Algorithm Foundations of Data Science

Lecture 3: Graph and Patterns

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Mar. 28, 2018

Outline

- Graph
 - Motivations
 - Patterns
- ② Graph Concepts
 - Graph types
 - Properties
 - Graph Modeling
- Network Generation

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- 3 Network Generation



Graphs - why should we care?











Networks in real world

- "YahooWeb graph": 1B vertices(Web sites), 6B edges (http links)
- Facebook, Twitter, etc: more than 1B users
- Food Web: all biologies, food chain
- Power-grid: vertices (plants or consumers), edges (power lines)
- Airline route: vertices (airports), edges (flights)
- Adoption: users purchase products, adopt services, etc.

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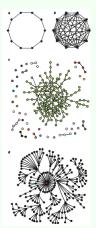
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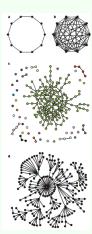
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- How to generate realistic graphs?
- How to get a "good" sample of a network?
- How to design an efficient algorithm to handle large-scale graphs?

Mar. 28, 2018

Steven H. S. proposes the model for complex networks in Nature 2001.

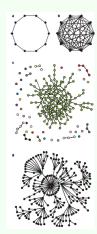


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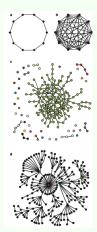
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- Regular network: each node has exactly the same number of edges.
- Random network: it is obtained by starting with a set of n isolated vertices and adding successive edges between them at random.
- Scale-free network: it grows via attaching new nodes to previously existing nodes randomly, while the probability is proportional to the degree of the target node, i.e., richly connected nodes tend to get richer, leading to the formation of hubs and a skewed degree distribution with a heavy tail. (Matthew Effect or Pareto's Law)

Are real graphs random?



Are real graphs random?



Looks random - right?
How does the Internet look like? Any rules?

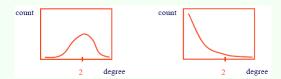
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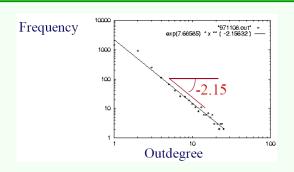
- Diameter: would you like to guess?
- In- and out- degree distributions: if average degree is 2, what is the most probable degree?
- Other (surprising) patterns?



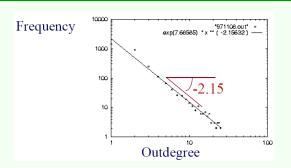
Outline

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- ② Graph Concepts
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Power-law I



Power-law I



Internet topology

- Out-degree distribution is plotted in log-log scale.
- It forms a line with a slope ~ -2.15
- $freq. = deg.^{-2.15}$



Due to Matthew effect, Pareto's law, "rich-get-richer", or the 80/20 principle, there are many settings with power law (Zipf's law).

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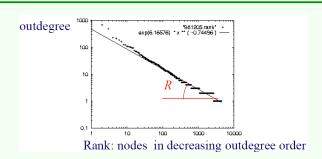
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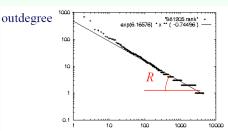
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- Business
 - 80% of a company's profits come from 20% of customers.
 - 80% of a company's complaints come from 20% of customers.
 - 80% of a company's profits come from 20% of the time staff spent
 - 80% of a company's sales are made by 20% of sales staff

Power-law II



Power-law II

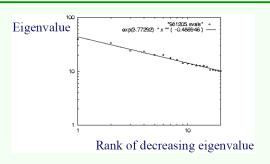


Rank: nodes in decreasing outdegree order

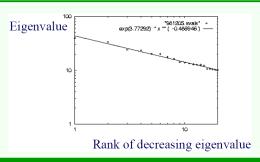
Rank of out-degrees

- Vertices are ranked in decreasing out-degree order, and plotted in log-log scale.
- It forms a line with a slope ~ -0.74
- $deg. = rank^{-0.74}$

