

The simplicial configuration model

A Sampling Method

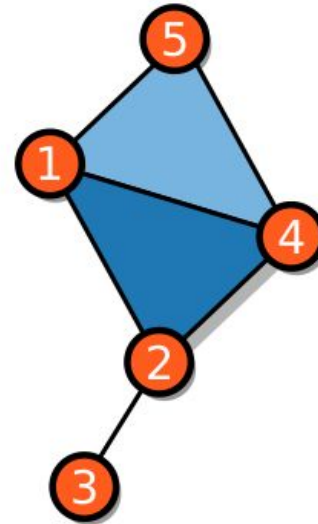
Alice Patania, Network Science Institute, Indiana University



A simplicial complex

A **simplicial complex** is a collection of simplices (non-empty finite sets ordered under inclusion).

It can be uniquely identified by its maximal simplices under inclusion (**facets**)



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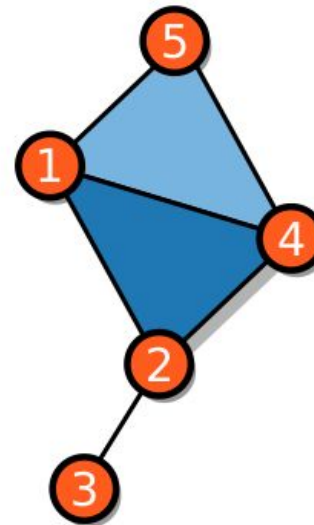
To every simplicial complex we can assign two sequences:

Degree sequence

Number of maximal simplices under inclusion incident on a node

Size sequence

Number of nodes contained in a maximal simplex



Simplicial degree and Facet size

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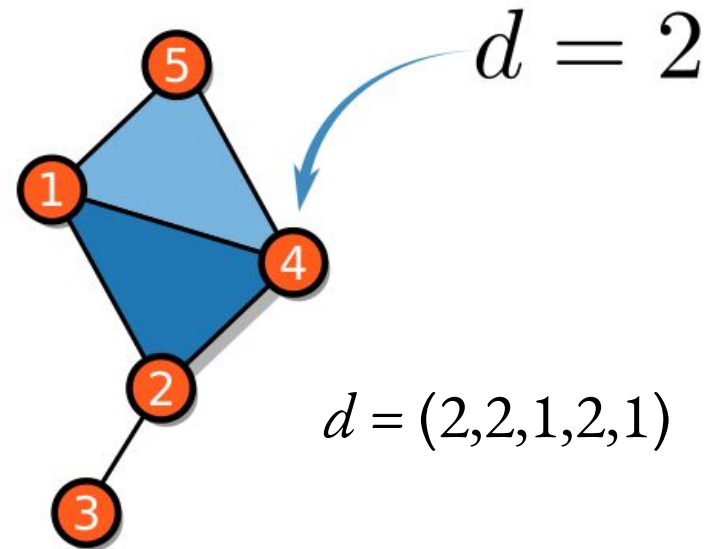
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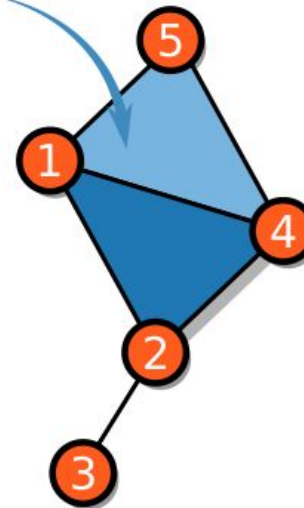
Degree sequence

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Size sequence

Number of nodes contained in a maximal simplex

$$s = 3$$



$$d = (2, 2, 1, 2, 1)$$

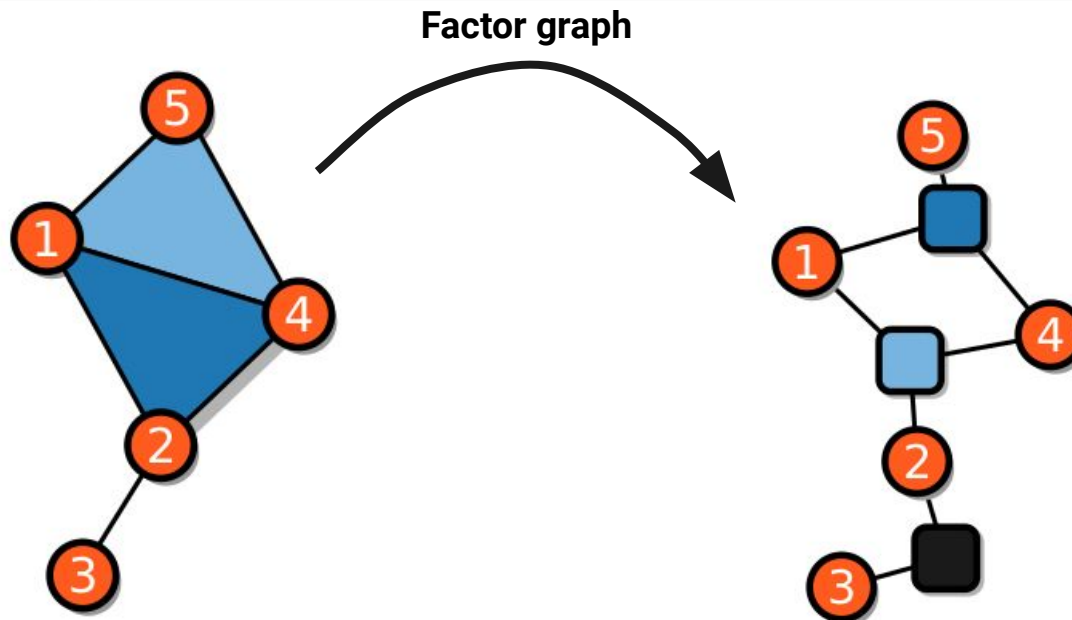
$$s = (3, 3, 2)$$

Bipartite graphs and Simplicial complexes

Theorem

For every Σ , $\exists G$, bipartite graph, s.t. one of its two one-mode projections G_V is the underlying graph of Σ .

Moreover, the facet size sequence of Σ is equal to the degree sequence of F .

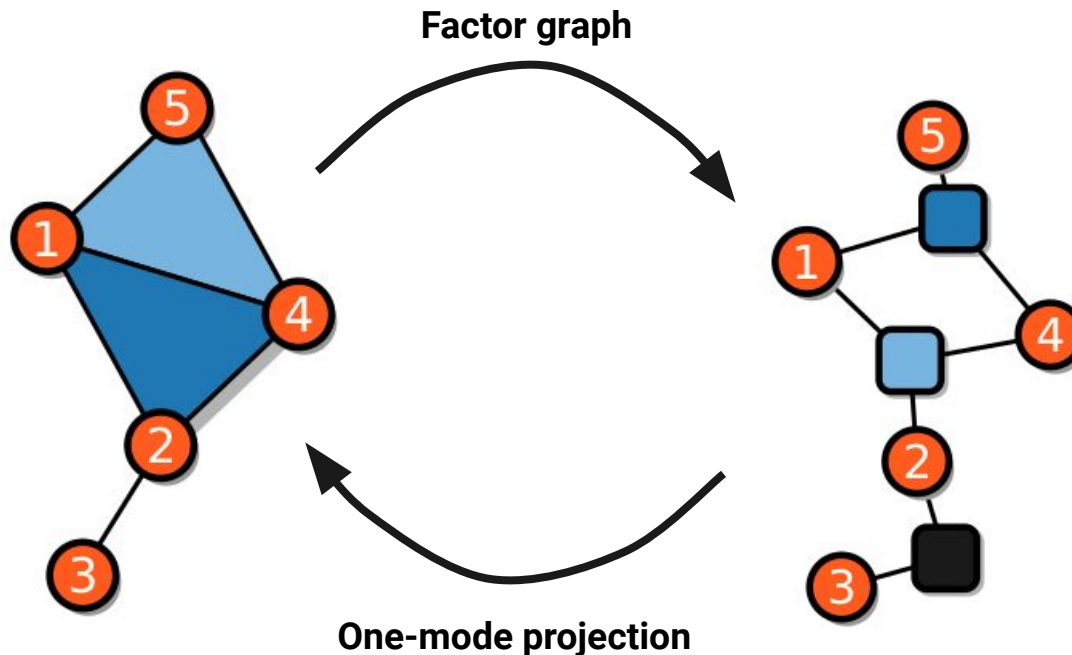


Bipartite graphs and Simplicial complexes

Theorem

Let G be a bipartite graph with vertex sets $\{F, V\}$, G_V its one-mode projections onto the vertex set V .

