On the Largest $k$th Eigenvalues of Trees*

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ABSTRACT

We consider the only remaining unsolved case $n \equiv 0 \pmod{k}$ for the largest $k$th eigenvalue of trees with $n$ vertices. We give complete solutions for the cases $k = 2, 3, 4, 5$ and give some necessary conditions for extremal trees in general cases.

1. INTRODUCTION

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

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

We call $\lambda_k(G)$ the $k$th eigenvalue of $G$.

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 $1 \leq k \leq [n/2]$. In this paper we always assume

*Research partially supported by the National Science Foundation of China.

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655 Avenue of the Americas, New York, NY 10010 SSDI 0024-3795(93)00236-S
that $1 \leq k \leq \lfloor n/2 \rfloor$.

There have been considerable attempts and some successes in finding the upper bounds for the eigenvalues of trees [1–4, 6]. An interesting unsolved problem in the study of the spectra of trees is to find "the best possible upper bound" for $k$th eigenvalues of trees of order $n$. In other words, let

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

and let

$$\overline{\lambda}_k(n) = \max\{\lambda_k(T) \mid T \in T_n\} \quad (1 \leq k \leq \lfloor n/2 \rfloor).$$

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

The case $k = 1$ was settled in 1957 [1], and it is now well known that $\lambda_1(T) \leq \sqrt{n-1}$ with equality if and only if $T$ is the star $K_{1,n-1}$. But the cases when $2 \leq k \leq \lfloor n/2 \rfloor$ are not completely solved yet. In 1986, Hong Yuan [3] showed that

$$\overline{\lambda}_k(n) = \sqrt{\left\lfloor \frac{n-2}{k} \right\rfloor} \quad [\text{if } n \equiv 1(\text{mod } k)]$$

We further improved Hong's bound and obtained in [4] the following.

**Theorem A [4].**

$$\lambda_k(T) \leq \sqrt{\left\lfloor \frac{n}{k} \right\rfloor - 1} \quad (T \in T_n, \quad 1 \leq k \leq \lfloor n/2 \rfloor). \quad (1.1)$$

*This bound is best possible for all $n \not\equiv 0(\text{mod } k)$ and for $k = 1$, while for $n \equiv 0(\text{mod } k), \quad k \neq 1$, the strict inequality in (1.1) holds.*

So now the only remaining unsolved case for $\overline{\lambda}_k(n)$ is the case $n \equiv 0(\text{mod } k), \quad 2 \leq k \leq \lfloor n/2 \rfloor$. For this case, we write $n = kt(t \geq 2)$ and let

$$\overline{T}_{k,t} = \{T \in T_{kt} \mid \lambda_k(T) = \overline{\lambda}_k(kt)\}. \quad (1.2)$$

The trees in $\overline{T}_{k,t}$ are called the *extremal trees*. Our main results in this paper are the determination of the function $\overline{\lambda}_k(kt)$ and the sets $\overline{T}_{k,t}$ for $k = 2, 3, 4, 5$. We also give several necessary conditions for the trees in $\overline{T}_{k,t}$ (Theorem 3.1 and Theorem 6.1).

The following lemmas will be crucial for the results of this paper:

**Lemma A [4].** For $T \in T_n$ and any positive integer $a$, there exists a
vertex $v \in V(T)$ such that there is one component of $T - v$ with order $\leq \max(n-1-a,a)$ and all the other components of $T - v$ have orders $\leq a$.

**Lemma B** (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

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

**2. The Largest Second Eigenvalues of Trees with Even Order $N = 2T$**

For the case $k = 2$, Neumaier [2] has shown that $\lambda_2(T) \leq \sqrt{(n-3)/2}$ if $T \in T_n$ with $n$ odd (which is just the case $k = 2$ in the bound (1.1)]. But this bound does not hold for even $n$, as was pointed out by Hong [3]—it is just the remaining unsolved case $n \equiv 0 \pmod k$ (as mentioned in Section 1) for $k = 2$. In this section, we will completely settle this case by determining the value $\lambda_2(2t)$ and the set of extremal trees $T_{2,t}$.

Let $G_0 \in T_t$ as in Figure 1. Then by [5, Corollary], we know that

$$\lambda_2(T) > \lambda_2(G_0) \quad (\text{for } T \in T_t \backslash \{K_{1,t-1}, G_0\}).$$

Using this and the fact that $\lambda_i(G_0) = 0(3 \leq i \leq t - 2)$, we have for $T \in T_t \backslash \{K_{1,t-1}, G_0\}$ that

$$2\lambda_1^2(T) = 2(t-1) - 2\lambda_2^2(T) - \sum_{i=3}^{t-2} \lambda_i^2(T) < 2(t-1) - 2\lambda_2^2(G_0) = 2\lambda_1^2(G_0).$$

Thus we obtain

$$\lambda_1(T) < \lambda_1(G_0) \quad (T \in T_t \backslash \{K_{1,t-1}, G_0\}), \quad (2.1)$$

namely, $\lambda_1(G_0)$ is the second largest value among the values $\{\lambda_1(T) \mid T \in T_t\}$.

**Remark 1.** (See [5]).

$$\lambda_1(G_0) = \sqrt{\frac{t-1 + \sqrt{(t-3)^2 + 4}}{2}}. \quad (2.2)$$
LEMMA 2.1. Let $G^{(1)}_{2,t}, G^{(2)}_{2,t}, G^{(3)}_{2,t} \subseteq T_{2t}$ as in Figure (2). Then we have

$$\lambda_2(T) \leq \lambda_1(G_0) \quad (T \in T_{2t} \setminus \{G^{(1)}_{2,t}, G^{(2)}_{2,t}, G^{(3)}_{2,t}\}).$$

(2.3)

Proof. Take $a = t - 1$ in Lemma A. Then there exists $v_1 \in V(T)$ such that one component $T_1$ of $T - v_1$ has order $\leq t$ and the rest of the components of $T - v_1$ have orders $\leq t - 1$.

Case 1. If $T_1 \not\cong K_{1,t-1}$, then $\lambda_1(T_1) \leq \max(\lambda_1(G_0), \sqrt{t-2}) = \lambda_1(G_0)$ [by (2.1)], so from Lemma B we have

$$\lambda_2(T) \leq \lambda_1(T - v_1) \leq \max(\lambda_1(T_1), \sqrt{t-2}) \leq \lambda_1(G_0).$$

Case 2. If $T_1 \cong K_{1,t-1}$. Let $v_2$ be the unique vertex in $T_1$ adjacent to $v_1$; then the component $T_2$ of $T - v_2$ containing $v_1$ has order $t$, and the rest of the components of $T - v_2$ have order $\leq t - 1$.

