

Graph mining - lesson 3

Tests and random graphs

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Sketch of this lesson

Issue at stake:

- ▶ short overview of different **random graph models**
- ▶ **tests** based on these models to assess the significance of numerical characteristics or of attributes



Notations for this class

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In the following, a **graph** $\mathcal{G} = (V, E, W)$ with:

- ▶ V : set of vertices $\{x_1, \dots, x_n\}$;
- ▶ E : set of (undirected) edges. $m = |E|$;
- ▶ W : weights on edges s.t. $W_{ij} \geq 0$, $W_{ij} = W_{ji}$ and $W_{ii} = 0$ (also called, *adjacency matrix*).



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If needed, attributes for the nodes will be denoted by $f_j(x_i)$ (j th attribute for node i) and attributes for the edges (other than the weights) by $g_j(x_i, x_{i'})$ (j th attribute for the edge $(x_i, x_{i'})$).



Outline

Some standard random graph models

Permutation tests

Permutation tests for testing vertex labels



Some well known models studied in this class...

- ▶ **Erdős-Rényi model** [Erdős and Rényi, 1959] first and simplest random graph model in which the probability to observe an edge between two vertices is uniform over all pairs of vertices
- ▶ **scale free model** [Barabási and Albert, 1999] network in which the degree distribution fits a power law
- ▶ **Stochastic Block Model** [Snijders and Nowicki, 1997] random graphs with a community structure



Erdős-Rényi model

2 closely related Erdős-Rényi models:

- ▶ $G(n, m)$ the first method consists to set a number of vertices, n , and a number of edges, m , and to choose one graph uniformly at random among the set of graphs with n vertices and m edges;
- ▶ $G(n, p)$ the second method consists to set a number of vertices, n , and the probability, p , to decide, for every pair of vertices, if an edge exists between the two vertices, independantly at random with probability p

Some properties of ER graphs $G(n, p)$

- ▶ $\mathbb{E}(\text{number of edges in } G(n, p)) = \binom{n}{2} p$
- ▶ degree distribution is binomial:

$$\mathbb{P}(d_i = k) = \binom{n-1}{k} p^k (1-p)^{n-1-k}$$

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- ▶ diameter $\sim \frac{\log n}{\log(np)}$ **[Albert and Barabási, 2002]**
- ▶ depending on whether $p < \frac{(1-\epsilon) \log n}{n}$ or $p > \frac{(1+\epsilon) \log n}{n}$,
 $\mathbb{P}(G(n, p) \text{ contains isolated vertices}) \xrightarrow{n \rightarrow +\infty} 1$ or
 $\mathbb{P}(G(n, p) \text{ is connected}) \xrightarrow{n \rightarrow +\infty} 1$



scale free model

Network is a network whose degree distribution (asymptotically) follows a **power law**:

$$\mathbb{P}(d_i = k) = k^{-\gamma}$$

for a $\gamma \in]2, 3[$ (in general).

