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Bounds of eigenvalues of graphs*

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Abstract

The eigenvalues of a graph are the eigenvalues of its adjacency matrix. This paper presents an algebraically defined invariant system of a graph. We get some bounds of the eigenvalues of graphs and propose a few open problems.

1. Introduction

Let G be a simple graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. Its adjacency matrix $A(G)=(a_{ij})$ is defined to be the $n \times n$ matrix (a_{ij}), where $a_{ij}=1$ if v_i is adjacent to v_j, and $a_{ij}=0$ otherwise. It follows immediately that if G is a simple graph, then $A(G)$ is a symmetric $(0,1)$ matrix in which every diagonal entry is zero. We shall denote the characteristic polynomial of G by

$$P(G)=\det(xI-A(G))=\sum_{i=0}^{n} a_i x^{n-i}.$$

Since $A(G)$ is a real symmetric matrix, its eigenvalues must be real, and may be ordered as

$$\lambda_1(A(G)) \geqslant \lambda_2(A(G)) \geqslant \cdots \geqslant \lambda_n(A(G)).$$

Denote $\lambda_i(A(G))$ simply by $\lambda_i(G)$. The sequence of n eigenvalues is called the spectrum of G. Spectra of graphs have appeared frequently in the mathematical literature. We shall now point out some reasons why graph spectra are important.

(1) Eigenvalues arise in a variety of applications, for example in quantum chemistry the skeletons of certain nonsaturated hydrocarbons are represented by graphs. The energy levels of the electrons in such a molecule are, in fact, the eigenvalues of

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the corresponding graph. The stability of the molecule as well as other chemically relevant facts are closely connected with the graph spectrum and the corresponding eigenvalues.

(2) Spectrum techniques are often used in the proofs of many theorems in graph theory and combinatorial theory, even though the statements of these theorems do not involve the spectra explicitly. One such example is the well-known 'friendship theorem'.

(3) The spectrum can be computed in polynomial time. This is regarded as an 'accessible' property of G. Conversely, some properties of G, like its chromatic number, are thought of as 'inaccessible' because to date no one knows how to compute them in polynomial time.

What kind of relationships might exist between the spectrum and the structure of G?

We know that the structure of a graph is not completely determined by its spectra. The two graphs shown in Fig. 1 are cospectral but not isomorphic.

There are many other examples of nonisomorphic cospectral graphs. For example, it is known that 'almost all' trees are cospectral.

For a few special classes of graphs, including the complete graphs, cycles, paths and the complete bipartite graphs, the known spectra are given in Table 1.

In general, eigenvalues of graphs are often difficult to evaluate for some classes of graphs, so it is sometimes useful to obtain bounds for them.

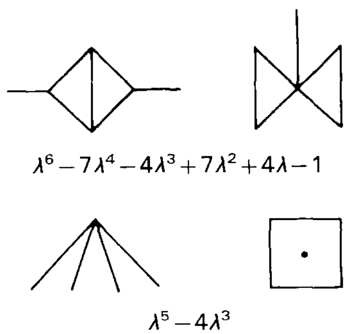


Fig. 1

Table 1
Spectra of some classes of graphs

Graph	Spectrum
Complete graph K_n	$n-1,-1,\dots,-1$
Cycle C_n	$2\cos(2\pi i/n)\quad(0\leqslant i\leqslant n-1)$
Path P_n	$2\cos(2\pi i/(n+1))\quad(1\leqslant i\leqslant n)$
Complete bipartite graph K_{ab} $(a+b=n)$	$\sqrt{ab},0,\dots,-\sqrt{ab}$

2. The spectral radius of graphs

The largest eigenvalue $\lambda_1(G)$ is often called the spectral radius of G. We now give some bounds for the spectral radius $\lambda_1(G)$.

Let G be a simple graph with n vertices and e edges.

(1) (Collatz and Sinogowitz [6]). If G is a connected graph of order n, then

$$2\cos(\pi/(n+1))=\lambda_1(P_n)\leqslant\lambda_1(G)\leqslant\lambda_1(K_n)=n-1.$$

The lower bound occurs only when G is the path P_n and the upper bound occurs only when G is the complete graph K_n.

