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On the largest kth eigenvalues of trees with $n \equiv 0 \pmod k$ ☆

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Abstract

We consider the only remaining unsolved case $n \equiv 0 \pmod k$ for the largest kth eigenvalue of trees with n vertices. In 1995, Jia-yu Shao gave complete solutions for the cases $k = 2, 3, 4, 5, 6$ and provided some necessary conditions for extremal trees in general cases (cf. [Linear Algebra Appl. 221 (1995) 131]). We further improve Shao's necessary condition in this paper, which can be seen as the continuation of [Linear Algebra Appl. 221 (1995) 131].
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1. Introduction

Let G be a graph of order n. The eigenvalues of G are defined as those of its adjacent matrix $A(G)$. Now, $A(G)$ is a symmetric $(0, 1)$ matrix, and so, the eigenvalues of $A(G)$ (or of G) are all real and can be ordered as

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

We call $\lambda_k(G)$ the kth *eigenvalue* of G.

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If T is a tree of order n, then T is bipartite, and its eigenvalues satisfy the relation $\lambda_i(T) = -\lambda_{n-i+1}(T)$ $(i = 1, 2, \ldots, n)$. So, it suffices to study those eigenvalues $\lambda_k(T)$ for $1 \leqslant k \leqslant [n/2]$. In this paper we always assume that $1 \leqslant k \leqslant [n/2]$.

An interesting unsolved problem in the study of the spectra of trees is to find "the best possible upper bound" for the kth eigenvalues of trees of order n. In other words, let

$$\Gamma_n = \{T \mid T \text{ is a tree of order } n\},$$

and let

$$\bar{\lambda}_k(n) = \max\{\lambda_k(T) \mid T \in \Gamma_n\} \quad (1 \leqslant k \leqslant [n/2]).$$

Then, the above problem asks to determine the function $\bar{\lambda}_k(n)$ and (if possible) find a tree $T \in \Gamma_n$ with $\lambda_k(T) = \bar{\lambda}_k(n)$.

There have been considerable attempts in studying this problem, and the remaining unsolved case for $\bar{\lambda}_k(n)$ is the case $n \equiv 0 \pmod k$, $7 \leqslant k \leqslant [n/2]$. For this case, we write $n = kt$ $(t \geqslant 2)$ and let

$$\bar{\Gamma}_{k,t} = \{T \in \Gamma_{kt} \mid \lambda_k(T) = \bar{\lambda}_k(kt)\}.$$

The trees in $\bar{\Gamma}_{k,t}$ are called the extremal trees.

To be clear, we give the same definitions as those in [1] below.

Definition 1. Let $X_{k,t}$ be the subset of trees in Γ_{kt} which consists of k disjoint stars $S_1, \ldots, S_k$ of the order $t\,(S_1 \cong S_2 \cong \cdots \cong S_k \cong K_{1,t-1})$ together with another $k-1$ edges $e_1, e_2, \ldots, e_{k-1}$ such that the two end vertices of each edge e_i $(i = 1, 2, \ldots, k-1)$ are noncentral vertices of different stars. We call $S_1, \ldots, S_k$ the *stars* of this tree $T \in X_{k,t}$, call the edges $e_1, \ldots, e_{k-1}$ the *nonstar edges* of T, and call the other edges the *star edges* of T.

Definition 2. We define the condensed tree $\widehat{T}$ of T as $V(\widehat{T}) = (S_1, S_2, \ldots, S_k)$, and there is an edge $[S_i, S_j]$ $(i \neq j)$ in $\widehat{T}$ if and only if there exists some nonstar edge of T with one end in S_i and the other end in S_j.

Definition 3. Define $X'_{k,t}$ as the subset of $X_{k,t}$ which consists of those trees T in $X_{k,t}$ such that for any star S_i of T, there is only one vertex in S_i incident to some nonstar edges of T.

