Wiener indices of maximal k-degenerate graphs

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Abstract

A graph is *maximal k-degenerate* if each induced subgraph has a vertex of degree at most k and adding any new edge to the graph violates this condition. In this paper, we provide sharp lower and upper bounds on Wiener indices of maximal k-degenerate graphs of order $n \geq k \geq 1$. A graph is *chordal* if every induced cycle in the graph is a triangle and chordal maximal k-degenerate graphs of order $n \geq k$ are *k-trees*. For k-trees of order $n \geq 2k+2$, we characterize all extremal graphs for the upper bound.

keywords: k-tree, maximal k-degenerate graph, Wiener index

1 Introduction

The *Wiener index* of a graph G, denoted by $W(G)$, is the the summation of distances between all unordered vertex pairs of the graph. The concept was first introduced by Wiener in 1947 for applications in chemistry [15], and has been studied in terms of various names and equivalent concepts such as the total status [11], the total distance [9], the transmission [13], and the *average distance* (or, *mean distance*) [8].

A graph with a property $\mathcal{P}$ is called *maximal* if it is complete or if adding an edge between any two non-adjacent vertices results in a new graph that does not have the property $\mathcal{P}$. Finding bounds on Wiener indices of maximal planar graphs of a given order has attracted attention recently, see [5, 6]. For a maximal planar graph of order $n \geq 3$, its Wiener index has a sharp lower bound $n^2 - 4n + 6$. An *Apollonian network* is a chordal maximal planar graph. Wiener indices of Apollonian networks of order $n \geq 3$ have a sharp upper bound $\lfloor \frac{1}{18}(n^3 + 3n^2) \rfloor$, which also holds for maximal planar graphs of order $3 \leq n \leq 10$, and was conjectured to be valid for all $n \geq 3$ in [5]. It was shown [6] that if G is a k-connected maximal planar graph of order n, then the mean distance $\mu(G) = \frac{W(G)}{\binom{n}{2}} \leq \frac{n}{3k} + O(\sqrt{n})$ for $k \in \{3, 4, 5\}$ and the coefficient of n is the best possible.

Let k be a positive integer. A graph is k-degenerate if its vertices can be successively deleted so that when deleted, they have degree at most k. Note that Apollonian networks are maximal 3-degenerate graphs. In this paper, we provide sharp lower and upper bounds for Wiener indices of maximal k-degenerate graphs of order n and some extremal graphs for all $n \geq k \geq 1$. The lower and upper bounds on Wiener indices are equal for maximal k-degenerate graphs whose order implies that they have diameter at most 2. The extremal graphs for the lower bound have a nice description for 2-trees. Maximal k-degenerate graphs with diameter at least 3 have order at least $2k + 2$. For k-trees of order $n \geq 2k + 2$, we charcterize all extremal graphs whose Wiener indices attain the upper bound. Our results generalize well-known sharp bounds on Wiener indices of some important classes of graphs such as trees and Apollonian networks.

2 Preliminaries

All graphs considered in the paper are simple graphs without loops or multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Then the order of G is $n = |V(G)|$ and the size of G is $|E(G)|$. Let K_n and P_n denote the clique and the path of order n respectively. Let $\overline{K}_n$ be the compliment of K_n, that is, the graph on n isolated vertices. Let $G + H$ be the graph obtained from G and H by adding all possible edges between vertices of G and vertices of H. A complete bipartite graph $K_{r,s}$ is $\overline{K}_r + \overline{K}_s$.

A graph is *connected* if there is a path between any two vertices of the graph. The *distance* between two vertices u, v of a graph G is the length of a shortest path joining u and v in G, and denoted by $d_G(u, v)$. The distance between two vertices from different components is infinite if G is disconnected. The *eccentricity* $e_G(u)$ of a vertex u in G is the maximum distance between u and other vertices of G. The set of all vertices with distance i from the vertex u in G is denoted by $N_G(u, i)$ for $1 \leq i \leq e_G(u)$. In particular, the set of all vertices adjacent to vertex u in G is denoted by $N_G(u)$, and its cardinality $|N_G(u)|$ is called the degree of vertex u. The *diameter* of G, denoted by $diam(G)$, is the maximum distance between any two vertices of G. A subgraph H of G is said to be *isometric* in G if $d_H(x, y) = d_G(x, y)$ for any two vertices x, y of H. The *status* (or, *transmission*) of a vertex u in G, denoted by $\sigma_G(u)$, is the summation of the distances between u and all other vertices in G.