Since $T \not\in \{G^{(1)}_{2,t}, G^{(2)}_{2,t}, G^{(3)}_{2,t}\}$ and $T_1 \cong K_{1,t-1}$, we must have $T_2 \not\cong K_{1,t-1}$. Then by the same argument as in case 1, we can obtain $\lambda_2(T) \leq \lambda_1(G_0)$.
It is easy to compute the characteristic polynomials of $G_{2,t}^{(1)}, G_{2,t}^{(2)}, G_{2,t}^{(3)}$ as follows:

\[
P(G_{2,t}^{(1)}; \lambda) = \lambda^{2t-6} \{ \lambda^6 - (2t - 1)\lambda^4 + (t^2 - 3)\lambda^2 - (t - 2)^2 \},
\]

\[
P(G_{2,t}^{(2)}; \lambda) = \lambda^{2t-4} \{ \lambda^4 - (2t - 1)\lambda^2 + t^2 - t - 1 \},
\]

\[
P(G_{2,t}^{(3)}; \lambda) = \lambda^{2t-4} \{ \lambda^4 - (2t - 1)\lambda^2 + (t - 1)^2 \}.
\]

Now let

\[
g(y) = y^3 + (t - 2)y^2 - 2y - 1.
\]

Then we can write $P(G_{2,t}^{(1)}; \lambda) = \lambda^{2t-6} g(\lambda^2 - (t - 1))$, and we have

\[
\lambda_2(G_{2,t}^{(1)}) = \sqrt{t - 1 + \lambda_2(g)}, \tag{2.4}
\]

\[
\lambda_2(G_{2,t}^{(2)}) = \sqrt{\frac{2t - 1 - \sqrt{5}}{2}}, \tag{2.5}
\]

\[
\lambda_2(G_{2,t}^{(3)}) = \sqrt{\frac{2t - 1 - \sqrt{4t - 3}}{2}}, \tag{2.6}
\]

where $\lambda_2(g)$ is the second largest real root of the cubic polynomial $g(y)$.

The following theorem asserts that $\lambda_2(G_{2,t}^{(1)})$ is the largest second eigenvalue of the trees in $T_{2t}$.

**Theorem 2.1.**

\[
\lambda_2(T) \leq \lambda_2(G_{2,t}^{(1)}) \quad (T \in T_{2t}) \tag{2.7}
\]

with equality if and only if $T \cong G_{2,t}^{(1)}$. Thus

\[
\overline{T}_{2,t} = \{ G_{2,t}^{(1)} \} \tag{2.8}
\]

and

\[
\overline{\lambda}_2(2t) = \lambda_2(G_{2,t}^{(1)}) = \sqrt{t - 1 + \lambda_2(g)}. \tag{2.9}
\]

**Proof.** Without loss of generality we may assume $t \geq 5$. Noting $g(0) < 0$ and $g(-\frac{1}{2}) > 0$, we have $\lambda_2(g) > -\frac{1}{2}$. So

\[
\lambda_2(G_{2,t}^{(3)}) < \lambda_2(G_{2,t}^{(2)}) < \sqrt{\frac{2t - 3}{2}} < \lambda_2(G_{2,t}^{(1)}). \tag{2.10}
\]
On the other hand, we have

\[ \lambda_1(G_0) < \sqrt{\frac{2t - 3}{2}} \quad (t \geq 5). \quad (2.11) \]

Combining (2.3), (2.10), and (2.11), we get the desired result.

We would like to mention here that Professor Hong Yuan had independently obtained the results in Theorem 2.1.

**Remark 2.** Let

\[ X_k(t) = \max \{X_1(T) \mid T \in T_{2t} \setminus \{G^{(1)}_{2,t}\}\}. \]

Then from (2.2), (2.3), (2.5), and (2.10) we have

\[ \lambda'_2(2t) = \lambda_2(G^{(2)}_{2,t}) \quad (t \geq 6). \quad (2.13) \]

This is also true for \( t = 2, 3, 5 \). But for \( t = 4 \), we have

\[ \lambda'_2(2t) \approx 1.564 > \lambda_2(G^{(2)}_{2,t}) \approx 1.543 \quad (t = 4). \quad (2.14) \]

3. **SOME NECESSARY CONDITIONS FOR EXTREMAL TREES**

Now we consider the general case where \( n = kt \ (t \geq 2, k \geq 2) \). First give some definitions and notation.

Let \( X_{k,t} \) be the subset of trees in \( T_{kt} \) which consists of \( k \) disjoint stars \( S_1, \ldots, S_k \) of order \( t(S_1 \cong S_2 \cong \cdots \cong S_k \cong K_{1,t-1}) \) together with another \( k - 1 \) edges \( e_1, \ldots, e_{k-1} \) such that the two end vertices of each edge \( e_i \) \((i = 1, \ldots, k - 1)\) 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 \( T \).

For example, we have \( X_{2,t} = \{G^{(1)}_{2,t}\} \).

**Lemma 3.1.** For \( k \geq 2 \), we have

\[ \lambda_k(T) \leq \lambda'_2(2t) \quad (T \in T_{kt} \setminus X_{k,t}). \quad (3.1) \]

**Proof.** The case \( k = 2 \) is Theorem 2.1. In general we use induction on \( k \). Take \( a = t - 1 \) and \( v_1 \in V(T) \) in Lemma A such that one component
$T_1$ of $T - v_1$ has order $\leq (k - 1)t$ and the rest of the components of $T - v_1$ have order $\leq t - 1$. If $T_1 \not\in X_{k-1,t}$, then for $|V(T_1)| = (k - 1)t$ we have $\lambda_{k-1}(T_1) \leq \lambda'_2(2t)$ by induction, while for, $|V(T_1)| < (k - 1)t$ we have from Theorem A that

$$\lambda_{k-1}(T_1) \leq \sqrt{\frac{|V(T_1)|}{k-1} - 1} \leq \sqrt{t-2}.$$ 

Thus

$$\lambda_k(T) \leq \lambda_{k-1}(T - v_1) \leq \max(\lambda_{k-1}(T_1), \sqrt{t-2}) \leq \lambda'_2(2t).$$

If $T_1 \in X_{k-1,t}$, take a star $S_t \cong K_{1,t-1}$ in $T_1$ such that $S_t$ does not contain the unique vertex in $T_1$ adjacent to $v_1$ and there is only one vertex (say $v_2$) in $S_t$ incident to some nonstar edge of $T_1$. Then one component $T_2$ of $T - v_2$ has order $(k - 1)t$. Now $T \not\in X_{k,t}$ and $T_1 \in X_{k-1,t}$ imply $T_2 \not\in X_{k-1,t}$, so using the same argument for $T_2$ as for $T_1$, we get $\lambda_k(T) \leq \lambda'_2(2t)$. 

For a graph $G$, let $q(G)$ be the number of edges in a maximal matching of $G$, 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

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

and

$$h_G(y) = m_G(y + a).$$

Then the characteristic polynomial of a tree $T \in \mathcal{T}_n$ is

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

and thus

$$\lambda_k(T) = \sqrt{\lambda_k(m_T)} = \sqrt{a + \lambda_k(h_T)} \quad (k \leq q(T))$$

where $\lambda_k(m_T)$ and $\lambda_k(h_T)$ are the $k$th largest real roots of the polynomials $m_T(x)$ and $h_T(y)$.