A considerable necessary condition for extremal trees obtained in [1] is that if $T \in \bar{\Gamma}_{k,t}$ $(k \geqslant 2, t \geqslant 5)$, then $T \in X_{k,t}$ and $\Delta(\widehat{T}) \leqslant 3$, where $\Delta(\widehat{T})$ is the maximal degree of the condensed tree $\widehat{T}$. In this paper, we establish a further necessary condition for extremal trees.

2. Some preliminary results

For a graph G, let $q(G)$ be the number of edges in a maximal matching of G, and let $a_j(G)$ be the number of j-matchings (the matchings with j-edges) of G. (We agree that $a_j(G) = 0$ for $j < 0$ and $j > q(G)$.) We also write

$$m_G(x) = \sum_{j=0}^{q(G)} (-1)^j a_j(G) x^{q(G)-j} \tag{2.1}$$

and

$$h_G(y) = m_G(y + a). \tag{2.2}$$

We call $h_G(y)$ the *key polynomial of G*. Then the characteristic polynomial of a tree $T \in \Gamma_n$ is

$$P(T, \lambda) = \lambda^{n-2q(T)} m_T(\lambda^2) = \lambda^{n-2q(T)} h_T(\lambda^2 - a), \tag{2.3}$$

and thus,

$$\lambda_k(T) = \sqrt{\lambda_k(m_T)} = \sqrt{a + \lambda_k(h_T)} \quad (k \leqslant q(T)), \tag{2.4}$$

where $\lambda_k(m_T)$ and $\lambda_k(h_T)$ are the kth largest real roots of the polynomials $m_T(x)$ and $h_T(y)$, respectively.

From now on, we always write

$$a = t - 1 \tag{2.5}$$

and let

$$f_u(y) = (y + a)y^2 - u(y + 1)^2, \tag{2.6}$$

$$g_1(y) = (y + a)y + 2(y + 2), \tag{2.7}$$

$$g_2(y) = 2(y + 1)^2 + (y + 2)y, \tag{2.8}$$

$$g_3(y) = (y + a)(y + 1)^2 - (y + 2)^2, \tag{2.9}$$

$$g_4(y) = 2(y + a)(y + 1) - 3(y + 3), \tag{2.10}$$

$$g_5(y) = (y + 1)^2 + (y + 2)y, \tag{2.11}$$

$$g_6(y) = (y + a)(y + 1)^2 - 4(y + 2)^2, \tag{2.12}$$

$$g_7(y) = (y + a)(y + 1) - 2(y + 3). \tag{2.13}$$

These polynomials will play an important role in our studies.

Lemma 1 (Cauchy interlacing theorem). *Let V' be a vertex subset with k vertices of the graph G. Let $G - V'$ be the subgraph of G obtained by deleting all the vertices in V' together with their incident edges. Then*

$$\lambda_i(G) \geqslant \lambda_i(G - V') \geqslant \lambda_{i+k}(G).$$

Lemma 2 [1]. *For $u > 0$, the cubic polynomial $f_u(y)$ has three real roots, which we can write as $\lambda_1(f_u) > \lambda_2(f_u) > \lambda_3(f_u)$. Furthermore, we have*

$$\lambda_3(f_u) \leqslant -1 < \lambda_2(f_u) < 0 < \lambda_1(f_u) \tag{2.14}$$

and

$$\lambda_2(f_\xi) < \lambda_2(f_u) \quad (\textit{for } 0 < u < \xi). \tag{2.15}$$

Lemma 3 [1]. *Let $T \in X'_{k,t}$ $(t \geqslant 2)$, and let $u_1 = \lambda_1(\widehat{T})$ be the largest eigenvalue of the condensed tree $\widehat{T}$. Then*

$$\lambda_k(T) = \sqrt{t - 1 + \lambda_2(f_{u_1})}. \tag{2.16}$$

The following lemma will be crucial for the results of this paper.

