Spectral characterization of graphs

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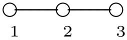
Notations

Let G be a simple connected graph of order n.

The adjacency matrix $A = (a_{ij})$ of G is a binary square matrix of order n with rows and columns indexed by the vertex set VG of G such that for any $i, j \in VG$, $a_{ij} = 1$ if i, j are adjacent in G.



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

Let $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$ denote the eigenvalues of A, and $\lambda_i(G) := \lambda_i(A)$.

Eigenvalues help us to realize the structure of a graph

Theorem

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

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 graph G,

$$(\lambda_n(G) - \lambda_1(G))/\lambda_n(G) \leq \chi(G) \leq \lambda_1(G) + 1.$$

□

Estimate the eigenvalues of a matrix by matrices of smaller sizes

It is well-known that

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

The following theorem generalizes this property.

Theorem (Cauchy interlacing theorem)

For $m < n$, and an $m \times n$ matrix S with $SS^\top = I$,

$$\lambda_i(A) \geq \lambda_i(SAS^\top),$$
$$\lambda_{n+1-i}(A) \leq \lambda_{m+1-i}(SAS^\top)$$

for $1 \leq i \leq m$. □

Example

Choose $S = [I\ 0]$ in block form and then $SAS^\top$ becomes the adjacency matrix of an induced subgraph of G.

List the eigenvalues of paths P_n and P_{n-1} of orders n and $n-1$ respectively:

$$\begin{array}{c} 2\cos\frac{\pi}{n+1} > 2\cos\frac{2\pi}{n+1} > 2\cos\frac{3\pi}{n+1} > \cdots > 2\cos\frac{(n-1)\pi}{n+1} > 2\cos\frac{n\pi}{n+1} \\ \searrow \quad 2\cos\frac{\pi}{n} > 2\cos\frac{2\pi}{n} > \qquad \cdots \qquad > 2\cos\frac{(n-1)\pi}{n} \nearrow \end{array}$$

The above method does not give us an upper bound of $\lambda_1(A)$.

Can we find a matrix M whose largest eigenvalue $\lambda_1(M)$ gives an upper bound of $\lambda_1(G)$?

Perron-Frobenius Theorem

Let $d_1 \geq d_2 \geq \cdots \geq d_n$ denote the degree sequence of G.

Theorem

$$\lambda_1(G) \leq d_1$$

with equality iff G is regular. □

Let $[d_1]$ be a 1×1 matrix. The above theorem says

$$\lambda_1(G) \leq \lambda_1([d_1]).$$

Another upper bound of $\lambda_1(G)$ is

Theorem (Stanley, 1987)

$$\lambda_1(G) \leq \frac{-1+\sqrt{1+8|EG|}}{2}$$

with equality if and only if G is the complete graph K_n. □

Equivalently, $\lambda_1(G)$ is bounded above by

$$\lambda_1\left(\begin{bmatrix} 0 & 1 & \cdots & & 1 & d_1-(n-1) \\ 1 & 0 & 1 & \cdots & 1 & d_2-(n-1) \\ \vdots & \ddots & \ddots & \ddots & \vdots & \\ & & & 1 & 0 & d_n-(n-1) \\ 1 & \cdots & & & 1 & d_{n+1}-n \end{bmatrix}_{(n+1)\times(n+1)}\right),$$

where $d_{n+1} := 0$, thinking of an isolated vertex being added.

An improvement of Stanley Theorem is

Theorem (Yuan Hong, Jin-Long Shu and Kunfu Fang, 2001)

$$\lambda_1(G) \le \frac{d_n - 1 + \sqrt{(d_n+1)^2 + 4(2|EG| - nd_n)}}{2},$$

with equality if and only if G is regular or there exists $2 \le t \le n$ such that $d_1 = d_{t-1} = n-1$ and $d_t = d_n$. □

