Some new results on distance-based graph invariants

M. H. Khalifeh

School of Mathematics, Statistics and Computer Science, University of Tehran, Tehran, I. R. Iran

H. Yousefi-Azari

School of Mathematics, Statistics and Computer Science, University of Tehran, Tehran, I. R. Iran

A. R. Ashrafi

Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran

S. G. Wagner

Department of Mathematical Sciences, Stellenbosch University, Stellenbosch 7602, South Africa

Abstract

We study distance-based graph invariants, such as the Wiener index, the Szeged index, and variants of these two. Relations between the various indices for trees are provided as well as formulas for line graphs and product graphs. This allows us, for instance, to establish formulas for the edge Wiener index of Hamming graphs, C_4-nanotubes and C_4-nanotori. We also determine minimum and maximum of certain indices over the set of all graphs with a given number of vertices or edges. Finally, we study the order of magnitude of the edge Wiener and edge Szeged index, responding negatively to a conjecture that is related to the maximization of the edge Szeged index.

Key words. Wiener index, Szeged index, trees, line graphs, product graphs

2000 AMS Subject Classification: 05C12; 05A15, 05A20, 05C05.

Email addresses: khalife@khayam.ut.ac.ir (M. H. Khalifeh), hyousefi@ut.ac.ir (H. Yousefi-Azari), ashrafi@kashanu.ac.ir (A. R. Ashrafi), swagner@sun.ac.za (S. G. Wagner).

1 Introduction and Notations

In this paper, we will consider distance-based graph invariants. A graph parameter Top with the property that $\mathrm{Top}(G) = \mathrm{Top}(H)$ whenever G and H are isomorphic is known as a *topological index* in the chemical literature. There are many examples of graph parameters, especially those based on distances, which are applicable in chemistry. The *Wiener index*, defined as the sum of all distances between pairs of vertices in a graph, is probably the first and most studied such graph invariant, both from a theoretical and practical point of view, see for instance [3,6,4,5,7,8,26].

Apart from the Wiener index, we will consider several related indices; to define them, we first introduce some notation. Throughout the paper, we only consider simple connected graphs. For a graph G, $V(G)$ and $E(G)$ denote the vertex and edge set, respectively. Furthermore, we use the following notations:

Definition 1.1 *Let G be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$, and let $\mathbb{N}^*$ denote the set of nonnegative integers. We use the following notations:*

$$\begin{aligned} d &: V \times V \longrightarrow \mathbb{N}^*, \\ D &: E \times E \longrightarrow \mathbb{N}^*, \\ d' &: V \times E \longrightarrow \mathbb{N}^*, \\ D' &: E \times V \longrightarrow \mathbb{N}^*, \end{aligned}$$

where for $u, v \in V$, $d(u, v)$ is defined as the length of a shortest path between u and v, and for edges $e = ab$ and $f = xy$,

$$d'(u, e) = D'(e, u) = \min\{d(u, a), d(u, b)\}$$

and

$$D(e, f) = \min\{D'(e, x), D'(e, y)\}.$$

Furthermore, we write

$$\begin{aligned} N_u(v) &= \{w \in V \mid d(u, w) > d(v, w)\}, \\ M_e(f) &= \{g \in E \mid D(e, g) > D(f, g)\}, \\ N'_u(v) &= \{e \in E \mid d'(u, e) > d'(v, e)\}, \\ M'_e(f) &= \{u \in V \mid D'(e, u) > D'(f, u)\}, \end{aligned}$$

and set $n_u(v) = |N_u(v)|$, $m_e(f) = |M_e(f)|$, $n'_u(v) = |N'_u(v)|$ and $m'_e(f) = |M'_e(f)|$. In all these definitions, equidistant vertices or edges are not counted.

This allows us to define the Wiener index of a graph formally as

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v).$$

Replacing d by D or d' yields the *edge Wiener index* and *vertex-edge Wiener index* respectively:

$$W_e(G) = \frac{1}{2} \sum_{g \in E(G)} \sum_{f \in E(G)} D(g,f),$$
$$W_{ev}(G) = \frac{1}{2} \sum_{f \in E(G)} \sum_{v \in V(G)} d'(v,f).$$

Another variant is known as the *Schultz index*:

$$W_+(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} \Big(\deg(u) + \deg(v)\Big) d(u,v).$$

In the important special case of trees, the Wiener index can be written as

$$\mathrm{Sz}(G) = \sum_{f=uv \in E(G)} n_u(v) n_v(u),$$

which is called the *Szeged index* [19] for general graphs. Again, it is possible to consider the *edge Szeged index* and *vertex-edge Szeged index* [10,12] by varying the definition:

$$\mathrm{Sz}_e(G) = \sum_{f=uv \in E(G)} n'_u(v) n'_v(u),$$
$$\mathrm{Sz}_{ev}(G) = \frac{1}{2} \sum_{f=uv \in E(G)} \Big(n'_u(v) n_v(u) + n'_v(u) n_u(v)\Big).$$

Finally, the *Padmakar-Ivan index* (PI index) is yet another distance-based graph parameter recently introduced by Padmakar Khadikar; its definition is very similar to that of the Szeged index, namely

$$PI(G) = \sum_{e=uv \in E(G)} \Big(n'_u(v) + n'_v(u)\Big),$$

see [12,14,18] for more details.

The special n-vertex graphs K_n (complete graph), P_n (path), S_n (star) and C_n (cycle) will repeatedly occur throughout the paper. For a graph G, a vertex v and a subgraph H of G, we write

$$d(v,H) = \sum_{u \in V(H)} d(v,u),$$

and we also define the quantities $d'(v,H)$, $D'(e,H)$ and $D(e,H)$ in a similar way (we will particularly often use the case when $H = G$). Finally, a subgraph H of G is called isometric, if for every $2-$subset $\{x,y\} \subseteq V(H)$, $d_G(x,y) = d_H(x,y)$. Other notations used are standard and taken mainly from [2,22].

2 Relations between indices

The aim of this section is to find relationships between the Wiener and edge Wiener index and other graph invariants such as the Schultz index and the Szeged index. The first part deals with trees, where it turns out that all these indices are closely related to each other. Then we present a relation between the edge Wiener index of a general graph and the Wiener index of its line graph. In the third part of this section, we investigate products of two or more graphs.

2.1 Trees

Theorem 2.1 *Let T be a tree with n vertices. The following equations are satisfied:*

(1) $W_{ev}(T) = W(T) - \binom{n}{2}$.
(2) $W_{ev}(T) = \frac{1}{4}W_+(T) - \frac{1}{2}\binom{n}{2}$,
(3) $W_e(T) = \frac{1}{4}W_+(T) - \frac{(3n-4)(n-1)}{4}$,

PROOF.

