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Distance Sequences to Bound the Harary Index and Other Wiener-Type Indices of a Graph

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Abstract

In this paper we obtain several new bounds on well-studied topological indices, among those sharp lower bounds on the Harary index and sharp upper bounds on the hyper-Wiener index and the multiplicative Wiener index for (i) graphs of given order and size (which solves a problem in the monograph [Xu, Das, Trinajstić, The Harary index of a graph, Springer (2015)]), (ii) κ-connected graphs, where κ is even, (iii) maximal outerplanar graphs, (iv) Apollonian networks, and (v) for trees in which all vertices have odd degree.

We use a novel approach to prove our bounds for a very general class of distance-based topological indices of graphs, which includes the Wiener index and most of its generalizations, including the Harary index, the hyper-Wiener index and the multiplicative Wiener index.

1 Introduction

Many topological indices in chemical and pure graph theory are based on distances between vertices. The best-known among the distance-based topological indices is the Wiener index $W(G)$, defined as

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

where $V(G)$ is the vertex set of G and $d_G(u,v)$ denotes the usual shortest path distance between vertices u and v of G. Two of the most important distance-based indices besides the Wiener index are the Harary index $H(G)$, defined as

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

and the hyper-Wiener index $\mathrm{WW}(G)$, defined as

$$\mathrm{WW}(G) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} \big(d_G(u,v)^2 + d_G(u,v)\big).$$

Bounds on these indices in terms of graph properties or other graph invariants have been the subject of intense study in the literature. Since the extremal graphs for distance-based topological indices like the Wiener index, Harary index and hyper-Wiener index coincide in many cases, it is natural to explore ways to prove extremal results for these topological indices in a unified way. This approach lead to the study of generalized Wiener indices, (also called Q-indices, see, for example, [9]), of the form

$$W_f(G) = \sum_{\{u,v\}\subseteq V(G)} f(d_G(u,v)),$$

where f is a real-valued function on the set of positive integers. For suitable choices of f, this definition includes many well-known distance-based indices, among others the Harary index, the variable Wiener index W_λ, where $\lambda \in \mathbb{R} \setminus \{0\}$, defined by $W_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u,v))^\lambda$ (see [28]), the hyper-Wiener index, the generalised hyper-Wiener index WW_λ, defined by $\mathrm{WW}_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{2}(d_G(u,v)^\lambda + d_G(u,v)^{2\lambda})$, where $\lambda \in \mathbb{R} \setminus \{0\}$ (see [42]), and the Tratch, Stankevich, Zefirov index $\sum_{\{u,v\}\subseteq V(G)} \frac{1}{3}\big(d_G(u,v) + \frac{1}{2} d_G(u,v)^2 + \frac{1}{6} d_G(u,v)^3\big)$ (see [32, 43]). While the multiplicative Wiener index, $\pi(G) = \prod_{\{u,v\}\subseteq V(G)} d_G(u,v)$ cannot be expressed in the form $W_f(G)$ for any f, the logarithm of $\pi(G)$ can.

This unified approach has yielded numerous general bounds on W_f. (The following results are stated for the case that f is an increasing function, corresponding results hold if f is decreasing.) In [37] the trees of given order that have the four largest and the four smallest values of W_f were determined. Considering trees with a given degree sequence, it was shown in [39, 45] that the so-called greedy tree minimizes W_f. In [13], extremal trees minimizing W_f among all trees with a given eccentric sequence are obtained. Unicyclic graphs with extremal values of W_f were considered in [38]. Sufficient conditions for graphs in terms of W_f to have vulnerability parameters (such as toughness, binding number, tenacity, integrity) at least a given value were obtained in [30]. Graphs with given independence number or matching number that are extremal with respect to W_f were considered in [10]. In recent years, sufficient conditions in terms of W_f that guarantee that graphs have certain Hamiltonian properties have attracted attention, see [4, 15, 33, 47, 48].

Other approaches to a unified treatment of topological indices on trees, that also includes some indices that were not distance-based, were taken in [44], where a partial order on the set of trees of given order is defined, and results for indices that are increasing or decreasing with respect to this partial order are obtained. This was further applied in [41]. In [3], the authors presented very general conditions on topological indices under which the greedy tree is always extremal among trees with a given degree sequence.