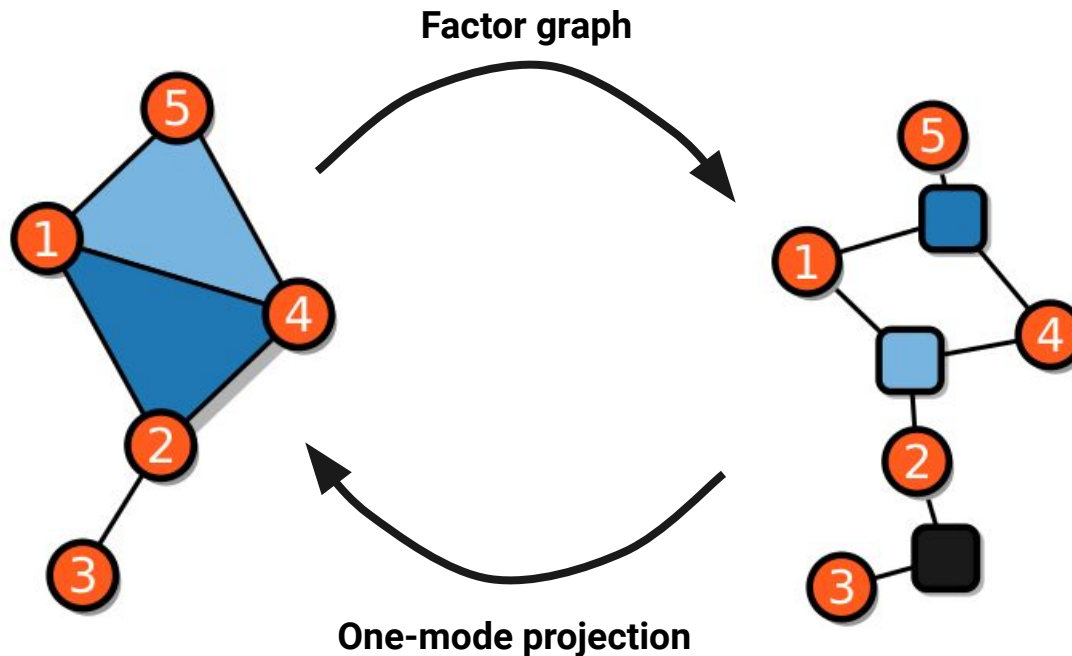
Then it exists a simplicial complex Σ whose underlying graph is G_V .



Bipartite graphs and Simplicial complexes

Idea

Use existing random models for bipartite graphs to construct a sampling method for SCM.



Existing approaches

— *this list is not exhaustive

Erdos-Renyi inspired:

Random pure simplicial complexes [Linial-Meshulam (2006)]

Random simplicial complexes [Kahle (2009)]

Multi-parameter random simplicial complexes [Costa-Farber (2015)]

Exponential random graphs inspired:

Exponential random simplicial complex [Zuev et al. (2015)]

Preferential attachment for simplicial complexes:

Network geometry with flavor [Bianconi-Rahmede (2016)]

Configuration model:

Configuration model for pure simplicial complexes [Courtney-Bianconi (2016)]

Configuration model

Idea

Use existing random models for bipartite graphs to construct a sampling method for SCM.

The **configuration model** is a generative model for random graphs with fixed number of nodes and degree sequence.

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This implies the following are fixed:

number of vertices (0-simplices) and number of maximal simplices
vertices' degree sequence and maximal simplices' size sequence

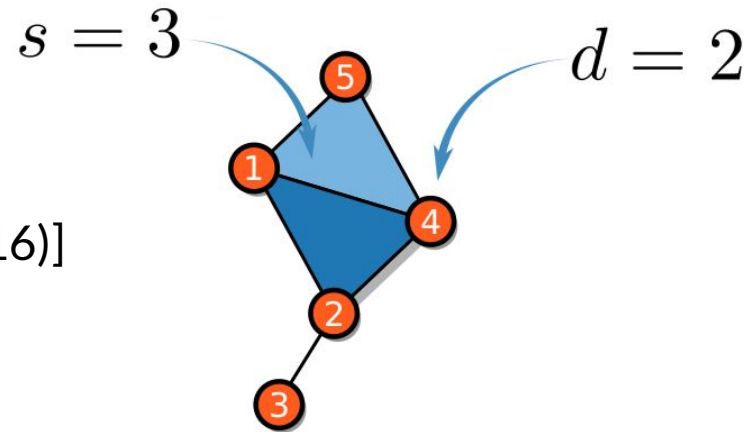
Simplicial degree and Facet size

The simplicial configuration model (SCM) is the distribution

$$\Pr(\mathbf{K}; \mathbf{d}, \mathbf{s}) = 1/|\Omega(\mathbf{d}, \mathbf{s})|$$

Where $\Omega(\mathbf{d}, \mathbf{s})$: number of simplicial complexes with sequences (\mathbf{d}, \mathbf{s})

This approach generalizes a method by
 [Courtney and Bianconi, Phys. Rev. E 93, (2016)]

