LARGE SCALE BIOLOGICAL NETWORKS

Part I

Complex network theory: An introduction

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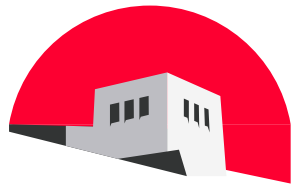
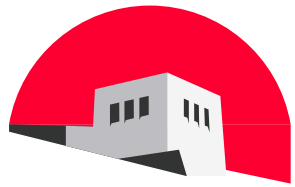
University of New Mexico, Albuquerque, USA

http://www.cs.unm.edu/~holme/



outline

- What systems can be modeled as networks?



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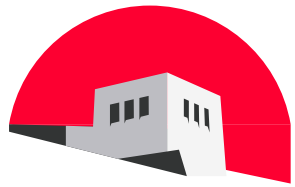
- What systems can be modeled as networks?
- Software and how to make network programs.



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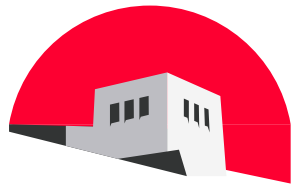
- What questions can we ask about a network?



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- What systems can be modeled as networks?
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- What questions can we ask about a network?
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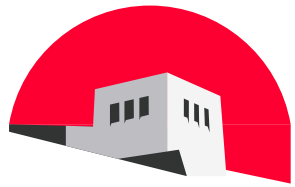

networked systems

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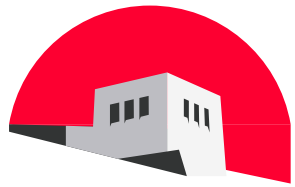

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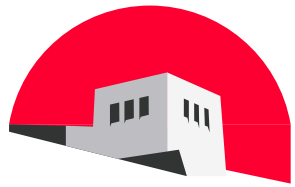
What systems can be modeled as networks?

Any system where many objects interact pairwise.



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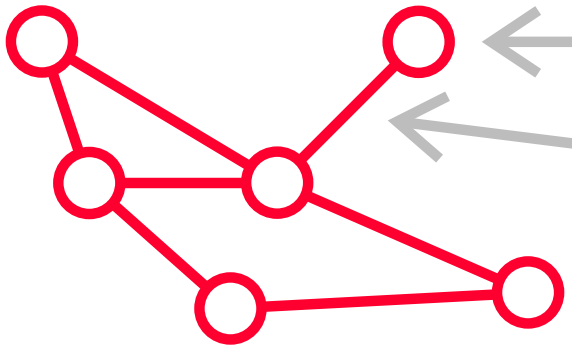

vertex, node, site, actor, agent

edge, link, tie, bond, arc

number of neighbors = *degree*

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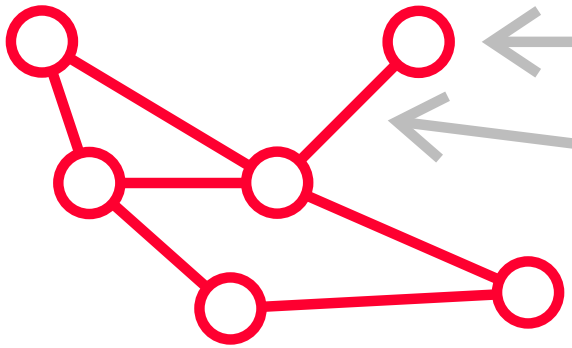

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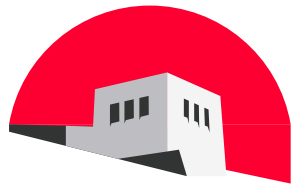

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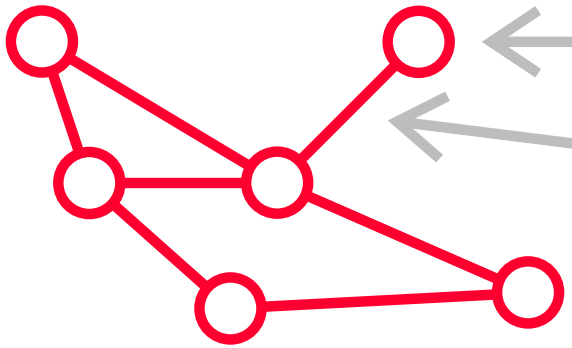

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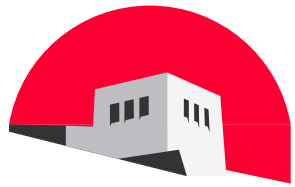
When is network modeling useful?
When the average degree is limited.



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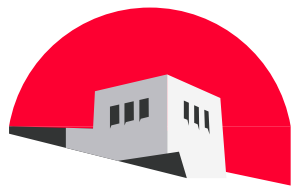
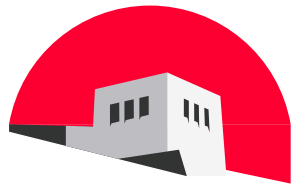


networked systems

constructing networks: example

1. Index the names.



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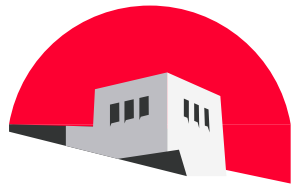
3. Construct a matrix with the number of hits H_{ij}.



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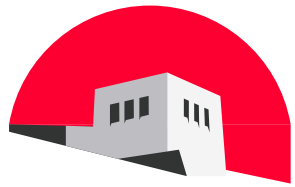
4. Let $h_i = \sum_j H_{ij}$.
5. If $w_{ij} = H_{ij} / \sqrt{h_i h_j} > \theta$ for a threshold θ make an edge between i and j.



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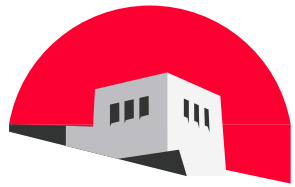
Things to ask oneself:



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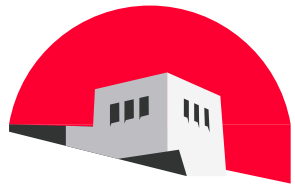

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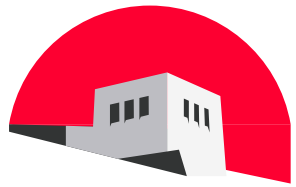
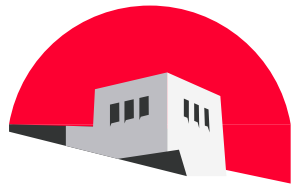


constructing networks: example

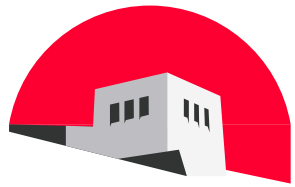
Things to ask oneself:

- What is my network, really? What do the edges really represent?
- Are there false edges? Missing edges?
- How does that affect my result?



analyzing the network

software:



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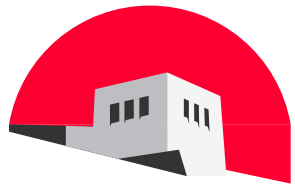

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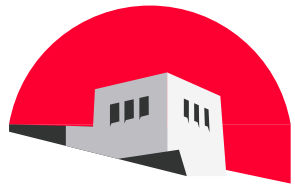

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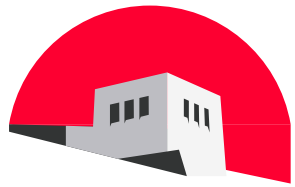

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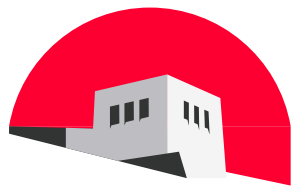

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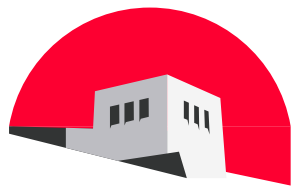

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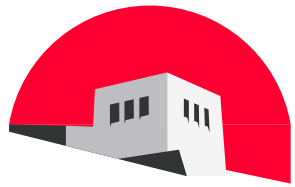
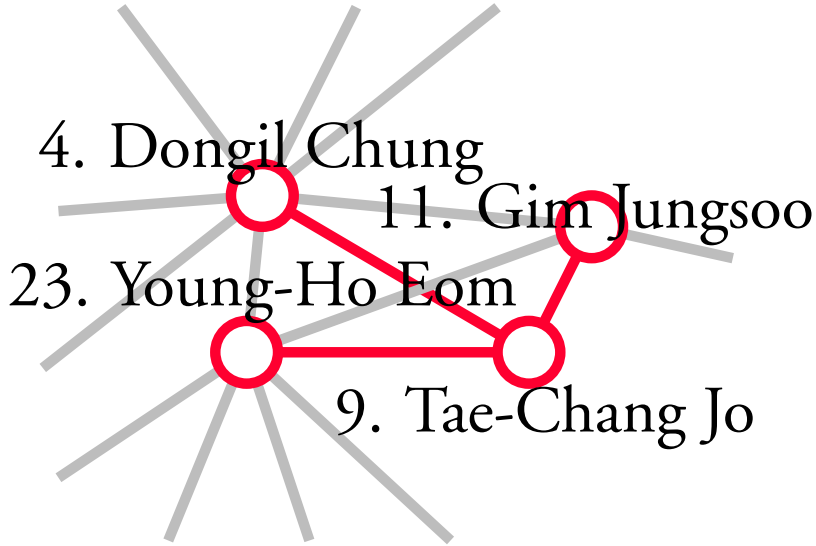
C, Matlab:

- You have to do most yourself . . .



internal representations



vertex 9, deg 3
neighbors 4, 11, 23

edge 31, one side 9
other side 23

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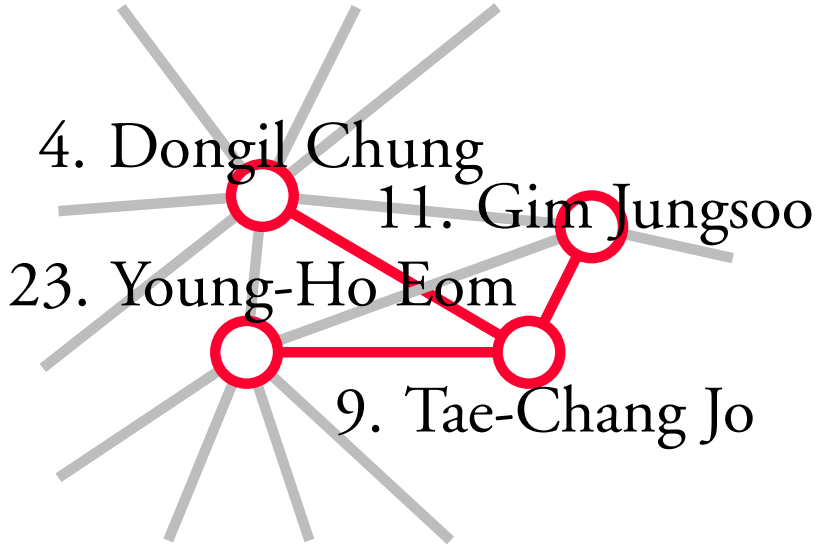