(2) (Collatz and Sinogowitz [6]). If G is a tree of order n, then

$$2\cos(\pi/(n+1))=\lambda_1(P_n)\leqslant\lambda_1(G)\leqslant\lambda_1(K_{1,n-1})=\sqrt{n-1}.$$

The lower bound occurs only when G is the path P_n, and the upper bound occurs only when G is the star $K_{1,n-1}$.

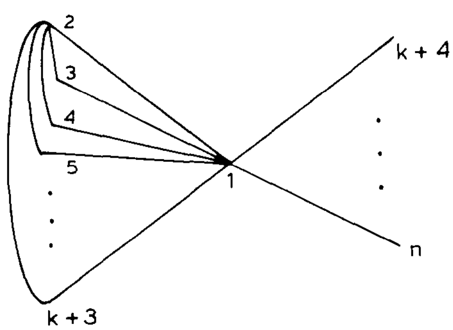
(3) (Hong [12]). If G is a connected unicyclic graph, then

$$2=\lambda_1(C_n)\leqslant\lambda_1(G)\leqslant\lambda_1(S_n^3),$$

where C_n denotes the cycle on n vertices and S_n^3 denotes the graph obtained from the star $K_{1,n-1}$ by joining the vertices of degree one. The lower bound occurs only when G is the cycle C_n, and the upper bound occurs only when G is the graph S_n^3.

(4) (Brualdi and Solheid [4]). Let G be a connected graph with n vertices and e edges having the largest possible spectral radius. Then G contains a star as a spanning tree. This fact can be used to determine the graphs with maximum spectral radius when $e\leqslant n+5$ and n is sufficiently large (see Fig. 2).

Conjecture 2.1 (Brualdi and Solheid [4]). For $e=n+k$, $k\neq 2$, the graph withe maximum spectral radius is as follows (n is sufficiently large):



$e=n+k$

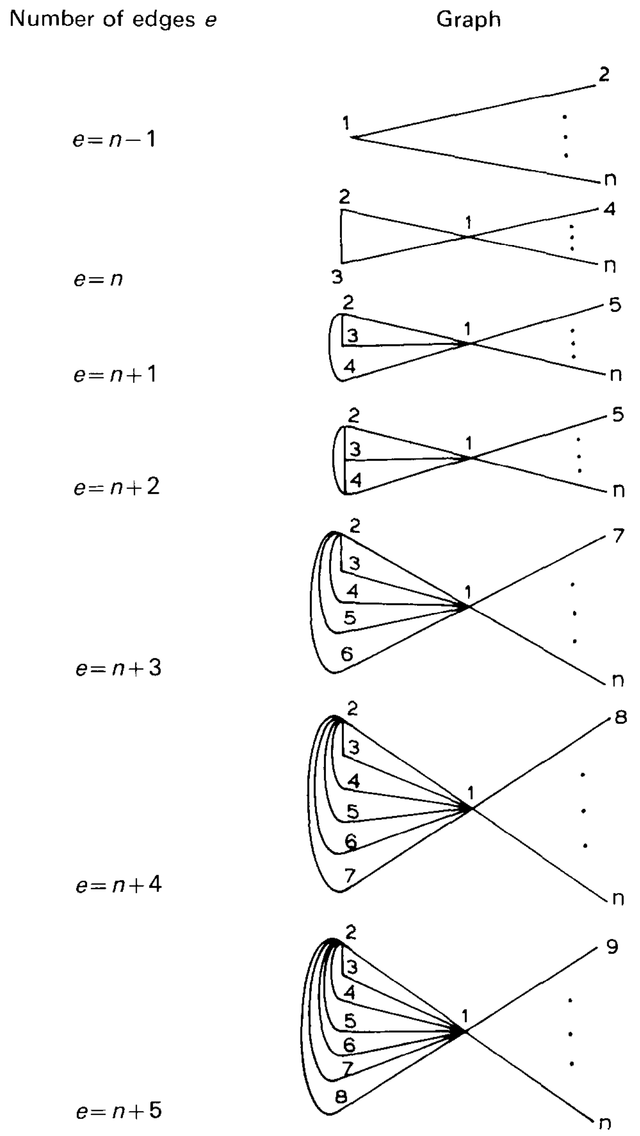


Fig. 2.

The graph is obtained from the star $k_{1,n-1}$ by adding the edges from vertex 2 to each of vertices $3, 4, \ldots, k+3$.

