Path-like Graphs Ordered by the Index

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Abstract

A path-like graph is a tree on n vertices and diameter $n - 3$. Let $\alpha = \sqrt{2}\sqrt{\left(\frac{9-\sqrt{33}}{36}\right)^{\frac{1}{3}} + \left(\frac{9+\sqrt{33}}{36}\right)^{\frac{1}{3}} + 1}$ (note $\alpha \in (2, \sqrt{2}\sqrt{1+\sqrt{2}})$). In this paper we first prove that all path-like graphs have the index in the interval $[2, \sqrt{2}\sqrt{1+\sqrt{2}})$. Next we totally order (with respect to the index) all path-like graphs which have the index in the interval $(\alpha, \sqrt{2}\sqrt{1+\sqrt{2}})$.

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1 Introduction

For the basic notions and terminology on spectral graph theory the readers are referred to [5] and [6]. To make the paper more self-contained, we will give here only a few basic facts. The *spectrum* of a graph G is the spectrum of $A(G)$, the adjacency matrix of G . Since $A(G)$ is symmetric, all roots of the characteristic polynomial $\Phi(G, x)$ ($= \det(xI - A(G))$) are real. The largest

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eigenvalue is called the *index*, or spectral radius of G , and denoted by $\rho(G)$. If G is connected, its index is a simple root of $\Phi(G, x)$. An interesting problem is to order the graphs in a prescribed class with respect to the index. The study of ordering graphs by the index was started by Collantz and Sinogowitz [3] in 1957. For the trees with n vertices, Lovasz and Pelican [9] determined the extreme cases by proving that the star $K_{1,n-1}$ has the largest index, and the path P_n the smallest index. In 1979, Li and Feng [8] gave two useful theorems which compare the indices of graphs under certain modifications. The study in this area has made great progress in the meantime.

Our aim here is to study the ordering of the graphs (with respect to the index) in the set $\mathcal{T}_{n,n-3}$, which consists of all the trees of order n and diameter $d = n - 3$. The idea to order such a type of graphs comes from [12]. In [4] and [2] the authors determined all graphs whose index is in the interval $(2, \sqrt{2 + \sqrt{5}})$, a large subclass of them is in the set $\mathcal{T}_{n,n-3}$ (see [1]).

In this paper we prove that all trees in $\mathcal{T}_{n,n-3}$ have index in the interval $[2, \sqrt{2}\sqrt{1 + \sqrt{2}})$, and we totally order the trees having index in the interval $(\alpha, \sqrt{2}\sqrt{1 + \sqrt{2}})$, where $\alpha = \sqrt{2}\sqrt{\left(\frac{9-\sqrt{33}}{36}\right)^{\frac{1}{3}} + \left(\frac{9+\sqrt{33}}{36}\right)^{\frac{1}{3}} + 1}$. For the remaining trees we give only a partial order.

2 Notation and Basic Tools

In $\mathcal{T}_{n,n-3}$ we can consider a large subset of *caterpillars* (trees in which a removal of all pendant vertices makes it a path) denoted by $\mathcal{T}_{n,n-3}^*$, which consists of all the trees of order n , diameter $d = n - 3$ and with two vertices of degree 3. In $\mathcal{T}_{n,n-3}^*$ we can say that the vertices of degree 3 are at position i and j ($i \neq j$) (see Fig. 1). We denote such caterpillars as $M_{i,j}^d$ where i and j ($0 < i < j < n - 3$) are the vertices of degree 3 on the path of length d . If the diameter is kept fixed, we will suppress it from our notation. Let k be the distance between the vertices of degree 3 in $M_{i,j}^d$; of course, $k = j - i$.

Fig. 1: The graph $M_{i,j}^d$

The graphs in $\mathcal{T}_{n,n-3} \setminus \mathcal{T}_{n,n-3}^*$ are the trees M_i^d ($1 \leq i \leq \lfloor \frac{d}{2} \rfloor$, $d = n - 3$) and N_i^d ($2 \leq i \leq \lfloor \frac{d}{2} \rfloor$, $d = n - 3$) defined in the following way: M_i^d is the caterpillar consisting of a path of length d having a vertex of degree 4 at position i , while

N_i^d is a tree consisting of a path of length d having a hanging path (of length 2) attached to position i (see also Fig. 2).

Fig. 2: Graphs in $\mathcal{T}_{n,n-3} \setminus \mathcal{T}_{n,n-3}^*$.

For $d \geq 4$, $\mathcal{T}_{n,n-3}$ is the (disjoint) union of these families of trees:

1. $\{M_{i,j}\}$, where $j - i = k$, i and j ($0 < i < j < n - 3$) are the vertices of degree 3 on the path of length $n - 3$, and $1 \leq i \leq \left\lfloor \frac{d-k}{2} \right\rfloor$ (Fig. 1).
2. $\{M_i\}$, where i is the only vertex of degree 4, and $1 \leq i \leq \left\lfloor \frac{d}{2} \right\rfloor$ (Fig. 2).
3. $\{N_i\}$, where i is the only vertex of degree 3, and $2 \leq i \leq \left\lfloor \frac{d}{2} \right\rfloor$ (Fig. 2).

