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journal homepage: www.elsevier.com/locate/laaSharp upper bounds on the second largest eigenvalues of connected graphs[☆]Mingqing Zhai^a, Huiqiu Lin^b, Bing Wang^{a,*}^a School of Mathematical Science, Chuzhou University, Anhui, Chuzhou 239012, China^b Department of Mathematics, East China Normal University, Shanghai 200241, China

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ABSTRACT

Let λ_2 be the second largest eigenvalue of a graph. Powers (1988) [4] gave some upper bounds of λ_2 for general graphs and bipartite graphs, respectively. Considering that these bounds are not always attainable for connected graphs, we present sharp upper bounds of λ_2 for connected graphs and connected bipartite graphs in this paper. Moreover, the extremal graphs are completely characterized.

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1. Introduction

Let G be a simple connected graph with n vertices and $A(G)$ be its adjacency matrix. Since $A(G)$ is a real symmetric matrix, its eigenvalues must be real and may be ordered as $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$. If G has a u, v -path, then the *distance* from u to v , written $d_G(u, v)$ or simply $d(u, v)$, is the least length of a u, v -path. The *eccentricity* of a vertex u , written $\epsilon(u)$, is defined as $\max_{v \in V(G)} d(u, v)$. The *center* of a graph G is the subgraph induced by the vertices of minimum eccentricity. Let $S_{a,b}^k$ denote the tree obtained from two disjoint stars $K_{1,a}$ and $K_{1,b}$ by joining a path of length $k - 1$ between their centers. Let $G \cup H$ denote disjoint union of two graphs G and H . The degree of a vertex u in a graph G , denoted by $d_G(u)$, is the number of neighbors of u in G . Let $G[S]$ be an induced subgraph of G with the vertex subset S .

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Since eigenvalues are often difficult to evaluate, it is sometimes useful to obtain bounds for them. Several bounds have been found for the second largest eigenvalues of certain graph classes. The following results are well-known.

Theorem 1.1 [3]. *Let T be a tree with n vertices. If n is odd, then $\lambda_2(T) \leq \sqrt{\frac{n-3}{2}}$. Equality holds if and only if T is isomorphic to one of $S^3_{\frac{n-3}{2}, \frac{n-3}{2}}$, $S^4_{\frac{n-5}{2}, \frac{n-3}{2}}$ and $S^5_{\frac{n-5}{2}, \frac{n-5}{2}}$.*

Theorem 1.2 [6]. *Let T be a tree with n vertices. If n is even, then $\lambda_2(T) \leq \lambda_2(S^4_{\frac{n-4}{2}, \frac{n-4}{2}})$. Equality holds if and only if $T \cong S^4_{\frac{n-4}{2}, \frac{n-4}{2}}$.*

For a general graph G , the following results are due to Powers and Hong.

Theorem 1.3 [4]. *If G is a bipartite graph with n vertices and $k = \lfloor \frac{n}{4} \rfloor$, then*

$$\lambda_2(G) \leq \begin{cases} k & \text{if } n = 4k \text{ or } 4k + 1; \\ \sqrt{k(k+1)} & \text{if } n = 4k + 2 \text{ or } 4k + 3. \end{cases}$$

Clearly, the bounds in Theorem 1.3 are always attainable. For $n = 4k + r$, where $r \in \{0, 1, 2, 3\}$, $K_{k, k+\lfloor \frac{r}{2} \rfloor} \cup K_{k, k+\lceil \frac{r}{2} \rceil}$ is an extremal graph.

Theorem 1.4 [2]. *Let G be a graph with n vertices. Then $\lambda_2(G) \leq \frac{n-2}{2}$. Equality holds if and only if $G \cong K_{\frac{n}{2}} \cup K_{\frac{n}{2}}$. Furthermore, if G is a connected graph, then $\lambda_2(G) \leq \frac{\sqrt{n^2-4}}{2} - 1$.*

However, if G is a connected graph with even n vertices, then both bounds of Theorems 1.3 and 1.4 are not attainable. This paper is focused on the sharp upper bounds of the second largest eigenvalues of connected graphs.