Equivalently, $\lambda_1(G)$ is bounded above by

$$\lambda_1\left(\begin{bmatrix} 0 & 1 & \cdots & & 1 & d_1 - n + 2 \\ 1 & 0 & 1 & \cdots & 1 & d_2 - n + 2 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ & & & 1 & 0 & d_{n-1} - n + 2 \\ 1 & \cdots & & & 1 & d_n - n + 1 \end{bmatrix}_{n\times n}\right).$$

Another version is

Theorem (Kinkar Ch. Das, 2011)

$$\lambda_1(G) \leq \frac{d_2 - 1 + \sqrt{(d_2+1)^2 + 4(d_1 - d_2)}}{2},$$

with equality if and only if either G is regular, or $d_1 = n-1$ and $d_2 = d_n$. □

Equivalently,

$$\lambda_1(G) \leq \lambda_1\left(\begin{bmatrix} 0 & d_1 \\ 1 & d_2 - 1 \end{bmatrix}_{2\times 2}\right).$$

The parameter ϕ_ℓ

For $1 \leq \ell \leq n$, let

$$\phi_\ell(G) := \lambda_1 \left(\begin{bmatrix} 0 & 1 & \cdots & & 1 & d_1 - \ell + 2 \\ 1 & 0 & 1 & \cdots & 1 & d_2 - \ell + 2 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ & & & 1 & 0 & d_{\ell-1} - \ell + 2 \\ 1 & \cdots & & & 1 & d_\ell - \ell + 1 \end{bmatrix}_{\ell \times \ell} \right)$$

$$= \frac{d_\ell - 1 + \sqrt{(d_\ell + 1)^2 + 4 \sum_{i=1}^{\ell-1} (d_i - d_\ell)}}{2}.$$

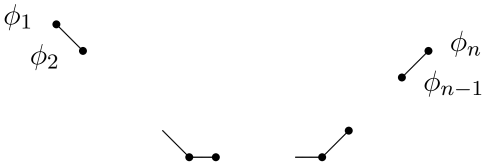
Theorem (Chia-an Liu, —, 2013)

For each $1 \le \ell \le n$,

$$\lambda_1(G) \le \phi_\ell(G),$$

with equality iff G *is regular or there exists* $2 \le t \le \ell$ *such that* $d_1 = d_{t-1} = n-1$ *and* $d_t = d_n$. □

Moreover, we show that the function $\phi_\ell(G)$ in variable ℓ is convex.



Small technical difficulty in the proof

The matrix

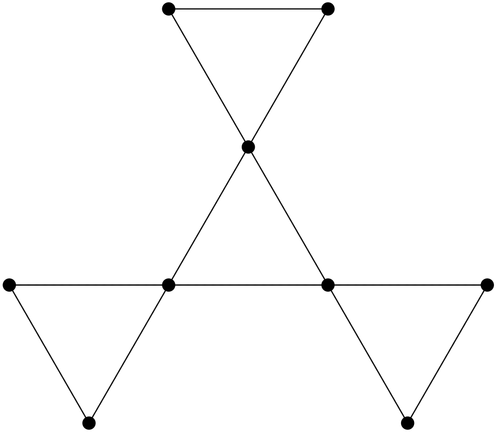
$$\begin{bmatrix} 0 & 1 & \cdots & & 1 & d_1-\ell+2 \\ 1 & 0 & 1 & \cdots & 1 & d_2-\ell+2 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ & & & 1 & 0 & d_{\ell-1}-\ell+2 \\ 1 & \cdots & & & 1 & d_\ell-\ell+1 \end{bmatrix}_{\ell\times\ell}$$

needs not to be nonnegative.

Our formal proof follows the idea of Jinlong Shu and Yarong Wu 2004, which applies Perron-Frobenius Theorem to $U^{-1}AU$ with some carefully selected diagonal matrix U.

