Large-scale structure of complex networks (Part 1)

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Networks/Graphs



- Points connected by lines
- ▶ Points: nodes/vertices/actors

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▶ Lines: links/edges/ties

- ▶ Social: Facebook, Friendships, Scientific collaborations
- ▶ **Biological**: Human brain, Metabolic reactions
- ▶ Technological: Internet, World-Wide-Web
- ▶ Transport: Airports-Air routes, Cities-Highways

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What are the nodes?

What are the links?

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Is this a network?



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Is this a network?



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Is this a network?



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▶ Sparse data



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- Sparse data
- ► Lack of regularity

- Sparse data
- Lack of regularity
- ▶ Lack of a better model

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Adjacency matrix

Adjacency matrix: Binary matrix of size $N\times N$

$$A_{ij} = \begin{cases} 1 & i \text{ and } j \text{ connected} \\ 0 & i \text{ and } j \text{ not connected} \end{cases}$$



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Degree

Degree of a vertex:

$$k_i = \sum_j A_{ij}$$

Average degree of the network:

$$\langle k \rangle = \frac{1}{N} \sum_{i} k_i$$



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▶ Complex: Edge of order and randomness

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▶ Complex: Edge of order and randomness

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Structure vs Processes

- ▶ Spreading of epidemics, rumors, ideas
- ► Traffic
- ▶ Neuronal dynamics

▶ Complex: Edge of order and randomness

Structure vs Processes

- ▶ Spreading of epidemics, rumors, ideas
- ► Traffic
- ▶ Neuronal dynamics

Structure is intersting on its own!

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Simplifications



- ► Simple
- ► Undirected
- ► Unweighted

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► Static

Large-scale structure of complex networks

Small-scale structures:

- ► degree
- local clustering
- centrality scores

Meso-scale structures:

- motifs
- vertex similarity
- rich-club effect

► Large-scale structures:

components and percolation

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- small-world effect
- ranking
- degree distribution
- assortative mixing
- community structure

Degree-distrbution



Total 10 vertices

 $p_1 = \frac{3}{10}$ $p_2 = \frac{2}{10}$ $p_3 = \frac{2}{10}$ $p_4 = \frac{2}{10}$ $p_5 = \frac{1}{10}$

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Degree distribution



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Metabolic network of the worm C-elegans



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Degree distribution of the real world networks



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Degree distribution of the real-world networks



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Power-laws and scale-free networks



$$\ln p(k) = -\alpha \ln k + c$$
$$p(k) = Ck^{-\alpha} \quad \forall k > k_{\min}$$

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How do we know that a given distribution is a power-law? (For $k > k_{\min}$)

Creating a log-log plot



Power-law is tricky!



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- ▶ Logarthmic binning: next bin is fixed multiple wider than the previous one
- Better but still noisy



Cumulative distribution

$$P(k) = \sum_{k'=k}^{\infty} p(k')$$

$$P(k) = C \sum_{k'=k}^{\infty} k'^{-\alpha} \approx C \int_{k}^{\infty} k'^{-\alpha} dk' = \frac{C}{\alpha - 1} k^{-(\alpha - 1)}$$

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A portion of the internet 1



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¹Taken from the website of Mark Newman

Calculation of the scaling exponent

$$\alpha = 1 + \frac{N}{\left[\sum_{i} \frac{k_i}{k_{\min} - \frac{1}{2}}\right]}$$

Statistical error on α

$$\sigma = \frac{\alpha - 1}{\sqrt{N}}$$

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Validating power-laws

"Power-law distributions in empirical data." Clauset, Shalizi, and Newman. SIAM review 51.4 (2009): 661-703.

Assortative mixing

Assortative mixing

Social network of school-children with two races: Black and White



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Assortative mixing

► Social networks: race, age, physical locations, language, income, educational level

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- Citation networks: topics of the study
- World Wide Web: contents of the webpages
- Internet: physical locations
Assortative mixing by enumerative characteristics

- Characteristics with a finite set of values
- ► No ordering
- ▶ Nationality, Gender, Race

Assortative mixing by scalar characteristics

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- ▶ Characteristics with a finite or infinite set of values
- Ordering
- ▶ Age, income, degree

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The network is **assortative** if a large fraction of the edges fall between vertices of the same type

If the opposite is true, the network is called **dissortative**

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▶ Fraction of edges connecting vertices of the same type?