2. Main results

Let $\mathcal{B}_{a,a}$ be the set of connected bipartite graphs obtained from two disjoint copies of complete bipartite graph $K_{\lfloor \frac{a}{2} \rfloor, \lceil \frac{a}{2} \rceil}$ by adding some edges from their vertices to an additional vertex u^* . Given a connected graph G , let X be an eigenvector corresponding to $\lambda_2(G)$ with its coordinate x_v corresponding to a vertex v . For any vertex subset $S \subseteq V(G)$, let $S^+ = \{v \in S : x_v > 0\}$. Similarly, we can define S^- and S^0 . Clearly, $S = S^+ \cup S^- \cup S^0$. For two disjoint subsets V_1 and V_2 of $V(G)$, denote by $E(V_1, V_2)$ the set of edges with one endpoint in V_1 and the other in V_2 .

Let V' be a subset of $V(G)$ with $|V'| = l$. Denoted by $G - V'$ the subgraph obtained from G by deleting all the vertices of V' together with their incident edges. If $V' = \{u\}$, we write $G - u$ for $G - \{u\}$. The following well-known result is the *Interlacing Theorem*, we cite it as our lemma.

Lemma 2.1 [1]. $\lambda_{i+l}(G - V') \leq \lambda_{i+l}(G) \leq \lambda_i(G - V')$, where $1 \leq i \leq n - l$.

Theorem 2.2. *Let $G = \langle S, T \rangle$ be a connected bipartite graph with n vertices, for some odd integer n .*

(i) *If $n = 4k + 1$, then $\lambda_2(G) \leq k$. Equality holds if and only if $G \in \mathcal{B}_{2k, 2k}$.*

(ii) *If $n = 4k + 3$, then $\lambda_2(G) \leq \sqrt{k(k+1)}$. Equality holds if and only if $G \in \mathcal{B}_{2k+1, 2k+1}$.*

Proof. If G is a complete bipartite graph, then $\lambda_2(G) = 0$. Hence, Theorem 2.2 holds. Considering the similarity and the convenience for illustrating, we only give the proof for the case of $n = 4k + 1$.

Now, suppose that G is not a complete bipartite graph. That is, $\lambda_2(G) > 0$. Let X be an eigenvector of $A(G)$ corresponding to $\lambda_2(G)$. Then we can partition S and T into $S = S^+ \cup S^- \cup S^0$ and $T = T^+ \cup T^- \cup T^0$,

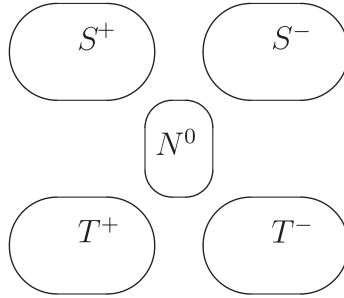


Fig. 1. The partition of a bipartite graph G.

respectively. For convenience, we write N^0 for $S^0 \cup T^0$ (see Fig. 1). Note that X must be orthogonal to the Perron vector of $A(G)$ and $\lambda_2(G) > 0$. Thus none of S^+, S^-, T^+ and T^- is empty.

Now consider a vertex $v \in S^+$ with maximal entry x_v . Note that $\lambda_2(G)x_v = \sum_{u \in N(v)} x_u$ and $N(v) \subseteq (T^+ \cup T^- \cup T^0)$, then we have

$$\lambda_2(G) \max_{v \in S^+} x_v \leq |T^+| \max_{v \in T^+} x_v. \tag{1}$$

Similarly, we have

$$\lambda_2(G) \max_{v \in T^+} x_v \leq |S^+| \max_{v \in S^+} x_v, \tag{2}$$

$$\lambda_2(G) \min_{v \in S^-} x_v \geq |T^-| \min_{v \in T^-} x_v, \tag{3}$$

and

$$\lambda_2(G) \min_{v \in T^-} x_v \geq |S^-| \min_{v \in S^-} x_v. \tag{4}$$

Note that $|S^+| + |T^+| + |S^-| + |T^-| \leq n = 4k + 1$. By multiplying (1) and (2) together, (3) and (4) together, respectively, we have

$$\lambda_2(G) \leq \min \left\{ \sqrt{|S^+||T^+|}, \sqrt{|S^-||T^-|} \right\} \leq \min \left\{ \frac{|S^+| + |T^+|}{2}, \frac{|S^-| + |T^-|}{2} \right\} \leq k. \tag{5}$$