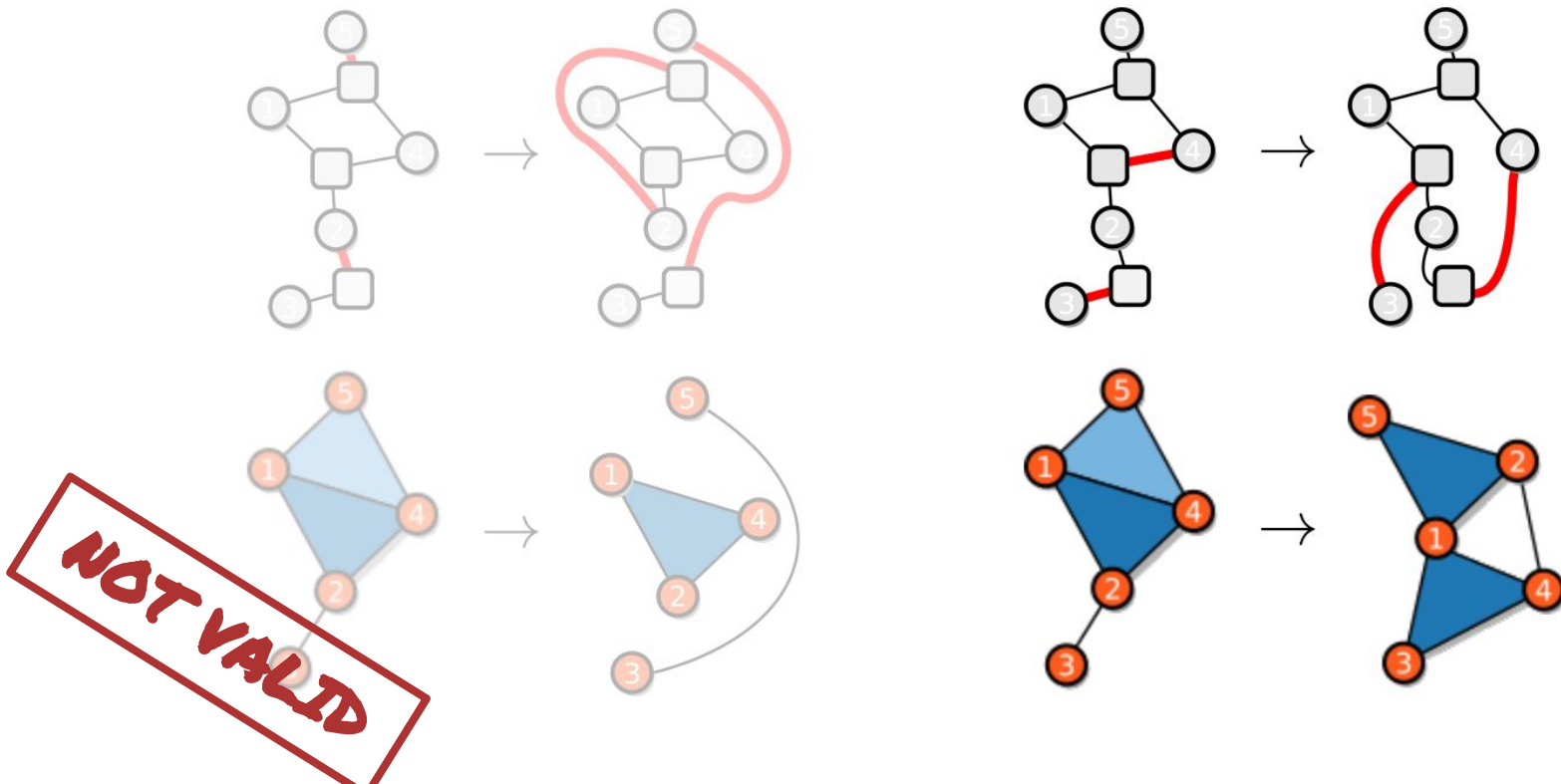


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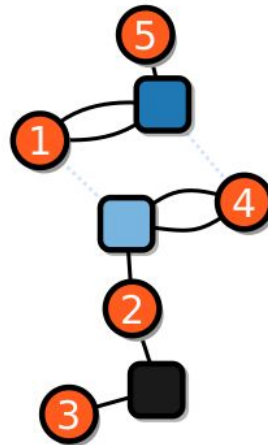


Adding constraints

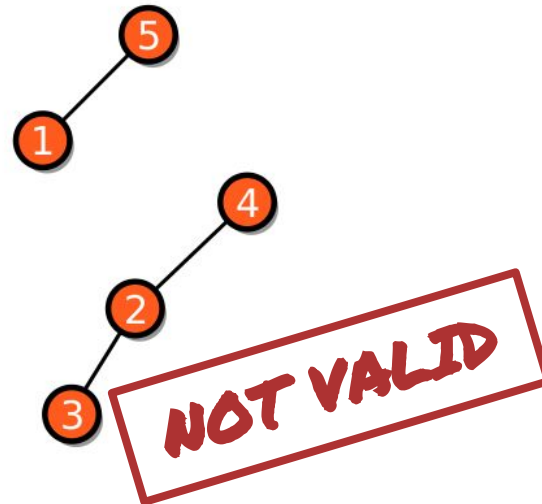
First constraint: **No multi-edges**

Multi-edges decrease the size of the maximal simplices.

Bipartite graph



Simplicial complex

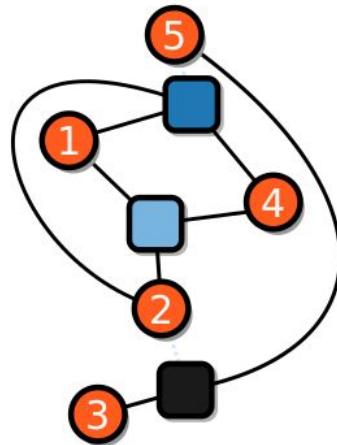


Adding constraints

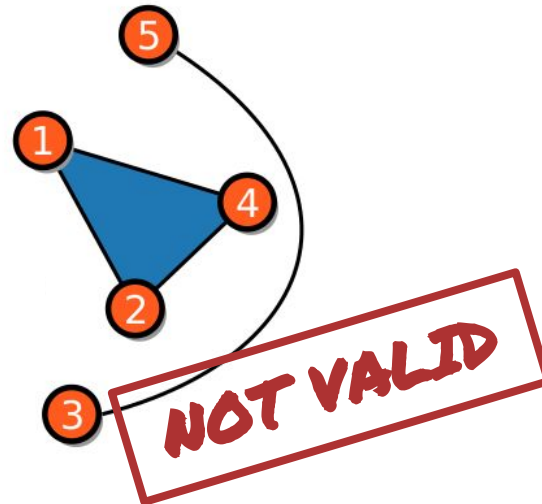
Second constraint: **No included neighborhoods**

Included neighborhoods violate the maximality assumption of the facets.

Bipartite graph



Simplicial complex



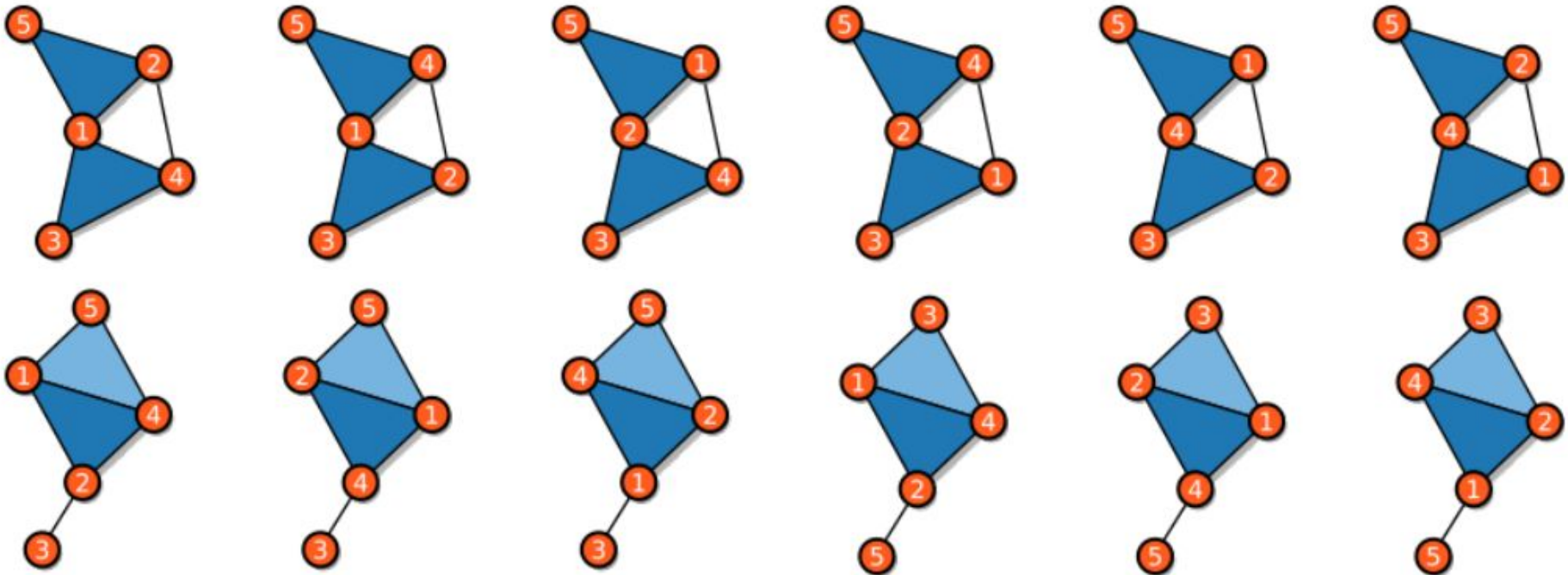
Adding constraints

Constraints:

No multi-edges

No included neighborhoods

Then the acceptable configurations for the toy example are the following:

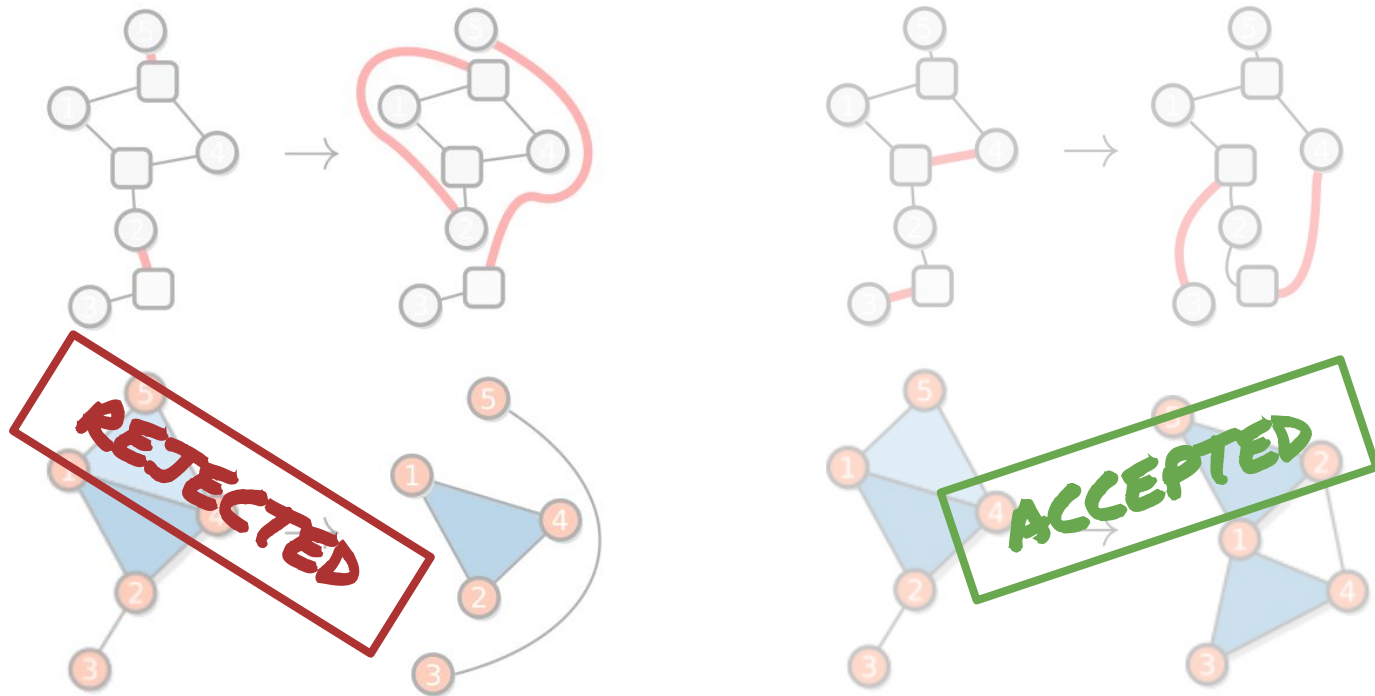


Bipartite graphs and Simplicial complexes

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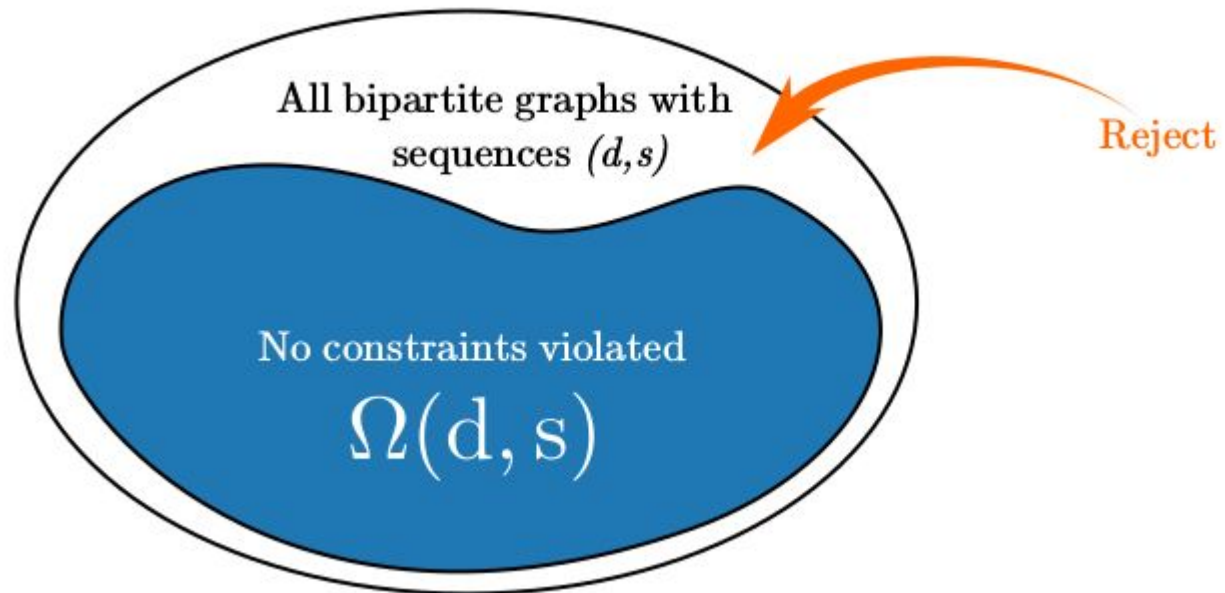


Adding constraints

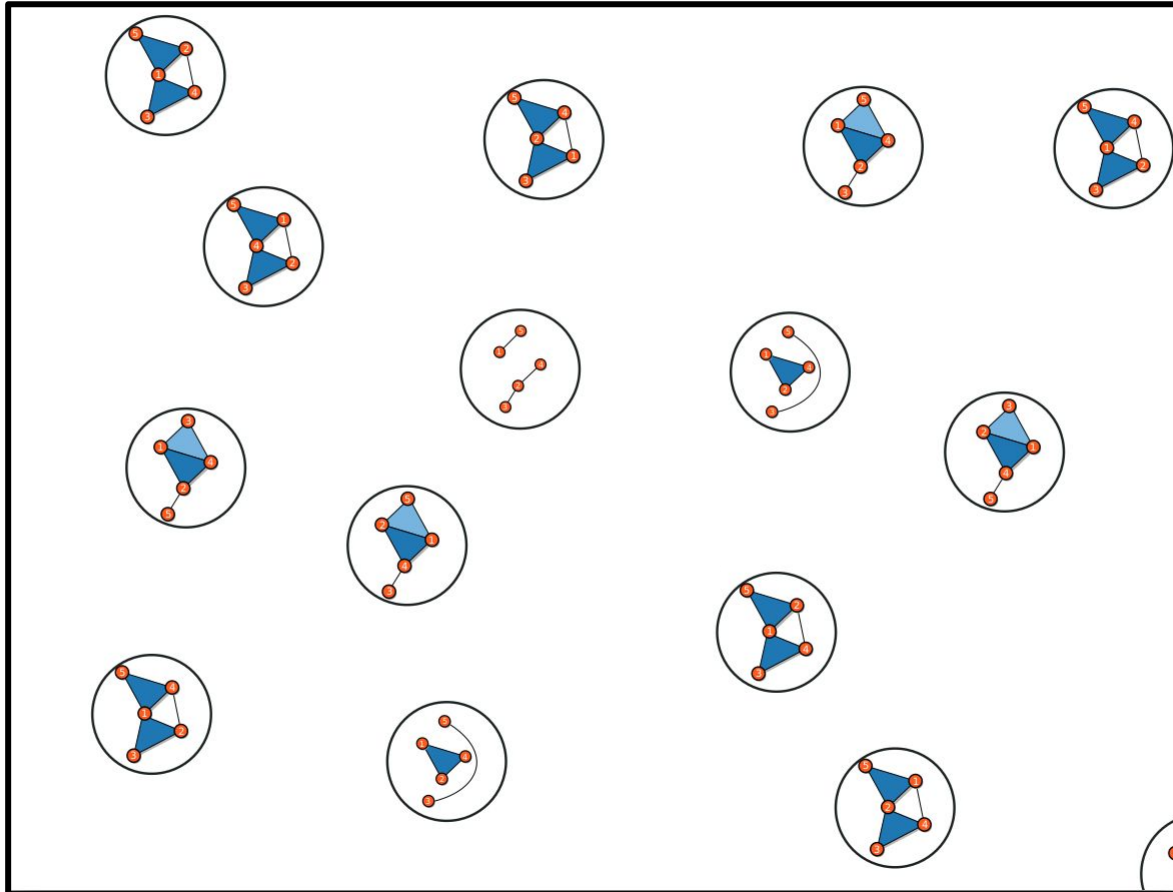
! Problem with rejection sampling: Far too many rejections!