Lemma 2.1 *[2, 9] Let G be a connected graph. Then*

(i) $W(G) \geq 2\binom{n}{2} - |E(G)|$, and the equality holds if and only if $diam(G) \leq 2$.

(ii) $W(G) \leq W(G - v) + \sigma_G(v)$ for any vertex v of G, and the equality holds if and only if $G - v$ is isometric in G.

(iii) $W(G) = \sum_{i=1}^{diam(G)} i \cdot d_i$, where d_i is the number of unordered vertex pairs with distance i in G.

We are interested in k-degenerate graphs and maximal k-degenerate graphs, introduced in [12]. A subclass of maximal k-degenerate graphs called k-trees [3] is particularly important.

A k-*tree* is a generalization for the concept of a tree and can be defined recursively: a clique K_k of order $k \geq 1$ is a k-tree, and any k-tree of order $n+1$ can be obtained from a k-tree of order $n \geq k$ by adding a new vertex adjacent to all vertices of a clique of order k, which is called the *root* of the newly added vertex, and we say that the newly added vertex is *rooted* at the specific clique. By definitions, the order of a maximal k-degenerate graph can be any positive integer, while the order of a k-tree is at least k. A graph is a k-*tree* if and only if it is a chordal maximal k-degenerate graph of order $n \geq k$ [1]. A graph is maximal 1-degenerate if and only if it is a tree [12]. It is known [14] that 2-trees form a special subclass of planar graphs extending the concept of maximal outerplanar graphs, and maximal outerplanar graphs are the only 2-trees that are outerplanar. Planar 3-trees are just Apollonian networks.

The k-*th power of a path* P_n, denoted by P_n^k, has the same vertex set as P_n and two distinct vertices u and v are adjacent in P_n^k if and only if their distance in P_n is at most k. Note that the order n of P_n^k can be any positive integer. When $n \geq k$, P_n^k is a special type of k-tree. For $n \geq 2$, P_n^k is an extremal graph for the upper bound on Wiener indices of maximal k-degenerate graphs of order n.

A graph is called k-*connected* if the removal of any $k-1$ vertices of the graph does not result in a disconnected or trivial graph. It is well-known that for a k-connected graph G of order n, $diam\,(G) \leq \frac{n-2}{k} + 1$. Since maximal k-degenerate graphs of order $n \geq k+1$ are k-connected [12], this bound holds for them, and a characterization of the extremal graphs (among maximal k-degenerate graphs) appears in [1].

Lemma 2.2 *[4, 10] Let G be a k-connected graph of order $n \geq k+1$ and $k \geq 1$. Then $\sigma_G(x) \leq (\lfloor \frac{n-2}{k} \rfloor + 1)(n - 1 - \frac{k}{2}\lfloor \frac{n-2}{k} \rfloor)$ for any vertex x of G. Moreover, $\sigma_G(x)$ attains the upper bound if and only if x satisfies both properties: (i) $e_G(x) = diam(G) = \lfloor \frac{n-2}{k} \rfloor + 1$, and (ii) $|N_G(x,i)| = k$ for all $1 \leq i \leq \lfloor \frac{n-2}{k} \rfloor$.*

If the graphs in consideration are maximal k-degenerate graphs, then the upper bound on vertex status in Lemma 2.2 can be achieved by any degree-k vertex of P_n^k for all $n \geq k+1$ and $k \geq 1$. Furthermore, the extremal graphs are exactly paths P_n when $k = 1$. If $k \geq 2$, then the extremal graphs can be different from P_n^k [1].

3 Sharp Bounds

Theorem 3.1 *Let G be a k-degenerate graph of order $n \geq k \geq 1$. Then*

$$W(G) \geq n^2 - (k+1)n + \binom{k+1}{2}.$$

The equality holds if and only if G is maximal k-degenerate with $diam(G) \leq 2$.