Now, we consider the condition that equality holds. Without loss of generality, we may assume that $|S^+ \cup T^+| \leq |S^- \cup T^-|$. If equalities hold in (5), then both (1) and (2) are equalities. This implies that

- (i) $E(S^+ \cup T^+, S^- \cup T^-) = \emptyset$;
- (ii) for any vertex $u \in S^+$, $x_u = \max_{v \in S^+} x_v$, and for any vertex $u \in T^+$, $x_u = \max_{v \in T^+} x_v$;
- (iii) $G[S^+ \cup T^+]$ is isomorphic to $K_{k,k}$.

If $N^0 = \emptyset$, then by (i), $G[S^+ \cup T^+]$ and $G[S^- \cup T^-]$ are two independent components of G . Since G is connected, $N^0 \neq \emptyset$. That is $|N^0| = 1$. Hence, $|S^-| + |T^-| = 2k$. Since $\lambda_2(G) = k$, by (5), we have $|S^-| = |T^-| = k$. Furthermore, both (3) and (4) are equalities. Similarly, we can observe that $G[S^- \cup T^-]$ is also isomorphic to $K_{k,k}$. Hence, $G \in \mathcal{B}_{2k,2k}$.

Now suppose that $G \in \mathcal{B}_{2k,2k}$. Note that $G - u^* \cong K_{k,k} \cup K_{k,k}$. Taking $V' = \{u^*\}$ and $i = 1$ in Lemma 2.1, we have

$$k = \lambda_2(G - u^*) \leq \lambda_2(G) \leq \lambda_1(G - u^*) = k.$$

Hence, $\lambda_2(G) = k$. This completes the proof. \square

Lemma 2.3 [5]. Let $e = uv$ be an edge of a graph G and $C(e)$ be the set of all the cycles containing e . Let $P(G, \lambda)$ be the characteristic polynomial of $A(G)$. Then

$$P(G, \lambda) = P(G - e, \lambda) - P(G - u - v, \lambda) - 2 \sum_{C \in C(e)} P(G - V(C), \lambda).$$

For two positive integers a, b with $a \geq b$, let $2K_{a,b} + e$ be the graph obtained from two disjoint copies of $K_{a,b}$ by joining an edge $e = uv$ between their partition sets of b vertices.

Lemma 2.4. $\lambda_2(2K_{k,k} + e) > \sqrt{k^2 - 1}$.

Proof. Clearly, the inequality holds for $k = 1$. Now let $k \geq 2$. By Lemma 2.3, we have $P(2K_{k,k} + e, \lambda) = \lambda^{4k-6} f(\lambda)g(\lambda)$, where

$$f(\lambda) = \lambda^3 - \lambda^2 - k^2\lambda + k^2 - k$$

and

$$g(\lambda) = \lambda^3 + \lambda^2 - k^2\lambda - k^2 + k.$$

Note that $f(\sqrt{k^2 - 1}) = -\sqrt{k^2 - 1} - k + 1 < 0$ and $g(\sqrt{k^2 - 1}) = -\sqrt{k^2 - 1} + k - 1 < 0$. This implies that both the largest roots of $f(\lambda)$ and $g(\lambda)$ are more than $\sqrt{k^2 - 1}$. Therefore, $\lambda_2(2K_{k,k} + e) > \sqrt{k^2 - 1}$.

Theorem 2.5. Let $G = \langle S, T \rangle$ be a connected bipartite graph with n vertices, for some even integer n .

(i) If $n = 4k$, then $\lambda_2(G) \leq \lambda_2(2K_{k,k} + e)$. Equality holds if and only if $G \cong 2K_{k,k} + e$.

(ii) If $n = 4k + 2$, then $\lambda_2(G) \leq \lambda_2(2K_{k,k+1} + e)$. Equality holds if and only if $G \cong 2K_{k,k+1} + e$.