In this paper we take an entirely different approach to distance-based topological indices by utilizing properties of distance sequences. The *distance sequence* $\mathcal{D}(G)$ of a connected graph G is the nondecreasing sequence of the distances between all unordered pairs of distinct vertices of G. The distance sequence was first considered in [11], where it was used to prove sharp bounds on the Wiener index of the strong product of graphs. We say that a topological index $I(G)$ is *distance-based* if it can be expressed in the form $I(G) = g(\mathcal{D}(G))$, where g is a function defined on the set of all finite sequences of positive integers. For example the Wiener index is a distance-based index, where $g(x_1 + x_2 + \cdots) = x_1 + x_2 + \cdots$. In this paper, the term index always means distance-based topological index.

We say that I is *increasing* (decreasing, nonincreasing, nondecreasing) if the function g, when restricted to sequences of a fixed length, is increasing (decreasing, nonincreasing, nondecreasing) in every coordinate. This definition includes as special cases the generalized Wiener index W_f, defined as $\sum_{\{u,v\}\subseteq V(G)} f(d_G(u,v))$, where f is an increasing or decreasing real function (which in turn includes well-known topological indices such as the Harary index and the hyper-Wiener index), but also, for example, the diameter of a graph, defined as the largest of the distances between its vertices.

An advantage of our approach is that it yields several new sharp bounds for distance-based topological indices for graph classes other than trees. We determine graphs that maximize (minimize) increasing (decreasing) distance-based topological indices among (i) graphs of given order and size, (ii) κ-connected graphs of given order, where κ is even, (iii) k-trees and maximal outerplanar graphs, and (iv) trees with all vertex degrees odd. As corollaries to our bounds we obtain several new bounds on the Harary index, the hyper-Wiener index and the multiplicative Wiener index. Our bound for graphs of given order and size resolves an open problem (Problem 6.1.2) from the monograph [51] on the Harary index.

This paper is organized as follows. In Section 2, we define the terminology and notation used in this paper. In Section 3 we introduce the distance sequence of graphs and prove basic properties. In the following sections we obtain extremal graphs for increasing or decreasing distance-based topological indices for various graph classes: graph of given order and size are considered in Section 4, graphs of given connectivity are considered in Section 5, maximal k-degenerate graphs (which as special cases contain k-trees, maximal outerplanar graphs and Apollonian networks, which are a subclass of maximal planar graphs) are considered in Section 6. Section 7 is on trees in which all vertices have odd degree.

2 Terminology and notation

If G is a graph, then we denote its vertex set and edge set by $V(G)$ and $E(G)$. The *order* and *size* of G are the number of vertices and edges, respectively, of G. If u, v are vertices of G, and $uv \in E(G)$, then we say that u is *adjacent* to v or that u is a *neighbor* of v, and that the edge uv is *incident* with u and v. The *degree* $\deg_G(v)$ of v is the number of its neighbors.

A graph is *connected*, if between any two of its vertices, u and v say, there is a (u, v)-path. The *distance* $d_G(u, v)$ between two vertices u and v in a connected graph is the minimum length, i.e., number of edges, of a (u, v)-path. If u is a vertex of G, then the *eccentricity* of u, denoted by $\mathrm{ecc}_G(u)$, is the distance from u to a vertex farthest from u.

If S is a set of vertices of G, then $G - S$ denotes the graph obtained from G by deleting all vertices in S and all edges incident with a vertex in S. The *connectivity* of a non-complete graph G is the minimum cardinality of a set $S \subseteq V(G)$ for which the graph $G - S$ is disconnected.

A graph G is *planar* if it can be embedded in the plane such that no two edges intersect. A graph is *outerplanar* if it can be embedded in the plane such that no two edges intersect, and every vertex is on the boundary of the exterior face. A graph G is *maximal planar* (*maximal outerplanar*) if it is planar (outerplanar), but after adding any edge it no longer has this property.