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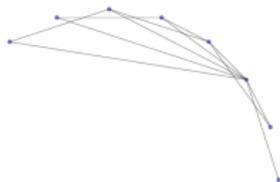
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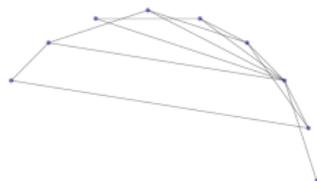
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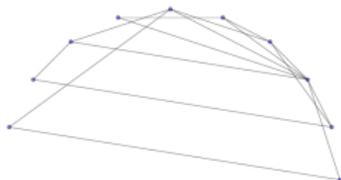
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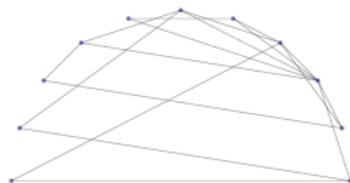
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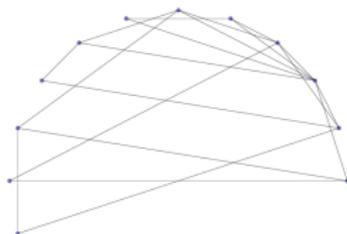
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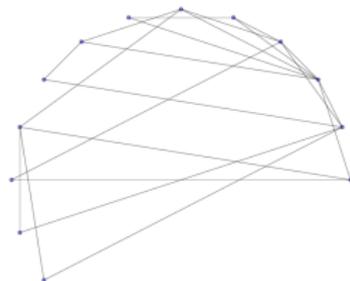
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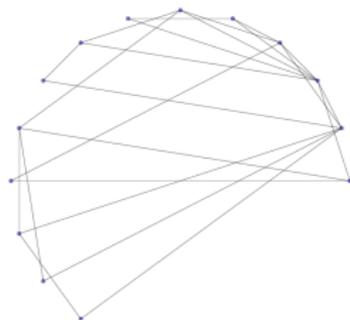
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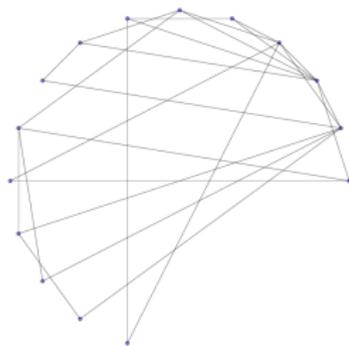
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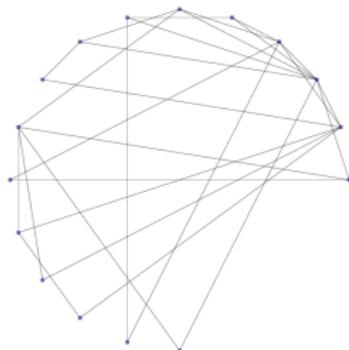
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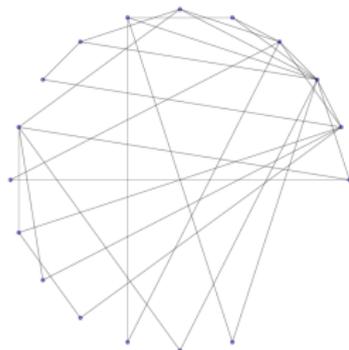
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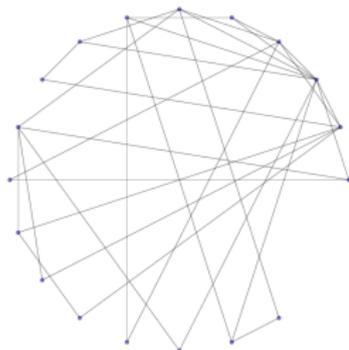
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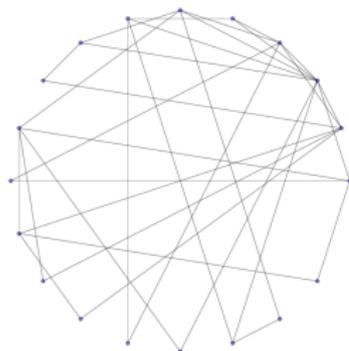
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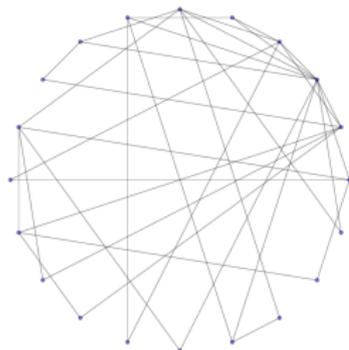
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Some properties of BA and scale free graphs

- ▶ Degree distribution of BA graph: scale free with $\gamma = 3$

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- ▶ Degree distribution of BA graph: scale free with $\gamma = 3$

- ▶ [Cohen and Havlin, 2003] depending on whether $\gamma < 3$, $\gamma = 3$ and $\gamma > 3$, the average shortest path length is of order $\log \log n$ (“ultra-small worlds”), $\frac{\log n}{\log \log n}$ or $\log n$



SBM

SBM with n vertices are random graphs for which a partition of the vertices, C_1, \dots, C_K is given, for which the probability that a vertex $x_i \in C_k$ and a vertex $x_j \in C_{k'}$ are connected, has a probability $\pi_{kk'} \in [0, 1]$.

