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Graphs for which the least eigenvalue is minimal, I[☆]

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Abstract

Let G be a connected graph whose least eigenvalue $\lambda(G)$ is minimal among the connected graphs of prescribed order and size. We show first that either G is complete or $\lambda(G)$ is a simple eigenvalue. In the latter case, the sign pattern of a corresponding eigenvector determines a partition of the vertex set, and we study the structure of G in terms of this partition. We find that G is either bipartite or the join of two graphs of a simple form.

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1. Introduction

Let $G = (V_G, E_G)$ be a simple graph, with vertex set V_G and edge set E_G. Its *order* is $|V_G|$, denoted by n, and its *size* is $|E_G|$, denoted by m. We write $u \sim v$ to indicate that vertices u and v are adjacent, and we write A_G for the (0, 1)-adjacency matrix of G. The zeros of $\det(xI - A_G)$ are called the *eigenvalues of G*; recall that they are real since A_G is symmetric. We write $\lambda(G)$ for the least eigenvalue of G.

There are many results in the literature concerning the largest eigenvalue (*spectral radius* or *index*) of simple graphs; see, e.g. [7] or [6]. Much less is known about the least eigenvalue. Recall first that the least eigenvalue of any graph is non-positive. It is equal to zero only for totally disconnected graphs. Otherwise, for graphs with at least one edge, it is less than or equal to -1 (by the Interlacing Theorem – see [4, p. 19]); it is equal to -1 if each component is a complete graph. For all other graphs it is less than or equal to $-\sqrt{2}$, the least eigenvalue of $K_{1,2}$ (again by the Interlacing Theorem). Graphs with least eigenvalue not less than -2 are studied extensively in the literature (see [8] for details). In this paper we study connected graphs whose least eigenvalue is minimal among graphs of prescribed order and size.

If we drop the requirement of connectedness, then the minimal least eigenvalue is attained by a graph with at most one non-trivial component (and our results apply to this component). To see this, note first that since the spectrum of a disconnected graph is the union of spectra of its components, we know that the least eigenvalue of a disconnected graph is the least eigenvalue of one of these components. Secondly, by the Interlacing Theorem, we have

$$\lambda(G \cdot H) \leqslant \min\{\lambda(G), \lambda(H)\} = \lambda(G \cup H); \tag{1}$$

here $G \cdot H$ denotes any coalescence of the graphs G and H [4, p. 158], and $G \cup H$ denotes the disjoint union of G and H. Therefore, if G is a disconnected graph with at least two non-trivial components, say G_1 and G_2, then a graph G' obtained from G by replacing $G_1 \cup G_2$ with $(G_1 \cdot G_2) \cup K_1$ is such that $\lambda(G') \leqslant \lambda(G)$. By extending this argument to the remaining non-trivial components we obtain a graph (of the same order and size, with just one non-trivial component) whose least eigenvalue cannot be larger than the least eigenvalue of G.

To make our statements more precise, let $G(n, m)$ be the set of graphs of order n and size m, and define

$$f(n, m) = \min\{\lambda(G) : G \in G(n, m)\},$$
$$g(n, m) = \min\{\lambda(G) : G \in G(n, m) \text{ and } G \text{ is connected}\}.$$

Then we have:

Proposition 1.1. *With the notation above*, $f(n, m) =$

$$\min\{g(k, m) : k \leqslant n \text{ and } G(k, m) \text{ contains at least one connected graph}\}.$$

Example 1.2. From [3,4,5] we see that $f(7, 9) = \lambda(K_{3,3} \cup K_1) = -3$, while $g(7, 9) \approx -2.92081$.

In view of Proposition 1.1 we shall be able to restrict our investigation to connected graphs. However, the scope of k in the formula of Proposition 1.1 can be further reduced, as we shall see in a further paper.

For graphs of given order, we have the following result of Constantine [2].

Theorem 1.3. *If G is a graph of order n then*

$$\lambda(G) \geqslant -\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil},$$

with equality if and only if $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Another relevant result appeared in [15]:

$$\lambda(G) \geqslant -\sqrt{m},$$

where m is the size of the graph G.

These results were improved by Favaron et al. [10]:

$$\lambda(G) \geqslant -\sqrt{\mathrm{MaxCut}(G)},$$

where $\mathrm{MaxCut}(G)$ is the size of a maximal bipartite subgraph of G.

