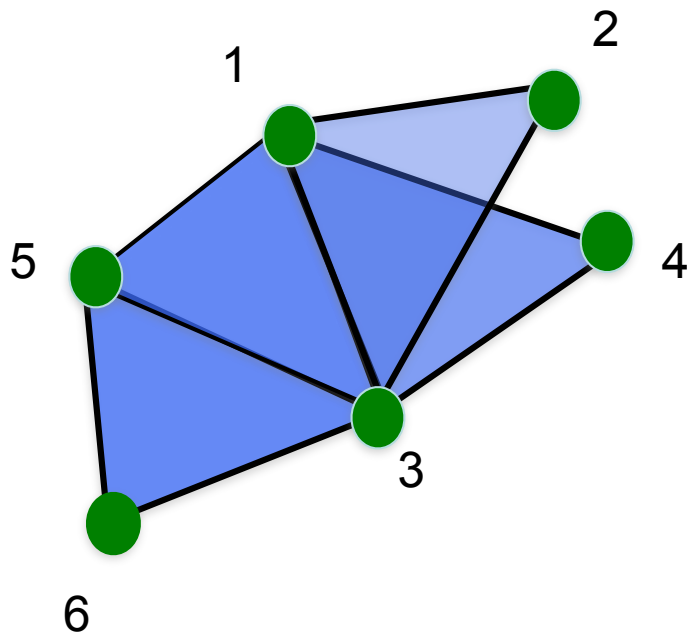


If a simplex α belongs to the simplicial complex \mathcal{K} then every face of α must also belong to \mathcal{K}

$$\mathcal{K} = \{[1], [2], [3], [4], [5], [6], \\ [1,2], [1,3], [1,4], [1,5], [2,3], \\ [3,4], [3,5], [3,6], [5,6], \\ [1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Dimension of a simplicial complex

The dimension of a simplicial complex \mathcal{K} is the largest dimension of its simplices



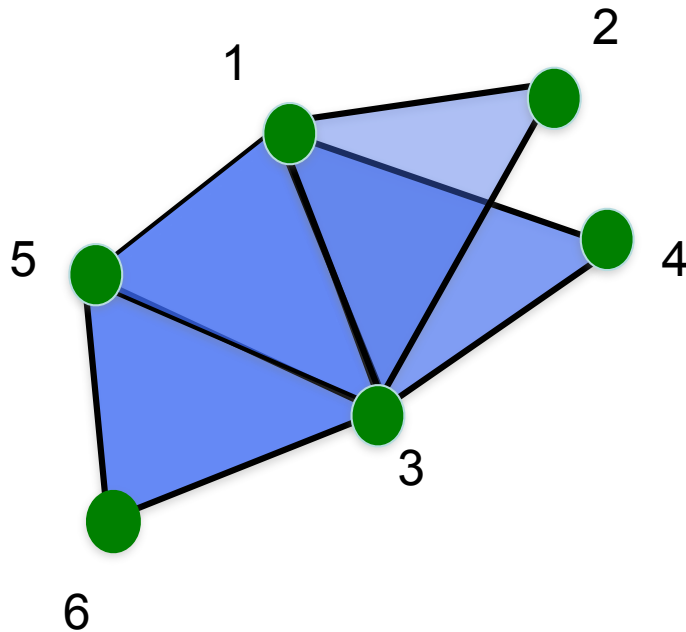
**This simplicial complex
has dimension 2**

$$\mathcal{K} = \{[1], [2], [3], [4], [5], [6], \\ [1,2], [1,3], [1,4], [1,5], [2,3], \\ [3,4], [3,5], [3,6], [5,6], \\ [1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Facets of a simplicial complex

FACET

A facet is a simplex of a simplicial complex that is not a face of any other simplex. Therefore a simplicial complex is fully determined by the sequence of its facets.



The facets of this simplicial complex are

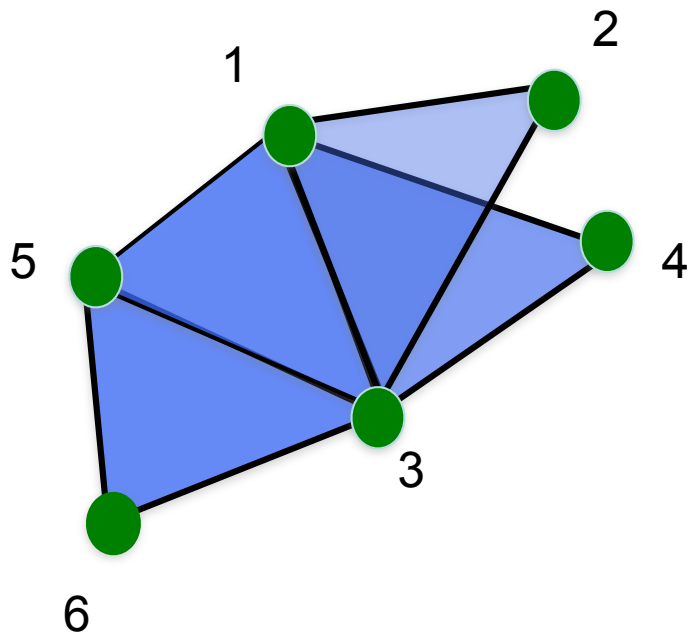
$$\mathcal{K} = \{[1,2,3], [1,3,4], [1,3,5], [3,5,6]\}$$