Let G be a graph and $k \in \mathbb{N}$. By the k-th *power* G^k of G we mean the graph on the same vertex set in which two vertices are adjacent if their distance is not more than k. If G and H are vertex disjoint graphs, then the *union* $G \cup H$ is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. If $G_1, G_2, \ldots, G_k$ are disjoint graphs, then the *sequential sum* $G_1 + G_2 + \cdots + G_k$ is the graph obtained from the disjoint union of $G_1, G_2, \ldots, G_k$ by by adding edges joining every vertex of G_i to every vertex of G_{i+1} for $i = 1, 2, \ldots, k - 1$.

We denote the path, the cycle, the complete graph and the edgeless graph on n vertices by P_n, C_n, K_n and $\overline{K_n}$, respectively.

Let $A = (a_1, a_2, \ldots, a_k)$ and $B = (b_1, b_2, \ldots, b_k)$ be nondecreasing sequences of integers, then we write $A \leq B$ if $a_i \leq b_i$ for $i = 1, 2, \ldots, k$. We write $A < B$ if $A \leq B$ and $A \neq B$. We denote the sequence obtained from the concatenation of A and B by arranging its elements in nondecreasing order by $A \odot B$. If $a, k \in \mathbb{N}$, then by $a^{(k)}$ we mean the sequence $(a, a, \ldots, a)$ of length k.

3 Distance sequences

Recall that the *distance sequence* $\mathcal{D}(G)$ of a connected graph G of order n is the nondecreasing sequence of the distances between all unordered pairs of distinct vertices of G. The distance sequence was first considered in [11]. The relation $\leq$ imposes a partial order on the distance sequences of connected graphs of given order.

If I is an nondecreasing (nonincreasing) index, then clearly $I(G_1) \leq I(G_2)$ ($I(G_1) \geq I(G_2)$) whenever G_1 and G_2 are connected graphs of the same order with $\mathcal{D}(G_1) \leq \mathcal{D}(G_2)$. Hence we have the following proposition.

Proposition 1. *Let $\mathcal{G}$ be a family of connected graphs, and for $n \in \mathbb{N}$ denote by $\mathcal{G}_n$ the set of all graphs in $\mathcal{G}$ of order n.*
(a) Let I be a nondecreasing index. If a graph $G_n \in \mathcal{G}_n$ satisfies $\mathcal{D}(G) \leq \mathcal{D}(G_n)$ for all $G \in \mathcal{G}_n$, then

$$I(G) \leq I(G_n) \quad \text{for all } G \in \mathcal{G}_n.$$

(b) Let I be an increasing index. If a graph $G_n \in \mathcal{G}_n$ satisfies $\mathcal{D}(G) < \mathcal{D}(G_n)$ for all $G \in \mathcal{G}_n - \{G_n\}$, then

$$I(G) < I(G_n) \quad \text{for all } G \in \mathcal{G}_n - \{G_n\}.$$

Corresponding inequalities hold if I is nonincreasing or decreasing.

If v is a vertex of a connected graph G, then $\mathcal{D}_G(v)$ denotes the nondecreasing sequence of the distances between v and all other vertices of G. The following lemma is a slightly more general version of the well-known fact that $W(G) \leq W(G - v) + t_G(v)$ if v is not a cut-vertex of G, where

$t_G(v)$ is the transmission of v, i.e., the sum of the distances between v and all other vertices of G.

Lemma 1. *Let G be a connected graph, and v a vertex of G which is not a cut-vertex. Then*

$$\mathcal{D}(G) \leq \mathcal{D}(G-v) \odot \mathcal{D}_G(v), \tag{1}$$

with equality if and only if $d_{G-v}(u,w) \leq 2$ for all $u,w \in N_G(v)$.

Proof. Let $\mathcal{D}'$ be the nondecreasing sequence of the distances in G between all pairs of vertices in $V(G)-\{v\}$. Then $\mathcal{D}(G) = \mathcal{D}' \odot \mathcal{D}_G(v)$. Since $d_G(u,w) \leq d_{G-v}(u,w)$ for all $u,w \in V(G)-\{v\}$, we have $\mathcal{D}' \leq \mathcal{D}(G-v)$. This proves (1).

Clearly, equality in (1) holds if an only if $d_G(u,w) = d_{G-v}(u,w)$ for all $u,w \in V(G)-\{v\}$, which in turn holds if and only if $d_G(u,w) = d_{G-v}(u,w)$ for all $u,w \in N_G(v)$. The latter holds if and only $d_{G-v}(u,w) \leq 2$ for all $u,w \in N_G(v)$. ■

4 Graphs of given order and size

In this section we present both, upper and lower bounds on indices for graphs of given order and size.