For any non-complete connected graph G of order $n \geqslant 4$ we have the bounds

$$-\frac{n}{2} \leqslant \lambda(G) < -\frac{1}{2}\left\{1 + \sqrt{1 + 4\frac{n-3}{n-1}}\right\}.$$

The lower bound follows from Theorem 1.3, and the upper bound is due to Yong [17]. Note also that as n tends to $+\infty$, the upper bound tends to $-\frac{\sqrt{5}+1}{2}$. This is the largest limit point for the least eigenvalue (see [12]); the second largest limit point is $-\sqrt{3}$. The families of graphs having these two numbers as limit points for the least eigenvalue are characterized in [9].

We mention also an earlier result of Hoffman [11]:

$$\lambda(G) \geqslant \frac{-\rho(G)}{\chi(G) - 1},$$

where $\rho(G)$ is the index of G and $\chi(G)$ is the chromatic number of G.

For K_{r+1}-free graphs G, of order n and size m, the upper bound

$$\lambda(G) < -\frac{2}{r}\left(\frac{2m}{n^2}\right)^r n$$

is established in [14].

Some lower bounds for graphs of fixed order and size also appear in the literature, for example in respect of planar graphs, or more generally in respect of graphs having prescribed Euler characteristic (see [13]).

We focus our attention on the structure of a graph G whose least eigenvalue is minimal among the connected graphs with prescribed order n and size m. In Section 2 we give some preliminary results, using Rayleigh quotients as a tool. In Section 3, we show that the least eigenvalue is simple when $m < \binom{n}{2}$, and show that in this case G is either bipartite or the join of two graphs of a simple form.

2. Preliminaries

For any unit vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$, we have $\lambda(G) \leqslant \mathbf{x}^{\mathrm{T}} A_G \mathbf{x}$, with equality if and only if $\mathbf{x}$ is an eigenvector of A_G corresponding to $\lambda(G)$ (see [7, Section 3.1]). Thus

$$\lambda(G) = \min_{||\mathbf{x}||=1} \mathbf{x}^{\mathrm{T}} A_G \mathbf{x} = \min 2\Sigma_{uv \in E_G} x_u x_v. \tag{2}$$

In what follows we assume that $\mathbf{x}$ is a unit eigenvector of A_G corresponding to $\lambda(G)$. Let G' be a graph obtained from G by relocating an edge, and let $A_{G'}$ be its adjacency matrix. Then from (2) we obtain:

$$\lambda(G') - \lambda(G) = \min_{||\mathbf{y}||=1} \mathbf{y}^{\mathrm{T}} A_{G'}\mathbf{y} - \mathbf{x}^{\mathrm{T}} A_G \mathbf{x} \leqslant \mathbf{x}^{\mathrm{T}}(A_{G'} - A_G)\mathbf{x}. \tag{3}$$

Lemma 2.1. *Let G' be the graph obtained from the graph G by rotating the edge rs (around r) to the non-edge position rt.*
Then

(i) $\lambda(G') < \lambda(G)$ *if* $x_r < 0$ *and* $x_s \leqslant x_t$, *or* $x_r = 0$ *and* $x_s \neq x_t$, *or* $x_r > 0$ *and* $x_s \geqslant x_t$;
(ii) $\lambda(G') \leqslant \lambda(G)$ *if* $x_r = 0$ *and* $x_s = x_t$.

Proof. From (3) we have

$$\lambda(G') - \lambda(G) \leqslant 2x_r(x_t - x_s). \tag{4}$$

In considering the relation (4), we distinguish two cases.

Case $x_r = 0$. Then $\lambda(G') \leqslant \lambda(G)$. If $x_s \neq x_t$ then $\lambda(G') < \lambda(G)$. For otherwise, if $\lambda = \lambda(G') = \lambda(G)$, then $\mathbf{x}$ must be an eigenvector of G' corresponding to its least eigenvalue (see (3)). Therefore, in G', we must have $\lambda x_r = \sum_{v\sim r} x_v$; but this cannot be the case when $x_s \neq x_t$. (Note that if $x_s = x_t$ then $\mathbf{x}$ as an eigenvector of G' corresponding to $\lambda(G)$, but $\lambda(G)$ is not necessarily the least eigenvalue of G'.)

Case $x_r \neq 0$. Without loss of generality, $x_r > 0$ (for otherwise, we may replace $\mathbf{x}$ by $-\mathbf{x}$). If $x_t < x_s$ then it follows at once from (4) that $\lambda(G') < \lambda(G)$. Assume next that $x_t = x_s$, so that certainly $\lambda(G') \leqslant \lambda(G)$. If $\lambda = \lambda(G') = \lambda(G)$ then, as above, $\mathbf{x}$ must be an eigenvector of G' corresponding to λ. This is impossible since, in G', we have $\lambda x_u \neq \sum_{v\sim u} x_v$ for u equal to s (or t).