**Example.** Let $S(n_1, \ldots, n_k) = K_{n_1} \cup \cdots \cup K_{n_k}$ be the disjoint union of $k$ stars. Then $q(S(n_1, \ldots, n_k)) = k$,

$$a_j(S(n_1, \ldots, n_k)) = \sum_{1 \leq r_1 < r_2 < \cdots < r_j \leq k} n_{r_1}n_{r_2}\cdots n_{r_j},$$

(3.6)
and so

\[ m_{S(n_1, \ldots, n_k)}(x) = \sum_{j=0}^{k} (-1)^j a_j(S(n_1, \ldots, n_k)) x^{k-j} \]

\[ = \prod_{i=1}^{k} (x - n_i). \quad (3.7) \]

For convenience we sometime abbreviate the notation as:

\[ S(a_{1_{r_1}}, a_{2_{r_2}}, \ldots, a_{j_{r_j}}) = S(a_{1_{(r_1)}}, a_{2_{(r_2)}}, \ldots, a_{j_{(r_j)}}). \quad (3.8) \]

Next we want to show the following necessary condition for a tree \( T \in T_{kt} \) to be extremal (i.e., in \( \bar{T}_{k,t} \)):

\[ \bar{T}_{k,t} \subseteq X_{k,t}. \]

For this purpose, it will suffice (by Lemma 3.1) to find a tree \( T \in X_{k,t} \) satisfying \( \lambda_k(T) > \lambda_2(2t) \). We will look for such \( T \) in the subset \( X'_{k,t} \) (see Definition 3.2 below) of \( X_{k,t} \).

**Definition 3.1.** Let \( S_1, \ldots, S_k \) be the \( k \) stars of the tree \( T \in X_{k,t} \). Then the condensed tree \( \hat{T} \) of \( T \) is defined as \( V(\hat{T}) = \{S_1, \ldots, S_k\} \), and there is an edge \([S_i, S_j](i \neq j)\) in \( \hat{T} \) if and only if there exists some nonstar edge of \( T \) with one end in \( S_i \) and the other end in \( S_j \).

It is obvious that \( T \in T_k \) for \( T \in X_{k,t} \).

**Definition 3.2.** The subset \( X'_{k,t} \) of the set \( X_{k,t} \) 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 \( T \).

For example, in Figure 3 below we have \( G^{(1)}_{3,t} \in X'_{3,t}, G^{(2)}_{3,t} \not\in X'_{3,t} \).

It is obvious that if \( \hat{T} \in X'_{k,t} \), then \( T \) is completely determined by its condensed tree \( \hat{T} \).

From now on, we always write

\[ a = t - 1 \quad (3.9) \]

and let (for \( u > 0 \))

\[ f_u(y) = (y + a)y^2 - u^2(y + 1)^2 \quad (a = t - 1). \quad (3.10) \]
The cubic polynomial \( f_u(y) \) will play an important role in our studies.

**Lemma 3.2.** 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

\[
\lambda_3(f_u) \leq -1 < \lambda_2(f_u) < 0 < \lambda_1(f_u)
\]  
(3.11)

and

\[
\lambda_2(f_\xi) < \lambda_2(f_u) \quad \text{(for} \quad 0 < u < \xi). 
\]  
(3.12)

**Proof.** The results are obvious for \( a = 1 \). Now for \( a \geq 2 \), we have \( f_u(0) = -u^2 < 0 \) and \( f_u(-1) = a - 1 > 0 \). Thus \( f_u(y) \) has three real roots, and (3.11) holds. Now if \( 0 < u < \xi \), then

\[
f_u(\lambda_2(f_\xi)) = (\xi^2 - u^2)\{\lambda_2(f_\xi) + 1\}^2 > 0
\]  
(3.13)

But \( \lambda_2(f_\xi) < 0 \) and \( f_u(y) \leq 0 \) for \( \lambda_2(f_u) \leq y < 0 \), so from (3.13) we must have \( \lambda_2(f_\xi) < \lambda_2(f_u) \).

**Lemma 3.3.** Let \( T \in X_{k,t}(t \geq 2) \), and let \( u_1 = \lambda_1(\widetilde{T}) \) be the largest eigenvalue of the condensed tree \( \widetilde{T} \). Then

\[
\lambda_k(T) = \sqrt{t - 1 + \lambda_2(f_{u_1})}.
\]  
(3.14)

**Proof.** Let \( q(\widetilde{T}) = q; \) then \( q(T) = q + k \). Since any \( j \)-matching of \( T \) is a combination of some \( i \)-matching of \( \widetilde{T} \) and some \((j - i)\)-matching of some \( S((a - 1)(2i)a^{(k-2i)}) \) for some \( 0 \leq i \leq j \), we have (where \( a = t - 1 \))

\[
a_j(T) = \sum_{i=0}^{j} a_i(\widetilde{T})a_{j-i}(S((a - 1)(2i)a^{(k-2i)})) \quad (0 \leq j \leq q + k),
\]

and

\[
\lambda_k(T) = \sqrt{t - 1 + \lambda_2(f_{u_1})}.
\]  
(3.14)
Here we have used the substitution \( j' = j - i \). Noting further that \( a_i(\hat{T}) = 0 \) for \( i > q \) and \( a_j(S((a - 1)^{(2i)}a^{(k - 2i)})) = 0 \) for \( j' > k \), we have

\[
m_T(x) = \sum_{i=0}^{q} (-1)^i a_i(\hat{T}) x^{q-i} \left( \sum_{j'=0}^{k} (-1)^{j'} a_{j'}(S((a - 1)^{(2i)}a^{(k - 2i)})) x^{k-j'} \right)
\]

So

\[
m_T(x) = \sum_{j=0}^{q+k} (-1)^j \left( \sum_{i=0}^{j} a_i(\hat{T}) a_{j-i}(S((a - 1)^{(2i)}a^{(k - 2i)})) \right) x^{q+k-j}
\]

\[
= \sum_{i=0}^{q+k} (-1)^i a_i(\hat{T}) x^{q-i} \left( \sum_{j'=0}^{q+k-i} (-1)^{j'} a_{j'}(S((a - 1)^{(2i)}a^{(k - 2i)})) x^{k-j'} \right)
\]

Here we have used the substitution \( j' = j - i \). Noting further that \( a_i(\hat{T}) = 0 \) for \( i > q \) and \( a_j(S((a - 1)^{(2i)}a^{(k - 2i)})) = 0 \) for \( j' > k \), we have

\[
m_T(x) = \sum_{i=0}^{q} (-1)^i a_i(\hat{T}) x^{q-i} \left( \sum_{j'=0}^{k} (-1)^{j'} a_{j'}(S((a - 1)^{(2i)}a^{(k - 2i)})) x^{k-j'} \right)
\]

\[
= \sum_{i=0}^{q} (-1)^i a_i(\hat{T}) x^{q-i} m_{S((a - 1)^{(2i)}a^{(k - 2i)})} (x)
\]

\[
= \sum_{i=0}^{q} (-1)^i a_i(\hat{T}) x^{q-i} (x - a + 1)^{2i} (x - a)^{k-2i}
\]

\[
= (x - a)^{k-2q} (x - a + 1)^{2q} \sum_{i=0}^{q} (-1)^i a_i(\hat{T}) \left( \frac{x(x - a)^2}{(x - a + 1)^2} \right)^{q-i}
\]

\[
= (x - a)^{k-2q} (x - a + 1)^{2q} m_{\hat{T}} \left( \frac{x(x - a)^2}{(x - a + 1)^2} \right).
\]