(1) Consider $v \in V(T)$. Define $f : E(T) \longrightarrow V(T) - \{v\}$ such that $f(e)$ is the end vertex of e with greater distance to v. Then f is bijective and so $d'(v,T) = d(v,T) - (n-1)$. This implies that

$$W_{ev}(T) = \frac{1}{2}\sum_{v \in V(T)} d'(v,T) = \frac{1}{2}\sum_{v \in V(T)} \Big(d(v,T) - (n-1)\Big) = W(T) - \binom{n}{2}.$$

(2) Consider an edge $e = u_1u_2 \in T$. By removing e from T, we obtain two new trees T_1 and T_2 with n_1 and n_2 vertices such that $u_1 \in V(T_1)$ and $u_2 \in V(T_2)$, respectively. Obviously, $n = n_1 + n_2$, and distances between u_1 and vertices of T_1 are shorter than distances between u_2 and vertices of T_1 (and the analogous statement holds for T_2). Thus,

$$D'(e,T) = d(u_1,T_1) + d(u_2,T_2).$$

Since paths between vertices of T are unique, we have $d(u_1, T_2) = d(u_2, T_2) + n_2$ and $d(u_2, T_1) = d(u_1, T_1) + n_1$. Therefore,

$$n + 2D'(e, T) = d(u_1, T) + d(u_2, T),$$

and since every vertex u is an endpoint of $\deg(u)$ edges, summing over all edges yields

$$W_{ev}(T) = \frac{1}{4} \sum_{u \in V(T)} \deg(u) d(u, T) - \frac{1}{2}\binom{n}{2}.$$

On the other hand, for every graph G,

$$\begin{aligned} W_+(G) &= \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} \Big(\deg(u) + \deg(v)\Big) d(u, v) \\ &= \frac{1}{2} \sum_{u \in V(G)} \deg(u) d(u, G) + \frac{1}{2} \sum_{v \in V(G)} \deg(v) d(v, G) \\ &= \sum_{u \in V} \deg(u) d(u, G), \end{aligned}$$

which proves the second part.

(3) By a similar argument as in the previous part,

$$D(e, T) = d'(u_1, T_1) + d'(u_2, T_2)$$

for any edge $e = u_1u_2$. Since T is a tree, we have $d'(u_2, T_2) = d(u_2, T_2) - (n_2 - 1)$ and $d'(u_1, T_1) = d(u_1, T_1) - (n_1 - 1)$. As in the proof of the previous part,

$$2D(u_1u_2, T) = d(u_1, T) + d(u_2, T) - (3n - 4).$$

Thus,

$$\begin{aligned} 4W_e(T) &= 2 \sum_{u_1u_2 \in E(T)} D(u_1u_2, T) \\ &= \sum_{u_1u_2 \in E(T)} \Big(d(u_1, T) + d(u_2, T) - (3n - 4)\Big) \\ &= \sum_{v \in V(T)} \deg(v) d(v, T) - (3n - 4)(n - 1), \end{aligned}$$

which finishes the proof of the final part. □

Corollary 2.2 *For a tree T with n vertices, $W_e(T) = \mathrm{Sz}_e(T)$.*

PROOF. By Theorem 2.1, parts (1) and (2),

$$W(T) = \frac{1}{4}W_+(T) + \frac{1}{2}\binom{n}{2},$$

and by combining this with part (3), we obtain

$$W(T) - W_e(T) = (n-1)^2.$$

It is a well-known fact that $W(T) = \mathrm{Sz}(T)$, see [5]. On the other hand, for every $e = uv \in E(T)$,

$$n'_u(v)n'_v(u) = \Big(n_u(v) - 1\Big)\Big(n_v(u) - 1\Big) = n_u(v)n_v(u) - n + 1.$$

Hence, by definition of Sz_e, $\mathrm{Sz}_e(T) = \mathrm{Sz}(T) - (n-1)^2$, which proves the result. $\square$

Corollary 2.3 *For a tree T with n vertices, $W_{ev}(T) = \mathrm{Sz}_{ev}(T)$.*

PROOF. This is similar to the previous proof. For any edge $e = uv$, we have

$$n'_u(v) = n_u(v) - 1.$$

Summing over all edges, we get

$$\mathrm{Sz}_{ev}(T) = \mathrm{Sz}(T) - \binom{n}{2} = W(T) - \binom{n}{2} = W_{ev}(T),$$

making use of Theorem 2.1 once again. $\square$

Remark. Alternatively, Corollaries 2.2 and 2.3 can be proved along the lines of the standard proof for the fact that $W = \mathrm{Sz}$ for trees: simply note that every edge $e = uv$ occurs exactly $n'_u(v)n'_v(u)$ times on a unique shortest path between two edges to prove Corollary 2.2. The proof for Corollary 2.3 is similar.

Remark. We can combine all our results to find the following chain of identities: for any tree T with n vertices,

$$\begin{aligned} W(T) &= W_e(T) + (n-1)^2 = W_{ev}(T) + \binom{n}{2} = \frac{1}{4}W_+(T) + \frac{1}{2}\binom{n}{2} \\ &= \mathrm{Sz}(T) = \mathrm{Sz}_e(T) + (n-1)^2 = \mathrm{Sz}_{ev}(T) + \binom{n}{2}. \end{aligned}$$

2.2 Line graphs

The line graph $L(G)$ of a graph G is defined as follows: each vertex of $L(G)$ represents an edge of G, and any two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G. One can also define iterated line graphs by setting $L^0(G) = G$, $L^1(G) = L(G)$ and generally $L^n(G) = L(L^{n-1}(G))$.

Theorem 2.4 *Suppose G is a connected graph. Then*

$$W(L(G)) - W_e(G) = \binom{|E(G)|}{2} = \binom{|V(L(G))|}{2}$$

and generally

$$W(L^n(G)) - W_e(L^{n-1}(G)) = \binom{|V(L^n(G))|}{2}.$$

PROOF. Suppose $a, b \in V(L(G))$, $a \neq b$. Then $a, b \in E(G)$ and $d_{L(G)}(a, b) = D_G(a, b) + 1$. Therefore,

$$W(L(G)) = \sum_{\{a,b\} \subseteq V(L(G))} d_{L(G)}(a, b) = \sum_{\{a,b\} \subseteq E(G)} \Big(D_G(a, b) + 1\Big) = W_e(G) + \binom{|E(G)|}{2},$$

and the theorem follows. □

2.3 Product graphs

The Cartesian product $G \times H$ of two graphs G and H has vertex set

$$V(G \times H) = V(G) \times V(H),$$

and $(a, x)(b, y)$ is an edge of $G \times H$ if either $a = b$ and $xy \in E(H)$, or if $ab \in E(G)$ and $x = y$.