Pure simplicial complex

PURE SIMPLICIAL COMPLEXES

A *pure d -dimensional simplicial complex* is formed by a set of d -dimensional simplices and their faces.

Therefore pure d -dimensional simplicial complexes admit as facets only d -dimensional simplices.

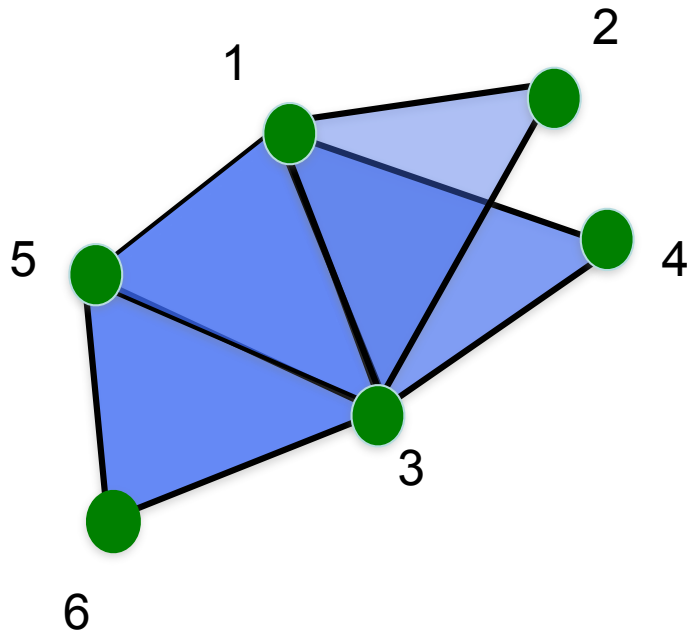


A pure d -dimensional simplicial complex is fully determined by an adjacency matrix tensor with $(d+1)$ indices.
For instance this simplicial complex is determined by the tensor

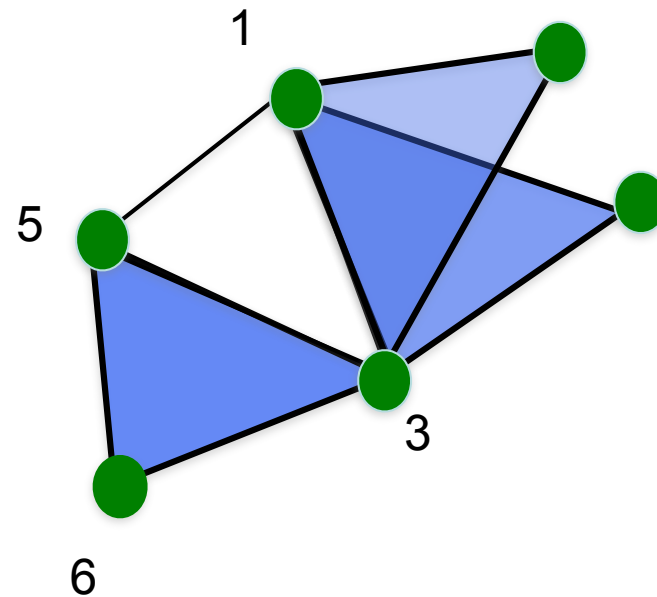
$$a_{rsp} = \begin{cases} 1 & \text{if } (r, s, p) \in \mathcal{K} \\ 0 & \text{otherwise} \end{cases}$$

Example

A simplicial complex \mathcal{K} is **pure** if it is formed by d -dimensional simplices and their faces

