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# A Survey on Graphs Extremal with Respect to Distance–Based Topological Indices

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## Abstract

This survey outlines results on graphs extremal with respect to distance–based indices, with emphasis on the Wiener index, hyper–Wiener index, Harary index, Wiener polarity index, reciprocal complementary Wiener index, and terminal Wiener index.

# 1 Introduction

Throughout this survey, the graphs considered will be assumed to be simple and connected. If $G = (V, E)$ is such a graph, then its vertex set is $V(G) = \{v_1, \dots, v_n\}$ and its edge set $E(G) = \{e_1, \dots, e_m\}$. This the number of vertices and edges of $G$ is denoted by $n$ and $m$, respectively.

The *distance* $d_G(u, v)$ (or simply $d(u, v)$ when no misunderstanding could occur) between the vertices $u$ and $v$ of $G$ is equal to the length of (number of edges in) a shortest path connecting $u$ and $v$. The number of vertex pairs of $G$, whose distance is $k$ is denoted by $d(G, k)$. Details on distance in graph theory can be found in the books [8, 15, 56], whereas on general distances in [29].

In the following we denote by $C_n$, $P_n$, $S_n$, and $K_n$ the cycle graph, the path graph, the star graph, and the complete graph of order $n$, respectively. Other undefined notation and terminology can be found in [5, 76].

The history of distance–based topological indices begins with year 1947, in which Harold Wiener [153] used the following formula to calculate the boiling point $t_B$ of alkanes:

$$t_B = a\,W(G) + b\,W_P(G) + c\ .$$

In this formula $a, b, c$ are constants for a given isomeric group, $W(G)$ is (in modern terminology, different from what Wiener originally used) equal to the sum of distances of all unordered vertex pairs in the molecular graph $G$, whereas $W_P(G)$ is the number of unordered vertex pairs at distance 3 in $G$, i.e., $d(G, 3)$. Initially, Wiener's ideas did not attract the attention of the chemical community, but as time passes, the quantity $W$ became one of the most popular molecular structure descriptors. It found numerous applications for designing quantitative structure–property relationships (QSPR) [28, 93]. Besides, it also was applied in crystallography, communication theory, facility location, cryptology, etc. [4, 73, 120]. Eventually, this graph invariant became known under the name *Wiener index* or *Wiener number*; for details see [129, 130].

Mathematicians started with the study of $W(G)$ almost three decades after chemists [43], initially without any knowledge of Wiener's earlier works. Anyway, also in contemporary mathematical literature $W(G)$ is usually referred to as the Wiener index [31, 32, 41, 53, 96, 134, 151]

Wiener himself named $W_P(G)$ *polarity number*, and this quantity is nowadays usually called the *Wiener polarity index* of $G$ [23–25, 37, 83, 100, 105, 106].

In the above specified notation, the Wiener index and the Wiener polarity index are defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) \tag{1}$$

$$W_P(G) = d(G,3)\ .$$

Note that the equation (1), explicitly using the graph–distance concept, was first given by Hosoya [81]. Wiener himself spoke of the number of carbon–carbon bonds separating two carbon atoms [153].

After the Wiener index was invented, a large number of other distance–based topological indices have been proposed and considered in the chemical and mathematico–chemical literature; for more information and additional references see [1, 30, 63, 64, 66, 67, 101, 107, 111, 112, 114, 116, 143, 144, 174]. All distance–based topological indices can be derived from the *distance matrix* or some closely related distance–based matrices; for more information on this matter see [12, 89–91, 116, 118, 127]. Much work has been devoted also to the eigenvalues of the distance and related matrices [16, 17, 139].

In this survey we shall restrict our considerations to only a few of distance–based topological indices, namely to the following:

- Wiener index $W$
- Wiener polarity index $W_P$
- hyper–Wiener index $WW$
- Harary index $H$
- reciprocal complementary Wiener index $RCW$
- terminal Wiener index $TW$

The **Wiener index and Wiener polarity index** were described above.

**Hyper–Wiener index**

In 1993, Milan Randić [126] introduced a distance–based quantity that he named hyper–Wiener index and denoted by $WW$. His definition could be applied only to trees, and was impossible to use for cycle–containing graphs. In 1995, Klein, Lukovits, and one of the present authors [95] showed that Randić's $WW$ (for trees) satisfies the identity

$$WW(G) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} \left[d_G(u,v) + d_G(u,v)^2\right] \tag{2}$$

which could be applied to all connected graphs. Since then, Eq. (2) is used as the definition of hyper–Wiener index.

**Harary index**

In 1993, Plavšić et al. [121] and Ivanciuc et al. [89] independently introduced the Harary index, named in honor of Frank Harary on the occasion of his 70th birthday. Actually, the Harary index was first defined in 1992 by Mihalić and Trinajstić [117] as:

$$H_{old}(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)^2} \ .$$

In spite of this, the Harary index is nowadays defined as [89, 121]:

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)} \ .$$

**Reciprocal complementary Wiener index**

In 2000, Ivanciuc et al. [88, 90] introduced the this topological index, defined it as:

$$RCW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d + 1 - d_G(u,v)}$$

where $d$ is the diameter of graph $G$ (i.e., the greatest distance between any two vertices).

**Terminal Wiener index**

The concept of terminal Wiener index was put forward by Petrović and two of the present authors [68]. Somewhat later, but independently, Székely, Wang, and Wu arrived at the same idea [140]. Let $V_1(G) \subset V(G)$ be the set of vertices of the graph $G$ whose degree is equal to one (the so-called pendent vertices or leaves). Then $TW$ is defined in full analogy with the Wiener index, Eq. (1), as

$$TW(G) = \sum_{\{u,v\} \subseteq V_1(G)} d_G(u,v) \ . \tag{3}$$

Thus, the terminal Wiener index consists of the sum of distances between pendent vertices. If the graph $G$ has no pendent vertex, or just one such vertex, then $TW(G) = 0$. The application of this molecular structure descriptor is purposeful mainly for graphs with many pendent vertices, especially trees [26, 27, 65, 78].

In Eq. (3) summation goes over pairs of vertices of degree 1. The terminal–Wiener–index concept was recently generalized [86] by considering pairs of vertices of some fixed degree $k > 1$.

Concluding this introductory section we remind that the distance–based topological indices $W$, $WW$, $H$, and $RCW$ can be expressed in terms of the numbers $d(G,k)$ of vertex pairs at distance $k$:

$$
\begin{aligned}
W(G) &= \sum_{k\geq 1} k\, d(G,k) \\
WW(G) &= \sum_{k\geq 1} \frac{k+k^2}{2}\, d(G,k) \\
H(G) &= \sum_{k\geq 1} \frac{1}{k}\, d(G,k) \\
RCW(G) &= \sum_{k\geq 1} \frac{1}{d+1-k}\, d(G,k)\ .
\end{aligned}
$$

In addition to this, as already mentioned, $W_P(G) = d(G,3)$.

* * * * *

In recent years, characterizing the extremal (maximal or minimal) graphs in a given set of graphs with respect to distance–based topological indices has become an important direction in chemical graph theory. Up to now, a number of nice results have been obtained along these lines. To our surprise, from a number of such results, we see that there exist close relations among the graphs extremal w.r.t. different distance–based topological indices. For some classes of graphs, the extremal graphs are identical. By collecting these extremal results and presenting them together, we hope to inspire the discovery of new results of this kind, as well as the elaboration of attractive and fundamental new proof techniques.

## 2 General graphs

In this section we report some extremal results with respect to the distance–based topological indices $W$, $WW$, $H$, $W_P$, and $RCW$ in different classes of general graphs.

Let $PK_{n,m}$ be the path–complete graph, obtained from the disjoint union of a path and a complete graph by the addition of edges between one end-vertex of the path and some, but not all, vertices of the complete graph.

**Theorem 2.1.** *Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then the following holds:*

(1) *The path–complete graph $PK_{n,m}$ is the unique graph with maximal Wiener index* [135] *(resp. diameter* [75]*). Any graph $G$ with diameter at most 2 has minimal Wiener index.*

(2) *If $G \ncong K_n$, then*

$$RCW(G) \leq \frac{n(n-1)}{2} - \frac{m}{2} .$$

*Equality holds if and only if the diameter of $G$ is 2* [172].

**Theorem 2.2.** ( [94]) *Let $a \geq 2$ be an positive integer and $G$ be any connected graph with $m$ edges where $\binom{a}{2} \leq m \leq \binom{a+1}{2}$. Then*

$$a(a+1) - m \leq W(G)$$

*with equality holding if and only if $G \cong G_0$, where $G_0$ is the graph obtained by deleting $\binom{a+1}{2} - m$ edges from the complete graph $K_{a+1}$ that are incident with a fixed vertex in it.*

Actually, in [43], the authors had also implicitly characterized the extremal graph maximizing the Wiener index among all connected graphs of order $n$ and with $m$ edges, which is just the result in Theorem 2.1 (1). Moreover, in [43] it was implicitly pointed out that the minimal Wiener index is attained at one connected graph in which any two distinct non-adjacent vertices have distance 2.

Denote by $G^{\circledast} = (V, E)$ a graph with diameter $d$ ($3 \leq d \leq 4$ and $|V(G^{\circledast})| \geq d+2$), such that for any two distinct vertices $u \in V(G^{\circledast}) \backslash V(P_{d+1})$ and $v \in V(G^{\circledast})$, $d_{G^{\circledast}}(u, v) = 1$ or 2, where $P_{d+1}$ is a path with $d+1$ vertices in $G^{\circledast}$. The two graphs depicted in Fig. 1 are of $G^{\circledast}$-type.

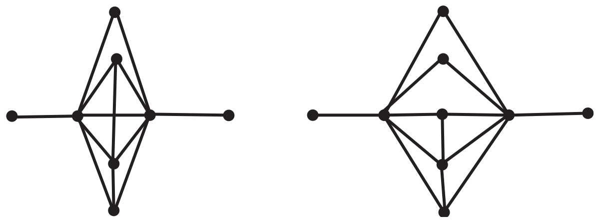

**Fig. 1.** Examples of graphs of $G^{\circledast}$-type.

**Theorem 2.3.** *Let $G$ be a connected graph with $n$ vertices, $m$ edges, and diameter $d$. Then*

(1) ([18]) $\frac{1}{6}(d-2)(d-1)d+n(n-1)-m \leq W(G) \leq \frac{1}{2}n(n-1)d-\frac{1}{3}(d-2)(d-1)d-(d-1)m$ *with the left equality holding if and only if $G$ is a graph with diameter $d \leq 2$, or $G \cong P_n$, or $G$ is isomorphic to some $G^{\circledast}$. The right equality holds if and only if $G$ is a graph with diameter $d \leq 2$ or $G \cong P_n$;*

(2) ([20]) $H(P_{d+1}) + \frac{n(n-1)+2(m-d)(d-1)}{2d} - \frac{d+1}{2} \leq H(G) \leq H(P_{d+1}) + \frac{n(n-1)+2m}{4} - \frac{d(d+3)}{4}$ *with the left equality holding if and only if $G$ is a graph with diameter $d \leq 2$ or $G \cong P_n$, and the right equality holding if and only if $G$ is a graph with diameter $d \leq 2$, or $G \cong P_n$, or $G$ is isomorphic to some $G^{\circledast}$.*

A connected graph $G$ is called a *cactus* if each block of $G$ is either an edge or a cycle. Denote by $Cat(n,t)$ the set of connected cacti possessing $n$ vertices and $t$ cycles. Let $C^0(n,t)$ be the cactus graph obtained from a star $S_n$ by adding $t$ independent edges between its leaves.

**Theorem 2.4.** *Among all graphs in $Cat(n,t)$, $C^0(n,t)$ is the unique graph having the minimal Wiener index* [102] *(resp. hyper–Wiener index* [51]*), and the maximal Harary index* [152].

Let $1 \leq k < n$ and $K_n^k$ be the graph obtained by attaching $k$ pendent vertices to one vertex of the complete graph $K_{n-k}$.

**Theorem 2.5.** *Among all connected graphs with $n$ vertices and $k$ cut edges, $K_n^k$ uniquely has the minimal Wiener index* [84,136,137,155] *(resp. hyper–Wiener index* [163]*) and the maximal Harary index* [163].

Note that the *kite graph* $K_{n,k}$ is obtained by identifying one vertex of $K_k$ with one pendent vertex of $P_{n-k+1}$ and the *Turán graph* $T_n(k)$ is a complete $k$-partite graph of order $n$ in which any two partition sets differ in size by at most one.

**Theorem 2.6.** *Among all connected graphs with $n$ vertices and clique number $k$,*

(1) *the Turán graph $T_n(k)$ uniquely has the minimal Wiener index* [50] *(resp. hyper–Wiener index* [50]*) and the maximal Harary index* [158];

(2) *the kite graph* $K_{n,k}$ *uniquely has the minimal Harary index* [158] *and the maximal Wiener index* [50] *(resp. hyper–Wiener index* [50]*).*

Moreover, in [12], the authors also determined some extremal bipartite graphs with respect to Harary index, that are all complete bipartite graphs. Hence these results can be viewed as special cases of Theorem 2.6 (1).

**Theorem 2.7.** *Among all connected graphs with* $n$ *vertices and chromatic number* $k$*,*

(1) *the Turán graph* $T_n(k)$ *uniquely has the minimal Wiener index* [50] *(resp. hyper–Wiener index* [50]*) and the maximal Harary index* [158]*;*

(2) *the kite graph* $K_{n,k}$ *uniquely has the maximal Wiener index* [50] *(resp. hyper–Wiener index* [50]*) and the minimal Harary index* [158].

The *broom* $B_{n,\Delta}$ is a tree obtained by attaching $\Delta - 1$ pendent vertices to one pendent vertex of the path $P_{n-\Delta+1}$.

**Theorem 2.8.** ( [138]) *For any connected graph* $G$ *with* $n$ *vertices and maximum degree* $\Delta$*, we have* $W(G) \leq W(B_{n,\Delta})$*, where the equality holds if and only if* $G \cong B_{n,\Delta}$*.*

The *dumbbell* $D(n, p, q)$ is a tree consisting of the path $P_{n-p-q}$ together with $p$ independent vertices adjacent to one pendent vertex of $P_{n-p-q}$ and $q$ independent vertices adjacent to the other pendent vertex of $P_{n-p-q}$. A *caterpillar* is a tree if by deleting all its pendent vertices it reduces to a path. Note that in the theory of benzenoid hydrocarbons, caterpillars are also called *Gutman trees* [39, 40, 58, 61, 82].

Suppose that $n \geq 2(a + b)$. Denote by $CP_n(a, b)$ a caterpillar obtained by attaching one pendent vertex to each of the first $a$ vertices in $P_{n-a-b}$ and one pendent vertex to each of the last $b$ vertices of $P_{n-a-b}$.

