Artificial Intelligence: Search & Mining

2015 人工知能:探索とマイニング

Graph Mining

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2015-06-02

Today's Agenda

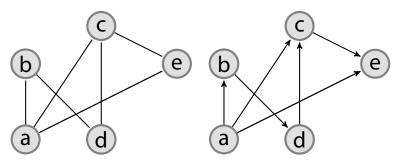
Graph Data

Properties of Graphs

Community Detection

Graph data

Graph G = (Vertices V, Edges E) Edges may be weighted, undirected or directed.



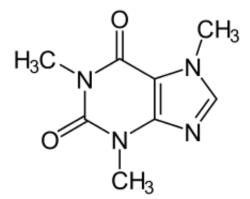


Figure : Chemical structure of caffeine

http://en.wikipedia.org/wiki/Caffeine#mediaviewer/File:Koffein_-_Caffeine.svg

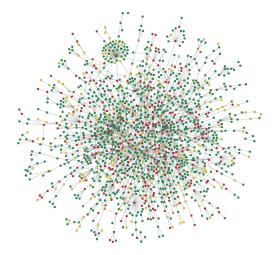


Figure : Yeast protein interaction network

http://www.nature.com/nature/journal/v411/n6833/full/411041a0.html

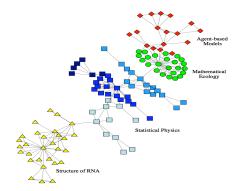


Figure : Collaboration graph among researchers

http://www.pnas.org/content/99/12/7821.full



Figure : Facebook Friendship Graph

https:

//www.facebook.com/notes/facebook-engineering/visualizing-friendships/469716398919

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Graph mining questions we might ask

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- Drug design
 - What are frequent sub-structures in a chemical database?
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- Biology research
 - What are the central proteins in a metabolic pathway, if any?
- Social network analysis
 - Does there exist distinct communities?
 - How do links form?
 - How do messages get disseminated?
- ► etc.

Tools/Concepts for answering graph mining questions

- Community Detection
- Graph Clustering
- Centrality Analysis, e.g. PageRank
- Link Prediction
- Frequent sub-graph mining
- Information diffusion on graphs
- ► Graph evolution, etc.

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- Small-World Phenomenon: 6 degrees of separation between any two people (Milgram experiment)

Characterizing Graphs: Degree

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- Degree distribution:
 - uniform or power-law?
 - are there popular hub vertices?

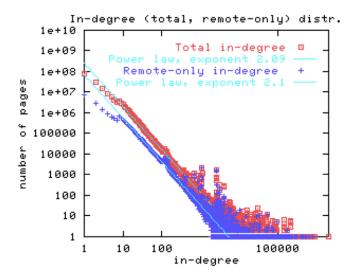
Power-law degree distribution is prevelant in real graphs

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- Consider Gaussian distribution: *p*(*d*) ∝ *exp*(−(*d* − μ)²): exponentially fast decay as d moves away from μ
- ► Power law: p(d) ∝ 1/d^β gives heavy-tail, i.e. vertices with very high degree can exist
 - straight-line on log-log plot: $\log(p(d)) = \beta \log(d)$

Power-law in WWW graphs



[Broder et. al., Graph Structure in the Web]

Characterizing Graphs: Clustering coefficient

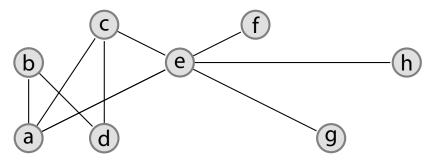
- Neighborhood of vertex v_i : $N_i = \{v_j : e_{ij} \in E \land e_{ji} \in E\}$
- Cluster coefficient of v_i:

$$C_{i} = \frac{|e_{jk} : v_{j} \in N_{i}, v_{k} \in N_{i}, e_{jk} \in E|}{|N_{i}|(|N_{i}| - 1)}$$

- i.e. percentage of triangles (i,j,k)
- Cluster coefficient C of graph = avg C_i

Quiz

What is the diameter? degree distribution? cluster coefficient of vertex *a*?