Proof. For convenience, we only elaborate our proof for the case of $n = 4k$. The case of $n = 4k + 2$ is analogous and hence omitted here.

The claim is trivial for $k = 1$. Now suppose that $k \geq 2$ and G^* is an extremal graph which has the maximum second largest eigenvalue among all connected bipartite graphs of order n . Then by Lemma 2.4, we have $\lambda_2(G^*) > \sqrt{k^2 - 1} > 1$. Let X be the eigenvector of $A(G^*)$ corresponding to $\lambda_2(G^*)$. Suppose $S = S^+ \cup S^- \cup S^0$ and $T = T^+ \cup T^- \cup T^0$ are two partition sets of G^* . Now, we give the following claims.

Claim 2.6. $|S^+| = |T^+| = |S^-| = |T^-| = k$.

Proof. Similar to the proof of Theorem 2.2, we have $\lambda_2(G^*) \leq \min\{\sqrt{|S^+||T^+|}, \sqrt{|S^-||T^-|}\}$. Note that $|S^+| + |T^+| + |S^-| + |T^-| \leq 4k$. If the claim does not hold, then $\lambda_2(G^*) \leq \sqrt{(k+1)(k-1)} = \sqrt{k^2 - 1}$, a contradiction. \square

Claim 2.7. Both $G[S^+ \cup T^+]$ and $G[S^- \cup T^-]$ are isomorphic to $K_{k,k}$.

Proof. Suppose to the contrary that $uv \notin E(G^*)$ for some $u \in S^+$ and $v \in T^+$. Then $\lambda_2(G^*)x_v \leq (k-1) \max_{w \in S^+} x_w$ and $\lambda_2(G^*) \max_{w \in S^+} x_w \leq (k-1) \max_{w \in T^+} x_w + x_v$. Hence

$$\left(\lambda_2(G^*) - \frac{k-1}{\lambda_2(G^*)} \right) \max_{w \in S^+} x_w \leq (k-1) \max_{w \in T^+} x_w. \tag{6}$$

By symmetry, we have

$$\left(\lambda_2(G^*) - \frac{k-1}{\lambda_2(G^*)} \right) \max_{w \in T^+} x_w \leq (k-1) \max_{w \in S^+} x_w. \tag{7}$$

Multiplying (6) and (7) together, we have $\lambda_2(G^*) - \frac{k-1}{\lambda_2(G^*)} \leq k - 1$. It is easy to see

$$\lambda_2(G^*) \leq \frac{k - 1 + \sqrt{(k - 1)(k + 3)}}{2} \leq \sqrt{k^2 - 1}, \tag{8}$$

a contradiction. Hence, $G[S^+ \cup T^+]$ is isomorphic to $K_{k,k}$. Similarly, we have $G[S^- \cup T^-] \cong K_{k,k}$. \square

Claim 2.8. $\max\{|E(S^+, T^-)|, |E(S^-, T^+)|\} \leq 1$.

Proof. Without loss of generality, assume $|E(S^+, T^-)| \leq |E(S^-, T^+)| = a$. For a vertex v and a subset U of $V(G^*)$, let $d_U(v)$ be the number of edges from v to U and $X_U = \sum_{u \in U} x_u$. For convenience, we write

$$X'_{S^-} = \sum_{v \in S^-} d_{T^+}(v)x_v \text{ and } X'_{T^+} = \sum_{v \in T^+} d_{S^-}(v)x_v, \text{ where } \sum_{v \in S^-} d_{T^+}(v) = \sum_{v \in T^+} d_{S^-}(v) = a.$$

Note that $\lambda_2(G^*)X'_{S^-} = aX_{T^-} + X'_{T^+}$ and $\lambda_2(G^*)X'_{T^+} = aX_{S^+} + X'_{S^-}$. We have

$$(\lambda_2(G^*) + 1)(X'_{T^+} - X'_{S^-}) = a(X_{S^+} - X_{T^-}).$$

Hence, for any integer $a \geq 2$,

$$\lambda_2(G^*)(X'_{T^+} - X'_{S^-}) = \frac{a\lambda_2(G^*)}{\lambda_2(G^*) + 1}(X_{S^+} - X_{T^-}) \geq X_{S^+} - X_{T^-}. \tag{9}$$