Recall that the average distance of a connected graph $G$ on $n$ vertices is defined as $\mu(G) = \binom{n}{2}^{-1} W(G)$. In [13, 14, 36], the extremal graph with maximal average distance are determined among all connected graphs with $n \geq 5$ vertices and matching number $\beta \geq 2$ and with domination number $\gamma$.

**Theorem 2.9.** ([13]) *If* $G$ *is a connected graph with* $n \geq 5$ *vertices and matching number* $\beta \geq 2$*, then*

$$\mu(G) \leq \mu\left(D\left(n, \lfloor (n+1)/2 - \beta \rfloor, \lceil (n+1)/2 - \beta \rceil\right)\right)$$

*with equality holding if and only if* $G \cong D(n, \lfloor (n+1)/2 - \beta \rfloor, \lceil (n+1)/2 - \beta \rceil)$*.*

**Theorem 2.10.** ([14]) *Let $G$ be any connected graph with $n$ vertices and domination number $\gamma$.*

(1) *If $\gamma \leq \frac{n}{3}$, then $\mu(G) \leq \mu(D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil))$ with equality holding if and only if $G \cong D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil)$.*

(2) *If $\gamma \geq \frac{n}{3}$, then $\mu(G) \leq \mu(CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor))$ with equality holding if and only if $G \cong CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor)$.*

If the order $n$ of the graph $G$ is fixed, then the extremal graph with respect to average distance is just the extremal one with respect to Wiener index, and vice versa. Therefore the following two corollaries can be deduced immediately from Theorems 2.9 and 2.10.

**Corollary 2.1.** *If $G$ is a connected graph with $n \geq 5$ vertices and matching number $\beta \geq 2$, then*

$$W(G) \leq W(D(n, \lfloor(n+1)/2 - \beta\rfloor, \lceil(n+1)/2 - \beta\rceil))$$

*with equality holding if and only if $G \cong D(n, \lfloor\frac{n+1}{2} - \beta\rfloor, \lceil\frac{n+1}{2} - \beta\rceil)$.*

**Corollary 2.2.** *Let $G$ be a connected graph of order $n$ with domination number $\gamma$.*

(1) *If $\gamma \leq \frac{n}{3}$, then $W(G) \leq W(D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil))$ with equality holding if and only if $G \cong D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil)$.*

(2) *If $\gamma \geq \frac{n}{3}$, then $W(G) \leq W(CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor))$ with equality holding if and only if $G \cong CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor)$.*

As usual, we denote by $\overline{G}$ the complement of the graph $G$. A graph $G$ is *self–complementary* if $G \cong \overline{G}$. It is well–known [5] that any self–complementary graph $G$ of order $n$ satisfies the condition $n \equiv 0$ *or* $1(mod\ 4)$. For $k \geq 1$, let $\mathcal{G}_{4k}$ be the set of all graphs whose structure is shown in Fig. 2, where $G_k$ is any graph of order $k$ and the double lines connecting two circled graphs indicate that all edges between them are present. In addition, let $\mathcal{G}_{4k+1}$ be the set of graphs obtained from a graph from $\mathcal{G}_{4k}$ by adding a new vertex adjacent to all vertices in the two copies of $G_k$ as indicated in Fig. 2. In [77], the self–complementary graphs with extremal average distance were determined. In view of the relation between Wiener index and average distance, we can obtain directly the following result.

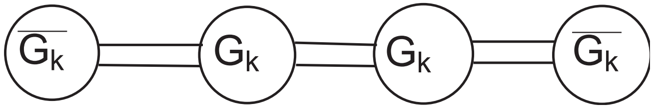


**Fig. 2.** The structure of the graphs belonging to the class $\mathcal{G}_{4k}$.

**Theorem 2.11.** ([77]) *Let $G$ be a self-complementary graph of order $n$.*

(1) *If $n \equiv 0(mod\ 4)$, then $\frac{3n(n-1)}{4} \leq W(G) \leq \frac{n(n-1)(13n-12)}{16n-16}$ with the left equality holding if and only if $G$ is a graph with diameter 2, and the right equality holding if and only if $G \in \mathcal{G}_{4k}$.*

(2) *If $n \equiv 1(mod\ 4)$, then $\frac{3n(n-1)}{4} \leq W(G) \leq \frac{n(n-1)(13n-1)}{16n}$ with the left equality holding if and only if $G$ is a graph with diameter 2, and the right equality holding if and only if $G \in \mathcal{G}_{4k+1}$.*

Recall that the circumference of a graph $G$ is the maximum length of any cycle in $G$. Denote by $C_k(\ell^1)$ the graph obtained by attaching a path of length $\ell$ to one vertex of cycle $C_k$. Let $n, \ell$ be two positive integers such that $(\ell-1) \mid (n-1)$. The graph $F^*_{n,\ell}$ is obtained by joining an isolated vertex $u$ to every vertices of $(n-1)/(\ell-1)$ copies of complete graphs $K_{\ell-1}$. In the following theorem, the extremal graphs with respect to Wiener index are characterized among all connected graphs with $n$ vertices and circumference $\ell$.

**Theorem 2.12.** ( [99]) *Let $G$ be a connected graph with $n$ vertices and circumference $\ell$.*

(1) *If $(\ell-1) \mid (n-1)$, then $W(G) \geq W(F^*_{n,\ell})$ with equality holding if and only if $G \cong F^*_{n,\ell}$.*

(2) *$W(G) \leq W(C_\ell((n-\ell)^1))$ with equality holding if and only if $G \cong C_\ell((n-\ell)^1)$.*

The well–known *Moore graph* is an $r$-regular graph with diameter $k$ whose order attains the upper bound

$$1 + r\sum_{i=0}^{k-1}(r-1)^i .$$

Hoffman and Singleton [79] proved that every $r$-regular Moore graph $G$ with diameter 2 must have $r \in \{2, 3, 7, 57\}$. They pointed out that $G \cong C_5$ if $r = 2$, $G$ is just Petersen graph for $r = 3$, whereas for $r = 7$, $G$ is the known under the name Hoffman–Singleton graph. For $r = 57$ it is not known whether such a graph does exist or not.

Recall that $M_1(G) = \sum_{v \in V(G)} d_G(v)^2$ is the well–known first Zagreb index of the graph $G$ (see [35, 62, 71, 72, 145]). In the following theorem we characterize the extremal connected triangle– and quadrangle–free graphs extremal with respect to Wiener index, hyper–Wiener index, and Harary index.

**Theorem 2.13.** *Let $G$ be a connected triangle– and quadrangle–free graph with $n$ vertices and $m$ edges. Then*

(1) ([173]) $\frac{3n(n-1)}{2} - \frac{1}{2} M_1(G) - m \leq W(G)$ *with equality holding if and only if $G$ is a graph of diameter $d \leq 3$;*

(2) ([171]) $3n(n-1) - \frac{3}{2} M_1(G) - 2m \leq WW(G)$ *with equality holding if and only if $G$ is a graph of diameter $d \leq 3$;*

(3) ([171]) $H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2}$ *with equality holding if and only if $G$ is a star or a Moore graph of diameter 2.*

Denote by $G_1 \vee G_2$ the *join* of two vertex disjoint graphs $G_1$ and $G_2$. Thus, $G_1 \vee G_2$ is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{v_1 v_2 : v_1 \in V(G_1), v_2 \in V(G_2)\}$.

By $\overline{G}$ we denote the complement of the graph $G$.

Obviously, either $G \cong C_3$ or $G \cong S_n$ holds for any connected graph $G$ with $n \geq 2$ vertices and matching number $\beta = 1$.

**Theorem 2.14.** ([45]) *Let $G$ be a connected graph with $n \geq 4$ vertices and matching number $\beta$, where $2 \leq \beta \leq \lfloor n/2 \rfloor$.*

(1) *If $\beta = \lfloor n/2 \rfloor$, then $WW(G) \geq WW(K_n)$ and $H(G) \leq H(K_n)$. Either equality holds if and only if $G \cong K_n$.*

(2) *If $2n/5 < \beta \leq \lfloor n/2 \rfloor - 1$, then $WW(G) \geq WW(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ and $H(G) \leq H(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$. Either equality holds if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.*

(3) *If $2 \leq \beta < 2n/5$, then $WW(G) \geq WW(K_\beta \vee \overline{K_{n-\beta}})$ and $H(G) \leq H(K_\beta \vee \overline{K_{n-\beta}})$. Either equality holds if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

(4) *If* $\beta = 2n/5$, *then* $WW(G) \geq WW(K_\beta \vee \overline{K_{n-\beta}}) = WW(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$ *and* $H(G) \leq H(K_\beta \vee \overline{K_{n-\beta}}) = H(K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}}))$. *Either equality holds if and only if* $G \cong K_\beta \vee \overline{K_{n-\beta}}$ *or* $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

**Theorem 2.15.** *Let* $G$ *be a connected graph with* $n$ *vertices and (edge)-connectivity* $k$, *where* $1 \leq k \leq n-1$. *Then,*

(1) ([74, 150]) $W(G) \geq W(K_k \vee (K_1 \cup K_{n-k-1}))$, *with equality holding if and only if* $G \cong K_k \vee (K_1 \cup K_{n-k-1})$;

(2) ([2]) $WW(G) \geq WW(K_k \vee (K_1 \cup K_{n-k-1}))$, *with equality holding if and only if* $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

By the definitions of the Wiener, hyper–Wiener, and Harary indices, one can easily see that any edge addition will decrease the Wiener index and the hyper–Wiener index, and will increase the Harary index. In other words:

**Proposition 2.1.** *Let* $G$ *be a connected graph with* $e \notin E(G)$. *Then,* $W(G) > W(G+e)$, $WW(G) > WW(G+e)$, *and* $H(G) < H(G+e)$.

Proposition 2.1 directly implies:

**Theorem 2.16.** *Let* $G$ *be a connected graph of order* $n$. *Then,*

(1) $W(G) \geq W(K_n)$, *where the equality holds if and only if* $G \cong K_n$;

(2) $WW(G) \geq WW(K_n)$, *where the equality holds if and only if* $G \cong K_n$;

(3) ([171]) $H(G) \leq H(K_n)$, *where the equality holds if and only if* $G \cong K_n$;

(4) ([172]) $RCW(G) \leq RCW(K_n)$, *where the equality holds if and only if* $G \cong K_n$.

Denote by $\mathcal{S}(K_n - ie)$ the set of graphs obtained by deleting $i$ edges from $K_n$. Clearly, $\mathcal{S}(K_n - 0e) = \{K_n\}$. The next theorem determines the first to $(k+1)$-th smallest Wiener and hyper–Wiener indices of graphs of order $n > 2k$.

**Theorem 2.17.** ([109]) *Suppose that* $n > 2k$. *For* $i = 0, 1, \ldots, k$, *the* $i$*-th smallest Wiener (resp. hyper–Wiener) indices of connected graphs of order* $n$ *are the graphs from* $\mathcal{S}(K_n - ie)$.

By the definition of Wiener polarity index, it easily follows:

**Theorem 2.18.** ([105]) *Let* $G$ *be a connected graph of order* $n$. *Then,* $W_P(G) \geq 0$, *where the equality holds if and only if the diameter of* $G$ *is less than 3.*

# 3 Trees

In this section, we outline some extremal results for the six distance–based topological indices $W$, $WW$, $H$, $W_P$, $RCW$, and $TW$, pertaining to trees.

**Theorem 3.1.** *Let $T$ be a tree of order $n$. Then,*

(1) ([43, 59, 69, 124]) $W(S_n) \leq W(T) \leq W(P_n)$, *with left (resp. right ) equality holding if and only if $T \cong S_n$ (resp. $T \cong P_n$) ;*

(2) ([59, 69]) $WW(S_n) \leq WW(T) \leq WW(P_n)$, *with left (resp. right ) equality holding if and only if $T \cong S_n$ (resp. $T \cong P_n$) ;*

(3) ([59, 157]) $H(P_n) \leq H(T) \leq H(S_n)$, *with left (resp. right ) equality holding if and only if $T \cong P_n$ (resp. $T \cong S_n$) ;*

(4) ([172]) $RCW(P_n) \leq RCW(T) \leq RCW(S_n)$, *with left (resp. right ) equality holding if and only if $T \cong P_n$ (resp. $T \cong S_n$).*

By Proposition 2.1, among all connected graphs, the extremal graphs with maximal Wiener and hyper–Wiener index, and with minimal Harary index must be a tree. Thus, by Theorem 3.1 we have:

**Corollary 3.1.** *Let $G$ be a connected graph of order $n$.*

(1) ([43]) $W(G) \leq W(P_n)$, *where the equality holds if and only if $G \cong P_n$ .*

(2) $WW(G) \leq WW(P_n)$, *where the equality holds if and only if $G \cong P_n$ .*

(3) ([171]) $H(G) \geq H(P_n)$ , *where the equality holds if and only if $G \cong P_n$ .*

(4) ([172]) $RCW(G) \geq RCW(P_n)$ , *where the equality holds if and only if $G \cong P_n$ .*

A tree of order $n$ is said to be a *bi-star* if it is obtained by attaching $n_1$ pendent vertices to one leaf of $P_2$ and $n_2$ pendent vertices to the other leaf of $P_2$ , where $n_1 + n_2 = n - 2$. This bi-star is denoted by $BS(n_1, n_2)$. Denote by $T^*(k_1, k_2, k_3, \ell_1, \ldots, \ell_m)$ a special tree with diameter 4 as shown in Fig. 3. Consider the set $\mathcal{T}^*$ of such trees

$$\mathcal{T}^* = \Big\{ T^*(k_1, k_2, k_3, \ell_1, \ldots, \ell_m) \Big\} \tag{4}$$

for which the conditions

$$k_1 + k_2 + k_3 + \sum_{i=1}^{m} \ell_i = n - m - 5$$

and

$$m + k_2 + 1 = \left\lfloor \frac{n-2}{2} \right\rfloor \quad \text{or} \quad \left\lceil \frac{n-2}{2} \right\rceil$$

are satisfied.