Loose upper bound :

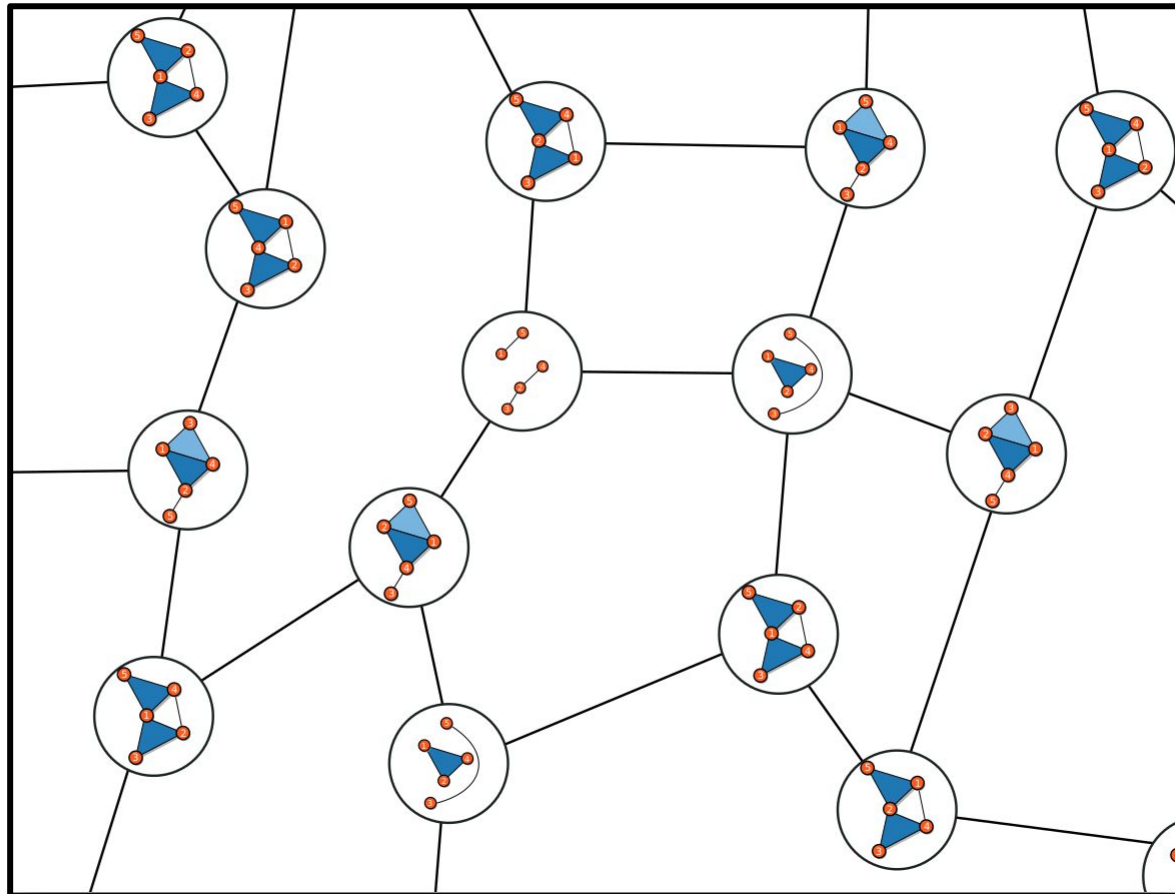
$$\Pr[\text{reject}] > \exp[-0.5(\langle d^2 \rangle / \langle d \rangle - 1)(\langle s^2 \rangle / \langle s \rangle - 1)]$$



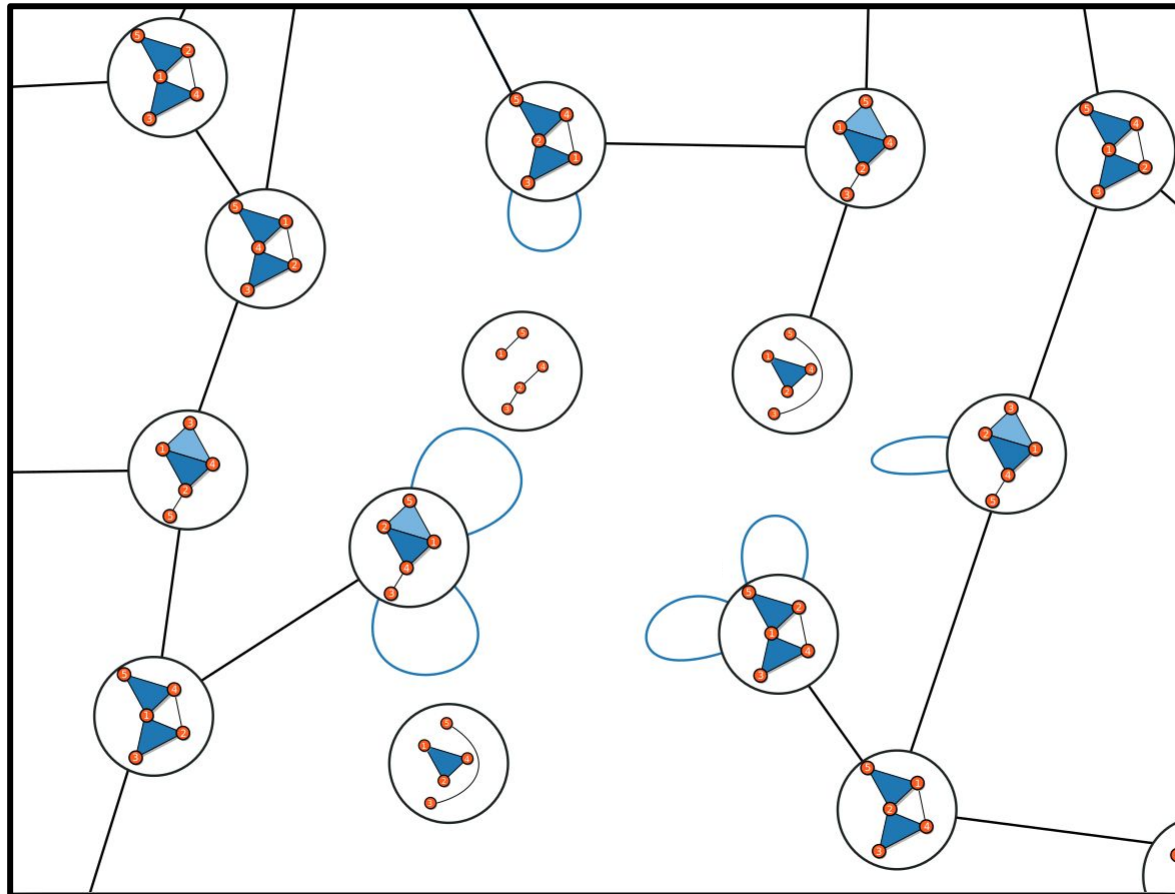
Markov Chain Monte Carlo sampling



Markov Chain Monte Carlo sampling



Markov Chain Monte Carlo sampling



MCMC sampling: The details

Move set

1. Pick $L \sim P$ random edges in bipartite graph
 P can be arbitrary, we use $P_{r|L} = Q = \exp(\lambda Q) / Z$
2. Rewire edges. If multi-edge or included neighbors, reject.