For a sequence $G_1, G_2, \cdots, G_n$ of graphs, we write

$$\bigotimes_{i=1}^{n} G_i = G_1 \times \cdots \times G_n$$

for the iterated product. If $G_1 = G_2 = ... = G_n = G$, we abbreviate $\bigotimes_{i=1}^{n} G_i$ by G^n.

It is well-known fact that the Cartesian product is commutative and associative. Moreover, $G \times H$ is connected if and only if G and H are connected.

There are quite a few examples of formulas for graph invariants of product graphs in the literature. To the best of our knowledge, Graovac and Pisanski were the first to consider this problem for the Wiener index, see [8]. Similar contributions are due to Klavžar, Rajapakse and Gutman [19] (for the Szeged index) and Klavžar [18] (for the PI index). Other examples include [13,14,16,17,27], where the first and second Zagreb index, PI and vertex PI index and edge Szeged index are considered. In the case of the Wiener index, Sagan, Yeh and Zhang [21] provided formulas for the Wiener for some other binary operations on graphs. In the following theorem we continue this program by providing a formula for the edge Wiener index of product graphs.

Theorem 2.5 *Let G and H be graphs with $V_1 = V(G)$, $V_2 = V(H)$, $E_1 = E(G)$ and $E_2 = E(H)$. Then*

$$\begin{aligned} W_e(G \times H) = &|V_2|^2 W_e(G) + |V_1|^2 W_e(H) + |E_2|^2 W(G) + |E_1|^2 W(H) \\ &+ 2|E_2||V_2|W_{ev}(G) + 2|E_1||V_1|W_{ev}(H). \end{aligned}$$

PROOF. Consider $(a,b)(c,d), (e,f)(g,h) \in E = E(G \times H)$. To determine the distance $D((a,b)(c,d),\ (e,f)(g,h))$, we consider the following four cases:

(1) $ac \in E_1,\ b = d\ ;\ eg \in E_1, f = h,$
(2) $ac \in E_1,\ b = d\ ;\ e = g, fh \in E_2,$
(3) $a = c,\ bd \in E_2\ ;\ e = g, fh \in E_2,$
(4) $a = c,\ bd \in E_2\ ;\ eg \in E_1, f = h.$

Since $G \times H \cong H \times G$, it is enough to consider Cases (1) and (2). By [11, Corollary 1.35], $d_{G\times H}((a,b),(e,f)) = d_G(a,e) + d_H(b,f)$. Therefore, we obtain in Case (1)

$$\begin{aligned} D_{G\times H}((a,b)(c,d),(e,f)(g,h)) &= \min\{d_G(a,e) + d_H(b,f), d_G(a,g) + d_H(b,f), \\ &\qquad d_G(c,e) + d_H(b,f), d_G(c,g) + d_H(b,f)\} \\ &= D_G(ac,eg) + d_H(b,f). \end{aligned}$$

Similarly,

$$\begin{aligned} D_{G\times H}((a,b)(c,d),(e,f)(g,h)) &= \min\{d_G(a,e) + d_H(b,f), d_G(a,g) + d_H(b,h), \\ &\qquad d_G(c,e) + d_H(d,f), d_G(c,g) + d_H(d,h)\} \\ &= \min\{d_G(a,e), d_G(c,e)\} + \min\{d_H(b,f), d_H(b,h)\} \\ &= D'_G(ac,e) + d'_H(b,fh) \end{aligned}$$

in Case (2).

As mentioned before, Cases (3) and (4) are analogous, and so we have

$$D_{G\times H}((a,b)(c,d),(e,f)(g,h)) = \begin{cases} D_H(bd,fh) + d_G(a,e) \\ d'_G(f,bd) + D'_H(eg,a) \end{cases}$$

in Cases (3) and (4), respectively. Obviously, $E(G \times H)$ is partitioned by the above four cases. Hence

$$\begin{aligned}
W_e(G\times H) &= \frac{1}{2}\sum_{(a,b)(c,d)\in E}\ \sum_{(e,f)(g,h)\in E} D_{G\times H}((a,b)(c,d),(e,f)(g,h)) \\
&= \frac{1}{2}\sum_{ac\in E_1}\sum_{b=d\in V_2}\sum_{eg\in E_1}\sum_{f=h\in V_2}\Big(D_G(ac,eg) + d_H(b,f)\Big) \\
&\quad + \frac{1}{2}\sum_{ac\in E_1}\sum_{b=d\in V_2}\sum_{e=g\in V_1}\sum_{fh\in E_2}\Big(D'_G(ac,e) + d'_H(b,fh)\Big) \\
&\quad + \frac{1}{2}\sum_{a=c\in V_1}\sum_{bd\in E_2}\sum_{e=g\in V_1}\sum_{fh\in E_2}\Big(D_H(bd,fh) + d_G(a,e)\Big) \\
&\quad + \frac{1}{2}\sum_{a=c\in V_1}\sum_{bd\in E_2}\sum_{eg\in E_1}\sum_{f=h\in V_2}\Big(d'_G(f,bd) + D'_H(eg,a)\Big) \\
&= |V_2|^2W_e(G) + |E_1|^2W(H) + |E_2||V_2|W_{ev}(G) + |E_1||V_1|W_{ev}(H) \\
&\quad + |V_1|^2W_e(H) + |E_2|^2W(G) + |E_1||V_1|W_{ev}(H) + |E_2||V_2|W_{ev}(G) \\
&= |V_2|^2W_e(G) + |V_1|^2W_e(H) + |E_2|^2W(G) + |E_1|^2W(H) \\
&\quad + 2|E_2||V_2|W_{ev}(G) + 2|E_1||V_1|W_{ev}(H).
\end{aligned}$$

This completes the proof. □

Theorem 2.6 *Let G and H be graphs with $V_1 = V(G)$, $V_2 = V(H)$, $E_1 = E(G)$, $E_2 = E(H)$, $V = V(G\times H)$ and $E = E(G\times H)$. Then*

$$W_{ev}(G\times H) = |V_1|^2W_{ev}(H) + |V_2|^2W_{ev}(G) + |E_1||V_1|W(H) + |E_2||V_2|W(G).$$