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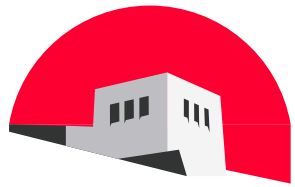

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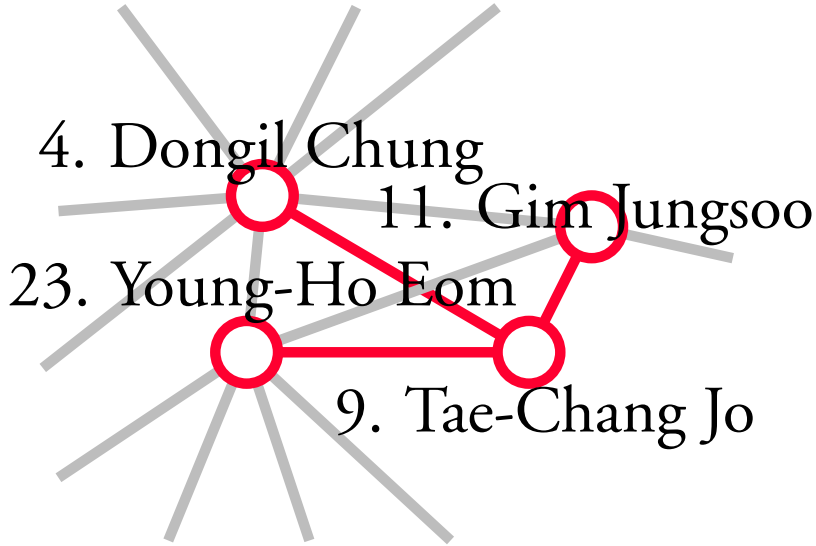

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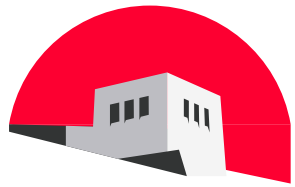

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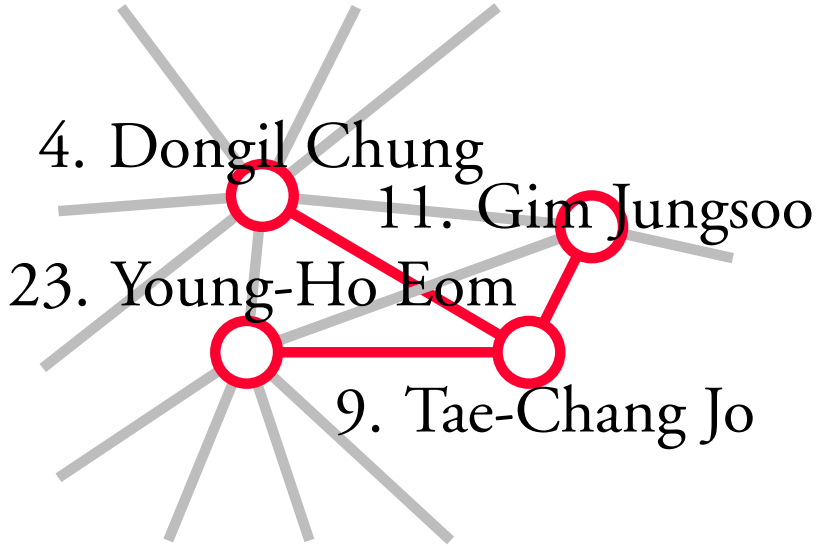

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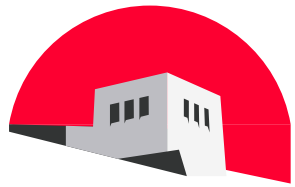

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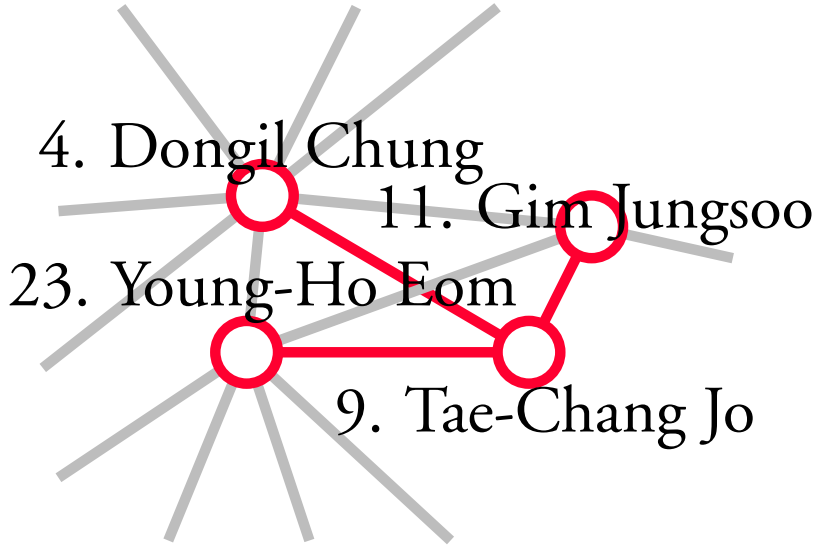

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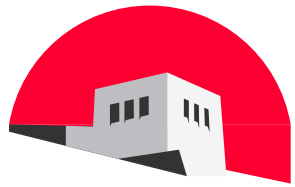
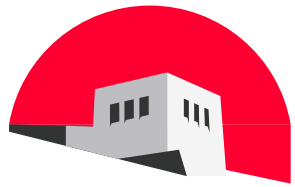


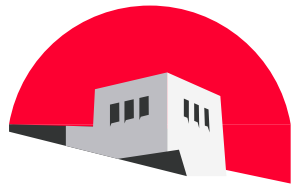
now what?

- We have a system represented as a network.
- We have the tools to analyze it.
- What questions can we ask?



network science

- **Measures of network structure.** How does a network that is too large to draw "look" like? Real-world networks have both randomness and structure. How can we quantify network structure?



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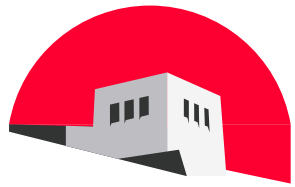

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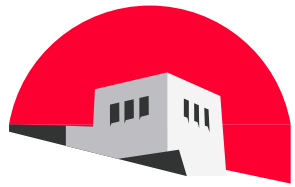

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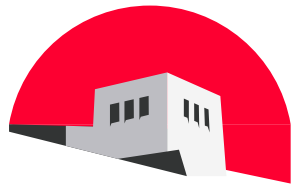

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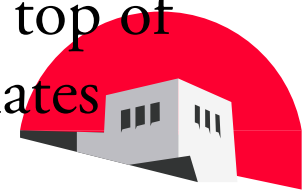
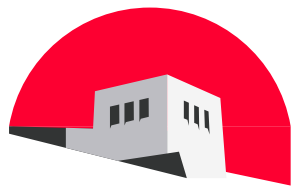
- **How does the network structure affect dynamic systems of the network?** Running dynamic simulations on top of the network and see how dynamic properties correlates with the network structure.



types of structural measures



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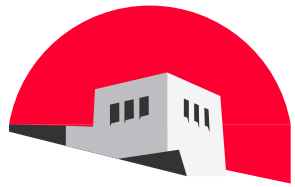
- Vertex measures.



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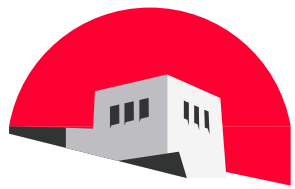
- Vertex measures.
- Edge measures.



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- Vertex measures.
- Edge measures.
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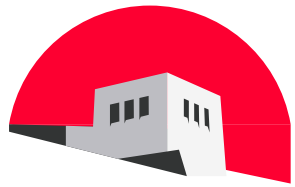
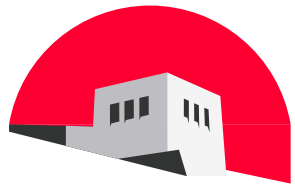


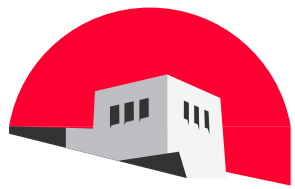
types of structural measures

- Vertex measures.
- Edge measures.
- Vertex-pair measures.
- Graph measures.