Power-law III



Power-law III

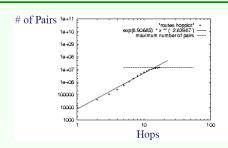


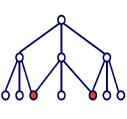
Rank of eigenvalues

- Eigenvalues of adjacency matrix (top 20) are ranked in decreasing order, and plotted in log-log scale.
- It forms a line with a slope ~ -0.48
- eigen. = $rank^{-0.48}$

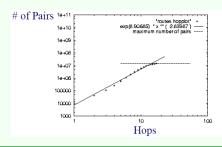
Patterns

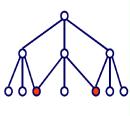
Power-law IV





Power-law IV

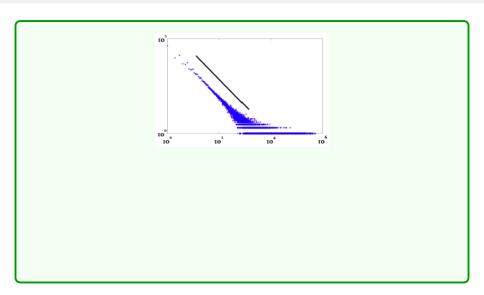




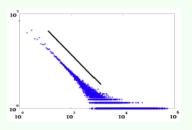
Hop plot

- How many neighbors within $1, 2, \dots, h$ hops? $(\sum_{i=1}^{h} avg.^{i})$
- ullet Pairs of vertices are plotted in log-log scale. It forms a line with a slope ~ 2.83
- pairs. = $hop^{2.83}$

Power-law V



Power-law V



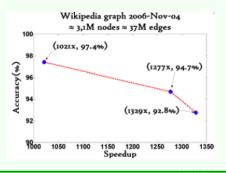
Counting of triangles

- X-axis: # of triangles a vertex participates in
- Y-axis: count of such vertices
- In log-log scale, the plot is almost linear.

Triangle law

How to count # triangles?

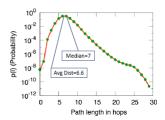
- Naive algorithm: 3-way join $(O(n^3))$.
- # triangles = $\frac{1}{6} \sum_{i=1}^{n} \lambda_i^3$. Why?
- Because of skewness, we only need the top few eigenvalues via using Lanczos algorithm.



Erdös number



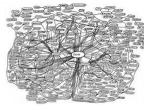


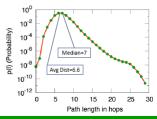


Patterns

Erdös number





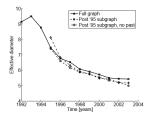


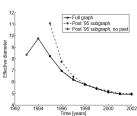
Small world - six degrees of separation

The world looks "small" when you think of how short a path of friends it takes to get from you to almost anyone else. Stanley Milgram and his colleagues in the 1960s did an experiment.

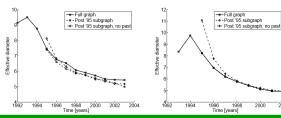
- 296 randomly chosen "starters" asked to forward a letter to a "target" person, a stockbroker in Boston's suburb.
- The six degrees of separation was also found by Jure Leskovec on Miscrosoft Instant Message.

Shrinking diameter





Shrinking diameter



Citation or patents networks

For citation network, they collected citations among Physics papers.

- 11 years data
 - 29,555 papers
 - 352,807 citations
- For each month, create a graph of all citations up to the month.
- The diameters are plotted in the figures.

Temporal evolution of graphs

Question

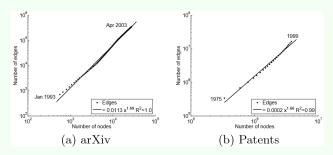
Let N(t) and E(t) be # nodes and # edges at time t, respectively. Suppose that N(t+1)=2N(t), what is your guess for E(t+1)?

Temporal evolution of graphs

Question

Let N(t) and E(t) be # nodes and # edges at time t, respectively. Suppose that N(t+1)=2N(t), what is your guess for E(t+1)?

- It is over-doubled, but obeying: $E(t) \sim N(t)^{\alpha}$ for all t, where $1 < \alpha < 2$.
- For tree (clique), $\alpha = 1$ ($\alpha = 2$).