The number $m_i := \frac{1}{d_i}\sum_{j\sim i} d_j$ is called the average 2-degree of i. List m_i in the decreasing ordering as

$$M_1 \geq M_2 \geq \cdots \geq M_n.$$



A non-regular graph with $M_1 = M_2 = \cdots = M_9 = 3$

Applying Perron-Frobenius Theorem to

$$\begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_n \end{pmatrix}^{-1} A \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_n \end{pmatrix},$$

we have

Theorem

$$\lambda_1(G) \leq M_1$$

with equality iff $M_1 = M_n$. □

An improvement of the upper bound M_1,

Theorem (Ya-hong Chen and Rong-yin Pan and Xiao-dong Zhang, 2011)

$$\lambda_1(G) \leq \frac{M_2 - a + \sqrt{(M_2 + a)^2 + 4a(M_1 - M_2)}}{2},$$

with equality iff $M_1 = M_n$, *where* $a = \max\{d_i/d_j \mid 1 \leq i, j \leq n\}$.

Equivalently,

$$\lambda_1(G) \leq \lambda_1 \left(\begin{bmatrix} 0 & M_1 \\ a & M_2 - a \end{bmatrix} \right).$$

Let $b \geq \max\{d_i/d_j \mid 1 \leq i, j \leq n, i \sim j\}$, and for $1 \leq \ell \leq n$, let

$$\psi_\ell(G) := \lambda_1 \left(\begin{bmatrix} 0 & b & \cdots & & b & M_1 - (\ell-2)b \\ b & 0 & b & \cdots & b & M_2 - (\ell-2)b \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ & & & b & 0 & M_{\ell-1} - (\ell-2)b \\ b & \cdots & & & b & M_\ell - (\ell-1)b \end{bmatrix}_{\ell \times \ell} \right)$$

$$= \frac{M_\ell - b + \sqrt{(M_\ell + b)^2 + 4b \sum_{i=1}^{\ell-1} (M_i - M_\ell)}}{2}.$$

Theorem (Yu-pei Huang, —, 2013)

For each $1 \leq \ell \leq n$,

$$\lambda_1(G) \leq \psi_\ell(G),$$

with equality iff $M_1 = M_n$. □

Problem: In the spirit of Cauchy interlacing theorem, give a uniform way to find a matrix M with $\lambda_1(A) \leq \lambda_1(M)$ that generalizes the above matrices.

Our second spectral characterization of graphs is related to distance-regular graphs.

We recall definition of DRGs and their basic properties.

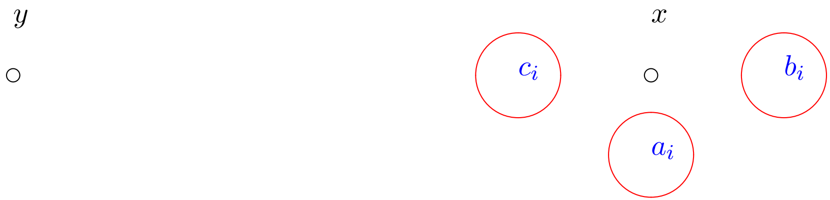
Distance-regular graphs

A graph G with diameter D is distance-regular if and only if for $i \leq D$,

$$
\begin{aligned}
c_i &:= |G_1(x) \cap G_{i-1}(y)|, \\
a_i &:= |G_1(x) \cap G_i(y)|, \\
b_i &:= |G_1(x) \cap G_{i+1}(y)|
\end{aligned}
$$

are constants subject to all vertices x, y with $\partial(x, y) = i$.

$\partial(x, y) = i$



Note that $a_i + b_i + c_i = b_0$ and $k := b_0$ is the valency of G.

Distance-Regular graphs, also called P-polynomial schemes, form an important subclass of association schemes.