Sharp lower bounds on nondecreasing/increasing indices (upper bounds on nonincreasing/decreasing indices) are known for several indices. They are a consequence of the following proposition. For $n,m \in \mathbb{N}$ with $n-1 \leq m < \binom{n}{2}$ we denote by $S_{n,m}$ a graph obtained from the star $K_1 + \overline{K_{n-1}}$ by adding $m-n+1$ edges. Clearly, $S_{n,m}$ has order n and size m, and diameter 2.

Proposition 2. *Let G be a connected graph of order n and size m.*
(a) If I be an nondecreasing index. then

$$I(G) \geq I(S_{n,m}).$$

If I is increasing, then equality holds if and only if $\text{diam}(G) \leq 2$.

(b) If I be an nonincreasing index. then

$$I(G) \leq I(S_{n,m}).$$

If I is decreasing, then equality holds if and only if $\mathrm{diam}(G) \leq 2$.

Proof. We only prove (a) as the proof of (b) is identical. It suffices to show that

$$\mathcal{D}(G) \geq \mathcal{D}(S_{n,m}),$$

where equality holds if and only if $\mathrm{diam}(G) \leq 2$.

Clearly, the statement holds if G is complete, so we may assume that $\mathrm{diam}(G) \geq 2$. If $\mathrm{diam}(G) = 2$, then $\mathcal{D}(G)$ has exactly m entries equal to 1, and $\binom{n}{2} - m$ entries equal to 2, so $\mathcal{D}(G) = \mathcal{D}(S_{n,m})$. If $\mathrm{diam}(G) > 2$, then $\mathcal{D}(G)$ has exactly m entries equal to 1, and $\binom{n}{2} - m$ entries greater or equal 2, where at least one entry is strictly greater than 2, so $\mathcal{D}(G) > \mathcal{D}(S_{n,m})$. ■

Proposition 2 implies several sharp bounds on indices in terms of order and size from the literature: lower bounds on the Wiener index [16], the variable Wiener index [25], the hyper-Wiener index [1] (the special case $m = n$, i.e., unicyclic graphs, was proved already in [27]), as well as an upper bound on the Harary index [51,52]. In addition to these, Proposition 2 implies the following bound on the multiplicative Wiener index.

Corollary 1. *If G is a connected graph of order n and size m, then $\pi(G) \geq 2^{\binom{n}{2}-m}$. Equality holds if and only if* $\mathrm{diam}(G) \leq 2$.

Sharp upper bounds on nondecreasing/increasing (or lower bounds on noninccreasing/decreasing) indices are less straightforward to obtain. For the Wiener index, Soltés [40] proved that, among all connected graphs of given order n and size m, the path-complete graph $PK_{n,m}$ (defined below) is the unique graph maximizing the Wiener index. No sharp upper bound on the hyper-Wiener index in terms of order and size is known, except for the special case $m = n$, i.e., for unicyclic graphs (see [49]). Upper bounds on the hyper-Wiener index in terms of order and size that also take into account eccentricities of vertices or diameter, were given in in [19] and [1], respectively. However, these bounds are not sharp in general. In their monograph [51], Xu, Das and Trinajstić posed the problem of determining a sharp lower bound on the Harary index in terms of order and size.

Theorem 3 below solves this problem not only for the Harary index, but for all increasing indices. Following Soltés [40], we define a path-complete graph as a graph obtained from the union of a path and a complete graph by joining one end of the path to one or more vertices of the complete graph.

It was observed in [40] that for given $n, m \in \mathbb{N}$ with $n-1 \leq m \leq \binom{n}{2}$ there exists a path-complete graph of order n and size m. (Indeed, P_n is a path-complete graph of size $n-1$. If G is a path-complete graph of order n and size $m < \binom{n}{2}$, then denote its path by P and its clique by K, and let v the the end of P adjacent to some vertices in K. We obtain a path-complete graph of order n and size $m+1$ by adding an edge from v to a vertex of K that v is not adjacent to yet. Note that we may assume that v is not adjacent to all vertices of K, otherwise we could include v in K, rather than in P.) Furthermore (see [40]) this graph is unique. We denote the unique path-complete graph of order n and size m by $PK_{n,m}$. The graph $PK_{9,16}$ is shown in Figure 1.