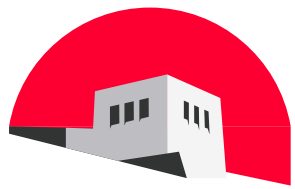
network null-models

- Network structures are always relative . . .



network null-models

- Network structures are always relative . . .
- . . . one has to be clear about what to compare with . . . a null model



network null-models

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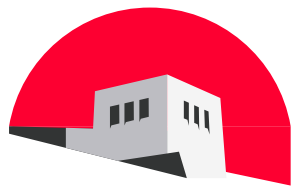
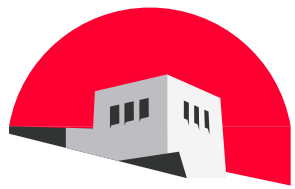
- *Null model 1:* random graphs (Poisson random graphs, Erdős-Rényi graphs)

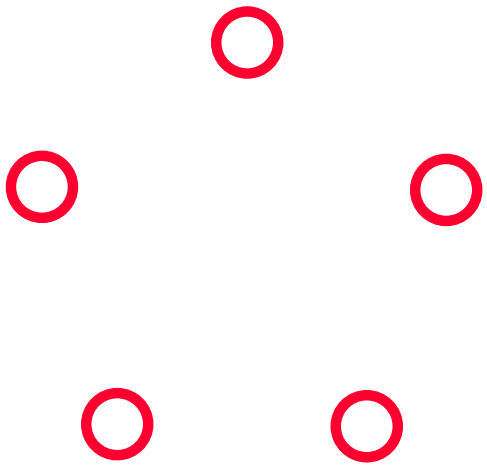


network null-models

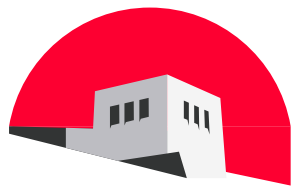
- Network structures are always relative . . .
- . . . one has to be clear about what to compare with . . . a null model
- *Null model 1:* random graphs (Poisson random graphs, Erdős-Rényi graphs)
- *Null model 2:* random graphs constrained to the set of degrees of the original graph



random graphs



for each pair of vertices,
with probability p, add an edge



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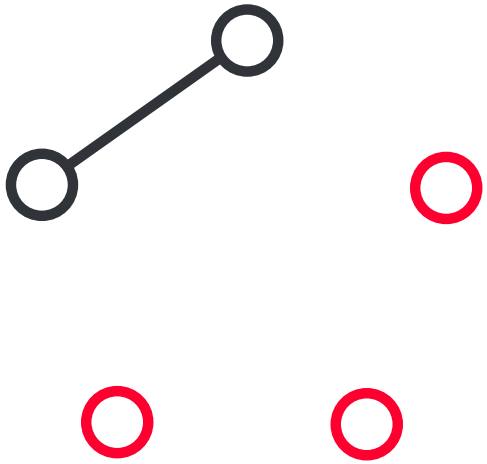

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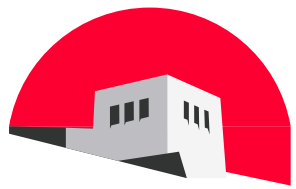

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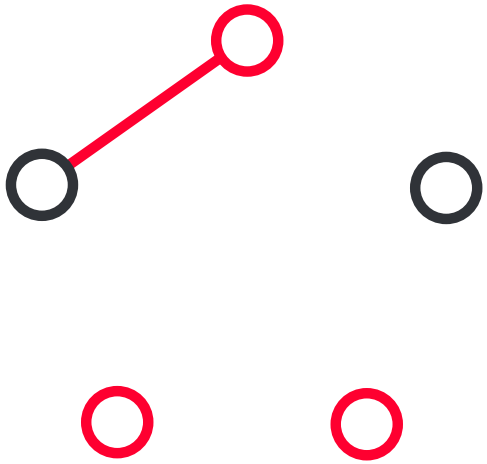

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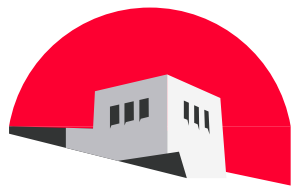

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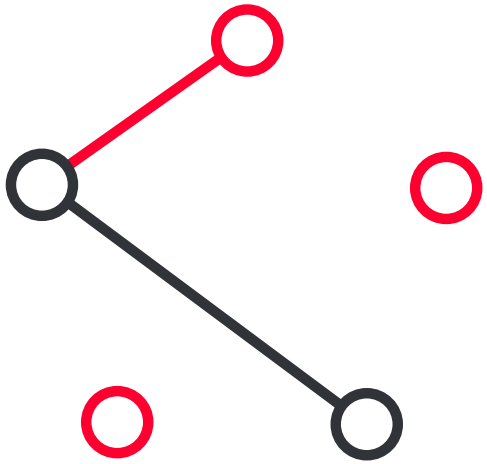

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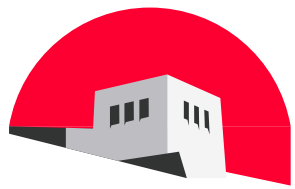

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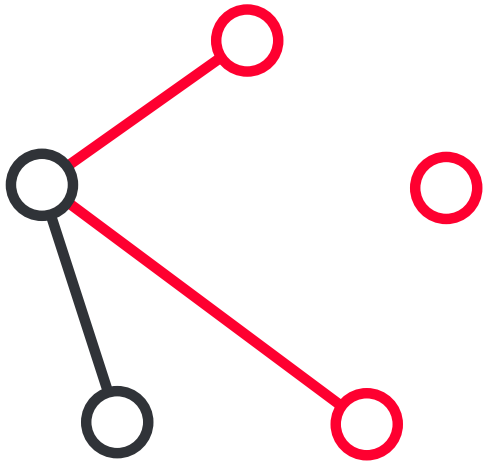

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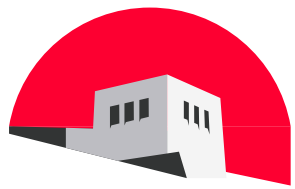

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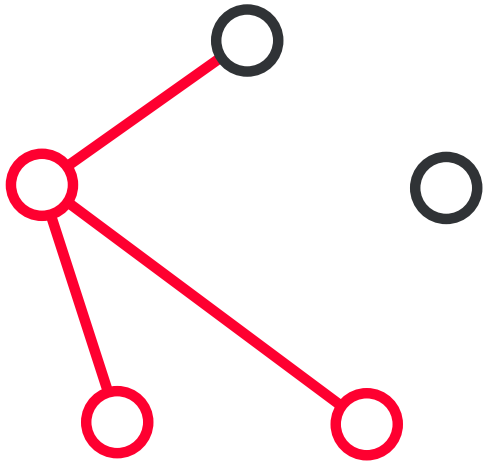

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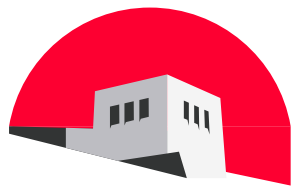

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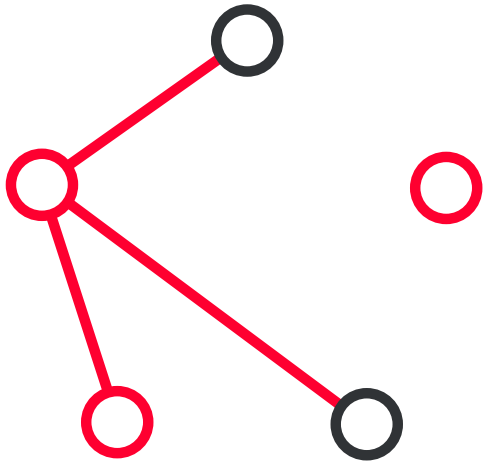

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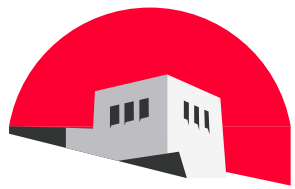

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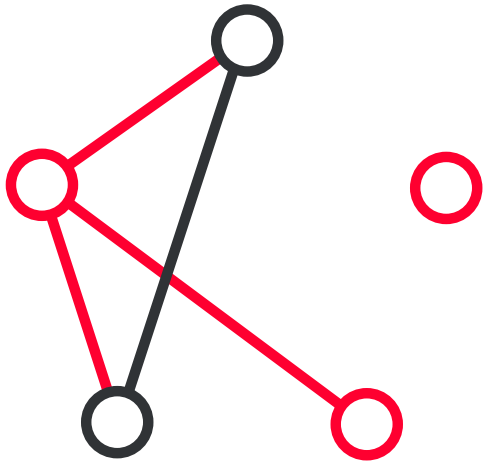

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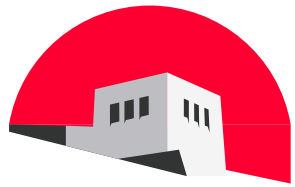

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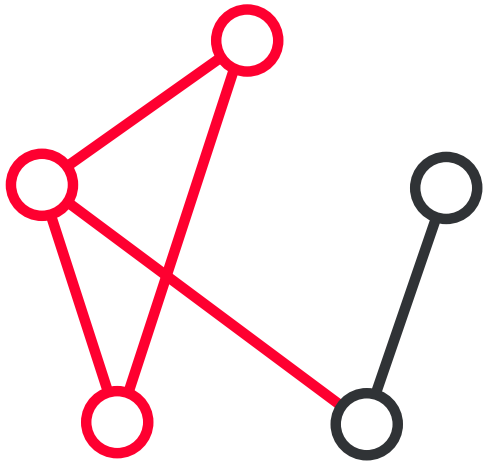

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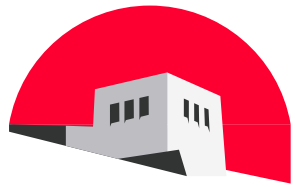

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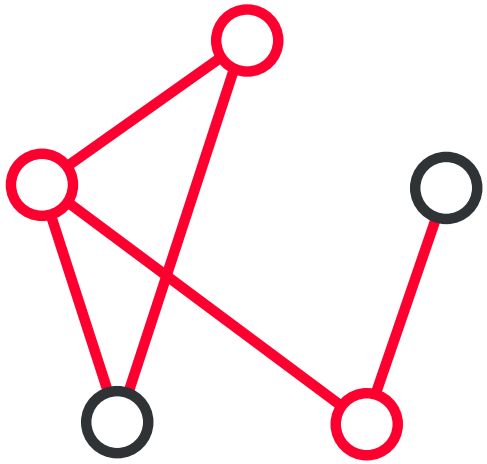

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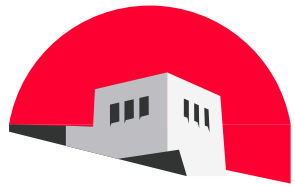

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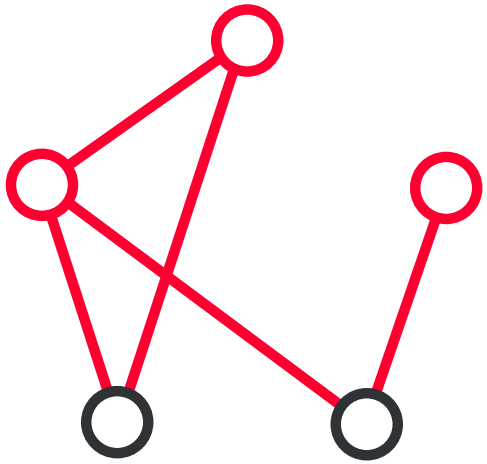

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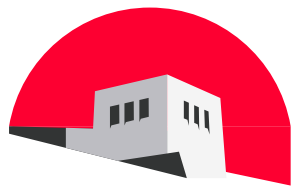