Lemma 4. *Let $f_2(y) = (y + a)y^2 - 4(y + 1)^2$. Then for $n \geqslant 8$, we have*

$$-1 + \frac{1}{\sqrt{3}} < \lambda_2(f_2) < 0 \tag{2.17}$$

and

$$g_i(\lambda_2(f_2)) > 0, \quad i = 2, 3, 4, \tag{2.18}$$

$$g_1(\lambda_2(f_2)) < 0. \tag{2.19}$$

Furthermore, for $a \geqslant 24$, we have

$$-1 + \frac{1}{\sqrt{2}} < \lambda_2(f_2) < 0 \tag{2.20}$$

and

$$g_i(\lambda_2(f_2)) > 0, \quad i = 2, 3, 4, 5, 6, 7, \tag{2.21}$$

$$g_1(\lambda_2(f_2)) < 0. \tag{2.22}$$

Proof. We need to prove only (2.17), (2.18) (for $i = 2$) and (2.19) here. The rest can be obtained in the same way.

For $a \geqslant 8$, we have

$$f_2(0) = -4 < 0 \quad \text{and} \quad f_2\left(-1 + \frac{1}{\sqrt{3}}\right) > 0.$$

From (2.14), we have $\lambda_3(f_2) < -1\lambda_2(f_2) < 0 < \lambda_1(f_2)$. So (2.17) holds.

Now, when $-1 + 1/\sqrt{3} < y < 0$, we have

$$g_2'(y) = 6(y + 1) > 0 \quad \text{and} \quad g_2\left(-1 + \frac{1}{\sqrt{3}}\right) > 0.$$

So

$$g_2(\lambda_2(f_2)) > 0.$$

Let $\lambda_1(y)$ be the larger root of $g_1(g) = 0$. Then the direct computations give

$$f_2(\lambda_1(g_1)) < 0.$$

Noticing the quality of the curve $f_2(y)$, we have

$$\lambda_2(f_2) < \lambda_1(g_1).$$

Thus, we can easily obtain (2.19). □

The seven trees shown in Fig. 1 will be important for our main results:
Now, let $W_1 \in \Gamma_6$, $W_2, W_6 \in \Gamma_7$, $W_3, W_5 \in \Gamma_8$, $W_4, W_7 \in \Gamma_9$ as in Fig. 1,

$$W = \{W_1, W_2, W_3, W_4, W_5, W_6, W_7\},$$

$$F_1 = \{T \in X_{6,t} \mid \widehat{T} = W_1\}, \quad F_1^* \in F_1 \cap X'_{6,t},$$

$$F_2 = \{T \in X_{7,t} \mid \widehat{T} = W_2\}, \quad F_2^* \in F_2 \cap X'_{7,t},$$

$$F_3 = \{T \in X_{8,t} \mid \widehat{T} = W_3\}, \quad F_3^* \in F_3 \cap X'_{8,t},$$

$$F_4 = \{T \in X_{9,t} \mid \widehat{T} = W_4\}, \quad F_4^* \in F_4 \cap X'_{9,t},$$

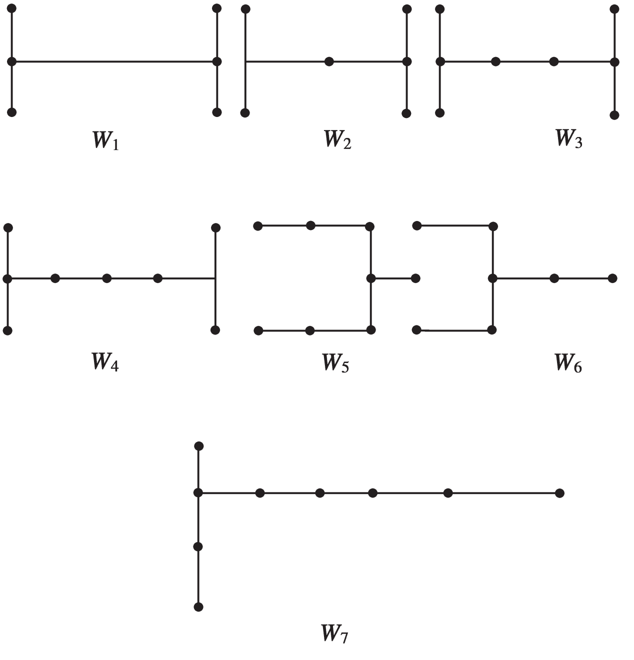

Fig. 1.