PROOF. We split the edge set of $G \times H$ into subsets

$$A = \{(c,d)(c,f) \in E(G\times H) \mid df \in E(H), c \in V(G)\}$$

and

$$B = \{(c,d)(e,d) \in E(G\times H) \mid ce \in E(G), d \in V(H)\}.$$

Using a similar argument as in the previous theorem, if $(c,d)(c,f) \in A$ then

$$d'_{G\times H}((a,b),(c,d)(c,f)) = d_G(a,c) + d'_H(b,df),$$

and if $(c,d)(e,d) \in B$ then

$$d'_{G\times H}((a,b),(c,d)(e,d)) = d_H(b,d) + d'_G(a,ce).$$

Therefore,

$$\begin{aligned}
W_{ev}(G\times H) &= \frac{1}{2}\sum_{(a,b)\in V}\ \sum_{(c,d)(e,f)\in E} d'_{G\times H}((a,b),(c,d)(e,f)) \\
&= \frac{1}{2}\sum_{a\in V_1}\sum_{b\in V_2}\sum_{c=e\in V_1}\sum_{df\in E_2}\Big(d_G(a,c)+d'_H(b,df)\Big) \\
&\quad+\frac{1}{2}\sum_{a\in V_1}\sum_{b\in V_2}\sum_{d=f\in V_2}\sum_{ce\in E_1}\Big(d_H(b,d)+d'_G(a,ce)\Big) \\
&= |V_1|^2W_{ev}(H)+|V_2|^2W_{ev}(G)+|E_1||V_1|W(H)+|E_2||V_2|W(G),
\end{aligned}$$

which completes the proof. □

The formulas provided in Theorem 2.5 and Theorem 2.6 can be generalized to the case of a product of n graphs. In the following, let $G_1, G_2, \ldots, G_n$ be a sequence of graphs, and let $G_{1,n}$ be their product, i.e.

$$G_{1,n} = \bigotimes_{i=1}^{n} G_i = G_1\times G_2\times\cdots\times G_n.$$

Furthermore, we set

$$G^i_{1,n} = \bigotimes_{j=1,j\neq i}^{n} G_j, \qquad 1\le i\le n$$

and write $V_{1,n}=V(G_{1,n})$, $V^i_{1,n}=V(G^i_{1,n})$, $E_{1,n}=E(G_{1,n})$, and $E^i_{1,n}=E(G^i_{1,n})$ for the sake of brevity.

For two arbitrary graphs G and H, one has $|V(G\times H)| = |V(G)|\times|V(H)|$ and $|E(G\times H)| = |V(G)|\times|E(H)|+|V(H)|\times|E(G)|$. An inductive argument shows that generally

$$|V_{1,n}| = \prod_{i=1}^{n}|V_i| \quad\text{and}\quad |E_{1,n}| = \sum_{i=1}^{n}|V^i_{1,n}||E_i|.$$

Corollary 2.7 *Let $G_1, G_2, \ldots, G_n$ be an arbitrary sequence of graphs. Then,*

$$W_{ev}(G_{1,n}) = \sum_{i=1}^{n}\Big(|V^i_{1,n}|^2W_{ev}(G_i)+|E^i_{1,n}||V^i_{1,n}|W(G_i)\Big).$$

PROOF. By induction on n; Theorem 2.6 provides the case $n=2$. For the induction step, we have

$$\begin{aligned}
W_{ev}(G_{n+1}\times G_{1,n}) &= |V_{1,n}|^2W_{ev}(G_{n+1})+|V_{n+1}|^2W_{ev}(G_{1,n}) \\
&\quad+|V_{1,n}||E_{1,n}|W(G_{n+1})+|V_{n+1}||E_{n+1}|W(G_{1,n}).
\end{aligned}$$

By a result of Klavžar, Rajapakse and Gutman [19], $W(G_{1,n}) = \sum_{i=1}^{n} |V_{1,n}^i|^2 W(G_i)$. Thus,

$$\begin{aligned} W_{ev}(G_{1,n+1}) &= |V_{1,n+1}^{n+1}|^2 W_{ev}(G_{n+1}) + |E_{1,n+1}^{n+1}||V_{1,n+1}^{n+1}|W(G_{n+1}) \\ &\quad + \sum_{i=1}^{n} \Big(|V_{n+1}|^2|V_{1,n}^i||E_{1,n}^i| + |V_{n+1}||E_{n+1}||V_{1,n}^i|^2\Big)W(G_i) \\ &\quad + |V_{n+1}|^2 \sum_{i=1}^{n} |V_{1,n}^i|^2 W_{ev}(G_i). \end{aligned}$$

By the formulas for $E_{1,n}$ and $V_{1,n}$, we have

$$\begin{aligned} |E_{1,n+1}^i||V_{1,n+1}^i| &= |V_{1,n+1}^i|(|E_{1,n}^i||V_{n+1}| + |V_{1,n}^i||E_{n+1}|) \\ &= |V_{n+1}|^2|V_{1,n}^i||E_{1,n}^i| + |V_{n+1}||E_{n+1}||V_{1,n}^i|^2, \end{aligned}$$

and so

$$W_{ev}(G_{1,n+1}) = \sum_{i=1}^{n+1} \Big(|V_{1,n+1}^i|^2 W_{ev}(G_i) + |E_{1,n+1}^i||V_{1,n+1}^i|W(G_i)\Big),$$

which completes the proof. $\square$

Using a similar argument as above, one can prove the following corollary of Theorem 2.5:

Corollary 2.8 *Let $G_1, G_2, \ldots, G_n$ be an arbitrary sequence of graphs. Then,*

$$W_e(G_{1,n}) = \sum_{i=1}^{n} \Big(|V_{1,n}^i|^2 W_e(G_i) + 2|E_{1,n}^i||V_{1,n}^i|W_{ev}(G_i) + |E_{1,n}^i|^2 W(G_i)\Big).$$

Combining the results of Theorem 2.4 and Corollary 2.8, one finally finds

Corollary 2.9 *Let $G_1, G_2, \ldots, G_n$ be an arbitrary sequence of graphs. Then,*

$$\begin{aligned} W(L(G_{1,n})) &= \sum_{i=1}^{n} \Big(V_{1,n}^i|^2 W(L(G_i)) + |V(L(G_{1,n}^i))|^2 W(G_i) \\ &\quad + 2|V(L(G_{1,n}^i))||V_{1,n}^i|W_{ev}(G_i)\Big) - \sum_{i=1}^{n} |V_{1,n}^i|^2 \binom{|V(L(G_i))|}{2} \\ &\quad + \binom{|V(L(G_{1,n}))|}{2}. \end{aligned}$$

Our final corollary treats the case that all graphs of the sequence are equal, i.e. $G_1 = \ldots = G_n = G$.

