MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **77** (2017) 635-654

ISSN 0340 - 6253

On Trees with Smallest Resolvent Energy[1]

Mohammad Ghebleh, Ali Kanso[2], Dragan Stevanović

Faculty of Science, Kuwait University, Safat 13060, Kuwait

mamad@sci.kuniv.edu.kw, akanso@sci.kuniv.edu.kw, dragance106@yahoo.com

(Received October 10, 2016)

Abstract

Let $P_{n-1}(a)$ be the tree obtained by attaching a pendent vertex at position a of the $(n-1)$-vertex path P_{n-1}. We prove here a conjecture of Gutman et al. [MATCH Commun. Math. Comput. Chem. 73 (2015), 267–270] that $P_{n-1}(a)$ has the a-th smallest resolvent Estrada index among all trees of order n, for $2 \leq a \leq \lfloor n/2 \rfloor$, and show that the analogous result also holds for the resolvent energy.

1 Introduction

Let $G = (V, E)$ be a simple graph. A walk of length k in G is a sequence of its vertices $W : v_0, \ldots, v_k$ such that $v_i v_{i+1}$ is an edge of G for each $i = 0, \ldots, k-1$. A walk W is closed if $v_0 = v_k$. Let $M_k(G, v)$ denote the number of closed walks of length k starting and ending at a vertex v of G. The sequence of numbers $M_k(G, v)$, $k \geq 2$, provides a certain glimpse into the density of edges in the vicinity of v. For example, $M_2(G, v)$ is equal to the degree of v, $M_3(G, v)$ is equal to twice the number of triangles containing v, while for larger values of k, $M_k(G, v)$ counts a mix of closed walks going up to the distance $\lfloor k/2 \rfloor$ from v. Since for practical purposes one usually wants to have a single numerical descriptor instead of an infinite sequence, Estrada and Highman [1, Section 3] proposed the use of a weighted series of the closed walk counts

$$f_c(G, v) = \sum_{k \geq 0} c_k M_k(G, v)\,,$$

[1]This work was supported and funded by Kuwait University Research Grant No. SM10/15.
[2]Corresponding author

where $(c_k)_{k\geq 0}$ is a predefined sequence of nonnegative weights that makes the above series convergent. Values $f_c(G,v)$ may then be considered as the closed walk based measure of vertex centrality, while

$$f_c(G)=\sum_{v\in V} f_c(G,v)=\sum_{k\geq 0} c_k M_k(G)\,, \tag{1}$$

where $M_k(G)=\sum_{v\in V} M_k(G,v)$ is the total number of closed walks of length k in G, represents a cumulative closed walk based descriptor of a graph.

The value $f_c(G)$ is closely related to the adjacency spectrum of G. Let $A(G)$ be the adjacency matrix of G, and let $\lambda_1(G)\geq\cdots\geq\lambda_n(G)$ be its eigenvalues. It is a folklore result that the number of walks of length k between the vertices u and v is equal to $A^k(G)_{u,v}$, easily proved by induction on k. Hence the number $M_k(G)$ of closed walks of length k represents the trace of $A^k(G)$, which is further equal to the k-th spectral moment $\sum_{i=1}^n \lambda_i^k(G)$, so that (1) may be rewritten as

$$f_c(G)=\sum_{i=1}^{n}\sum_{k\geq 0} c_k\lambda_i^k(G)\ . \tag{2}$$

Estrada's original suggestion [2] for the sequence $(c_k)_{k\geq 0}$ was $c_k=1/k!$, which puts more emphasis on shorter closed walks and ensures the convergence as

$$f_c(G)=\sum_{i=1}^{n}\sum_{k\geq 0}\frac{\lambda_i^k(G)}{k!}=\sum_{i=1}^{n} e^{\lambda_i(G)}\ .$$

This so-called Estrada index $EE(G)=\sum_{i=1}^n e^{\lambda_i(G)}$ has been initially applied in measuring the degree of protein folding [2, 3, 4], the centrality of complex networks [5] and the branching of molecular graphs [6, 7]. It has been steadily gaining popularity in mathematical chemistry community, as Zentralblatt now reports more than a hundred research articles on the Estrada index.

A more recent suggestion for $(c_k)_{k\geq 0}$ was made in [1]. In order to downweight shorter closed walks, Estrada and Highman suggested the use of $c_k=1/(n-1)^k$, inspired by the ratio of the numbers of closed walks of length k between the pairs of vertices in G and in the complete graph K_n. This latter choice defines the so-called resolvent Estrada index

$$EE_r(G)=\sum_{k\geq 0}\frac{M_k(G)}{(n-1)^k}\,, \tag{3}$$

which can also be represented in terms of eigenvalues as

$$EE_r(G)=\sum_{i=1}^{n}\frac{n-1}{n-1-\lambda_i(G)}$$

when G is not a complete graph. Some bounds on $EE_r(G)$ have been obtained in [8] and [9]. Chen and Qian [10] showed that the star S_n has the maximum resolvent Estrada index among trees of order n, followed by a number of trees similar to the star, and on the other hand, Gutman et al. [11] showed that the path P_n has the minimum resolvent Estrada index among trees of order n. Let $P_{n-1}(a)$ be the tree obtained by attaching a pendent vertex at position a of the $(n-1)$-vertex path P_{n-1}. Gutman et al. [11] further showed that $P_{n-1}(2)$ has the second smallest resolvent Estrada index for $n \geq 4$, while $P_{n-1}(3)$ has the third smallest resolvent Estrada index for $n \geq 6$, and proposed the following conjecture.

Conjecture 1 ([11])**.** *For $2 \leq a \leq \lfloor n/2 \rfloor$, the tree $P_{n-1}(a)$ has the a-th smallest resolvent Estrada index among trees of order n.*

Another suggestion $c_k = 1/n^{k+1}$ appears in [12, 13], where it defines the closely related resolvent energy

$$ER(G) = \frac{1}{n} \sum_{k \geq 0} \frac{M_k(G)}{n^k}, \tag{4}$$

which can also be represented in terms of eigenvalues as

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n - \lambda_i(G)} .$$

Gutman et al. [12, 13] establish a number of bounds on the resolvent energy and characterize trees, unicyclic and bicyclic graphs with smallest and largest resolvent energies.

While researching Estrada index with a former PhD student [15], one of the present authors made a conjecture analogous to Conjecture 1 about trees with smallest Estrada indices, although it had not been published. Motivated by similarity in conjectured structure of trees with smallest Estrada and resolvent Estrada indices, and the fact that both of these indices are defined in terms of the numbers of closed walks, we now turn our attention to the following partial order of graphs.