Why primates have unusually big brains?

Social group size (and a lot of social behaviour as wel) correlates with relative neocortex volume.

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• Our relationships form a hierarchically inclusive series of circles of increasing size but decreasing intensity.

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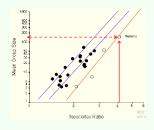
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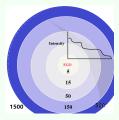
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Social group size (and a lot of social behaviour as wel) correlates with relative neocortex volume.

- Our relationships form a hierarchically inclusive series of circles of increasing size but decreasing intensity.
- 150 is the limitation on reciprocated relationships.
- 1500 is the limitation on memory for faces?



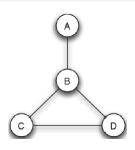


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- **Graph Concepts**
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Graph types

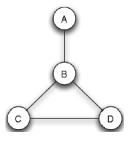


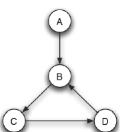
Undirected graph

A undirected graph on 4 vertices

- Degree: # edges connected to the vertex
- Degree 0 vertex: isolated vertex

Graph types





Undirected graph

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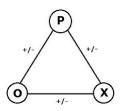
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Directed graph

A directed graph on 4 vertices

- In-degree: # incoming edges to the vertex
- Out-degree: # outgoing edges to the vertex
- Degree: in-degree + outdegree

Graph types cont.

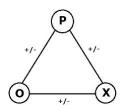


Signed graph

A signed graph on 3 vertices

- Positive-degree: # edges associated with positive labels
- Negative-degree: # edges associated with negative labels

Graph types cont.





Signed graph

A signed graph on 3 vertices

- Positive-degree: # edges associated with positive labels
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Bipartite graph

Users interact on social platforms

- Reply network
- Retweet network
- Adoption network

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Path

Path is a sequence of nodes with the property that each consecutive pair in the sequence is connected by an edge

- Simple path does not repeat nodes.
- The length of path is the number of nodes in the path



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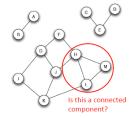
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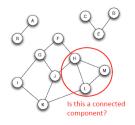
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Cycle

Cycle is a path with at least three edges, in which the first and last nodes are the same. Every edge in the 1970 Arpanet belongs to a cycle, and this was by design. Why?



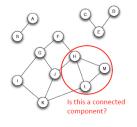




Connected component

A connected component is a subset of nodes s.t.:

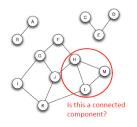
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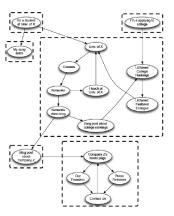


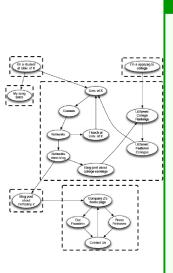
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- Every node in the subset has a path to every other; and
- The subset is not part of some larger set with the property that every node can reach every other.

A graph is connected if for every pair of nodes, there is a path between them, i.e., the whole graph is a connected component.

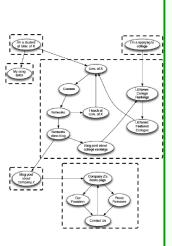




Strongly connected component

A *directed graph* is strongly connected if there is a path from every node to every other node.

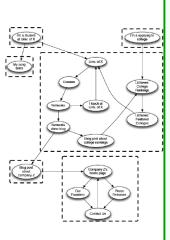
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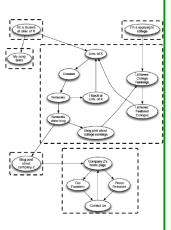
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- In a strongly connected component, there are followers and followees for each node.



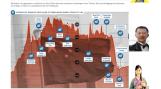
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- SCCs can be treated as super-nodes.









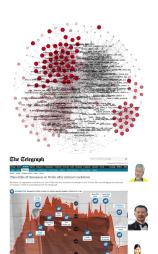
The Telegraph The Te



Giant connected component

A connected component that contains a significant fraction of all the nodes.