$$F_5 = \{T \in X_{8,t} \mid \widehat{T} = W_5\}, \quad F_5^* \in F_5 \cap X'_{8,t},$$

$$F_6 = \{T \in X_{7,t} \mid \widehat{T} = W_6\}, \quad F_6^* \in F_6 \cap X'_{7,t},$$

$$F_7 = \{T \in X_{9,t} \mid \widehat{T} = W_7\}, \quad F_7^* \in F_7 \cap X'_{9,t},$$

and

$$F = F_1 \cup F_2 \cup F_3 \cup F_4 \cup F_5 \cup F_6 \cup F_7.$$

From [2, Table 2], we know that the largest eigenvalue of each $W_i\,(i = 1, 2, \ldots, 7)$ is 2. Then by Lemma 3

$$\begin{aligned}\lambda_6(F_1^*) &= \lambda_7(F_2^*) = \lambda_8(F_3^*) = \lambda_9(F_4^*)\\ &= \lambda_8(F_5^*) = \lambda_7(F_6^*) = \lambda_9(F_7^*)\\ &= \sqrt{t - 1 + \lambda_2(f_2)},\end{aligned} \tag{2.23}$$

where $t \geqslant 2$.

Theorem 5. *For $t \geqslant 4$, we have*

$$\lambda_6(T) < \lambda_6(F_1^*), \quad T \in F_1 \backslash \{F_1^*\}, \tag{2.24}$$

$$\lambda_7(T) < \lambda_7(F_2^*), \quad T \in F_2 \backslash \{F_2^*\}, \tag{2.25}$$

$$\lambda_8(T) < \lambda_8(F_3^*), \quad T \in F_3 \backslash \{F_3^*\}, \tag{2.26}$$

$$\lambda_9(T) < \lambda_9(F_4^*), \quad T \in F_4 \backslash \{F_4^*\}, \tag{2.27}$$

$$\lambda_8(T) < \lambda_8(F_5^*), \quad T \in F_5 \backslash \{F_5^*\}, \tag{2.28}$$

$$\lambda_7(T) < \lambda_8(F_6^*), \quad T \in F_6 \backslash \{F_6^*\}, \tag{2.29}$$

$$\lambda_9(T) < \lambda_9(F_7^*), \quad T \in F_7 \backslash \{F_7^*\}. \tag{2.30}$$

Proof. The proofs follow from extensive calculations (available from the authors on request), and Lemmas 4 and 5.1 in [1]. □

3. A further necessary condition for extremal trees

Let P_k, J_k and $L_k \in \Gamma_k$ as in Fig. 2,

$$M_9 = \{T \in \Gamma_9 \mid \Delta(T) = 3\} \backslash \{J_9\}, \tag{3.1}$$

and

$$M_{9,t} = \{T \in X_{9,t} \mid \widehat{T} \in M_9\}. \tag{3.2}$$

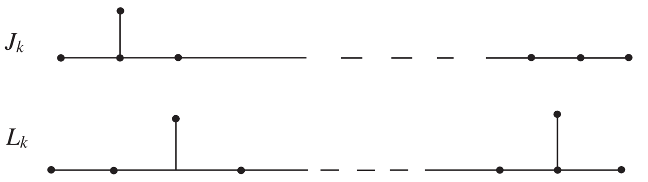

Fig. 2.