Definition 2. *For two graphs G and H we write $G \preceq H$ if $M_k(G) \leq M_k(H)$ for each $k \geq 0$. Further, $G \prec H$ if $G \preceq H$ and there exists $k' \geq 0$ such that $M_{k'}(G) < M_{k'}(H)$.*

Thus

$$G \preceq H \Longrightarrow EE(G) \leq EE(H), EE_r(G) \leq EE_r(H) \text{ and } ER(G) \leq ER(H) , \tag{5}$$

while

$$G \prec H \Longrightarrow EE(G) < EE(H), EE_r(G) < EE_r(H) \text{ and } ER(G) < ER(H) \ . \tag{6}$$

The partial order $\preceq$ enables the comparison of spectral radii of graphs as well. The Perron-Frobenius theorem [16] states that $\lambda_1(G) = \max_i |\lambda_i(G)|$, so that

$$\lambda_1(G) = \lim_{k\to\infty} \sqrt[2k]{M_{2k}(G)} \ .$$

(We include only closed walks of even length above, as bipartite graphs do not have closed walks of odd length.) Thus

$$G \preceq H \Longrightarrow \lambda_1(G) \leq \lambda_1(H) \ . \tag{7}$$

However, due to the appearance of the limit above, $G \prec H$ does not necessarily imply $\lambda_1(G) < \lambda_1(H)$.

Certainly, not all trees are comparable by $\preceq$: one of the smallest pairs of incomparable trees is depicted in Fig. 1. Nevertheless, we will show that trees $P_{n-1}(j)$ precede almost all other trees in $\preceq$-order.

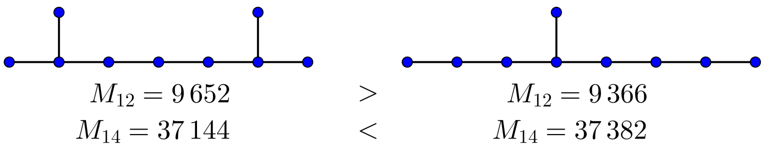

Figure 1. A pair of trees incomparable by $\preceq$.

Let us now define a few further trees. First, let F_n be the tree obtained from the path P_{n-2} by attaching a pendent path of length two at position 3 in P_{n-2} (see Fig. 2 for an example).

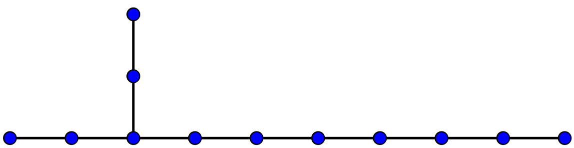

Figure 2. The tree F_n for $n = 12$.

Next, let $\mathcal{Q}_n$ denote the set of trees of order n that may be obtained from the path P_k for some $k \leq n$ by attaching at most three new pendent edges to the leaves of P_k and at most one new pendant edge to its internal vertices. Note that this implies that $\mathcal{Q}_n$ also contains $P_n, P_{n-1}(2), P_{n-1}(3), \ldots, P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$. In order to distinguish them from other trees in $\mathcal{Q}_n$, we further denote $\mathcal{Q}_n^* = \mathcal{Q}_n \setminus \{P_n, P_{n-1}(2), P_{n-1}(3), \ldots, P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)\}$. Fig. 3 illustrates a few trees from $\mathcal{Q}_{12}^*$ in which the attached pendent edges are shown in red (dashed line).

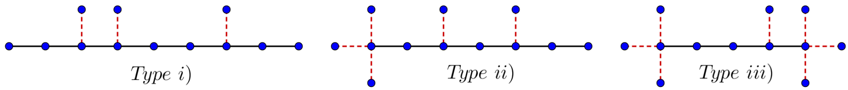

Figure 3. A few trees from $\mathcal{Q}_{12}^*$.

The rest of the paper may be summarized as follows. In the next section we show that

$$P_n \prec P_{n-1}(2) \prec P_{n-1}(3) \prec \cdots \prec P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \prec F_n$$

and further that

$$F_n \preceq T\,,$$

whenever T is a tree of order n such that $T \notin \mathcal{Q}_n$. Due to (6), this shows that $P_{n-1}(2), P_{n-1}(3), \ldots, P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$ have smaller resolvent Estrada indices (and ordinary Estrada indices and resolvent energies) than any tree not in $\mathcal{Q}_n$. Trees in $\mathcal{Q}_n^*$ need not be $\preceq$-comparable to $P_{n-1}(2), P_{n-1}(3), \ldots, P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$—see the example of incomparable trees depicted in Fig. 1. In Section 3 we bound the contribution of longer closed walks to the resolvent Estrada index and resolvent energy in terms of the spectral radius. The small spectral radius of trees in $\mathcal{Q}_n^*$ will then enable us to focus on short closed walks to show that trees in $\mathcal{Q}_n^*$ have larger resolvent Estrada indices and resolvent energies than $P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$, thus completing the proof of Conjecture 1 and proving an analogous result for the resolvent energy.

2 Trees not in $\mathcal{Q}_n$

The following lemma appears as Theorem 3.2 in [15].

Lemma 3. *Let u be a vertex of a nontrivial connected graph G, and for nonnegative integers p and q let $G(u; p, q)$ denote the graph obtained from G by attaching two pendent paths of lengths p and q, respectively, at u. If $1 \leq p \leq q$, then*

$$G(u; p-1, q+1) \prec G(u; p, q)\ .$$

Repeated application of Lemma 3 further shows that

$$G(u;0,p+q) \prec G(u;p,q)\,, \tag{8}$$

where $G(u;0,p+q)$ is the result of replacing two pendent paths of lengths p and q attached at u with a single path of length $p+q$.

Corollary 4. *For each $n \geq 4$,*

$$P_n \prec P_{n-1}(2) \prec P_{n-1}(3) \prec P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \ . \tag{9}$$

Proof. Let u be a vertex of the path P_2 on two vertices. Then

$$\begin{aligned} P_n &\cong P_2(u;0,n-2)\,, \\ P_{n-1}(2) &\cong P_2(u;1,n-3)\,, \\ P_{n-1}(3) &\cong P_2(u;2,n-4)\,, \\ &\cdots \\ P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) &\cong P_2\left(u;\left\lfloor \frac{n}{2} \right\rfloor - 1, \left\lceil \frac{n}{2} \right\rceil - 1\right) \ . \end{aligned}$$

The chain of inequalities (9) now follows from Lemma 3. ■

We will now extend the chain (9) with an additional term. Note that we exclude the case $n = 6$ below, as $P_5(3) = F_6$.