Similar to [Miklós–Erdős–Soukup, Electron. J. Combin., 20, (2013)]

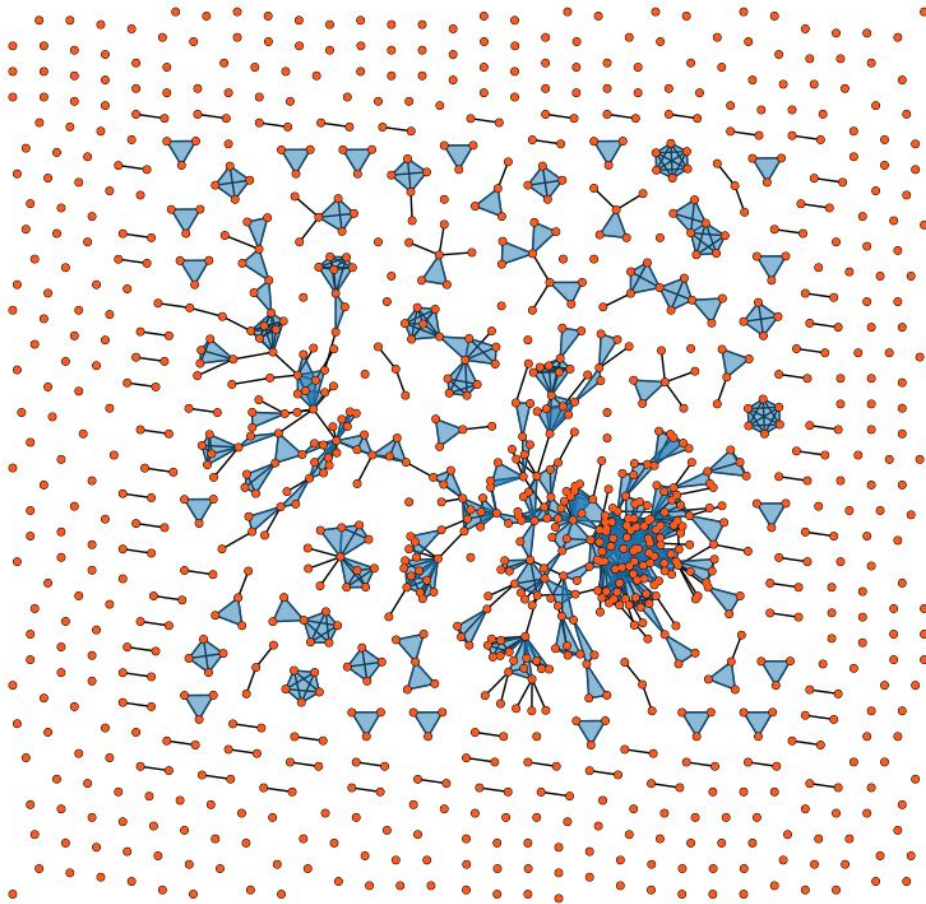
- MCMC is uniform over $\Omega(d, s)$
- Move set yields aperiodic chain
- Move set connects the space

Results - True systems

Disease regulation dataset

(facets : *genes*, nodes : *human diseases*)

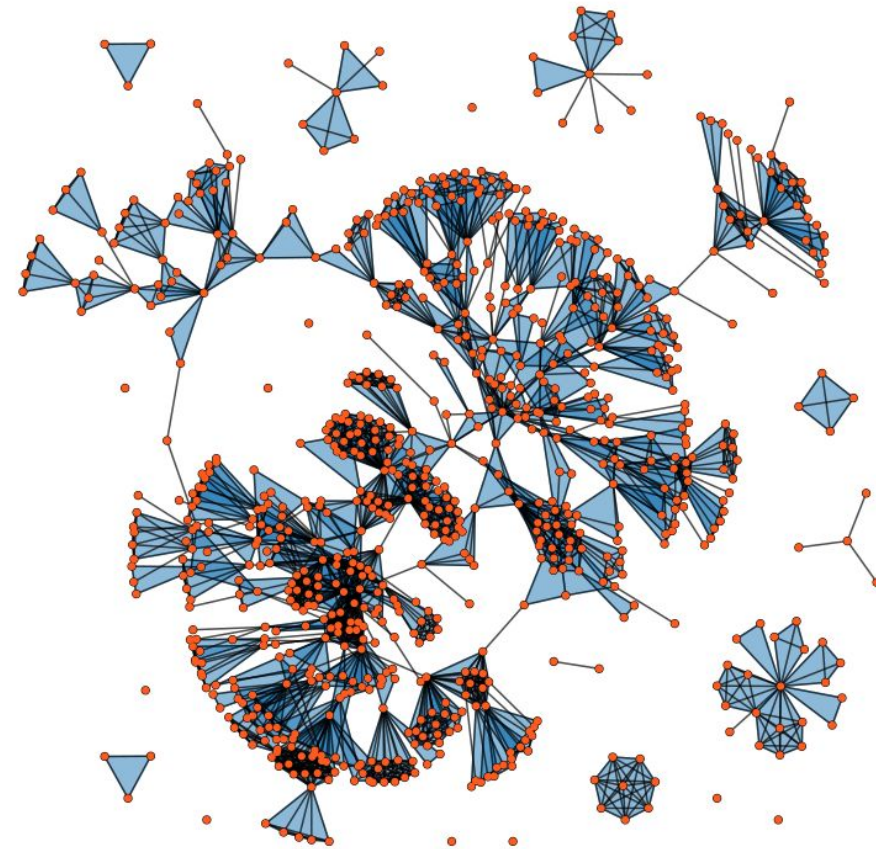
[Goh et al., PNAS, **104**, (2007)]



Crimes in St-Louis (true system)

(facets : *people*, nodes : *crimes*)

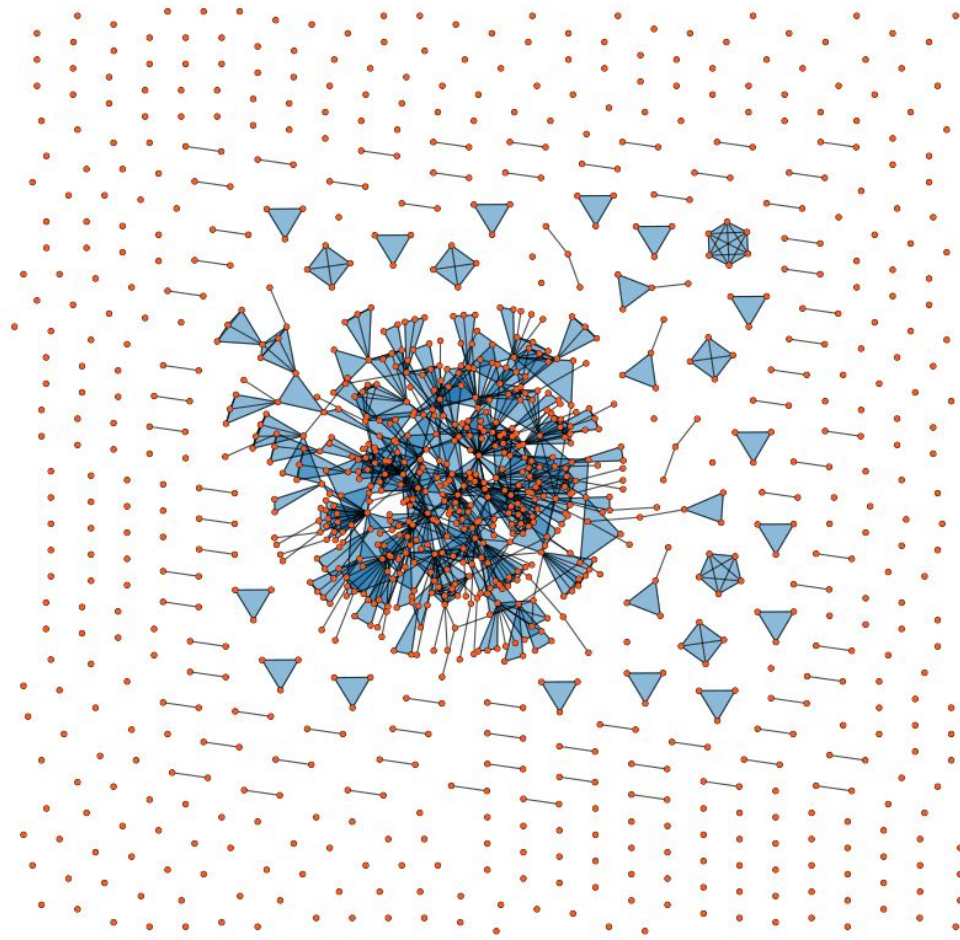
[Rosenfeld et al., (1991)]