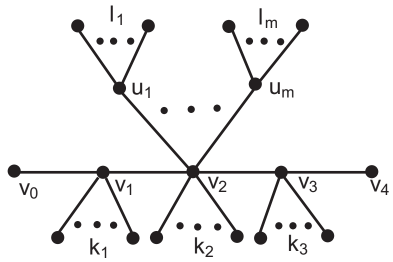


**Fig. 3.** The tree $T^*(k_1, k_2, k_3, \ell_1, \ldots, \ell_m)$ from Eq. (4) and Theorems 3.2, 3.9.

**Theorem 3.2.** ([37]) *Let $T$ be a tree of order $n$. Then*

$$0 \le W_P(T) \le \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$$

*where the left equality holds if and only if $T \cong S_n$ and the right equality holds if and only if $T$ is either a bi-star $BS(\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$ or a tree in the set $\mathcal{T}^*$.*

Although until the present moment a generally accepted measure of branching does not exist, there are several properties that any proposed measure has to satisfy [3, 52, 70, 115, 125, 128, 131, 146, 147]. Basically, a topological index ($TI$) acceptable as a measure of branching must satisfy the inequalities

$$TI(S_n) < TI(T) < TI(P_n) \quad \text{or} \quad TI(P_n) < TI(T) < TI(S_n)$$

for any tree $T$ of order $n \ge 5$ different from $S_n$ and $P_n$. From Theorem 3.1, we find that the four indices $W$, $WW$, $H$ and $RCW$ satisfy the basic requirement to be branching measures. On the other hand, Theorem 3.2 implies that $W_P$ is not a branching index.

Taking Theorem 3.1 into consideration, we naturally ask: *Which trees have the extremal distance–based topological indices among the trees of order* $n$ *different from* $S_n$ *and* $P_n$ *?*

In order to approach this problem, we first introduce some necessary notations and definitions.

A vertex $v$ of a tree $T$ is called a *branching point* if $d(v) \geq 3$. Let $T_n(n_1, n_2, \dots, n_m)$ be the tree of order $n$ obtained by inserting, respectively, $n_1 - 1, \dots, n_m - 1$ vertices into the $m$ edges of the star $S_{m+1}$, where $n_1 + \cdots + n_m = n - 1$.

Assume that $T$ is a tree of order $n$ with exactly two branching points $v_1$ and $v_2$ with $d(v_1) = r$ and $d(v_2) = t$. The orders of $r-1$ components, which are paths, of $T - v_1$ are $p_1, \dots, p_{r-1}$, the order of the component which is not a path of $T - v_1$ is $p_r = n - p_1 - \cdots - p_{r-1} - 1$. The orders of $t-1$ components, which are paths, of $T - v_2$ are $q_1, \dots, q_{t-1}$, the order of the component which is not a path of $T - v_2$ is $q_t = n - q_1 - \cdots - q_{t-1} - 1$. We denote this tree by $T = T_n(p_1, \dots, p_{r-1}; q_1, \dots, q_{t-1})$, where $r \leq t$, $p_1 \geq \cdots \geq p_{r-1}$ and $q_1 \geq \cdots \geq q_{t-1}$.

For convenience, when considering the trees

$$T_n(n_1, n_2, \dots, n_k, \dots, n_m) \quad \text{or} \quad T_n(p_1, \dots, p_k, \dots, p_{r-1}\,;\, q_1, \dots, q_k, \dots, q_{t-1})$$

we use the symbols $n_k^{\ell_k}$ or $p_k^{\ell_k}$ (resp. $q_k^{\ell_k}$) to indicate that the number of $n_k$ or $p_k$ (resp. $q_k$) is $\ell_k > 1$ in the following. For example, $T_{16}(2,2,3,3,5)$ will be written as $T_{16}(2^2, 3^2, 5^1)$.

Let $T_2, T_3, \dots, T_8$ be the trees of order $n \geq 14$ depicted in Fig. 4, and $T_D$ the tree depicted in Fig. 5.

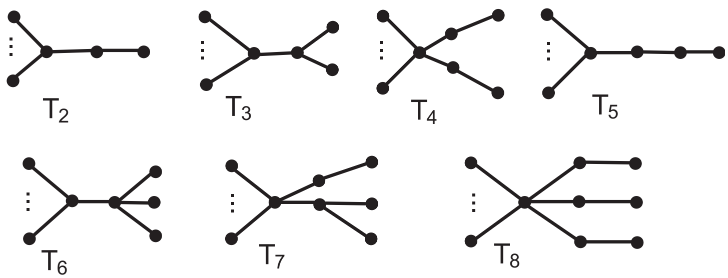


**Fig. 4.** The trees $T_2, T_3, \dots, T_8$ encountered in Theorems 3.3 and 3.4.

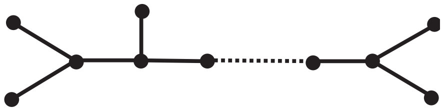

**Fig. 5.** The tree $T_D$ encountered in Theorem 3.3 .

The following two theorems present trees extremal with respect to $W$, $WW$, $H$, and $RCW$ among the trees of order $n$ different from $S_n$ and $P_n$. These results may be viewed as a extensions of Theorem 3.1.

**Theorem 3.3.** (1) ([22, 108]) *Suppose that $T$ is a tree of order $n \geq 28$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} W(P_n) &> W(T_n(n-3,1^2)) > W(T_n(n-4,2,1)) > W(T_n(1^2;1^2)) \\ &> W(T_n(n-5,3,1)) > W(T_n(n-4,1^3)) > W(T_n(1^2;2,1)) \\ &> W(T_n(n-6,4,1)) > W(T_n(n-5,2^2)) > W(T_n(1^2;n-5,1)) \\ &> W(T_n(1^2;3,1)) > W(T_n(2,1;2,1)) > W(T_n(1^2;1^3)) \\ &> W(T_n(n-7,5,1)) > W(T_n(1^2;n-6,1)) > W(T_n(1^2;4,1)) \\ &> W(T_n(n-5,2,1^2)) > W(T_n(1^2;2^2)) > W(T_n(2,1;3,1)) \\ &> W(T_D) > W(T)\ . \end{aligned}$$

(2) ([104]) *Suppose that $T$ is a tree of order $n \geq 20$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} WW(P_n) &> WW(T_n(n-3,1^2)) > WW(T_n(n-4,2,1)) > WW(T_n(1^2;1^2)) \\ &> WW(T_n(n-5,3,1)) > WW(T_n(n-4,1^3)) > WW(T_n(1^2;2,1)) \\ &> WW(T_n(n-6,4,1)) > WW(T_n(n-5,2^2)) > WW(T_n(1^2;n-5,1)) \\ &> WW(T_n(1^2;3,1)) > WW(T_n(2,1;2,1)) > WW(T_n(1^2;1^3)) \\ &> WW(T_n(n-7,5,1)) > WW(T_n(1^2;n-6,1))) > WW(T)\ . \end{aligned}$$

(3) ([157]) *Suppose that $T$ is a tree of order $n \geq 16$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} H(P_n) &< H(T_n(n-3,1^2)) < H(T_n(n-4,2,1)) < H(T_n(1^2;1^2)) \\ &< H(T_n(n-5,3,1)) < H(T_n(1^2;2,1)) < H(T_n(n-4,1^3)) < H(T)\ . \end{aligned}$$

(4) ([9]) *Suppose that $T$ is a tree of order $n \geq 7$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} RCW(P_n) &< RCW(T_n(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor, 1)) \\ &< RCW(T_n(\lceil n/2 \rceil, \lfloor (n-4)/2 \rfloor, 1)) < RCW(T) \ . \end{aligned}$$

**Theorem 3.4.** (1) ([33, 57, 110]) *Suppose that $T$ is a tree of order $n \geq 24$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} W(T) &> W(T_5) > W(T_8) = W(T_7) > W(T_6) > W(T_4) \\ &> W(T_3) > W(T_2) > W(S_n) \ . \end{aligned}$$

(2) ([104]) *Suppose that $T$ is a tree of order $n \geq 18$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} WW(T) &> WW(T_5) > WW(T_8) > WW(T_7) > WW(T_6) > WW(T_4) \\ &> WW(T_3) > WW(T_2) > WW(S_n) \ . \end{aligned}$$

(3) ([157]) *Suppose that $T$ is a tree of order $n \geq 14$, different from those occurring in the below inequalities. Then,*

$$\begin{aligned} H(T) &< H(T_8) < H(T_7) < H(T_6) < H(T_5) < H(T_4) \\ &< H(T_3) < H(T_2) < H(S_n) \ . \end{aligned}$$

Recall that a chemical tree is a tree with maximum degree not greater than 4. By Theorem 3.3, we find that the extremal trees with greatest Wiener and hyper–Wiener indices, and the ones with smallest Harary and reciprocal complementary Wiener indices are chemical trees. Recently, Deng [23] determined the maximal values for Wiener polarity index in the class of chemical trees, but, disappointedly, he did not characterize the corresponding extremal chemical tree(s).

**Theorem 3.5.** ([105]) *Let $T$ be a tree of order $n$ different from $S_n$. Then, $W_P(T) \geq W_P(D(n, n-k-b, b))$, where the equality holds if and only if $T \cong D(n, n-k-b, b)$ with $k \geq 3$ and $n-k \geq b \geq 0$.*

In the subsequent two theorems we assume that $n-1 = kq + r$ with $0 \leq r < k$, that is, $q = \lfloor n/k \rfloor$. Then, obviously, $n-1 = k\lfloor n/k \rfloor + r = (k-r)\lfloor n/k \rfloor + r\lceil n/k \rceil$.

**Theorem 3.6.** ([7, 42, 133]) *Let $T$ be a tree with $n$ vertices and $k$ pendent vertices, where $2 \le k \le n-2$. Then,*

$$W\left(T_n\left(\left\lceil\frac{n}{k}\right\rceil^r, \left\lfloor\frac{n}{k}\right\rfloor^{k-r}\right)\right) \le W(T) \le W\left(D\left(n, \lfloor k/2\rfloor, \lceil k/2\rceil\right)\right)$$

*with the left equality holding if and only if $T \cong T_n(\lceil n/k\rceil^r, \lfloor n/k\rfloor^{k-r})$ and the right equality holding if and only if $T \cong D(n, \lfloor k/2\rfloor, \lceil k/2\rceil)$.*

**Theorem 3.7.** *Let $T$ be a tree with $n$ vertices and $k$ pendent vertices, where $2 \le k \le n-2$.*

(1) ([168]) $WW(T_n(\lceil n/k\rceil^r, \lfloor n/k\rfloor^{k-r})) \le WW(T)$, *with equality holding if and only if $T \cong T_n(\lceil n/k\rceil^r, \lfloor n/k\rfloor^{k-r})$.*

(2) ([87]) $H(T) \le H(T_n(\lceil n/k\rceil^r, \lfloor n/k\rfloor^{k-r}))$, *with equality holding if and only if $T \cong T_n(\lceil n/k\rceil^r, \lfloor n/k\rfloor^{k-r})$.*

**Theorem 3.8.** ([123]) *Suppose that $T$ is a tree with $n$ vertices and $k$ pendent vertices where $3 \le k \le n-2$. Then*

$$RCW(T) \ge RCW\left(T_n\left(\left\lceil\frac{n-k+1}{2}\right\rceil, \left\lfloor\frac{n-k+1}{2}\right\rfloor, 1^{k-2}\right)\right)$$

*with equality if and only if $T \cong T_n(\lceil\frac{n-k+1}{2}\rceil, \lfloor\frac{n-k+1}{2}\rfloor, 1^{k-2})$.*

**Theorem 3.9.** ([24]) *Suppose that $T$ is a tree with $n$ vertices and $k$ pendent vertices, where $3 \le k \le n-2$.*

(1) *If $\lceil n/2\rceil \le k \le n-2$, then $W_P(T) \le \lceil\frac{n-2}{2}\rceil\lfloor\frac{n-2}{2}\rfloor$ with equality holding if and only if $T$ is either a bi-star $BS(\lceil\frac{n-2}{2}\rceil, \lfloor\frac{n-2}{2}\rfloor)$ or a tree in the set $\mathcal{T}^*$.*

(2) *If $3 \le k < \lceil n/2\rceil$, then $W_P(T) \le k^2 - 3k + n - 1$ with equality holding if and only if $T$ is a starlike tree in which the lengths of all pendent chains are at least 2.*

Combining Proposition 2.1 and Corollaries 2.1 and 2.2, we naturally arrive at the following two corollaries.

**Corollary 3.2.** *If $T$ is a tree with $n \ge 5$ vertices and matching number $\beta \ge 2$, then*

$$W(T) \le W\left(D\left(n, \left\lfloor\frac{n+1}{2} - \beta\right\rfloor, \left\lceil\frac{n+1}{2} - \beta\right\rceil\right)\right)$$

*with equality holding if and only if $T \cong D(n, \lfloor\frac{n+1}{2} - \beta\rfloor, \lceil\frac{n+1}{2} - \beta\rceil)$.*

**Corollary 3.3.** *Let $T$ be a tree with $n$ vertices and domination number $\gamma$.*

(1) *If $\gamma \leq \frac{n}{3}$, then $W(T) \leq W(D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil))$ with equality holding if and only if $T \cong D(n, \lfloor\frac{n+2-3\gamma}{2}\rfloor, \lceil\frac{n+2-3\gamma}{2}\rceil)$.*

(2) *If $\gamma \geq \frac{n}{3}$, then $W(T) \leq W(CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor))$ with equality holding if and only if $T \cong CP_n(\lceil\frac{3\gamma-n}{2}\rceil, \lfloor\frac{3\gamma-n}{2}\rfloor)$.*

Let $A_{n,\beta}$ be the tree obtained by attaching a pendent vertex to each of $\beta-1$ noncentral vertices of the star $S_{n-\beta+1}$. Clearly, the matching number of $A_{n,\beta}$ is $\beta$, and there is exactly one tree with $n$ vertices and matching number $\beta = 1$, which is just the star $S_n$. Recently, the minimal Wiener and hyper–Wiener indices and the maximal Harary index in the class of trees with $n$ vertices and matching number $\beta \geq 2$ were determined.

**Theorem 3.10.** *Let $T$ be a tree with $n$ vertices and matching number $2 \leq \beta \leq \lfloor n/2\rfloor$.*

(1) ([38]) *$W(A_{n,\beta}) \leq W(T)$, where the equality holds if and only if $T \cong A_{n,\beta}$.*

(2) ([168]) *$WW(A_{n,\beta}) \leq WW(T)$, where the equality holds if and only if $T \cong A_{n,\beta}$.*

(3) ([19, 87]) *$H(T) \leq H(A_{n,\beta})$, where the equality holds if and only if $T \cong A_{n,\beta}$.*

For a bipartite graph $G$ of order $n$ with matching number $\beta$ and independence number $\alpha$, it is well known that $\alpha + \beta = n$ (see, e.g., [5, 76]). Therefore the following corollary can be easily obtained from Theorem 3.10.

**Corollary 3.4.** ([19, 87, 168]) *Let $T$ be a tree with $n$ vertices and independence number $\alpha$. Then,*

(1) *$W(A_{n,n-\alpha}) \leq W(T)$, with equality holding if and only if $T \cong A_{n,n-\alpha}$;*

(2) *$WW(A_{n,n-\alpha}) \leq WW(T)$, with equality holding if and only if $T \cong A_{n,n-\alpha}$;*

(3) *$H(T) \leq H(A_{n,n-\alpha})$, with equality holding if and only if $T \cong A_{n,n-\alpha}$.*

As the following two results show, the extremal reciprocal complementary Wiener index in the class of trees with $n$ vertices and matching number $\beta$ (resp. independence number $\alpha$) appears to have a much more complex structure.