Lemma 5. *For each $n \geq 7$,*

$$P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \prec F_n \ . \tag{10}$$

Proof. We calculate characteristic polynomials of $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)$ and a subgraph of F_n in order to derive an important relation between their spectral moments. For this task we use the result of Schwenk [14], who has shown that

$$\phi(G,\lambda) = \phi(G-uv,\lambda) - \phi(G-u-v,\lambda) \tag{11}$$

whenever uv is a cut edge of G.

Case 1. Suppose that n is even, $n = 2b$, $b \geq 4$, so that $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \cong P_2(u;b-1,b-1)$. We also have $F_n \cong P_3(v;2,2b-5)$, where v is the vertex of degree three in F_n. Let $P_3(v;2,b-2)$ denote a subgraph of F_n, obtained by deleting the farthest $b-3$ edges from the branch of F_n of length $2b-5$. (Examples of $P_2(u;b-1,b-1)$ and $P_3(v;2,b-2)$ are depicted in Fig. 4.)

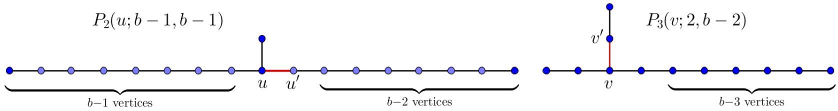

Figure 4. Trees $P_2(u; b-1, b-1)$ and $P_3(v; 2, b-2)$.

Let u' be a neighbor of u on one of the branches of length $b-1$ in $P_2(u; b-1, b-1)$. Then by (11)

$$\begin{aligned}\phi(P_2(u; b-1, b-1), \lambda) &= \phi(P_2(u; b-1, b-1) - uu', \lambda) - \phi(P_2(u; b-1, b-1) - u - u', \lambda) \\ &= \phi(P_{b+1}, \lambda)\phi(P_{b-1}, \lambda) - \phi(P_1, \lambda)\phi(P_{b-1}, \lambda)\phi(P_{b-2}, \lambda) \\ &= \phi(P_{b-1}, \lambda)\left[\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda)\right] \ .\end{aligned}$$

On the other hand, denoting by v' a neighbor of v on one of the branches of length two in $P_3(v; 2, b)$, we get

$$\begin{aligned}\phi(P_3(v; 2, b-2), \lambda) &= \phi(P_3(v; 2, b-2) - vv', \lambda) - \phi(P_3(v; 2, b-2) - v - v', \lambda) \\ &= \phi(P_2, \lambda)\phi(P_{b+1}, \lambda) - \phi(P_1, \lambda)\phi(P_2, \lambda)\phi(P_{b-2}, \lambda) \\ &= \phi(P_2, \lambda)\left[\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda)\right] \ .\end{aligned}$$

Hence the characteristic polynomials $\phi(P_2(u; b-1, b-1), \lambda)$ and $\phi(P_3(v; 2, b-2), \lambda)$ have a common factor $\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda)$. If $Sp(\phi)$ denotes the set of roots of the polynomial ϕ, this implies

$$\begin{aligned}Sp(\phi(P_2(u; b-1, b-1), \lambda)) = Sp(\phi(P_{b-1}, \lambda)) \ &\cup \ Sp(\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda)) \, , \\ Sp(\phi(P_3(v; 2, b-2), \lambda)) = Sp(\phi(P_2, \lambda)) \ &\cup \ Sp(\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda)) \, ,\end{aligned}$$

and consequently, for each $k \geq 0$,

$$\begin{aligned}M_k(P_2(u; b-1, b-1)) &= M_k(P_{b-1}) + \sum_{\lambda \in Sp(\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda))} \lambda^k \, , \\ M_k(P_3(v; 2, b-2)) &= M_k(P_2) + \sum_{\lambda \in Sp(\phi(P_{b+1}, \lambda) - \lambda\phi(P_{b-2}, \lambda))} \lambda^k \ .\end{aligned}$$

Thus

$$M_k(P_2(u; b-1, b-1)) - M_k(P_3(v; 2, b-2)) = M_k(P_{b-1}) - M_k(P_2) \ . \tag{12}$$

Suppose now that one pendent edge of P_{b-1} is colored green, while the remaining $b-3$ edges are colored red. The expression $M_k(P_{b-1}) - M_k(P_2)$ then represents the number of closed walks of length k in P_{b-1} that contain at least one red edge.

Suppose further that the edges of $F_n = P_3(v; 2, 2b-5)$ are also colored (see Fig. 5): the last $b-3$ edges of the branch of length $2b-5$ are colored red (dashed line), the preceding edge of that branch is colored green (dotted line), while the remaining edges are colored black. The subgraph induced by the black and green edges is then $P_3(v; 2, b-2)$, while the subgraph determined by the green and red edges is P_{b-1}. The closed walks of length k

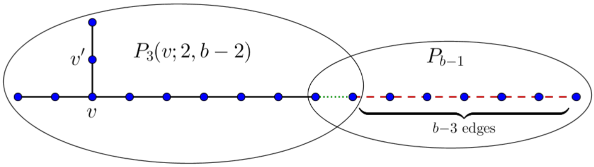

Figure 5. The black and green edges of F_n induce $P_3(v; 2, b-2)$, while the green and red edges induce P_{b-1} .

in F_n may now be partitioned into those closed walks that belong to the black-green subgraph $P_3(v; 2, b-2)$ and those that contain at least one red edge. The closed walks that contain at least one red edge may be further partitioned into $M_k(P_{b-1}) - M_k(P_2)$ walks that contain only green and red edges and those that contain both black and red edges. Thus from (12) we see that for each $k \geq 0$,

$$M_k(F_n) \geq M_k(P_3(v; 2, b-2) + (M_k(P_{b-1}) - M_k(P_2)) = M_k(P_2(u; b-1, b-1)) \ . \quad (13)$$

Moreover, strict inequality holds for $k \geq 6$ as F_n then contains closed walks with both black and red edges. Hence

$$P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) = P_2(u; b-1, b-1) \prec F_n$$

holds for even n.