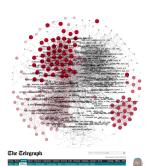
 When a network (e.g., friendship network) contains a giant component, it almost always contains only one.

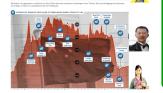


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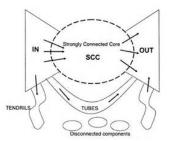


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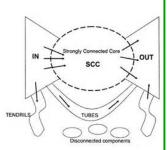
- When a network (e.g., friendship network) contains a giant component, it almost always contains only one.
- The other connected components are very small by comparison.
- The largest connected component would break apart into three distinct components if this node were removed [related to robustness of network].

Web giant component



200 M pages, 1.5 B hyperlinks

Web giant component

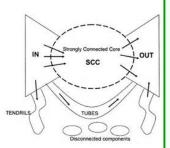


200 M pages, 1.5 B hyperlinks

Web graph

Web contains a giant strongly connected component (containing home pages of many of the major commercial, governmental, and nonprofit organizations)

Web giant component



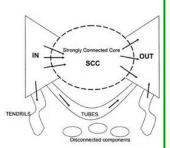
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 IN: nodes that can reach the giant SCC but cannot be reached from it, i.e., nodes that are "upstream" of it.

Web giant component

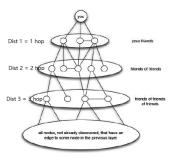


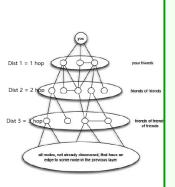
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Web graph

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- IN: nodes that can reach the giant SCC but cannot be reached from it, i.e., nodes that are "upstream" of it.
- OUT: nodes that can be reached from the giant SCC but cannot reach it, i.e., nodes are "downstream" of it.

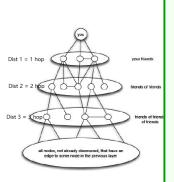




Distance or Geodesic distance

The distance between two vertices in a graph is the number of edges in a shortest path.

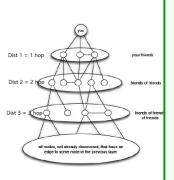
 Diameter is the length of the "longest shortest path" between any two vertices of a graph.



Distance or Geodesic distance

The distance between two vertices in a graph is the number of edges in a shortest path.

- Diameter is the length of the "longest shortest path" between any two vertices of a graph.
- Erdös number is bounded by diameter of a graph.



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- Erdös number is bounded by diameter of a graph.
- Research community is a small world [Duncan Watts and Steven Strogatz 1998].

Definition

$$L=\frac{1}{\frac{1}{2}n(n+1)}\sum_{i>j}d_{ij},$$

where n denotes # of nodes, and d_{ij} is the shortest distance between nodes i and j.

Mean Geodesic distance includes distance to itself.

Definition

$$L=\frac{1}{\frac{1}{2}n(n+1)}\sum_{i\geq j}d_{ij},$$

where n denotes # of nodes, and d_{ij} is the shortest distance between nodes i and j.

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- Mean Geodesic distance includes distance to itself.
- Can be computed in O(mn) using breadth first search, where m denotes # of edges.
- What happens if the network has multiple connected components?
- Harmonic mean (can have multiple connected components):