**Theorem 3.11.** ([123]) *Let $T$ be a tree with $n$ vertices and matching number $\beta \geq 2$.*

(1) *If $\beta = \lfloor n/2 \rfloor$, then $RCW(T) \geq RCW(P_n)$, with equality if and only if $T \cong P_n$;*

(2) *If $\beta \leq \lfloor n/2 \rfloor - 1$ and $\beta$ is odd, then $RCW(T) \geq RCW(T_n(\beta^2, 1^{n-2\beta-1}))$, with equality if and only if $T \cong T_n(\beta^2, 1^{n-2\beta-1})$.*

(3) *If $\beta \leq \lfloor n/2 \rfloor - 1$ and $\beta$ is even, then $RCW(T) \geq RCW(T_n(\beta+1, \beta-1, 1^{n-2\beta-1}))$, with equality if and only if $T \cong T_n(\beta+1, \beta-1, 1^{n-2\beta-1})$.*

**Corollary 3.5.** *Let $T$ be a tree with $n$ vertices and independence number $\alpha$.*

(1) *If $\alpha = \lceil n/2 \rceil$, then $RCW(T) \geq RCW(P_n)$, with equality if and only if $T \cong P_n$;*

(2) *If $\alpha \geq \lceil n/2 \rceil + 1$ and $n - \alpha$ is odd, then $RCW(T) \geq RCW(T_n((n-\alpha)^2, 1^{2\alpha-n-1}))$, with equality if and only if $T \cong T_n((n-\alpha)^2, 1^{2\alpha-n-1})$;*

(3) *If $\alpha \geq \lceil n/2 \rceil + 1$ and $n - \alpha$ is even, then $RCW(T) \geq RCW(T_n(n-\alpha+1, n-\alpha-1, 1^{2\alpha-n-1}))$, with equality if and only if $T \cong T_n(n-\alpha+1, n-\alpha-1, 1^{2\alpha-n-1})$.*

For $2 \leq \Delta \leq n-1$, the *Volkmann tree* $V_{n,\Delta}$ is defined as follows [52, 53, 97]:
If $n = \Delta + 1$, then $V_{n,\Delta}$ is just a star of order $n$.
For $n > \Delta + 1$, define $n_i$ as

$$n_i = 1 + \sum_{j=1}^{i} \Delta(\Delta-1)^j$$

for $i = 1, 2, \ldots$, and choose $k$ such that $n_{k-1} < n \leq n_k$.
Then, calculate the parameters $m$ and $h$ so that

$$m = \frac{n - n_{k-1}}{\Delta - 1} \qquad \text{and} \qquad h = n - n_{k-1} - (\Delta-1)m\ .$$

The vertices of $V_{n,\Delta}$ are arranged into $k+1$ levels. In level 0, there is only one vertex labeled as $v_{0,1}$. In level $i$ for $i = 1, 2, \ldots, k-1$, there are $\Delta(\Delta-1)^i$ vertices labeled as $v_{i,1}, v_{i,2}, \ldots, v_{i,\Delta(\Delta-1)^i}$. These are connected (in that order) to the vertices in level $i$, so that $\Delta - 1$ vertices from level $i$ are adjacent to each vertex from level $i-1$. At level $k$ there are $n - n_{k-1}$ vertices, labeled as $v_{k,1}, v_{k,2}, \ldots, v_{k,n-n_{k-1}}$. They are connected (in that order) to the vertices in level $k-1$, so that $\Delta - 1$ vertices from level $k$ are adjacent to vertices $v_{k-1,1}, v_{k-1,1}, \ldots, v_{k-1,m}$. The remaining $h$ vertices at level $k$ (if any) are connected to the vertex $v_{k-1,m+1}$ in level $k-1$.

In Fig. 6 we illustrate the structure of the Volkmann trees $V_{n,\Delta}$ by the example with $n = 22$ and $\Delta = 4$.

**Theorem 3.12.** ([53,92,97]) *Let $T$ be a tree with $n$ vertices and maximum degree at most $\Delta \geq 3$. Then*

$$W(V_{n,\Delta}) \leq W(T) \leq W(P_n)$$

*with the left equality holding if and only if $T \cong V_{n,\Delta}$ and the right equality holding if and only if $T \cong P_n$ .*

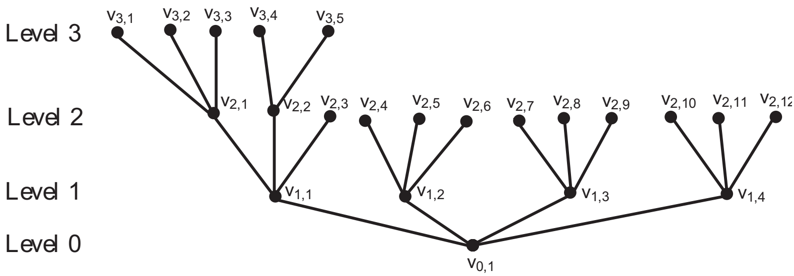


**Fig. 6.** The Volkmann tree $V_{22,4}$ with its vertices labeled.

Which are the extremal trees of order $n$ with respect to the indices $W$, $WW$, $H$, and $RCW$ is the maximum degree $\Delta$ is fixed? In the following theorem, we will give a partial answer to this question.

Recall that $B_{n,\Delta}$ is a broom as defined in Section 2.

**Theorem 3.13.** *Let $T$ be a tree with $n$ vertices and maximum degree $\Delta \geq 3$. Then*

(1) ([32]) $W(T) \leq W(B_{n,\Delta})$, *with equality holding if and only if $T \cong B_{n,\Delta}$ .*

(2) ([168]) $WW(T) \leq WW(B_{n,\Delta})$, *with equality holding if and only if $T \cong B_{n,\Delta}$ .*

(3) ([87, 149]) $H(B_{n,\Delta}) \leq H(T) \leq H(V_{n,\Delta})$, *with the left equality holding if and only if $T \cong B_{n,\Delta}$, and the right equality holding if and only if $T \cong V_{n,\Delta}$ .*

(4) ([123]) $RCW(T) \geq RCW(T_n(\lceil \frac{n-\Delta+1}{2} \rceil, \lfloor \frac{n-\Delta+1}{2} \rfloor, 1^{\Delta-2}))$, *with equality holding if and only if $T \cong T_n(\lceil \frac{n-\Delta+1}{2} \rceil, \lfloor \frac{n-\Delta+1}{2} \rfloor, 1^{\Delta-2})$.*

Define the following auxiliary sets:

$$V^{(\Delta)}(T) = \{v \in V(T) \mid d_T(v) = \Delta\} \qquad \text{and} \qquad N^{(\Delta)}(T) = \bigcup_{u \in V^{(\Delta)}(T)} N_T(u)$$

where $N_T(u)$ denotes the set of first neighbors of the vertex $u$ in the graph $T$.

Let $h = n - (\Delta + 1)$ and $T_0 = S_{\Delta+1}$. Let $T_i$ be a tree obtained from $T_{i-1}$ by attaching a pendent vertex to one vertex of $N^{(\Delta)}(T_{i-1}) \setminus V^{(\Delta)}(T_{i-1})$, where $i = 1, 2, \ldots, h$. Then we can construct a tree $T_h$ after $h$ steps, and the set of all $T_h$'s is denoted by $\mathcal{T}^{\Delta}$.

**Theorem 3.14.** ([100]) *Let $T$ be a tree with $n$ vertices and maximum degree $\Delta$, where $3 \leq \Delta \leq n-3$. Then,*

$$W_P(D(n, \Delta-1, \ell)) \leq W_P(T) \leq W_P(T^{\Delta})$$

*with the right equality holding if and only if $T \cong T^{\Delta} \in \mathcal{T}^{\Delta}$ and the left equality holding if and only if $T \cong D(n, \Delta-1, \ell)$, where $0 \leq \ell \leq \min\{\Delta-1, n-\Delta-2\}$.*

Let $C_{n,d}$ be the tree obtained from a path $P_{d+1} = v_0 v_1 \ldots v_d$, by attaching $n-d-1$ pendent vertices to the vertex $v_{\lfloor d/2 \rfloor}$.

**Theorem 3.15.** *Let $T$ be a tree with $n$ vertices and diameter $d$, where $3 \leq d \leq n-2$. Then*

(1) ([103, 154]) *$W(C_{n,d}) \leq W(T)$, with equality holding if and only if $T \cong C_{n,d}$;*

(2) ([48, 168]) *$WW(C_{n,d}) \leq WW(T)$, with equality holding if and only if $T \cong C_{n,d}$;*

(3) ([87]) *$H(T) \leq H(C_{n,d})$, with equality holding if and only if $T \cong C_{n,d}$;*

(4) ([9]) *$RCW(T) \geq RCW(C_{n,d})$, with equality holding if and only if $T \cong C_{n,d}$.*

Note that, in [19], some extremal trees with respect to Harary index are characterized in terms of order $n$, diameter $d$, first Zagreb index $M_1$, and second Zagreb index $M_2$.

By Theorem 3.2, the extremal tree maximizing the Wiener polarity index in the class of trees with $n$ vertices and diameter 3 or 4 is determined. The following theorem characterizes the trees with maximal Wiener polarity index when the diameter is greater than 4.

Denote by $CT_n(k_1, k_2, \ldots, k_{d-1})$ the tree (a caterpillar) of order $n$ obtained by attaching $k_i$ pendent vertices to the vertex $v_i$ of $P_{d+1} = v_0 v_1 \ldots v_d$ for $i = 1, 2, \ldots, d-1$.

**Theorem 3.16.** ([25]) *Let $T$ be a tree with $n$ vertices and diameter $d$.*

(1) *If $d \geq 3$, then $W_P(T^{(0)}) \leq W_P(T)$, with equality if and only if $T \cong T^{(0)}$, where $T^{(0)} \cong D(n,r,t)$ with $r+t = n-d+1$ $(t \geq r \geq 1)$ for $d \geq 4$ and $T^{(0)} \cong B_{n,n-3}$ for $d = 3$.*

(2) *If $d \geq 5$, then $W_P(T) \leq W_P(CT_n(0,0,\ldots,0,k_i,k_{i+1},k_{i+2},0,\ldots,0,0))$, with equality if and only if $T \cong CT_n(0,0,\ldots,0,k_i,k_{i+1},k_{i+2},0,\ldots,0,0)$, where $1 \leq i \leq d-5$ and $k_{i+1} = \lfloor \frac{n-d-1}{2} \rfloor$ or $\lceil \frac{n-d-1}{2} \rceil$.*

The following theorems present the minimal Wiener and reciprocal complementary Wiener indices among non-caterpillars with $n$ vertices and diameter $d$, where $4 \leq d \leq n-3$.

**Theorem 3.17.** ([113]) *Let $T$ be a non-caterpillar tree with $n$ vertices and diameter $d$, where $4 \leq d \leq n-3$. Then, $W(T_n(\lceil \frac{d}{2} \rceil, \lfloor \frac{d}{2} \rfloor, 2, 1^{n-d-3})) < W(T)$.*

**Theorem 3.18.** ([123]) *Let $T$ be a non-caterpillar tree of order $n \geq 7$. Then,*

$$RCW\left(T_n\left(\left\lceil \frac{n-3}{2} \right\rceil, \left\lfloor \frac{n-3}{2} \right\rfloor, 2\right)\right) \leq RCW(T)\ .$$

The *degree sequence* of a tree is the sequence of the degrees (in non-increasing order) of its vertices. Suppose that the degrees of non-leaf vertices are given, the so-called *greedy tree* is formed by the following “greedy algorithm” [134, 151]:

($i$) Label the vertex with the greatest degree by $v$ (the root).

($ii$) Label the neighbors of $v$ by $v_1, v_2, \ldots$, such that $d(v_1) \geq d(v_2) \geq \cdots$.

($iii$) Label the neighbors of $v_1$ (except $v$) by $v_{11}$, $v_{12}, \ldots$ such that they take all the greatest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \cdots$. Then do the same for $v_2, v_3, \ldots$.

($iv$) Repeat ($iii$) for all the newly labeled vertices, always starting with the neighbors of the labeled vertex with greatest degree whose neighbors are not yet labeled.

As an example, in Fig. 7 is depicted the greedy tree with degree sequence $\pi = (4,4,3,3,3,3,2,2,1,1,1,1,1,1,1,1,1,1)$.

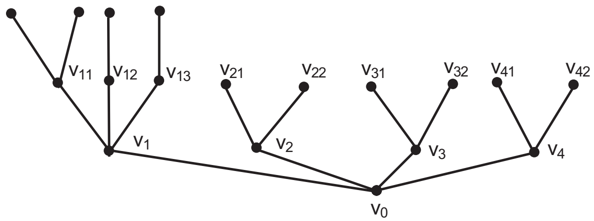


**Fig. 7.** A greedy tree.

If $T$ is a caterpillar obtained from the path $P = v_1 v_2 \dots v_k$ by attaching $y_i$ $(y_i \geq 1)$ pendent vertices to the vertex $v_i$ , $i \in \{1, k\}$ and attaching $y_j - 1$ $(y_i \geq 1)$ pendent vertices to $v_j$ for $j \in \{2, \dots, k-1\}$, then we denote the resultant tree by $T(y_1, y_2, \dots, y_k)$ [169]. Clearly, the degree sequence of $T(y_1, y_2, \dots, y_k)$ is

$$\pi = (y_1 + 1, y_2 + 1, \dots, y_k + 1, 1, \dots, 1) \; .$$

For example, the caterpillar $T(5, 3, 2, 1)$ is depicted in Fig. 8. Its degree sequence is $\pi = (6, 4, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1)$.

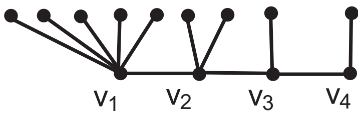


**Fig. 8.** The caterpillar $T(5, 3, 2, 1)$.

**Theorem 3.19.** *Given the degree sequence and the number of vertices, the greedy tree minimizes the Wiener index* ([134, 151, 170]) *and also maximizes the Harary index* ([149]). *In addition, the same greedy tree maximizes the Wiener polarity index* ([106]).

Let $\mathbb{T}_{n,\pi,p}$ be the class of trees on $n$ vertices and $p$ leaves, with degree sequence $\pi = (d_1, d_2, \dots, d_n)$, where $d_1 \geq d_2 \geq \cdots \geq d_n$ .

