Èdouard Lucas:

The theory of recurrent sequences is an inexhaustible mine which contains all the properties of numbers; by calculating the successive terms of such sequences, decomposing them into their prime factors and seeking out by experimentation the laws of appearance and reproduction of the prime numbers, one can advance in a systematic manner the study of the properties of numbers and their application to all branches of mathematics.

Applications of Linear Algebra to Graph Theory and Network Science

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Department of Mathematics and Statistics

ILAS Vodcast
April 2023

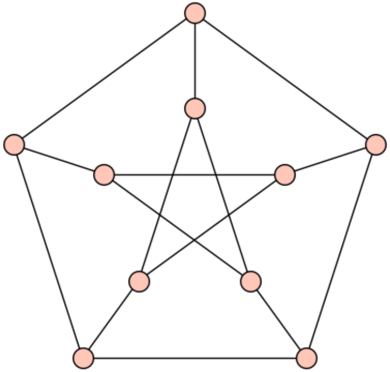
Outline

- **Goals:**
  - Introduce graph theory and social network modeling
  - Investigate connections with linear algebra
  - Inspire interest in exploring further
- **Format:**
  - Overview of ideas and connections
  - A couple of proofs and examples
  - Computational notebooks and resources
- **Topics:**
  - Introduction to graphs networks
  - Graph Matrices
  - Centrality
  - Clustering
  - Dynamics
  - Random Models
- **Resources:**
  - `https://github.com/ILAS_Networks`

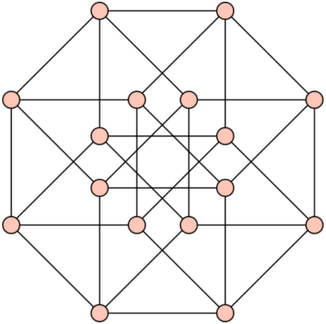
Graph Theory

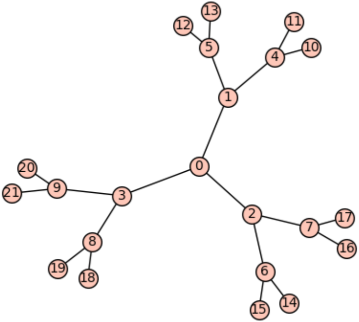
Definition (Graph)

A Graph $G = (V, E)$ is a set of nodes V and a set of edges $E \subseteq V \times V$.



Graph Examples

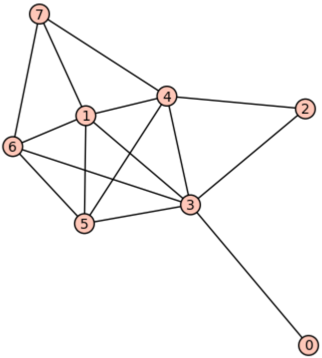




Example Graph Questions

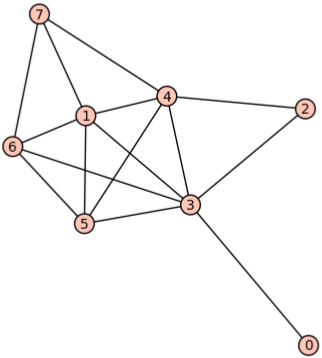
- Are there Hamiltonian/Eulerian Paths? If so, how many?
- Are there perfect matchings? If so, how many?
- Is it possible color the nodes with k colors so that no neighboring nodes are the same color?
- What is the largest set of nodes that share no edges?
- How many edges/vertices must be removed to disconnect the graph?
- Is it possible to embed the graph in the plane without any edges crossing?
- How many spanning trees does the graph have?
- What is the automorphism group of the graph?
- ...