$$L^{-1} = \frac{1}{\frac{1}{2}n(n+1)} \sum_{i>j} d_{ij}^{-1}$$



Summarization

	network	type	n	m	z	ℓ	α	$C^{(1)}$	$C^{(2)}$	r	Ref(s).
social	film actors	undirected	449 913	25 516 482	113.43	3.48	2.3	0.20	0.78	0.208	20, 416
	company directors	undirected	7 673	55 392	14.44	4.60	_	0.59	0.88	0.276	105, 323
	math coauthorship	undirected	253 339	496 489	3.92	7.57	_	0.15	0.34	0.120	107, 182
	physics coauthorship	undirected	52 909	245 300	9.27	6.19	_	0.45	0.56	0.363	311, 313
	biology coauthorship	undirected	1520251	11 803 064	15.53	4.92	_	0.088	0.60	0.127	311, 313
	telephone call graph	undirected	47 000 000	80 000 000	3.16		2.1				8, 9
	email messages	directed	59912	86 300	1.44	4.95	1.5/2.0		0.16		136
	email address books	directed	16 881	57 029	3.38	5.22	_	0.17	0.13	0.092	321
	student relationships	undirected	573	477	1.66	16.01	_	0.005	0.001	-0.029	45
	sexual contacts	undirected	2810				3.2				265, 266
information	WWW nd.edu	directed	269 504	1497135	5.55	11.27	2.1/2.4	0.11	0.29	-0.067	14, 34
	WWW Altavista	directed	203549046	2130000000	10.46	16.18	2.1/2.7				74
	citation network	directed	783 339	6716198	8.57		3.0/-				351
	Roget's Thesaurus	directed	1 022	5 103	4.99	4.87	-	0.13	0.15	0.157	244
	word co-occurrence	undirected	460 902	17000000	70.13		2.7		0.44		119, 157
biological	Internet	undirected	10697	31 992	5.98	3.31	2.5	0.035	0.39	-0.189	86, 148
	power grid	undirected	4941	6594	2.67	18.99	_	0.10	0.080	-0.003	416
	train routes	undirected	587	19603	66.79	2.16	_		0.69	-0.033	366
	software packages	directed	1 439	1723	1.20	2.42	1.6/1.4	0.070	0.082	-0.016	318
	software classes	directed	1 377	2 213	1.61	1.51	-	0.033	0.012	-0.119	395
	electronic circuits	undirected	24097	53 248	4.34	11.05	3.0	0.010	0.030	-0.154	155
	peer-to-peer network	undirected	880	1 296	1.47	4.28	2.1	0.012	0.011	-0.366	6, 354
	metabolic network	undirected	765	3 686	9.64	2.56	2.2	0.090	0.67	-0.240	214
	protein interactions	undirected	2 115	2240	2.12	6.80	2.4	0.072	0.071	-0.156	212
	marine food web	directed	135	598	4.43	2.05	-	0.16	0.23	-0.263	204
	freshwater food web	directed	92	997	10.84	1.90	-	0.20	0.087	-0.326	272
	neural network	directed	307	2359	7.68	3.97	-	0.18	0.28	-0.226	416, 421

Outline

- - Motivations
 - Patterns
- **Graph Concepts**
 - Graph types
 - Properties
 - Graph Modeling
- Network Generation



Adjacency matrix

Definition

Given a finite graph G = (V, E), an adjacency matrix A is a $|V| \times |V|$ matrix, whose elements indicate whether pairs of vertices are adjacent or not in the graph.

- The adjacency matrix is a (0,1)-matrix with zeros on its diagonal.
- If the graph is undirected, the adjacency matrix is symmetric.

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The adjacency matrix A of a bipartite graph whose two parts have r and s vertices can be written in the form

$$A = \begin{pmatrix} 0_{r,r} & B \\ B & 0_{5,5} \end{pmatrix}.$$

- 4 ロ ト 4 回 ト 4 重 ト 4 重 ト 9 回

Storing a graph

Adjacency lists

An adjacency list is a collection of unordered lists used to represent a graph G. Each list describes the set of neighbors of a vertex in the graph.

1	2	1	4			1	2	-1	
1	11	0	2			3	4	1	
1	10	1	3	5		5	6	-1	
2	3	2	4	5		7	8	-1	
3	4	0	3			7	9	-1	
4	5	2	3	6	8	10	11	1	
5	6	5	7			12	13	1	
5	8	6	8			14	15	1	
5	11	5	7			16	17	1	
(a	a)		(k)		(c)			

Markov chain

Suppose that G = (V, E) is a graph of n vertices with vertex set V and edge set $E \subset V \times V$. Let $N(x) = \{y | (x, y) \in E\}$, and degree of vertex x denote as d(x) = |N(x)|.

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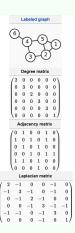
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For each $x \in V$, the transition matrix P(y|x) is $\frac{1}{d(x)}$ if $y \in N(x)$, and P(y|x) = 0 otherwise.