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Some results describe the conditions for which the **partition can be recovered** (for a number of vertices that tends to $+\infty$), according to the relation between the intra/inter-block probabilities.



Comparison with random graphs...

Erdos-Renyi model with the same number of nodes and the same number of edges than the original graph $G(n, m)$



Comparison with random graphs...

Erdos-Renyi model with the same number of nodes and the same number of edges than the original graph $G(n, m)$

Method: compare the observed values with those of a large number of randomly generated random graphs (with no loop, only connected graphs are kept)



Results of the comparison with random graphs...

For $B = 500$ graphs (only connected graphs are kept), we have:

| | density | transitivity | diameter | radius | girth | cohesion |
|-----|----------------|----------------|--------------|-----------|-----------|-------------|
| X | Min. :0.0725 | Min. :0.0541 | Min. :4.00 | Min. :3 | Min. :3 | Min. :1.0 |
| X.1 | 1st Qu.:0.0725 | 1st Qu.:0.0673 | 1st Qu.:4.00 | 1st Qu.:3 | 1st Qu.:3 | 1st Qu.:2.0 |
| X.2 | Median :0.0725 | Median :0.0719 | Median :4.00 | Median :3 | Median :3 | Median :3.0 |
| X.3 | Mean :0.0725 | Mean :0.0719 | Mean :4.11 | Mean :3 | Mean :3 | Mean :2.5 |
| X.4 | 3rd Qu.:0.0725 | 3rd Qu.:0.0765 | 3rd Qu.:4.00 | 3rd Qu.:3 | 3rd Qu.:3 | 3rd Qu.:3.0 |
| X.5 | Max. :0.0725 | Max. :0.0895 | Max. :5.00 | Max. :3 | Max. :3 | Max. :4.0 |

which has to be compared to 0.072, 0.56, 18, 9, 3 and 1.

- ▶ the transitivity is much larger;
- ▶ the diameter and the radius are much larger also;
- ▶ the cohesion is smaller.

The first remark indicates a **stronger local connectivity** in my NVV network than in ER models with same number of nodes and edges. Large radius and diameter are explained by an isolated branch in the network.



Comparison with random graphs...

Scale free model: Barabási and Albert model is used with a number of edges added at each step which is chosen so that the final number of edges resembles that of the original graph (4 edges, which gives 478 edges in the final graph, compared to 535 in the real NVV network).



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For $B = 500$ graphs, we have:

| | density | transitivity | diameter | radius | girth | cohesion |
|-----|----------------|---------------|-----------|--------------|-----------|-----------|
| X | Min. :0.0648 | Min. :0.102 | Min. :4 | Min. :2.00 | Min. :3 | Min. :4 |
| X.1 | 1st Qu.:0.0648 | 1st Qu.:0.116 | 1st Qu.:4 | 1st Qu.:3.00 | 1st Qu.:3 | 1st Qu.:4 |
| X.2 | Median :0.0648 | Median :0.121 | Median :4 | Median :3.00 | Median :3 | Median :4 |
| X.3 | Mean :0.0648 | Mean :0.121 | Mean :4 | Mean :2.97 | Mean :3 | Mean :4 |
| X.4 | 3rd Qu.:0.0648 | 3rd Qu.:0.125 | 3rd Qu.:4 | 3rd Qu.:3.00 | 3rd Qu.:3 | 3rd Qu.:4 |
| X.5 | Max. :0.0648 | Max. :0.139 | Max. :5 | Max. :3.00 | Max. :3 | Max. :4 |

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Limits of the previous approaches

Until now, we have compared the real graph to graphs randomly generated according to a given random model but:

- ▶ this approach only gives information about **global characteristics** of the observed graph;
- ▶ none of the distributions of the current characteristics is preserved during the process, especially not the **degree distribution** which is central for controlling local/global connectivity, counts of specific patterns...



A null model closer to the real graph...