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- Maximize: Actual number of edges between the same type minus the number of expected edges between the same types

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- ▶ Fraction of edges connecting vertices of the same type?
- Maximize: Actual number of edges between the same type minus the number of expected edges between the same types

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▶ Has value 0 in trivial cases

Number of edges between the same types

 c_i : the class or type of vertex i

 n_c : total number of types

Total number of edges between the vertices of the same type:

$$\sum_{\text{edges}(i,j)} \delta(i,j) = \frac{1}{2} \sum_{i,j} A_{ij} \delta(c_i, c_j)$$

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Expected number of edges between the same types

- ▶ Half-edges or stubs, degrees preserved
- ▶ For a given stub at vertex i, there are 2m 1 stubs to which it can connect to
- Probability of connecting vertex j is $\frac{k_j}{2m}$
- Expected number of edges between *i* and *j* is $\frac{k_i k_j}{2m-1}$
- Expected number of edges between all the pairs of the same type:

$$\frac{1}{2}\sum_{ij}\frac{k_ik_j}{2m}\delta(c_i,c_j)$$

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$$\frac{1}{2}\sum_{i,j}A_{ij}\delta(c_i, c_j) - \frac{1}{2}\sum_{ij}\frac{k_ik_j}{2m}\delta(c_i, c_j) = \frac{1}{2}\sum_{ij}\left(A_{ij} - \frac{k_ik_j}{2m}\right)\delta(c_i, c_j)$$

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$$\frac{1}{2}\sum_{i,j}A_{ij}\delta(c_i, c_j) - \frac{1}{2}\sum_{ij}\frac{k_ik_j}{2m}\delta(c_i, c_j) = \frac{1}{2}\sum_{ij}\left(A_{ij} - \frac{k_ik_j}{2m}\right)\delta(c_i, c_j)$$

$$Q = \frac{1}{2m} \sum_{ij} \left(A_{ij} - \frac{k_i k_j}{2m} \right) \delta(c_i, c_j)$$

Q is called the **modularity** of the network w.r.t. to c

$$B_{ij} = A_{ij} - \frac{k_i k_j}{2m}$$

Normalized modularity

Modularity is not 1 even for a perfectly mixed network.

Normalized modularity

Modularity is not 1 even for a perfectly mixed network.

$$Q_{\max} = \frac{1}{2m} \left(2m - \sum_{ij} \frac{k_i k_j}{2m} \delta(c_i, c_j) \right)$$

Normalized modularity

Modularity is not 1 even for a perfectly mixed network.

$$Q_{\max} = \frac{1}{2m} \left(2m - \sum_{ij} \frac{k_i k_j}{2m} \delta(c_i, c_j) \right)$$



Quantification for scalar characteristics

 x_i : a scalar value for vertex i

$$r = \frac{\sum_{ij} (A_{ij} - k_i k_j/2m) x_i x_j}{\sum_{ij} (k_i \delta_{ij} - k_i k_j/2m) x_i x_j}$$

Degree-correlations/Degree-assortativity

- ▶ Using degree itself as a scalar property of the nodes
- Degree is the property of the network structure
- One property (degree) dictating the others (position of the edges)

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Network	n	r
Physics coauthorship (a)	52 909	0.363
Biology coauthorship (a)	1 520 251	0.127
Mathematics coauthorship (b)	253 339	0.120
Film actor collaborations (c)	449913	0.208
Company directors (d)	7 673	0.276
Internet (e)	10697	-0.189
World-Wide Web (f)	269 504	-0.065
Protein interactions (g)	2115	-0.156
Neural network (h)	307	-0.163
Marine food web (i)	134	-0.247
Freshwater food web (j)	92	-0.276

²Newman, M.E.J., Assortative Mixing in Networks, PRL, 89, 20. \mathbb{R}

Random graph models

- Better way to describe the structure of the networks
- ▶ Generative models of networks
- ▶ Probabilistic models capable of generating an observed data

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▶ Certain properties can be fixed for generative models





- Mean of x = 9
- Variance of x = 11
- Mean of y = 7.5
- Variance of y = 4.125
- Correlation = 0.816

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Anscombe's quartet!

Random graph models (RGMs)

- Erdős-Rényi model
- Configuration model
- Stochastic-block model
- ▶ Degree-corrected SBM
- Equitable random graphs
- Hierarchical block models
- ▶ Random graphs with expected degrees

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- Microcanonical SBM
- Poisson SBM

Erdős-Rényi model (ER model/G(n, p))

- Fix n and the average degree c
- Connect every pair of nodes with a probability $p = \frac{c}{n-1}$
- Number of graphs in the ensemble: $2^{\binom{n}{2}}$
- ▶ ER model: Every member of the ensemble is equally likely



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Properties of the ER model

Average properties of the ensemble

$$=\sum_{G}P(G)m(G)=\frac{1}{\Omega}\sum_{G}m(G)$$

Properties of the ER model

Degree distribution

- Given vertex can connect to remaining n-1 vertices
- Probability of connecting to particular k vertices:

$$p^k(1-p)^{n-1-k}$$

• There are $\binom{n-1}{k}$ ways to choose k vertices

$$p_k = \binom{n-1}{k} p^k (1-p)^{n-1-k} = e^{-c} \frac{c^k}{k!}$$

The giant component



What is the size of the largest component?

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The giant component

- Giant component: size is an extensive function of the network size
- Transition between the two extremes with p: gradual or sudden?
- Size of the giant component as a function of p can be calculated exactly in the limit

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 \boldsymbol{u} : Fraction of vertices not in the giant component

When is a vertex i not in the giant component?