Corollary 2.10 *Let G be a graph with $E = E(G)$ and $V = V(G)$. The edge Wiener index of G^n, the vertex-edge Wiener index of G^n and the Wiener index of $(L(G^n))^m$ are given by*

(1)

$$W_e(G^n) = n|E||V|^{2n-3}\Big(\frac{|V|}{|E|}W_e(G)+2(n-1)W_{ev}(G)+\frac{|E|}{|V|}(n-1)^2W(G)\Big),$$

(2)

$$W_{ev}(G^n) = n|V|^{2n-2}\Big(W_{ev}(G) + (n-1)\frac{|E|}{|V|}W(G)\Big),$$

(3)

$$\begin{aligned} W((L(G^n))^m) = m\left(n|V(G)|^{n-1}|E(G)|\right)^{2m-2} \\ \cdot\Bigg(n|E||V|^{2n-3}\Big(\frac{|V|}{|E|}W_e(G) + 2(n-1)W_{ev}(G) \\ + \frac{|E|}{|V|}(n-1)^2W(G)\Big) + \binom{n|V(G)|^{n-1}|E(G)|}{2}\Bigg). \end{aligned}$$

PROOF. The three formulas follow from Corollaries 2.7, 2.8 and 2.9. □

Example. Consider the graph G whose vertices are the $N-$tuples $b_1b_2\cdots b_N$ with $b_i \in \{0, 1, \cdots, n_i - 1\}, n_i \geq 2$, and let two vertices be adjacent if the corresponding tuples differ in precisely one place. Such a graph is called a Hamming graph and denoted by $H_{n_1,n_2,\cdots,n_N}$. A Hamming graph with $n_1 = n_2 = ... = n_N = 2$ is called a hypercube of dimension N and denoted by Q_N. It is a well-known fact that Hamming graphs can be written as

$$H_{n_1,n_2,\cdots,n_N} = \bigotimes_{i=1}^{N} K_{n_i}.$$

Corollary 2.8 allows us to compute the edge Wiener index of a Hamming graph. To this end, simply note that

$$W_e(K_{n_i}) = 3\binom{n_i}{4}, \quad W_{ev}(K_{n_i}) = \frac{3}{2}\binom{n_i}{3}, \quad \text{and} \quad W(K_{n_i}) = \binom{n_i}{2}.$$

This gives us

$$\begin{aligned} &W_e(H_{n_1,n_2,\cdots,n_N}) \\ &= \frac{\left(\prod_{i=1}^{N} n_i\right)^2}{8}\Bigg(N(N^2 + 2N + 4) - (N^2 + 2N + 3)\sum_{i=1}^{N}\frac{1}{n_i} + 2(N + 1)\sum_{i,j=1}^{N}\frac{n_i}{n_j} \end{aligned}$$

$$- (2N^2+2N+1)\sum_{i=1}^{N} n_i + N\sum_{i,j=1}^{N} n_in_j - \sum_{i,j,k=1}^{N} \frac{n_in_j}{n_k}\Bigg).$$

Thus for a hypercube Q_N, $W_e(Q_N) = N(N-1)^2 2^{2(N-2)}$, and by Corollary 2.10, $W(L(Q^N)) = N2^{2N-4}\Big(N^2+1-2^{2-N}\Big)$.

Example. As our final example, we consider graphs of the form $C_n \times C_m$, $P_n \times C_m$, and $P_n \times P_m$. Note that C_4-nanotubes and -nanotori are special cases of these general graph products. In order to apply Theorem 2.5, we need to know the Wiener, edge Wiener and vertex-edge Wiener indices of path and cycle graphs, which are given in Table 2.3. We obtain the following formulas for the edge Wiener indices of these graphs:

$$\begin{aligned}
W_e(C_{2m}\times C_{2n}) &= 4mn\Big(m(2n-1)^2+n(2m-1)^2\Big),\\
W_e(C_{2m+1}\times C_{2n+1}) &= 2(2m+1)(2n+1)\Big((2m+1)n^2+(2n+1)m^2\Big),\\
W_e(C_{2m+1}\times C_{2n}) &= (2m+1)n\Big(8m^2n+(2m+1)(2n-1)^2\Big),\\
W_e(P_n\times C_{2m+1}) &= \frac{2m+1}{6}\Big(3m^2(2n-1)^2+(8n^3-24n^2+22n-9)m\\
&\quad + (4n^3-12n^2+14n-6)\Big),\\
W_e(P_n\times C_{2m}) &= m\Big(2mn-(m+n)\Big)^2+\frac{4m^2(n-1)}{3}\Big(2n^2-4n+3\Big),\\
W_e(P_n\times P_m) &= n^2\binom{m-1}{3}+(n-1)^2\binom{m+1}{3}+2n(n-1)\binom{m}{3}\\
&\quad + m^2\binom{n-1}{3}+(m-1)^2\binom{n+1}{3}+2m(m-1)\binom{n}{3}.
\end{aligned}$$

$W_e(C_{2k}) = k(k-1)^2$	$W(C_{2k}) = k^3$	$W_{ev}(C_{2k}) = k^2(k-1)$
$W_e(C_{2k+1}) = (2k+1)\binom{k}{2}$	$W(C_{2k+1}) = (2k+1)\binom{k+1}{2}$	$W_{ev}(C_{2k+1}) = (2k+1)\frac{k^2}{2}$
$W_e(P_k) = \binom{k-1}{3}$	$W(P_k) = \binom{k+1}{3}$	$W_{ev}(P_k) = \binom{k}{3}$

Table 1
The Wiener, edge Wiener and vertex-edge Wiener indices of cycles and paths.

3 Extremal results

In this section, we provide the extremal values attained by some of our indices, taken over the set of all graphs with a fixed number of vertices or edges. We denote the set of all connected graphs with n vertices by $\mathcal{G}(n)$ and the set of all connected graphs with m edges by $\mathcal{G}_m$. The following theorem provides the minimum value of the edge Wiener index over all graphs with n vertices (cf. [9]).