Sketch of statistical tests on graphs

1. sample at random within the set of graphs **with the same degree distribution** than the observed graph (B times)
2. compute a numerical statistics for each of these randomly generated graphs
3. compare the observed value of the statistics and its **distribution** over the random graphs, **a p-value can be derived** (for B large enough)



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Two main approaches to sample at random with fixed degrees:

- ▶ configuration model [**Bender and Canfield, 1978**]
- ▶ **permutation approach** [**Rao et al., 1996, Roberts Jr., 2000**]

Sampling at random within the set of graphs with a given degree distribution

Aim:

- ▶ all graphs can **exhaustively** be sampled
- ▶ all graphs have the **same probability to be sampled**

⇒ MCMC approach

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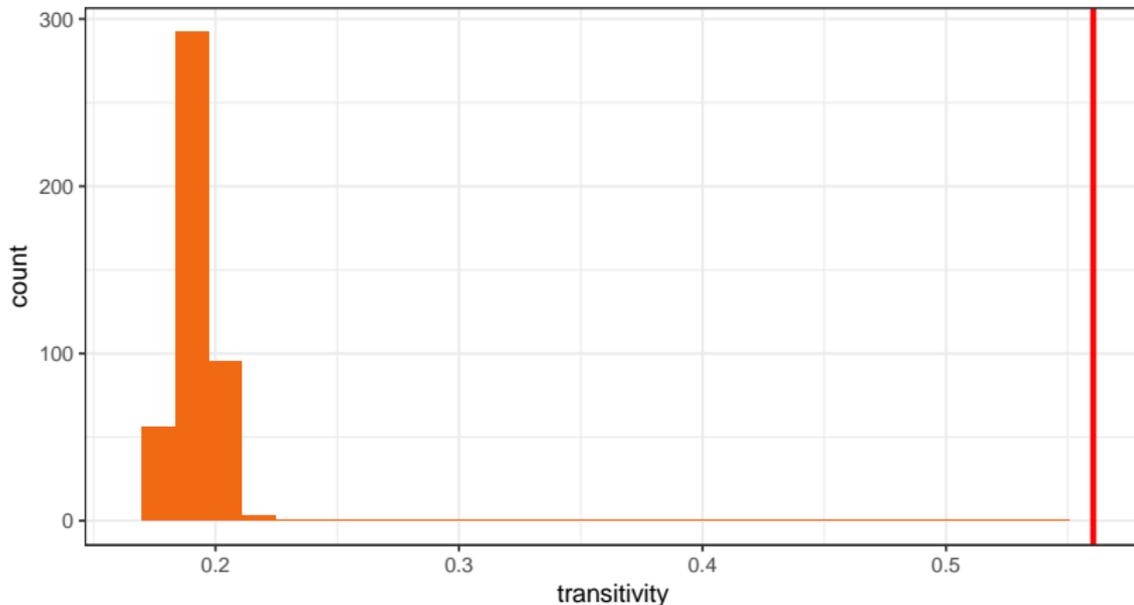
⇒ MCMC approach

Method:

- 1: Start from the observed graph \mathcal{G}
- 2: **for** $t = 1 \rightarrow T|E|$ **do**
- 3: Select uniformly at random two edges $e^1 = (x_i^1, x_j^1)$ and $e^2 = (x_i^2, x_j^2) \in E$
- 4: $E' \leftarrow E \setminus \{e^1, e^2\} \cup \{e_s^1, e_s^2\}$ with $e_s^1 = (x_i^1, x_j^2)$ and $e_s^2 = (x_i^2, x_j^1)$
- 5: **if** $\mathcal{G}' = (V, E')$ is simple and connected **then**
- 6: $\mathcal{G} \leftarrow \mathcal{G}'$
- 7: **end if**
- 8: **end for**
- 9: **return** \mathcal{G}

In practice... (for the transitivity)

transitivity of random graphs with degree distribution as NVV



Again, this is evidence for a strong local connectivity in the network.