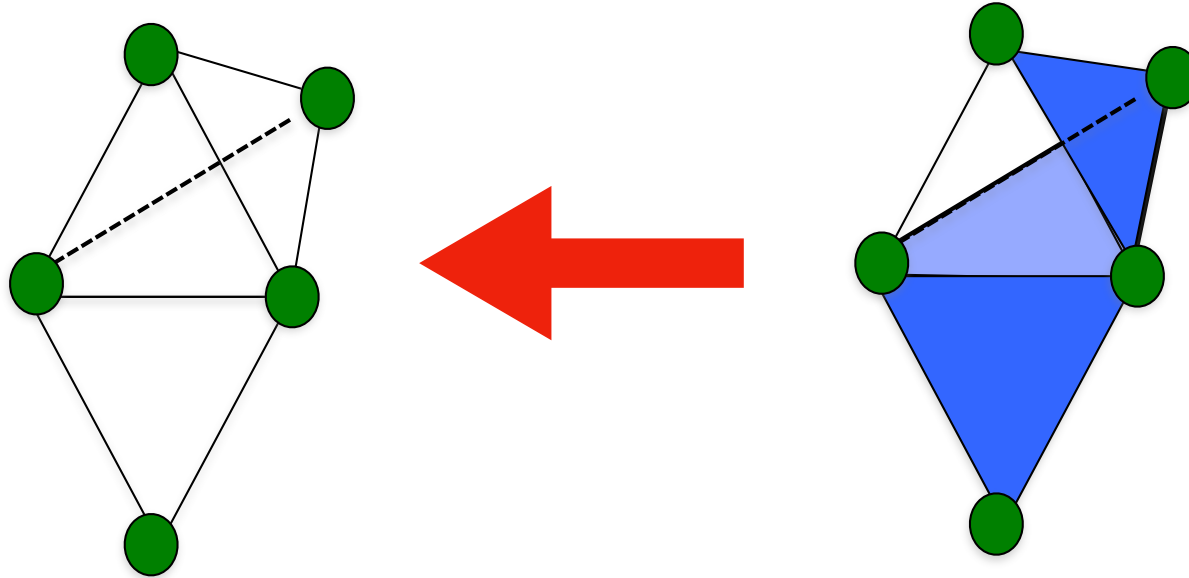


PURE SIMPLICIAL COMPLEX



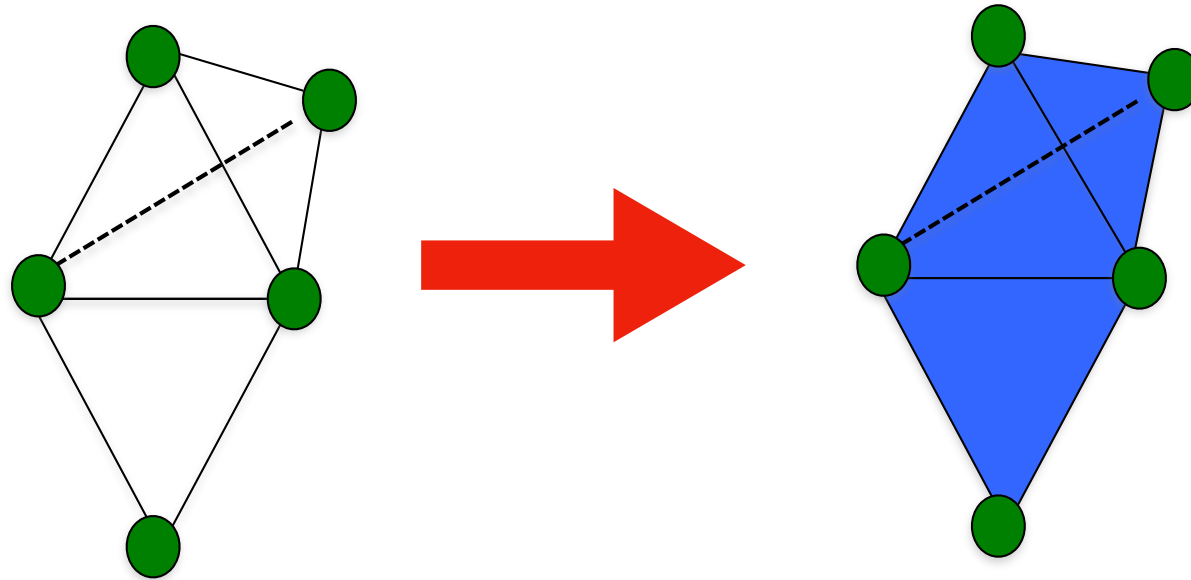
**SIMPLICIAL COMPLEX
THAT IS NOT PURE**

Simplicial complex skeleton



From a simplicial complex is possible to generate a network called the **simplicial complex skeleton** by considering only the nodes and the links of the simplicial complex