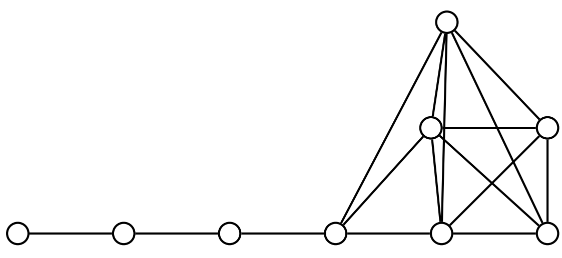

Figure 1. The graph $PK_{9,16}$.

Using Soltés' approach, it was shown in [11] that the distance sequence of $PK_{n,m}$ is maximal with respect to the partial order $\leq$ among the distance sequences of all connected graphs of order n and size m.

Lemma 2. *[11] Let G be a connected graph of order n and size m. Then*

$$\mathcal{D}(G) \leq \mathcal{D}(PK_{n,m}).$$

As a direct consequence of Lemma 2 and Proposition 1 we obtain the following theorem.

Theorem 3. *Let G be a connected graph of order n and size m.*
(a) If I is an nondecreasing index, then

$$I(G) \leq I(PK_{n,m}).$$

(b) If I is a nonincreasing index, then

$$I(G) \geq I(PK_{n,m}).$$

Corollary 2. *Among connected graphs of given order and size, the path-complete graph has minimum Harary index, minimum variable Wiener index for $\lambda < 0$, maximum hyper-Wiener index, maximum variable Wiener index for $\lambda > 0$, and maximum multiplicative Wiener index.*

5 Graphs of given connectivity

In this section we consider graphs of given connectivity κ. Several sharp lower bounds for nondecreasing/increasing (or sharp upper bounds for non-increasing/decreasing) indices of given order and connectivity are known in the literature. The following proposition provides a short, unified proof for many of these results. For given $n, \kappa \in \mathbb{N}$ with $1 \leq \kappa \leq n-2$ define the graph $H_{n,\kappa}$ as $K_1 + K_\kappa + K_{n-1-\kappa}$.

Proposition 4. *Let G be a graph of order n and connectivity κ.*
(a) If I is a nondecreasing index, then

$$I(G) \geq I(H_{n,\kappa}).$$

If I is increasing, then equality holds if and only if $G = H_{n,\kappa}$.

(b) If I is an nonincreasing index, then

$$I(G) \leq I(I_{n,\kappa}).$$

If I is decreasing, then equality holds if and only if $G = H_{n,\kappa}$.

Proof. Let G be a graph of order n with $\kappa(G) = \kappa$. We only prove (a) as the proof of (b) is identical. By Proposition 1 it suffices to show that

$$\mathcal{D}(G) \geq \mathcal{D}(H_{n,\kappa}),$$

with equality only if $G = H_{n,\kappa}$.

Let $S \subseteq V(G)$ be a set of κ vertices such that $G - S$ is disconnected. The graph $G - S$ has $n - \kappa$ vertices and at least two components, hence it contains at least $n - \kappa - 1$ pairs of nonadjacent vertices. It follows that $\mathcal{D}$ contains at least $n - \kappa - 1$ entries greater than 1. Hence

$$\mathcal{D}(G) \geq (1^{(\binom{n}{2}-n+\kappa+1)}, 2^{(n-\kappa-1)}) = \mathcal{D}(H_{n,\kappa}).$$

Equality implies that $G - S$ has exactly two components which contain 1 and $n - \kappa - 1$ vertices, and that any two vertices of G are adjacent, unless they belong to two different components of $G - S$, which in turn implies that $G = H_{n,\kappa}$. ■

Proposition 4 implies several known sharp bounds on indices for graphs of given order and connectivity: a lower bound on the Wiener index (see [24]), a lower bound on the hyper-Wiener index (see [6]), a lower bound on the general hyper-Wiener index (see [42]) and an upper bound on the Harary index (see [20]), as well as a following new bound.