The following results will be useful further on.

Theorem 2.1. [8] *Let $G(m, n)$ be a graph obtained from a non-trivial connected graph G by adding to a fixed vertex two hanging paths whose lengths are m and n . If $m \geq n \geq 1$ then $\rho(G(m, n)) > \rho(G(m + 1, n - 1))$.*

In order to state the next result we need more definitions. An *internal path* $v_0, v_1, \dots, v_s$ in a graph is a path connecting the vertices v_0 and v_s (possibly with $v_0 = v_s$) for which $\deg(v_0), \deg(v_s) \geq 3$, while $\deg(v_i) = 2$ for $0 < i < s$. In addition, let $T_n = M_{1,n-4}^{n-3}$ (the *double snake*).

Theorem 2.2. [6] *Let G' be a graph obtained from a connected graph G by inserting in an edge e a vertex of degree 2. Then, if G is not a tree T_n , or a cycle C_n , we have:*

- (i) *if e lies on an internal path then $\rho(G') < \rho(G)$;*
- (ii) *if e does not lie on an internal path then $\rho(G') > \rho(G)$.*

If $G = T_n$, and $G' = T_{n+1}$ or $G = C_n$, and $G' = C_{n+1}$ then $\rho(G') = \rho(G) = 2$.

The study of limit points for the eigenvalues of a graph was initiated by Hoffman in [7], where he posed the problem of finding the limit points of the eigenvalues of graphs. The following theorem (along with Theorem 3.3) will be used to calculate the limit points for the index of trees in $\mathcal{T}_{n,n-3}$.

Theorem 2.3. [7] *Let G be a rooted graph with a vertex u as its root, and let G_n be the graph obtained from G by attaching to u a hanging path of length n . Then the limit point for the index of G_n is equal to the greatest root of the equation:*

$$\frac{1}{2}(x + \sqrt{x^2 - 4})\Phi(G, x) - \Phi(G - u, x) = 0.$$

Theorem 2.4. [10] *Let G be a (simple) graph and v one of its vertices. Denote by $\mathcal{C}(v)$ the set of all cycles in G containing v . Then we have:*

$$\Phi(G, x) = x\Phi(G - v, x) - \sum_{w \sim v} \Phi(G - v - w, x) - 2 \sum_{C \in \mathcal{C}(v)} \Phi(G - V(C), x).$$

We assume that $\Phi(G, x) = 1$ if G is the empty graph (i.e. with 0 vertices).

We recall that $\rho(G') < \rho(G)$ whenever G' is a proper subgraph of a connected graph G . Furthermore, the following description of the largest eigenvalue of any hermitian matrix A holds (see, for example, [6], p. 49):

$$\rho(A) = \max_{\|\mathbf{x}\|=1} \mathbf{x}^T A \mathbf{x} \quad (\mathbf{x} \in \mathbf{R}^n). \quad (1)$$

We note here that the maximum is attained in (1) if and only if $\mathbf{x}$ is an eigenvector (for the largest eigenvalue) of A . Next, since A is a non-negative matrix, the corresponding eigenvector can be taken to be non-negative. In addition, if G is connected (i.e. if A is irreducible) then $\mathbf{x}$ can be taken to be positive. We will refer to $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$, as the Perron eigenvector of a (labeled) graph G (generally, it need not be of unit length). Then (for all simple graphs) we have

$$\rho x_i = \sum_{i \sim j} x_j \quad (i = 1, 2, \dots, n). \quad (2)$$

In fact, (2) is an *eigenvalue equation* for the i -th vertex (corresponding to the index).

Consider now the trees from $\mathcal{T}_{n,n-3}^*$. To get a better insight into this set we will arrange it as in Table I. Firstly, for a fixed $d (= n - 3)$, we indicate $M_{i,j}^d$ (for short) by $M_{i,j}$. Let $k = j - i$ be a gap between vertices of degree 3 (in $M_{i,j}$). For a fixed k ($1 \leq i \leq d - 2$), we have a row in the table that consists of all graphs $M_{i,i+k}$, $1 \leq i \leq \frac{d-k}{2}$. Next, for a fixed i , we have a column in which all trees $M_{i,j}$ are placed.

$k = d - 2$	$M_{1,d-1}$					
$k = d - 3$	$M_{1,d-2}$					
$k = d - 4$	$M_{1,d-3}$	$M_{2,d-2}$				
$k = d - 5$	$M_{1,d-4}$	$M_{2,d-3}$				
$\dots$	$\dots$	$\dots$	$\dots$			
k	$M_{1,k+1}$	$M_{2,k+2}$	$\dots$	$M_{\lfloor \frac{d-k}{2} \rfloor, \lfloor \frac{d+k}{2} \rfloor}$		
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	
$k = 1$	$M_{1,2}$	$M_{2,3}$	$\dots$	$\dots$	$\dots$	$M_{\lfloor \frac{d-1}{2} \rfloor, \lfloor \frac{d+1}{2} \rfloor}$

Table I

The class $\mathcal{T}_{n,n-3}$ is largely covered by the class $\mathcal{T}_{n,n-3}^*$. In the next section a partial ordering with respect to the index for the class $\mathcal{T}_{n,n-3}^*$ will be given.