(9) implies at least one of the following inequalities:

$$-\lambda_2(G^*)X'_{S^-} \geq X_{S^+}; \tag{10}$$

$$\lambda_2(G^*)X'_{T^+} \geq -X_{T^-}.$$

Without loss the generality, suppose that (10) holds. Note that $\lambda_2(G^*)X_{S^+} \leq kX_{T^+}$ and $\lambda_2(G^*)X_{T^+} = kX_{S^+} + X'_{S^-}$. We have

$$(\lambda_2^2(G^*) - k^2)X_{S^+} \leq kX'_{S^-} \leq -\frac{k}{\lambda_2(G^*)}X_{S^+} \leq -X_{S^+},$$

since by Theorem 1.3 $\lambda_2(G^*) \leq k$. So $\lambda_2^2(G^*) - k^2 + 1 \leq 0$. That is, $\lambda_2(G^*) \leq \sqrt{k^2 - 1}$, a contradiction. Hence, Claim 2.8 holds.

If $|E(S^+, T^-)| = |E(S^-, T^+)| = 1$, then $G \cong H$ (see Fig. 2), where both $H[S^+ \cup T^+]$ and $H[S^- \cup T^-]$ are isomorphic to $K_{k,k}$. By symmetry, we have

$$x_{u_1} = x_{u_2} = -x_{v_1} = -x_{v_2}.$$

In addition, all coordinates x_w , for $w \in S^+ \cup T^+ \setminus \{u_1, u_2\}$, are equal and we may denote them by x_{u_0} . Then

$$\lambda_2(G^*)x_{u_0} = (k - 1)x_{u_0} + x_{u_1}$$

and

$$\lambda_2(G^*)x_{u_1} = (k - 1)x_{u_0} + x_{u_2} + x_{v_2} = (k - 1)x_{u_0}.$$

Hence,

$$\lambda_2^2(G^*) - (k - 1)\lambda_2(G^*) - (k - 1) = 0.$$

By (8), we have $\lambda_2(G^*) \leq \sqrt{k^2 - 1}$, a contradiction. So two disjoint copies of $K_{k,k}$ in G^* can be connected with just one edge. That is, $G \cong 2K_{k,k} + e$. This completes the proof. \square

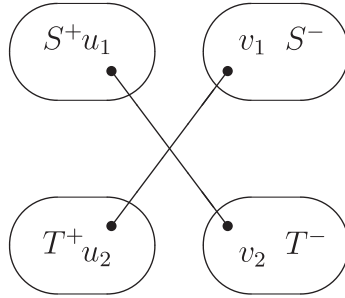


Fig. 2. The graph H.

For odd n , let $2\mathcal{K}_{\frac{n-1}{2}} \bullet \mathcal{K}_1$ be the set of connected graphs obtained from two disjoint copies of complete graph $K_{\frac{n-1}{2}}$ by adding some edges from their vertices to an additional vertex. Besides, for even n , let $2K_{\frac{n}{2}} + e$ be the graph obtained from two disjoint copies of $K_{\frac{n}{2}}$ by joining an edge between them. Similar to the proof of connected bipartite graphs, we have the following results.

Theorem 2.9. *Let G be a connected graph with n vertices.*

- (i) *If n is odd, then $\lambda_2(G) \leq \frac{n-3}{2}$. Equality holds if and only if $G \in 2\mathcal{K}_{\frac{n-1}{2}} \bullet \mathcal{K}_1$.*
- (ii) *If n is even, then $\lambda_2(G) \leq \lambda_2(2K_{\frac{n}{2}} + e)$. Equality holds if and only if $G \cong 2K_{\frac{n}{2}} + e$.*

For any connected graph (particularly, for any connected bipartite graph) with an even number of vertices, we can find that the bounds of Theorems 2.5 and 2.9 are better than those of Theorems 1.3 and 1.4.

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