Using random graphs to assess the relevance of the clustering

Method:

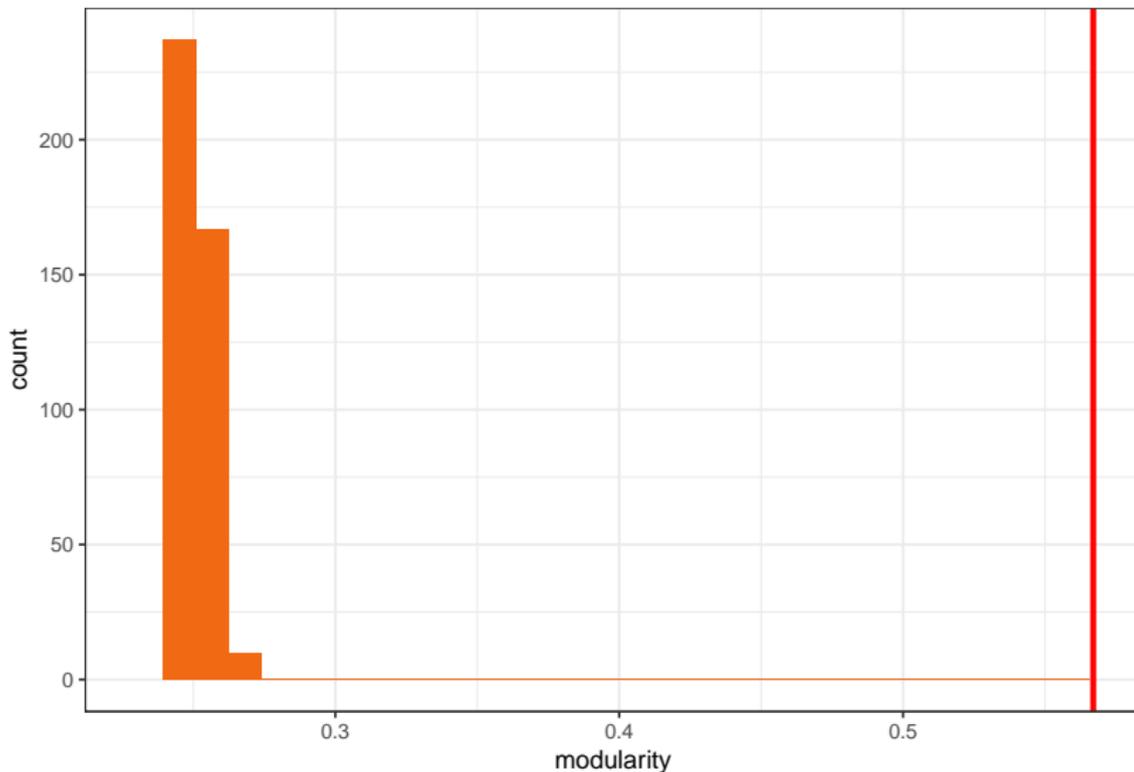
- ▶ Find the clustering associated to the maximum modularity.

- ▶ Compare this modularity with the distribution of maximum modularities over B random graphs obtained by edge permutation.



Relevance of the clustering of NVV

modularity of random graphs with degree distribution as NVV



More on random graphs generation

Sometimes, one wants to compare the observed graph with a more sophisticated (constrained) null model (taking into account some additional information on edges or nodes for instance):

- ▶ This can be achieved using the same principle and throwing away the random graphs which do not satisfy the constraints.

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Sometimes, one wants to compare the observed graph with a more sophisticated (constrained) null model (taking into account some additional information on edges or nodes for instance):

- ▶ This can be achieved using the same principle and throwing away the random graphs which do not satisfy the constraints. **Warning:** The more sophisticated the model is, the more costly the simulation would be. For instance, only removing graphs with multiple edges and graphs which are not connected leads to **throw away** 53 graphs during the previous generation process.
- ▶ **Possible solution:** [Tabourier and Cointet, 2011] use **multiple edge switching** to improve such simulations.



Outline

Some standard random graph models

Permutation tests

Permutation tests for testing vertex labels



General setting

A label $f(x_i)$ is given for all vertices in the graph.