Corollary 3. *Let G be a graph of order n and connectivity κ. Then*

$$\pi(G) \geq 2^{n-\kappa-1},$$

with equality only if $G = H_{n,\kappa}$.

As for graphs of given order and size, a sharp upper bound for graphs of given order and connectivity κ, is known only for the Wiener index and for even κ (see [17]), but not for any of the other indices mentioned above. We now give a sharp upper bound on nondecreasing indices (a sharp lower bound on nonicreasing indices) for graphs of order n and connectivity κ, where κ is even.

In [11] it was shown that, for even κ, the distance sequence of the $\frac{\kappa}{2}$-th power of the cycle C_n, is maximal, with respect to the partial order $\leq$, among the distance sequences of all κ-connected graphs of order n.

Lemma 3. *[11] Let $\kappa \in \mathbb{N}$ be even. If G is a κ-connected graph of order n, then*

$$\mathcal{D}(G) \leq \mathcal{D}(C_n^{\kappa/2}).$$

For the special case $\kappa = 2$, i.e., for 2-connected graphs, it is easy to see that equality in Lemma 3 implies that G is 2-regular, so for $\kappa = 2$ equality holds if and only if $G = C_n$.

As a direct consequence of Lemma 3 and Proposition 1 we obtain the following theorem.

Theorem 5. *Let G be a κ-connected graph of order n, where κ is even.*
(a) If I is an nondecreasing index, then

$$I(G) \leq I(C_n^{\kappa/2}).$$

(b) If $\kappa = 2$ and I is a increasing index, then

$$I(G) \geq I(C_n^{\kappa/2}),$$

with equality if and only if G is a cycle.
(c) Corresponding statements hold if G is nonincreasing or decreasing.

Theorem 5 implies, for example that for even κ the graph $C_n^{\kappa/2}$ minimizes the Harary index and maximizes the hyper-Wiener index and the multiplicative Wiener index among all κ-connected graphs of order n. For $\kappa = 2$, the unique extremal graph is a cycle.

The above results apply only to even values of κ. We do not know if similar results hold for κ-connected graphs where κ is odd. Apart from an asymptotically sharp upper bound on the Wiener index (see [12]), no good bound on any distance-based topological index appears to be in known.

6 Maximal (outer)planar graphs, k-trees and k-degenerate graphs

In this section we consider maximal outerplanar graphs and a subclass of maximal planar graphs, Apollonian networks, which we define below. We prove our results in a more general setting, for maximal k-degenerate graphs.

Let $k \in \mathbb{N}$. A k-tree (see [5]) is a graph defined as follows. The complete graph K_{k+1} is a k-tree. If G is a k-tree, then the graph obtained from G by adding a new vertex and joining it to the vertices of a k-clique is also a k-tree. The 1-trees are exactly the trees. A graph G is k-degenerate if every induced subgraph of G contains a vertex of degree at most k (see [35]). A k-degenerate graph is maximal k-degenerate if adding any edge yields a graph that is no longer k-degenerate. It was shown in [7] that every k-tree is a maximal k-degenerate graph.

It is easy to see that for $k \leq n-1$ the graph P_n^k, i.e., the k-th power of the path P_n, is a k-tree and thus maximal k-degenerate. Bickle and Che [8] showed that the graph P_n^k maximizes the Wiener index among all maximal k-degenerate graphs, and thus among all k-trees, of order n. Modifying their proof slightly, we prove that this holds not only for the Wiener index, but for all nondecreasing indices.

Lemma 4 ([7]). *Every maximal k-degenerate graph is k-connected.*

As a direct consequence of Lemma 4 and Proposition 1 we obtain the following theorem.

Theorem 6. *Let $k, n \in \mathbb{N}$ with $1 \leq k \leq n-1$ and let G be a maximal k-degenerate graph of order n.*
(a) If I is a nondecreasing index, then

$$I(G) \leq I(P_n^k).$$

(b) If I is a nonincreasing index, then

$$I(G) \geq I(P_n^k).$$

Proof. By Proposition 1 it suffices to prove that for every maximal k-degenerate graph of order n, we have

$$\mathcal{D}(G) \leq \mathcal{D}(P_n^k). \tag{2}$$

Let k be fixed. We prove (2) by induction on n. If $n = k+1$, then $G = K_{k+1}$, so $G = P_n^k$ and (2) holds.