Clique complex



**From a network is possible to generate a simplicial complex by
Assuming that each clique is a simplex**

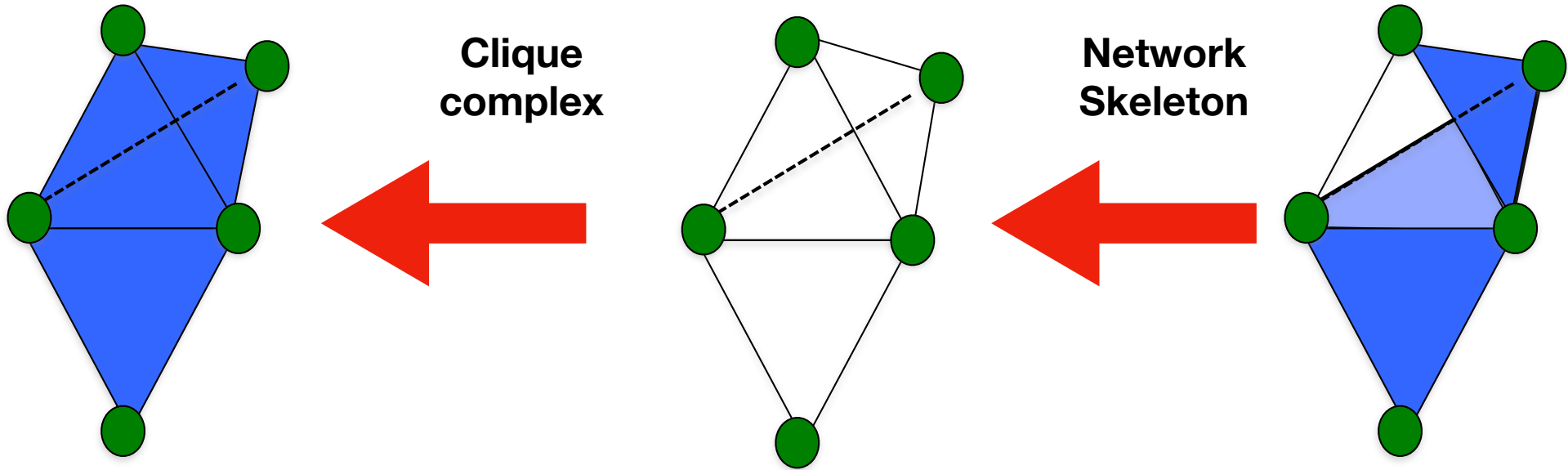
Note:

Poisson networks have a clique number that is 3 and actually on a finite expected number of triangles in the infinite network limit

However

Scale-free networks have a diverging clique number, therefore the clique complex of a scale-free network has diverging dimension. (Bianconi, Marsili 2006)

Concatenation of the operations

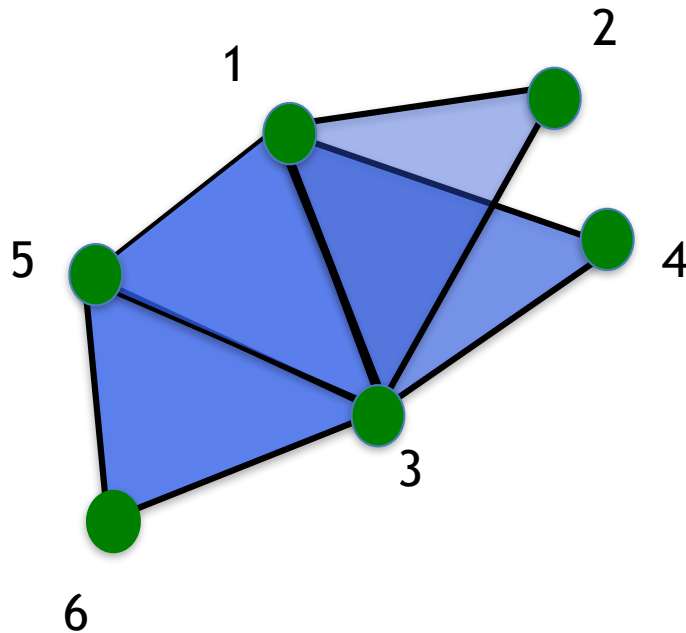


Attention!

By concatenating the operations you are not guaranteed to return to the initial simplicial complex

Generalized degrees

The generalized degree $k_{d,m}(\alpha)$ of a m -face α in a d -dimensional simplicial complex is given by the number of d -dimensional simplices incident to the m -face α .

