Spectral Graph Theory and Its Applications

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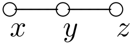
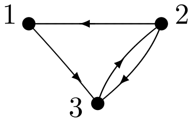
Adjacency matrix

Let Γ be a graph (or a digraph) of order n without loops. The adjacency matrix A of Γ is a matrix of size n with rows and columns indexed by the vertices of Γ such that

$$A_{xy} = \begin{cases} 1, & \text{if } xy \text{ is an edge;} \\ 0, & \text{otherwise.} \end{cases}$$



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



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

If all eigenvalues of a matrix M of order n are reals, we order them by

$$\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M).$$

Eigenvalues help us to realize the structure of a graph

Theorem

For a simple undirected graph Γ of order n, Γ is bipartite if and only if $\lambda_1(A) = -\lambda_n(A)$. □

The above simple fact in Spectral Graph Theory has real-world application.

Dongbo Bu, et al., Topological structure analysis of the protein-protein interaction network in budding yeast, Nucleic Acids Research, 2003, Vol. 31, No. 9, 2443-2450.

Eigenvalues help us to solve problems in Combinatorics

Let $\chi(G)$ denote the chromatic number of G.

Theorem (Wilf Theorem(1967) and Hoffman(1970))

For a simple undirected graph Γ with adjacency matrix A,

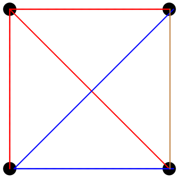
$$(\lambda_n(A) - \lambda_1(A))/\lambda_n(A) \le \chi(A) \le \lambda_1(A) + 1.$$

□

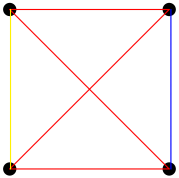
Graph decomposition

Definition

An edge decomposition of a graph Γ is a partition of the edges of Γ.



$$K_4 = K_{1,3} + K_{1,2} + K_{1,1}$$



$$K_4 = K_{2,2} + K_{1,1} + K_{1,1}$$

Sylvester's law of inertia

Let Γ be an undirected graph with n vertices. Let n_+ (resp. n_-) denote the the number of positive (resp. negative) eigenvalues of the adjacency matrix A of Γ with repetitions.

Theorem (Graham, Pollak, 1971)

Suppose Γ *has an edge decomposition into* r *complete bipartite graphs. Then* $r \geq \max\{n_+, n_-\}$.

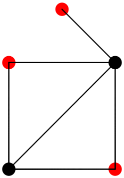
Independent number

Definition

Let Γ be a simple undirected graph.

1. A coclique (independent set) in Γ is a set of pairwise nonadjacent vertices.
2. The independent number $\alpha(\Gamma)$ in Γ is the size of the largest coclique in Γ.

Γ :



$$\alpha(\Gamma) = 3.$$

Theorem (Cvetković, 1971)

$$\alpha(\Gamma) \leq \min(n - n_+, n - n_-),$$

where n_+ (resp. n_-) is the number of positive (resp. negative) eigenvalues of adjacency matrix A of Γ.

Theorem (Hoffman, unpublished)

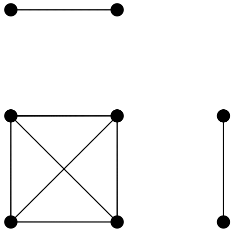
If Γ is k-regular with $k > 0$, then

$$\alpha(\Gamma) \leq \frac{-n\lambda_n(A)}{k - \lambda_n(A)}.$$

Definition

1. If Γ and Γ' have adjacency matrices A and A' respectively, then their strong product $\Gamma \boxtimes \Gamma'$ has adjacency matrix $(I+A)\otimes(I+A')-I$.
2. The ℓ-th strong power Γ^ℓ of Γ has adjacency matrix $(\otimes^\ell(I+A))-I$.

Γ



$\Gamma \boxtimes \Gamma'$ $\quad\quad$ Γ'

$$(I+\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix})\otimes(I+\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}) = \begin{pmatrix}1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\end{pmatrix}.$$

Shannon capacity

Definition

1. $c(\Gamma) := \limsup_{\ell \to \infty} \alpha(\Gamma^\ell)^{1/\ell}$, where $\alpha(\Gamma)$ is the independent number of Γ.
2. $\log c(\Gamma)$ is called the Shannon capacity of Γ.