3 Main Tools

The main result of [1] reads as follows:

Theorem 3.1. *Let $G_i^d = M_{i,i+k}^d$. Then, for any fixed d it holds:*

- (i) *if $d > 2(k-1)$ then $\rho(G_i^d) < \rho(G_j^d)$ for all $1 \leq i < j \leq \left\lfloor \frac{d-k}{2} \right\rfloor$*
- (ii) *if $d < 2(k-1)$ then $\rho(G_i^d) > \rho(G_j^d)$ for all $1 \leq i < j \leq \left\lfloor \frac{d-k}{2} \right\rfloor$*
- (iii) *if $d = 2(k-1)$ then $\rho(G_i^d) = \rho(G_j^d)$ for all $1 \leq i < j \leq \left\lfloor \frac{d-k}{2} \right\rfloor$*

The consequence of the previous theorem is that the trees within the rows of Table I are totally ordered with respect to the index. So we next need to order trees from different rows. The following theorem gives a partial answer to this question; more precisely, it gives, a total ordering of the trees, with respect to the index for the diagonal entries (i, j) , $(i+1, j)$, $(i+2, j), \dots$, and for the column entries.

Theorem 3.2. *For any $d \geq 5$ the following holds:*

- (i) $\rho(M_{i-1,j}) < \rho(M_{i,j})$, with $1 < i < j$;
- (ii) $\rho(M_{i,j}) < \rho(M_{i,j-1})$, with $1 \leq i < j-1$.

Theorem 3.3 (Limit point technique). *Let P_{k+3} ($k \geq 0$) be a path (whose vertex labels are $u_0, u_1, \dots, u_{k+2}$). Let $G_r^{(k)}$ be the graph obtained from this path by attaching to the vertices u_1 , and u_{k+1} , a hanging path of length $r - 1$. Then*

$$\lim_{r \rightarrow \infty} \rho(G_r^{(k)}) = \bar{\rho}$$

where $\bar{\rho}$ is the greatest solution to the equation

$$\left(\rho - \frac{1}{\rho} - d_k\right) \frac{\rho + \sqrt{\rho^2 - 4}}{2} - 1 = 0, \quad (3)$$

with $d_0 = \frac{\rho}{2}$, $d_k = \frac{\sinh(k-1)t + \sinh t}{\sinh kt}$ for $k > 0$, where $t = \ln \frac{\rho + \sqrt{\rho^2 - 4}}{2}$.

Proof. We first label the vertices of a graph $G_r^{(k)}$. Firstly, the vertices originating from the path P_{k+3} are labeled as above. The vertices of the hanging paths are labeled from its terminal vertices by $1, 2, \dots, r$ and $1', 2', \dots, r'$, respectively (so $r = u_1$ and $r' = u_{k+1}$; in addition, we put $v = u_0$ and $v' = u_{k+2}$). If $k = 0$ we get that $r \equiv r' \equiv u_1$, while if $k = 1$ we haven't any vertex between r and r' . Since $G_r^{(k)}$ is symmetric with respect to the center, we have $x_1 = x_{1'}$, $x_2 = x_{2'}$, ..., $x_r = x_{r'}$, $x_v = x_{v'}$ and $x_{u_i} = x_{u_{k+2-i}}$, where $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ is its Perron eigenvector.

Considering the eigenvalue equation (see (2)) for vertices from 1 up to r , we obtain $\rho x_1 = x_2$, $\rho x_i = x_{i-1} + x_{i+1}$, where $1 < i < r$. Therefrom we get

$$\rho x_1 = x_2 = \frac{a x_r + c x_1}{b}, \quad x_{r-1} = \frac{c x_r + a x_1}{b},$$

where $a = \sinh t$, $b = \sinh(r-1)t$ and $c = \sinh(r-2)t$.

If $k = 0$, let us consider the eigenvalue equation at vertex r : then $\rho x_r = 2x_{r-1} + 2x_v$ ($x_v = \frac{1}{\rho} x_r$). Combining the above equations we obtain

$$\rho x_r = 2 \frac{c x_r + \frac{a^2}{\rho b - c} x_r}{b} + \frac{2}{\rho} x_r$$

and by simple calculations we get

$$\left[\left(\frac{\rho}{2} - \frac{1}{\rho}\right) \frac{b}{c} - 1\right] \left(\rho \frac{b}{c} - 1\right) = \frac{a^2}{c^2}.$$

Next, letting r tend to infinity (since $\lim_{r \rightarrow \infty} \frac{a}{c} = 0$ and $\lim_{r \rightarrow \infty} \frac{b}{c} = \frac{\rho + \sqrt{\rho^2 - 4}}{2} = e^t$), it follows that $\bar{\rho}$ must satisfy the equation (with $d_0 = \frac{\rho}{2}$)

$$\left(\rho - \frac{1}{\rho} - d_0\right) \frac{\rho + \sqrt{\rho^2 - 4}}{2} - 1 = 0.$$

Analogously, if $k = 1$ then the eigenvalue equation (2) for r becomes

$$\rho x_r = x_{r-1} + x_{r'} + \frac{1}{\rho} x_r$$

and, since $x_r = x_{r'}$, we obtain in a similar way that $\bar{\rho}$ must satisfy the equation

$$\left(\rho - \frac{1}{\rho} - d_1\right) \frac{\rho + \sqrt{\rho^2 - 4}}{2} - 1 = 0,$$

where $d_1 = 1 = \frac{\sinh(k-1)t + \sinh t}{\sinh kt}$, with $k = 1$.