Proof. By Lemma 2.1 (i), $W(G) \geq 2\binom{n}{2} - |E(G)|$ and the equality holds if and only if G has diameter at most 2. By Proposition 3 in [12], a k-degenerate graph G of order $n \geq k$ has $|E(G)| \leq kn - \binom{k+1}{2}$. Moreover, a k-degenerate graph G of order $n \geq k$ is maximal if and only if $|E(G)| = kn - \binom{k+1}{2}$, [1]. Therefore, $W(G) \geq n(n-1) - kn + \binom{k+1}{2} = n^2 - (k+1)n + \binom{k+1}{2}$, and the equality holds exactly when G is maximal k-degenerate with $diam(G) \leq 2$. □

This bound is sharp since for $k \leq n \leq k+1$, the only maximal k-degenerate graph is K_n. For $n \geq k+2$, $K_k + \overline{K}_{n-k}$ achieves the bound.

Theorem 3.2 *Let G be a maximal k-degenerate graph of order $n \geq 2$ and $D = \left\lfloor \frac{n-2}{k} \right\rfloor$. Then*

$$W(G) \leq W\left(P_n^k\right) = \sum_{i=0}^{D} \binom{n-ik}{2} = \binom{n}{2} + \binom{n-k}{2} + \ldots + \binom{n-Dk}{2}.$$

Proof. We show $W(G) \leq W\left(P_n^k\right)$ using induction on order n. When $2 \leq n \leq k+2$, P_n^k is the only such graph, so it is extremal. Let G be a maximal k-degenerate graph of order $n \geq k+3$, and assume the result holds for all maximal k-degenerate graphs of smaller orders. By [12], G has a vertex v of degree k and $G-v$ is a maximal k-degenerate graph. Thus $W(G-v) \leq W\left(P_{n-1}^k\right)$.

Label vertices of P_n^k along the path P_n as $v_1, v_2, \ldots, v_n$ where $n \geq k+3$. It is clear that P_n^k is k-connected and $\sigma_{P_n^k}(v_n)$ achieves the bound in Lemma 2.2. By Lemma 2.1(iii), $W(G) \leq W(G-v) + \sigma_G(v) \leq W\left(P_n^k - v_n\right) + \sigma_{P_n^k}(v_n) = W\left(P_n^k\right)$.

Note $W\left(P_n^k\right) = \binom{n}{2}$ when $2 \leq n \leq k+1$, so that the formula holds then. In P_n, there are $n-i$ pairs of vertices with distance i. Now distances $rk-k+1$ through rk in P_n become r in P_n^k. Since $diam\left(P_n^k\right) = D+1$, by Lemma 2.1(iii),

$$\begin{aligned}
W\left(P_n^k\right) =& 1(n-1) + \ldots + 1(n-k) \\
&+ 2(n-k-1) + \ldots + 2(n-2k) \\
&+ 3(n-2k-1) + \ldots + 3(n-3k) \\
&+ \ldots \\
&+ D(n-(D-1)k-1) + \ldots + D(n-Dk) \\
&+ (D+1)(n-Dk-1) + \ldots + (D+1)1 \\
=& (n-1+\ldots+1) + (n-k-1+\ldots+1) + (n-2k-1+\ldots+1) \\
&+ \ldots + (n-(D-1)k-1+\ldots+1) + (n-Dk-1+\ldots+1) \\
=& \binom{n}{2} + \binom{n-k}{2} + \binom{n-2k}{2} + \ldots + \binom{n-(D-1)k}{2} + \binom{n-Dk}{2}
\end{aligned}$$

□

We now provide a closed form expression for $W\left(P_n^k\right)$ for all $n \geq 2$.

Corollary 3.3 *Let $n \geq 2$ and $n-2 \equiv i \mod k$ for $0 \leq i \leq k-1$. Then*

$$W\left(P_n^k\right) = \frac{n^3}{6k} + \frac{(k-1)n^2}{4k} + \frac{(k-3)n}{12} + \frac{-2i^3 + 3i^2(k-3) - i\left(k^2-9k+12\right) - 2k^2 + 6k - 4}{12k}.$$