**Theorem 3.20.** ([169]) *Let $T$ be the tree with maximum Wiener index in $\mathbb{T}_{n,\pi,n-5}$ .*

(1) *If $d_1 > d_2 + d_3$, then $T \cong T(d_1 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$.*

(2) *If $d_1 = d_2 + d_3$, then either $T \cong T(d_1 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$ or $T \cong T(d_1 - 1, d_4 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$.*

(3) *If* $d_1 < d_2 + d_3$, *then* $T \cong T(d_1 - 1, d_4 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$.

**Theorem 3.21.** ([169]) *Let* $T$ *be the tree with maximum Wiener index in* $\mathbb{T}_{n,\pi,n-6}$ .

(1) *If* $d_1 > d_2 + d_3 + d_4 - 2$, *then* $T \cong T(d_1 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$.

(2) *If* $d_1 = d_2 + d_3 + d_4 - 2$, *then either* $T \cong T(d_1 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$ *or* $T \cong T(d_1 - 1, d_5 - 1, d_6 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$.

(3) *If* $d_2 + d_3 - 1 < d_1 < d_2 + d_3 + d_4 - 2$, *then* $T \cong T(d_1 - 1, d_5 - 1, d_6 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$.

(4) *If* $d_2 + d_3 - 1 = d_1$, *then either* $T \cong T(d_1 - 1, d_5 - 1, d_6 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$ *or* $T \cong T(d_1 - 1, d_4 - 1, d_6 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$.

(5) *If* $\max\{d_2 + d_3 - d_4, d_2 + \frac{1}{3}(d_5 - d_6)\} < d_1 < d_2 + d_3 - 1$, *then* $T \cong T(d_1 - 1, d_4 - 1, d_6 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$.

(6) *If* $d_1 = d_2 + d_3 - d_4 > d_2 + \frac{1}{3}(d_5 - d_6)$, *then either* $T \cong T(d_1 - 1, d_4 - 1, d_6 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$ *or* $T \cong T(d_1 - 1, d_4 - 1, d_5 - 1, d_6 - 1, d_3 - 1, d_2 - 1)$.

(7) *If* $d_1 = d_2 + \frac{1}{3}(d_5 - d_6) > d_2 + d_3 - d_4$, *then either* $T \cong T(d_1 - 1, d_4 - 1, d_6 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$ *or* $T \cong T(d_1 - 1, d_3 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_2 - 1)$.

(8) *If* $d_1 = d_2 + d_3 - d_4 = d_2 + \frac{1}{3}(d_5 - d_6)$, *then* $T \in \{T(d_1 - 1, d_4 - 1, d_6 - 1, d_5 - 1, d_3 - 1, d_2 - 1), T(d_1 - 1, d_4 - 1, d_5 - 1, d_6 - 1, d_3 - 1, d_2 - 1), T(d_1 - 1, d_3 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_2 - 1)\}$.

(9) *If* $d_2 + \frac{1}{3}(d_5 - d_6) \leq d_1 < d_2 + d_3 - d_4$ *or* $d_1 \leq d_2 + \frac{1}{3}(d_5 - d_6) < d_2 + d_3 - d_4$, *then* $T \cong T(d_1 - 1, d_4 - 1, d_5 - 1, d_6 - 1, d_3 - 1, d_2 - 1)$.

(10) *If* $d_2 + d_3 - d_4 \leq d_1 < d_2 + \frac{1}{3}(d_5 - d_6)$ *or* $d_1 \leq d_2 + d_3 - d_4 < d_2 + \frac{1}{3}(d_5 - d_6)$, *then* $T \cong T(d_1 - 1, d_3 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_2 - 1)$.

(11) *If* $d_1 < d_2 + \frac{1}{3}(d_5 - d_6) = d_2 + d_3 - d_4$, *then either* $T \cong T(d_1 - 1, d_3 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_2 - 1)$ *or* $T \cong T(d_1 - 1, d_4 - 1, d_5 - 1, d_6 - 1, d_3 - 1, d_2 - 1)$.

Although the extremal trees with maximal Wiener index are determined in $\mathbb{T}_{n,\pi,p}$ when $p$ is large enough, as pointed out in [169], the problem of characterizing the trees maximizing the Wiener index in $\mathbb{T}_{n,\pi,p}$ for any $p$ is still open. For the newest results on this matter see [132].

Let $\mathcal{T}_m^{(4)}$ be the set of trees with $m$ edges and diameter 4. Denote by $S_m^{(t)}(c_1, c_2, \ldots, c_k)$ the tree with $m$ edges obtained by attaching $c_1 - 1, c_2 - 1, \ldots, c_t - 1$ pendent vertices to $t$ leaves of the star $S_{t+1}$; for an example see Fig. 9. From [148], we know that any tree from $\mathcal{T}_m^{(4)}$ must be of the form $S_m^{(t)}(c_1, c_2, \ldots, c_k)$.

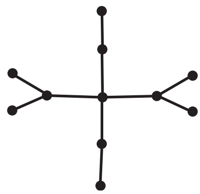

**Fig. 9.** The tree $S_{10}^{(4)}(3, 3, 2, 2)$.

**Theorem 3.22.** ([148]) *Let $T$ be a tree from $\mathcal{T}_m^{(4)}$. Then*

$$W(T) \leq W(S_m^{(t)}(k, \ldots, k, k+1, \ldots, k+1))$$

*with equality holding if and only if $T \cong S_m^{(t)}(k, \ldots, k, k+1, \ldots, k+1)$ where $k = \lfloor \sqrt{m} \rfloor$. In the tree $S_m^{(t)}(k, \ldots, k, k+1, \ldots, k+1)$, $t = k$, the term $k$ appears $k^2 + k - m$ times and the term $k+1$ appears $m - k^2$ times provided $k^2 + k > m$. If $t = k+1$, then the term $k$ appears $k^2 + 2k + 1 - m$ times and the term $k+1$ appears $m - k^2 - k$ times.*

We end this section by outlying extremal results on the terminal Wiener index $TW$, defined via Eq. (3).

In the introductory part, we already pointed out that is reasonably to investigate $TW$ only for graphs possessing two or more pendent vertices. Therefore, to date, results on extremal values of $TW$ are established only for trees. All results that are presented below have been published in [68].

The proofs of all theorems on $TW$ presented here are based on the following lemma:

**Lemma 3.1.** [68] *Let $T$ be an $n$-vertex tree with $k$ pendent vertices. Let $e$ be an edge of $T$. Denoting by $p_1(e)$ and $p_2(e)$ the numbers of pendent vertices of $T$, lying of the two sides of $e$, the terminal Wiener index can be calculated as*

$$TW(T) = \sum_e p_1(e) \cdot p_2(e)$$

*with summation going over all edges of $T$.*

**Theorem 3.23.** *Let $T$ be an $n$-vertex tree. Then, $TW(T) \geq n-1$. Equality is attained if and only if $T \cong P_n$ .*

A tree is said to be *starlike* if it possesses a single vertex of degree greater than two. If the degree of this vertex is $d \geq 3$, then the respective tree is referred to as *starlike of degree $d$*.

**Theorem 3.24.** *Among $n$-vertex trees with a fixed number $k$ of pendent vertices, $k \geq 3$ , the starlike trees of degree $k$ possess minimal $TW$ equal to $(n-1)(k-1)$ .*

The problem of characterizing trees with maximal $TW$ values is more complex than in the case of trees with minimal $TW$. Nonetheless, this problem has been completely solved in [68].

**Theorem 3.25.** *Let $T$ be an $n$-vertex tree with a fixed number $k$ of pendent vertices, $k \geq 4$ . The trees whose all non–pendent edges ($e'$) satisfy the condition $p_1(e') \cdot p_2(e') = \lfloor k/2 \rfloor \lceil k/2 \rceil$ have maximal $TW$. The terminal Wiener index of these trees is equal to*

$$TW = k(k-1) + (n-1-k) \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil .$$

The characterization of trees possessing maximal $TW$ among all trees is given by the following theorem:

**Theorem 3.26.** *Within the class of $n$-vertex trees, the trees having maximal $TW$ obey to one of the following conditions:*

(1) *If $3 \leq n \leq 9$ , then the star $S_n$ has the maximal terminal Wiener index, equal to $(n-1)(n-2)$ .*

(2) *If $n = 3s$ , where $s \geq 4$ , then the tree with $k = 2s+2$ pendent vertices has maximal terminal Wiener index, equal to $s^3 + 3s^2 + s - 1$ . This tree is unique.*

(3) *If $n = 3s+1$, where $s \geq 3$ , then the trees with $k = 2s+2$ and $k = 2s = 3$ pendent vertices have maximal terminal Wiener indices, equal to $s^3 + 4s^2 + 3s$ . There are $\lceil s/2 \rceil$ distinct trees of this kind.*

(4) *If $n = 3s+2$, where $s \geq 3$ , then the trees with $k = 2s+3$ pendent vertices have maximal terminal Wiener indices, equal to $s^3 + 5s^2 + 6s + 2$ . There are $\lceil (s-1)/2 \rceil$ distinct trees of this kind.*

The trees described in Theorems 3.25 and 3.26 can be constructed as follows:

**(a)** If the number of pendent vertices ($k$) is even and $4 \leq k \leq n-1$, then the unique tree with maximal $TW$ is obtained from the path $P_{n-k}$ by attaching to each of its terminal vertices $k/2$ new pendent vertices.

**(b)** If the number of pendent vertices ($k$) is odd and $5 \leq k \leq n-1$, then the tree with maximal $TW$ is obtained from the path $P_{n-k}$ by attaching to each of its terminal vertices $(k-1)/2$ new pendent vertices, and by attaching one more pendent vertex to some vertex of $P_{n-k}$. There exist $\lceil (n-k)/2 \rceil$ distinct trees of this kind.

**(c)** If the number of pendent vertices $k = n-1$, then the tree with maximal $TW$ is the star $S_n$.

Recently Lin [98] considered trees in which all vertices have odd degrees, and determined the species with smallest and greatest Wiener index. The trees of this kind, with the first few smallest and first few greatest Wiener indices have also been determined [54,55]. Connected graphs in which all vertices have even degrees (which, of course, are not trees) are said to be Eulerian. Eulerian graphs extremal with respect to the Wiener index were characterized in [60].

More results on trees with extremal Wiener and terminal Wiener indices [11], and Harary indices [164] were also recently communicated.

# 4 Unicyclic and bicyclic graphs

In this section we report some extremal results for the distance–based topological indices, with restriction to unicyclic or bicyclic graphs.

Recall that a unicyclic graph is a connected graph with $n$ vertices and $n$ edges, and a bicyclic graph is a connected graph with $n$ vertices and $n+1$ edges. If $n = 3$, then there is exactly one unicyclic graph, i.e., $C_3$. If $n = 4$, there is precisely one bicyclic graph, obtained by deleting one edge from $K_4$. Thus, we only need to consider unicyclic graphs of order $n \geq 4$ and bicyclic graphs of order $n \geq 5$.

In order to characterize the unicyclic graphs extremal w.r.t. the distance–based topological indices, we first introduce some necessary notations.

Denote by $C_k(n_1^{\ell_1}, n_2^{\ell_2}, \ldots, n_m^{\ell_m})$ the unicyclic graph obtained by attaching $\ell_1$ paths of length $n_1$, $\ell_2$ paths of length $n_2, \ldots, \ell_m$ paths of length $n_k$, respectively, to one vertex of $C_k$, where $n_1 > n_2 > \cdots > n_m$. Note that the graph $C_k(\ell^1)$, defined in Section 2, is a special case of $C_k(n_1^{\ell_1}, n_2^{\ell_2}, \ldots, n_m^{\ell_m})$. For example, the graph $C_5(4^1, 3^2, 2^2)$ is shown in Fig. 10.

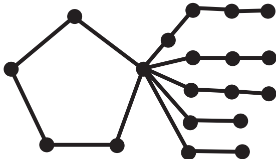

**Fig. 10.** The graph $C_5(4^1, 3^2, 2^2)$.

There are exactly two unicyclic graphs of order 4, namely $C_4$ and $C_3(1^1)$. We have $W(C_4) = W(C_3(1^1))$, $WW(C_4) = WW(C_3(1^1))$, $RCW(C_4) = RCW(C_3(1^1))$, $H(C_4) = H(C_3(1^1))$, and $W_P(C_4) = W_P(C_3(1^1)) = 0$.

**Theorem 4.1.** *Let $G$ be a unicyclic graph of order $n \geq 5$.*

(1) ([141, 167]) $W(C_3(1^{n-3})) \leq W(G) \leq W(C_3((n-3)^1))$, *where the left equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n = 5$, and the right equality holds if and only if $G \cong C_3((n-3)^1)$.*

(2) ([46, 156]) $WW(C_3(1^{n-3})) \leq WW(G) \leq WW(C_3((n-3)^1))$, *where the left equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n = 5$, and the right equality holds if and only if $G \cong C_3((n-3)^1)$.*

(3) ([160]) $H(C_3((n-3)^1)) \leq H(G) \leq H(C_3(1^{n-3}))$, *where the left equality holds if and only if $G \cong C_3((n-3)^1)$, and the right equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n = 5$.*

From Theorem 2.1 (2), we easily deduce the following:

**Corollary 4.1.** *Let $G$ be a unicyclic or bicyclic graph. Then, $RCW(G)$ attains its maximal value if and only if the diameter of $G$ is 2.*

This corollary further implies:

**Theorem 4.2.** *Let $G$ be a unicyclic graph of order $n \geq 5$. Then,*

$$RCW(G) \leq RCW(C_3(1^{n-3}))$$

*where the equality holds if and only if $G \cong C_3(1^{n-3})$ for $n \geq 6$ and $G \cong C_3(1^{n-3})$ or $G \cong C_5$ for $n = 5$.*

Let $C_k^{(s)}(p^1, q^1)$ be the unicyclic graph obtained by attaching two paths of lengths $p$ and $q$, respectively, to two vertices of $C_k$ whose distance is $s$ , $s \leq \lfloor k/2 \rfloor$.

**Theorem 4.3.** ([9]) *Let $G$ be a unicyclic graph of order $n \geq 7$. Then*

$$RCW\left(C_4^{(2)}\left(\lceil (n-4)/2 \rceil^1, \lfloor (n-4)/2 \rfloor^1\right)\right) \leq RCW(G)$$

*with equality holding if and only if $G \cong C_4^{(2)}\left(\lceil (n-4)/2 \rceil^1, \lfloor (n-4)/2 \rfloor^1\right)$.*

A unicyclic graph is said to be a *cycle–caterpillar* if by deleting all its pendent vertices it reduces it to a cycle [159]. Denote by $U_g$ a cycle–caterpillar obtained by attaching $k_1 > 0$, $k_2 = \lceil (n-g)/2 \rceil$ or $\lfloor (n-g)/2 \rfloor$, and $k_3 > 0$ pendent vertices to three consecutive vertices $v_1$, $v_2$ and $v_3$ of $C_g$ with $g \geq 4$. Let $U_3$ be a cycle–caterpillar obtained by attaching $k_i$ pendent vertices to the vertex $v_i$ (where $i = 1, 2, 3$) of the cycle $C_3 = v_1 v_2 v_3 v_1$ with $|k_i - k_j| \leq 1$ for $i, j \in \{1, 2, 3\}$.