Theorem 6. *Let* M_9, $M_{9,t}$ *as* (3.1), (3.2). *Then for* $t \geqslant 4$, *we have*

$$\lambda_9(T) \leqslant \sqrt{t-1+\lambda_2(f_2)}, \quad T \in M_{9,t}. \tag{3.3}$$

Proof. For $T \in M_{9,t}$, it is obvious that $\widehat{T}$ has an induced subgraph isomorphic to some $W_i \in W$, $1 \leqslant i \leqslant 7$, and thus, there exists a vertex set $V^* \subset V(T)$ such that

$$\begin{aligned} T - V^* = W^* \dot{\cup} \overbrace{K_{1,t-2} \dot{\cup} \cdots \dot{\cup} K_{1,t-2}} \dot{\cup} \overbrace{K_{1,t-3} \dot{\cup} \cdots \dot{\cup} K_{1,t-3}} \\ \dot{\cup} \overbrace{K_{1,t-4} \dot{\cup} \cdots \dot{\cup} K_{1,t-4}}, \end{aligned} \tag{3.4}$$

where $W^* \in F$, $\widehat{W}^* = W_i$ and n_1, n_2, n_3 are the three finite integers. By Theorem 5 and from (2.23) $\lambda_k(W^*) \leqslant \sqrt{t-1+\lambda_2(f_2)}$ for some k $(6 \leqslant k \leqslant 9)$. So, by the Cauchy interlacing theorem, we have

$$\begin{aligned} \lambda_9(T) &\leqslant \lambda_k(T - V^*) \\ &\leqslant \max\{\lambda(W^*), \sqrt{t-2}, \sqrt{t-3}, \sqrt{t-4}\} \\ &\leqslant \sqrt{t-1+\lambda_2(f_2)}. \qquad \square \end{aligned} \tag{3.5}$$

Lemma 7. *Let*

$$M_k = \{T \in \Gamma_k \mid \Delta(T) = 3\} \backslash \{J_k, L_k\} \quad (k \geqslant 10).$$

Then, for $T \in M_k$, *T has an induced subgraph isomorphic to some* $T_9^0 \in M_9$.

Proof. The proof is trivial. □

Theorem 8. *For* $t \geqslant 4$, $k \geqslant 10$, *let* $M_{k,t} = \{T \in X_{k,t} \mid \widehat{T} \in M_k\}$. *Then*

$$\bar{\Gamma}_{k,t} \cap M_{k,t} = \emptyset. \tag{3.6}$$

Proof. For $T \in M_{k,t}$, by Lemma 7, we have that $\widehat{T}$ has an induced subgraph isomorphic to some $T_9^0 \in M_9$.Thus, as the proof of Theorem 6, we have

$$\lambda_k(T) \leqslant \sqrt{t-1+\lambda_2(f_2)}. \tag{3.7}$$

On the other hand, by [1]

$$\bar{\lambda}_k(kt) \geqslant \sqrt{t-1+\lambda_2(f_{\lambda_1(P_k)})} = \sqrt{t-1+\lambda_2\left(f_{2\cos\frac{\pi}{k+1}}\right)} \tag{3.8}$$

and from (2.15)

$$\sqrt{t-1+\lambda_2\left(f_{2\cos\frac{\pi}{k+1}}\right)} \geqslant \sqrt{t-1+\lambda_2(f_2)}. \tag{3.9}$$

Combining (3.6)–(3.8), we obtain (3.5). □

Remark 1. We have also verified that (3.5) holds for $k = 7, 8, 9$. So, for $k \geqslant 7$ and $t \geqslant 4$, if we denote by

$$P_{k,t} = \{T \in X_{k,t} \mid \widehat{T} = P_k\},$$

$$J_{k,t} = \{T \in X_{k,t} \mid \widehat{T} = J_k\},$$

and

$$L_{k,t} = \{T \in X_{k,t} \mid \widehat{T} = L_k\},$$

then, from the previous results and Theorem 8, it suffices to find the extremal trees in $P_{k,t} \cup J_{k,t} \cup L_{k,t}$.

4. Some further discussions

In this section, we establish some further results about the left problem of finding the extremal trees in $J_{k,t}$.