Note that

\[
m_{\hat{T}}(x) = \prod_{i=1}^{q} (x - u_i^2), \quad (3.15)
\]

where \( u_1 > u_2 > \cdots > u_q > 0 \) are the \( q \) positive eigenvalues of \( \hat{T} \). So we have

\[
m_T(x) = (x - a)^{k-2q} (x - a + 1)^{2q} \prod_{i=1}^{q} \left( \frac{x(x - a)^2}{(x - a + 1)^2} - u_i^2 \right)
\]

\[
= (x - a)^{k-2q} \prod_{i=1}^{q} \left\{ x(x - a)^2 - u_i^2(x - a + 1)^2 \right\}.
\]

Thus by definition,

\[
h_T(y) = m_T(y + a) = y^{k-2q} \prod_{i=1}^{q} \left\{ y^2(y + a) - u_i^2(y + 1)^2 \right\}
\]
\[ y^{k-2q} \prod_{i=1}^{q} f_{u_i}(y). \]  

(3.16)

Now from (3.11) we see that \( h_T(y) \) has \( q \) positive roots and \( k - 2q \) zero roots, so \( \lambda_k(h_T) \) is the \( q \)th largest negative root of \( h_T(y) \). By (3.11) and (3.12), we further see that

\[ \lambda_k(h_T) = \min\{\lambda_2(f_{u_1}), \ldots, \lambda_2(f_{u_q})\} = \lambda_2(f_{u_1}), \]  

(3.17)

so from (3.5) we obtain (where \( a = t - 1 \))

\[ \lambda_k(T) = \sqrt{t - 1 + \lambda_2(f_{u_1})}. \]

An immediate consequence of Lemma 3.2 and Lemma 3.3 is:

**Corollary 3.1.** Let \( T* \in X'_k \), with \( \hat{T}^* = P_k \) (a path with \( k \) vertices). Then

\[ \lambda_k(T) < \lambda_k(T^*) \quad \text{for} \quad T \in X'_k \backslash \{T^*\}. \]  

(3.18)

**Corollary 3.2.**

\[ \lambda_k(T^*) > \lambda'_2(2t) \quad (t \geq 5). \]  

(3.19)

**Proof.** Let

\[ u_1 = \lambda_1(\hat{T}^*) = \lambda_1(P_k) = 2 \cos \frac{\pi}{k+1}. \]

Then

\[ \lambda_k(T^*) = \sqrt{t - 1 + \lambda_2(f_{u_1})}, \]  

(3.20)

and from (2.13),

\[ \lambda'_2(2t) = \lambda_2(G_{2,t}^{(2)}) = \sqrt{t - 1 + \frac{1 - \sqrt{5}}{2}} \quad (t \geq 5). \]

We want \( \lambda_2(f_{u_1}) > (1 - \sqrt{5})/2 \). Now

\[ f_{u_1}(y) = y^2(y + a) - 4 \left( \cos^2 \frac{\pi}{k+1} \right) (y + 1)^2, \]
\[ f_{u_1} \left( \frac{1 - \sqrt{5}}{2} \right) > 0 \quad \text{for} \quad a = t - 1 \geq 3, \]

and \((1 - \sqrt{5})/2 < 0\), so \((1 - \sqrt{5})/2 < \lambda_2(f_{u_1})\).

Now we can obtain the following necessary condition for extremal trees.

**Theorem 3.1.** For \( k \geq 2 \) and \( t \geq 3(t \neq 4) \), we have

\[ \overline{T}_{k,t} \subseteq X_{k,t}. \]

**Proof.** The case \( t \geq 5 \) follows from Lemma 3.1 and Corollary 3.2. The case \( t = 3 \) and \( k = 2 \) can be checked directly (see [7]), so we only need to consider the case \( t = 3 \) and \( k \geq 3 \).

Let \( T^* \in X'_{k,3} \) as in Corollary 3.1 (now \( t = 3 \)). Then from (3.20) and (3.12) we have

\[ \lambda_k(T^*) = \sqrt{t - 1 + \lambda_2(f_{u_1})} = \sqrt{2 + \lambda_2(f_{\lambda_1(p_k)})} \geq \sqrt{2 + \lambda_2(f_2)}, \tag{3.21} \]

where \( f_2(y) = y^2(y + 2) - 4(y + 1)^2 \) (now \( a = t - 1 = 2 \)). By studying Table 2 in [7, Appendix] for the case \( k = 3 \) (\( n = kt = 9 \)), we find the following fact:

\[ \lambda_3(T) < 1.160 \quad (T \in \mathcal{T}_9 \setminus X_{3,3}), \]

so by using a similar inductive argument to the one for Lemma 3.1 we can show that

\[ \lambda_k(T) < 1.160 \quad (T \in \mathcal{T}_k \setminus X_{k,3}, \quad k \geq 3). \tag{3.22} \]

On the other hand, by direct computation we have

\[ f_2(-0.6544) = (0.6544)^2(1.3456) - 4 \times (0.3456)^2 \]
\[ \geq (0.65)^2 \times \frac{4}{3} - 4 \times (0.35)^2 > 0, \]

so \( \lambda_2(f_2) > -0.6544 \), and thus \( 1.160 \approx \sqrt{2 + \lambda_2(f_2)} \). Combining this with (3.21) and (3.22), we have

\[ \lambda_k(T) < \lambda_k(T^*) \quad (T \in \mathcal{T}_k \setminus X_{k,3}, \quad k \geq 3), \]

and so we obtain

\[ \overline{T}_{k,3} \subseteq X_{k,3} \quad (k \geq 3). \]
Using Lemma 3.3, we can also derive a lower bound for $\bar{\lambda}_k(kt)$ and prove that $\bar{\lambda}_k(kt)$ is a decreasing function of $k$ (when $t$ is fixed).

**Theorem 3.2.**

$$\sqrt{t - 2} < \bar{\lambda}_k(kt) < \sqrt{t - 1} \quad (t \geq 2).$$

**Proof.** The upper bound is just a part of the conclusions in Theorem A. For the lower bound, from (3.11) we have $\lambda_2(f_u) > -1$, so

$$\bar{\lambda}_k(kt) \geq \lambda_k(T^*) = \sqrt{t - 1 + \lambda_2(f_u)} > \sqrt{t - 2}.$$

Thus by the Cauchy interlacing theorem we have

$$\lambda_{k+1}(T) \leq \sqrt{[\frac{|V(T_1)|}{k}]} - 1 \leq \sqrt{t - 2} < \bar{\lambda}_k(kt).$$

Thus by the Cauchy interlacing theorem we have

$$\lambda_{k+1}(T) \leq \lambda_k(T - v) \leq \max(\lambda_k(T_1), \sqrt{t - 2}) \leq \bar{\lambda}_k(kt) \quad (T \in T_{(k+1)t}).$$

It follows that $\bar{\lambda}_{k+1}((k + 1)t) \leq \bar{\lambda}_k(kt)$. 