Adjacency Matrix



$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

Degree Matrix



$$D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

Laplacian Matrix (D-A)

$$L = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & -1 & -1 & -1 & -1 & -1 \\ 0 & 0 & 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & -1 & -1 & 6 & -1 & -1 & -1 & 0 \\ 0 & -1 & -1 & -1 & 5 & -1 & 0 & -1 \\ 0 & -1 & 0 & -1 & -1 & 4 & -1 & 0 \\ 0 & -1 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & -1 & 0 & 0 & -1 & 0 & -1 & 3 \end{bmatrix}$$

Notation and Structural Results

- Notation:
  - $G = (V, E)$
  - Number of nodes: $|V| = n$
  - Number of edges: $|E| = m$
  - There is an edge between u and v: $u \sim v$
  - The geodesic distance between two nodes: $d(u, v)$
  - Eigenvalues of A: $|\lambda_1| \geq |\lambda_2| \cdots \geq |\lambda_n|$
- $(A^k)_{i,j}$ counts the number of walks of length k starting at node i and ending at node j.
- When A is a connected graph it is irreducible and hence satisfies the non-negative Perron-Frobenius theorem

Spectral Graph Theory

F. Chung: *Spectral Graph Theory*, AMS, (1997).

"Roughly speaking, half of the main problems of spectral theory lie in deriving bounds on the distributions of eigenvalues. The other half concern the impact and consequences of the eigenvalue bounds as well as their applications."

R. Brualdi: *The Mutually Beneficial Relationship of Graphs and Matrices*, CBMS, (2011)

Graphs and matrices enjoy a fascinating and mutually beneficial relationship. This interplay has benefited both graph theory and linear algebra. In one direction, knowledge about one of the graphs that can be associated with a matrix can be used to illuminate matrix properties and to get better information about the matrix. [...] Going the other way, linear algebraic properties of one of the matrices associated with a graph can be used to obtain useful combinatorial information about the graph.

Diameter and Multiplicity

Theorem

The diameter of G is bounded above by the number of distinct eigenvalues of A.

Proof.

Let k be the number of distinct eigenvalues of A. Since A is diagonalizable, k is also the degree of the minimal polynomial of A. Thus, the set $\{I, A, A^2, \ldots, A^k\}$ is linearly dependent and in particular $A^k = \sum_{i=0}^{k-1} \alpha_i A^i$ for some constants α_i. In order to obtain a contradiction, assume that there is a pair of vertices $u, v \in V$ with $d(u, v) = k$. Then $(A^k)_{u,v} > 0$ but $(A^i)_{u,v} = 0$ for all $0 \leq i \leq k-1$, which is a contradiction. ☺

Bounding λ_1

Theorem

Let δ and Δ be the minimum and maximum degrees of nodes in G and λ_1 be the leading eigenvalue . Then $\delta \leq \lambda_1 \leq \Delta$.

Proof.

Let v be an eigenvector for λ_1 and k be the index of a maximal entry of v, so $v_k = \max_i v_i$. Consider the kth row of $Av = \lambda_1 v$:

$$\lambda_1 v_k = (Av)_k = \sum_{i \sim k} v_i \leq \sum_{i \sim k} v_k = deg(v_k) v_k \leq \Delta v_k.$$

To see the other inequality consider the quadratic form:

$$\lambda_1 = \sup_{||v||=1} v^T A v \geq (\frac{1}{n}) 1^T A 1 = (\frac{1}{n}) \sum_{i=1}^{n} \sum_{j=1}^{n} A_{i,j} = \frac{2|E|}{n} \geq \delta.$$

☺

Laplacian Properties

- L is positive semi-definite since it can be factored at VV^T where V is an incidence matrix for the graph
- The all ones vector is an eigenvector with eigenvalue 0 for L. The dimension of the 0 eigenspace is the number of connected components of G.
- The smallest non-zero eigenvalue is called the algebraic connectivity or Fiedler value and we'll see this has
- Kirchoff's theorem: The number of spanning trees in a graph is given by the value of any cofactor of the Laplacian.

What is a social network?

Definition (Social Network)

A social network is represented by a collection of "nodes" representing individual actors and a set of "edges" representing a binary relationship between the actors.

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Example

What kinds of systems can social networks describe?

- What could be represented by nodes?
  - **University Students**
- What type of edges could connect them?
  - **In a class together**
  - **Facebook friends**
  - **Speak at least twice a week**

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Definition (Social Network)

Mathematically, a social network is represented by a collection of “nodes” representing individual actors and a set of “edges” representing a binary relationship between the actors.

Example

What kinds of systems can social networks describe?