Finally, let $k > 1$. Since $\rho u_j = x_{j-1} + x_{j+1}$, $1 < j < k+1$, by noticing that $x_r = x_{u_1} = x_{u_{k+1}}$, we obtain

$$x_{u_2} = x_{u_k} = \frac{ax_r + c'x_r}{b'},$$

where $c' = \sinh(k-1)t$ and $b' = \sinh kt$. Consider now equation (2) at the vertex r . Then $\rho x_r = x_{r-1} + x_v + x_{u_2}$ ($x_v = \frac{1}{\rho} x_r$). Combining the above equations we get

$$\left(\rho \frac{b}{c} - 1\right) \left[\left(\rho - \frac{1}{\rho} - d_k\right) \frac{b}{c} - 1\right] = \frac{a^2}{c^2}.$$

Therefrom $\bar{\rho}$ must satisfy the equation

$$\left(\rho - \frac{1}{\rho} - d_k\right) \frac{\rho + \sqrt{\rho^2 - 4}}{2} - 1 = 0,$$

where $d_k = \frac{\sinh(k-1)t + \sinh t}{\sinh kt}$.

This completes the proof. $\square$

Some values of $\mathbf{d_k}$: $d_0 = \frac{\rho}{2}$; $d_1 = 1$; $d_2 = \frac{2}{\rho}$; $d_3 = \frac{1}{\rho-1}$; $d_4 = \frac{\rho}{\rho^2-2}$;
 $d_5 = \frac{\rho-1}{\rho^2-\rho-1}$; $d_6 = \frac{\rho^2-2}{\rho(\rho^2-3)}$; $\dots$.

The following corollary now easily follows:

Corollary 3.4. *We have:*

- (i) $\sqrt{2}\sqrt{1+\sqrt{2}} \approx 2.19736$ is the limit point for the index of the graphs $M_{\lfloor \frac{d}{2} \rfloor}$;

(ii) $\gamma = \frac{(188-12\sqrt{93})^{\frac{1}{3}}}{6} + \frac{(188+12\sqrt{93})^{\frac{1}{3}}}{6} + \frac{1}{3} \approx 2.14789$ is the limit point for the index of the graphs $M_{\lfloor \frac{d-1}{2} \rfloor, \lfloor \frac{d+1}{2} \rfloor}$;

(iii) $\frac{3}{2}\sqrt{2} \approx 2.12132$ is the limit point for the index of the graphs $M_{\lfloor \frac{d-2}{2} \rfloor, \lfloor \frac{d+2}{2} \rfloor}$;

(iv) $\beta \approx 2.10476$ is the limit point for the index of the graphs $M_{\lfloor \frac{d-3}{2} \rfloor, \lfloor \frac{d+3}{2} \rfloor}$;

(v) $\alpha = \sqrt{2}\sqrt{\left(\frac{9-\sqrt{33}}{36}\right)^{\frac{1}{3}} + \left(\frac{9+\sqrt{33}}{36}\right)^{\frac{1}{3}}} + 1 \approx 2.09355$ is the limit point for the index of the graphs $M_{\lfloor \frac{d-4}{2} \rfloor, \lfloor \frac{d+4}{2} \rfloor}$.

Proof. We will prove only (i). The largest root of the equation (3), for $k = 0$, is $\sqrt{2}\sqrt{1 + \sqrt{2}}$. By Theorem 3.3 we get

$$\rho(M_{\lfloor \frac{d}{2} \rfloor}) < \sqrt{2}\sqrt{1 + \sqrt{2}}$$

Additional claims come by calculating the largest root of (3) for $d_1 = 1$, $d_2 = \frac{2}{\rho}$, $d_3 = \frac{1}{\rho - 1}$ and $d_4 = \frac{\rho}{\rho^2 - 2}$, respectively. $\square$

Theorem 3.5. *We have:*

(i) $\frac{3}{2}\sqrt{2}$ is the limit point for the index of the graphs M_1 ;

(ii) α is the limit point for the index of the graphs $N_{\lfloor \frac{d}{2} \rfloor}$ and $M_{1,2}$;

(iii) $\sqrt{2 + \sqrt{5}}$ is the limit point for the index of the graphs N_2 , and of the graphs $M_{i,i+k}$, with $d = 2(k - 1)$.