Case 2. Now let n be odd, $n = 2b-1$, $b \geq 4$, so that $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \cong P_2(u; b-1, b-2)$, while $F_n \cong P_3(v; 2, 2b-6)$. Similarly as in the previous case, we can see that

$$M_k(P_2(u; b-1, b-1)) \geq M_k(P_2(u; b-1, b-2)) + (M_k(P_{b-1}) - M_k(P_{b-2})) \qquad (14)$$

by coloring a pendent edge of one of the branches of length $b-1$ in $P_2(u; b-1, b-1)$ in red (dashed line), the preceding $b-3$ edges of the same branch in green (dotted line), and the remaining edges in black (see Fig. 6). The closed walks of length k of $P_2(u; b-1, b-1)$ may then be partitioned into the closed walks contained within the black-green subgraph

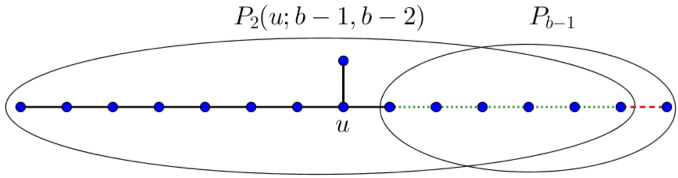

Figure 6. The black and green edges induce $P_2(u; b-1, b-2)$, while the green and red edges induce P_{b-2}.

$P_2(u; b-1, b-2)$ and the closed walks than contain at least one red edge. The latter may further be partitioned into the $M_k(P_{b-1}) - M_k(P_{b-2})$ closed walks that contain green and red edges only and the remaining closed walks that contain both red and black edges. The inequality in (14) is strict for $k \geq 2(b-1)$ when closed walks with both red and black edges start to appear in $P_2(u; b-1, b-1)$.

Now from (12) and (14) we get

$$\begin{aligned} M_k(P_2(u; b-1, b-2)) &\leq M_k(P_2(u; b-1, b-1)) - M_k(P_{b-1}) + M_k(P_{b-2}) \\ &= [M_k(P_3(v; 2, b-2)) + M_k(P_{b-1}) - M_k(P_2)] - M_k(P_{b-1}) + M_k(P_{b-2}) \\ &= M_k(P_3(v; 2, b-2)) + M_k(P_{b-2}) - M_k(P_2) \ . \end{aligned}$$

By adapting the proof of (13) from the case of $F_n \cong P_3(v; 2, 2b-5)$ for even n to the case of $F_n \cong P_3(v; 2, 2b-6)$ for odd n, we see that

$$M_k(P_3(v; 2, b-2)) + M_k(P_{b-2}) - M_k(P_2) \leq M_k(P_3(v; 2, 2b-6)) \, ,$$

which finally yields

$$M_k\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right) = M_k(P_2(u; b-1, b-2)) \leq M_k(P_3(v; 2, 2b-6)) = M_k(F_n)$$

with strict inequality for $k \geq 6$. Hence

$$P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \prec F_n$$

holds for odd n as well. ■

Remark. As a consequence of walk counting in Lemma 5 we easily get that

$$\lambda_1\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right) \leq \lambda_1(F_n) \ .$$

Note that it would be very hard to obtain this inequality in a different way, due to the diminishing difference between these two spectral radii and the fact that both are bounded from above by $\sqrt{2+\sqrt{5}} \approx 2.058171027271492$ (see [17, 18]). For example, already for $n = 75$ we have an agreement in the first eight of their digits after the decimal point:

$$\begin{aligned} \lambda_1\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right) &\approx 2.05817102402 \\ \lambda_1(F_n) &\approx 2.05817102727. \end{aligned}$$

■

Corollary 4 and Lemma 5 yield the chain of inequalities

$$P_n \prec P_{n-1}(2) \prec P_{n-1}(3) \prec P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right) \prec F_n \,. \tag{15}$$

The fact that $P_n, P_{n-1}(2), P_{n-1}(3), \ldots, P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)$ have smaller resolvent Estrada indices (and ordinary Estrada indices and resolvent energies) than trees not in $\mathcal{Q}_n$ now follows from (5), (15) and the following theorem.

Theorem 6. *If T is a tree of order $n \geq 6$ such that $T \notin \mathcal{Q}_n$, then $F_n \preceq T$.*

Proof. If T has no vertices of degree larger than two, then T is the path P_n which belongs to $\mathcal{Q}_n$, yielding a contradiction. Hence T has at least one vertex of degree at least three.

Let v be a vertex of degree $d \geq 3$, and let $T_1, \ldots, T_d$ be the connected components of $T - v$. Let n_i be the order of the subtree T_i, $i = 1, \ldots, d$. Within each subtree T_i we may repeatedly replace any two paths of lengths p and q attached at a vertex of degree at least three at the largest distance from v with a single path of length $p + q$, until the subtree T_i itself becomes the path P_{n_i}. Due to (8), each such path replacing transformation produces a smaller tree in $\prec$-order. After all the subtrees T_i become paths, this sequence of transformations produces a tree T' such that $T' - v = P_{n_1} \cup \cdots \cup P_{n_d}$ and $T' \preceq T$.

If $d > 3$, we may continue applying this transformation in T' by replacing any pair of paths P_{n_i} and P_{n_j} attached at v with a single path $P_{n_i+n_j}$, until the degree of v becomes three. This sequence of transformations then produces a tree T'' such that $T'' - v = P_{m_1} \cup P_{m_2} \cup P_{m_3}$ for some $m_1 \leq m_2 \leq m_3$ and $T'' \preceq T'$. (If $d = 3$, then set $T'' = T'$.) Here the numbers m_1, m_2 and m_3 represent the sums of the three subsets that partition the set $\{n_1, \ldots, n_d\}$, depending on which paths have been replaced together. In addition, note that T'' may be equivalently denoted as $P_{m_1+1}(v; m_2, m_3)$, $P_{m_2+1}(v; m_1, m_3)$ or $P_{m_3+1}(v; m_1, m_2)$.

If $2 \leq m_1$ then from the repeated application of Lemma 3 we have

$$\begin{aligned} P_{m_1+1}(v; 2, m_2+m_3-2) &\preceq P_{m_1+1}(v; m_2, m_3) = T'' , \\ P_3(v; m_1, m_2+m_3-2) &= P_{m_1+1}(v; 2, m_2+m_3-2) , \\ F_n \cong P_3(v; 2, m_1+m_2+m_3-2) &\preceq P_3(v; m_1, m_2+m_3-2) . \end{aligned}$$

Hence $F_n \preceq T'' \preceq T' \preceq T$.