**Theorem 3.3.** For fixed $t \geq 2$, we have

$$\bar{\lambda}_k(kt) \geq \bar{\lambda}_{k+1}((k + 1)t) \quad (k = 1, 2, \ldots).$$

**Proof.** Let $T \in T_{(k+1)t}$. Take $a = t - 1$ and $v \in V(T)$ in Lemma A such that one component $T_1$ of $T - v$ has order $\leq kt$ and the rest of the components have orders $\leq t - 1$. If $|V(T_1)| = kt$, then surely $\lambda_k(T_1) \leq \bar{\lambda}_k(kt)$. If $|V(T_1)| < kt$, we also have

$$\lambda_k(T_1) \leq \sqrt{[\frac{|V(T_1)|}{k}]} - 1 \leq \sqrt{t - 2} < \bar{\lambda}_k(kt).$$

4. **The Cases $K = 3$ and $K = 4$**

We first settle the case $k = 3$ by determining the value $\bar{\lambda}_3(3t)$ and the extremal tree set $\mathcal{F}_{3,t}$. We see from Theorem 3.1 that $\mathcal{F}_{3,t} \subseteq X_{3,t}$, but by definition we find (see Figure 3).

$$X_{3,t} = \{G_{3,t}^{(1)}, G_{3,t}^{(2)}\}. \quad (4.1)$$
So it will suffice to compare \( \lambda_3(G_{3,t}^{(1)}) \) and \( \lambda_3(G_{3,t}^{(2)}) \).

**Lemma 4.1.**

\[
\lambda_3\left(G_{3,t}^{(2)}\right) < \lambda_3\left(G_{3,t}^{(1)}\right) \quad (t \geq 3).
\]  

**Proof.** Write \( T_i = G_{3,t}^{(i)} \) \((i = 1, 2)\). Then \( q(T_2) = 5, q(T_1) = 4, \) and \( a_j(T_2) = a_j(T_1) + a_{j-2}(S(a-1, a-1, a-2)) \). \((4.3)\)

Thus

\[
m_{T_2}(x) = \sum_{j=0}^{5} (-1)^j a_j(T_1)x^{5-j} + \sum_{j=0}^{5} (-1)^j a_{j-2}(S(a-1, a-1, a-2))x^{5-j}
\]

\[
= x m_{T_1}(x) + m_{S(a-1, a-1, a-2)}(x)
\]

\[
= x m_{T_1}(x) + (x-a+1)^2(x-a+2),
\]

so

\[
h_{T_2}(y) = m_{T_2}(y+a) = (y+a)h_{T_1}(y) + (y+1)^2(y+2). \quad (4.4)
\]

Now \( T_1 \in X_{3,t}^{1} \), so by Lemma 3.3, (3.16), and (3.17) we have

\[
h_{T_1}(y) = y f_{\sqrt{2}}(y),
\]

\[
-1 < \lambda_3(h_{T_1}) < 0, \quad (4.5)
\]

and \( \lambda_3(h_{T_1}) \), is the largest negative root of \( h_{T_1}(y) \), which implies that

\[
h_{T_1}(y) \geq 0 \quad \text{[for \ } \lambda_3(h_{T_1}) \leq y \leq 0]\]

So by (4.4) and (4.6) we have

\[
h_{T_2}(y) > 0 \quad \text{[for \ } \lambda_3(h_{T_1}) \leq y \leq 0]\]  

(4.7)

On the other hand, \( \lambda_3(T_2) = \sqrt{t-1 + \lambda_3(h_{T_2})} < \sqrt{t-1} \) by (3.5) and Theorem 3.2, so \( \lambda_3(h_{T_2}) < 0 \) is a negative root of \( h_{T_2}(y) \). Combining this with (4.7), we have \( \lambda_3(h_{T_2}) < \lambda_3(h_{T_1}) \) and thus obtain

\[
\lambda_3(T_2) = \sqrt{a + \lambda_3(h_{T_2})} < \sqrt{a + \lambda_3(h_{T_1})} = \lambda_3(T_1).
\]

From Lemma 4.1, Theorem 3.1, and (4.1), we immediately get the following solution for \( k = 3 \).
THEOREM 4.1. For $t \geq 5$, we have

$$\overline{T}_{3,t} = \{G_{3,t}^{(1)}\}$$

and

$$\overline{\lambda}_3(3t) = \lambda_3(G_{3,t}^{(1)}) = \sqrt{t - 1 + \lambda_2(f_{\sqrt{2}})},$$

where $f_{\sqrt{2}}(y) = y^2(y + a) - 2(y + 1)^2$ \((a = t - 1)\).

Next we consider the case $k = 4$ \((t \geq 5)\). From Theorem 3.1 we have

$$\overline{T}_{4,t} \subseteq X_{4,t},$$

while by definition we find that \(x_{4,t} = \{c_1, \ldots, c_t\}\).

(4.8)

LEMMA 4.2. For any $1 \leq i, j \leq 6$, we have

$$\lambda_5(T_i) \leq \lambda_4(T_i) \leq \lambda_3(T_j).$$

(4.9)

Proof. Take an induced subgraph $H_i$ of $T_i$ which is a disjoint union of four stars, each of which has order $\geq t - 1$ (the existence of such $H_i$ can be seen from the structure of $T_i$). Then

$$\lambda_4(T_i) \geq \lambda_4(H_i) \geq \sqrt{t - 2}. \quad (4.10)$$

On the other hand, we have from Theorem A that

$$\lambda_5(T_j) \leq \sqrt{\left[\frac{4t}{5}\right] - 1} \leq \sqrt{t - 2} \quad (4.11)$$

So we get the first inequality in (4.9).

Next we take an induced subgraph $F_j$ of $T_j$ with order $3t$ (by deleting some suitable star of $T_j$) such that $F_j$ is either a disjoint union of three stars $K_{1,t-1}$ or a disjoint union of a $K_{1,t-1}$ and $G_{2,t}^{(1)}$. Then by Theorem 3.3 we obtain

$$\lambda_3(T_j) \geq \lambda_3(F_j) \geq \lambda_2(G_{2,t}^{(1)}) = \overline{\lambda}_2(2t) \geq \overline{\lambda}_4(4t) \geq \lambda_4(T_i),$$

(4.12)

which gives the second inequality in (4.9).
COROLLARY 4.1. For $1 \leq i, j \leq 6$, $i \neq j$, we have:

1. If $h_{T_j}(\lambda_4(h_{T_i})) > 0$, then $\lambda_4(h_{T_i}) > \lambda_4(h_{T_j})$.
2. If $h_{T_j}(\lambda_4(h_{T_i})) < 0$, then $\lambda_4(h_{T_i}) < \lambda_4(h_{T_j})$.

Proof. From (4.9) we have that

$$\lambda_5(h_{T_i}) \leq \lambda_4(h_{T_i}) \leq \lambda_3(h_{T_i}).$$

Now all the roots of $h_{T_i}(y)$ are real, since all the eigenvalues of $T_i$ are real, so

$$h_{T_i}(y) = \prod_{k=1}^{q(T_i)} \left\{ y - \lambda_k(h_{T_i}) \right\}.$$
Write \( b = \lambda_4(h_{T_j}) \). If \( h_{T_j}(b) > 0 \), then from (4.13) we have
\[
\lambda_1(h_{T_j}) \geq \lambda_2(h_{T_j}) \geq \lambda_3(h_{T_j}) > b > \lambda_5(h_{T_j}) \geq \cdots
\]
and so
\[
b - \lambda_4(h_{T_j}) = h_{T_j}(b) \cdot \left( \prod_{k=1}^{3} \{b - \lambda_k(h_{T_j})\} \right)^{-1} \left( \prod_{k=5}^{n} \{b - \lambda_k(h_{T_j})\} \right)^{-1} < 0.
\]
Thus (1) follows, and similar arguments will prove (2).