Proof. The limit point for the index of the graphs M_1 , $M_{1,2}$ and N_2 follows from Theorem 2.3 (see [7]). The limit point of $N_{\lfloor \frac{d}{2} \rfloor}$ can be obtained by a similar calculus of Theorem 3.3. The limit point of $M_{i,i+k}$, with $d = 2(k - 1)$, is the main result in [1]. $\square$

Theorem 3.6. *For any n , all trees in $\mathcal{T}_{n,n-3}$ have index in the interval $[2, \sqrt{2}\sqrt{1 + \sqrt{2}}]$.*

Proof. Let us consider separately the graphs of the type $M_{i,j}^d$, M_i^d and N_i^d . Firstly, $\rho(M_{i,j}^d) \geq 2$ because it is obtained from a double snake by adding some vertices. Secondly, from Theorem 2.1, $\rho(M_i^d) \geq \rho(M_1^d) \geq \rho(M_1^2) = 2$. Thirdly, from Theorem 2.1, $\rho(N_i^d) \geq \rho(N_2^d) \geq (N_2^4) = 2$.

Since the graph $M_{\lfloor \frac{d}{2} \rfloor}$ has the maximum index (see [11]) and $\rho(M_{\lfloor \frac{d}{2} \rfloor}) < \sqrt{2}\sqrt{1 + \sqrt{2}}$ (by Corollary 3.4(i)), the proof follows. $\square$

Remark 3.7 (Complete order in $\mathcal{T}_{n,n-3}$, $n \leq 10$). *We now list the graphs in $\mathcal{T}_{n,n-3}$, $5 \leq n \leq 10$, in decreasing order with respect to the index.*

$d = 2$ *The only graph is the star M_1^2 ;*

$d = 3$ $\rho(M_1^3) > \rho(M_{1,2}^3)$;

$d = 4$ $\rho(M_2^4) > \rho(M_1^4) > \rho(M_{1,2}^4) > \rho(M_{1,3}^4) = \rho(N_2^4)$;

$d = 5$ $\rho(M_2^5) > \rho(M_1^5) > \rho(M_{2,3}^5) > \rho(M_{1,2}^5) > \rho(M_{1,3}^5) > \rho(N_2^5) > \rho(M_{1,4}^5)$;

$d = 6$ $\rho(M_3^6) > \rho(M_2^6) > \rho(M_1^6) > \rho(M_{2,3}^6) > \rho(M_{1,2}^6) > \rho(M_{2,4}^6) > \rho(M_{1,3}^6) > \rho(N_3^6) > \rho(N_2^6) > \rho(M_{1,4}^6) > \rho(M_{1,5}^6)$;

$d = 7$ $\rho(M_3^7) > \rho(M_2^7) > \rho(M_{3,4}^7) > \rho(M_1^7) = {}^3\rho(M_{2,3}^7) > \rho(M_{2,4}^7) > \rho(M_{1,2}^7) > \rho(M_{1,3}^7) > \rho(N_3^7) > \rho(M_{2,5}^7) > \rho(M_{1,4}^7) > \rho(N_2^7) > \rho(M_{1,5}^7) > \rho(M_{1,6}^7)$.

From now on we should consider only the case $d > 7$ (i.e. $n > 10$).

To conclude this section we give the following Table III which collects the results from Corollary 3.4 and Theorem 3.5:

k	limit point for ρ
0	$\sqrt{2}\sqrt{1+\sqrt{2}}$
1	$\gamma \approx 2,14789$
2	$\frac{3}{2}\sqrt{2}$
3	$\beta \approx 2,10476$
4	$\alpha \approx 2,09355$
$\frac{d+2}{2}$	$\sqrt{2+\sqrt{5}}$
$d-2$	2

tree	limit point for ρ
M_1	$\frac{3}{2}\sqrt{2}$
$M_{1,2}$	$\alpha \approx 2,09355$
$N_{\lfloor \frac{d}{2} \rfloor}$	$\alpha \approx 2,09355$
N_2	$\sqrt{2+\sqrt{5}}$

Table III

4 Ordering of the Trees in $\mathcal{T}_{n,n-3}$ with index in $(\frac{3}{2}\sqrt{2}, \sqrt{2}\sqrt{1+\sqrt{2}})$

Recall first that we can assume throughout this section that $d > 7$ (i.e. $n > 10$). We first prove:

Theorem 4.1. *If $d > 7$ and $2 \leq i \leq \frac{d-1}{2}$, then $\rho(M_1) < \rho(M_{i,i+1})$.*

³The polynomial $x^6 - 6x^4 + 7x^2 - 1$ divides both characteristic polynomials and the index of both graphs is its greatest root.

Proof. Let us first prove that $\rho(M_1^d) < \rho(M_{2,3}^8)$. Indeed by Theorem 3.5 we have that the limit point for the index of the trees M_1 is $\frac{3}{2}\sqrt{2}$, which is smaller than $\rho(M_{2,3}^8) \approx 2.12243$. Further, by Theorem 2.2(ii) and Theorem 3.1(i), it follows that $\rho(M_{2,3}^8) \leq \rho(M_{i,i+1}^8) \leq \rho(M_{i,i+1}^d)$ ($i \geq 2, d \geq 8$), and this completes the proof. $\square$

Theorem 4.2. *If $d > 7$ and $1 \leq i \leq \frac{d}{2} - 1$, then $\rho(M_1) > \rho(M_{i,i+2})$.*

Proof. By Theorem 3.1(i) we have to prove the claim just for $i = \lfloor \frac{d-2}{2} \rfloor$.