- What could be represented by nodes?
  - **Academic Departments**
- What type of edges could connect them?
  - **Located in same building**
  - **Students who major in both**
  - **Crosslisted courses**

Starting Example

Definition (Ego Network)

An ego network is a social network centered at a particular individual containing their connections and the connections between their "friends."

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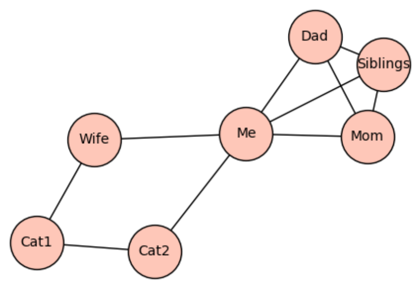
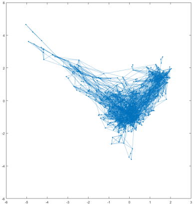
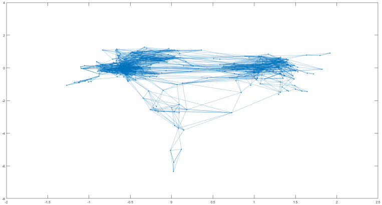


World Trade Web

Karnataka Village Data



Village 5



Village 61

Figure: Two of the Karnataka Village networks

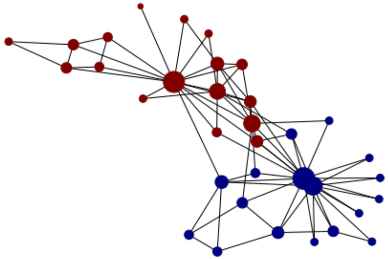
A. Banerjee, A.G. Chandrasekhar, E. Duflo, and M.O. Jackson, The Diffusion of Microfinance. Science, (2013).

Common Properties of Social Networks

Example (What features distinguish social networks?)

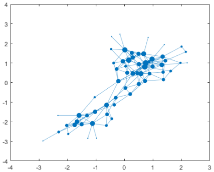
- Transitivity
- Community structure
- Small average path length
- Long–tailed degree distribution
- Hubs
- . . .

Karate Club

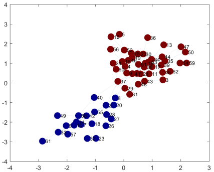


Zachary, Wayne W. “An Information Flow Model for Conflict and Fission in Small Groups.” Journal of Anthropological Research, 33, 452–473, (1977).

Dolphins



Centrality



Clustering

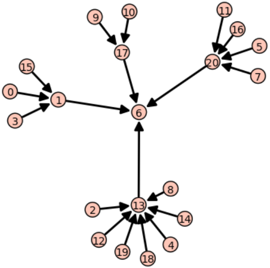
Figure: Dolphin social network[1]

[1] D. Lusseau, K. Schneider, O. Boisseau, Patti Haase, E. Slooten, and S. Dawson, The bottlenose dolphin community of Doubtful Sound features a large proportion of long-lasting associations, Behavioral Ecology and Sociobiology 54 (2003), 4, 396–405.

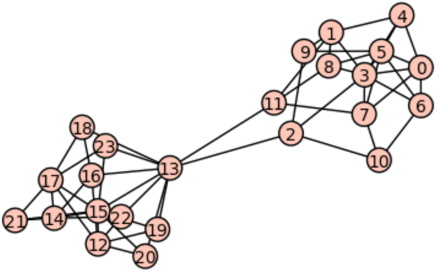
Network Examples

- Internet
  - Nodes: Hardware
  - Edges: Physical Connections
- WWW
  - Nodes: Webpages
  - Edges: Links
- Neuroscience
  - Nodes: Brain areas
  - Edges: Functional Connections
- Food webs
  - Nodes: Species
  - Edges: Predation
- World Trade
  - Nodes: Countries
  - Edges: Trade Agreements
- Banking
  - Nodes: Banks
  - Edges: Loans
- Genetics
  - Nodes: Genes/Proteins
  - Edges: Functional Interactions
- Recommendations
  - Nodes: People/Products
  - Edges: Ratings/Consumption