(5) (Brualdi and Hoffman [3]). If $e=\binom{k}{2}$, then

$$\lambda_1(G) \leqslant k-1,$$

where the equality holds iff G is a disjoint union of the complete graph K_k and some isolated vertices.

(6) (Stanley [19])

$$\lambda_1(G) \leqslant (-1+\sqrt{1+8e})/2$$

where the equality occurs iff $e=\binom{k}{2}$ and G is a disjoint union of the complete graph K_k and some isolated vertices.

(7) (Hong [15]). If G is a connected graph, then

$$\lambda_1(G) \leqslant \sqrt{2e-n+1}, \tag{**}$$

where the equality holds iff G is one of the following graphs:

(a) the star $K_{1,n-1}$;

(b) the complete graph K_n.

Proof. Let A_i denote the ith row of A and d_i the ith row sum of A. Let $X=(x_1, x_2, \ldots, x_n)^T$ be an unit length eigenvector of A corresonding to the eigenvalue $\lambda_1(A)$. For $i=1,2,\ldots,n$, let $X(i)$ denote the vector obtained from X by replacing those components x_j by 0 such that $a_{ij}=0$. Since $AX=\lambda_1 X$, we have

$$A_i X(i) = A_i X = \lambda_1(A) x_i.$$

By the Cauchy–Schwartz inequality, for $i=1,2,\ldots,n$, we have

$$\lambda_1(A)^2 x_i^2 = |A_i X(i)|^2 \leqslant |A_i|^2 |X(i)|^2 = d_i\left(1-\sum_{j:\, a_{ij}=0} x_j^2\right).$$

Summing the above inequalities we obtain

$$\lambda_1(A)^2 \leqslant 2e - \sum_{i=1}^n d_i \sum_{j:\, a_{ij}=0} x_j^2.$$

Now

$$\begin{aligned}\sum_{i=1}^n d_i \sum_{j:\, a_{ij}=0} x_j^2 &= \sum_{i=0}^n d_i x_i^2 + \sum_{i=1}^n d_i \sum_{j:\, a_{ij}=0 \quad j\neq i} x_j^2 \\ &\leqslant \sum_{i=0}^n d_i x_i^2 + \sum_{i=1}^n \sum_{j:\, a_{ij}=0 \quad j\neq i} x_j^2 \\ &= \sum_{i=0}^n d_i x_i^2 + \sum_{i=1}^n (n-1-d_i) x_i^2 \\ &= n-1. \end{aligned} \tag{*}$$

Therefore, we have

$$\lambda_1(A) \leqslant \sqrt{2e-n+1}. \tag{**}$$

In order for equality to hold, all inequalities in the above argument must be equalities. In particular, from (*) we must have that

$$\sum_{i=1}^{n} d_i \sum_{j:a_{ij}=0} \sum_{i\neq j} x_j^2 = \sum_{i=1}^{n} \sum_{j:a_{ij}=0} \sum_{i\neq j} x_j^2.$$

Hence, either $d_i=1$ or $d_i=n-1$ $(1\leqslant i\leqslant n)$, which implies either

(a) G is the star $K_{1,n-1}$, or

(b) G is the complete graph K_n.

Conversely, it is easy to verify that the equality is satisfied by the graphs $K_{1,n-1}$ and K_n.

Remark. Inequality (**) holds for all graphs without isolated vertices. Since $e=\binom{k}{2}$ implies $(-1+\sqrt{1+8e})/2=k-1$ and $e\leqslant\binom{k}{2}$ *implies* $(\sqrt{2e-n+1}\leqslant(-1+\sqrt{1+8e})/2$, the upper bound in (7) is an improvement on the upper bound in (6) while the upper bound in (5) is a special case of the upper bound in (6).

Now let D be a digraph, let $d^+(v)$ and $d^-(v)$ be the out-degree and in-degree, respectively, of the vertex v in D. A digraph is said to be 'balanced' if $d^+(v)=d^-(v)$ for every vertex v in D. An undirected graph G can be considered as a symmetric diagraph $D=D(G)$, such that there are two arcs (u,v) in D for every edge (u,v) in G.

Let D be a balanced strongly connected digraph with n vertices and m arcs. Let A be the adjacency matrix of D. Then the spectral radius $\lambda_1(D)$ of $A(D)$ satisfies

$$\lambda_1(D)\leqslant\sqrt{m-n+1}$$

with equality iff D is the star $K_{1,n-1}$ or the complete graph K_n.