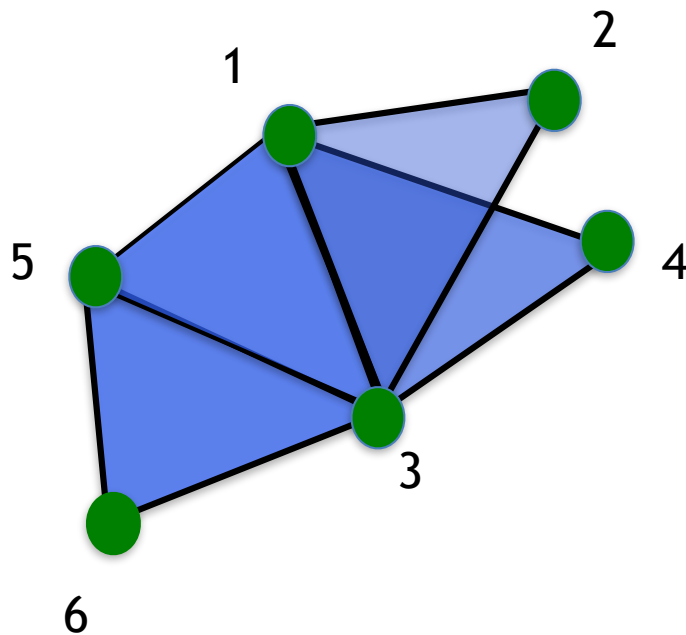


$k_{2,0}(\alpha)$ Number of triangles incident to the node α

$k_{2,1}(\alpha)$ Number of triangles incident to the link α

Generalized degree

The generalized degree $k_{d,m}(\alpha)$ of a m -face α in a d -dimensional simplicial complex is given by the number of d -dimensional simplices incident to the m -face α .

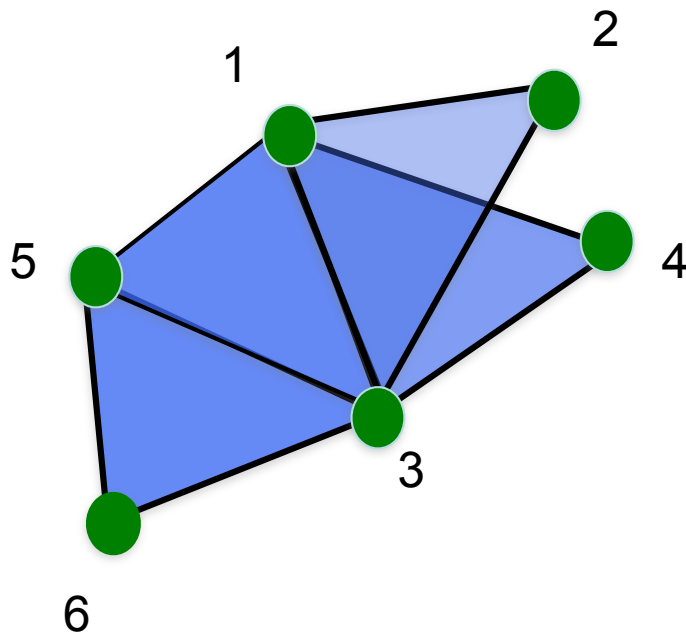


i	$k_{2,0}(i)$
1	3
2	1
3	4
4	1
5	2
6	1

(i,j)	$k_{2,1}(i,j)$
(1,2)	1
(1,3)	3
(1,4)	1
(1,5)	1
(2,3)	1
(3,4)	1
(3,5)	2
(3,6)	1
(5,6)	1

Pure simplicial complex

A simplicial complex \mathcal{K} is **pure** if it is formed by d -dimensional simplices and their faces



A pure d -dimensional simplicial complex is fully determined by an adjacency matrix tensor with $(d+1)$ indices. For instance this simplicial complex is determined by the tensor

$$a_{rsp} = \begin{cases} 1 & \text{if } (r, s, p) \in \mathcal{K} \\ 0 & \text{otherwise} \end{cases}$$

Combinatorial properties of the generalised degrees

The generalized degrees $k_{d,m}(\alpha)$ of a pure d -dimensional simplicial complex can be defined in terms of the adjacency tensor \mathbf{a} as

$$k_{d,m}(\alpha) = \sum_{\alpha' \in \mathcal{Q}_d(N) | \alpha' \supseteq \alpha} a_{\alpha'}$$

The generalized degrees obey a nice combinatorial relation as they are not independent of each other.

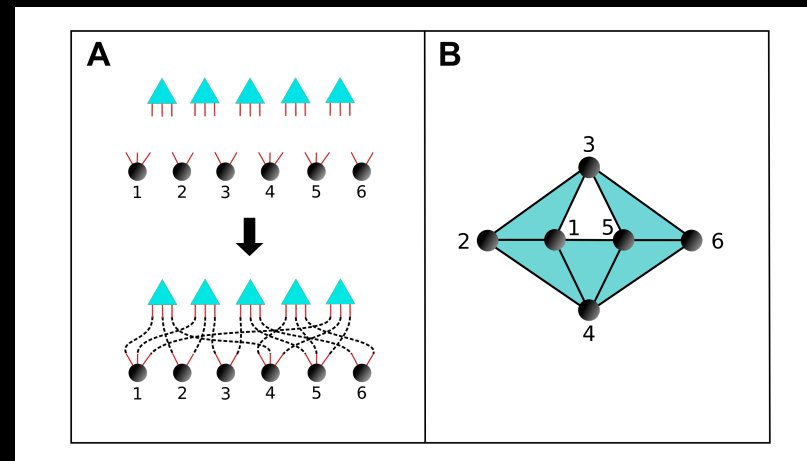
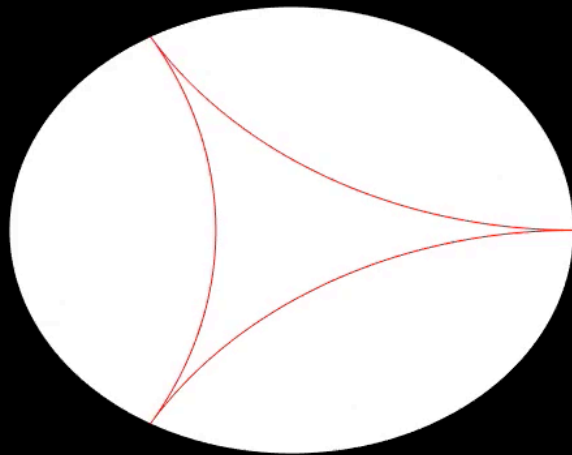
In fact for $m' > m$ we have