Network Questions



Centrality



Clustering

Centrality

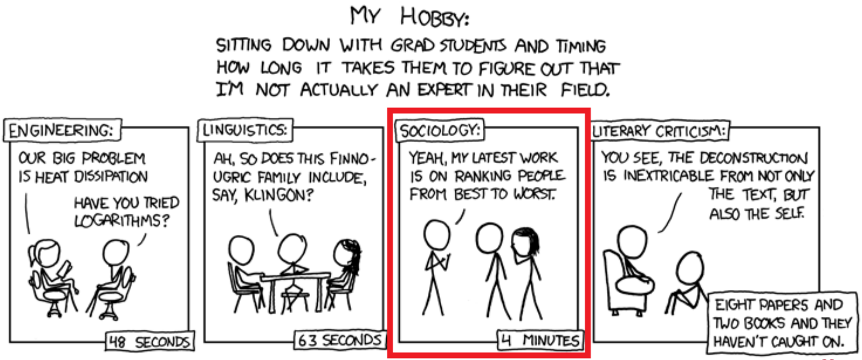
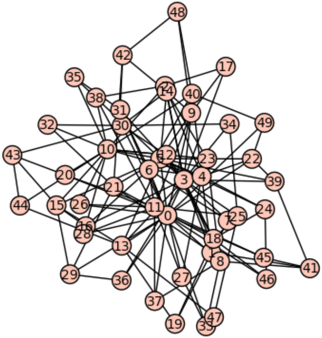


Figure: Relevant comic by Randall Munroe[1] (emphasis mine).

[1] https://xkcd.com/451/

Harder Question



Eigenvector Centrality

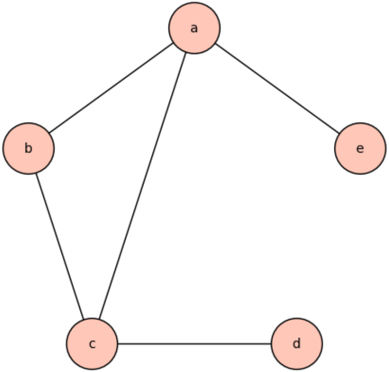
- Naively: You are popular if you have lots of friends
- Intuitively: You are popular if your friends are popular
- Formally: Your popularity should be proportional to the sum of your friends' popularities.
- Mathematically: Given a vector v whose entries represent the initial popularity of each node in the network we seek a solution to:

$$v_i = \lambda \sum_{i \sim j} v_j = \sum_{j=1}^{n} A_{i,j} v_j$$

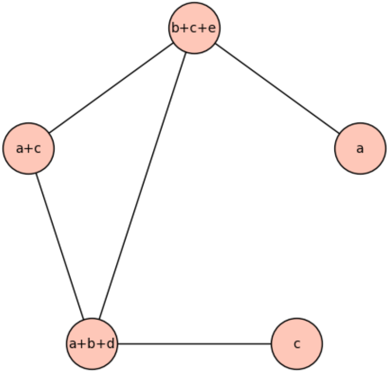
or equivalently:

$$v = \lambda A v$$

Adjacency Action



Before



After

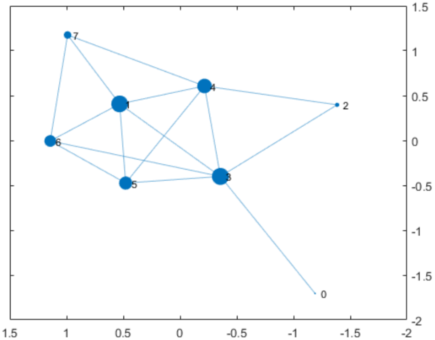
Eigenvector Centrality Extensions

- Many real-world networks have a directed structure, in which case we might have ‘sinks’ in the adjacency dynamics that will eventually absorb all of the popularity
- To address this, we might continually pump popularity into the system at each step
- Katz Centrality: For some parameter $\alpha < \lambda_1$ compute

$$K_i = \sum_{k=0}^{\infty} \sum_{j=1}^{n} \alpha^k (A^k)_{i,j}$$

- PageRank: We can also compute a similar centrality score proportional to the stationary distribution of a random walk on the (di)graph. The pagerank is equivalent to normalizing our adjacency matrix by degree and then allowing some small probability of randomly hopping to any node in the network.