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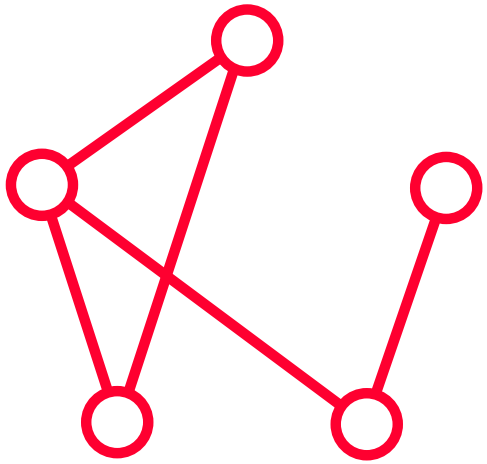

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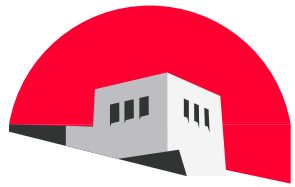
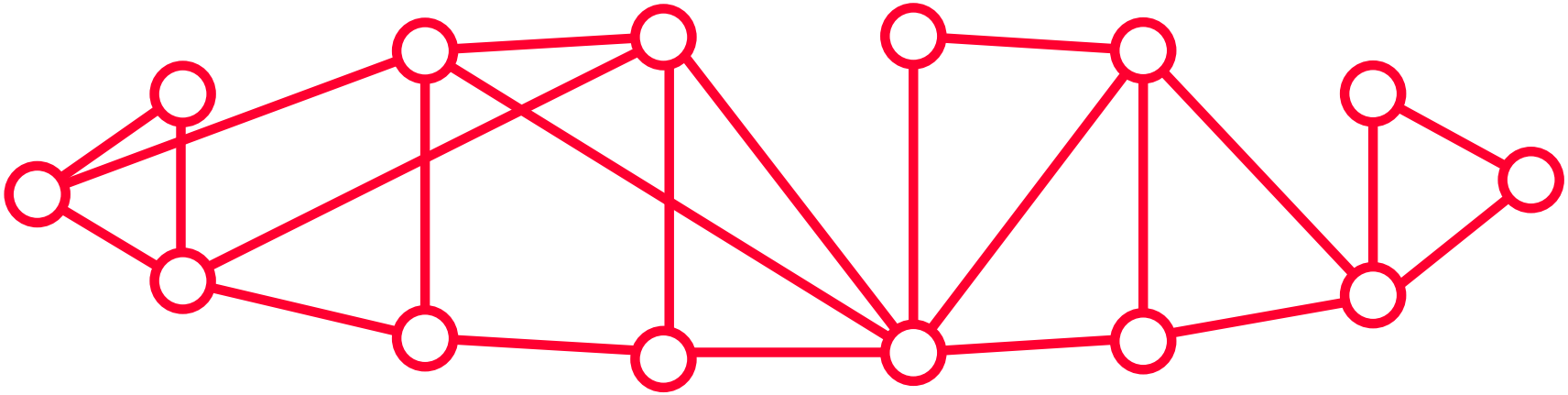
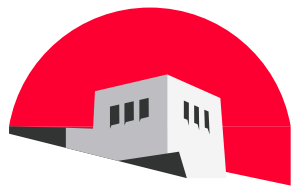


random rewiring



start from the original graph
choose edge pairs, and swap them



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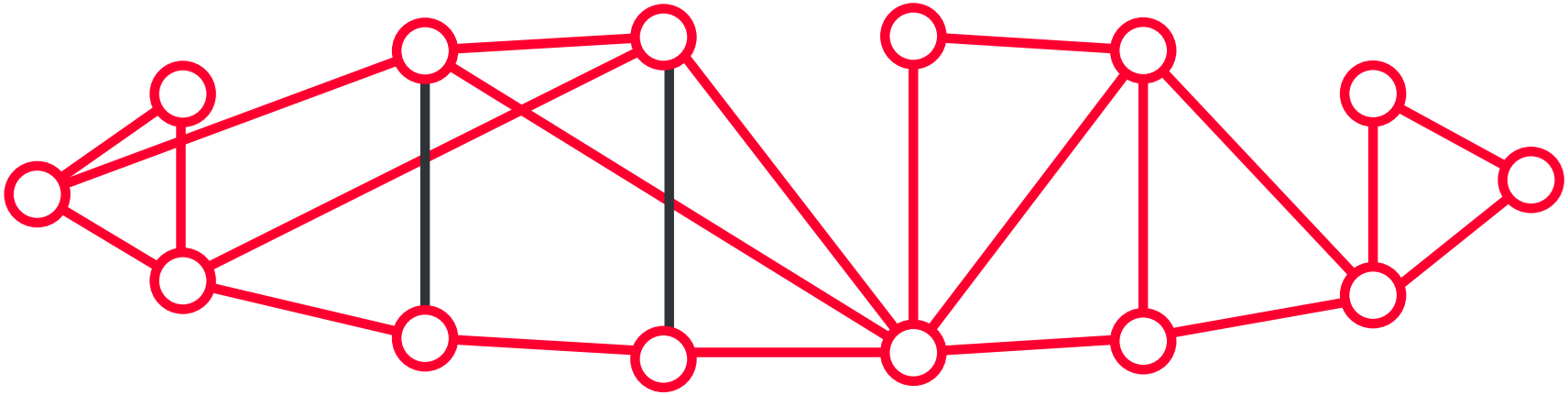

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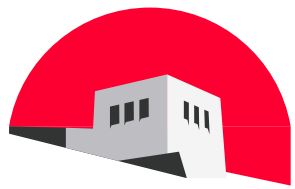

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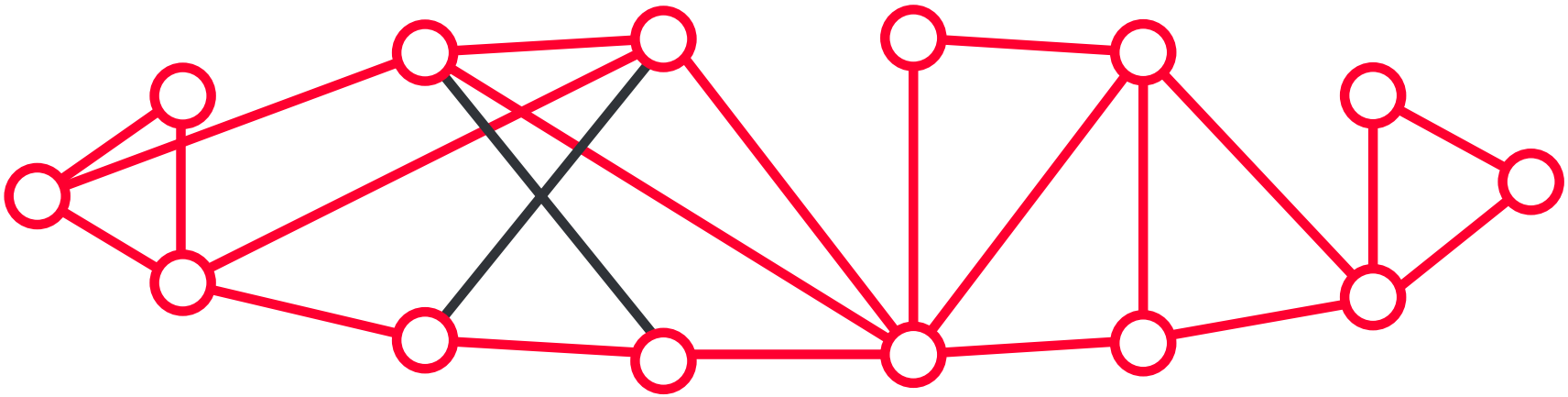

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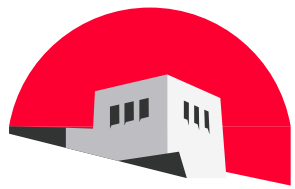

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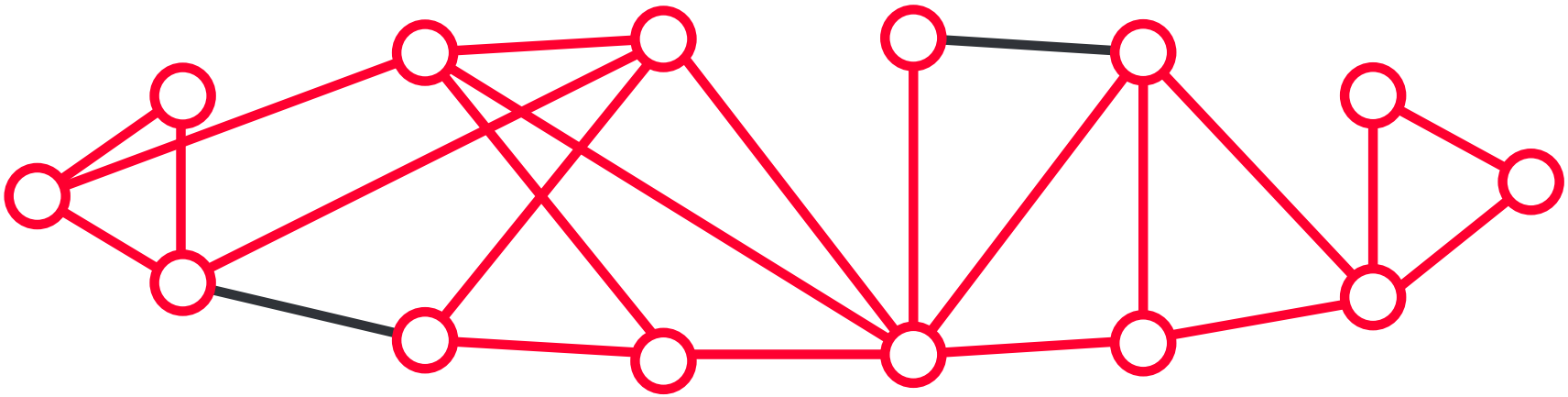

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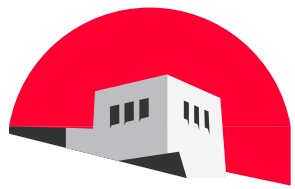