This completes the proof. □

Lemma 2.2. *Let G' be the graph obtained from the graph G by relocating the edge ab to the non-edge position cd, where $\{a, b\} \cap \{c, d\} = \emptyset$. Then*

(i) $\lambda(G') < \lambda(G)$ *if* $x_c x_d < x_a x_b$;
(ii) $\lambda(G') \leqslant \lambda(G)$ *if* $x_c x_d = x_a x_b$, *and in this situation*, $\lambda(G') = \lambda(G)$ *only if* $x_a = x_b = x_c = x_d = 0$.

Proof. From (3) we have

$$\lambda(G') - \lambda(G) \leqslant 2(x_c x_d - x_a x_b). \tag{5}$$

It follows immediately that $\lambda(G') < \lambda(G)$ if $x_c x_d < x_a x_b$. Suppose that $x_c x_d = x_a x_b$. Then $\lambda(G') \leqslant \lambda(G)$ from (5), and (as before) if $\lambda = \lambda(G') = \lambda(G)$ then $\mathbf{x}$ is an eigenvector of G' corresponding to λ. Now all the eigenvalue equations $\lambda x_u = \sum_{v\sim u} x_v$ are satisfied in G' only when x_a, x_b, x_c and x_d are all equal to 0.

This completes the proof. □

Remark. In Lemmas 2.1(ii) and 2.2(ii), we do not know whether strict inequality ($\lambda(G') < \lambda(G)$) can occur.

3. Structural considerations

Throughout this section, G denotes a non-trivial connected graph of order n and size m whose least eigenvalue is minimal. We let $(x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ be an eigenvector $\mathbf{x}$ corresponding to $\lambda(G)$, and we consider the partition of V_G induced by the sign pattern of the entries of $\mathbf{x}$. Accordingly, we define

$V^-(\mathbf{x}) = \{u \in V_G : x_u < 0\}$, the set of *negative vertices* with respect to $\mathbf{x}$;
$V^0(\mathbf{x}) = \{u \in V_G : x_u = 0\}$, the set of *zero vertices* with respect to $\mathbf{x}$;
$V^+(\mathbf{x}) = \{u \in V_G : x_u > 0\}$, the set of *positive vertices* with respect to $\mathbf{x}$.

We first prove:

Lemma 3.1. *If* $V^0(\mathbf{x}) \neq \emptyset$ *then* $\deg(u) = n - 1$ *for any vertex* $u \in V^0(\mathbf{x})$.

Proof. Assume the contrary, and let r be a vertex in $V^0(\mathbf{x})$ such that $\deg(r) < n - 1$. Let $S_r = \{s \in V_G : s \sim r\}$, and $T_r = \{t \in V_G : t \not\sim r, t \neq r\}$. Note that $S_r \neq \emptyset$ because G is connected and non-trivial. Now choose a vertex s from S_r and a vertex t from T_r. Let G' be the graph obtained from G by rotating the edge rs around r to rt.

Assume first that G' is connected for any choice of s and t. If $x_s \neq x_t$ for some s and t then $\lambda(G') < \lambda(G)$ by Lemma 2.1(i). This contradicts the choice of G, and so $x_s = x_t$ for any choice of s and t. But then $x_v = c$ for any $v \neq r$, where c is a real constant. Now $\lambda(G)x_r = \sum_{v \in S_r} x_v = \deg(r)c$. Since $\deg(r) \neq 0$ and $x_r = 0$, we conclude that $c = 0$ and hence $\mathbf{x} = \mathbf{0}$, a contradiction.

Now suppose that, for some choice of s and t, the graph G' is disconnected. Then rs must be a bridge in G, and s, t lie in different components G_s, G_t of G', respectively. Let t' be a vertex (if any) in G_s different from s. Note that $t' \in T_r$, for otherwise there exists an r–s path in G avoiding the bridge rs. If $x_s \neq x_{t'}$, then we obtain a contradiction by applying the above argument to t' instead of t (note that the corresponding graph G' is now connected). Consequently, $x_u = x_s$ for every $u \in V_{G_s}$. By the eigenvalue equation for the vertex s, applied in G, we obtain $\lambda(G)x_s = (\deg(s) - 1)x_s$, whence $x_s = 0$. Therefore, G_t contains a vertex u such that $x_u \neq 0$. Now the graph G'' obtained from G by rotating sr to su is connected, and $\lambda(G'') < \lambda(G)$ by Lemma 2.1(i).