Toy Eigenvector Centrality



$$v = \begin{bmatrix} 0.1052 \\ 0.4470 \\ 0.2022 \\ 0.4508 \\ 0.4155 \\ 0.3926 \\ 0.3683 \\ 0.2873 \end{bmatrix}$$

Clustering Definitions

- Spectral clustering
  - Minimize Inter–Community Edges
  - Minimize $s^T Ls$ with $s \in \{\pm 1\}^n$

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- Markov Stability
  - Given a partition $(V_1, V_2, \ldots, V_\ell)$ maximize (for fixed t) $r(t, V) = \sum_{i=1}^{\ell} \sum_{v_y, v_z \in V_i} C(t)_{y,z}$
  - Discrete: $C(t) = \Pi S^t - \pi^T \pi$ where π is the steady state vector and Π is the diagonal matrix of π
  - Continuous: $C(t) = \Pi e^{-t(I-S)} - \pi^T \pi$ where π is the steady state vector and Π is the diagonal matrix of π

Spectral Clustering Setup

We can think of this as minimizing the damage done to the network by removing the edges between clusters. Investigating the 2-partition case, we can begin by constructing a vector v to represent the desired partition, with entries of 1 assigned to nodes in one component and entries of -1 assigned to the other component. This gives that $v_i v_j = 1$ if and only if i and j are in the same component. We can now formulate the damage condition algebraically as

$$\mathrm{damage}(v) = \frac{1}{2}\sum_{i,j}\frac{1}{2}(1 - v_i v_j)A_{i,j}.$$

Proceeding by algebraic manipulation, we can reduce this expression to

$$\begin{aligned} \frac{1}{2}\sum_{i,j}\frac{1}{2}(1 - v_i v_j)A_{i,j} &= \tfrac{1}{4}(\textstyle\sum_{i,j} A_{i,j} - v_i v_j A_{i,j}) \\ &= \tfrac{1}{4}\textstyle\sum_{i,j} v_i \deg(i) v_j \delta_{i,j} - v_i A_{i,j} v_j) \\ &= \tfrac{1}{4} v^T D v - v^T A v \\ &= \tfrac{1}{4} v^T L v \end{aligned}$$

Spectral Clustering II

- Solving this problem exactly across all binary vectors is:
  - NP-hard
  - usually irrelevant (separating a leaf)
- Instead, we can solve a relaxed problem with $v \in \mathbb{R}^n$ with $||v|| = 1$ and $v \perp 1$
- In this case our solution is just given by a Raleigh quotient
- The continuous solution is thus given by the eigenvector corresponding to the Fiedler value and we can recover a binary solution by setting the positive values to 1 and the negative values to -1
- Ratio and Normalized cuts also address the irrelevancy issue
- We'll explore the case of more than two parts on the computational side

Dynamics on Networks

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  - Discretized version of Laplacian heat diffusion
  - **Fiedler value**: smallest non–zero eigenvalue
- Random Walk
  - Matrix: AD^{-1}
  - Stochastic, regular if G is connected
  - Transition matrix of associated Markov process
  - Convergence governed by second largest eigenvalue

Diffusion Dynamics

Given a vector of initial heat values v the change in temperature at node i with respect to time is given by

$$\frac{dv_i}{dt} = -K \sum_{i \sim j} v_i - v_j$$

or

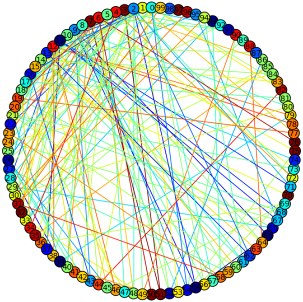
$$\frac{dv}{dt} = -KLv$$

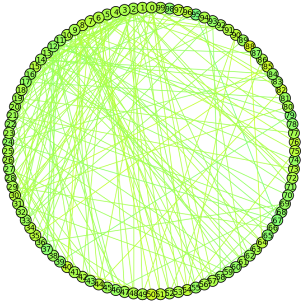
where L is the graph Laplacian. This is a symmetric, positive semi–definite matrix so the value at time t is

$$v(t) = \sum_{i=1}^{n} c_i v^i e^{-\lambda_i t}$$

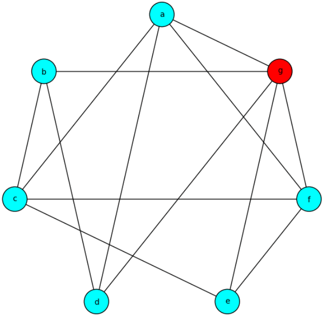
where the (v^i, λ_i) are eigenpairs for L.