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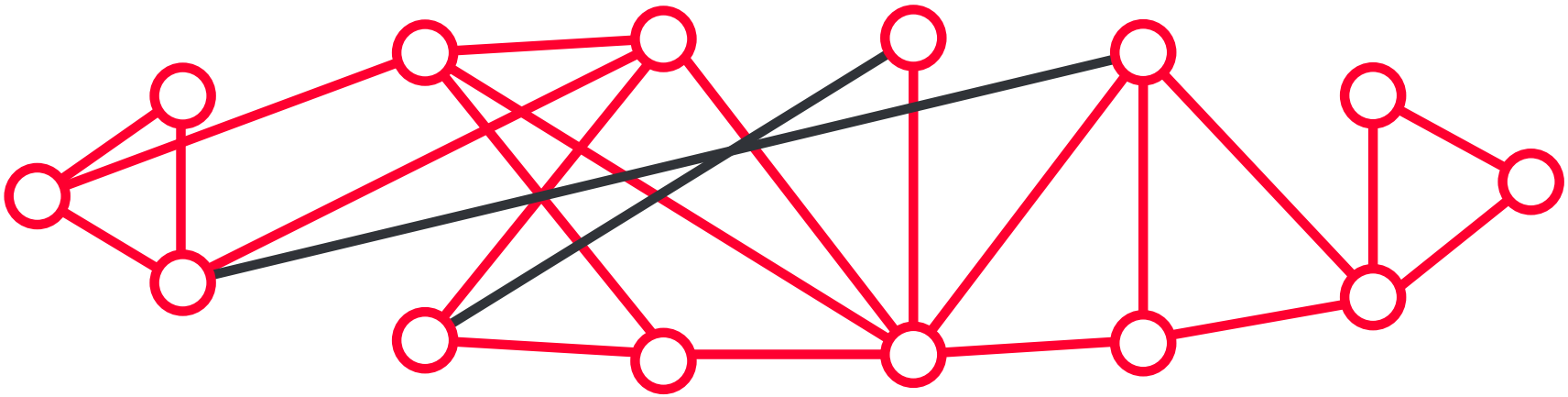

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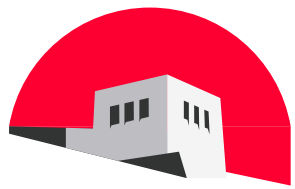

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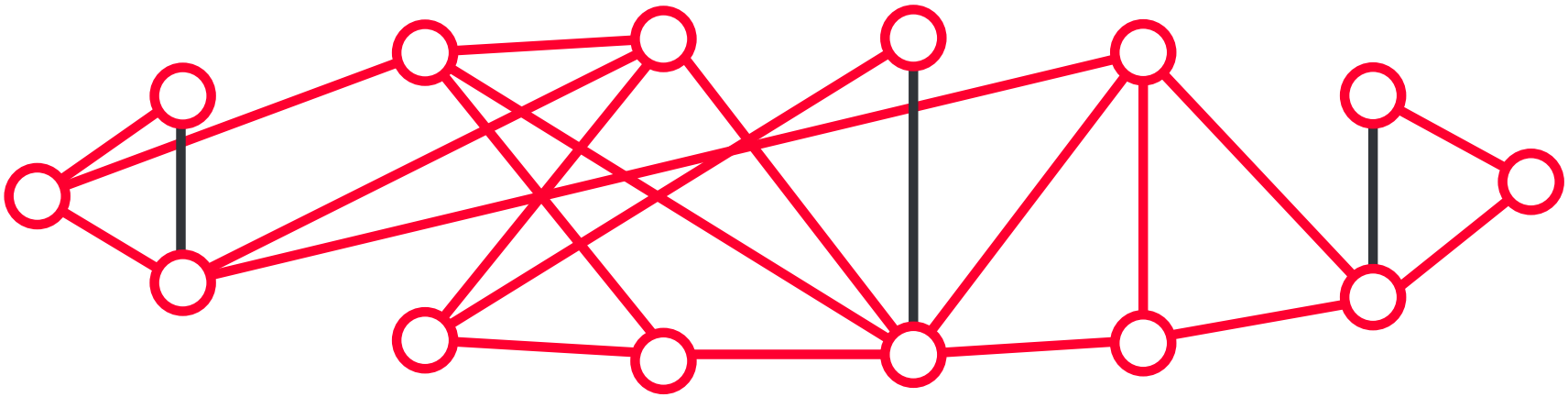
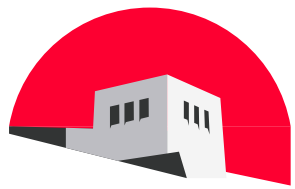


start from the original graph
for ergodicity, edge triples have to be swapped too



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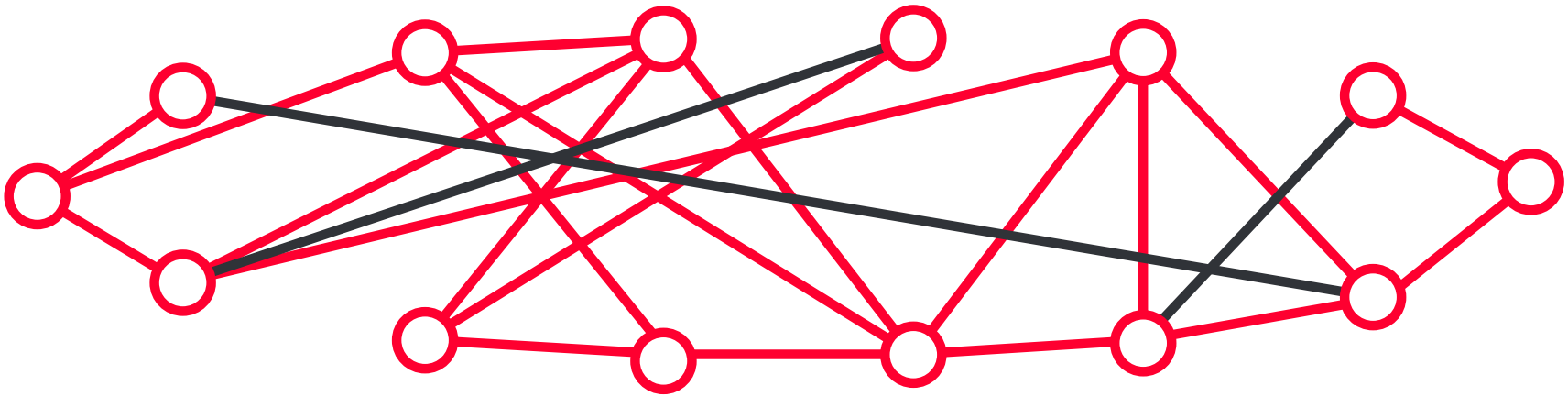

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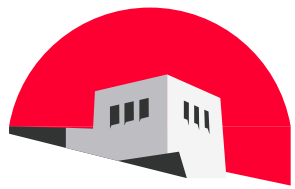

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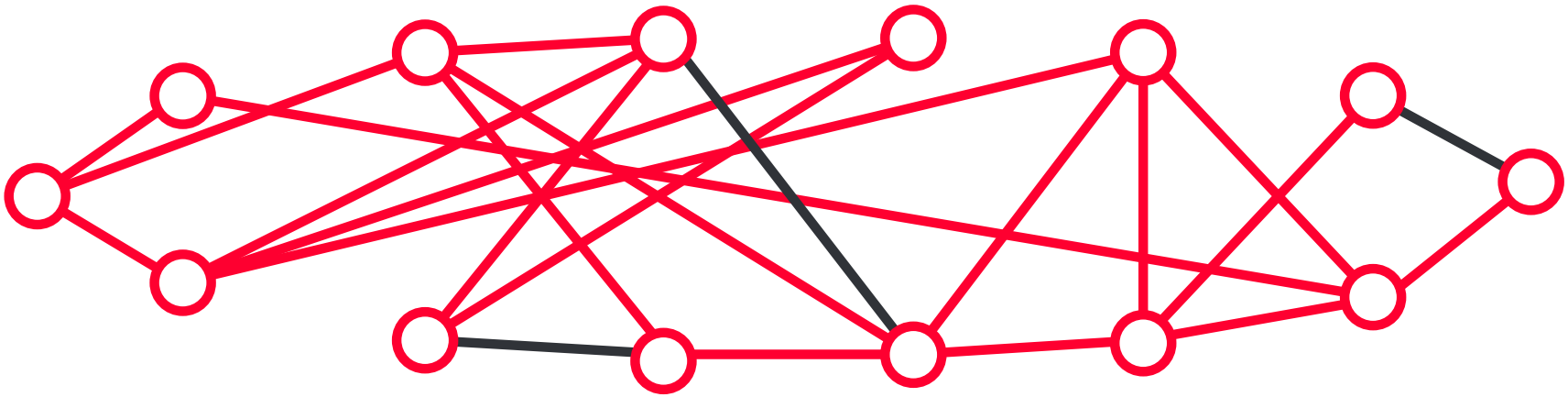

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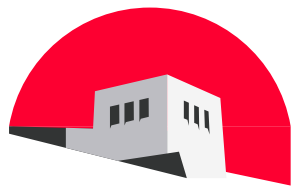

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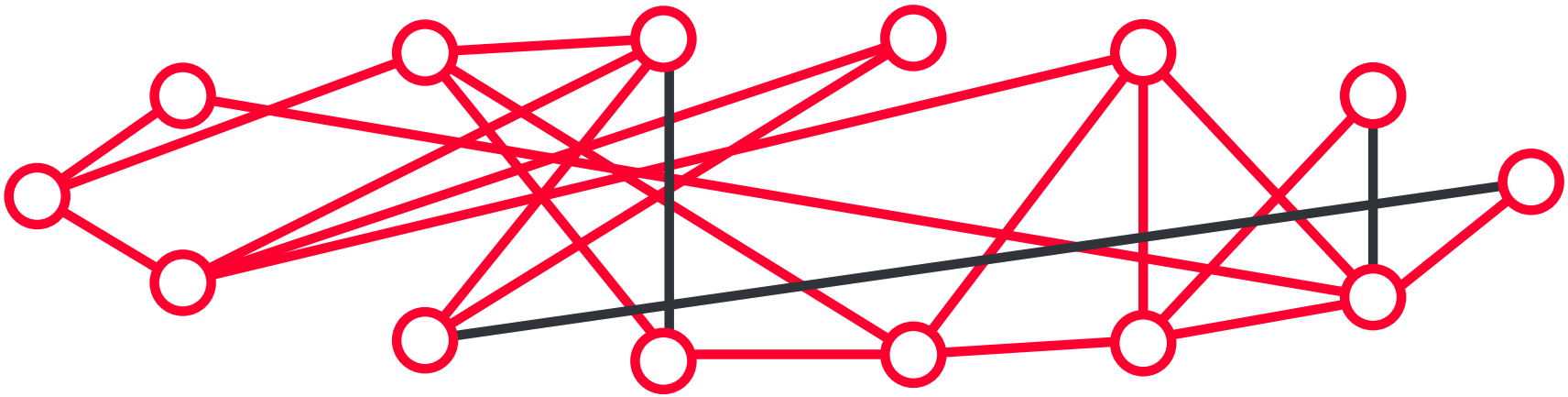