Results - Random instances

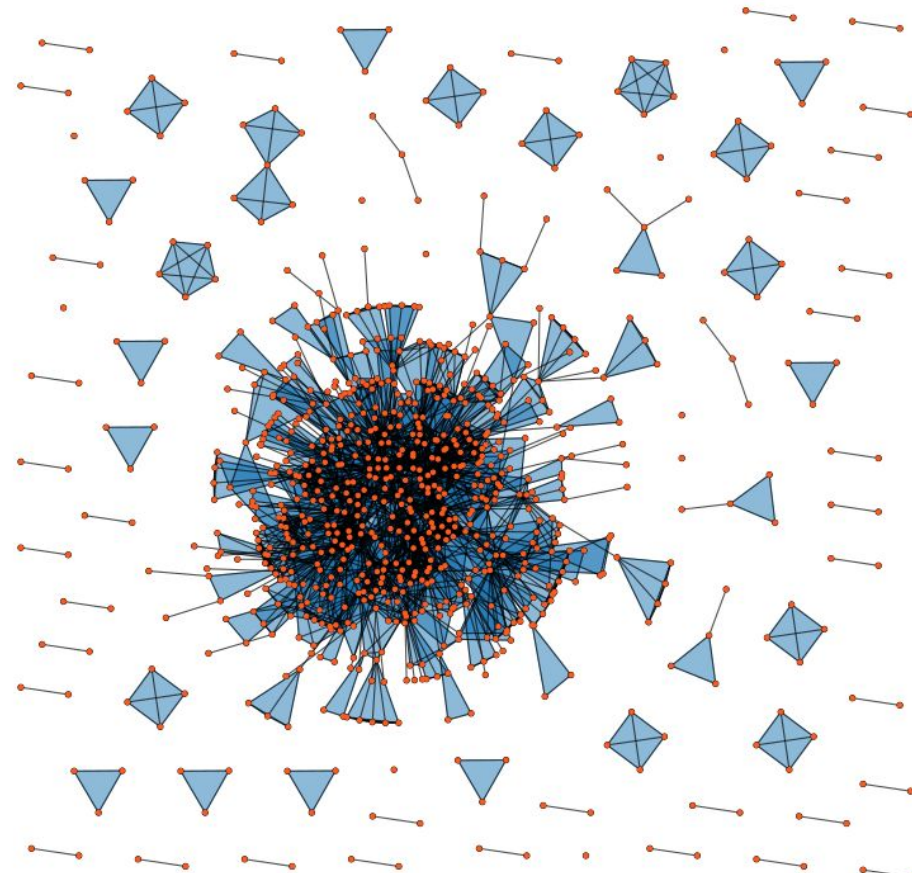
Disease regulation dataset (random instance)

(facets : *genes*, nodes : *human diseases*)
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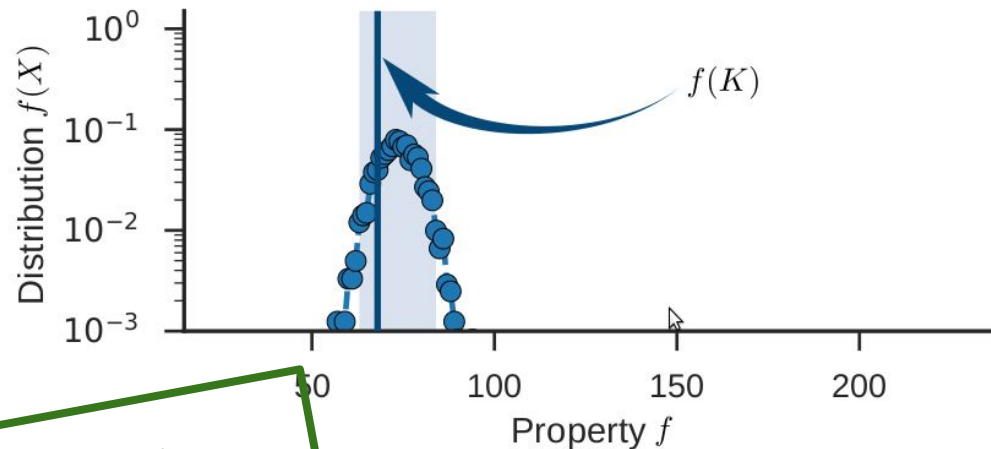
How to assess the significance
of the properties of a simplicial complex?

Building a null model

Concept for a null model

Null model

Is the quantity $f(X)$ close to $f(K)$ for random simplicial complexes $X \sim \text{SCM}(d(K), s(K))$?



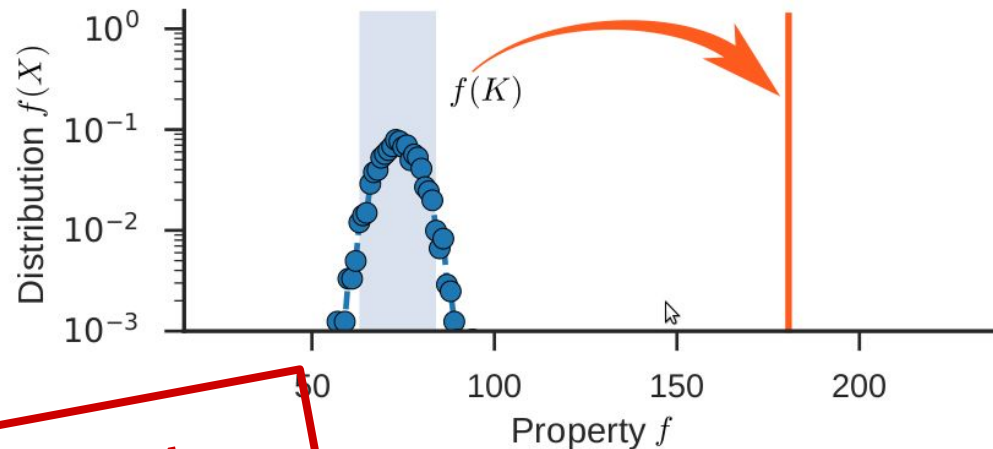
$$\Pr(|f(X) - f(K)| < 1) \approx 1$$

K is typical, the local quantities (d, s) explain f .

Concept for a null model

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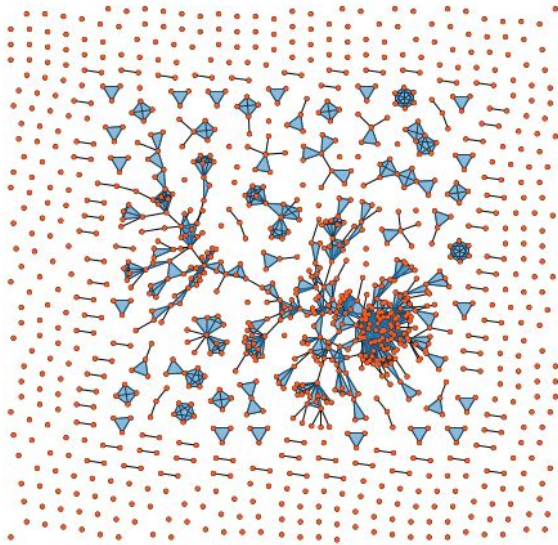


$$\Pr(|f(K) - f(X)| < 1) \ll 1$$

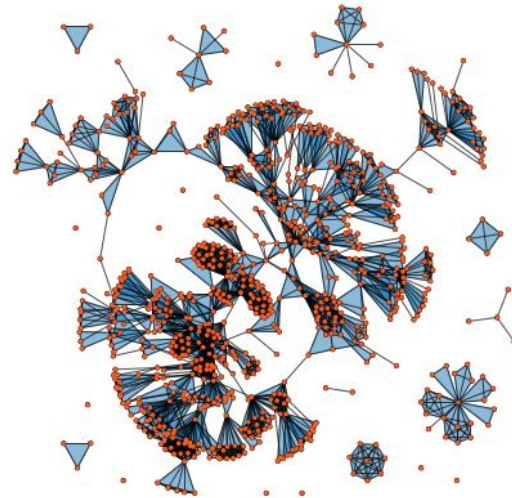
K is atypical, K is organized beyond the local scale.