Lemma 9. *Let P_k, J_k $k \geqslant 4$ as in Fig.* 2. *We have*

$$\lambda_i(J_k) = 2\cos\frac{(2i-1)\pi}{2k-2}, \quad i = 1, 2, \ldots, k, \tag{4.1}$$

i.e.

$$\lambda_i(J_k) = \lambda_{2i-1}(P_{2k-3}). \tag{4.2}$$

Proof. From Fig. 2, we can write

$$A(J_k) = \begin{pmatrix} A & \alpha \\ \alpha^{\mathrm{T}} & 0 \end{pmatrix},$$

where A is the adjacent matrix of P_{k-1}, $\alpha = (0, 1, 0, \ldots, 0)^{\mathrm{T}}$.

Let $J_k(\lambda) = \det(\lambda I - A(J_k))$. Then, we have the recursive relation as follows:

$$J_k(\lambda) = \lambda J_{k-1}(\lambda) - J_{k-2}(\lambda),$$

since $x_{1,2} = \lambda \pm \sqrt{\lambda^2 - 4}/2$ are the two roots of $x^2 - \lambda x + 1 = 0$, we have

$$J_k(\lambda) = c_1 x_1^k + c_2 x_2^k. \tag{4.3}$$

On the other hand,

$$J_4(\lambda) = \lambda^3 - 3\lambda^2 = c_1 x_1^4 + c_2 x_2^4, \tag{4.4}$$

$$J_5(\lambda) = \lambda^5 - 4\lambda^3 + 2\lambda = c_1x_1^5 + c_2x_2^5. \tag{4.5}$$

Combining (4.4) and (4.5), we have

$$c_1 = \frac{J_5(\lambda) - J_4(\lambda)x_2}{x_1^5 - x_1^4x_2}, \quad c_2 = \frac{J_5(\lambda) - J_4(\lambda)x_1}{x_2^5 - x_2^4x_1}. \tag{4.6}$$

From (4.3) and (4.6), we have

$$J_k(\lambda) = \frac{J_5(\lambda) - J_4(\lambda)x_2}{x_1 - x_2}x_1^{k-4} + \frac{J_5(\lambda) - J_4(\lambda)x_1}{x_2 - x_1}x_2^{k-4}.$$

Let

$$\lambda_i = 2\cos\frac{(2\mathrm{i} - 1)\pi}{2k - 2}.$$

Then the direct computations give

$$J_k(\lambda_i) = 0, \quad i = 1, 2, \ldots, k.$$

Thus we obtain (4.1). Noticing

$$\lambda_i(P_k) = 2\cos\frac{\mathrm{i}\pi}{k + 1},$$

we have (4.2). □

Theorem 10. *If there is no extremal tree in $J_{k,t}$, then there is no extremal tree in $J_{s,t}$ for $k + 1 \leqslant s \leqslant 2k - 2$.*

Proof. By Lemma 9, we have

$$\lambda_1(J_k) = \lambda_1(P_{2k-3}), \quad \lambda_1(J_s) > \lambda_1(J_k),$$

and

$$\lambda_1(P_s) > \lambda_1(P_k), \quad k + 1 \leqslant s \leqslant 2k - 2.$$

So, from (2.15), we have

$$\sqrt{t - 1 + \lambda_2(f_{\lambda_1(J_k)})} < \sqrt{t - 1 + \lambda_2(f_{\lambda_1(P_{2k-3})})} < \sqrt{t - 1 + \lambda_2(f_{\lambda_1(P_s)})}.$$

On the other hand, obviously $J_s(k + 1 \leqslant s \leqslant 2k - 2)$ has J_k as its induced subgraph. Thus, by the same reasoning as Theorem 8, we conclude that there is no extremal tree in $J_{s,t}$ $(k + 1 \leqslant s \leqslant 2k - 2)$. □

Acknowledgement

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[2] D.M. Cretkvoic, M. Doob, H. Sachs, Spectra of Graphs, Academic, New York, 1980 (Appendix, Table 2).