"Association schemes are the frameworks on which coding theory, design theory and other theories developed in a unified and satisfactory way. .... There are many mathematical objects whose essence is that of association schemes and many different names are given to the essentially the same mathematical concept: Adjacency algebra, Bose-Mesner algebra, centralizer ring, Hecke ring, Schur ring, character algebra, hypergroup, probabilistic group, etc" ———Eiichi Bannai and Tatsuro Ito

Distance matrices

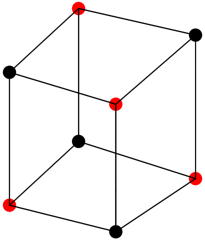
The matrices that we are concerned are square matrices with rows and columns indexed by the vertex set VG. Let α be an eigenvector of A corresponding to $\lambda_1(G)$ normalized to $\alpha^\top \alpha = n$. For each i let A_i be the matrix with entries

$$(A_i)_{xy} = \begin{cases} \alpha_x \alpha_y, & \text{if } \partial(x,y) = i; \\ 0, & \text{else.} \end{cases}$$

A_i is called i-th distance matrix of Γ. Note $A_0 = I$ and $A_{-1} = A_{D+1} = 0$.

If G is regular then $\alpha = (1, 1, \ldots, 1)^\top$, so A_i is binary and $A_1 = A$.

G



$$A_2 = \begin{pmatrix} 0&1&1&1&0&0&0&0\\ 1&0&1&1&0&0&0&0\\ 1&1&0&1&0&0&0&0\\ 1&1&1&0&0&0&0&0\\ 0&0&0&0&0&1&1&1\\ 0&0&0&0&1&0&1&1\\ 0&0&0&0&1&1&0&1\\ 0&0&0&0&1&1&1&0 \end{pmatrix},$$

$A_0 = I,$

$$A_1 = \begin{pmatrix} 0&0&0&0&1&1&1&0\\ 0&0&0&0&1&1&0&1\\ 0&0&0&0&1&0&1&1\\ 0&0&0&0&0&1&1&1\\ 1&1&1&0&0&0&0&0\\ 1&1&0&1&0&0&0&0\\ 1&0&1&1&0&0&0&0\\ 0&1&1&1&0&0&0&0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0 \end{pmatrix}.$$

Three-term recurrence relation of DRGs

Theorem

Let G be a regular graph. Then the following are equivalent.

1. *G is distance-regular;*
2. $AA_i = b_{i-1}A_{i-1} + a_iA_i + c_{i+1}A_{i+1} \qquad 0 \le i \le D$;
3. *there exist a unique sequence of polynomials $p_0(x) = 1$, $p_1(x) = x$, $\ldots$, $p_D(x)$ such that $\deg(p_i) = i$ and $A_i = p_i(A)$.*

□

The polynomials $p_0(x) = 1$, $p_1(x) = x$, $\ldots$, $p_D(x)$ are called distance polynomials of a DRG, but they can be reconstructed in a general graph.

Let G a general graph G with adjacency matrix A and minimal polynomial of degree $d+1$. Since A is symmetric, A has $d+1$ distinct eigenvalues. The number d is called the spectral diameter of G.

Define an inner product on the space of real polynomials of degrees at most d by

$$\langle f(\lambda), g(\lambda)\rangle = \frac{1}{n}\mathrm{trace}\left(f(A)g(A)^\top\right).$$

Then there exists a unique sequence of orthogonal polynomials $p_0(x)=1$, $p_1(x)$, ..., $p_d(x)$ such that

$$\deg(p_i)=i, \qquad \text{and} \qquad \langle p_i(x), p_i(x)\rangle = p_i(\lambda_1).$$

The number

$$p_d(\lambda_1)$$

is called the spectral excess of G; while the number

$$\delta_D := \frac{1}{n}\mathrm{trace}(A_D A_D^\top)$$

is called the excess of G. It is well-known that $d \geq D$.

When G is regular

$$\delta_D = \frac{1}{n} \sum_{x \in V(G)} |G_D(x)|$$

is the average number of vertices which have distance the diameter to a vertex.

Spectral Excess Theorem

Theorem (M.A. Fiol, E. Garriga and J.L.A. Yebra, 1996)

If G is regular then

$$\delta_D \leq p_d(\lambda_1),$$

with equality iff G is distance-regular. □

Short proofs are given by [E.R. van Dam, 2008] and [M.A. Fiol, S. Gago and E. Garriga, 2010].