Let $n > k+1$ and let G be a maximal k-degenerate graph of order n. Since G is k-degenerate, G contains a vertex v of degree at most k. Since G is k-connected by Lemma 4, it follows that $G - v$ is connected. Also, $G - v$ is maximal k-degenerate. By our induction hypothesis we have

$$\mathcal{D}(G - v) \leq \mathcal{D}(P_{n-1}^k). \tag{3}$$

Let $i \in \{1, 2, \dots, \mathrm{ecc}_G(v) - 1\}$. Deleting the set of vertices at distance exactly i from v disconnects G. Since G is k-connected, this implies that are at least k vertices at distance i from v in G. Letting $s = \lfloor \frac{n-1}{k} \rfloor$, we thus obtain

$$\mathcal{D}_G(v) \leq (1^{(k)}, 2^{(k)}, \dots, (s)^{(k)}, (s+1)^{(n-1-sk)}). \tag{4}$$

Let w be an end vertex of the path P_n. It is easy to verify that $\mathcal{D}_{P_n^k}(w) = (1^{(k)}, 2^{(k)}, \dots, (s)^{(k)}, (s+1)^{(n-1-sk)})$. Now Lemma 1 in conjunction with (3) and (4) yields

$$\mathcal{D}(G) \leq \mathcal{D}(G - v) \odot \mathcal{D}_G(v) \leq \mathcal{D}(P_{n-1}^k) \odot \mathcal{D}_{P_n^k}(w) = \mathcal{D}(P_n^k),$$

which is (2), as desired. ∎

Since every k-tree is maximal k-degenerate, and P_n^k is a k-tree, Theorem 6 yields that P_n^k maximizes every nondecreasing (minimizes every nondecreasing) index for k-trees of order n.

It is well-known that every maximal outerplanar graph is a 2-tree. Among the maximal planar graphs, the planar 3-trees, also called Apollonian networks, are of interest here. They can be thought of as planar graphs that are obtained from a triangle by successively inserting a new vertex into a face of length three and joining the new vertex to the three vertices on this face by edges. It is easy to verify that the 2-tree P_n^2 is maximal outerplanar, and the 3-tree P_n^3 is an Apollonian network for $n \geq 3$. Hence we have the following corollary.

Corollary 4. *(a) Let G be a maximal outerplanar graph of order $n \geq 3$. If I is a nondecreasing (resp. nonincreasing) index, then*

$$I(G) \leq I(P_n^2) \quad (\textit{resp. } I(G) \geq I(P_n^2)).$$

(b) Let G be an Apollonian network of order $n \geq 3$. If I is a nondecreasing (resp. nonincreasing) index, then

$$I(G) \leq I(P_n^3) \quad (\textit{resp. } I(G) \geq I(P_n^3)).$$

Corollary 4 implies, for example, that among all maximal outerplanar graphs of order n, the graph P_n^2 has minimum Harary index and maximum hyper-Wiener index as well as maximum multiplicative Wiener index. Also, among all Apollonian networks of order n, the graph P_n^3 has minimum Harary index and maximum hyper-Wiener index as well as maximum multiplicative Wiener index.

Corollary 4(b) also contains as a special case a sharp upper bound on the Wiener index of Apollonian networks, which was proved by Bickle and Che [8].

We do not know if the conclusion of Corollary 4(b) holds for all maximal planar graphs. If this is the case, this would yield, among others, a sharp bound on Harary index and hyper-Wiener index for maximal planar graphs.

7 Trees with all degrees odd

In this section we consider trees in which every vertex has odd degree. We refer to such trees as odd trees. The minimum and maximum Wiener index of odd trees was determined by [36]. For further results on the Wiener index of odd trees see [21, 22]. For other indices, the maximum or minimum value for odd trees appears not to have been investigated.

It follows from the handshake lemma that odd trees have even order. Let $n \in \mathbb{N}$ be even, $n \geq 4$. Let S_n be the star of order n. If $n \geq 4$ define the tree T_n as the tree obtained from a path $P_{n/2+1}$ by attaching a leaf to each internal vertex of the path. Clearly, T_n is an odd tree of order n.