Question: Are the labels “related” to the graph structure? *e.g.*

- ▶ connected nodes tend to have similar labels;
- ▶ OR connected nodes tend to have opposite labels.



Join Count Statistics

First case: binary labels $f(x_i) \in \{0, 1\}$



Join Count Statistics

First case: binary labels $f(x_i) \in \{0, 1\}$

General form:

$$JC = \frac{1}{2} \sum_{i \neq j} W_{ij} \xi_i \xi_j$$

where ξ_i is either $f(x_i)$ or $1 - f(x_i)$.

Join Count Statistics

First case: binary labels $f(x_i) \in \{0, 1\}$

Derived statistics:

- ▶ Number of “1” labels in the neighbor of a vertex labelled “1”

$$JC_1 = \frac{1}{2} \sum_{i,j: f(x_i)=f(x_j)=1} W_{ij}$$

- ▶ Number of “0” labels in the neighbor of a vertex labelled “0”

$$JC_0 = \frac{1}{2} \sum_{i,j: f(x_i)=f(x_j)=0} W_{ij}$$

- ▶ Number of “1” labels in the neighbor of a vertex labelled “0” (and the opposite)

$$JC_{0-1} = \sum_{i,j: f(x_i)=0, f(x_j)=1} W_{ij}$$

Interpretation

Basic interpretation: If JC_1 is “large” (“small”) then vertices labelled “1” in the network tend to be connected with vertices labelled the same way (or tend not to be related to vertices labelled “1”).



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Statistical significance: When is JC_1 significantly large or small?

- ▶ **Method 1:** [Noether, 1970] proves the asymptotic normal distribution of JC_1 : requires additional assumptions on the network and not valid for small networks;



Interpretation

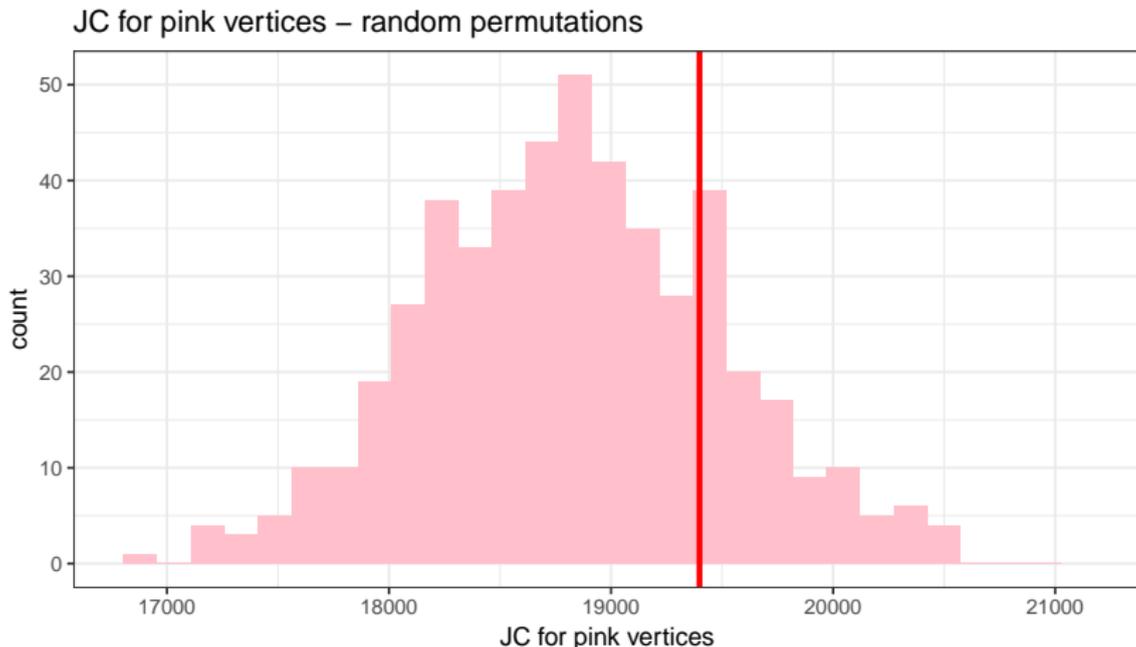
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Statistical significance: When is JC_1 significantly large or small?