Theorem (Lovász, 1979)

Let Γ be k-regular of order n with adjacency matrix A. Then

$$c(\Gamma) \le -n\lambda_n(A)/(k - \lambda_n(A)).$$

Diameter bounds

Theorem (Chung, 1989)

Let Γ be a k-regular graph on $n \geq 3$ vertices with diameter D and adjacency matrix A. Let $\lambda = \max_{i>1} |\lambda_i(A)|$. Then

$$D \leq \left\lceil \frac{\log(n-1)}{\log(k/\lambda)} \right\rceil .$$

The larger k/λ the more random the graph Γ is.

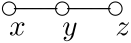
Almost every graph has diameter 2.

Laplace and signless Laplace matrices

Let Γ be a simple undirected graph. Let D denote a diagonal matrix with rows and columns indexed by vertices of Γ such that

$$D_{xx} = \text{degree of } x.$$

Then $L = D - A$ is called the Laplace matrix of Γ, and $|L| = D + A$ is called signless Laplace matrix Γ.



$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, L = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}, |L| = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{pmatrix}.$$

Sometimes the matrices

$$D^{-1}A, \qquad I - D^{-1/2}AD^{-1/2}$$

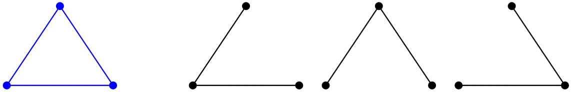
are also of interest.

Theorem

The number of bipartite components of Γ *is the nullity of* $|L|$.

Tree

1. A tree is an undirected graph without cycles.
2. A spanning tree of an undirected graph Γ is a subgraph of Γ which is a tree and contains all vertices of Γ.



K_3 has three spanning trees.

Laplacian spectrum tells the number of spanning trees

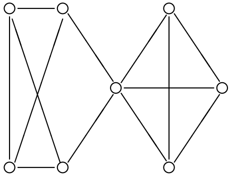
Theorem (Cayley, 1889)

$$\tau(\Gamma) = \frac{1}{n}\lambda_1(L)\lambda_2(L)\cdots\lambda_{n-1}(L).$$

Connectivity and algebraic connectivity

Definition

The connectivity of Γ, written $\kappa(\Gamma)$, is the minimum size of a vertex set S such that $\Gamma - S$ is disconnected or has only one vertex.



$\kappa(\Gamma) = 1$

Theorem

$$\kappa(\Gamma) \geq \lambda_{n-1}(L).$$

$\lambda_{n-1}(L)$ is called the algebraic connectivity of Γ.

Conductance

Definition

Let Γ be a simple undirected graph of order n.

1. For a subset S of the vertex set $V\Gamma$, define

$$\partial S := \{xy \in E\Gamma \mid x \in S, y \notin S\}.$$

2. The value

$$\Phi(\Gamma) := \min_{|S| \leq n/2} \frac{|\partial S|}{|S|}$$

is called the conductance or isoperimetric number of Γ.

Theorem

$$\Phi(\Gamma) \geq \lambda_{n-1}(L)/2.$$

The bisection width of a graph

The bisection width of a graph Γ is the value

$$\min_{S \subseteq V\Gamma, |S| = \lfloor |V\Gamma|/2 \rfloor} |\partial S|.$$

Theorem

The bisection width of a graph Γ is at least $\lambda_{n-1}(L)\lfloor |V\Gamma|/4 \rfloor$.

Example

The n-cube has $\lambda_{n-1}(L) = 2$, and has bisection width 2^{n-1}, reaching the equality.

$\mathrm{bip}(\Gamma)$

$$\mathrm{bip}(\Gamma) := \max_{S \subseteq V\Gamma, |S| \leq |V\Gamma|/2} |\partial S|$$

is the maximum number of edges in a spanning bipartite subgraph of Γ.

Proposition

$\mathrm{bip}(\Gamma) \leq n\lambda_1(L)/4$, *where* $n = |V\Gamma|$.