For any other vertex j:

- 1. i is not connected to j
- 2. i is connected to j but j is not in the giant component

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The giant component

 \boldsymbol{u} : Fraction of vertices not in the giant component

When is a vertex i not in the giant component?

For any other vertex j:

- 1. *i* is not connected to $j \Rightarrow$ **probability** = 1 p
- 2. *i* is connected to *j* but *j* is not in the giant component \Rightarrow **probability** = *pu*

Thus, the probability of not being connected to the giant component through vertex j is (1 - p + pu)

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$$u = (1 - p + pu)^{n-1}$$

$$u = \left(1 - \frac{c}{n-1} + p\frac{c}{n-1}\right)^{n-1} = \left[1 - \frac{c}{n-1}(1-u)\right]^{n-1}$$
$$u = e^{-c(1-u)}$$

Let S be the size of the giant component

$$\therefore 1 - S = e^{-cS}$$

Graphical solution for the giant component



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$$\left.\frac{d}{dS}(1-e^{-cS})\right|_{S=0} = 1$$

$$\therefore c e^{-cS}\Big|_{S=0} = 1$$

$$\therefore c = 1$$

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c < 1 and c > 1



Network science researchers



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Small components



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Two giant components?

Distinct pairs (i, j) with i in S_1 and j in S_2 : $S_1n \times S_2n = S_1S_2n^2$

Probability that there is no edge between the two:

$$q = (1-p)^{S_1 S_2 n^2} = \left(1 - \frac{c}{n-1}\right)^{S_1 S_2 n^2} \sim e^{-cS_1 S_2 n}$$

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Sizes of the small components

π_s : probability that a randomly chosen vertex belongs to component of size s

$$\sum_{s=1}^{\infty} = 1 - S$$

Small-components are trees!

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Tree graph



- ► A graph without loops
- ▶ n vertices and n-1 edges
- Removal of any vertex or edge witll disconnect the graph

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Small components

Small components are trees

$$\binom{s}{2} - (s-1) = \frac{1}{2}(s-1)(s-2)$$

The total number of extra edges:

$$\frac{1}{2}(s-1)(s-2)\frac{c}{n-1} \to 0$$

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For degree 3 vertex,

$$P(s|k=3) = \pi_{s_1}\pi_{s_2}\pi_{s_3}$$
$$s_1 + s_2 + s_3 = s - 1$$

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For degree 3 vertex,

$$P(s|k=3) = \pi_{s_1}\pi_{s_2}\pi_{s_3}$$
$$s_1 + s_2 + s_3 = s - 1$$
$$P(s|k) = \sum_{s_1=0}^{\infty} \sum_{s_2=0}^{\infty} \cdots \sum_{s_k=0}^{\infty} \left[\prod_{j=1}^k \pi_{s_j}\right] \delta(s-1, \sum_j s_j)$$

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For degree 3 vertex,

$$P(s|k = 3) = \pi_{s_1} \pi_{s_2} \pi_{s_3}$$

$$s_1 + s_2 + s_3 = s - 1$$

$$P(s|k) = \sum_{s_1=0}^{\infty} \sum_{s_2=0}^{\infty} \cdots \sum_{s_k=0}^{\infty} \left[\prod_{j=1}^k \pi_{s_j} \right] \delta(s - 1, \sum_j s_j)$$

$$\pi_s = \sum_{k=0}^{\infty} p_k P(s|k)$$

$$< s >= \sum_{s=0}^{\infty} s \pi_s$$

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$$< s >= \frac{1}{1-c+cS}$$

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$$\langle s \rangle = \frac{1}{1 - c + cS}$$

$$R = \frac{2}{2 - c + cS}$$

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$$< s >= \frac{1}{1 - c + cS}$$

$$R = \frac{2}{2 - c + cS}$$

$$R = \frac{2}{2 - c + cS}$$

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- ▶ Model with a given degree sequence
- ▶ More realistic and more flexible
- Can be solved exactly in the limit

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• Specify
$$k_i$$
 for $i = 1, 2, \cdots, n$

 Every vertex i has k_i half-edges/stubs

•
$$\sum_{i} k_i = 2m$$

- Randomly connect stubs to each other
- Every matching appears with equal probability



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Do all graphs appear with equal probability?

Do all graphs appear with equal probability?

More than one matchings can correspond to the same graph



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Number of matchings for the network N: $N(\{k_i\}) = \prod_i k_i!$

Thus, networks do occur with equal probability!

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$$N = \frac{\prod_i k_i!}{\prod_{i < j} A_{ij}! \prod_i A_{ii}!!}$$

$$n!! = n(n-2)(n-4)\cdots 2$$

Graphs do not appear with equal probability!

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Summary

- ▶ Many real networks have fat-tailed degree distributions
- ▶ Naturally occuring networks tend be dissortative by degree
- ▶ Social networks tend to be assortative by degree
- Random graphs provide a powerful way to describe the large-scale structure of complex networks

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