Theorem 3.1 *Let $G \in \mathcal{G}(n)$ be a graph, where $n \geq 4$. Then $W_e(G) \geq 0$, with equality if and only if $G \cong S_n$, i.e. if G is a star graph with exactly n vertices.*

PROOF. It is clear that $W_e(S_n) = 0$, so it is enough to prove that $W_e(G) = 0$ implies $G \cong S_n$. Assume the contrary, i.e. $W_e(G) = 0$ and G is not isomorphic to S_n. Consider two edges ab and ac. Since every other edge is adjacent to both ab and ac, either $G \cong K_3$ (if bc is also an edge of G), which is excluded, or all edges are incident with a, i.e. $G \cong S_n$. $\square$

The proof of the following theorem can be found in [3,7]:

Theorem 3.2 *For every $G \in \mathcal{G}(n)$, $W(G) < W(P_n)$ if and only if $G \ncong P_n$.*

For the set $\mathcal{T}(n)$ of all trees with n vertices, the results given in Section 2.1 immediately yield the following result:

Corollary 3.3 *Suppose* Top *is one of W, W_e, W_{ev}, W_+,* Sz*,* Sz_e*,* Sz_{ev}*. Then*

$$\mathrm{Top}(S_n) = min\{\mathrm{Top}(G) \mid G \in \mathcal{T}(n)\}$$

and

$$\mathrm{Top}(P_n) = max\{\mathrm{Top}(G) \mid G \in \mathcal{T}(n)\}.$$

PROOF. This follows immediately from Theorems 3.1 and 3.2 and the results of Section 2.1. $\square$

Combining Theorems 3.2 and 2.4, one obtains immediately that the maximum of the Wiener index and the edge Wiener index over the set $\mathcal{G}_m$ are $W(P_{m+1})$ and $W_e(P_{m+1})$ respectively. It is also easy to see that if $m = \binom{n}{2}$ for some positive integer n, $W(K_n)$ is the minimum of the Wiener index over $\mathcal{G}_m$. The following theorem generalizes this observation:

Theorem 3.4 *If $G \in \mathcal{G}_m$ such that $\binom{a}{2} < m \leq \binom{a+1}{2}$, then*

$$W(G) \geq a(a+1) - m.$$

PROOF. Suppose that $G \in \mathcal{G}(n)$. Then clearly $m \leq \binom{n}{2}$, implying that $n \geq a+1$. Furthermore, at most m pairs of vertices have distance 1, while the remaining pairs contribute a distance of at least 2 to the Wiener index. This implies

$$W(G) \geq m + 2\left(\binom{a+1}{2} - m\right) = a(a+1) - m.$$

This lower bound is actually attained: consider a complete graph K_{a+1} and remove $\binom{a+1}{2} - m$ edges that are incident with a fixed vertex of K_{a+1}. Then, all distances are either 1 or 2, with the minimum possible number of 2's. $\Box$

We remark that it is actually possible to construct more examples of graphs for which the bound in Theorem 3.4 is attained by the same approach. Let us now turn to the Szeged and edge Szeged index.

Theorem 3.5 *Let G be a graph on n vertices. Then $\mathrm{Sz}(G) \geq \binom{n}{2}$ with equality if and only if $G \cong K_n$.*

PROOF. By [19, Theorem 3.1], $W(G) \leq \mathrm{Sz}(G)$. Suppose G is a non-complete graph with n vertices. Since K_n is the only graph in which all vertices are adjacent to each other, $\mathrm{Sz}(G) \geq W(G) > W(K_n) = \binom{n}{2} = \mathrm{Sz}(K_n)$. Therefore, $\mathrm{Sz}(G) = \mathrm{Sz}(K_n)$ implies that $G = K_n$. $\Box$

As in Theorem 3.1, it can be shown that if $G \in \mathcal{G}_m$ and $m > 3$, $\mathrm{Sz}_e(G) \geq 0$ with equality if and only if G is a star. In the following, we provide a sharp upper bound for the edge Szeged index in terms of the number of edges.

Theorem 3.6 *Let $G \in \mathcal{G}_m$ be a graph. Then*

$$\mathrm{Sz}_e(G) \leq \frac{m(m-1)^2}{4}$$

with equality if and only if m is odd and $G \cong C_m$, i.e. G is a cycle.

PROOF. Suppose $e = uv \in E(G)$. Then $n'_u(v) + n'_v(u) \leq m-1$ and so $n'_u(v)n'_v(u) \leq \frac{(m-1)^2}{4}$. Therefore,

$$\mathrm{Sz}_e(G) = \sum_{e=uv} n'_u(v)n'_v(u) \leq \frac{m(m-1)^2}{4}.$$

It is not difficult to see that this bound is actually attained if m is odd and $G \cong C_m$. Conversely, suppose that $\mathrm{Sz}_e(G) = \frac{m(m-1)^2}{4}$. Then for any edge

$e = uv \in E(G)$,

$$n'_u(v)n'_v(u) = \frac{(m-1)^2}{4},$$

and so G does not have vertices of degree 1 (since the above product would be 0 for the corresponding edge). This implies that G is not a tree and by [11, Proposition 1.25], it contains an isometric cycle $C : u_1u_2 \cdots u_nu_1$. If n is even then for every edge u_iu_{i+1} of C,

$$n'_{u_i}(u_{i+1}) + n'_{u_{i+1}}(u_i) \leq m-2 < m-1,$$

a contradiction. We now assume that n is odd and $G \ncong C_n$. Since G is connected, there exists a vertex v connected to one of the vertices of C_n, say u_1. Then $d'(u_{\frac{n+1}{2}}, u_1v) = d'(u_{\frac{n+3}{2}}, u_1v)$ and so

$$n'_{u_{\frac{n+3}{2}}}(u_{\frac{n+1}{2}}) + n'_{u_{\frac{n+1}{2}}}(u_{\frac{n+3}{2}}) \leq m-2 < m-1,$$

which is a contradiction again. This completes the proof. □

Let us remark that this result is closely related to the following:

Theorem 3.7 (see [1, Theorem 2]) *If $G \in \mathcal{G}_m$, then $PI(G) \leq m(m-1)$ with equality if and only if G is a tree or an odd cycle.*

Theorem 3.8 *Let G be a graph. Then*

$$|E(G)| \leq \mathrm{Sz}(G) \leq \frac{|E(G)||V(G)|^2}{4}$$

and the lower bound is attained if and only if $G \cong K_n$ for some n. Moreover, the upper bound is only attained if

- *G is bipartite,*
- *$|V(G)|$ is even, and*
- *G has no vertices of degree 1.*

PROOF. By definition,

$$2 \leq n_u(v) + n_v(u) \leq |V(G)|$$

for any edge $e = uv$, and so

$$|E(G)| \leq \mathrm{Sz}(G) \leq \frac{|E(G)||V(G)|^2}{4}.$$

By Theorem 3.5, the lower bound can only be attained if G is a complete graph. On the other hand,

$$n_u(v) + n_v(u) = |V(G)|$$

can only hold for all edges $e = uv$ of G if G is bipartite (since otherwise G contains an isometric odd cycle). By the same argument as in the proof of Theorem 3.6, there cannot be vertices of degree 1. Finally, if $|V(G)|$ is odd, then

$$n_u(v)n_v(u) \leq \frac{|V(G)|(|V(G)| - 1)}{4}$$

for every edge $e = uv \in E(G)$, which finishes the proof. $\square$

Remark. A related question is known as the inverse problem: given an integer n, it is possible to find a graph in some class (e.g. the class of trees) such that its Wiener index (or any other topological index) is exactly n. It was conjectured by Lepović and Gutman that every positive integer n is the Wiener index of some tree, with the exception of 49 specific numbers smaller than 160, see [20]. This was verified independently in [24] and [25].