Now we compute the polynomials \( h_{T_i}(y)(i = 1, \ldots, 6) \). First we have
\[
q(T_1) = q(T_2) = q(T_6) = 6, \quad q(T_4) = 5, \quad q(T_3) = q(T_5) = 7; \quad (4.15)
\]
and (where \( a = t - 1 \))
\[
\begin{align*}
a_j(T_1) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})) + a_{j-2}(S((a-1)^{(4)})), \\
a_j(T_2) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})) + a_{j-2}(S((a-1)^{(4)})) + a_{j-2}s(a,a-1,a-1,a-2), \\
a_j(T_3) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})) + a_{j-2}(S((a-1)^{(4)})) + 2a_{j-2}s(a,a-1,a-1,a-2) + a_{j-3}(S((a-1)^{(2)}(a-2)^{(2)})}, \\
a_j(T_4) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})), \\
a_j(T_5) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})) + 2a_{j-2}s(a,a-1,a-1,a-2), \\
a_j(T_6) &= a_j(S(a^{(4)})) + 3a_{j-1}(S(a^{(2)}(a-1)^{(2)})) + 3a_{j-2}s(a,a-1,a-1,a-2) + a_{j-3}(S((a-3)(a-1)^{(3)})).
\end{align*}
\]
Thus we have
\[
m_{T_1}(x) = \sum_{j=0}^{6} (-1)^{j} a_j(T_1)x^{6-j} = x^2 \sum_{j=0}^{4} (-1)^{j} a_j(S(a^{(4)}))x^{4-j}
\]
\[-3x \sum_{j=0}^{4} (-1)^j a_j \left( S(a^{(2)}(a-1)^{(2)}) \right) x^{4-j} \]
\[+ \sum_{j=0}^{4} (-1)^j a_j \left( S((a-1)^{(4)}) \right) x^{4-j} \]
\[= x^2(x-a)^4 - 3x(x-a)^2(x-a+1)^2 + (x-a+1)^4 \]
and so
\[h_{T_1}(y) = m_{T_1}(y+a) = (y+a)^2 y^4 - 3(y+a)y^2(y+1)^2 + (y+1)^4. \quad (4.16)\]

Similarly,
\[h_{T_2}(y) = (y+a)^2 y^4 - 3(y+a)y^2(y+1)^2 \]
\[+ (y+1)^4 + y(y+1)^2(y+2), \quad (4.17)\]
\[h_{T_3}(y) = (y+a)^3 y^4 - 3(y+a)^2 y^2(y+1)^2 + (y+a)(y+1)^4 \]
\[+ 2(y+a)y(y+1)^2(y+2) - (y+1)^2(y+2)^2, \quad (4.18)\]
\[h_{T_4}(y) = (y+a)^4 y^4 - 3(y+a)^2 y^2(y+1)^2 \]
\[+ 3(y+a)y(y+1)^2 \times (y+2) - (y+3)(y+1)^3. \quad (4.19)\]

**Lemma 4.3.** For \( t \geq 3 \), we have
\[\lambda_4(h_{T_i}) < \lambda_4(h_{T_1}) \quad (i = 2, 3, 4, 5, 6). \quad (4.22)\]

**Proof.** By Theorem A and (4.10), we have
\[\sqrt{t-2} \leq \lambda_4(T_i) = \sqrt{t-1 + \lambda_4(h_{T_1})} < \sqrt{t-1} \quad (i = 1, \ldots, 6). \quad (4.23)\]
Also clearly \( h_{T_1}(-1) \neq 0 \), so we always have
\[-1 < \lambda_4(h_{T_i}) < 0 \quad (i = 1, \ldots, 6). \quad (4.24)\]
Now
\[h_{T_2}(y) = h_{T_1}(y) + y(y+1)^2(y+2), \]
so
\[h_{T_2}(\lambda_4(h_{T_1})) < 0, \]
and thus (by Corollary 4.1)

$$\lambda_4(h_{T_2}) < \lambda_4(h_{T_1}).$$

(4.25)

Also

$$h_{T_3}(y) = (y + a)h_{T_2}(y) + (y + a)y(y + 1)^2(y + 2) - (y + 1)^2(y + 2)^2,$$

so

$$h_{T_3}(\lambda_4(h_{T_2})) < 0$$

and

$$\lambda_4(h_{T_3}) < \lambda_4(h_{T_2}).$$

(4.26)

Also

$$h_{T_4}(y) = (y + a)h_{T_4}(y) + (y + 1)^4,$$

so

$$h_{T_4}(\lambda_4(h_{T_4})) > 0$$

and

$$\lambda_4(h_{T_4}) < \lambda_4(h_{T_1}).$$

(4.27)

Also

$$h_{T_5}(y) = (y + a)h_{T_4}(y) + 2y(y + 1)^2(y + 2),$$

so

$$h_{T_5}(\lambda_4(h_{T_4})) < 0$$

and

$$\lambda_4(h_{T_5}) < \lambda_4(h_{T_4}).$$

(4.28)

Also

$$h_{T_6}(y) = (y + a)h_{T_5}(y) + (y + a)y(y + 1)^2(y + 2) - (y + 3)(y + 1)^3,$$

so

$$h_{T_6}(\lambda_4(h_{T_5})) < 0$$

and

$$\lambda_4(h_{T_6}) < \lambda_4(h_{T_5}).$$

(4.29)

Combining (4.25)–(4.29), we obtain (4.22).

Note that $T_1 = G_{4,1}^{(1)} \in X_{4,t}^t$ and $\widehat{T_1} = P_4$, so by (3.20) we have

$$\lambda_4(T_1) = \sqrt{t - 1 + \lambda_2(f_{\lambda_1(P_4)})},$$
where $\lambda_1(P_4) = 2\cos(\pi/5)$. Thus we obtain:

**Theorem 4.2.** For $t \geq 5$, we have

$$\overline{T}_{4,t} = \{G_{4,t}^{(1)}\}$$

and

$$\overline{\lambda}_4(4t) = \lambda_4(G_{4,t}^{(1)}) = \sqrt{t - 1 + \lambda_2(f_2\cos(\pi/5))}.$$