- ▶ **Method 1:** [Noether, 1970] proves the asymptotic normal distribution of JC_1 : requires additional assumptions on the network and not valid for small networks;
- ▶ **Method 2: Monte Carlo approach:** Randomly permute the values $f(x_i)$ over the vertices, B times (where B is large) and obtain the empirical distribution of JC_1 . Compare with the true JC_1 .
⇒ Estimation of the distribution of JC_1 given the network and the numbers of labels “1” and “0”.



FB network and connection gender

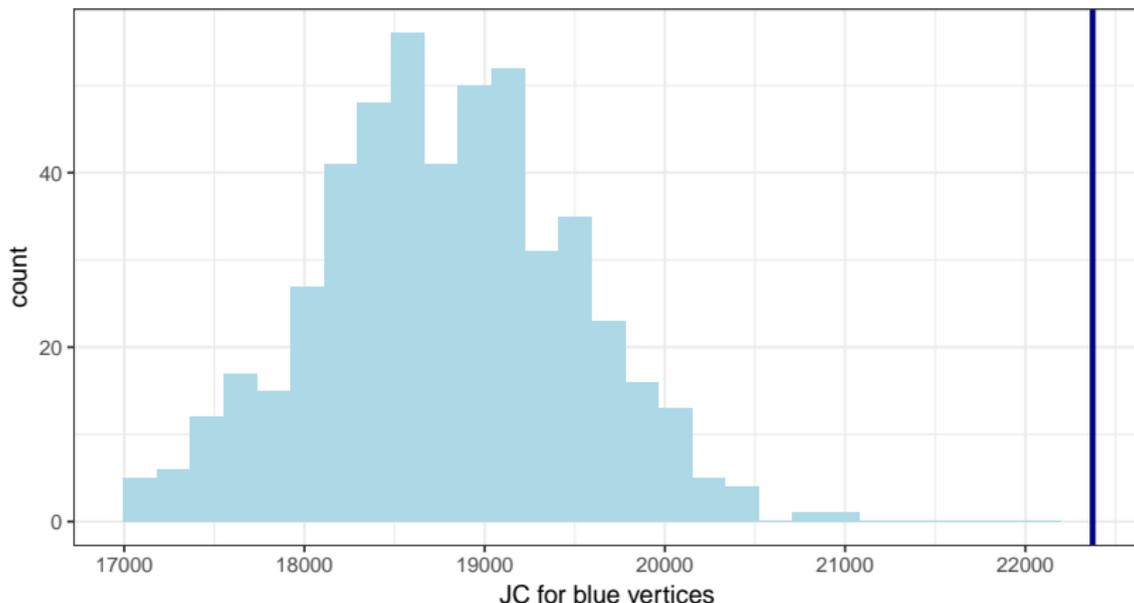


girls tend not to be particularly more connected with other girls than what could be expected by random choice



FB network and connection gender

JC for blue vertices – random permutations



boys tend to be more connected with other boys than what could be expected by random choice



Continuous labels with Moran's I

[Moran, 1950] proposes to measure spatial correlation with the I statistics:

$$I = \frac{\frac{1}{2m} \sum_{i \neq j} W_{ij} \overline{f(x_i) f(x_j)}}{\frac{1}{n} \sum_i \overline{f(x_i)}^2}$$

where $m = \frac{1}{2} \sum_{i \neq j} W_{ij}$ and $\overline{f(x_i)} = f(x_i) - \bar{f}$ with $\bar{f} = \frac{1}{n} \sum_i f(x_i)$.



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Interpretation: When I is “large”, vertices tend to be connected to other vertices having similar labels; when I is “small”, vertices tend to be connected to other vertices having opposite labels. Average I means that there is no special relation between labels and the graph structure.



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Deriving a test for I : again, asymptotic normality can be proved or using a Monte Carlo simulation is also possible.





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