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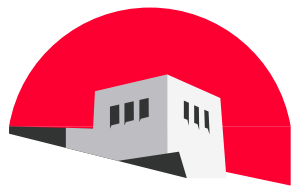
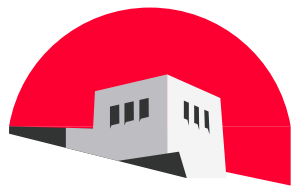


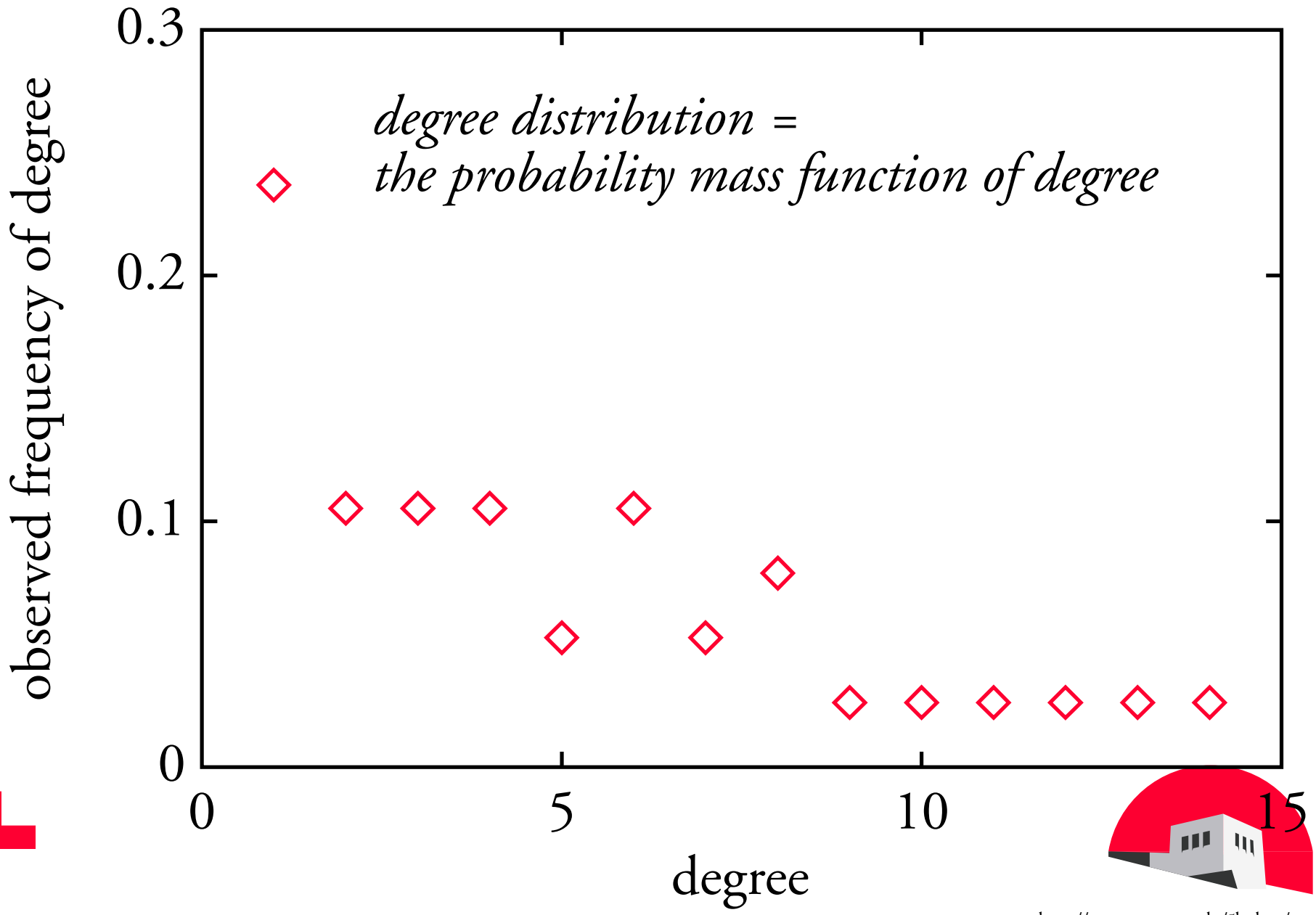
component sizes

giant component 38 vertices

$S = 38$, $s = 38/46 \approx 0.82\cdots$

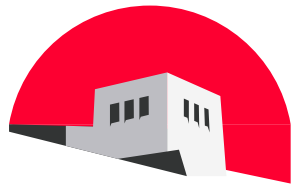


degree distribution



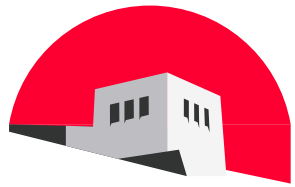
degree distribution

- If the degree distribution looks like a power-law it is called a *scale-free network*.



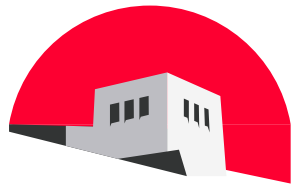
degree distribution

- If the degree distribution looks like a power-law it is called a *scale-free network*.
- This does not necessarily mean system is self-similar. There can be scales visible in other network quantities.

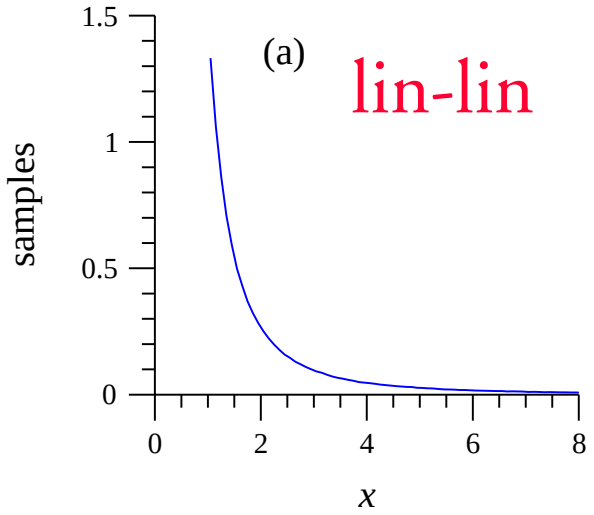


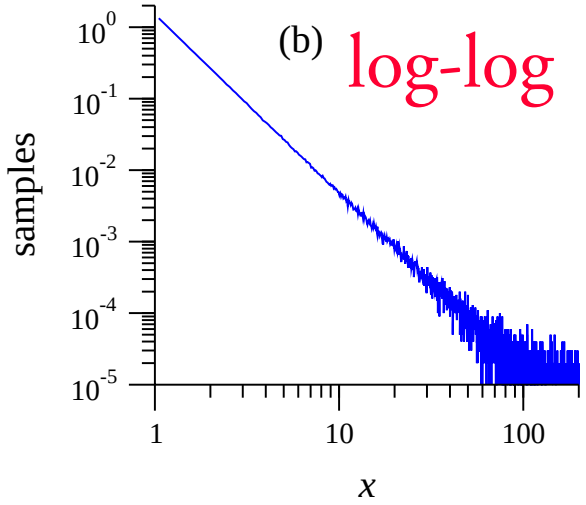
degree distribution

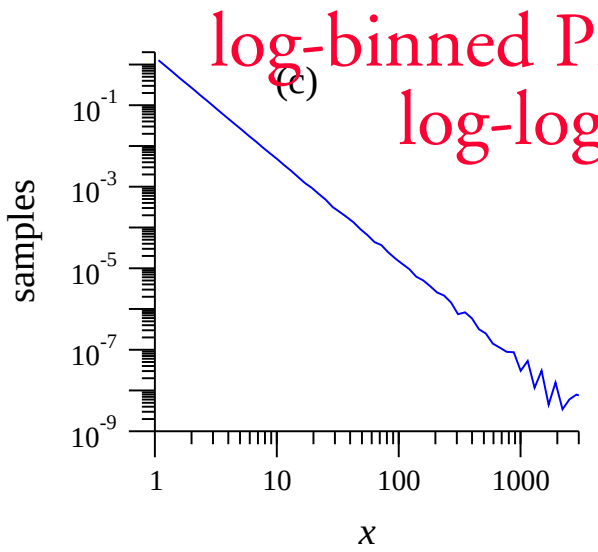
- If the degree distribution looks like a power-law it is called a *scale-free network*.
- This does not necessarily mean system is self-similar. There can be scales visible in other network quantities.
- Exactly where to draw the line between scale-free / not scale-free networks is not known.