Erdős-Rényi model of random graph

- Start with N vertices
- Connect every pair of vertices with probability p

Graph will have about pN(N-1)/2 edges distributed randomly

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- ► Diameter = log(N) → "small world"
- Degree distribution = Poisson(*pN*), not power-law
- Clustering coefficient = p, no hierarchical clusters

Properties of Real-world Graphs

From: Albert & Barabási, Statistical mechanics of complex networks, 2002

Data	WWW	Co-Author	Movie
	[Broder]	[Newman]	[Watts]
size V	2×10^8	56,627	225,226
avg degree	7.5	173	61
power-law β	2.71, 2.1	1.2	n/a
avg distance ℓ	16	4	3.65
$\ell_{random graph}$	8.85	2.12	2.99
cluster coeff C	n/a	0.726	0.79
Crandomgraph	n/a	0.003	0.00027

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Given a graph G=(V,E), find subsets of V that form communities

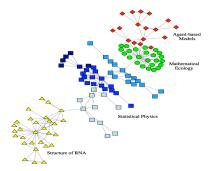


Figure : Do you see distinct communities of researchers in this collaboration graph?

http://www.pnas.org/content/99/12/7821.full

A Method for Community Detection Betweenness of edge (A,B) = # pairs of endpoints X & Y such that (A,B) lies on the shortest path between X and Y

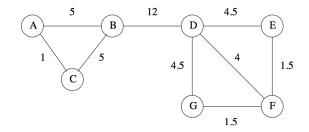


Figure : Betweenness example

All figures in this section come from http://infolab.stanford.edu/~ullman/mmds/ch10.pdf

A Method for Community Detection To detect communities, delete edges with high betweeness

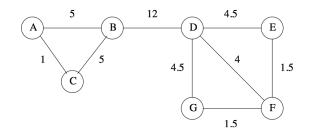


Figure : (B,D) has highest betweeness. So communities are {A,B,C} and {D,E,G,F}

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Betweenness Calculation: Girvan-Newman Algorithm

 Run breadth-first search from a vertex
 Label each vertex and edge with the # of shortest paths that passes through it.

Repeat for each vertex, sum edge scores / 2.

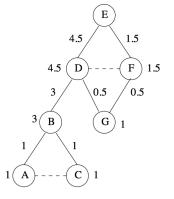


Figure : BFS from E

Betweenness Calculation: preparation

label from top-down: - root: 1 - other vertex: sum of parent labels result: for each X, # of shortest paths from E to X is known

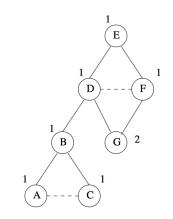


Figure : top-down labeling (preparation)

Betweenness Calculation: vertex/edge labeling in detail label from bottom-up:

- leaf vertex: 1
- internal vertex: 1 + children edge scores
- edge: a fraction of the child vertex score
- fraction computed by # of
- shortest paths to child
- through edge (preparation)

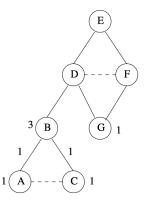
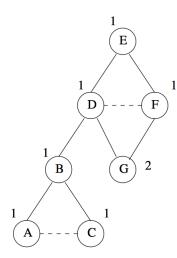


Figure : bottom-up labeling



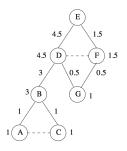
E 4.5 1.5 4.5 D F 1.5 0.5 0.5 3 3 В G C

Figure : top-down labeling (preparation)

Figure : bottom-up labeling: score indicates # of shortest paths from E that passes through.

Wrap-up: Community Detection by Betweenness

- Betweenness calculation by BFS
- To find community, delete edges with high betweenness
- Cost: O(|E|) per BFS & labeling, so O(|V||E|) total
- Many other methods available!



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 - a method based on betweenness