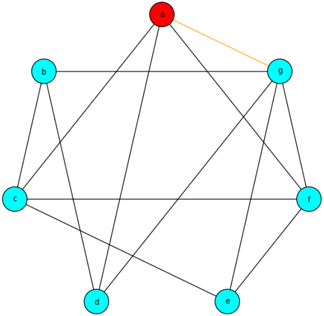
Diffusion Animation



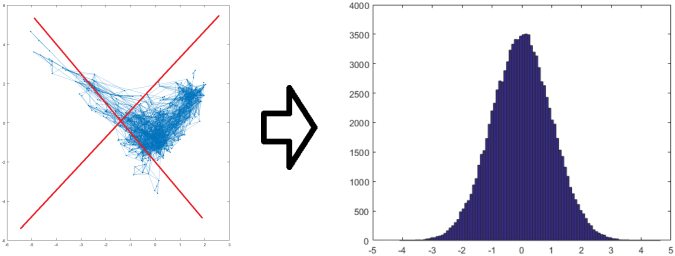


Random Walk Dynamics





Random Models



Null Models

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A random network, parameterized to match some features of a given network, used to compare “expected” network measures.

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Example (How to grow a network?)

- Ego networks
  - Start with a single node
  - Attach that node to k other nodes
  - Add edges between the each pair of friends with probability p
- ?

Dot Product Graphs

Definition (Dot Product Graph)

G is a dot product graph of dimension d if there exists a map $f : V(G) \to \mathbb{R}^d$ such that $(i, j) \in E(G)$ if and only if $\langle f(i), f(j)\rangle > 1$.

---

[1] C. Fiduccia, E. Scheinerman, A. Trenk, and J. Zito: Dot Product Representations of Graphs, Discrete Mathematics, 181, 1998, 113–138.

[2] R. Kang, L. Lovasz, T. Muller, and E. Scheinerman: Dot Product Representations of Planar Graphs, Electronic Journal of Combinatorics, 18, (2011), 1–14.

[3] Sphere and Dot Product Representations of Graphs: Discrete Computational Geometry, 47, (2012), 548–568.

[4] B. Li and G. Chang: Dot Product Dimension of Graphs, Discrete Applied Mathematics, 166, (2014), 159–163

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- Initial work: Fiduccia et al. (1998)[1]
- Planar graphs: Kang et al. (2011)[2]
- NP–Hard: Kang and Muller (2012)[3]
- $\frac{n}{2}$ critical graphs: Li and Chang (2014)[4]

---

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RDPM

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RDPM

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(RDPM 5): Form an adjacency matrix, A, form a network with $A_{j,\ell}$ drawn from $\text{Bernoulli}(\langle X_j, X_\ell\rangle)$ for $j \neq \ell$ and $A_{j,j} = 0$ for all $1 \leq j \leq n$.

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- Angle – Community assignment
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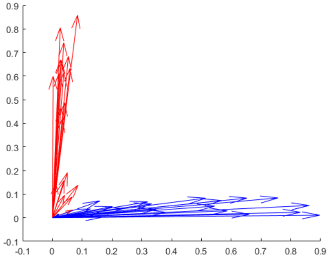
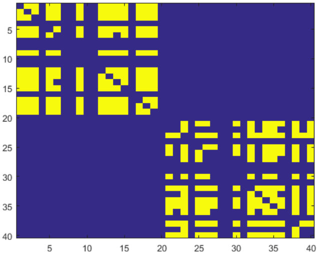
Angle – Community Assignment