Base on the short proofs, the regularity assumption of G is dropped in the Spectral Excess Theorem by [Guang-Siang Lee, ——, 2012].

Application

The odd girth of a graph is the smallest length of an odd cycle in the the graph.

Corollary (E.R. van Dam and W.H. Haemers, 2011)

A regular graph with odd girth $2d+1$ is a generalized odd graph. □

The above corollary generalizes the spectral characterization of generalized odd graphs [Tayuan Huang, 1994], [Tayuan Huang and Chao Rong Liu, 1999].

The regularity assumption is dropped in the above corollary by [Guang-Siang Lee, ——, 2012].

Near DRGs

Similar to the definition of excess, one can define

$$\delta_i := \frac{1}{n}\mathrm{trace}(A_i A_i^\top),$$

and want to characterize the graphs satisfying $\delta_i = p_i(\lambda_1)$ for some i.

A bipartite graph with bipartitin $V(G) = X \cup Y$ is biregular if there exist distinct integers $k \neq k'$ such that every $x \in X$ has degree k, and every $y \in Y$ has degree k'.

Proposition

Let G be a connected graph. Then $\delta_1 \geq p_1(\lambda_1)$, and the following statements are equivalent.

(i) $\delta_1 = p_1(\lambda_1)$,

(ii) $A_1 = p_1(A)$,

(iii) *G is regular or G is bipartite biregular.*

Theorem (Guang-Siang Lee, ——, 2013)

Let G be a connected bipartite graph with bipartition $X \cup Y$ and assume that the spectral diameter d is odd. Then the following are equivalent.

(i) $\delta_i = p_i(\lambda_1)$ *for even* i;

(ii) $\delta_{d-1} = p_{d-1}(\lambda_1)$;

(iii) G *is* 2*-partially distance-regular and both of the halved graphs* G^X *and* G^Y *are distance-regular* $\lfloor d/2 \rfloor$.

We shall provide two graphs that satisfy the above equivalent conditions, but are not distance-regular graphs.

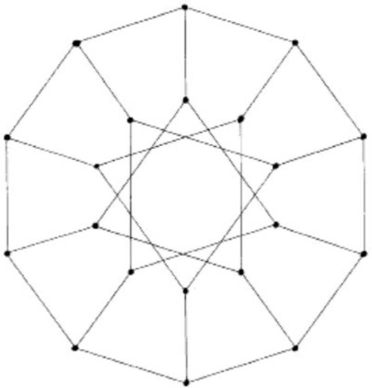
Example (W.H. Haemers and E. Spence, 1995)

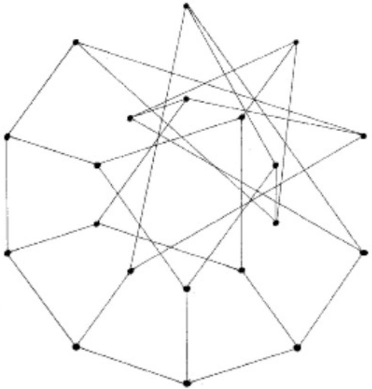
Consider the regular bipartite graphs G on 20 vertices obtained from the Desargues graph (the bipartite double of the Petersen graph) by the GM-switching. One can check (by Maple) that $D = d = 5$, sp $G = \{3^1, 2^4, 1^5, (-1)^5, (-2)^4, (-3)^1\}$, and

$$A_i = p_i(A) \qquad \text{iff} \qquad i \in \{0, 1, 2, 4\}.$$

Then G is not distance-regular.

Desargues graph and its cospectral mate

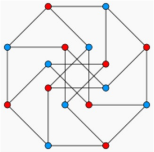




Example (D. Marušič and T. Pisanski, 2000)

Consider the Möbius-Kantor graph G. One can check (by Maple) that $D = 4 < 5 = d$, and

$$A_i = p_i(A) \qquad \text{iff} \qquad i \in \{0, 1, 2, 4\}.$$



Möbius-Kantor graph

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Thanks for your attention.

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