Let us now consider when we can direct path replacing transformations so as to arrive at $2 \leq m_1$. Suppose, without loss of generality, that $1 \leq n_1 \leq n_2 \leq \cdots \leq n_d$. First, if $d \geq 6$ then we can set $m_1 = n_1 + n_2 \geq 2$, $m_2 = n_3 + n_4 \geq 2$ and $m_3 = n_5 + \cdots + n_d \geq 2$. Next, if $d = 5$ and $n_5 \geq 2$ then we can similarly set $m_1 = n_1 + n_2 \geq 2$, $m_2 = n_3 + n_4 \geq 2$ and $m_3 = n_5 \geq 2$. The remaining case $n_1 = \cdots = n_5 = 1$ corresponds to T'' being a star, which has the largest number of closed walks of any even length among all trees of the given order [19], so that necessarily $F_n \preceq T''$. Further, if $d = 4$ and $2 \leq n_3$ then we can set $m_1 = n_1 + n_2 \geq 2$, $m_2 = n_3 \geq 2$ and $m_3 = n_4 \geq 2$. Finally, if $d = 3$ then $m_1 = n_1$, $m_2 = n_2$, $m_3 = n_3$, so that $2 \leq m_1$ is equivalent to $2 \leq n_1$.

From the previous paragraph we see that we have $F_n \preceq T''$ unless it happens that for each vertex of degree at least three in T holds either $d = 3$ and $n_1 = 1$ or $d = 4$ and $n_1 = n_2 = n_3 = 1$. Since $n_i = 1$ corresponds to a pendent edge, we see that the tree obtained after removing all pendent edges from such T necessarily results in some path P_k: vertices of degree three in T have their degree reduced to two, while vertices of degree four have their degree reduced to one (and consequently there may be at most two vertices of degree four in T). This, however, implies that $T \in \mathcal{Q}_n$, which is contradictory to the assumption of this theorem. ∎

3 Trees in $\mathcal{Q}_n$

As we can see from the example depicted in Fig. 1, trees in $\mathcal{Q}_n^*$ need not be $\preceq$-comparable to $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)$, so that Conjecture 1 has to be tackled in a different way for them. Thanks to the fact that trees in $\mathcal{Q}_n$ have small spectral radius, the following simple bound turns out to be sufficient for its resolution.

Lemma 7. *For graphs G and H of order n, let $\max\{\lambda_1(G), \lambda_1(H)\} \leq \Lambda$. Then*

$$\left| \sum_{k \geq k_0} \frac{M_k(G) - M_k(H)}{(n-1)^k} \right| \leq \frac{n(n-1)}{n-1-\Lambda} \left(\frac{\Lambda}{n-1} \right)^{k_0} . \tag{16}$$

Proof. Since $|\lambda_i(G)| \leq \lambda_1(G) \leq \Lambda$ for each $i = 1, \ldots, n$, we have that

$$|M_k(G)| = \left|\sum_{i=1}^{n} \lambda_i(G)^k\right| \leq \sum_{i=1}^{n} |\lambda_i(G)|^k \leq n\Lambda^k$$

and, similarly, $|M_k(H)| \leq n\Lambda^k$. Since both $M_k(G)$ and $M_k(H)$ are nonnegative, we get

$$-n\Lambda^k \leq -M_k(H) \leq M_k(G) - M_k(H) \leq M_k(G) \leq n\Lambda^k \ .$$

Hence

$$\begin{aligned} \left|\sum_{k\geq k_0} \frac{M_k(G) - M_k(H)}{(n-1)^k}\right| &\leq \sum_{k\geq k_0} \frac{|M_k(G) - M_k(H)|}{(n-1)^k} \\ &\leq n \sum_{k\geq k_0} \left(\frac{\Lambda}{n-1}\right)^k \\ &= \frac{n(n-1)}{n-1-\Lambda}\left(\frac{\Lambda}{n-1}\right)^{k_0} \ . \end{aligned}$$

■

A tree is a bipartite graph which does not contain closed walks of odd length, so that its resolvent Estrada index is equal to

$$EE_r(T) = n + \frac{2(n-1)}{(n-1)^2} + \frac{M_4(T)}{(n-1)^4} + \frac{M_6(T)}{(n-1)^6} + \sum_{k\geq 8} \frac{M_k(T)}{(n-1)^k}\,,$$

thanks to $M_0(T) = n$ and $M_2(T) = 2(n-1)$. For two trees T and S of order n we therefore have

$$EE_r(T) - EE_r(S) = \frac{M_4(T) - M_4(S)}{(n-1)^4} + \frac{M_6(T) - M_6(S)}{(n-1)^6} + \sum_{k\geq 8} \frac{M_k(T) - M_k(S)}{(n-1)^k} \ .$$

If Λ is a common upper bound for the spectral radii of T and S, we get from Lemma 7 that

$$\begin{aligned} EE_r(T) - EE_r(S) \ \in \ & \left[\frac{M_4(T) - M_4(S)}{(n-1)^4} + \frac{M_6(T) - M_6(S)}{(n-1)^6} - \frac{n(n-1)}{n-1-\Lambda}\left(\frac{\Lambda}{n-1}\right)^8, \right. \\ & \left. \frac{M_4(T) - M_4(S)}{(n-1)^4} + \frac{M_6(T) - M_6(S)}{(n-1)^6} + \frac{n(n-1)}{n-1-\Lambda}\left(\frac{\Lambda}{n-1}\right)^8 \right] \ . \end{aligned}$$

This yields the following useful lemma.

Lemma 8. *Let T and S be two trees of order n such that $\Lambda \geq \max\{\lambda_1(T), \lambda_1(S)\}$. If*

$$(n-1)^2[M_4(T) - M_4(S)] + [M_6(T) - M_6(S)] > \frac{n\Lambda^8}{(n-1)(n-1-\Lambda)}\,,$$

then $EE_r(T) > EE_r(S)$.

Similarly to Lemmas 7 and 8, we can prove the following two lemmas on the resolvent energy.

Lemma 9. *For graphs G and H of order n, let* $\max\{\lambda_1(G), \lambda_1(H)\} \leq \Lambda$. *Then*

$$\left| \sum_{k \geq k_0} \frac{M_k(G) - M_k(H)}{n^{k+1}} \right| \leq \frac{n}{n-\Lambda} \left(\frac{\Lambda}{n} \right)^{k_0} . \tag{17}$$

Lemma 10. *Let T and S be two trees of order n such that* $\Lambda \geq \max\{\lambda_1(T), \lambda_1(S)\}$. *If*

$$n^2[M_4(T) - M_4(S)] + [M_6(T) - M_6(S)] > \frac{\Lambda^8}{n-\Lambda} ,$$

then $ER(T) > ER(S)$.