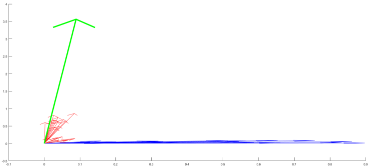


Vectors



Graph

Magnitude – Centrality



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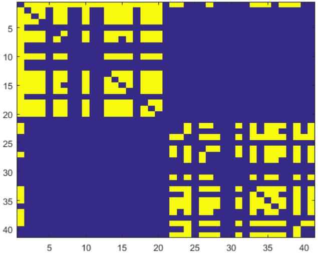
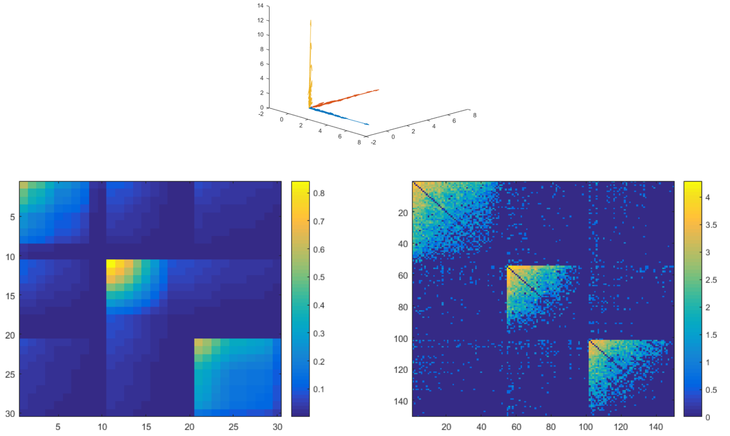


Graph

Multi-Resolution Communities



Network Properties

- Initial work: Kraetzel et al. (2005)[5]
- General distributions: Young and Sceinerman (2007)[6]

[5] M. Kraetzel, C. Nickel, and E. Scheinerman: *Random Dot Product Networks: A model for social networks*, Preliminary Manuscript, (2005).

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Statistical Applications

- Inverse problem: Scheinerman and Tucker (2010)[7]
  - Iterative SVD for approximating $A_{i,j} = \langle X_i, X_j \rangle$
  - Angular k-means
- MAP/Conic Programming: Wu, Palmer, and DeFord (2022)

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- Spectral Embedding and Statistics: Priebe Lab (2012–present)
  - Adjacency embedding[8]
  - Hypothesis testing[9]
  - Limit theorems[10]

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Edge Parameterized Models

Theorem

Let n be a fixed positive integer. For each pair (i, j) with $1 \leq i < j \leq n$ let $a_{i,j} = a_{j,i} \in \mathbb{R}$. Then there exist n real numbers $a_{\ell,\ell}$ for $1 \leq \ell \leq n$ such that the matrix $A_{i,j} = a_{i,j}$ is positive definite.

Proof.

Let the $a_{i,j}$ be selected arbitrarily. For $1 \leq \ell \leq n$ choose $a_{\ell,\ell} \in \mathbb{R}$ so that $a_{\ell,\ell} > \sum_{j \neq \ell} |a_{j,\ell}|$. Form a matrix A with $A_{i,j} = a_{i,j}$. This is a real symmetric matrix and so by the spectral theorem A has real eigenvalues. Applying Gershgorin's Circle Theorem to A gives that the eigenvalues of A lie in the closed disks centered at $a_{\ell,\ell}$ with radius $\sum_{j \neq \ell} |a_{j,\ell}|$. Intersecting these disks with the real line gives that the eigenvalues of A must lie in $\bigcup_{\ell=1}^{n} \left[a_{\ell,\ell} - \sum_{j \neq \ell} |a_{j,\ell}|, a_{\ell,\ell} + \sum_{j \neq \ell} |a_{j,\ell}| \right] \subseteq \mathbb{R}^{+}$. Thus, all eigenvalues of A are positive and A is positive definite. ☺

Edge Parameterized Models

Corollary

Any generative network model, on a fixed number of nodes n, where the edge weight between each pair of nodes is drawn independently from a fixed probability distribution, possibly with different parameters for each pair, can be realized under the WRDPN.

Proof.