It is natural to ask the same problem for other indices. For the edge Wiener index, however, the problem is not particularly difficult. To see why, consider a star S_{n+2} with $n + 2$ vertices and add a new vertex v to one of the leaves of this star to obtain a new tree S'_{n+2}. If e is the unique edge incident with v, then

$$D(e, S'_{n+2}) = n,$$

and all other edges of S'_{n+2} have mutual distance 0. Hence,

$$W_e(S'_{n+2}) = n,$$

which shows that there is a tree for any given value of the edge Wiener index. Since $\mathrm{Sz}_e(T) = W_e(T)$ for any tree T, the same conclusion holds for the edge Szeged index. It is quite believable that the Schultz index can be treated along the same lines as the Wiener index; we leave this as an open problem.

4 The order of magnitude of certain indices

In [10], the authors conjectured that the complete graph K_n has the largest edge-Szeged index among all n-vertex graphs. However, this was disproved by Vukičević [23] by virtue of the following sequence $\{G_n\}_{n\geq 9}$ of graphs:

$$E(G_n) = \{v_{i,j}v_{k,l} \mid i - k \ \equiv 1 \ (mod\ 9)\}$$

and

$$V(G_n) = \{v_{i,j} \mid (i,j) \in S\},$$

where

$$S = \left\{(i,j) \mid i \in \{0,1,3,4,6\}, \quad 1 \le j \le \left\lfloor \frac{n-3}{6} \right\rfloor \right\} \cup \left\{(i,1) \mid i \in \{2,5,8\}\right\}$$
$$\cup \left\{(7,j) \mid 1 \le j \le n-3-5\left\lfloor \frac{n-3}{6} \right\rfloor \right\}.$$

According to Vukičević, a tedious calculation shows that for these graphs, $\lim_{n\to\infty} \frac{\mathrm{Sz}_e(G_n)}{n^6} = \frac{3}{6^6}$. It was conjectured in [23] that the constant $\frac{3}{6^6}$ is maximal, i.e. for every sequence $\{F_n\}_{n\ge1}$ of graphs, where $F_n \in \mathcal{G}(n)$,

$$\limsup_{n\to\infty} \frac{\mathrm{Sz}_e(F_n)}{n^6} \le \frac{3}{6^6}.$$

In this section, we present an entire family of counterexamples for this conjecture by studying compositions of graphs.

Let us briefly define the composition of graphs: suppose G_1 and G_2 are graphs with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2, respectively. The composition $G = G_1[G_2]$ has vertex set $V(G_1[G_2]) = V_1 \times V_2$, and $u = (u_1, u_2)$ is adjacent to $v = (v_1, v_2)$ whenever

- u_1 is adjacent to v_1, or
- $u_1 = v_1$ and u_2 is adjacent with v_2,

see [11, p. 22]. Composition of graphs is generally not commutative, but it is associative. Moreover, the composition $G_1[G_2]$ of two graphs is connected if and only if G_1 is connected.

As shown in [15], if Q and F are arbitrary graphs, and if $ab \in E(Q)$, then for an edge $(a,u)(b,v) \in E(Q[F])$ in $Q[F]$ we have

$$\begin{aligned} n'_{(b,v)}((a,u))n'_{(a,u)}((b,v)) \ge& \\ &\Big((n_b(a)-1)|E(F)| + (n'_b(a) - \deg(a) + 1)|V(F)|^2\Big) \\ &\quad \cdot \Big((n_a(b)-1)|E(F)| + (n'_a(b) - \deg(b) + 1)|V(F)|^2\Big). \end{aligned}$$

Therefore,

$$\begin{aligned} \mathrm{Sz}_e(Q[F]) =& \sum_{u\in V(F)} \sum_{v\in V(F)} \sum_{ab\in E(Q)} n'_{(b,v)}((a,u))n'_{(a,u)}((b,v)) \\ &+ \sum_{a\in V(Q)} \sum_{uv\in E(F)} n'_{(b,v)}((a,u))n'_{(a,u)}((b,v)) \\ \ge& \sum_{u\in V(F)} \sum_{v\in V(F)} \sum_{ab\in E(Q)} \Big(\Big((n_b(a)-1)|E(F)| + (n'_b(a) - \deg(a) + 1)|V(F)|^2\Big) \end{aligned}$$

$$\cdot\Big((n_a(b)-1)|E(F)| + (n'_a(b)-\deg(b)+1)|V(F)|^2\Big)\Big).$$

We immediately obtain the following theorem:

Theorem 4.1 *Fix a graph $Q \in \mathcal{G}(p)$, and consider a sequence F_n of graphs such that $F_n \in \mathcal{G}(\lfloor \frac{n}{p} \rfloor)$ for all n. Suppose that either*

- *there is an edge $ab \in E(Q)$ such that $n'_b(a) - \deg(a) + 1 > 0$ and $n'_a(b) - \deg(b) + 1 > 0$, or*
- *there is an edge $ab \in E(Q)$ such that $n_b(a) > 1$ and $n_a(b) > 1$, and $|E(F_n)| \geq \frac{n^2}{\beta}$ for a fixed constant β.*

Then

$$\liminf_{n\to\infty} \frac{\mathrm{Sz}_e(Q[F_n])}{n^6} > 0.$$

Remark. We remark that the first condition is satisfied if Q contains an isometric cycle C_r with $r > 4$ or if $\operatorname{diam} Q > 4$. The second condition for Q is satisfied if Q contains an isometric cycle C_r with $r > 3$ or if $\operatorname{diam} Q \geq 3$.

In the following, we choose $Q = C_r$ for some integer r. Using the above inequality again, we obtain

Theorem 4.2 *For any sequence G_n of graphs with $G_n \in \mathcal{G}(\lfloor \frac{n}{r} \rfloor)$, we have*

$$\liminf_{n\to\infty} \frac{\mathrm{Sz}_e(C_r[G_n])}{n^6} \geq \begin{cases} \frac{(r-4)^2}{4r^5} & 2 \mid r, \\ \frac{(r-3)^2}{4r^5} & 2 \nmid r. \end{cases}$$

For $r = 5$, we obtain $\frac{1}{3125}$ as a lower bound, which already gives us a counterexample for Vukičević's conjecture [23], since $\frac{1}{3125} > \frac{3}{6^6} = \frac{1}{15552}$.