$$k_{d,m}(\alpha) = \frac{1}{\binom{d-m}{m'-m}} \sum_{\alpha' \in \mathcal{Q}_d(N) | \alpha' \supseteq \alpha} k_{d,m'}(\alpha').$$

Simplicial complex models of arbitrary dimension

**Emergent Hyperbolic Geometry
Network Geometry with Flavor (NGF)
[Bianconi Rahmede ,2016 & 2017]**

**Maximum entropy model
Configuration model
of simplicial complexes
[Courtney Bianconi 2016]**



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Information theory of ensembles of simplicial complexes

Entropy of ensembles of simplicial complexes

To every simplicial complex \mathcal{K} of N nodes we associate a probability

$$P(\mathcal{K})$$

The entropy of the ensemble of simplicial complexes is given by

$$S = - \sum_{\mathcal{K}} P(\mathcal{K}) \ln P(\mathcal{K})$$

Constraints

We might consider simplicial complex ensemble
with given
Expected generalized degrees of the nodes
or
Given generalized degrees of the nodes

Soft constraints

$$\sum_{\mathcal{K}} P(\mathcal{K}) \left[\sum_{\alpha \supset i} a_{\alpha} \right] = \bar{k}_{d,0}(i)$$

Hard constraints

$$\sum_{\alpha \supset i} a_{\alpha} = k_{d,0}(i)$$

[Courtney & Bianconi (2015)]

Maximum entropy ensembles

The maximum entropy ensembles
of simplicial complexes
are characterized by a probability measure given by

Soft constraints

$$P(\mathcal{K}) = \frac{1}{Z} e^{-\sum_i \lambda_i \sum_{\alpha \supset i} a_\alpha}$$

Hard constraints

$$P(\mathcal{K}) = \frac{1}{\mathcal{N}} \delta \left(k_{d,0}(i), \sum_{\alpha \supset i} a_\alpha \right)$$

[Courtney & Bianconi (2015)]

Marginal probability

The marginal probability of a d-dimensional simplex μ is given by

$$p_\alpha = \frac{e^{-\sum_{r \subset \alpha} \lambda_r}}{1 + e^{-\sum_{r \subset \alpha} \lambda_r}}$$

In presence of a maximum degree K (the structural cutoff)
the marginal can be written as

$$p_\alpha = d! \frac{\prod_{r \subset \alpha} k_{d,0}(r)}{(\langle k_{d,0}(r) \rangle N)^d} \quad \text{where} \quad K = \left[\frac{(\langle k_{d,0}(r) \rangle N)^d}{d!} \right]^{1/(d+1)}$$

[Courtney & Bianconi (2015)]

Case d=1

The marginal probability of a 1-dimensional simplex μ is given by

$$p_{ij} = \frac{e^{-\lambda_i - \lambda_j}}{1 + e^{-\lambda_i - \lambda_j}}$$

In presence of a maximum degree K (the structural cutoff)
the marginal can be written as

$$p_{ij} = \frac{k_{d,0}(i)k_{d,0}(j)}{(\langle k_{d,0}(r) \rangle N)} \quad \text{where} \quad K = [(\langle k_{d,0}(r) \rangle N)]^{1/2}$$

[Courtney & Bianconi (2015)]

Case d=2

The marginal probability of a 2-dimensional simplex μ is given by

$$p_{ijr} = \frac{e^{-\lambda_i - \lambda_j - \lambda_r}}{1 + e^{-\lambda_i - \lambda_j - \lambda_r}}$$

In presence of a maximum degree K (the structural cutoff)
the marginal can be written as

$$p_{ijr} = 2 \frac{k_{d,0}(i)k_{d,0}(j)k_{d,0}(r)}{(\langle k_{d,0}(r) \rangle N)^2} \quad \text{where} \quad K = \frac{(\langle k_{d,0}(r) \rangle N)^{2/3}}{2^{1/3}}$$