First suppose that d is even (so $d = 2r$). Let $G_1 = M_1^r$ and $G_2 = M_{r-1,r+1}^{2r}$. By Theorem 2.4 applied to the vertex of degree 4 in G_1 we get $\Phi(G_1, x) = x^4\Phi(P_{r-1}, x) - 3x^2\Phi(P_{r-1}, x) - x^3\Phi(P_{r-2}, x)$. Analogously, we get that $x\Phi(P_{r-1}, x) = \Phi(P_r, x) + \Phi(P_{r-2}, x)$ and $x\Phi(P_r, x) = \Phi(P_{r+1}, x) + \Phi(P_{r-1}, x)$. By a few substitutions we obtain

$$\Phi(G_1, x) = x^2[\Phi(P_{r+1}, x) - 2\Phi(P_{r-1}, x)].$$

In particular, we get that the index of G_1 is a root of $\Phi(P_{r+1}, x) - 2\Phi(P_{r-1}, x)$. Next, by Theorem 2.4, applied to the central vertex in G_2 , we get $\Phi(G_2, x) = x\Phi^2(P_{r+1}, x) - 2x\Phi(P_{r+1}, x)\Phi(P_{r-1}, x)$. Therefrom (by a few substitutions) we obtain

$$\Phi(G_2, x) = x\Phi(P_{r+1}, x)[\Phi(P_{r+1}, x) - 2\Phi(P_{r-1}, x)].$$

Since $\rho(G_2) > \rho(P_{r+1})$, the index of G_2 must be a root of $\Phi(P_{r+1}, x) - 2\Phi(P_{r-1}, x)$.

Finally, we have $\rho(M_1^{2r}) > \rho(G_1) = \rho(G_2) = \rho(M_{r-1,r+1}^{2r})$, as required.

Now suppose that d is odd (so $d = 2r - 1$). Then $\rho(M_1^{2r-1}) > \rho(M_1^r) = \rho(M_{r-1,r+1}^{2r}) > \rho(M_{r-2,r}^{2r-1})$, as required.

This completes the proof. $\square$

Remark 4.3. *As a consequence of Theorem 3.5, $\rho(N_i), \rho(M_{1,2}) < \rho(M_1)$, with $2 \leq i \leq \lfloor \frac{d}{2} \rfloor$. In fact the limit point for the index of $N_{\lfloor \frac{d}{2} \rfloor}$ and $M_{1,2}$ is strictly less than the index of M_1^7 .*

Remark 4.4. *We recall the Main Result in [12]: For $d > 7$ the ordering for the first $\lfloor \frac{d}{2} \rfloor$ indices is the following:*

$$\rho(M_{\lfloor \frac{d-1}{2} \rfloor, \lfloor \frac{d+1}{2} \rfloor}) < \rho(M_2) < \cdots < \rho(M_{\lfloor \frac{d}{2} \rfloor}).$$

We are now in position to state the Main Result of this section:

Theorem 4.5. *For $d > 7$ we have*

$$\rho(M_1) < \rho(M_{2,3}) < \cdots < \rho(M_{\lfloor \frac{d-1}{2} \rfloor, \lfloor \frac{d+1}{2} \rfloor}) < \rho(M_2) < \cdots < \rho(M_{\lfloor \frac{d}{2} \rfloor}).$$

Note, $\rho(M_1)$ is the greatest index not in the interval $(\frac{3}{2}\sqrt{2}, \sqrt{2}\sqrt{1+\sqrt{2}})$, then it is the greatest index in the interval $(\alpha, \frac{3}{2}\sqrt{2})$. Also note that no graph has the index equal to $\frac{3}{2}\sqrt{2}$, since this is not an algebraic integer.

5 Ordering of the Trees in $\mathcal{T}_{n,n-3}$ with index in $(\alpha, \frac{3}{2}\sqrt{2})$

In this section we also assume that $d > 7$ (i.e. $n > 10$). To simplify the proof of the following theorems let us denote by $A_{r,q}$ (as in [1]) the tree depicted in Fig. 3.

Fig. 3: The graph $A_{r,q}$

Theorem 5.1. *If $d > 7$ then $\rho(M_{1,2}^d) = \rho(N_{d-1}^{2d-2})$.*

Proof. By Theorem 2.4, applied to the vertex of degree 1 which is adjacent to the vertex labeled 1 (in $M_{1,2}^d$), we get

$$\Phi(M_{1,2}^d, x) = x(\Phi(A_{2,d-2}, x) - \Phi(P_d, x)).$$

By Theorem 2.4, applied to the vertex of degree 2 adjacent to the vertex of degree 1 and the vertex of degree 3, we obtain $\Phi(A_{2,d-2}, x) = x^2\Phi(P_d, x) - \Phi(P_d, x) - x^2\Phi(P_{d-2}, x)$ and therefrom