Results on Betti numbers of real data sets

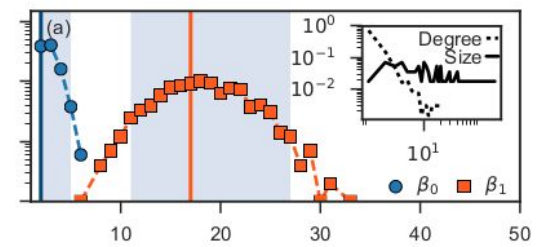
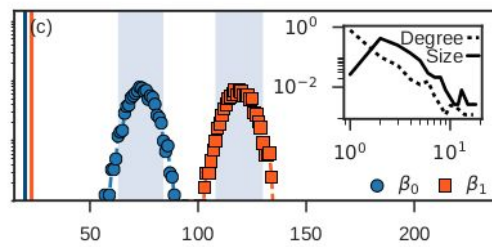
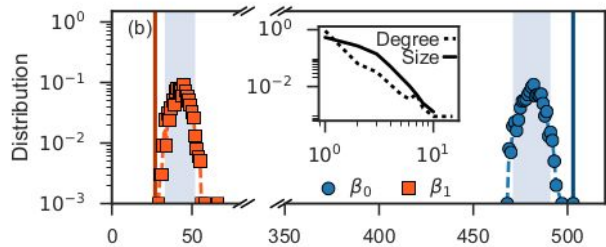
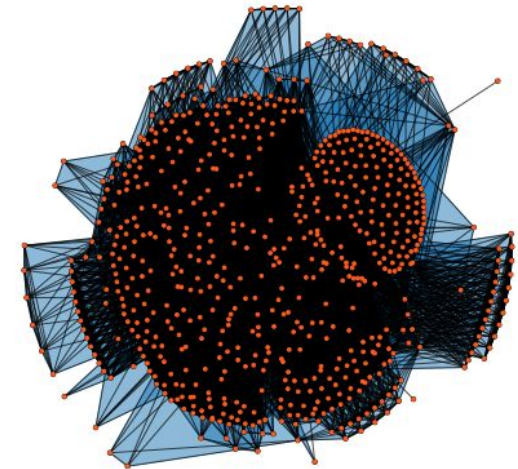
Diseases



Crime

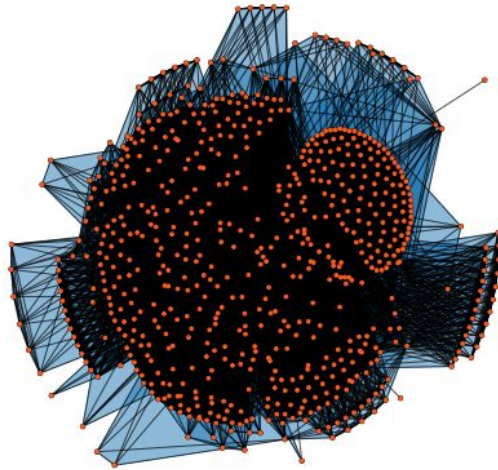


Pollinators

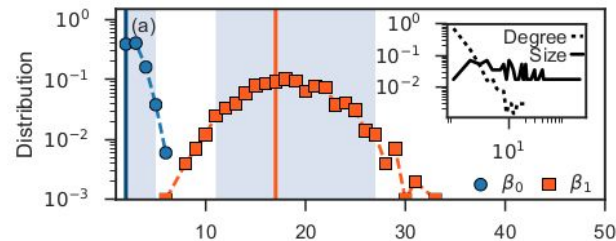
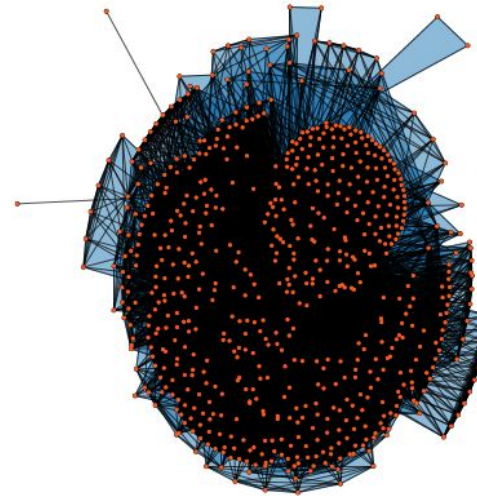


Results on Betti numbers of real data sets

Pollinators (*real*)



Pollinators (*random*)



Our contribution

Code : github.com/jg-you/scm

(1) J.-G. Young, G. Petri, F. Vaccarino and A. Patania, Phys. Rev. E 96 (3), 032312 (2017)

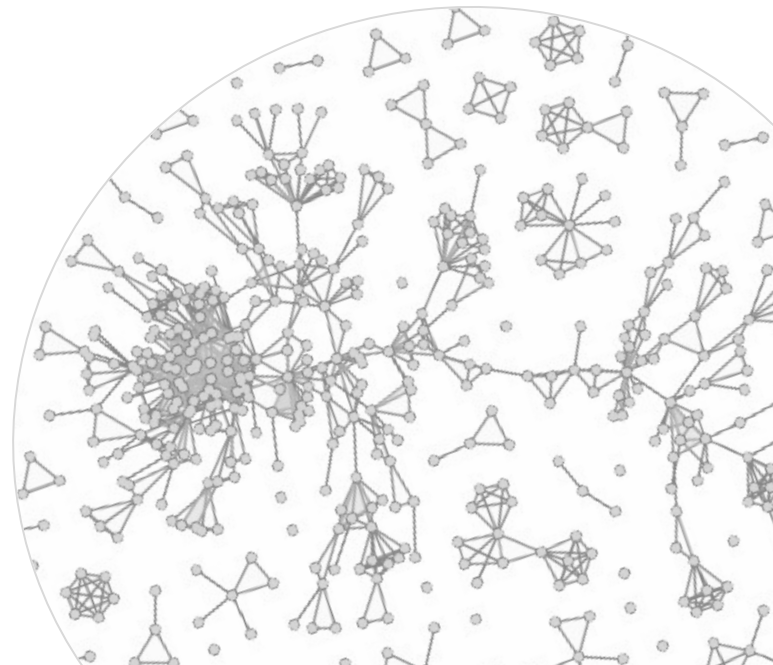
Equilibrium random ensembles

(2) O. Courtney and G. Bianconi, Phys. Rev. E 93, (2016)

(3) K. Zuev, O. Eisenberg and K. Krioukov, J. Phys. A 48, (2015)

Sampling

(4) B. K. Fosdick, et al., arXiv :1608.00607 (2016)



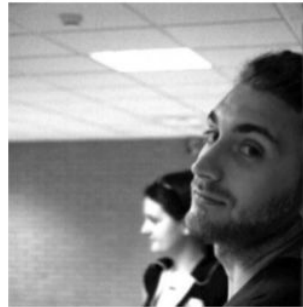
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Francesco Vaccarino



Giovanni Petri



Jean-Gabriel Young

Thank You for the Attention