- Let X be a random walk on G, if G is connected then X is irreducible
- X has period 2 if and only if G is bipartite, in which case the parts are the cyclic classes of X.
- Let $D = diag(d_1, d_2, \dots, d_n)$ be a diagonal matrix, and $P = D^{-1}A$.

Definition Labeled graph

Definition



Given a graph G, (Combinatorial) Laplacian of G:

$$L = D - A$$
, i.e.,
$$L(u, v) = \begin{cases} d_v, & \text{if } u = v; \\ -1, & \text{if } u \text{ and } v \text{ are adjacent }; \\ 0, & \text{otherwise.} \end{cases}$$

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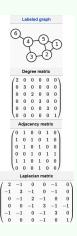
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If G is an undirected graph G, and its Laplacian matrix L with eigenvalues $\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$, then

• *L* is singular and symmetric(existing $\lambda_i = 0$).

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Definition

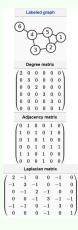


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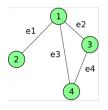
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- The second smallest eigenvalue is called algebraic connectivity.
- For weighted graph G, Laplacian can be defined in a same manner.

Incidence matrix

Definition

An incidence matrix B is a $|V| \times |E|$ matrix that shows the relationship between vertices and edges of graph G = (V, E).



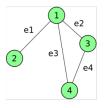
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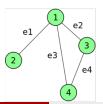
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- Each column corresponds to an edge $e = (v_i, v_j)$ (with i < j), where the value of an entry is 1 in the row corresponding to v_i , and entry -1 in the row corresponding to v_j .
- $L = BB^T$. Thus, L is positive semidefinite and has nonnegative eigenvalues since $\mathbf{x}^T L \mathbf{x} = \mathbf{x}^T BB^T \mathbf{x} = (B^T \mathbf{x})^T (B^T \mathbf{x}) \geq 0$ $(\lambda_i \geq 0)$.



$$\begin{pmatrix} 1 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{pmatrix}$$

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- P has an eigenvalue $1 \lambda_i$, where λ_i is an eigenvalue of \mathcal{L} .
- The regularization of graph G: $F^T \mathcal{L}F = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \left(\frac{f_i}{\sqrt{d_{ii}}} \frac{f_j}{\sqrt{d_{ij}}} \right)^2.$

Properties of normalized Laplacian [WebScience 2013]

Properties

The eigenvalues of the normalized Laplacian matrix of graph G with n vertices satisfy the following properties:

- $0 \le \lambda_2 \le \frac{n}{n-1} \le \lambda_n \le 2$.
- $\lambda_2 = \cdots = \lambda_n = \frac{n}{n-1}$ if and only if G is a clique.
- $\lambda_n = 2$ if and only if G is a bi-clique.
- G has at least i connected components if and only if $\lambda_j = 0$, for $j = 1, 2, \dots, i$.
- The mean of eigenvalues $\lambda_2, \lambda_3, \dots, \lambda_n$ of a network G with n vertices is $\frac{n}{n-1}$.
- The variance of eigenvalues $\lambda_2, \lambda_3, \dots, \lambda_n$ of a network G with n vertices is $\frac{1}{n-1} \sum_{i=1}^n \sum_{j \neq i}^n \frac{A_{ij}}{d(v_i)d(v_j)} \frac{n}{(n-1)^2}$ (R-energy).



Network generation

Generators

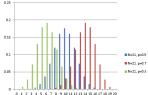
- Erdös-Renyi model
- Preferential attachment
- Variations + extensions
 - Copying model
 - Triad-closing
 - Butterfly model
- Recursion Kronecker generator



Random network generator: Erdös-Renyi model

Erdös-Renyi model is known as the random graph model, which generates undirected random graphs.

- Parameters: N (# vertices) and p (prob. of forming an edge)
- For each possible node pair, the approach generates an edge with probability p. Thus, # edges $=\frac{pN(N-1)}{2}$.
- Degree distribution:
 - $P(\text{node has degree k}) = \binom{N-1}{k} p^k (1-p)^{N-1-k}$
 - Follows binomial distribution with mean (N-1)p and variance (N-1)p(1-p) (not power-law distribution).