$$\Phi(M_{1,2}^d, x) = x[(x^2 - 2)\Phi(P_d, x) - x^2\Phi(P_{d-2}, x)].$$

Let us now consider the tree N_{d-1}^{2d-2} . Making use of Theorem 2.4 at the vertex of degree 3, and by noticing that $\Phi(P_t, x) = x\Phi(P_{t-1}, x) - \Phi(P_{t-2}, x)$ we obtain that $\Phi(N_{d-1}^{2d-2}, x) = \Phi(P_{d-1}, x)[x\Phi(P_2, x)\Phi(P_{d-1}, x) - 2\Phi(P_2, x)\Phi(P_{d-2}, x) - x\Phi(P_{d-1}, x)] = \Phi(P_{d-1}, x)[(x^2 - 1)(\Phi(P_d, x) + \Phi(P_{d-2}, x)) - 2(x^2 - 1)\Phi(P_{d-2}, x) - \Phi(P_d, x) - \Phi(P_{d-2}, x)]$, and consequently that

$$\Phi(N_{d-1}^{2d-2}, x) = \Phi(P_{d-1}, x)[(x^2 - 2)\Phi(P_d, x) - x^2\Phi(P_{d-2}, x)].$$

Since both trees $M_{1,2}^d$ and N_{d-1}^{2d-2} have their index as the largest root of the polynomial $(x^2 - 2)\Phi(P_d, x) - x^2\Phi(P_{d-2}, x)$, the proof follows. $\square$

Theorem 5.2. *If $d > 7$ then $\rho(M_{1,2}^d) = \rho(M_{d-2,d+2}^{2d})$.*

Proof. From the proof of the previous theorem we have

$$\Phi(M_{1,2}^d, x) = x[(x^2 - 2)\Phi(P_d, x) - x^2\Phi(P_{d-2}, x)].$$

Consider then the graph $M_{d-2,d+2}^{2d}$. By Theorem 2.4, applied to the (unique) central vertex, we get

$$\begin{aligned}\Phi(M_{d-2,d+2}^{2d}, x) &= x\Phi^2(A_{1,d-2}, x) - 2\Phi(P_d, x)\Phi(A_{1,d-2}, x) = \\ &= \Phi(A_{1,d-2}, x)[x\Phi(A_{1,d-2}, x) - 2\Phi(P_d, x)].\end{aligned}$$

By Theorem 2.4, applied to the vertex of degree 1 and adjacent to the vertex of degree 3 in the graph $A_{1,d-2}$, we get

$$\begin{aligned}\Phi(M_{\lfloor \frac{d-4}{2} \rfloor, \lfloor \frac{d+4}{2} \rfloor}^{2d}, x) &= \Phi(A_{1,d-2}, x)[x(x\Phi(P_d, x) - x\Phi(P_{d-2}, x)) - 2\Phi(P_d, x)] = \\ &= \Phi(A_{1,d-2}, x)[(x^2 - 2)\Phi(P_d, x) - x^2\Phi(P_{d-2}, x)].\end{aligned}$$

The rest of the proof follows by the same arguments as in Theorem 5.1. $\square$

Corollary 5.3. *If $d > 7$ then $\rho(M_{1,2}^d) > \rho(N_{\lfloor \frac{d}{2} \rfloor}^d) > \rho(M_{\lfloor \frac{d-4}{2} \rfloor, \lfloor \frac{d+4}{2} \rfloor}^d)$.*

Proof. Let us consider the first inequality. By Theorem 5.1 $\rho(M_{1,2}^d) = \rho(N_{d-1}^{2d-2})$. By Theorem 2.2(ii) we also have that $\rho(N_{d-1}^{2d-2}) > \rho(N_{\lfloor \frac{d}{2} \rfloor}^d)$. So the first inequality follows. Consider next the second inequality. First suppose that d is even (so $d = 2r$). Then, by Theorems 2.2(ii), 5.1 and 5.2, the following holds: $\rho(N_r^{2r}) = \rho(M_{1,2}^{r+1}) = \rho(M_{r-1,r+3}^{2r+2}) > \rho(M_{r-2,r+2}^{2r})$, and we are done. Next suppose that d is odd (so $d = 2r + 1$). Then the following holds: $\rho(N_r^{2r+1}) > \rho(N_r^{2r})$, $\rho(N_r^{2r}) = \rho(M_{1,2}^{r+1}) = \rho(M_{r-1,r+3}^{2r+2}) > \rho(M_{r-2,r+2}^{2r+1})$, so the second inequality follows. This completes the proof. $\square$

Remark 5.4. *Note that from the previous corollary, for the ordering of the trees in $\mathcal{T}_{n,n-3}$ having the index in the interval $(\alpha, \frac{3}{2}\sqrt{2})$, we should only consider the graphs $M_{i,i+2}$ and $M_{i,i+3}$, excluding the graphs $M_{1,3}$ and $M_{1,4}$. Indeed, if $d > 7$ then $\rho(N_i^d) < \rho(M_{1,2}^d)$ ($i \geq 2$), $\rho(M_{1,4}^d) < \rho(M_{1,3}^d) < \rho(M_{1,2}^d)$, $\rho(M_{i,i+k}^d) < \rho(M_{1,2}^d)$ ($i \geq 1, k \geq 4$), and $\rho(M_{1,2}^d) < \alpha$.*