Next we have to provide an upper bound on the spectral radius of trees in $\mathcal{Q}_n$. We first observe that, as a tree obtained by attaching at most three new pendent edges to the leaves of a path and at most one new pendant edge to its internal vertices, every tree in $\mathcal{Q}_n$ is an induced subgraph of the tree Q depicted in Fig. 7. To bound the spectral

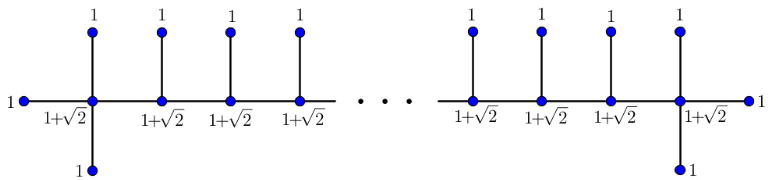

Figure 7. A tree containing all trees in $\mathcal{Q}_n^*$ as its subtrees.

radius of Q, we will resort to the following result from [20], restated in more familiar terms.

Theorem 11 ([20]). *If G is a connected graph with adjacency matrix A, then the system of inequalities*

$$Ax \leq \Lambda x \tag{18}$$

has a solution for real Λ and non-negative x if and only if $\lambda_1(G) \leq \Lambda$.

Let A be the adjacency matrix of Q and recall that for each vertex u of Q

$$(Ax)_u = \sum_{v \sim u} x_v ,$$

where the sum goes over all neighbors of u in Q. It is straightforward to check that the system (18) is satisfied for $\Lambda = 1 + \sqrt{2}$ and the vector x, whose components are depicted in Fig. 7. As a matter of fact, equality holds in (18) for each vertex of Q, except for the two vertices of degree four for which we have strict inequality. Hence

$$\lambda_1(Q) \leq \Lambda\,,$$

and since the spectral radius is edge-monotone, also $\lambda_1(T) \leq \Lambda$ for each tree $T \in \mathcal{Q}_n$.

Now that we have a common upper bound on the spectral radius of trees in $\mathcal{Q}_n$, we can move on to estimate their numbers of closed walks of lengths 4 and 6. From [21] we have that

$$M_4(G) = 2 \sum_{u \in V(G)} d_u^2 - 2m + 8q\,, \tag{19}$$

where d_u is the degree of the vertex u, m is the number of edges and q is the number of quadrangles in G. Certainly, $m = n-1$ and $q = 0$ in a tree T, so that (19) for trees reduces to

$$M_4(T) = 2 \left(\sum_{u \in V(G)} d_u^2 - n + 1 \right).$$

Closed walks of length six may, in general, go over the cycles of length 4 and 6 in a graph. However, as we are interested in trees only, each closed walk $u = u_0, u_1, \ldots, u_6 = u$ may have only one of the forms depicted in Fig. 8. They are classified according to whether the vertices u_2 and u_4 are equal to u and to each other (vertices that are not specified beneath each drawing may be mutually equal even if they are depicted as different in the drawing).

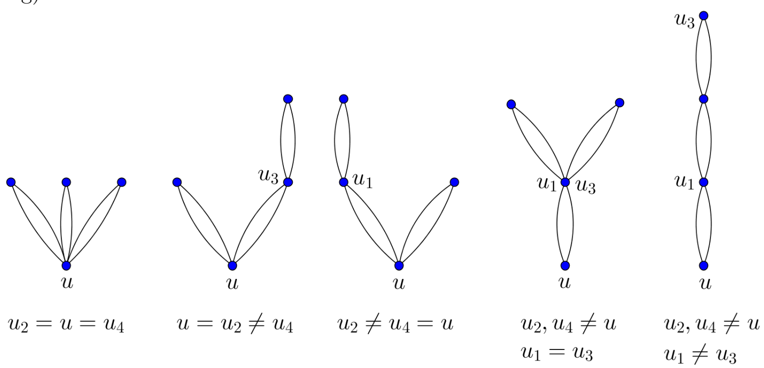

Figure 8. Five types of closed walks of length six in trees.

Clearly, there are $\sum_{u \in V(T)} d_u^3$ walks of the first type $u_2 = u = u_4$. Walks of the second type $u_2 = u \neq u_4$ are most easily counted with the help of adjacent vertices u and u_3:

there are d_u choices for u_1 and since $u_4 \neq u$, there are $d_{u_3} - 1$ choices for the vertex u_4, so that the total number of walks of this type is

$$\sum_{u \in V(T)} \sum_{\{u_3:\ uu_3 \in E(T)\}} d_u(d_{u_3} - 1) = 2 \sum_{uu_3 \in E(T)} d_u d_{u_3} - \sum_{u \in V(T)} d_u^2 \ .$$

as each edge of T gets counted twice in the first double sum—once as (u, u_3) and once as (u_3, u), while each degree d_u gets subtracted d_u times. In the same way, counting over the pairs of adjacent vertices u and u_1 (instead of u_3), we see that there are also

$$2 \sum_{uu_1 \in E(T)} d_u d_{u_1} - \sum_{u \in V(T)} d_u^2$$

walks of the third type $u_2 \neq u = u_4$. Closed walks of the fourth type may be counted by the adjacent pair (u, u_1): for each choice of the neighbor u_1 of u, there are $d_{u_1} - 1$ choices for each of $u_2 \neq u$ and $u_4 \neq u$, so that the total number of walks of this type is

$$\sum_{u \in V(T)} \sum_{\{u_1:\ uu_1 \in E(T)\}} (d_{u_1} - 1)^2 = \sum_{u_1 \in V(T)} d_{u_1}(d_{u_1} - 1)^2 = \sum_{u_1 \in V(T)} d_{u_1}^3 - 2 \sum_{u_1 \in V(T)} d_{u_1}^2 + 2m \ .$$