Theorem 7. *Let T be an odd tree of order n, where $n \geq 4$.*
(a) If I is a nondecreasing index, then

$$I(G) \leq I(T_n).$$

(b) If I is a nonincreasing index, then

$$I(G) \geq I(T_n).$$

Proof. By Proposition 1 it suffices to prove that for every odd tree T of order n, $n \geq 4$ we have

$$\mathcal{D}(T) \leq \mathcal{D}(T_n). \tag{5}$$

We prove (5) by induction on n. If $n = 4$, then $T_4 = S_4$ is, up to isomorphism, the only odd tree of order 4, so (5) holds for $n = 4$.

Now assume that $n \geq 6$, and that (5) holds for all odd trees of order less than n. Let P be a longest path in T. Let v_1 be its end vertex and w the unique neighbor of v. Since $\deg_T(w)$ is odd, vertex w has at least one other leaf neighbor v_2. Consider the tree $T - \{v_1, v_2\}$. Observe that $T - \{v_1, v_2\}$ is an odd tree. We express $\mathcal{D}(T)$ in terms of $\mathcal{D}(T - \{v_1, v_2\}$ and $\mathcal{D}_{T-v_2}(v_1)$. Clearly, v_1 and v_2 have the same distance sequence in T, and $\mathcal{D}_T(v_1) = \mathcal{D}_T(v_2) = \mathcal{D}_{T-v_2}(v_1) \odot (2)$. Hence

$$\mathcal{D}(T) = \mathcal{D}_{T-\{v_1,v_2\}} \odot \mathcal{D}_{T-v_2}(v_1) \odot \mathcal{D}_{T-v_2}(v_1) \odot (2). \tag{6}$$

We bound the terms on the right hand side of (6) separately. Applying our inductive hypothesis to the odd tree $T - \{v_1, v_2\}$ yields

$$\mathcal{D}(T - \{v_1, v_2\}) \leq \mathcal{D}(T_{n-2}). \tag{7}$$

Consider $\mathcal{D}_{T-v_2}(v_1)$. Apart from the neighbor w of v in T', every internal vertex of T' has degree at least 3. This implies that there are at least two vertices at distance j from v_1 for every $j \in \{3, 4, \ldots, \text{ecc}_{T-v_2}(v_1)\}$. Hence,

$$\mathcal{D}_{T'}(v_1) \leq (1, 2, 3^{(2)}, 4^{(2)}, \ldots, (\frac{n}{2})^{(2)}). \tag{8}$$

Substituting (7) and (8) into (6), we obtain

$$\begin{aligned}
\mathcal{D}(T) &\leq \mathcal{D}(T_{n-2}) \oplus (1, 2, 3^{(2)}, 4^{(2)}, \ldots, (\frac{n}{2})^{(2)}) \\
&\quad \oplus (1, 2, 3^{(2)}, 4^{(2)}, \ldots, (\frac{n}{2})^{(2)}) \odot (2) \\
&= \mathcal{D}(T_{n-2}) \oplus (1^{(2)}, 2^{(3)}, 3^{(4)}, 4^{(4)}, \ldots, (\frac{n}{2})^{(4)}).
\end{aligned}$$

It is easily verified that $\mathcal{D}(T_n) = \mathcal{D}(T_{n-2}) \oplus (1^{(2)}, 2^{(3)}, 3^{(4)}, 4^{(4)}, \ldots, (\frac{n}{2})^{(4)})$ for $n \geq 6$. Hence we obtain that $\mathcal{D}(T) \leq \mathcal{D}(T_n)$, which is (5). ■

Corollary 5. *Among all odd trees of order n, the tree T_n maximizes the hyper-Wiener index and the multiplicative Wiener index, and minimizes the Harary index.*

8 Conclusion

In this paper we considered graphs of given order and size, graphs of given order and (even) connectivity, maximal k-degenerate graphs of given order, and odd trees of given order. We proved that in each of these graph classes there is a graph whose distance sequence is maximal or minimal withe respect to the partial order $\leq$. This yielded new sharp bounds on increasing or decreasing distance-based topological indices. It would be interesting to find other graph classes in which a similar approach yields bounds on distance based topological indices.

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