Theorem 5.5. *If $d > 7$ then $\rho(M_{3,5}) > \alpha$, and $\rho(M_{3,5}) > \rho(M_{i,i+3})$.*

Proof. Consider the first inequality. Since $\rho(M_{3,5}^8) \approx 2.101 (> \alpha)$ we are done. For the second inequality, we observe that for $d = 8$ we have that $\rho(M_{3,5}^8) > \rho(M_{2,5}^8) \approx 2.07431$. For $d \geq 9$ $\rho(M_{3,5}^9) \approx 2.10672 (> \beta)$ (see Corollary 3.4). This completes the proof. $\square$

From Theorem 5.5 we have that, for any $d > 7$,

$$\rho(M_{3,5}) < \cdots < \rho(M_{\lfloor \frac{d-2}{2} \rfloor, \lfloor \frac{d+2}{2} \rfloor}) < \rho(M_1). \quad (4)$$

Theorem 5.6. *If $d > 15$ then*

$$(i) \quad \rho(M_{2,5}) < \rho(M_{1,2}) < \alpha;$$

$$(ii) \quad \rho(M_{2,4}), \rho(M_{3,6}) > \alpha;$$

$$(iii) \quad \rho(M_{4,7}) < \rho(M_{2,4}) < \rho(M_{5,8}).$$

Proof. First consider (i). By Theorem 2.3 we have that $\rho(M_{2,5}^d) < 2.0879 < \rho(M_{1,2}^7) < \alpha$, so (i) follows. For (ii), observe that $\rho(M_{2,4}^8) \approx 2.09529 (> \alpha)$ and $\rho(M_{3,6}^{12}) \approx 2.09456 (> \alpha)$. Finally, for (iii), by making use of Theorem 2.3, we get that $\rho(M_{4,7}^d) < 2.10037$ and $\rho(M_{2,4}^d) < 2.10192$. Since $\rho(M_{2,4}^{11}) \approx 2.10100$ and $\rho(M_{5,8}^{16}) \approx 2.10216$, we have $\rho(M_{4,7}^d) < \rho(M_{2,4}^{11}) < \rho(M_{2,4}^d) < \rho(M_{5,8}^{16}) \leq \rho(M_{5,8}^d)$. This completes the proof. $\square$

If $d > 15$, by collecting the above results, we obtain the Main Result of this section which reads:

Theorem 5.7. *If $d > 15$ then*

$$\begin{aligned} \rho(M_{1,2}) < \rho(M_{3,6}) < \rho(M_{4,7}) < \rho(M_{2,4}) < \rho(M_{5,8}) < \cdots < \rho(M_{\lfloor \frac{d-3}{2} \rfloor, \lfloor \frac{d+3}{2} \rfloor}) < \\ < \rho(M_{3,5}) < \rho(M_{4,6}) < \cdots < \rho(M_{\lfloor \frac{d-2}{2} \rfloor, \lfloor \frac{d+2}{2} \rfloor}) < \rho(M_1). \end{aligned}$$

Taking the Main Result of [12] and the Main Results in Sections 4 and 5, we totally order the graphs in $\mathcal{T}_{n,n-3}$ (for $d > 15$) having their index in the interval $(\alpha, \sqrt{2}\sqrt{1+\sqrt{2}})$. Note that $M_{1,2}$ has the index less than α .

Now we list the chain of inequalities for $7 < d \leq 15$ for the graphs having index greater than α up to the index of the graph $M_{3,5}$ (see (4)):

$$8 \leq d \leq 10 \quad \rho(M_{1,2}) < \rho(M_{2,4}) < \rho(M_{3,5})$$

$$d = 11 \quad \rho(M_{1,2}) = {}^4\rho(M_{3,6}) < \rho(M_{4,7}) < \rho(M_{2,4}) < \rho(M_{3,5})$$

$$d = 12 \quad \rho(M_{1,2}) < \rho(M_{3,6}) < \rho(M_{4,7}) < \rho(M_{2,4}) < \rho(M_{3,5})$$

$$13 \leq d \leq 14 \quad \rho(M_{1,2}) < \rho(M_{3,6}) < \rho(M_{4,7}) < \rho(M_{5,8}) < \rho(M_{2,4}) < \rho(M_{3,5})$$

$$d = 15 \quad \rho(M_{1,2}) < \rho(M_{3,6}) < \rho(M_{4,7}) < \rho(M_{5,8}) = {}^4\rho(M_{2,4}) < \rho(M_{6,9}) < \rho(M_{3,5})$$

⁴The two graphs are cospectral.

We observe that $\rho(M_{1,2})$ is the greatest index not in the interval $(\alpha, \sqrt{2}\sqrt{1+\sqrt{2}})$, while in the interval $(2, \alpha)$ the graph $M_{1,2}$ will be the tree having the greatest index.

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