5. THE CASE $K = 5$

Let $T^* \in X_{5,t}'$ with $\overline{T^*} = P_5$ as in Corollary 3.1. Note also $G_{4,t}^{(4)} \in X_{4,t}'$ with $G_{4,t}^{(4)} = K_{1,3}$. So by Lemma 3.3 we have

$$\lambda_5(T^*) = \sqrt{t - 1 + \lambda_2(f_1(P_5))}$$

and

$$\lambda_4(G_{4,t}^{(4)}) = \sqrt{t - 1 + \lambda_2(f_1(K_{1,3}))}.$$

Now $\lambda_1(P_5) = 2\cos(\pi/6) = \sqrt{3} = \lambda_1(K_{1,3})$, so we have

$$\lambda_5(T^*) = \lambda_4(G_{4,t}^{(4)}). \quad (5.1)$$

**Lemma 5.1.** If $T \in X_{5,t}$ and $\overline{T} \neq P_5$, then

$$\lambda_5(T) \leq \lambda_5(T^*).$$

**Proof.** By assumption $\overline{T} \in T_5 \backslash\{P_5\}$, so $\overline{T}$ has an induced subgraph isomorphic to $K_{1,3}$, and thus there exists a vertex $v \in V(T)$ such that $T - v = H \cup K_{1,t-2}$, where $H \in X_{4,t}$ and $H = K_{1,3}$. By (4.8) we have $H \in \{G_{4,t}^{(4)}, G_{4,t}^{(5)}, G_{4,t}^{(6)}\}$, where $\lambda_4(G_{4,t}^{(6)}) < \lambda_4(G_{4,t}^{(5)}) < \lambda_4(G_{4,t}^{(4)})$ [see (4.28), (4.29)]. So by the Cauchy interlacing theorem we have

$$\lambda_5(T) \leq \lambda_4(T - v) \leq \max(\lambda_4(H), \sqrt{t - 2}) \leq \lambda_4(G_{4,t}^{(4)}) = \lambda_5(T^*).$$
Now let (see Figure 5)

\[ Y_{5,t} = \{ T \in X_{5,t} \mid \hat{T} = P_3 \} = \{ G_{5,t}^{(1)}, G_{5,t}^{(2)}, \ldots, G_{5,t}^{(6)} \}. \]  
(5.2)

Write \( G_i = G_{5,t}^{(i)}(i = 1, \ldots, 6) \). From Lemma 5.1, we need to compare \( \lambda_5(G_i)(i = 1, \ldots, 6) \), or equivalently to compare those \( \lambda_5(h_{G_i})(i = 1, \ldots, 6) \).

For any \( T \in X_{k,t} \), by deleting a vertex \( v \) in a star corresponding to a pendant vertex (vertex with degree 1) of \( \hat{T} \) such that \( v \) is also incident to some nonstar edge of \( T \), and using induction on \( k \), we can find an induced subgraph \( H \) of \( T \) such that \( H \) is a disjoint union of \( k \) stars \( K_{1,t-2} \). So we always have

\[ \lambda_k(T) \geq \lambda_k(H) = \sqrt{t - 2} \quad (T \in X_{k,t}). \]  
(5.3)

It follows as in the case \( k = 4 \) that

\[ \lambda_6(G_j) \leq \sqrt{t - 2} \leq \lambda_5(G_i) \quad (1 \leq i, j \leq 6). \]  
(5.4)
On the other hand, by deleting a suitable star (the middle star in Figure 5) of each \( G_j \) we can find an induced subgraph \( F_j \) of \( G_j \) such that \( F_j \cong G_{2,t}^{(1)} \cup G_{2,t}^{(1)} \), and thus

\[
\lambda_4(G_j) \geq \lambda_4(F_j) = \lambda_2(G_{2,t}^{(1)}) = \lambda_2(2t) \geq \lambda_5(5t) \geq \lambda_5(G_i). \tag{5.5}
\]

Therefore (as in case \( k = 4 \))

\[
\lambda_6(h_{G_i}) \leq \lambda_5(h_{G_i}) \leq \lambda_4(h_{G_i}) \quad (1 \leq i, j \leq 6) \tag{5.6}
\]
and we have (as in Corollary 4.1) that

- if \( h_{G_j}(\lambda_5(h_{G_i})) > 0 \), then \( \lambda_5(h_{G_i}) > \lambda_5(h_{G_j}) \); \tag{5.7}
- if \( h_{G_j}(\lambda_5(h_{G_i})) < 0 \), then \( \lambda_5(h_{G_i}) < \lambda_5(h_{G_j}) \). \tag{5.8}

Also we have, as in \( k = 4 \), that

\[-1 < \lambda_5(h_{G_i}) < 0 \quad (i = 1, \ldots, 6). \tag{5.9}\]

Now we compute

\[
h_{G_1}(y) = (y + a)^2y^5 - 4(y + a)y^3(y + 1)^2 + 3y(y + 1)^4, \tag{5.10}
\]
\[
h_{G_2}(y) = (y + a)^2y^5 - 4(y + a)^2y^3(y + 1)^2 + 3(y + a)y(y + 1)^4 + (y + a)y^2(y + 1)^2(y + 2) - (y + 1)^4(y + 2), \tag{5.11}
\]
\[
h_{G_3}(y) = (y + a)^2y^5 - 4(y + a)y^3(y + 1)^2 + 3y(y + 1)^4 + 3y^2(y + 1)^4(y + 2), \tag{5.12}
\]
\[
h_{G_4}(y) = (y + a)^3y^5 - 4(y + a)^2y^3(y + 1)^2 + 3(y + a)y(y + 1)^4 + 2(y + a)y^2(y + 1)^2(y + 2) - (y + 1)^4(y + 2)
- y(y + 1)^2(y + 2)^2, \tag{5.13}
\]
\[
h_{G_5}(y) = (y + a)^3y^5 - 4(y + a)^2y^3(y + 1)^2 + 3(y + a)y(y + 1)^4 + 2(y + a)y^2(y + 1)^2(y + 2) - 2(y + 1)^4(y + 2), \tag{5.14}
\]
\[
h_{G_6}(y) = (y + a)^4y^5 - 4(y + a)^3y^3(y + 1)^2 + 3(y + a)^2y(y + 1)^4 + 3(y + a)^2y^2(y + 1)^2(y + 2) - 2(y + a)(y + 1)^4(y + 2)
- 2(y + a)y(y + 1)^2(y + 2)^2 + (y + 1)^2(y + 2)^3. \tag{5.15}
\]

Note that \( h_{G_1}(y) = yf_{\sqrt{3}}(y)f_1(y) \) and \( f_{\sqrt{3}}(\lambda_5(h_{G_1})) = 0 \), and we have

\[
h_{G_2}(y) = (y + a)h_{G_1}(y) + f_{\sqrt{3}}(y)(y + 1)^2(y + 2) + 2(y + 1)^4(y + 2),
\]
From (5.16)-(5.20) and (5.9) we get

\[ h_{G_i}(\lambda_5(h_{G_i})) > 0 \quad (i = 2, 3, 4, 5, 6) \]

and thus obtain

\[ \lambda_5(h_{G_i}) < \lambda_5(h_{G_1}) \quad (i = 2, 3, 4, 5, 6). \]  

Combining Lemma 5.1 (where \( T^* = G_1 = G_{5,t}^{(1)} \)) and (5.21), we have:

**Theorem 5.1.** For \( t \geq 5 \),

\[ \bar{\lambda}_5(5t) = \lambda_5(G_{5,t}^{(1)}) = \sqrt{t - 1 + \lambda_2(f_{\sqrt{3}})}. \]