We now give some open problems on the spectral radius of a graph.

Problem 1: Let G be a connected planar graph with n vertices. We already know [15] that

$$2\cos(\pi/(n+1))=\lambda_1(P_n)\leqslant\lambda_1(G)\leqslant\lambda_1(G^*)\leqslant\sqrt{5n-11},$$

where G^* is the maximum planar graph (a planar graph G^* is called maximal planar graph if, for every pair of nonadjacent vertices u and v of G^*, the graph G^*+uv is nonplanar on n vertices. What is the spectral radius of a graph G^*?

Problem 2: Let G be a connected graph with n vertices and chromatic number k. We already know that

$$k-1\leqslant\lambda_1(G)\leqslant(k-1)n/k.$$

what is the best possible lower bound?

Problem 3: Let G be a simple connected nonregular graph with n vertices and e edges. We denote by $\delta(G)$ and $\Delta(G)$ the minimum and the maximum degree, respectively, of G. If G has the smallest possible spectral radius, is it true that $\Delta-\delta\leqslant 1$?

Problem (proposed by Brualdi and Li [2]): Let T_n denote a tourament with n vertices and $A(T_n)=(a_{ij})$, the adjacency matrix of T_n, where $a_{ij}=1$ if there is an arc from v_i to v_j and 0 otherwise. Is it true that $\lambda_1(\tilde{T}_n)<\lambda_1(T_n)\leqslant\lambda_1(\bar{T}_n)$ where

$$A(\tilde{T}_n)=\begin{pmatrix} 0 & 1 & 0 & & & & & & 0 \\ 0 & 0 & 1 & 0 & & & & & \\ 1 & 0 & 0 & 1 & 0 & & & & \\ & 1 & 0 & 0 & 1 & . & & & \\ & & . & . & . & . & . & & \\ & & & . & . & . & . & . & \\ & & & & . & . & . & & 0 \\ & & & & & . & . & . & 1 \\ 1 & & & & & & 1 & 0 & 0 \end{pmatrix},$$

$$A(\bar{T}_n)=\left(\begin{array}{cccccc|cccccc} 0 & 1 & & & & 1 & 0 & 0 & . & . & . & 0 \\ 0 & 0 & 1 & & & & 1 & 0 & 0 & . & . & \\ & 0 & 0 & 1 & \mathbf{1} & & & 1 & 0 & 0 & . & . \\ & & . & . & . & & & & . & . & . & . \\ & & & . & . & . & & & & . & . & . \\ & \mathbf{0} & & & . & . \; 1 & & \mathbf{1} & & & . \; . & 0 \\ 0 & & & & 0 & 0 & 1 & & & & 1 & 0 \\ \hline 1 & 0 & & & & 0 & 0 & 1 & & & & 1 \\ 1 & 1 & 0 & & & & 0 & 0 & 1 & & & \\ . & 1 & 1 & 0 & \mathbf{0} & & & 0 & 0 & 1 & \mathbf{1} & \\ . & . & . & . & . & & & & . & . & . & \\ . & . & . & . & . & . & & & & . & . & . \\ & & & & . \; . & 0 & & \mathbf{0} & & & . \; . & 1 \\ 1 & . & . & . & 1 & 1 & 0 & & & & 0 & 0 \end{array}\right).$$

3. Some results on $\lambda_i(G)$

(1) (Brigham and Dutton [1]).

$$-\sqrt{(2e(i-1)/n(n-i+1))}\leqslant\lambda_i(G)\leqslant\sqrt{(2e(n-i)/ni)}\quad(1\leqslant i\leqslant n).$$

(2) (Constantine [7], Hong [14] and Powers [17]). Let G be a simple graph with n vertices. Then

$$\lambda_n(G)\geqslant-\sqrt{(n/2)[(n+1)/2]},$$

where $[x]$ denotes the largest integer not greater than x. The equality holds iff G is the complete bipartite graph $K_{[n/2][(n+1)/2]}$.