Proof. We have

$$
\begin{aligned}
W\left(P_n^k\right) &= \sum_{i=0}^{D} \binom{n-ik}{2} = \sum_{i=0}^{D} \frac{1}{2}\left(n-ik\right)\left(n-ik-1\right) \\
&= \sum_{i=0}^{D} \left[\left(\frac{n^2}{2}-\frac{n}{2}\right)+\left(\frac{k}{2}-kn\right)i+\frac{k^2}{2}i^2\right] \\
&= \sum_{i=0}^{D} \left(\frac{n^2}{2}-\frac{n}{2}\right)+\sum_{i=0}^{D}\left(\frac{k}{2}-kn\right)i+\sum_{i=0}^{D}\frac{k^2}{2}i^2 \\
&= \left(D+1\right)\left(\frac{n^2}{2}-\frac{n}{2}\right)+\frac{D\left(D+1\right)}{2}\left(\frac{k}{2}-kn\right)+\frac{D\left(D+1\right)\left(2D+1\right)}{6}\frac{k^2}{2} \\
&= \frac{k^2}{6}D^3+\left(\frac{k}{4}+\frac{k^2}{4}-\frac{kn}{2}\right)D^2+\left(\frac{k}{4}+\frac{k^2}{12}-\frac{n}{2}-\frac{kn}{2}+\frac{n^2}{2}\right)D-\frac{n}{2}+\frac{n^2}{2}
\end{aligned}
$$

Since $D=\left\lfloor\frac{n-2}{k}\right\rfloor$, $n-2=Dk+i$ for $0\le i\le k-1$. Substituting $D=\frac{n-2-i}{k}$ into the above and simplifying, we obtain the formula. □

If $1\le k\le 5$, this formula can be reduced to $W\left(P_n^k\right)=\left\lfloor\frac{2n^3+3(k-1)n^2+k(k-3)n}{12k}\right\rfloor$. Formulas for small values of k and the beginnings of the resulting sequences are given in the following table. These sequences occur (shifted) in OEIS. For $1\le k\le 3$, they have many different combinatorial interpretations.

k	$W\left(P_n^k\right)$	Sequence	OEIS
1	$\frac{n^3-n}{6}$	0, 1, 4, 10, 20, 35, 56, 84, 120, 165, ...	A000292
2	$\left\lfloor\frac{n^3+1.5n^2-n}{12}\right\rfloor$	0, 1, 3, 7, 13, 22, 34, 50, 70, 95, ...	A002623
3	$\left\lfloor\frac{n^3+3n^2}{18}\right\rfloor$	0, 1, 3, 6, 11, 18, 27, 39, 54, 72, ...	A014125
4	$\left\lfloor\frac{n^3+4.5n^2+2n}{24}\right\rfloor$	0, 1, 3, 6, 10, 16, 24, 34, 46, 61, ...	A122046
5	$\left\lfloor\frac{n^3+6n^2+5n}{30}\right\rfloor$	0, 1, 3, 6, 10, 15, 22, 31, 42, 55, ...	A122047

4 Extremal Graphs

Any graph of order n and diameter 1 is a clique and has Wiener index $\binom{n}{2}$. Any maximal k-degenerate graph of diameter 1 is K_n, $2\le n\le k+1$, which is also P_n^k. Recall that a graph G of order n and diameter 2 has $W(G)=n(n-1)-|E(G)|$, and a maximal k-degenerate graph G of order $n\ge k$ has $|E(G)|=kn-\binom{k+1}{2}$. Then any maximal k-degenerate graph of order $n\ge k$ and diameter 2 has $W(G)=n(n-1)-kn+\binom{k+1}{2}=\binom{n}{2}+\binom{n-k}{2}$. Therefore, when $k\le n\le 2k+1$, the lower bound given in Theorem 3.1 and the upper bound given in Theorem 3.2 are the same, and any maximal k-degenerate graph of order n has this value for its Wiener index.

Maximal 1-degenerate graphs are just trees and so all maximal 1-degenerate graphs of diameter 2 are just stars. For $k \geq 2$, the graphs $K_k + \overline{K}_{n-k}$ are maximal k-degenerate graphs of diameter 2, but there are others.

We are able to characterize 2-trees of diameter 2. But the situation becomes complicated as k gets larger.