This final contradiction completes the proof. $\square$

Theorem 3.2. *Let G be a connected graph whose least eigenvalue $\lambda(G)$ is minimal among the connected graphs of order n and size $m < \binom{n}{2}$. Then $\lambda(G)$ is a simple eigenvalue of G.*

Proof. Suppose that $\lambda(G)$ has multiplicity at least two. Then, for any vertex $u \in V_G$, there exists an eigenvector $\mathbf{x}$ whose uth entry is equal to zero (so that $u \in V^0(\mathbf{x})$ and $V^0(\mathbf{x}) \neq \emptyset$). Since G is not complete, we may choose u to be a vertex such that $\deg(u) < n - 1$. Now we have a contradiction to Lemma 3.1, and the proof follows. $\square$

As an immediate consequence of Theorem 3.2 we see that if G is not complete then the partition of V_G induced by the sign pattern of any eigenvector corresponding to $\lambda(G)$ is unique (note that only the role of negative and positive vertices can be exchanged). Accordingly, in what follows we assume that $m < \binom{n}{2}$, and write $V_G = V^- \cup V^0 \cup V^+$.

Given $U \subseteq V_G$, denote by $\langle U \rangle$ the subgraph of G induced by the vertices in U. We write $G \nabla H$ for the *join* (or *complete product*) of two graphs [4, p. 54]. Using Lemma 3.1 we can now describe the general structure of G: If $V^0 \neq \emptyset$ then $K = \langle V^0 \rangle$ is a complete graph and $G = K \nabla H$, where $H = \langle V^- \cup V^+ \rangle$.

In what follows we focus our attention on the graph H, and we write $H^- = \langle V^- \rangle$, $H^+ = \langle V^+ \rangle$. These subgraphs of H are non-empty since the eigenspaces of $\lambda(G)$ and $\rho(G)$ are orthogonal and the latter is spanned by a positive eigenvector; in contrast, V^0 can be an empty set.

A graph G is called a *nested split graph*[2] if its vertices can be ordered so that $jq \in E_G$ implies $ip \in E_G$ whenever $i \leqslant j$ and $p \leqslant q$.

Proposition 3.3. *Both H^+ and H^- are nested split graphs.*

Proof. Let $V^+ = \{1, 2, \ldots, k\}$ where $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_k$. We shall prove that $jq \in E_G$ implies that $ip \in E_G$ whenever $1 \leqslant i \leqslant j \leqslant k$ and $1 \leqslant p \leqslant q \leqslant k$. Asume for a contradiction that

$$1 \leqslant i \leqslant j \leqslant k, \quad 1 \leqslant p \leqslant q \leqslant k, \quad jq \in E_G, \quad ip \notin E_G.$$

Delete jq and add ip, to obtain the graph G'. Now

$$0 \leqslant \lambda(G') - \lambda(G) = 2(x_i - x_j)x_p + 2(x_p - x_q)x_j \leqslant 0,$$

and so $x_i = x_j$, $x_p = x_q$. Moreover $\mathbf{x}$ is an eigenvector corresponding to $\lambda(G') = \lambda(G)$. This is a contradiction, since q has lost a neighbour from V^+. Hence H^+ is a nested split graph. In a similar way we can derive the same conclusion for H^-. □

Lemma 3.4. *If V^+ or V^- induces an edge ij, then $pq \in E_G$ for all $p \in V^-, q \in V^+$.*

Proof. Otherwise we can remove ij and add an edge between V^- and V^+ to reduce $2\Sigma x_u x_v$. □

Accordingly, we arrive at the following conclusion.

Proposition 3.5. *If at least one of the graphs H^- or H^+ is not a totally disconnected graph then $H = H^- \nabla H^+$; otherwise, H is a bipartite graph (not necessarily a complete bipartite graph).*

In addition we have:

Lemma 3.6. *If $V^0 \neq \emptyset$ then $H = H^- \nabla H^+$.*

Proof. If $H \neq H^- \nabla H^+$ then we obtain a contradiction by applying Lemma 2.2(i) to four vertices chosen as follows. First, let c and d be two non-adjacent vertices taken from V^- and V^+, respectively; secondly, choose a from V^0 and b from $V^- \cup V^+$. By Lemma 3.1, a is adjacent to b, and ab is not a bridge. Moreover, $x_c x_d < x_a x_b$. If we replace the edge ab with cd then we obtain a connected graph G' for which $\lambda(G') < \lambda(G)$ by Lemma 2.2(i). This contradicts the minimality of $\lambda(G)$, and so every vertex of H^- is adjacent to every vertex of H^+.