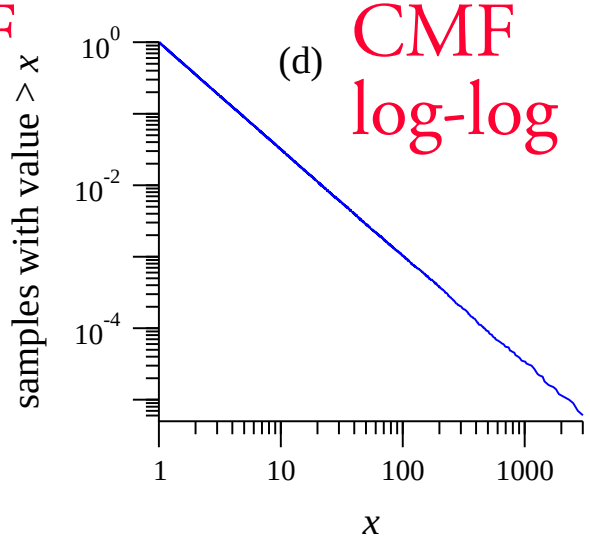


plotting power-laws

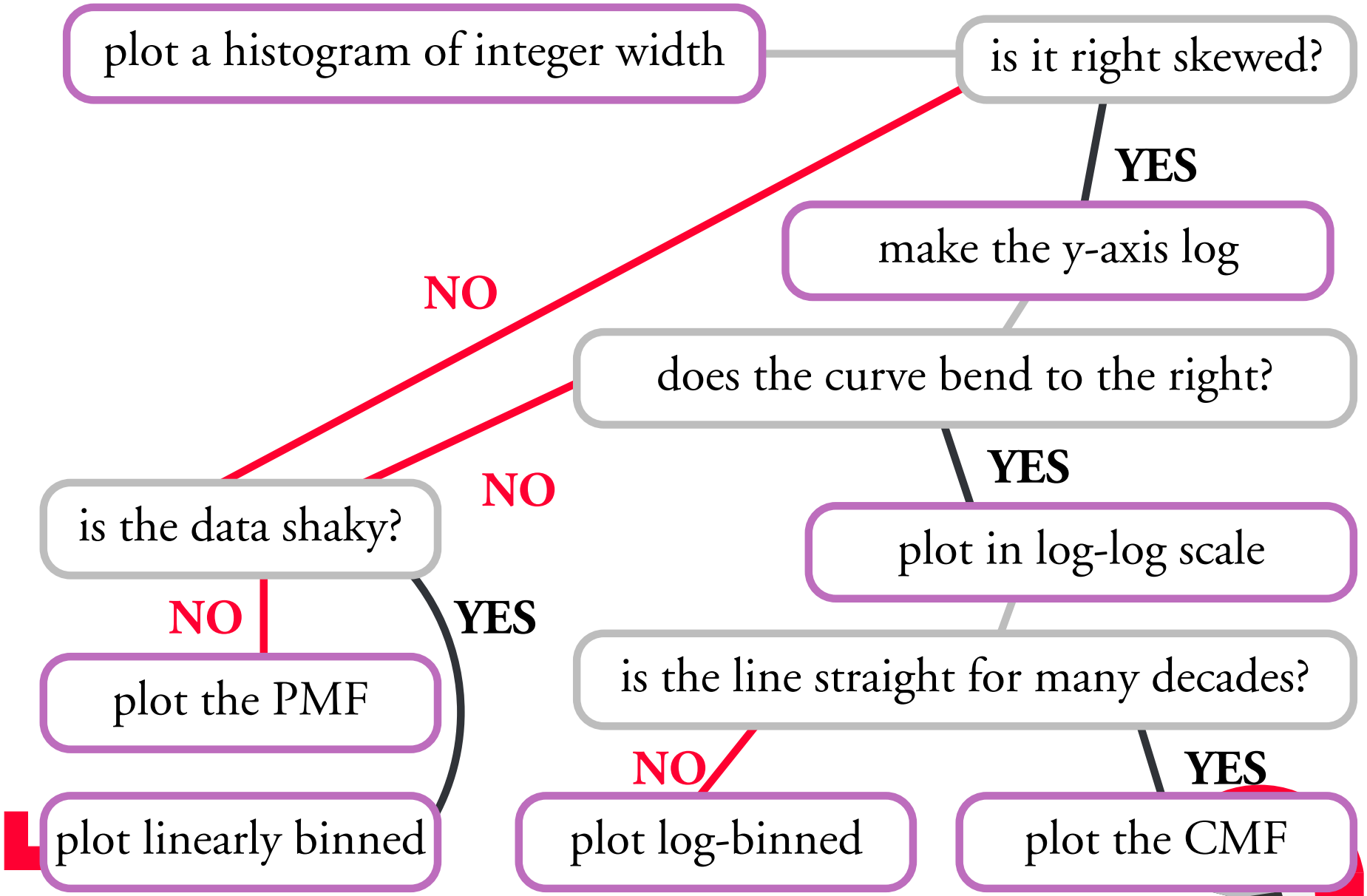






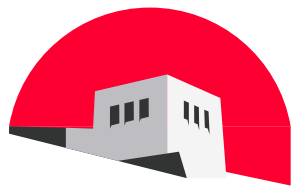


plotting degree distributions



assortative mixing coefficient

Are high-degree vertices connected to other high-degree vertices? Or are they vertices primarily connected to low-degree vertices.



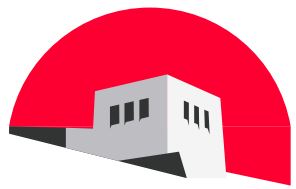
assortative mixing coefficient

Are high-degree vertices connected to other high-degree vertices? Or are they vertices primarily connected to low-degree vertices.

The **assortative mixing coefficient**:

$$r = \frac{4\langle k_1\, k_2\rangle - \langle k_1 + k_2\rangle^2}{2\langle k_1^2 + k_2^2\rangle - \langle k_1 + k_2\rangle^2}$$

where k_i is the degree of the i'th argument of the edges as they appear in an enumeration of the edges.



assortative mixing coefficient

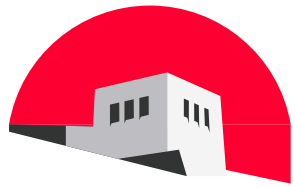
Are high-degree vertices connected to other high-degree vertices? Or are they vertices primarily connected to low-degree vertices.

The **assortative mixing coefficient**:

$$r = \frac{4\langle k_1\, k_2\rangle - \langle k_1 + k_2\rangle^2}{2\langle k_1^2 + k_2^2\rangle - \langle k_1 + k_2\rangle^2}$$

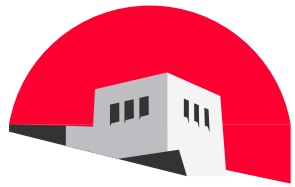
where k_i is the degree of the i'th argument of the edges as they appear in an enumeration of the edges.

In the SSCB name network: $r = 0.023$. In the null-model: $r = -0.23$.



clustering coefficient

How many triangles are there in the network?

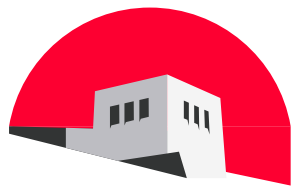


clustering coefficient

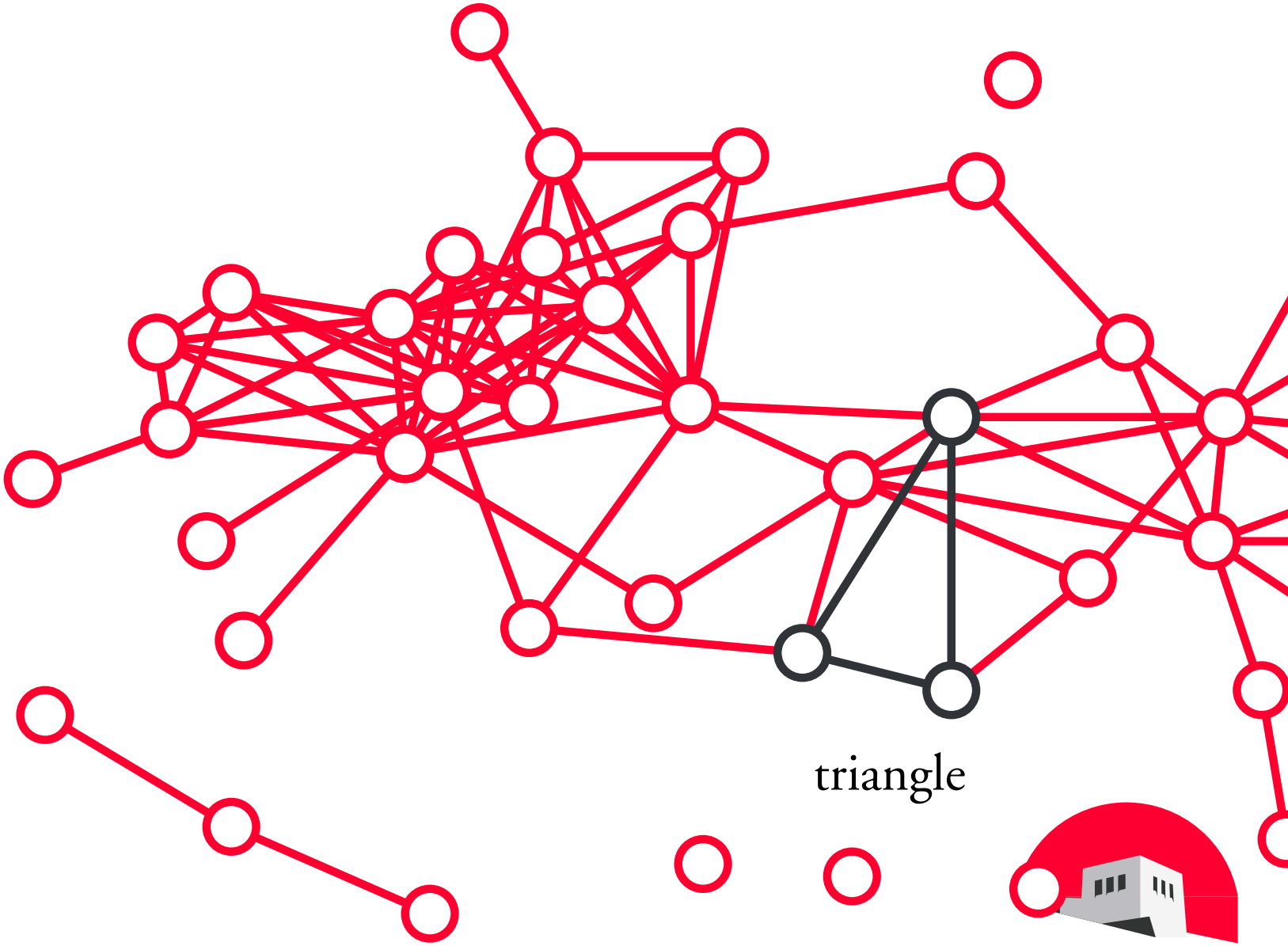
How many triangles are there in the network?