Closed walks of the fifth type may be counted by the adjacent pair (u_1, u_2): for each choice of the neighbor u_1 of u, there are $d_{u_1} - 1$ choices for u_2 and $d_{u_2} - 1$ choices for u_3. Hence the total number of walks of this type is

$$\begin{aligned} \sum_{u \in V(T)} \sum_{\{u_1:\ uu_1 \in E(T)\}} \sum_{\{u_2:\ u_1u_2 \in E(T)\}} (d_{u_2} - 1) &= 2 \sum_{u_1u_2 \in E(T)} (d_{u_1} - 1)(d_{u_2} - 1) \\ = \ 2 \sum_{u_1u_2 \in E(T)} d_{u_1} d_{u_2} - \sum_{u_1 \in V(T)} d_{u_1}^2 - \sum_{u_3 \in V(T)} d_{u_3}^2 + 2m \ . \end{aligned}$$

Finally, adding these quantities together we see that

$$M_6(T) = 2 \sum_{u \in V(T)} d_u^3 - 6 \sum_{u \in V(T)} d_u^2 + 6 \sum_{uv \in E(T)} d_u d_v + 4m \ . \tag{20}$$

Now we can move forward to compare the closed walks of lengths 4 and 6 between $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)$ and the trees in $\mathcal{Q}_n^*$. Tree $P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)$ has one vertex of degree 3, three leaves and $n-4$ vertices of degree 2, so that

$$M_4\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right) = 6n - 6 \quad \text{and} \quad M_6\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right) = 20n - 14 \ .$$

If T is a tree in $\mathcal{Q}_n^*$, then it has one of the three types depicted in Fig. 3, depending on the number of vertices of degree 4 that it contains:

Type i) For a tree $T \in \mathcal{Q}_n^*$ with no vertices of degree 4, if it has $k \geq 2$ vertices of degree 3, then it has $k+2$ leaves and $n-2k-2$ vertices of degree 2, so that

$$M_4(T) = 6n + 4k - 10 \geq 6n - 2 \; . \tag{21}$$

It further contains k edges between vertices of degrees 3 and 1, two edges that connect path leaves to vertices of degree either 2 or 3, and $n-k-3$ edges that connect vertices of degrees either 2 or 3 on the path. The edge on the right from each vertex of degree 3 on the path will contribute at least $3 \cdot 2$ to the sum $\sum_{uv \in E(T)} d_u d_v$. Regardless of how the vertices of degree 3 are distributed, there will be at least $k-1$ such edges, while the remaining $n-2k-2$ will contribute at least $2 \cdot 2$. Hence $\sum_{uv \in E(T)} d_u d_v \geq 4n + k - 10$, so that

$$M_6(T) \geq 20n + 18k - 56 \geq 20n - 20 \; . \tag{22}$$

Hence

$$(n-1)^2 [M_4(T) - M_4(S)] + [M_6(T) - M_6(S)] \geq 4(n-1)^2 - 6 \; .$$

The inequality

$$4(n-1)^2 - 6 > \frac{n\Lambda^8}{(n-1)(n-1-\Lambda)}$$

for $\Lambda = 1 + \sqrt{2}$ is satisfied for $n \geq 9$, so that from Lemma 8 we have

$$EE_r(T) > EE_r\left(P_{n-1}\left(\left\lfloor \frac{n}{2} \right\rfloor\right)\right)$$

for each tree T of this type with at least 9 vertices.

Type ii) For a tree $T \in \mathcal{Q}_n^*$ with one vertex of degree four, if it has $k \geq 0$ vertices of degree three, then it has $k+4$ leaves and $n-2k-5$ vertices of degree two, so that

$$M_4(T) = 6n + 4k + 2 \geq 6n + 2 \, ; \tag{23}$$

Similarly as in the previous case, we get $\sum_{uv \in E(T)} d_u d_v \geq 4n + k - 4$, so that

$$M_6(T) \geq 20n + 18k - 32 \geq 20n - 32 \; . \tag{24}$$

Hence

$$(n-1)^2 [M_4(T) - M_4(S)] + [M_6(T) - M_6(S)] \geq 8(n-1)^2 - 18 \; .$$

The inequality

$$8(n-1)^2 - 18 > \frac{n\Lambda^8}{(n-1)(n-1-\Lambda)}$$

is satisfied for $n \geq 8$, so that from Lemma 8

$$EE_r(T) > EE_r\left(P_{n-1}\left(\left\lfloor\frac{n}{2}\right\rfloor\right)\right)$$

for each tree T of this type with at least 8 vertices.

Type iii) For a tree $T \in \mathcal{Q}_n^*$ with two vertices of degree four, if it has $k \geq 0$ vertices of degree three, then it has $k+6$ leaves and $n-2k-8$ vertices of degree two, so that

$$M_4(T) = 6n + 4k + 14 \geq 6n + 14\ . \tag{25}$$

In this case we get $\sum_{uv\in E(T)} d_u d_v \geq 4n + k + 2$, so that

$$M_6(T) \geq 20n + 18k + 112 \geq 20n + 112\ . \tag{26}$$

Hence

$$(n-1)^2[M_4(T) - M_4(S)] + [M_6(T) - M_6(S)] \geq 20(n-1)^2 + 126.$$

The inequality

$$20(n-1)^2 + 126 > \frac{n\Lambda^8}{(n-1)(n-1-\Lambda)}$$

is satisfied for $n \geq 6$, so that from Lemma 8

$$EE_r(T) > EE_r\left(P_{n-1}\left(\left\lfloor\frac{n}{2}\right\rfloor\right)\right)$$

for all trees T of this type.

Hence it remains to computationally check trees of the first type with at most 8 vertices and trees of the second type with at most 7 vertices. There are 11 such trees in total, depicted in Fig. 9, all of which have resolvent Estrada index larger than that of $P_{n-1}\left(\left\lfloor\frac{n}{2}\right\rfloor\right)$. This resolves Conjecture 1 for trees in $\mathcal{Q}_n^*$ as well, so that we finally have

Theorem 12. *For $2 \leq a \leq \lfloor n/2 \rfloor$, the tree $P_{n-1}(a)$ has the a-th smallest resolvent Estrada index among trees of order n.*

Lemma 10, together with the estimates (21)-(26) for the numbers of closed walks of lengths 4 and 6, implies that

$$ER(T) > ER\left(P_{n-1}\left(\left\lfloor\frac{n}{2}\right\rfloor\right)\right)$$