Let $S_{i,t-k}$ be the unicyclic graph of order $t-k+i$ obtained by attaching $t-k$ pendent vertices to one pendent vertex of $C_3(1^{i-3})$, where $i \geq 4$ and $t-k \geq 1$. Let $S_{i,n-k,k-i}$ be the unicyclic graph of $n$ obtained by attaching $k-i \geq 1$ pendent vertices to a pendent vertex of $S_{i,n-k}$ which is at distance 2 to the vertex of $C_3(1^{i-3})$ with maximum degree. See Fig. 11 for two illustrative examples.

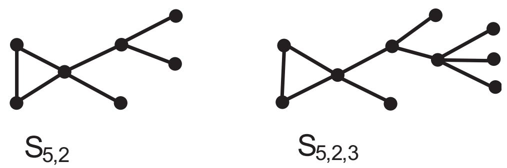


**Fig. 11.** Examples of graphs $S_{i,t-k}$ and $S_{i,n-k,k-i}$ .

Denote by $S_3(1^{n-4}, 1^1)$ the unicyclic graph obtained by attaching $n-4$ pendent vertices to one vertex of $C_3$ and one pendent vertex to another vertex of $C_3$.

As pointed out in [105], the minimal Winer polarity index of unicyclic graphs on $n$ vertices is attained by $C_3(1^{n-3})$ or $C_4$ or $C_5$ . In the following two theorems, we present the extremal unicyclic graphs with the greatest and second smallest Wiener polarity indices among unicyclic graphs of order $n$.

**Theorem 4.4.** ([83]) *Let $G$ be the unicyclic graph with the maximal Wiener polarity index in the class of unicyclic graphs of order $n \geq 5$.*

(1) *If $n = 5$, then $G \cong S_{4,1}$.*

(2) *If $n = 6$, then $G \cong S_{4,2}$.*

(3) *If $n = 7$, then $G \cong U_7$.*

(4) *If $n = 8$, then $G \in \{U_7, S_{5,3}, S_{4,3,1}\}$.*

(5) *If $n = 9$, then $G \in \{U_7, U_5, U_3, S_{4,3,2}, S_{5,3,1}, S_{4,4,1}, S_{6,3}, S_{5,4}\}$.*

(6) *If $n = 10$, then $G \in \{U_5, U_3, S_{4,4,2}, S_{5,4,1}, S_{6,4}\}$.*

(7) *If $n = 11$, then $G \cong U_5$ or $G \cong U_3$.*

(8) *If $n \geq 12$, then $G \cong U_3$.*

**Theorem 4.5.** ([105]) *Let $G$ be a unicyclic graph with minimal Wiener polarity index among unicyclic graphs of order $n \geq 5$, different from $C_3(1^{n-3})$ and $C_5$. Then $G$ is either in the set $\{S_3(1^{n-4}, 1^1), C_4(1^{n-4}), C_5(1^1)\}$ or is $C_4(1^t, 0, 1^{n-4-t}, 0)$ with $1 \leq t \leq \lfloor n/2 \rfloor - 2$, where $C_4(1^t, 0, 1^{n-4-t}, 0)$ is a cycle–caterpillar obtained by attaching $t$ pendent vertices to a vertex $v$ of $C_4$ and $n-4-t$ pendent vertices to another vertex of $C_4$ not adjacent to $v$.*

In the subsequent theorem, the unicyclic graph with the second smallest reciprocal complementary Wiener index among all the unicyclic graphs of order $n \geq 7$ is characterized.

**Theorem 4.6.** ([9]) *Let $G$ be a unicyclic graph of order $n \geq 7$, different from $C_4^{(2)}(\lceil \frac{n-4}{2} \rceil^1, \lfloor \frac{n-4}{2} \rfloor^1)$.*

(1) *If $n$ is odd and $n \leq 11$, then $RCW(C_3^{(1)}(\lceil \frac{n-3}{2} \rceil^1, \lfloor \frac{n-3}{2} \rfloor^1)) \leq RCW(G)$, with equality holding if and only if $G \cong C_3^{(1)}(\lceil \frac{n-3}{2} \rceil^1, \lfloor \frac{n-3}{2} \rfloor^1)$.*

(2) *If $n$ is even or $n \geq 13$, then $RCW(C_4^{(2)}(\lceil \frac{n-2}{2} \rceil^1, \lfloor \frac{n-6}{2} \rfloor^1)) \leq RCW(G)$, with equality holding if and only if $G \cong C_4^{(2)}(\lceil \frac{n-2}{2} \rceil^1, \lfloor \frac{n-6}{2} \rfloor^1)$.*

For $2 \leq \beta \leq \lfloor n/2 \rfloor$, we denote by $U_{n,m}$ the unicyclic graph obtained by attaching $n - 2m + 1$ pendent edges and $m - 2$ pendent paths of length 2 to one vertex of $C_3$, see Fig. 12.

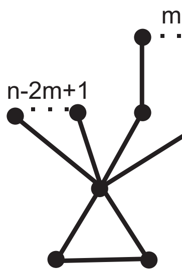


**Fig. 12.** The graph $U(n,m)$.

There is exactly one unicyclic graph with $n$ vertices and matching number $\beta = 1$, which is $C_3$. In the following, we describe the unicyclic graphs extremal with respect to Wiener, hyper–Wiener, and Harary indices among unicyclic graphs with $n$ vertices and matching number $\beta \geq 2$.

**Theorem 4.7.** *Let $G$ be a unicyclic graph with $n \geq 9$ vertices and matching number $\beta$.*

(1) ([38]) *If $\beta \geq 2$, then $W(U_{n,\beta}) \leq W(G)$, with equality holding if and only if $G \cong U_{n,\beta}$.*

(2) ([44]) *If $\beta \geq 2$, then $WW(U_{n,\beta}) \leq WW(G)$, with equality holding if and only if $G \cong U_{n,\beta}$.*

(3) ([161]) *If $\beta \geq 3$, then $H(G) \leq H(U_{n,\beta})$, with equality holding if and only if $G \cong U_{n,\beta}$.*

Let $B'_{n,\Delta}$ be the graph obtained by adding a new edge between two pendent vertices of the broom $B_{n,\Delta}$. In the next theorem the graph with maximal Wiener index in the class of unicyclic graphs of order $n$ and with maximum degree $\Delta$ is completely determined. If $\Delta = 2$, then there is only one unicyclic graph, which is just $C_n$. Therefore, we may assume that $3 \leq \Delta \leq n-1$.

**Theorem 4.8.** ([34]) *Let $G$ be a graph with $n$ vertices and maximum degree $\Delta$, $3 \leq \Delta \leq n-1$. Then*

$$W(G) \leq W(B'_{n,\Delta})$$

*with equality holding if and only if $G \cong B'_{n,\Delta}$.*

Denote by $\mathcal{U}_{n,g}$ the set of unicyclic graphs with $n$ vertices and girth $g$. Let $C_g^{(1)}(1^1, 1^{n-g-1})$ be a graph obtained by attaching $n-g-1$ pendent vertices and a single pendent vertex to two adjacent vertices of $C_g$. For $3 \le g \le n-3$, let $C_g^*((n-g)^1)$ be the graph obtained by attaching a pendent vertex to the unique neighbor of the pendent vertex of $C_g((n-g-1)^1)$.

**Theorem 4.9.** ([167]) *Let $G \in \mathcal{U}_{n,g}$ with $n \ge 6$ and $3 \le g \le n-2$. Then*

$$W(C_g(1^{n-g})) \le W(G) \le W(C_g((n-g)^1))$$

*where the left equality holds if and only if $G \cong C_g(1^{n-g})$, and the right equality holds if and only if $G \cong C_g((n-g)^1)$.*

**Theorem 4.10.** ([47]) *Let $G \in \mathcal{U}_{n,g} \setminus \{C_g(1^{n-g}), C_g((n-g)^1)\}$ with $n \ge 13$ and $3 \le g \le n-2$. Then the following holds:*

(1) *$W(G) \le W(G_1^*)$ with equality holding if and only if $G \cong G_1^*$ where*

$$G_1^* \cong C_g^{(\lfloor g/2 \rfloor)}(1^1, (n-g-1)^1) \qquad \text{and} \qquad G_1^* \cong C_g^*((n-g)^1)$$

*for $g \in \{3, 4, n-3, n-2\}$ and $5 \le g \le n-4$, respectively.*

(2) *$W(C_g^{(1)}(1^1, 1^{n-g-1})) \le W(G)$ with equality if and only if $G \cong C_g^{(1)}(1^1, 1^{n-g-1})$.*

**Corollary 4.2.** ([47]) *Let $G_0$ and $G_1$ be the unicylic graphs with minimal Wiener index and with maximal Wiener index, respectively, among all unicyclic graphs of order $n \ge 7$ different from $C_3(1^{n-3})$ and $C_3((n-3)^1)$. Then*

(1) *$G_0 \cong C_4(1^{n-4})$ or $G_0 \cong C_3^{(1)}(1^1, 1^{n-4})$;*

(2) *$G_1 \cong C_4((n-4)^1)$ or $G_1 \cong C_3^{(1)}(1^1, (n-4)^1)$.*

Note that the result in Corollary 4.2 has been independently obtained also in [141].

Let $U_{n,g}(k)$ be the element of $\mathcal{U}_{n,g}$, obtained by attaching $k$ paths of almost equal lengths to one vertex of $C_g$. Let, in addition, $U_{n,g}^*(k)$ be the graph in $\mathcal{U}_{n,g}$ obtained by attaching $k$ paths of almost equal lengths $q_1, q_2, \ldots, q_k$ to only one pendent vertex of $U_{g+q_0,g}(1)$ with $q_i - q_0 - g \le 1$ for $i = 1, 2, \ldots, k$. Recall that $A_{n,\beta}$ is the same graph as defined before.

If $g$ is odd, let $C_{n,g}^*(\beta)$ be the graph in $\mathcal{U}_{n,g}$ obtained by identifying a vertex of a cycle $C_g$ of odd order $g$ with the vertex of $A_{n-g+1,\beta-\frac{g-1}{2}}$ of degree $n-\beta-\frac{g-1}{2}$. When $g$ is even, let $C_{n,g}^*(\beta)$ be the graph in $\mathcal{U}_{n,g}$ obtained by identifying the vertex $u_1$ in a cycle $C_g = u_1u_2u_3\ldots u_gu_1$ of even order $g$ with the vertex of $A_{n-g,\beta-\frac{g}{2}}$ of degree $n-\beta-\frac{g}{2}$, and by attaching a pendent vertex to the vertex $u_2$ in $C_g$.

**Theorem 4.11.** ([80]) *Let $3 \leq g \leq n-1$ and $G$ be a graph in $\mathcal{U}_{n,g}$ with $k$ pendent vertices.*

(1) *If $1 \leq k \leq n-3$ and $g > \lfloor (n-g)/k \rfloor$, then $W(G) \geq W(U_{n,g}(k))$, with equality holding if and only if $G \cong U_{n,g}(k)$.*

(2) *If $2 \leq k \leq n-3$ and $g \leq \lfloor (n-g)/k \rfloor$ ; $n-g \neq 0(mod\ k)$, then $W(G) \geq W(U^*_{n,g}(k))$, with equality holding if and only if $G \cong U^*_{n,g}(k)$.*

(3) *If $2 \leq k \leq n-3$ and $n = (k+1)g$, then $W(G) \geq W(U_{n,g}(k)) = W(U^*_{n,g}(k))$, with equality holding if and only if $G \cong U_{n,g}(k)$ or $G \cong U^*_{n,g}(k)$.*

**Theorem 4.12.** ([10]) *Let $3 \leq g \leq n-1$ and $G$ be a graph in $\mathcal{U}_{n,g}$ with matching number $\beta \geq 3g/2$. Then*

$$W(G) \geq W(C^*_{n,g}(\beta))$$

*with equality holding if and only if $G \cong C^*_{n,g}(\beta)$.*

Further results on extremal Wiener indices of unicyclic graphs can be found in [60,119].

Let $\mathcal{B}(n)$ be the set of bicyclic graphs of order $n$. The structure of cycles in $G \in \mathcal{B}(n)$ can be divided into the following three cases (see [162]):

(I) The two cycles $C_p$ and $C_q$ in $G$ have only one common vertex $v$.

(II) The two cycles $C_p$ and $C_q$ in $G$ are linked by a path of length $\ell > 0$.

(III) The two cycles $C_{\ell+k}$ and $C_{\ell+m}$ in $G$ have a common path of length $\ell > 0$.

The bicyclic graphs $C_{p,q}$ , $C_{p,\ell,q}$ , and $\theta_{k,\ell,m}$ (where $1 \leq \ell \leq min\{k,m\}$), corresponding to the above three cases will be referred to as the *base subgraphs* of $G \in \mathcal{B}(n)$ of type (I), (II), and (III), respectively. These are depicted in Fig. 13.

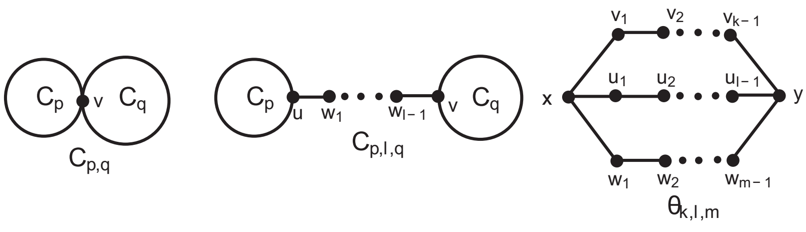


**Fig. 13.** The base graphs of type (I), (II), and (III).

For $n \geq 5$, let $B_n^{(1)}$ and $B_n^{(2)}$ be the bicyclic graphs shown in Fig. 14. In Fig. 15 are depicted the graphs $\theta_{2,1,3}$ and $\theta_{2,2,3}$, which are bicyclic with diameter 2. It is easy to see that $\theta_{2,1,3} \notin \{B_n^{(1)}, B_n^{(2)}\}$ and $\theta_{2,2,3} \notin \{B_n^{(1)}, B_n^{(2)}\}$.

