Matrix methods in the analysis of complex networks

Introduction

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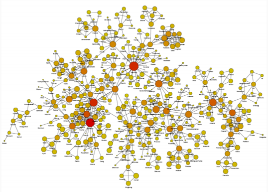
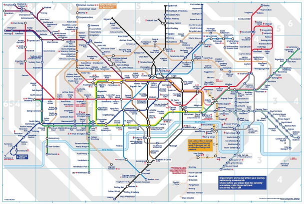
Outline

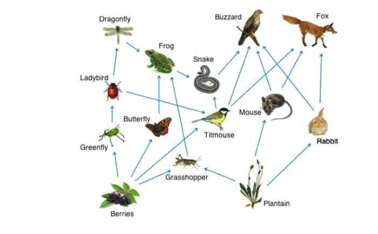
- An introduction to complex network analysis
- Classic and spectral centrality indices
- Random walks: classic and second-order
- Meso-scale structures and community detection

…with an emphasis on matrix techniques.

Complex networks







A complex network is a mathematical representation of a complex system: objects + relationships.

Network science

It's a branch of data science

The analysis of complex networks includes various aspects:

- Empirical — What it is made of? How it works?
- Structure
  - Microscopic (node level): quantify importance/participation of individual nodes
  - Mesoscopic (subnetwork level): Identify communities, split/partition networks into regions
  - Macroscopic (networks as a whole): Quantify macroscopic properties
- Dynamics — Modeling processes on networks: diffusion, formation, navigation, routing, degradation...
- Control — optimization.

Graphs and networks

A network (or graph) is a collection of vertices joined by edges: $\mathcal{G} = (V, E)$ where $E \subseteq V \times V$. Edges represent dyadic relationships between nodes.

Edges can be directed $(i \to j)$ or undirected $(i \sim j)$. In some cases they can be associated to a weight, which indicates length/strength/cost... of that edge $\rightsquigarrow$ weighted graph.

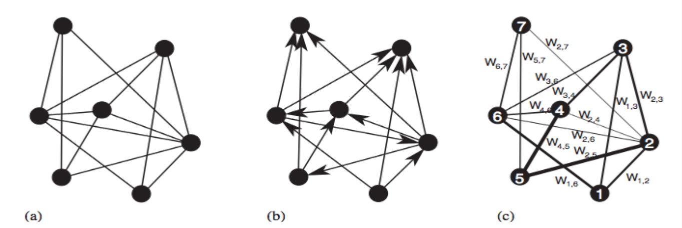


Figure 1: (a) A graph. (b) A digraph. (c) A weighted graph.

Formal definitions

A loop in $\mathcal{G}$ is an edge from a node to itself. Loops are often ignored or excluded.

A simple graph is an unweighted graph without multiple edges or loops.

A walk of length k in $\mathcal{G}$ is a set of nodes $v_1, v_2, \ldots, v_k, v_{k+1}$ such that $(v_i, v_{i+1}) \in E$ for all $1 \leq j \leq k$. A closed walk is a walk where $v_1 = v_{k+1}$.

A path is a walk with no repeated nodes. The geodetic distance $d(v_i, v_j)$ between two nodes is the length of the shortest path connecting v_i and v_j. We let $d(v_i, v_j) = \infty$ if no such path exists.

An undirected, loopless graph is a simple graph.

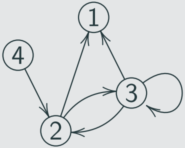
Formal definitions

A graph with $|V| = n$ is characterized by its adjacency matrix $A \in \mathbb{R}^{n \times n}$,

$$A_{ij} = \begin{cases} 1 & i \to j \qquad \text{i.e., } (i,j) \in E \\ 0 & i \not\to j \qquad \text{i.e., } (i,j) \notin E. \end{cases}$$

Example

$\mathcal{G}$:



$$\rightsquigarrow \qquad A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

If edges are weighted then A_{ij} is the weight of edge $i \to j$
(weighted adjacency matrix, or weight matrix)

Formal definitions

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Theorem

The number of walks of length k that originate at node i and terminate at node j is $(A^k)_{ij}$.

For example, the number of closed walks of length k is

$$\sum_{i=1}^{n} (A^k)_{ii} = \mathrm{trace}(A^k) = \sum_{i=1}^{n} \lambda_i^k.$$

Formal definitions: degrees

- If $\mathcal{G} = (V, E)$ is undirected, the degree d_i of node $i \in V$ is the number of edges incident to i in $\mathcal{G}$. In other words, d_i is the number of immediate neighbors of i in $\mathcal{G}$:

$$d_i = \sum_{i=1}^{n} A_{ij}, \qquad d = Ae,$$

  where $e = (1, \dots 1)^{\mathrm{T}}$.