We would also like to point out that by direct verifications as in (5.16)-(5.21), we can actually show that the strict inequality holds in Lemma 5.1. Thus we also have

\[ \bar{T}_{5,t} = \{G_{5,t}^{(1)}\}. \]  

6. SOME FURTHER NECESSARY CONDITIONS FOR EXTREML TRES

A further necessary condition for \( T \in \bar{T}_{k,t} \) which is stronger than \( \bar{T}_{k,t} \subseteq X_{k,t} \) is that if \( T \in \bar{T}_{k,t} \), then \( T \in X_{k,t} \) and \( \Delta(\hat{T}) \leq 3 \), where \( \Delta(\hat{T}) \) is the maximal degree of the condensed tree \( \hat{T} \). We will prove this in Theorem 6.1.
Let (see Figure 6)

\[ W_{5,t} = \{H_1, H_2, \ldots, H_5\} = \{T \in X_{5,t} \mid \hat{T} = K_{1,4}\} \quad (6.1) \]

**Lemma 6.1.** For \( t \geq 3 \), we have

\[ \lambda_5(H_1) > \lambda_5(H_i) \quad (i = 2, 3, 4, 5; \quad k = 1, 2, \ldots). \quad (6.2) \]

**Proof.** We have \( H_1 \in X'_{5,t} \) and \( \hat{H}_1 = K_{1,4} \), so by Lemma 3.3 we have

\[ \lambda_5(H_1) = \sqrt{t - 1 + \lambda_2(f_{\lambda_1(K_{1,4})})}. \]

By (3.20) we also have

\[ \lambda_k(kt) \geq \sqrt{t - 1 + \lambda_2(f_{\lambda_1(P_k)})}. \]

Now

\[ \lambda_1(K_{1,4}) = 2 > \lambda_1(P_k) = 2 \cos \frac{\pi}{k+1}, \]
so \( \lambda_2(f_{\lambda_1(K_{1,4}}) < \lambda_2(f_{\lambda_1(P_5)}) \) and \( \lambda_k(kt) > \lambda_5(H_1) \).

On the other hand, direct computations give

\[
\begin{align*}
    h_{H_1}(y) &= (y + a)y^5 - 4y^3(y + 1)^2, \\
    h_{H_2}(y) &= (y + a)^2y^5 - 4(y + a)y^3(y + 1)^2 + 3y^2(y + 1)^2(y + 2), \\
    h_{H_3}(y) &= (y + a)^2y^5 - 4(y + a)y^3(y + 1)^2 + 4y^2(y + 1)^2(y + 2), \\
    h_{H_4}(y) &= (y + a)^3y^5 - 4(y + a)^2y^3(y + 1)^2 + 5(y + a)y^2(y + 1)^2 \\
    &\quad \times (y + 2) - 2y(y + 1)^3(y + 3), \\
    h_{H_5}(y) &= (y + a)^4y^5 - 4(y + a)^3y^3(y + 1)^2 + 6(y + a)^2y^2(y + 1)^2 \\
    &\quad \times (y + 2) - 4(y + a)y(y + 1)^3(y + 3) + (y + 1)^4(y + 4).
\end{align*}
\]

Using similar arguments to (5.6) and (5.9), we also have

\[-1 < \lambda_5(h_{H_i}) < 0 \quad (i = 1, \ldots, 5) \tag{6.8}\]

and

\[
\lambda_6(H_j) \leq \lambda_5(H_i) < \sqrt{t - 1} \leq \lambda_4(F_j) \leq \lambda_4(H_j) \quad (i, j = 1, 2, \ldots, 5), \tag{6.9}
\]

where \( F_j \) is an induced subgraph of \( H_j \) which is a disjoint union of four stars \( K_{1,t-1} \). Then we verify that

\[ h_{H_{i+1}}(\lambda_5(h_{H_i})) > 0 \quad (i = 1, 2, 3, 4), \]

and so, by the same reasoning as before, we obtain

\[ \lambda_5(H_5) < \lambda_5(H_4) < \lambda_5(H_3) < \lambda_5(H_2) < \lambda_5(H_1). \]

Lemma 6.1 implies that if \( T \in \overline{T}_{5,t} \) then \( T \in X_{5,t} \) and \( \Delta(\overline{T}) \leq 3. \) Now the following theorem shows that this holds for general \( k. \)

**Theorem 6.1.** Let

\[ Z_{k,t} = \{T \in X_{k,t} | \Delta(T) \leq 3\}. \tag{6.10} \]

Then for \( k \geq 2 \) and \( t \geq 5 \), we have

\[ \overline{T}_{k,t} \subseteq Z_{k,t}. \tag{6.11} \]
Proof. The case \( k = 2, 3, 4, 5 \) follows from the preceding results. In general we show the following inequality for \( k \geq 5 \) by using induction on \( k \):

\[
\lambda_k(T) \leq \lambda_5(H_1), \quad T \in X_{k,t} \setminus Z_{k,t}.
\] (6.12)

For \( k = 5 \), (6.12) follows from (6.2). For \( k \geq 6 \) and \( T \in X_{k,t} \setminus Z_{k,t} \), we have \( \hat{T} \in T_k \) with \( \Delta(\hat{T}) \geq 4 \), so by deleting a suitable vertex \( v \) in a suitable star of \( T \) corresponding to a pendant vertex of \( \hat{T} \), we will have

\[
T - v = T_1 \cup K_{1,t-2}
\] (6.13)

with \( T_1 \in X_{k-1,t} \) and \( \Delta(\hat{T}_1) \geq 4 \); therefore \( T_1 \in X_{k-1,t} \setminus Z_{k-1,t} \). Now by induction \( \lambda_{k-1}(T_1) \leq \lambda_5(H_1) \) and so

\[
\lambda_k(T) \leq \lambda_{k-1}(T - v) \leq \max(\lambda_{k-1}(T_1), \sqrt{t-2}) \leq \lambda_5(H_1).
\]

Thus (6.12) holds. Combining this with Lemma 6.1, we have

\[
\lambda_k(T) < \lambda_k(kt) \quad (T \in X_{k,t} \setminus Z_{k,t}),
\] (6.14)

and so (6.11) holds.

From the results in cases \( k = 2, 3, 4, 5 \) and the necessary conditions given in Theorem 6.1, it is quite reasonable to propose the following conjecture:

**Conjecture.** For \( t \geq 2 \), we have

\[
\overline{\mathcal{T}}_{k,t} = \{G^{(1)}_{k,t}\}
\]

and

\[
\overline{\lambda}_k(kt) = \sqrt{t-1 + \lambda_2(f_{\lambda_1(P_k)})},
\]

where

\[
f_{\lambda_1(P_k)}(y) = f_{2\cos(\pi/(k+1))}(y) = y^2(y + t - 1) - 4\left(\cos^2\frac{\pi}{k + 1}\right)(y + 1)^2,
\]

and \( \{G^{(1)}_{k,t}\} \) is the tree in Figure 7.

**Remark.** We have also verified that this conjecture is true for the case \( k = 6 \).
REFERENCES

3 Hong Yuan, The kth largest eigenvalue of a tree, Linear, Algebra Appl. 73:151–155 (1986).

Received 22 October 1990