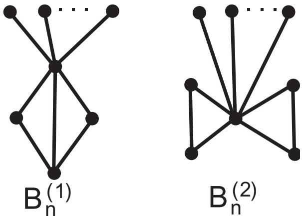


**Fig. 14.** Bicyclic graphs used in Theorem 4.13.

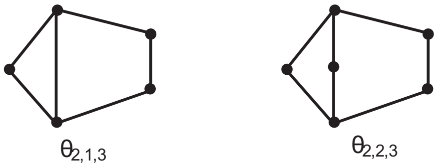


**Fig. 15.** Bicyclic graphs with diameter 2.

For $n \geq 5$, let $B_n^{(0)}$ be the graph obtained by attaching a path of length $n-4$ to one vertex of degree 2 of $\theta_{2,1,2}$. In the following two theorems, we characterize the bicyclic graphs extremal w.r.t. $W$, $WW$, and $H$ in the class $\mathcal{B}(n)$. Note that, in [142], the authors have determined the extremal graphs with respect to Wiener index among bicyclic graphs containing two disjoint cycles.

**Theorem 4.13.** *Let $G$ be a bicyclic graph of order $n \geq 5$ and $i \in \{1,2\}$. Then we have:*

(1) ([49]) $W(B_n^{(i)}) \leq W(G)$, *with equality holding if and only if* $G \cong B_n^{(i)}$ *for* $n \geq 7$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,2,3}$ *for* $n = 6$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,1,3}$ *or* $G \cong K_{2,3}$ *for* $n = 5$;

(2) ([49]) $WW(B_n^{(i)})) \leq WW(G)$, *with equality holding if and only if* $G \cong B_n^{(i)}$ *for* $n \geq 7$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,2,3}$ *for* $n = 6$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,1,3}$ *or* $G \cong K_{2,3}$ *for* $n = 5$;

(3) ([160]) $H(G) \leq H(B_n^{(i)})$, *with equality holding if and only if* $G \cong B_n^{(i)}$ *for* $n \geq 7$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,2,3}$ *for* $n = 6$ *and* $G \cong B_n^{(i)}$ *or* $G \cong \theta_{2,1,3}$ *or* $G \cong K_{2,3}$ *for* $n = 5$.

**Remark 4.1.** *It needs to be pointed out that the extremal graph $\theta_{2,2,3}$ has been overlooked in* [49]*. But, clearly, it is an extremal graph, since its diameter is 2.*

**Theorem 4.14.** *Let $G$ be a bicyclic graph of order $n \geq 5$.*

(1) ([49]) $W(G) \leq W(B_n^{(0)})$, *where the equality holds if and only if* $G \cong B_n^{(0)}$.

(2) ([49]) $WW(G) \leq WW(B_n^{(0)})$, *where the equality holds if and only if* $G \cong B_n^{(0)}$.

(3) ([160]) $H(B_n^{(0)}) \leq H(G)$, *where the equality holds if and only if* $G \cong B_n^{(0)}$.

From Corollary 4.1, in view of the structure of bicyclic graphs with diameter 2, we obtain the following:

**Theorem 4.15.** *Let $G$ be a bicyclic graph of order $n \geq 5$ and $i \in \{1, 2\}$. Then,*

$$RCW(G) \leq RCW(B_n^{(i)})$$

*where the equality holds if and only if $G \cong B_n^{(i)}$ for $n \geq 7$ and $G \cong B_n^{(i)}$ or $G \cong \theta_{2,2,3}$ for $n = 6$ and $G \cong B_n^{(i)}$ or $G \cong \theta_{2,1,3}$ or $G \cong K_{2,3}$ for $n = 5$.*

Denote by $L_{n,i}$ the graph obtained by attaching a path of length $i$ to a vertex of degree 2 of $\theta_{2,1,2}$, and then attaching another path of order $n-4-i$ to the other vertex of degree 2 of $\theta_{2,1,2}$. The following theorem characterizes the bicyclic graphs with the smallest and second smallest reciprocal complementary Wiener indices.

**Theorem 4.16.** ([9]) *Let $G$ be a bicyclic graph of order $n \geq 7$, different from $L_{n,\lfloor (n-4)/2 \rfloor}$ and $L_{n,\lfloor (n-6)/2 \rfloor}$. Then*

$$RCW\left(L_{n,\lfloor (n-4)/2 \rfloor}\right) < RCW\left(L_{n,\lfloor (n-6)/2 \rfloor}\right) < RCW(G) \ .$$

# 5 Concluding remarks

In the above sections, we have collected many results on graphs extremal with regard to Wiener, hyper–Wiener, Harary, Wiener polarity, and reciprocal complementary Wiener indices. In this section, we would like to outline a few concluding remarks.

**Remark 5.1.** As mentioned in Section 1, the Wiener index and the Wiener polarity index were defined simultaneously. The Wiener polarity index seems less well–known than the

Wiener index, and even less well–known than the hyper–Wiener index, Harary index, and reciprocal complementary Wiener index, which were conceived much later. So far, results on Wiener polarity index are much fewer than those on other distance–based topological indices. Therefore, there are many extremal problems w.r.t. Wiener polarity index that have been left unsolved. Moreover, it would be interesting to study the relation between Winer polarity index and the other topological indices. By doing so, we might envisage the major differences between $W_P$ and the other distance–based indices.

**Remark 5.2.** Since the diameter is included in the reciprocal complementary Wiener index, it is much more difficult to deal with it than with the Harary index. But, to our surprise, sometimes in a given set of graphs, the graph with maximal Harary index is just the same that with minimal reciprocal complementary Wiener index (see, e.g., Theorem 3.15). Thus, it would be an interesting problem to find the other classes of graphs, in which the graph with maximal (resp. minimal) Harary index is just the one with minimal (resp. maximal) reciprocal complementary Wiener index. Furthermore, the reciprocal forms of the other distance–based topological indices would also be worthy of consideration.

**Remark 5.3.** When studying the extremal trees, unicyclic, and bicyclic graphs, with respect to distance–based topological indices, we find that in many cases (especially for $W$, $WW$, and $H$), the extremal unicyclic graph is obtained by adding a new edge to the extremal tree, and the extremal bicyclic graph is obtained by adding a new edge to the extremal unicyclic graph (cf. Theorems 3.1 and 4.1). It is therefore natural to ask: *Can the unicyclic graphs with given graphic parameters extremal w.r.t. the three indices $W$, $WW$, and $H$ be obtained by adding a new edge to the extremal tree with the same graphic parameters? What about the transition from the unicyclic to the bicyclic case?* Examples corroborating our idea are found in Theorems 3.10, 4.7, 3.13 (1), and 4.8. However, finding the answer to this problem in the general case is still an open and challenging task.

Other interesting remarks on Wiener index, hyper–Wiener index, and Harary index can be found in [157]. So far there is a great number of results on graphs extremal with respect to the Wiener index. But there are fewer results on graphs extremal with respect to other distance–based topological indices ($WW$, $H$, $RCW$, $W_P$, $TW$, and so on). In line with this remark, in the future one should focus more attention to the extremal problems of other distance–based topological indices, especially when some additional conditions on the graphs are given.

In spite of the great number of extremal results on the Wiener index, there still are some open problems. We mention here the characterization of extremal graphs with given radius (for some partial results see [85, 150, 166]), and with given diameter ( for partial but incomplete results see [21, 122, 165] and in Theorem 2.3). Similarly, some interesting and attractive problems on other distance–based topological indices also remain open.

Recently, Brückler et al. [6] introduced a general distance–based topological index, called $Q$-index. The $Q$-index is defined as

$$Q(G) = \sum_{k \geq 1} f(k)\, d(G, k)$$

where $f$ is a function such that $f(0) = 0$ and $d(G, k)$ is the number of vertex pairs at distance $k$. The Wiener, hyper–Wiener, Harary, and reciprocal complementary Wiener indices are all special cases of the $Q$-index.

We would like to end this survey with the following remark.

**Remark 5.4.** Suppose that some property of the function $f$ is given, enabling one to characterize the extremal graphs (with respect to the $Q$-index) in some particular sets of graphs. By comparing this results with the existing results for $W$, $WW$, $H$, $RCW$, $\ldots$, in may be that some interesting and fundamental mathematical unified properties of the distance–based topological indices could be envisaged.

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# References

[1] A. T. Balaban, Topological indices based on topological distances in molecular graphs, *Pure Appl. Chem.* **55** (1983) 199–206.

[2] A. Behtoei, M. Jannesari, B. Taeri, Maximum Zagreb index, minimum hyper–Wiener index and graph connectivity, *Appl. Math. Lett.* **22** (2009) 1571–1576.

[3] S. H. Bertz, Branching in graphs and molecules, *Discr. Appl. Math.* **19** (1988) 65–83.

[4] D. Bonchev, The Wiener number – some applications and new developments, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry – Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 58–88.

[5] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan, New York, 1976.

[6] F. M. Brückler, T. Došlić, A. Graovac, I. Gutman, On a class of distance–based molecular structure descriptors, *Chem. Phys. Lett.* **503** (2011) 336–338.

[7] K. Burns, R. C. Entringer, A graph–theoretic view of the United States postal service, in: Y. Alavi, A. J. Schwenk (Eds.), *Graph Theory, Combinatorics, and Algorithms*, Wiley, New York, 1995, pp. 323–334.

[8] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.

[9] X. Cai, B. Zhou, Reciprocal complementary Wiener numbers of trees, unicyclic graphs and bicyclic graphs, *Discr. Appl. Math.* **157** (2009) 3046–3054.

[10] Y. H. Chen, X. D. Zhang, The Wiener index of unicyclic graphs with girth and matching number, *Ars Combin.* **104** (2012) 115–128.

[11] Y. H. Chen, X. D. Zhang, On Wiener and terminal Wiener indices of trees, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 591–602.

[12] Z. Cui, B. Liu, On Harary matrix, Harary index and Harary energy, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 815–823.

[13] P. Dankelmann, Average distance and independence number, *Discr. Appl. Math.* **51** (1994) 75–83.

[14] P. Dankelmann, Average distance and domination number, *Discr. Appl. Math.* **80** (1997) 21–35.

[15] P. Dankelmann and S. Mukwembi, The distance concept and distance in graphs, in: I. Gutman and B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 3–48.

[16] K. C. Das, On the largest eigenvalue of the distance matrix of a bipartite graph, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 667–672.

[17] K. C. Das, Maximum eigenvalue of the reciprocal distance matrix, *J. Math. Chem.* **47** (2010) 21–28.

[18] K. C. Das, I. Gutman, Estimating the Wiener index by means of number of vertices, number of edges, and diameter, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 647–660.

[19] K. C. Das, K. Xu, I. Gutman, On Zagreb and Harary indices, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 301–314.

[20] K. C. Das, B. Zhou, N. Trinajstaić, Bounds on Harary index, *J. Math. Chem.* **46** (2009) 1377–1393.

[21] E. De La Viña, B. Waller, Spanning trees with many leaves and average distance, *El. J. Combin.* **15** (2008) R33.

[22] H. Deng, The trees on $n > 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 393–402.

[23] H. Deng, On the extremal Wiener polarity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 305–314.

[24] H. Deng, H. Xiao, The maximum Wiener polarity index of trees with $k$ pendants, *Appl. Math. Lett.* **23** (2010) 710–715.

[25] H. Deng, H. Xiao, F. Tang, On the extremal Wiener polarity index of trees with a given diameter, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 257–264.

[26] X. Deng, J. Zhang, Equiseparability on terminal Wiener index, in: A. V. Goldberg, Y. Zhou (Eds.), *Algorithmic Aspects in Information and Management*, Springer, Berlin, 2009, pp. 166–174.

[27] X. Deng, J. Zhang, Equiseparability on terminal Wiener index, *Appl. Math. Lett.* **25** (2012) 580–585.

[28] J. Devillers, A. T. Balaban (Eds.),*Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[29] M. M. Deza, E. Deza, *Dictionary of Distances*, Elsevier, Amsterdam, 2006.

[30] M. V. Diudea, I. Gutman, Wiener–type topological indices, *Croat. Chem. Acta* **71** (1998) 21–51.

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

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

[33] H. Dong, X. Guo, Ordering trees by their Wiener indices, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 527–540.

[34] H. Dong, B. Zhou, Maximum Wiener index of unicyclic graphs with fixed maximum degree, *Ars Combin.* **103** (2012) 407–416.

[35] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex–degree–based molecular structure descriptors, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 613–626.

[36] J. K. Doyle, J. E. Graver, Mean distance in a graph, *Discr. Appl. Math.* **17** (1977) 147–154.

[37] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 235–244.

[38] Z. Du, B. Zhou, Minimum Wiener indices of trees and unicyclic graphs of given matching number, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 101–112.

[39] S. El–Basil, Gutman trees, *J. Chem. Soc. Faraday Trans. 2*, **82** (1986) 299–316.

[40] S. El-Basil, Caterpillar (Gutman) trees in chemical graph theory, in: I. Gutman, S. J. Cyvin (Eds.), *Advances in the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, 1990, pp. 273–289.

[41] M. Eliasi, G. Raeisi, B. Taeri, Wiener index of some graph operations, *Discr. Appl. Math.* **160** (2012) 1333–1344.

[42] R. C. Entringer, Bounds for the average distance–inverse degree product in trees, in: Y. Alavi, D. R. Lick, A. J. Schwenk (Eds.), *Combinatorics, Graph Theory, and Algorithms*, New Issues Press, Kalamazoo, 1999, pp. 335–352.

[43] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czech. Math. J.* **26** (1976) 283–296.

[44] L. Feng, The hyper–Wiener index of unicyclic graphs with given matching number, *Ars Combin.* **100** (2011) 9–17.

[45] L. Feng, A. Ilić, Zagreb, Harary and hyper–Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* **23** (2010) 943–948.

[46] L. Feng, A. Ilić, G. Yu, The hyper–Wiener index of unicyclic graphs, *Util. Math.* **82** (2010) 215–226.

[47] L. Feng, A. Ilić, G. Yu, On the second maximal and minimal Wiener index of unicyclic graphs with given girth, *Ars Combin.* **104** (2012) 13–22.

[48] L. Feng, W. Liu, The hyper–Wiener index of graphs with given diameter, *Util. Math.* **88** (2012) 3–12.

[49] L. Feng, W. Liu, K. Xu, The hyper–Wiener index of bicyclic graphs, *Util. Math.* **84** (2011) 97–104.

[50] L. Feng, G. Yu, W. Liu, The hyper–Wiener index of graphs with a given chromatic (clique) number, *Util. Math.* **88** (2012) 399–407.

[51] L. Feng, G. Yu, W. Liu, On the hyper–Wiener index of cacti, *Util. Math.*, in press.

[52] M. Fischermann, I. Gutman, A. Hoffmann, D. Rautenbach, D. Vidović, L. Volkmann, Extremal chemical trees, *Z. Naturforsch.* **57a** (2002) 49–52.

[53] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Discr. Appl. Math.* **122** (2002) 127–137.

[54] B. Furtula, Odd–vertex–degree trees maximizing Wiener index, *Kragujevac J. Math.* **37** (2013) 129–134.

[55] B. Furtula, I. Gutman, H. Lin, More trees with all degrees having extremal Wiener index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 293–296.