This completes the proof. □

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[2] This term comes from [1] with an equivalent definition. The present definition is used in [7], where the graphs in question were called graphs with a *stepwise* adjacency matrix.

It follows from Lemmas 3.1 and 3.6 that when $V^0 \neq \emptyset$, G has the form $K\nabla L$, where K and L are nested split graphs, the vertices of K are non-negative, and those of L are non-positive. Here $V_K = V^+ \cup X$ and $V_L = V^- \cup Y$, where $X \cup Y$ is an arbitrary bipartition of V_0. Combining this observation with Proposition 3.5, we can state our main structural result as follows:

Theorem 3.7. *Let G be a connected graph whose least eigenvalue $\lambda(G)$ is minimal among the connected graphs of order n and size $m\left(0 < m < \binom{n}{2}\right)$. Then G is either*

(i) *a bipartite graph, or*
(ii) *a join of two nested split graphs (not both totally disconnected).*

Remark. In case (i) of Theorem 3.7, the vertices of G from one colour class are negative, while those from the other are positive. The graphs which arise in this case will be discussed in part II of this paper.

In case (ii) of Theorem 3.7, it remains to determine the graph(s) with minimal least eigenvalue λ among the non-bipartite graphs which are the join of two nested split graphs. As a possible pointer to the solution of this problem we discuss such graphs under the assumption that $V_0 \neq \emptyset$. Then we may write

$$A_G = \begin{pmatrix} J-I & J & J \\ J & A & J \\ J & J & B \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} \mathbf{0} \\ \mathbf{y} \\ -\mathbf{z} \end{pmatrix},$$

where J denotes an all-1 matrix of appropriate size, $A = A_{H^+}$, $B = A_{H^-}$ and all entries of $\mathbf{y}$ and $\mathbf{z}$ are positive. From the relation $A_G\mathbf{x} = \lambda\mathbf{x}$ we deduce:

$$J\mathbf{y} - J\mathbf{z} = \mathbf{0}, \quad A\mathbf{y} - J\mathbf{z} = \lambda\mathbf{y}, \quad J\mathbf{y} - B\mathbf{z} = -\lambda\mathbf{z}.$$

It follows that $J\mathbf{x} = \mathbf{0}$ (i.e. λ is a non-main eigenvalue of G) and

$$(J - I - A)\mathbf{y} = (-1-\lambda)\mathbf{y}, (J - I - B)\mathbf{z} = (-1-\lambda)\mathbf{z}.$$

Hence $-1-\lambda = \rho(\overline{H^+}) = \rho(\overline{H^-})$, and this common index is maximal.

Now assume further that $\binom{n}{2} - m$ is even, say $\binom{n}{2} - m = 2h$, and that $n > 2d + 2$, where d is the largest integer such that $\binom{d}{2} \leqslant h$. Recall from [16] that there is a unique graph $G(h)$ with maximal index among the graphs with h edges and no isolated vertices: if $\binom{d}{2} = h$ then $G(h) = K_d$, and if $\binom{d}{2} < h$ then $G(h)$ is obtained from K_d by adding a vertex of degree $h - \binom{d}{2}$. Note that both $G(h)$ and its complement are nested split graphs.

We claim that $G = \overline{N \cup G(h) \cup G(h)}$, where N consists of the appropriate number of isolated vertices (namely $n - 2d$ or $n - 2d - 2$). Otherwise, we can reduce λ by replacing each of $\overline{H^+}$ and $\overline{H^-}$ in $\overline{G}$ with $G(h)$, and adjusting the number of isolated vertices accordingly. To see this, suppose that $\overline{H^+}$ has p edges and $\overline{H^-}$ has q edges. Then $p + q = 2h$ and without loss of generality, $q \leqslant h$. Then we have

$$\rho(\overline{H^-}) \leqslant \rho(G(q)) \leqslant \rho(G(h)).$$

If $\rho(\overline{H^-}) = \rho(G(h))$ then $q = h$ and $\overline{H^-} = G(h)$; in this situation, $p = h$ and similarly $\overline{H^+} = G(h)$. This contradiction shows that our replacements result in a strict decrease in λ. We conclude that (under our assumptions) $H^+ = H^- = \overline{G(h)}$, a graph that consists of isolated vertices and at most one star. $\square$

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