The **clustering coefficient**:

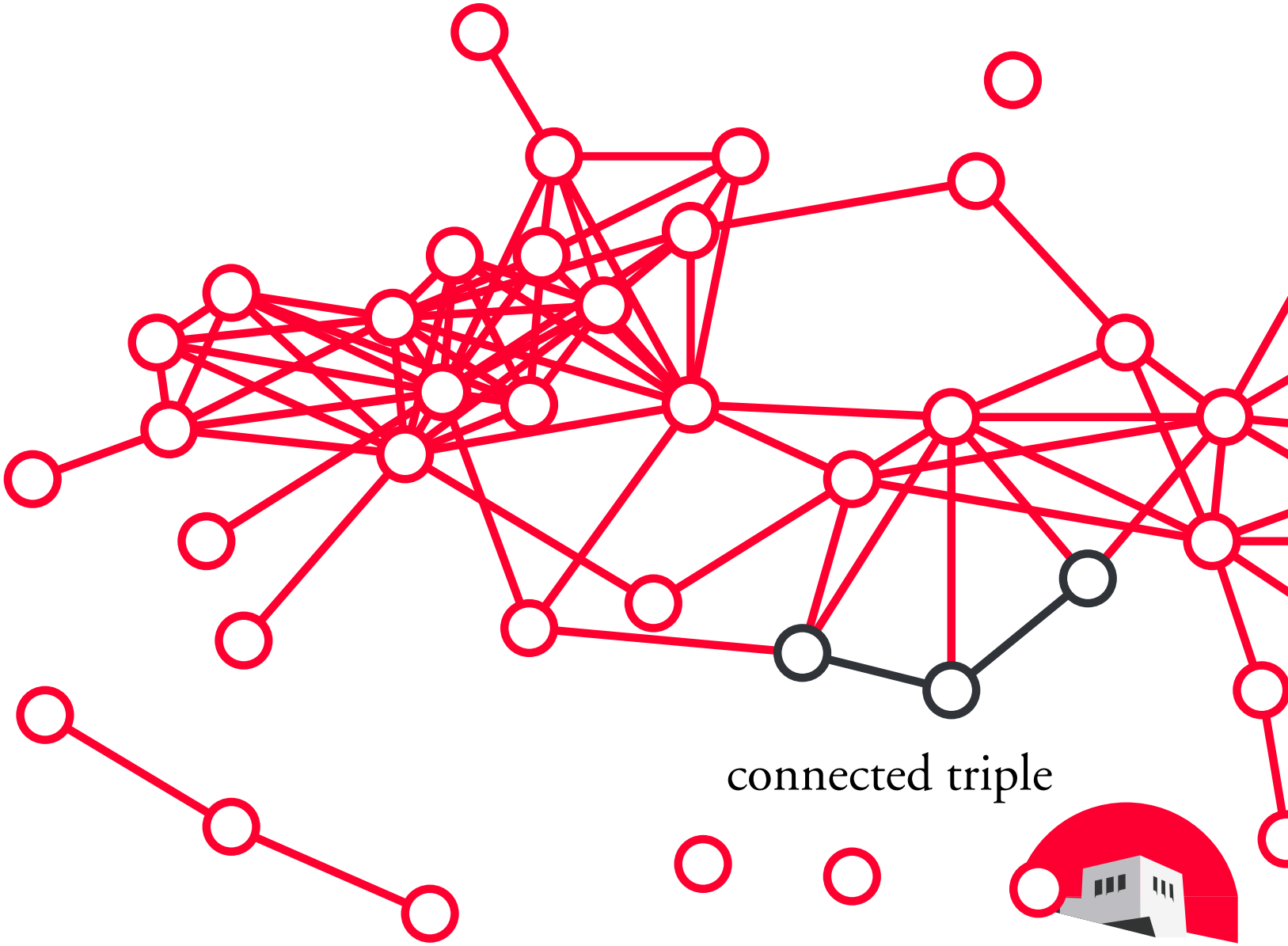
$$C = \frac{\text{the number of triangles}}{3 \times \text{the number of connected triples of vertices}}$$



clustering coefficient



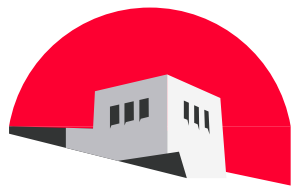
clustering coefficient



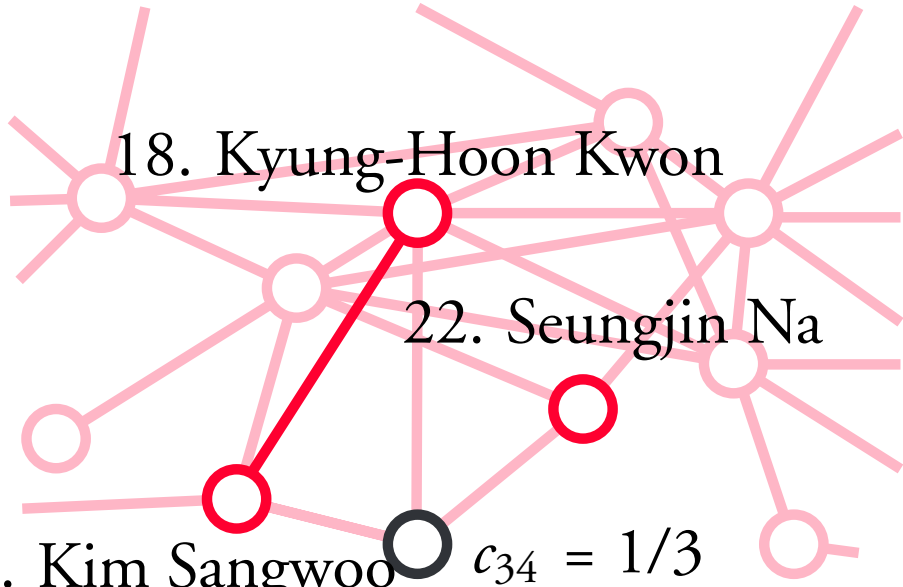
clustering coefficient

Clustering coefficient for the SSCB name network: $C = 0.51$. In the null-model: $C = 0.23$.

The SSCB name network have high clustering and positive assortative mixing coefficient—the same as many social networks.

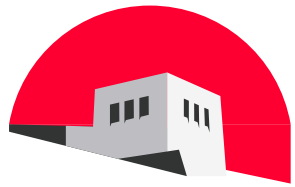


local clustering coefficient



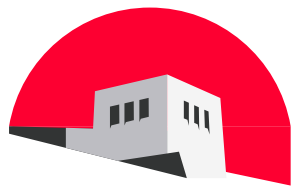
$c_{34} = 1/3$

$$c_i = (\#\text{ edges in neighborhood of } i) / \frac{k_i}{2}$$



centrality measures

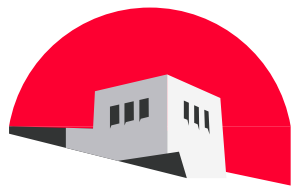
Closeness centrality: $C_C(i)$ The reciprocal average distance from i to all other vertices.



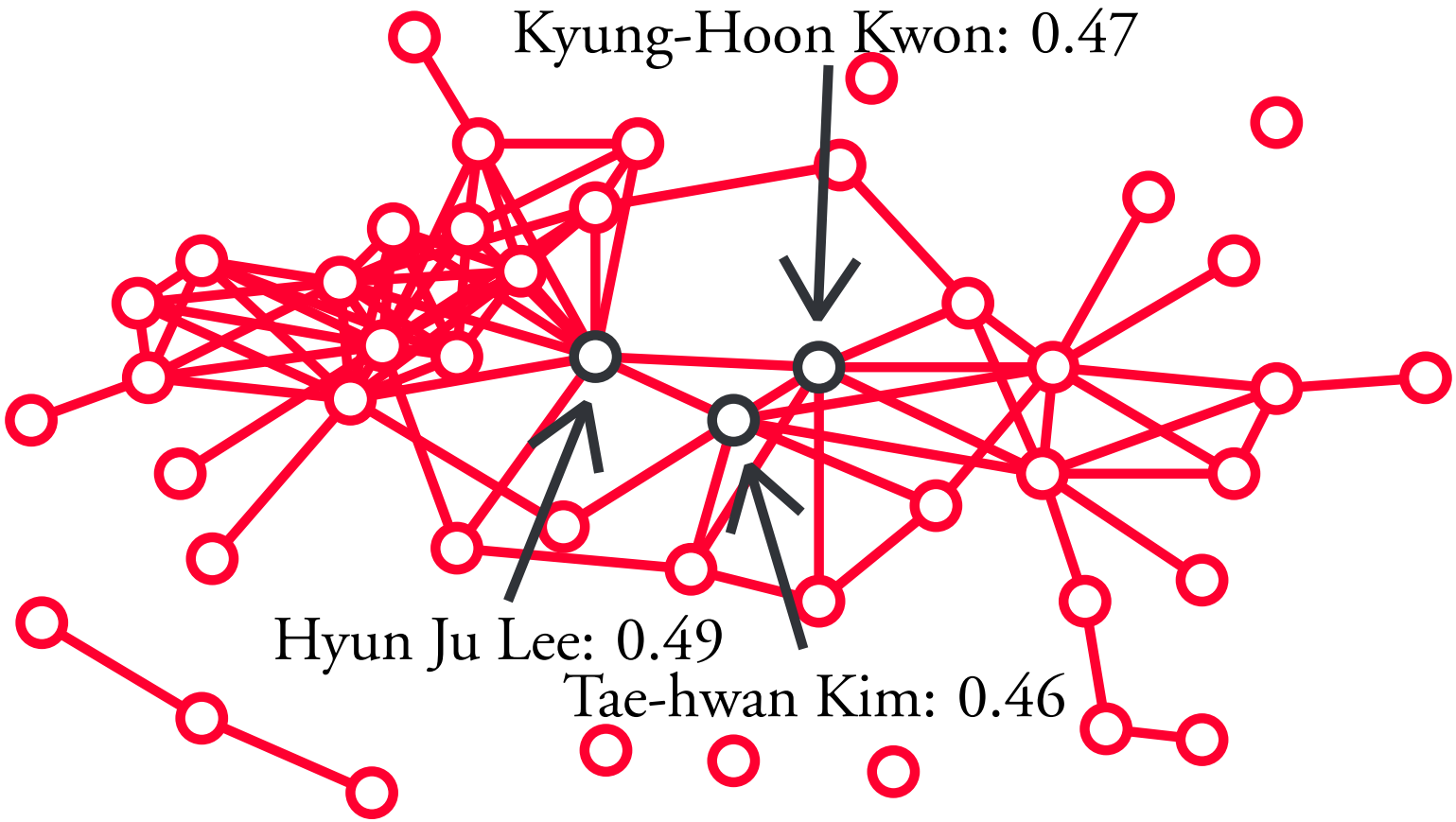
centrality measures

Closeness centrality: $C_C(i)$ The reciprocal average distance from i to all other vertices.

Betweenness centrality: $C_B(i)$ The number of shortest paths between pairs of vertices in the network passing through i.



closeness



betweenness