Furthermore, it is not difficult to show the following:

Theorem 4.3 *For $r > 3$, we have*

$$\lim_{n\to\infty} \frac{\mathrm{Sz}_e(C_r[K_{\lfloor \frac{n}{r} \rfloor}])}{n^6} = \begin{cases} \frac{(3r-10)^2}{16r^5} & 2 \mid r, \\ \frac{9(r-3)^2}{16r^5} & 2 \nmid r. \end{cases}$$

We note that the lower bound is larger than $\frac{3}{6^6}$ for $3 < r < 18$. Of course the question remains for which graphs in $\mathcal{G}(n)$ the maximum of Sz_e is attained, and how this maximum behaves for $n \to \infty$.

It is natural to ask similar questions for the edge Wiener index. In the following, we show that the maximal order of magnitude is n^5:

Theorem 4.4 *For any graph $G \in \mathcal{G}(n)$, the inequality $W_e(G) \leq \frac{n^5}{8}$ holds. On the other hand, there is a sequence of graphs H_n such that $H_n \in \mathcal{G}(n)$ and $\lim_{n\to\infty} \frac{W_e(H_n)}{n^5} > 0$.*

PROOF. Since G has at most $\binom{n}{2}$ edges, there are at most $\binom{\binom{n}{2}}{2} \leq \frac{n^4}{8}$ pairs of edges, and since all distances are $\leq n$, the inequality follows immediately. On the other hand, let H_n be constructed from two copies of $K_{\lfloor \frac{2n}{5} \rfloor}$ connected by a simple path of length $n - 2\lfloor \frac{2n}{5} \rfloor + 1$. Then it is not difficult to show that

$$\lim_{n\to\infty} \frac{W_e(H_n)}{n^5} = \frac{4}{3125} > 0,$$

which proves the theorem. □

5 Concluding Remarks

In this final section, we would like to present a conjecture and an open problem related to the results of this paper. First of all, we believe that the upper bound in Theorem 3.8 is only attained under stronger conditions than those we were able to prove:

Conjecture 5.1 *For a connected graph G, $\mathrm{Sz}(G) = \frac{|E(G)||V(G)|^2}{4}$ if and only if G is bipartite and regular.*

While Theorem 3.1 settles the problem of determining the minimum value of the edge Wiener index, the analogous question for the maximum is not as straightforward, and we leave this as in interesting open problem to consider:

Problem 5.2 *What is the maximum value of the edge Wiener index on $\mathcal{G}(n)$ and for which graph(s) is the maximum attained?*

Acknowledgment

The third author was in part supported by a grant from the Center of Excellence of Algebraic Methods and Applications of the Isfahan University of Technology.

References

[1] A. R. Ashrafi, B. Manoochehrian and H. Yousefi-Azari, On the PI polynomial of a graph, Util. Math., **71** (2006), 97–108.

[2] M. V. Diudea, I. Gutman and L. Jantschi, Molecular Topology, Huntington, NY, 2001.

[3] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math., **66**(2001), 211–249.

[4] A. A. Dobrynin and I. Gutman, Solving a problem connected with distances in graphs, Graph Theory Notes of New York, **28**(1995), 21–23.

[5] A. A. Dobrynin, I. Gutman and G. Domotor, A Wiener-type graph invariant for some bipartite graphs, Appl. Math. Lett., **8**(5)(1995), 57–62.

[6] A. A. Dobrynin, I. Gutman, S. Klavžar and P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math., **72**(2002), 247–294.

[7] R. C. Entringer, D. E. Jackson and D. A. Snyder, Distance in graphs. Czechoslovak Math. J., **26**(101) (1976), no. 2, 283–296.

[8] A. Graovac and T. Pisanski, On the Wiener index of a graph, J. Math. Chem. **8**(1991), 53–62.

[9] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes of New York, **27** (1994), 9–15.

[10] I. Gutman and A. R. Ashrafi, The edge version of the Szeged index, Croat. Chem. Acta (in press).

[11] W. Imrich and S. Klavžar, Product graphs: structure and recognition, John Wiley & Sons, New York, USA, 2000.

[12] P. V. Khadikar, On a Novel Structural Descriptor PI, Nat. Acad. Sci. Lett., **23**(2000), 113–118.

[13] M. H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi and I. Gutman, The edge Szeged index of product graphs, Croat. Chem. Acta **81**(2008) (in press).

[14] M. H. Khalifeh, H. Yousefi-Azari and A.R. Ashrafi, Vertex and Edge PI Indices of Cartesian Product Graphs, Disc. Appl. Math. (in press).

[15] M. H. Khalifeh, H. Yousefi-Azari and A.R. Ashrafi, A matrix method for computing Szeged and vertex PI indices of join and composition of graphs, Linear Algebra Appl. (in press).

[16] M. H. Khalifeh, H. Yousefi-Azari and A.R. Ashrafi, The hyper-Wiener index of graph operations, Computers and Mathematics with Applications (in press).

[17] M. H. Khalifeh, H. Yousefi-Azari and A.R. Ashrafi, The First and Second Zagreb Indices of some Graph Operations, Disc. Appl. Math. (in press).

[18] S. Klavžar, On the PI Index: PI-Partitions and Cartesian Product Graphs, MATCH Commun. Math. Comput. Chem., **57**(3)(2007), 573–586.

[19] S. Klavžar, A. Rajapakse and I. Gutman, The Szeged and the Wiener index of graphs, Appl. Math. Lett., **9**(1996), 45–49.

[20] M. Lepović and I. Gutman, A Collective Property of Trees and Chemical Trees, J. Chem. Inf. Comput. Sci., **38**(1998), 823-826.

[21] B. E. Sagan, Y. -N. Yeh and P. Zhang, The Wiener Polynomial of a Graph, Int. J. Quantum Chem., **60**(1996), 959–969.

[22] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL. 1992.

[23] D. Vukičević, Note on the graphs with the greatest edge-Szeged index, MATCH Commun. Math. Comput. Chem. (in press).

[24] S. G. Wagner, A class of trees and its Wiener index, Acta Appl. Math. **91** (2006), 119–132.

[25] H. Wang and G. Yu, All but 49 Numbers are Wiener Indices of Trees, Acta Appl Math **92** (2006), 15-20.

[26] H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc., **69**(1947), 17–20.

[27] H. Yousefi-Azari, B. Manoochehrian and A. R. Ashrafi, The PI index of product graphs, Appl. Math. Lett., **21**, 624–627.