[Courtney & Bianconi (2015)]

Entropy of simplicial complex ensembles

Canonical ensemble

Microcanonical ensemble

$$S = - \sum_{\alpha \in \mathcal{S}_d(N)} [p_\alpha \ln p_\alpha + (1 - p_\alpha) \ln(1 - p_\alpha)]$$

$$\Sigma = \ln \mathcal{N}$$

Non-equivalence of the ensembles

$$\Sigma = S - \Omega$$

[Courtney & Bianconi (2015)] generalizing [Anand & Bianconi (2009)-(2010)] for simple networks

Non-equivalence of ensembles

In the uncorrelated simplicial complex limit we have

$$\Sigma = \ln \mathcal{N} = S - \Omega$$

Where Ω is extensive and given by

$$\Omega = - \sum_{r=1}^N \ln \frac{1}{k_{d,0}(r)!} (k_{d,0}(r))^{k_{d,0}(r)} e^{-k_{d,0}(r)}$$

[Courtney & Bianconi (2015)]

Asymptotic expression
for the number
of simplicial complexes
with given
generalized degree of the nodes

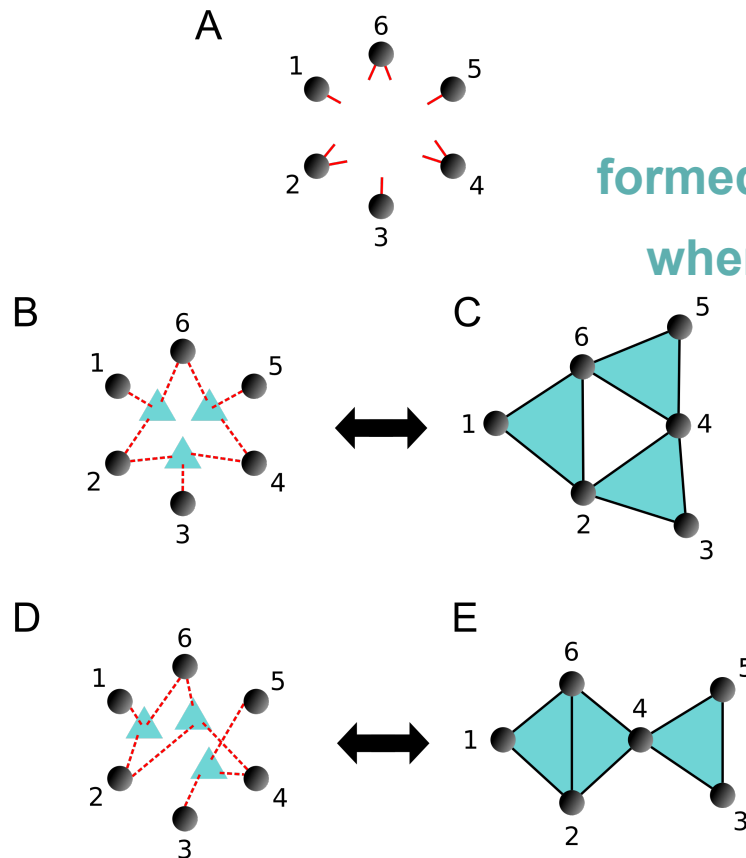
$$\mathcal{N} \sim \frac{[(\langle k \rangle N)!]^{d(d+1)}}{\prod_{r=0}^N k_{d,0}(r)!} \frac{1}{(d!)^{\langle k \rangle N / (d+1)}} \exp \left(-\frac{d!}{2(d+1)(\langle k \rangle N)^{d-1}} \left(\frac{\langle k^2 \rangle}{\langle k \rangle} \right)^{d+1} \right)$$

[Courtney & Bianconi (2015)]