- For a directed graph, we define the in-degree of node i as the number d_i^{in} of edges ending in i, and the out-degree of i as as the number d_i^{out} of edges originating at i. In terms of the (nonsymmetric) adjacency matrix,

$$d^{in} = A^{\mathrm{T}} e, \qquad d^{out} = Ae,$$

  Hence, the column sums of A give the in-degrees and the row sums give the out-degrees.

Graph isomorphisms

Any renumbering of the graph nodes results in a symmetric permutation $A \mapsto PAP^{\mathrm{T}}$ of the adjacency matrix of the graph.

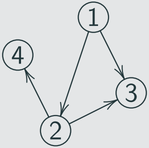
Isomorphic graphs: $\mathcal{G}_1 \simeq \mathcal{G}_2$

Two graphs $\mathcal{G}_1 = (V_1, E_1)$ and $\mathcal{G}_2 = (V_2, E_2)$ are isomorphic if there is an invertible map $\phi : V_1 \mapsto V_2$ such that

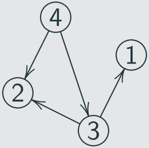
$$(i, j) \in E_1 \quad \Longleftrightarrow \quad (\phi(i), \phi(j)) \in E_2.$$

Example

$\mathcal{G}_1$:



$\mathcal{G}_2$:



V_1	1	2	3	4
V_2	4	3	2	1

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Equivalently: The graphs $\mathcal{G}_1$ and $\mathcal{G}_2$ with adjacency matrices A_1 and A_2 are isomorphic if there is a permutation matrix P such that $A_2 = PA_1P^{\mathrm{T}}$.

Graph automorphism

Let A be the adjacency matrix of $\mathcal{G}$. If there exists a permutation matrix P such that $A = PAP^{\mathrm{T}}$ then P is an automorphism of $\mathcal{G}$.

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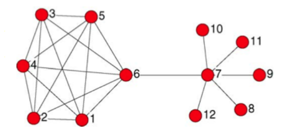
Nodes that are permuted by automorphisms are said to be similar or equivalent, and are collected into orbits.

Example. This graph has a lot of automorphisms:



Orbits: $\{1,2,3,4,5\}, \{6\}, \{7\}, \{8,9,10,11,12\}$.

Graph isomorphisms

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Topological index

A topological index (or network topology measure) is a function $\tau : \{\mathcal{G}\} \mapsto \mathbb{R}$ such that

$$\mathcal{G}_1 \simeq \mathcal{G}_2 \implies \tau(\mathcal{G}_1) = \tau_(\mathcal{G}_2).$$

Let $\mathcal{G} = (V, E)$. A centrality index is a function $f : V \mapsto \mathbb{R}$ which quantifies some kind of "importance" or "participation" of individual nodes.

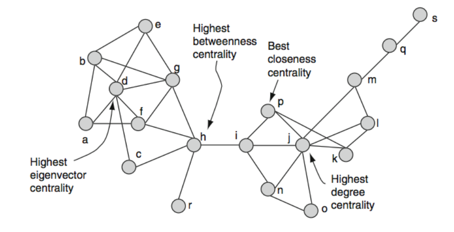
Centrality index

A centrality index is a family of functions $f_{\mathcal{G}} : V \mapsto \mathbb{R}$ such that if ϕ is a graph isomorphism between $\mathcal{G}_1$ and $\mathcal{G}_2$ and $\phi(i) = j$ then $f_{\mathcal{G}_2}(j) = f_{\mathcal{G}_1}(i)$.

In other words, if c is the vector of node centralities of a graph $\mathcal{G}$ with adjacency matrix A and $\mathcal{G}'$ is a graph with adjacency matrix $A' = PAP^{\mathrm{T}}$ with P a permutation matrix, then the vector of node centralities for $\mathcal{G}'$ is given by $c' = Pc$.

Freeman's centrality indices

- Degree Number of each node's connections
- Closeness Inverse average geodetic distance of a node from every other node
- Betweenness Fraction of shortest (geodetic) paths passing through a given node.



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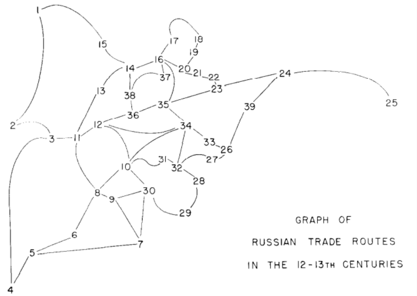
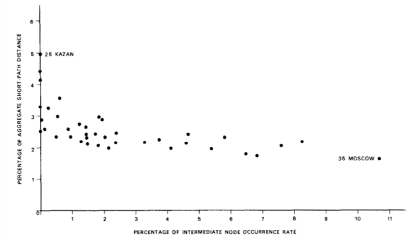
Moscow's rise in medieval Russia