Scale-free network generator

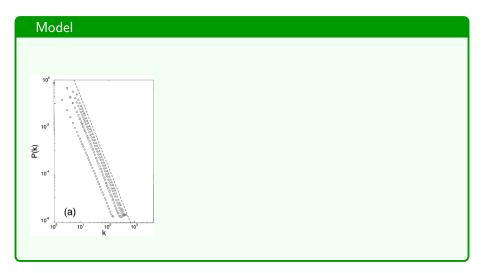
Preferential attachment model

The more connected a node is, the more likely it is to receive new links (namely, Rich gets Richer, Matthew Effect or Paretos Law, etc.).

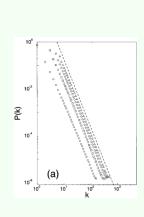
- Price model
- Barabasi Albert model

Price model for citation networks

- Each new paper is generated with m citations (mean).
- New papers cite previous papers with probability proportional to their indegree (citations).
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 - Power law with exponent $\alpha = 2 + \frac{1}{m}$ [Science 1965]

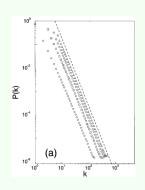






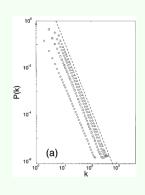
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- For each new node, connect it to m existing nodes i with a probability p_i , where $p_i = \frac{k_i}{\sum_j k_j}$, where k_i is degree of node i.
- Results in a single connected component with power-law degree distribution with $\alpha=3$ [Reviews of Modern Physics 2003].

$$S = U \bigotimes V = \begin{pmatrix} u_{11}V & u_{12}V & \cdots & u_{1m}V \\ u_{21}V & u_{22}V & \cdots & u_{2m}V \\ \cdots & \cdots & \cdots \\ u_{n1}V & u_{n2}V & \cdots & u_{nm}V \end{pmatrix}$$

Given two matrices $U \in \mathbb{R}^{n \times m}$ and $V \in \mathbb{R}^{p \times q}$, the Kronecker product matrix $S \in \mathbb{R}^{np \times mq}$ is given by

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- $|A \bigotimes B| = |A|^m |B|^n$ and $Tr(A \bigotimes B) = Tr(A) Tr(B)$ if $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{m \times m}$.

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- We define k-th Kronecker power of A_1 as $A_1^{[k]}$ (abbreviated to A_k), where $A_k = A_1^{[k]} = A_{k-1} \bigotimes A_1$.

Kronecker model cont.

Model

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Kronecker model cont.

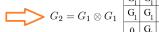
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Instead of a single property of the network, Kronecker model can fit multiple properties of a network, which makes them interesting for fitting.

- Deterministic Kronecker model: it begins with an initiator graph G_1 with N_1 nodes, and produces successively larger graphs G_2, \dots, G_n such that the k-th graph G_k has $N_k = N_1^k$.
- Stochastic Kronecker model: it starts with a $N_1 \times N_1$ probability matrix $\Theta = [\theta_{ij}]$, where the element $\theta_{ij} \in [0,1]$ is the probability that edge (i,j) is present.

1	1	0
1	1	1
0	1	1









Sources for generator

Generators

- Erdös Renyi: http://ladamic.com/netlearn/NetLogo501/ ErdosRenyiDegDist.html
- BRITE: http://wwwcsbuedu/brite/
- INET: http://topology.eecs.umich.edu/inet
- Kronecker:
 - christos@cs.cmu.edu
 - http://www.cc.gatech.edu/dimacs10/archive/ kronecker.shtml
 - http://www.cc.gatech.edu/dimacs10/archive/ kronecker.shtml

Take-home messages

- Graph
 - Motivations
 - Patterns
- Graph aspects
 - Graph types
 - Properties
 - Graph modeling
- Network generation
 - Erdös Renyi model
 - Barabasi Albert model
 - Kronecker model