Configuration model of simplicial complexes

We consider an ensemble of pure simplicial complexes

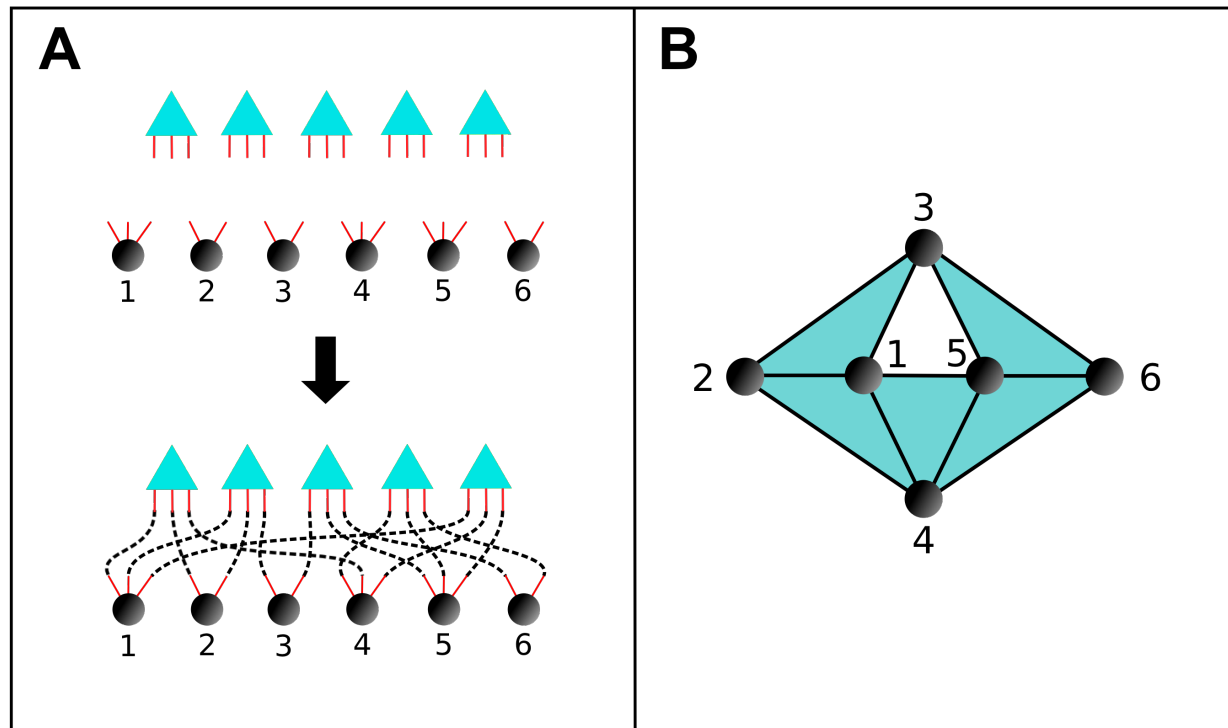
formed by d -dimensional simplices and their faces where each node has given generalized degree



- Given the generalized degree of the nodes there are in general multiple ways to realize the simplicial complex.
- The information encoded in the constraints is captured by the entropy of the ensemble

[Courtney & Bianconi (2015)]

Construction of a random simplicial complex



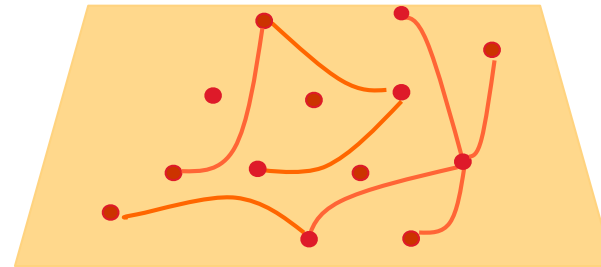
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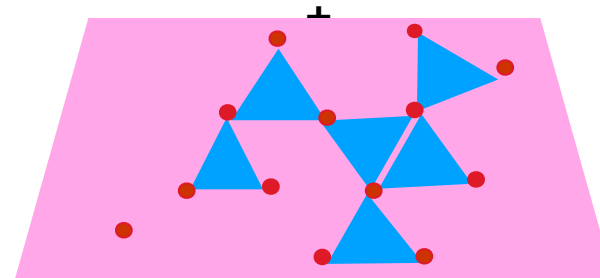
From models of pure simplicial complexes to models of hypergraphs

Pure 1-dimensional
simplicial complex



+

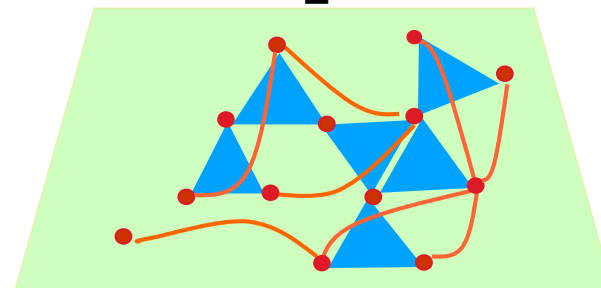
Pure 2-dimensional
simplicial complex



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HYPERGRAPH



Conclusions

- **Simplicial complexes capture the many-body interactions of complex systems and reveal the hidden geometry and topology of data**
- **Pure simplicial complexes can be represented by tensors**
- **The generalised degrees allow to capture important combinatorial properties of simplicial complexes**
- **Maximum entropy models of simplicial complexes are unbiased models with given (expected) generalised degrees**

Maximum entropy models for complex networks

London Taught Course (PhD Level)
on You Tube at

[https://www.youtube.com/channel/
UCsHAVdCU5XLaBYDXoINYZvg](https://www.youtube.com/channel/UCsHAVdCU5XLaBYDXoINYZvg)