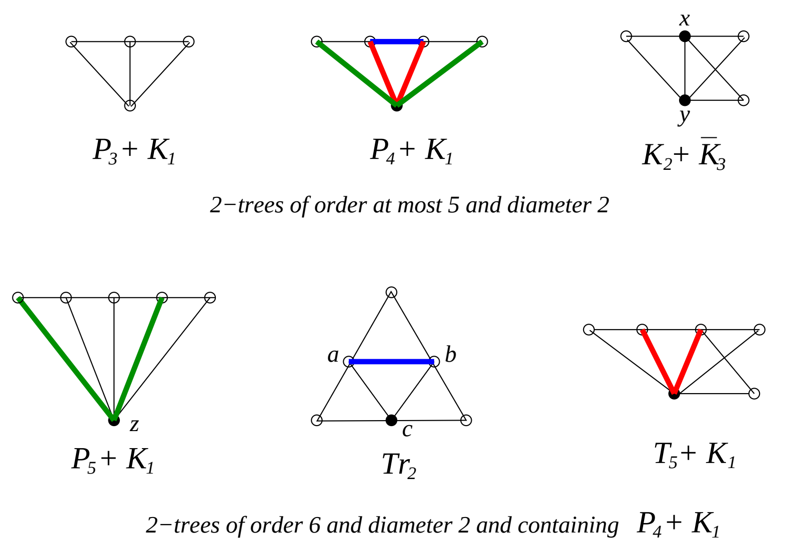

Figure 1: Examples of 2-trees.

Proposition 4.1 *Let G be a 2-tree with diameter 2. Then G is isomorphic to $T + K_1$ for a tree T, or a graph formed by adding any number of vertices adjacent to pairs of vertices of K_3. In particular, the maximal outerplanar graphs with diameter 2 are fans $P_{n-1} + K_1$ and the triangular grid Tr_2. See Figure 1.*

Proof. By its recursive definition, the diameter of 2-trees cannot decrease as order increases. Any 2-tree with diameter 2 must have order at least 4. There is a unique 2-tree with diameter 2 and order 4, $P_4^2 = P_3 + K_1$. The 2-trees of diameter 2 and order 5 are $P_5^2 = P_4 + K_1$ and $K_2 + \overline{K}_3 = K_{1,3} + K_1$.

It is easily seen that 2-tree not containing $P_4 + K_1$ is $K_{1,r} + K_1$ because any additional vertices must be rooted at the edge xy of $K_2 + \overline{K}_3$, see Figure 1. Let G be a 2-tree of order at least 6 and with diameter 2 containing $P_4 + K_1$. Then it cannot contain P_6^2, the smallest 2-tree with diameter 3. It is easy to check that G has three possibilities.

Case 1. G contains $P_5 + K_1$. Then any additional vertices must be rooted on edges incident with K_1 (the vertex z), or else it will contain P_6^2.

Case 2. G contains the triangular grid graph Tr_2. Then the only edges that can be used as roots are those of the central clique K_3 (the triangle abc), or else it will contain P_6^2.

Case 3. G roots all additional vertices on the edges between vertices of degree 3 and 4 in $P_4 + K_1$.

Graphs in Case 1 and Case 3 can be described as $T + K_1$, where T is a tree. Graphs in Case 2 are formed by adding vertices rooted at edges from a fixed clique K_3.

Maximal planar graphs are exactly the 2-trees that are outerplanar [14]. A graph is outerplanar if and only if it does not contain a subdivision of K_4 or $K_{2,3}$ [7]. Thus any maximal outerplanar graph with diameter 2 is either a fan $P_{n-1}+K_1$ or the triangular grid Tr_2. □

Since any maximal k-degenerate graph of order $n \geq k+1$ is k-connected and $diam(G) \leq \lfloor \frac{n-2}{k} \rfloor + 1$ for a k-connected graph G of order n, any maximal k-degenerate graph of diameter at least 3 has order $n \geq 2k+2$.

Theorem 4.2 *Let G be a k-tree of order $n \geq 2k+2$ and $k \geq 1$. Then $W(G) = \sum_{i=0}^{\lfloor \frac{n-2}{k} \rfloor} \binom{n-ik}{2}$ exactly when $G = P_n^k$.*

Proof. We use induction on order n. By the recursive definition of a k-tree, G can be constructed from a clique K_k, and the i-th vertex added is adjacent to at least $k-i+1$ vertices of the above clique. Thus the smallest order of a k-tree with diameter 3 is $n = 2k+2$, and the only such k-tree is P_{2k+2}^k. So, the result holds for the base case when $n = 2k+2$.