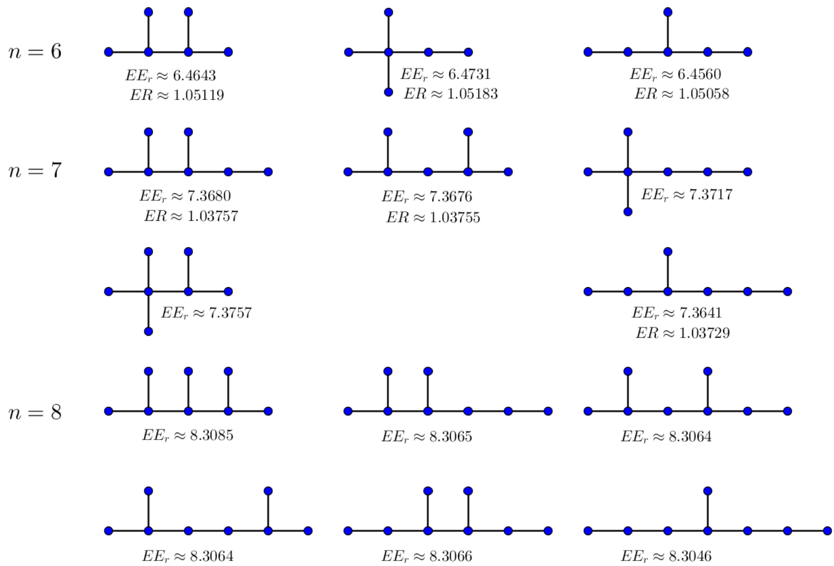

Figure 9. Trees in $\mathcal{Q}_n^*$ to which Lemma 8 cannot be applied. Their resolvent Estrada indices and resolvent energies are shown beneath the drawings. Trees $P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$, $6 \le n \le 8$, are shown for comparison.

holds for trees in $\mathcal{Q}_n^*$ of the first type with at least 8 vertices, of the second type with at least 7 vertices, and for all trees of the third type (see Fig. 3). The remaining four trees in $\mathcal{Q}_6^*$ and $\mathcal{Q}_7^*$ also have resolvent energy larger than that of the corresponding $P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$, as shown in Fig. 9. Hence we also have

Theorem 13. *For $2 \le a \le \lfloor n/2 \rfloor$, the tree $P_{n-1}(a)$ has the a-th smallest resolvent energy among trees of order n.*

4 Concluding remarks

We have resolved Conjecture 1 in Sections 2 and 3 by applying different approaches to trees not in $\mathcal{Q}_n^*$ and trees in $\mathcal{Q}_n^*$. The fact that trees not in $\mathcal{Q}_n^*$ are $\preceq$-comparable to F_n enabled us to conclude that $P_n, P_{n-1}(2), \ldots, P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$ are the smallest trees for any invariant defined as a weighted series of closed walk numbers with nonnegative coefficients, including the Estrada index, the resolvent Estrada index, the resolvent energy and the spectral radius (allowing equality instead of strict inequality in the latter case).

On the other hand, trees in $\mathcal{Q}_n^*$ are, in principle, not $\preceq$-comparable to $P_{n-1}\left(\lfloor \frac{n}{2} \rfloor\right)$. The appropriate choices of coefficients $c_k = 1/(n-1)^k$ in the definition of the resolvent Estrada index and $c_k = 1/n^{k+1}$ in the definition of the resolvent energy enabled us to use a simple spectral bound on the tail of defining series in Lemmas 7 and 9, and to focus solely on closed walks of lengths 4 and 6 in Lemmas 8 and 10. Such approach, unfortunately, cannot be used with the Estrada index or the spectral radius, so that new methods have to be found in order to deduce results for the Estrada index and the spectral radius analogous to those presented here for the resolvent Estrada index and the resolvent energy.

References

[1] E. Estrada, D. J. Highman, Network properties revealed through matrix functions, *SIAM Rev.* **52** (2010) 696–714.

[2] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

[3] E. Estrada, Characterization of the folding degree of proteins, *Bioinf.* **18** (2002) 697–704.

[4] E. Estrada, Characterization of the amino–acids contributions to the folding degree of proteins, *Proteins Struct. Func. Bioinf.* **54** (2004) 727–737.

[5] E. Estrada, Topological structural classes of complex networks, *Phys. Rev. E* **75** (2007) #016103.

[6] E. Estrada, J. A. Rodríguez-Valázquez, M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.* **106** (2006) 823–832.

[7] I. Gutman, B. Furtula, V. Marković, B. Glišić, Alkanes with greatest Estrada index, *Z. Naturforsch.* **62a** (2007) 495–498.

[8] M. Benzi, P. Boito, Quadrature rule–based bounds for functions of adjacency matrices, *Lin. Algebra Appl.* **433** (2010) 637–652.

[9] X. Chen, J. Qian, Bounding the resolvent Estrada index of a graph, *J. Math. Study* **45** (2012) 159–166.

[10] X. Chen, J. Qian, On resolvent Estrada index, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 163–174.

[11] I. Gutman, B. Furtula, X. Chen, J. Qian, Graphs with smallest resolvent Estrada indices, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 267–270.

[12] I. Gutman, B. Furtula, E. Zogić, E. Glogić, Resolvent energy of graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 279–290.

[13] I. Gutman, B. Furtula, E. Zogić, E. Glogić, Resolvent energy, in: I. Gutman, X. Li (Eds.), *Energies of Graphs – Theory and Applications*, Univ. Kragujevac, Kragujevac, 2016, pp. 277–290.

[14] A. J. Schwenk, Computing the characteristic polynomial of a graph, in: R. A. Bari, F. Harary (Eds.), *Graphs and Combinatorics*, Springer–Verlag, Berlin, 1974, pp. 153–172.

[15] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* **47** (2010) 305–314.

[16] D. Stevanović, *Spectral Radius of Graphs*, Acad. Press, Amsterdam, 2015.

[17] D. M. Cvetković, M. Doob, I. Gutman, On graphs whose spectral radius does not exceed $\sqrt{2+\sqrt{5}}$, *Ars Comb.* **14** (1982) 225–239.

[18] A. E. Brouwer, A. Neumaier, The graphs with spectral radius between 2 and $\sqrt{2+\sqrt{5}}$, *Lin. Algebra Appl.* **114-115** (1989) 273–276.

[19] H. Deng, A proof of a conjecture on the Estrada index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 599–606.

[20] W. E. Pruitt, Eigenvalues of non-negative matrices, *Ann. Math. Stat.* **35** (1964) 1797–1800.

[21] I. Gutman, Some topological properties of benzenoid systems, *Croat. Chem. Acta* **46** (1974) 209–215.