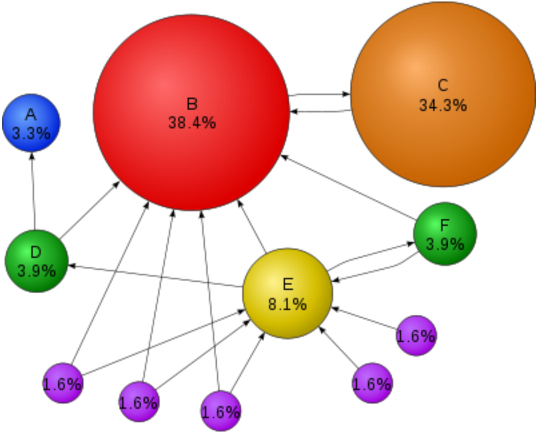
How to compute eigenvalues in practice?

$$\lambda_1 = \max_{\substack{x \in \mathbb{R}^n \\ x^\top x = 1}} x^\top A x, \qquad \lambda_n = \min_{\substack{x \in \mathbb{R}^n \\ x^\top x = 1}} x^\top A x.$$

Eigenvectors are also used in applications.

PageRank (http://en.wikipedia.org/wiki/PageRank)

PageRank was developed at Stanford University by Larry Page (hence the name Page-Rank) and Sergey Brin as part of a research project about a new kind of search engine.



Let A denote the adjacency matrix of a directed webgraph of order n and J is the all ones matrix of size n. Let d_i denote the out-degree of the node i, and D is a diagonal matrix with ii entry

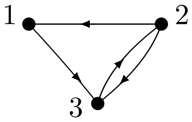
$$D_{ii} = \begin{cases} d_i, & \text{if } d_i \neq 0; \\ 1, & \text{if } d_i = 0. \end{cases}$$

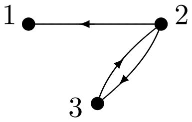
Then the positive left eigenvector of

$$M := \frac{1-0.85}{n} J + 0.85 D^{-1} A$$

corresponding to $\lambda_1(M)$ is used in the PageRank.

Example





$$M = \frac{1-0.85}{3}J + 0.85D^{-1}A = \begin{pmatrix} 0.05 & 0.05 & 0.9 \\ 0.475 & 0.05 & 0.475 \\ 0.05 & 0.9 & 0.05 \end{pmatrix}$$

has eigenvalue 1 with left eigenvector $P = (0.215, 0.388, 0.397)$.

$$M = \frac{1-0.85}{3}J + 0.85D^{-1}A = \begin{pmatrix} 0.05 & 0.05 & 0.05 \\ 0.475 & 0.05 & 0.475 \\ 0.05 & 0.9 & 0.05 \end{pmatrix}$$

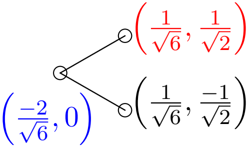
has eigenvalue 0.747 with left eigenvector $P = (0.297, 0.405, 0.297)$.

Google PageRank

Graph drawing

$$L = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

	Eigenvalues	eigenvectors
$\lambda_1(L)$	3	$x = \left(\frac{1}{\sqrt{6}}, \frac{-2}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right)$
$\lambda_2(L)$	1	$y = \left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}}\right)$
$\lambda_3(L)$	0	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$



1. $\sum x_i = 0 = \sum y_i$ (即質心在原點).
2. $\begin{pmatrix} x \\ y \end{pmatrix} \begin{pmatrix} x^\top & y^\top \end{pmatrix} = I_2$ (某種讓點分散一點的要求).
3. 在以上兩條件下使得 $\sum_{e_{ij} \in E\Gamma} (x_i - x_j)^2 + (y_i - y_j)^2$ 能得最小值 (此值已知為 $\lambda_1(L) + \lambda_2(L) = 4$).

Once a graph has been drawn nicely, one might want to study the graph in this particular drawing, e.g. how to cluster the vertices according to some given rule, how to cut the graph into two parts, etc.

How to compute eigenvector

We might normalize a matrix M so that 1 is an eigenvalue. Then starting for any vector x, the sequence

$$x, Mx, M^2x, M^3x, \cdots$$

will approach an eigenvector of M corresponding to the eigenvalue 1, provided the limit exists.

"Most introductory linear algebra courses impart the belief that the way to compute the eigenvalues of a matrix is to find the zeros of its characteristic polynomial. For matrices with order greater than two, this is false. Generally, the best way to obtain eigenvalues is to find eigenvectors."
(page 171, Algebraic Graph Theory by Chris Godsil and Gordon Royle.)