[56] W. Goddard, O. R. Oellermann, Distance in graphs, in: M. Dehmer (Ed.), *Structural Analysis of Complex Networks*, Birkhäuser, Dordrecht, 2011, pp. 49–72.

[57] X. Guo, H. Dong, Ordering trees by their Wiener indices, *J. Xiamen Univ. (Nat. Sci.)* **44** (2005) 297–298.

[58] I. Gutman, Topological properties of benzenoid systems - An identity for the sextet polynomial, *Theor. Chim. Acta* **45** (1977) 309–315.

[59] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128–132.

[60] I. Gutman, R. Cruz, J. Rada, Wiener index of Eulerian graphs, *Discr. Appl. Math.*, in press.

[61] I. Gutman, S. J. Cyvin, *Introdution to the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, 1989, p. 112.

[62] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[63] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010.

[64] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010.

[65] I. Gutman, B. Furtula, A survey on terminal Wiener index, in: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010, pp. 173–190.

[66] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012.

[67] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Applications*, Univ. Kragujevac, Kragujevac, 2012.

[68] I. Gutman, B. Furtula, M. Petrović, Terminal Wiener index, *J. Math. Chem.* **46** (2009) 522–531.

[69] I. Gutman, W. Linert, I. Lukovits, A. A. Dobrynin, Trees with extremal hyper–Wiener index: Mathematical basis and chemical applications, *J. Chem. Inf. Comput. Sci.* **37** (1997) 349–354.

[70] I. Gutman, M. Randić, Algebraic characterization of skeletal branching, *Chem. Phys. Lett.* **47** (1977) 15–19.

[71] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[72] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. III. Total $\pi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[73] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A** (1993) 651–661.

[74] I. Gutman, S. Zhang, Graph connectivity and Wiener index, *Bull. Acad. Serbe Sci. Arts* **133** (2006) 1–5.

[75] F. Harary, The maximum connectivity of a graph, *Proc. Nat. Acad. Sci. U.S.A.* **48** (1962) 1142–1146.

[76] F. Harary, *Graph Theory*, Addison–Wesley, Reading, 1969.

[77] G. R. T. Hendry, On mean distance in certain classes of graphs, *Networks* **19** (1989) 451–457.

[78] A. Heydari, I. Gutman, On the terminal Wiener index of thorn graphs, *Kragujevac J. Sci.* **32** (2010) 57–64.

[79] A. J. Hoffman, R. R. Singleton, On Moore graphs with diameters 2 and 3, *IBM J. Res. Develop.* **4** (1960) 497–504.

[80] Y. Hong, H. Liu, X. Wu, On the Wiener index of unicyclic graphs, *Haceteppe J. Math. Statist.* **40** (2011) 63–68.

[81] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.

[82] H. Hosoya, I. Gutman, Kekulé structures of hexagonal chains – some unusual connections, *J. Math. Chem.* **44** (2008) 559–568.

[83] H. Hou, B. Liu, Y. Huang, The maximum Wiener polarity index of unicyclic graphs, *Appl. Math. Comput.* **218** (2012) 10149–10157.

[84] H. Hua, Wiener and Schultz molecular topological indices of graphs with specified cut edges, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 643–651.

[85] A. Ilić, A. Ilić, D. Stevanović, On the Wiener index and Laplacian coefficients of graphs with given diameter or radius, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 91–100.

[86] A. Ilić, M. Ilić, Generalizations of Wiener polarity index and terminal Wiener index, *Graphs Comb.* **29** (2013) 1403–1416.

[87] A. Ilić, G. Yu, L. Feng, The Harary index of trees, *Util. Math.* **87** (2012) 21–32.

[88] O. Ivanciuc, QSAR comparative study of Wiener descriptors for weighted molecular graphs, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1412–1422.

[89] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices, *J. Math. Chem.* **12** (1993) 309–318.

[90] O. Ivanciuc, T. Ivanciuc, A. T. Balaban, The complementary distance matrix, a new molecular graph metric, *ACH Models Chem.* **137** (2000) 57–82.

[91] D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry*, Univ. Kragujevac, Kragujevac, 2007.

[92] F. Jelen, E. Triesch, Superdominance order and distance of trees with bounded maximum degree, *Discr. Appl. Math.* **125** (2003) 225–233.

[93] M. Karelson, *Molecular Descriptors in QSAR/QSPR*, Wiley/Interscience, New York, 2000.

[94] M. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, S. Wagner, Some new results on distance–based graph invariants, *Eur. J. Comb.* **30** (2009) 1149–1163.

[95] D. J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper–Wiener index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **35** (1995) 50–52.

[96] M. Knor, P. Potočnik, R. Škrekovski, The Wiener index in iterated line graphs, *Discr. Appl. Math.* **160** (2012) 2234–2245.

[97] W. Li, X. Li, I. Gutman, Volkmann trees and their molecular structure descriptors, in: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010, pp. 231–246.

[98] H. Lin, Extremal Wiener index of trees with all degrees odd, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 287–292.

[99] X. Lin, On the Wiener index and circumference, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 331–336.

[100] B. Liu, H. Hou, Y. Huang, On the Wiener polarity index of trees with maximum degree or given number of leaves, *Comput. Math. Appl.* **60** (2010) 2053–2057.

[101] B. Liu, M. Liu, Some recent results on the variable Wiener index of graphs, in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 231–282.

[102] H. Liu, M. Lu, A unified approach to cacti for different indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 193–204.

[103] H. Liu, X. Pan, On the Wiener index of trees with fixed diameter, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 85–94.

[104] M. Liu, B. Liu, Trees with the seven smallest and fifteen greatest hyper–Wiener indices, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 151–170.

[105] M. Liu, B. Liu, On the Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 293–304.

[106] M. Liu, B. Liu, The second Zagreb indices and Wiener polarity indices of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 439–450.

[107] M. Liu, B. Liu, A survey on recent results of variable Wiener index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 491–520.

[108] M. Liu, B. Liu, Q. Li, Erratum to 'The trees on $n > 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees', *MATCH Commun. Math. Comput. Chem.* **64** (2010) 743–756.

[109] M. Liu, X. Tan, The first to $(k+1)$-th smallest Wiener (hyper–Wiener) indices of connected graphs, *Kragujevac J. Math.* **32** (2009) 109–115.

[110] S. Liu, L. Tong, Y. Yeh, Trees with the minimum Wiener number, *Int. J. Quantum Chem.* **78** (2000) 331–340.

[111] B. Lučić, I. Lukovits, S. Nikolić, N. Trinajstić, Distance–related indexes in the quantitative structure–property relationship modeling, *J. Chem. Inf. Comput. Sci.* **41** (2001) 527–535.

[112] B. Lučić, S. Nikolić, N. Trinajstić, Distance–related molecular descriptors, *Internet El. J. Mol. Design* **7** (2008) 195–206.

[113] W. Luo, B. Zhou, On ordinary and reverse Wiener indices of non-caterpillars, *Math. Comput. Model.* **50** (2009) 188–193.

[114] A. K. Madan, H. Dureja, Eccentricity based descriptors for QSAR/QSPR, in: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010, pp. 91–138.

[115] Z. Marković, V. Ivanov–Petrović, I. Gutman, Extremely branched alkanes, *J. Mol. Struct. (Theochem)* **629** (2003) 303–306.

[116] Z. Mihalić, S. Nikolić, N. Trinajstić, Comparative study of molecular descriptors derived from the distance matrix, *J. Chem. Inf. Comput. Sci.* **32** (1992) 28–36.

[117] Z. Mihalić, N. Trinajstić, A graph–theoretical approach to structure–property relationships, *J. Chem. Educ.* **69** (1992) 701–712.

[118] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, The distance matrix in chemistry, *J. Math. Chem.* **11** (1992) 223–258.

[119] R. Nasiri, H. Yousefi–Azari, M. R. Darafsheh, Remarks on the Wiener index of unicyclic graphs, *J. Appl. Math. Comput.* **41** (2013) 49–59.

[120] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: Development and applications, *Croat. Chem. Acta* **68** (1995) 105–129.

[121] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.

[122] J. Plesník, On the sum of all distances in a graph or digraph, *J. Graph Theory* **8** (1984) 1–24.

[123] X. Qi, B. Zhou, Extremal properties of reciprocal complementary Wiener numbers of trees, *Comput. Math. Appl.* **62** (2011) 523–531.

[124] J. Rada, Variation of the Wiener index under tree transformations, *Discr. Appl. Math.* **148** (2005) 135–146.

[125] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[126] M. Randić, Novel molecular descriptor for structure–property studies, *Chem. Phys. Lett.* **211** (1993) 478–483.

[127] D. H. Rouvray, The role of the topological distance matrix in chemistry, in: N. Trinajstić (Ed.), *Mathematics and Computational Concepts in Chemistry*, Horwood, Chichester, 1986, pp. 295–306.

[128] D. H. Rouvray, The challenge of characterizing branching in molecular species, *Discr. Appl. Math.* **19** (1988) 317–338.

[129] D. H. Rouvray, Harry in the limelight: The life and times of Harry Wiener, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry – Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 1–15.

[130] D. H. Rouvray, The rich legacy of half century of the Wiener index, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry – Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 16–37.

[131] E. Ruch, I. Gutman, The branching extent of graphs, *J. Combin. Inf. System Sci.* **4** (1979) 285–295.

[132] N. S. Schmuck, S.G. Wagner, H. Wang, Greedy trees, caterpillars, and Wiener–type graph invariants, *Comput. Math. Appl.* **68** (2012) 273–292.

[133] R. Shi, The average distance of trees, *Systems Sci. Math. Sci.* **6** (1993) 18–24.

[134] A. V. Sills, H. Wang, On the maximal Wiener index and related questions, *Discr. Appl. Math.* **160** (2012) 1615–1623.

[135] L. Šoltés, Transmission in graphs: a bound and vertex removing, *Math. Slovaca* **41** (1991) 11–16.

[136] P. Šparl, D. Vukičević, J. Žerovnik, Graphs with minimal value of Wiener and Szeged number, *Int. J. Chem. Model.* **4** (2012) 127–134.

[137] P. Šparl, J. Žerovnik, Graphs with given number of cut-edges and minimal value of Wiener number, *Int. J. Chem. Model.* **3** (2011) 131–137.

[138] D. Stevanović, Maximizing Wiener index of graphs with fixed maximum degree, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 71–83.

[139] D. Stevanović, A. Ilić, Spectral properties of distance matrix of graphs, in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 139–176.

[140] L. A. Székely, H. Wang, T. Wu, The sum of distances between the leaves of a tree and the 'semi-regular' property, *Discr. Math.* **311** (2011) 1197–1203.

[141] Z. Tang, H. Deng, The $(n, n)$-graphs with the first three extremal Wiener indices, *J. Math. Chem.* **43** (2008) 60–74.

[142] Z. Tang, H. Deng, The graphs with minimal and maximal Wiener indices among a class of bicyclic graphs, *J. Nat. Sci. Hunan Norm. Univ.* **31** (2008) 27–30.

[143] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[144] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

[145] N. Trinajstić, S. Nikolić, A. Miličević, I. Gutman, On Zagreb indices, *Kem. Ind.* **59** (2010) 577–589 (in Croatian).

[146] D. Vukičević, Which generalized Randić indices are suitable measures of branching?, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 443–452.

[147] D. Vukičević, Which generalized Randić indices are suitable measures of molecular branching?, *Discr. Appl. Math.* **158** (2010) 2056–2065.

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

[149] S. Wagner, H. Wang, X. Zhang, Distance–based graph invariants of trees and the Harary index, *Filomat* **27** (2013) 39–48.

[150] H. B. Walikar, V. S. Shigehalli, H. S. Ramane, Bounds on the Wiener number of a graph, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 117–132.

[151] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **156** (2009) 2647–2654.

[152] H. Wang, L. Kang, On the Harary index of cacti, *Util. Math.*, in press.

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

[154] S. Wang, X. Guo, Trees with extremal Wiener indices, *MATCH Commum. Math. Comput. Chem.* **60** (2008) 609–622.

[155] X. Wu, H. Liu, On the Wiener index of graphs, *Acta Appl. Math.* **110** (2010) 535–544.

[156] R. Xing, B. Zhou, X. Qi, Hyper–Wiener index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 315–328.

[157] K. Xu, Trees with the seven smallest and eight greatest Harary indices, *Discr. Appl. Math.* **160** (2012) 321–331.

[158] K. Xu, K. C. Das, On Harary index of graphs, *Discr. Appl. Math.* **159** (2011) 1631–1640.

[159] K. Xu, K. C. Das, Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 257–272.

[160] K. Xu, K. C. Das, Extremal unicyclic and bicyclic graphs with respect to Harary index, *Bull. Malays. Math. Sci. Soc.* **36** (2013) 373–383.

[161] K. Xu, K. C. Das, H. Hua, M. V. Diudea, Maximal Harary idnex of unicyclic graphs with given matching number, *Studia Univ. Babeş–Bolyai – Chemia*, **58** (2013) 71–86.

[162] K. Xu, I. Gutman, The largest Hosoya index of bicyclic graphs with given maximum degree, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 795–824.

[163] K. Xu, N. Trinajstić, Hyper–Wiener and Harary indices of graphs with cut edges, *Util. Math.* **84** (2011) 153–163.

[164] K. Xu, J. Wang, H. Liu, The Harary index of ordinary and generalized quasi–tree graphs, *J. Appl. Math. Comput.*, in press.

[165] S. Yamaguchi, A note on Wiener index, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 645–648.

[166] Z. You, B. Liu, Note on the minimal Wiener index of connected graphs with $n$ vertices and radius $r$, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 343–344.

[167] G. Yu, L. Feng, On the Wiener index of unicyclic graphs with given girth, *Ars Combin.* **94** (2010) 361–369.

[168] G. Yu, L. Feng, A. Ilić, The hyper–Wiener index of trees with given parameters, *Ars Combin.* **96** (2010) 395–404.

[169] X. Zhang, Y. Liu, M. Han, The maximum Wiener index of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 661–682.

[170] X. Zhang, Q. Xiang, L. Xu, R. Pan, The Wiener index of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 623–644.

[171] B. Zhou, X. Cai, N. Trinajstić, On Harary index, *J. Math. Chem.* **44** (2008) 611–618.

[172] B. Zhou, X. Cai, N. Trinajstić, On reciprocal complementary Wiener number, *Discr. Appl. Math.* **157** (2009) 1628–1633.

[173] B. Zhou, I. Gutman, Relations between Wiener, hyper–Wiener and Zagreb indices, *Chem. Phys. Lett.* **394** (2004) 93–95.

[174] B. Zhou, N. Trinajstić, Mathematical properties of molecular descriptors based on distances, *Croat. Chem. Acta* **83** (2010) 227–242.