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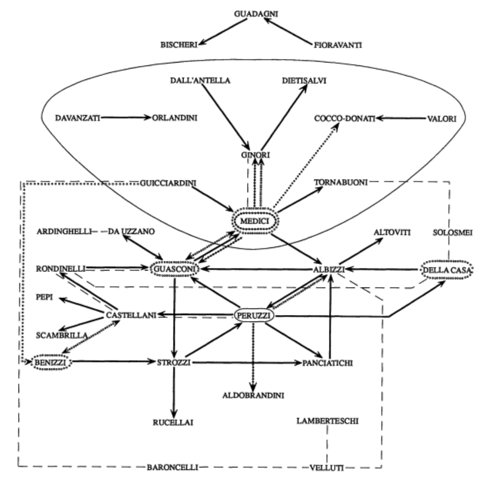
The prominence of the Medici in Renaissance Florence



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How many centralities?

The CentiServer web site `www.centiserver.org/centrality/` lists 400^+ centrality indices.

> *Social prediction tasks benefit by combining many different types of information; [...] adding your new solution to an ensemble of existing solutions enables better predictions for some tricky problems.*
>
> David Gleich, *ACM Crossroads*, 19 (2013), 32–36.

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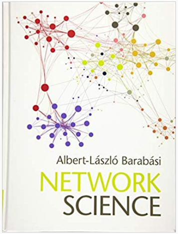

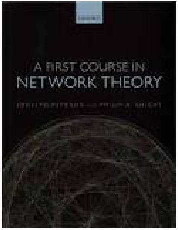

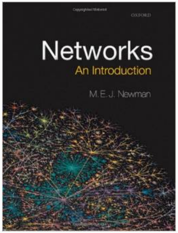

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A summary of Perron–Frobenius theory

Perron Thm. (1907)

Let $A > O$ and let $\rho(A)$ be its spectral radius.
Then $\rho(A)$ is a simple, dominant eigenvalue of A.
Moreover, $\rho(A) > 0$ and $Ax = \rho(A)x$ with $x > 0$.

Remarks:

- $\rho(A)$ is an eigenvalue.
- If λ is another eigenvalue then $|\lambda| < \rho(A)$.
- If y is an eigenvector of $\rho(A)$, that is, $Ay = \rho(A)y$, then y must be a multiple of x.

A summary of Perron–Frobenius theory

Frobenius Thm. (1913)

Let $A \geq O$ and irreducible. Let $\rho(A)$ be its spectral radius.
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Remarks:

- A positive eigenvector associated to $\rho(A)$ is a Perron vector. Moreover, $\rho(A)$ is the Perron eigenvalue of A.
- If $A \geq O$ then $\rho(A)$ may not be dominant; see $A = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$.

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Definition

A matrix $A \geq O$ is primitive if $A^k > O$ for some integer $k \geq 1$.

Corollary

Let $O \leq A \in \mathbb{R}^{n \times n}$. If A is primitive
then $\rho(A)$ is a simple, dominant eigenvalue of A.
Moreover, $\rho(A) > 0$ and $Ax = \rho(A)x$ with $x > 0$.

A summary of Perron–Frobenius theory

Other results in the Perron–Frobenius theory:

- Let $A \geq O$. If $Ax = \lambda x$ and $x > 0$ then $\lambda = \rho(A)$.
- Let $A \geq O$, $r_i = \sum_{j=1}^{n} A_{ij}$ and $c_i = \sum_{j=1}^{n} A_{ji}$. Then

$$\min_i r_i \leq \rho(A) \leq \max_i r_i, \qquad \min_i c_i \leq \rho(A) \leq \max_i c_i.$$

- Let $O \leq A \leq B$. Then $\rho(A) \leq \rho(B)$.

The power method

The power method is a simple iterative method to compute the Perron eigenpair of a nonnegative matrix A.

Unnormalized version

- Choose $x_0 \geq 0$
- For $k = 1, 2, 3 \dots$
  - Compute $x_k = Ax_{k-1}$

Normalized version

- Choose $x_0 \geq 0$, $\|x_0\| = 1$
- For $k = 1, 2, 3 \dots$
  - Compute $y_k = Ax_{k-1}$
  - Set $x_k = y_k / \|y_k\|$

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- If $\rho(A)$ is simple and dominant then x_i approaches a Perron eigenvector.
- Convergence ratio is $|\lambda_2|/\lambda_1$.
- Define $\lambda^{(k)} = e^{\mathrm{T}} A x_k / e^{\mathrm{T}} x_k$. Then $\lambda^{(k)}$ converges to $\rho(A)$.
- Of course, the iteration must be terminated!
  - Set a maximum number for iterations
  - Stop when $\lambda^{(k)}$ "converges."