Proof. Let $X=(x_1,x_2,\dots,x_n)^T$ be an unit length eigenvector of $A(G)$, corresponding to the eigenvalue $\lambda_n(G)$. Without loss of generality, we assume that $x_1,x_2,\dots,x_a$ are positive and $x_{a+1},\dots,x_n$ are nonpositive. Let $b=n-a$, then $\lambda_n(G)$ is the smallest eigenvalue of $A(G)$, and we have

$$\begin{aligned}\lambda_n(G)=\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j &\geqslant \sum_{x_kx_l<0} a_{kl}x_kx_l\\ &\geqslant \lambda_n(K_{ab})\\ &\geqslant \lambda_n(K_{[n/2][(n+1)/2]})\\ &= -\sqrt{[n/2]\cdot[(n+1)/2]}.\end{aligned}$$

In order for the equality to hold, all inequalities in the above argument must be equalities. It follows that the equality holds if and only if G is the complete bipartite graph $K_{[n/2][(n+1)/2]}$.

(3) (Hong [13]). Let G be a tree, then

$$0\leqslant\lambda_i(G)\leqslant\sqrt{[(n-2)/i]}\quad(2\leqslant i\leqslant[n/2]),$$

where $[x]$ denotes the largest integer not greater than x. The upper bound is best possible for $n\equiv 1 \pmod{i}$.

(4) (Godsil [11]). Let F be a forest of order $2s$ with a perfect matching. Then

$$\lambda_s(F)\geqslant\lambda_s(P_{2s})$$

with equality iff $F\cong P_{2s}$, where P_{2s} is the path on $2s$ vertices.

(5) (Hong [16]). Let F be a forest with n vertices, $\lambda(F)$ be the smallest positive eigenvalue of F, and t the largest integer not greater than $n/2$. Then

$$\lambda(F)\geqslant\lambda_t(P_{2t})=2\cos(t\pi/(2t+1)),$$

where P_{2t} is a path on $2t$ vertices. The equality holds iff n is even and $F\cong P_n$.

Denote by $S_{\Delta}^{n-\Delta}$ $(\Delta\leqslant n-2)$ the tree with n vertices obtained from the star $K_{1,\Delta-1}$ and the path $P_{n-\Delta}$ by connecting a vertex of degree one on $P_{n-\Delta}$ with the vertex of degree $\Delta-1$ on $K_{1,\Delta-1}$.

(6) (Hong [16]). Let T be a tree with n vertices which is neither the star $K_{1,n-1}$ nor the tree S_{n-2}^2. Then $\lambda_2(T)\geqslant 1$.

Conjecture (Hong [16]). Let T be a tree of order n with the size of the maximum matching q. If $k\leqslant q$, then

$$\lambda_k(T)\geqslant\lambda_k(S_{n-2k+2}^{2k-2})$$

with equality iff $T\cong S_{n-2k+2}^{2k-2}$.

(7) (Chen and Cao [5]). Let F be a forest with edge-independence number q. Then for $1 \leqslant i \leqslant [q/2]$

$$\lambda_{[(q+1)/2]+i}(F) \geqslant 2\cos(2\pi i/(4i+1)) \quad \text{for even } q,$$

$$\lambda_{[(q+1)/2]+i}(F) \geqslant 2\cos(2(i+1)\pi/(4i+3)) \quad \text{for odd } q,$$

where $[x]$ denotes the largest integer not greater than x.

(8) (Shao [18]). Let G be a tree on n vertices. Then

$$\lambda_i(G) \leqslant \sqrt{[n/i]-1} \quad (2 \leqslant i \leqslant [n/2]),$$

where $[x]$ denotes the largest integer not greater than x. The upper bound is the best possible for $n \not\equiv 0 (\mathrm{mod}\, i)$.

(9) (Hong [14] and Powers [17])

$$-1 \leqslant \lambda_2(G) \leqslant (n-2)/2.$$

The lower bound occurs only when G is the complete graph K_n and the upper bound occurs only when n is even and $G \cong 2K_{n/2}$.

Let G be a simple connected graph with $n \geqslant 2$ vertices. Then

$$\begin{aligned} -1 \leqslant \lambda_2(G) &\leqslant -1-\lambda_n(K_{[n/2],[(n+1)/2]}-e) \\ &\leqslant \sqrt{(n^2-4)/4}-1, \end{aligned}$$

where e is an edge of $K_{[n/2],[(n+1)/2]}$.

Problem: Find the best possible lower and upper bounds for the kth eigenvalue of graphs with n vertices.

For other results on the bounds of eigenvalues of graphs, see [8–10].

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