Let G be a k-tree of order $n \geq 2k+3$ that maximizes $W(G)$, and assume the result holds for all k-trees of order $n-1$. By the recursive definition of a k-tree, G has a vertex v of degree k such that $G-v$ is a k-tree. By Lemma 2.1(ii), $W(G) \leq W(G-v) + \sigma_G(v)$.

Maximizing $W(G-v)$ requires that $G-v$ is the extremal graph P_{n-1}^k. Number the vertices of $G-v$ along the path from 1 to $n-1$. Since k-trees of order at least $k+1$ are k-connected, $\sigma_G(v)$ is maximized when $N_G(v) = \{1, 2, ..., k\}$ (or $N_G(v) = \{n-k, ..., n-1\}$) since it achieves the bound in Lemma 2.2. When $n \geq 2k+3$, any other choice for $N_G(v)$ has $|N_G(v, 2)| > k$, so $\sigma_G(v)$ is not maximized. Thus $G = P_n^k$, and Theorem 3.2 provides the formula. □

Note that for $k > 1$, there is a unique extremal graph for k-trees to achieve the upper bound in Theorem 3.2 when $k \leq n \leq k+2$ or $n \geq 2k+2$, but not when $k+3 \leq n \leq 2k+1$.

By Theorem 3.1, Theorem 3.2 and Corollary 3.3, we have the following sharp bounds on Wiener indices of maximal k-degenerate graphs for $1 \leq k \leq 3$.

Corollary 4.3 *Let G be a maximal k-degenerate graph of order $n \geq k \geq 1$.*

1. *If $k = 1$, then G is a tree and $n^2 - 2n + 1 \leq W(G) \leq \frac{n^3}{6} - \frac{n}{6}$. The extremal graphs for the bounds are exactly $K_1 + \overline{K}_{n-1}$ and P_n respectively, see [9].*

2. *If $k = 2$, then $n^2 - 3n + 3 \leq W(G) \leq \frac{n^3}{12} + \frac{n^2}{8} - \frac{n}{12} - \frac{1}{16} + \frac{(-1)^n}{16}$.*

   For 2-trees, the extremal graphs for the lower bound are characterized in Proposition 4.1; the extremal graphs for the upper bound are P_n^2 and $K_2 + \overline{K}_3$ (of order 5), see Theorem 4.2.

   For maximal outerplanar graph of order $n \geq 3$ (that is, outerplanar 2-trees), the extremal graphs for the lower bound are fans $P_{n-1} + K_1$ and the triangular grid graph Tr_2 if $n = 6$; and the extremal graphs for the upper bound are P_n^2.

3. *If* $k = 3$*, then* $n^2 - 4n + 6 \le W(G) \le \lfloor \frac{n^3}{18} + \frac{n^2}{6} \rfloor$.

For 3*-trees, it is easily checked that the extremal graphs for the upper bound are* P_n^3*,* $K_3 + \overline{K}_3$ *of order 6 and four others of order* 7 *which are* $K_3 + \overline{K}_4$*,* $K_2 + T_5$*, where* T_5 *is the tree of order 5 that is neither a path nor a star,* $P_5 + K_2$*, and the graph formed from* K_4 *by adding degree* 3 *vertices inside* 3 *regions. See Figure 2.*

For Apollonian networks (planar 3*-trees), the upper bound was given in [5]. The extremal graphs for the upper bound are* P_n^3 *and the last two graphs of order* 7 *in Figure 2.*

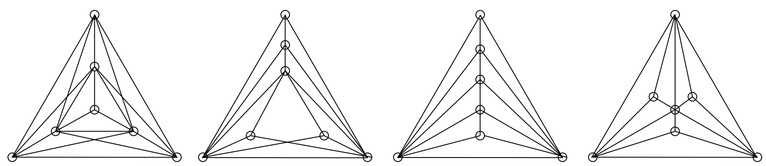

Figure 2: Examples of 3-trees of order 7.

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