Let P be the k–parameter distribution from which the edge weights are drawn and for $1 \leq i \leq k$ let $a^i_{j,\ell} = a^i_{\ell,j}$ be the value of the ith parameter between nodes j and ℓ. Applying Theorem 1 to the collection $a^i_{j,\ell} = a^i_{\ell,j}$ gives a positive definite matrix A^i. Thus, there exists an $n \times n$ matrix X^i such that $(X^i)^T X^i = A$.
To form the WRDPM that matches the given generative model we take $d_i = n$ for all $1 \leq i \leq k$ and to each node $1 \leq j \leq n$ assign the collection of vectors given by the jth columns of the X^i for $1 \leq i \leq k$. ☺

Examples

- Erdos–Renyi
  - Single vector for W
  - Simplest null model

[11] J. Ranola, S. Ahn, M. Sehl, D. Smith, and K. Lange: *A Poisson Model for random multigraphs*, Bioinformatics, 26, (2010), 2004–2011.

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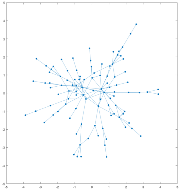
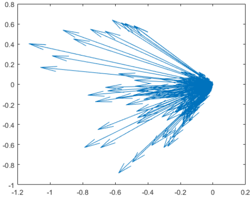
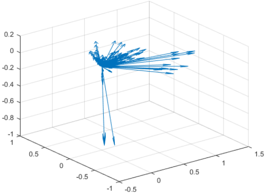
Unweighted Collaboration Network



Collaboration Network



Unweighted 2–Embedding

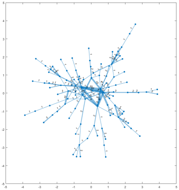


Unweighted 3–Embedding

[12]

[12] V. Batagelj and A. Mrvar: *Pajek datasets*, (2006), URL: http://vlado.fmf.uni-lj.si/pub/networks/data/.

Weighted Collaboration Network



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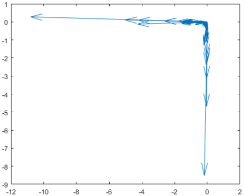
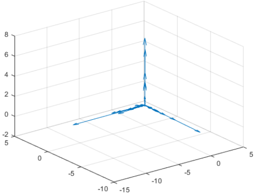


Weighted 2–Embedding



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[13]

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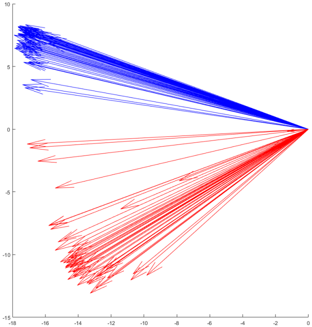
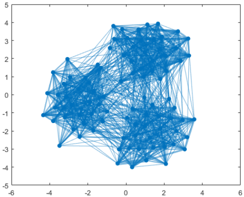
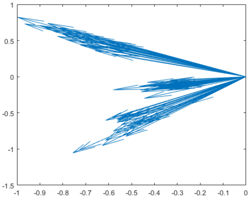
Voting Data



Dimension Example



Weighted Network



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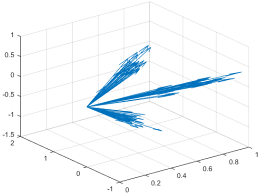

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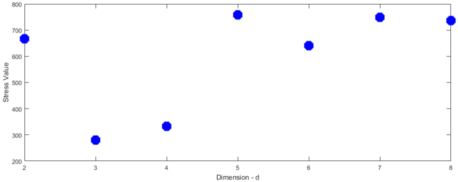

Stress Function

Coauthorship Revisited

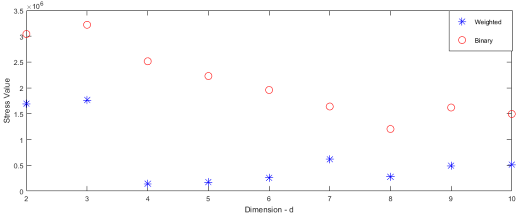

Figure: Comparison of stress values for the computational geometry coauthorship network between the weighted and unweighted realizations. The weighted embedding significantly outperforms the binarized model.

Resources

- Spectral Graph Theory (Chung)
- The Mutually Beneficial Relationship of Graphs and Matrices (Brualdi)
- Networks (Newman)
- Network Analysis and Modeling (Clauset)
- https://github.com/drdeford/ILAS_Networks
- https://github.com/drdeford/CISER2023NetworkX/
- https://github.com/drdeford/JMM2021NetworkX

Conclusion

Thanks!