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

has eigenvalues

$$0, 0, 0, a.$$

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = 4 \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

Hence $a = 4$.

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = 4 \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

$$\left(4\right)\left(1\right) = 4\left(1\right).$$

4 is the common row sum of

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

$$\begin{pmatrix} 3 & 2 & 1 & 1 \\ 2 & 2 & 2 & 1 \\ 4 & 2 & 0 & 1 \\ -2 & 1 & 13 & 5 \end{pmatrix} \begin{pmatrix} a \\ a \\ a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ a \\ a \\ b \end{pmatrix}.$$

$$\begin{pmatrix} 6 & 1 \\ 12 & 5 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}.$$

Find the eigenvalues of

$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 3 & 1 & 0 & -2 \end{pmatrix}.$$

Try

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 3 & 1 & 0 & -1 \end{pmatrix}.$$

The latter has eigenvalues $0, 0, a+1, b+1$, so the first one has eigenvalues $-1, -1, a, b$.

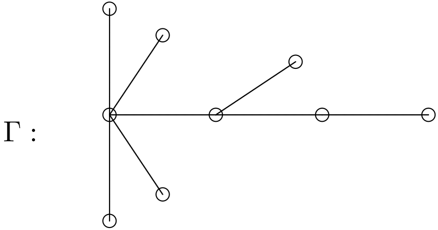
$$\begin{pmatrix} 2 & 1 \\ 4 & -2 \end{pmatrix} \text{ has eigenvalues } a = 2\sqrt{2}, b = -2\sqrt{2}.$$

Find the eigenvalues of

$$\begin{pmatrix} 0 & 1 & 1 & 3 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & -2 \end{pmatrix}.$$

Considering transpose, the eigenvalues are

$$-1, -1, 2\sqrt{2}, -2\sqrt{2}.$$



The graph has degree sequence $5, 3, 2, 1, 1, 1, 1, 1, 1$.

Theorem

The eigenvalue $\lambda_1(A)$ of $A(\Gamma)$ is at most

$$1+\sqrt{6}=\lambda_1\left(\begin{pmatrix}0 & 5\\ 1 & 2\end{pmatrix}\right).$$

Row-sums of the above 2×2 matrix are $5=d_1, 3=d_2$.

Proof.

Naming the vertices so that in the positive right eigenvector $(x_1, x_2, \ldots, x_9)^\top$ we have $x_1, x_2 \geq x_i$ for $i \geq 2$. Then

$$A \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_2 \end{pmatrix} \geq A \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_9 \end{pmatrix} = \lambda_1(A) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_9 \end{pmatrix}.$$

Considering the first two rows,

$$\lambda_1(A) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \leq \begin{pmatrix} I_2 & \mathbf{0} \end{pmatrix} A \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_2 \end{pmatrix} \leq \begin{cases} \begin{pmatrix} 0 & 5 \\ 1 & 3-1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, & \text{if } 1 \sim 2; \\ \begin{pmatrix} 0 & 5 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, & \text{if } 1 \not\sim 2. \end{cases}$$

Let (y_1, y_2) be the positive left eigenvector of

$$\begin{cases} \begin{pmatrix} 0 & 5 \\ 1 & 3-1 \end{pmatrix}, & \text{if } 1 \sim 2; \\ \begin{pmatrix} 0 & 5 \\ 0 & 3 \end{pmatrix}, & \text{if } 1 \not\sim 2. \end{cases}$$

Then

$$\begin{aligned} &(y_1, y_2)\lambda_1(A) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \leq &(y_1, y_2) \max \left\{ \lambda_1 \left(\begin{pmatrix} 0 & 5 \\ 1 & 3-1 \end{pmatrix} \right), \lambda_1 \left(\begin{pmatrix} 0 & 5 \\ 0 & 3 \end{pmatrix} \right) \right\} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ = &\max\{(1+\sqrt{6}), 3\}(y_1, y_2) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \end{aligned}$$

Deleting the positive value $y_1 x_1 + y_2 x_2$, we have

$$\lambda_1(A) \leq 1 + \sqrt{6}.$$

Stay here to see a more general result in the next talk.

Thanks for your attention.