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ORIGINAL PAPER

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 summation of distances between all unordered vertex pairs of the graph. The concept was first introduced by Wiener in 1947 for applications in chemistry [17], and has been studied in terms of various names and equivalent concepts such as the total status [13], the total distance [10], the transmission [16], and the *average distance* (or, *mean distance*) [9].

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 [7, 8, 12]. For a maximal planar graph of order $n \geq 3$, its Wiener index has a sharp lower bound $n^2 - 4n + 6$. An *Apollonian*

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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 [7]. Recently, the conjecture was confirmed in [12]. With an extra condition on vertex connectivity, it was shown [8] 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 $n \geq k \geq 1$. When the lower and upper bounds on Wiener indices are equal for maximal k-degenerate graphs of order n, their diameters are at most 2, which implies that $k \leq n \leq 2k + 1$. The extremal graphs for the lower bound have a nice description for 2-trees of diameter at most 2. 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 characterize 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 1 [4, 10] *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 [14]. A subclass of maximal k-degenerate graphs called k-trees [1] 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 $n \geq k$ [2]. A graph is maximal 1-degenerate if and only if it is a tree [14]. It is known [15] 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 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 [14], this bound holds for them, and a characterization of the extremal graphs (among maximal k-degenerate graphs) appears in [2].

The following upper bound on vertex status of a k-connected graph of order n can be obtained by the fact that $\sigma_G(x) = \sum_{i=1}^{e_G(x)} i \cdot |N_G(x,i)|$ [4, 10]. An equivalent upper bound formula was first appeared in [11, Remark 2.6.1]. without reference papers available.

Lemma 2 [6, 11] *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) $e_G(x) = \text{diam}(G) = \lfloor \frac{n-2}{k} \rfloor + 1$, *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 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 [2].

3 Sharp Bounds

Theorem 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 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 [14], 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 $|E(G)| = kn - \binom{k+1}{2}$, [2]. 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 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*

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

Proof We show that $W(G) \leq W\left(P_n^k\right)$ 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 that the result holds for all maximal k-degenerate graphs of smaller orders. By [14], 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. By Lemma 1 (ii), $W(G) \leq W(G-v) + \sigma_G(v) \leq W\left(P_n^k - v_n\right) + \sigma_{P_n^k}(v_n) = W\left(P_n^k\right)$.

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 1 (iii),

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

□

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

Corollary 1 *Let $n \geq 2$ and $n-2 \equiv j \bmod k$ for $0 \leq j \leq k-1$. Then*

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

Proof We have

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

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

If $1 \leq k \leq 5$, 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 the On-Line Encyclopedia of Integer Sequences (OEIS). For $1 \leq k \leq 3$, they have many different combinatorial interpretations, which are listed in OEIS.

k	$W(P_n^k)$	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 1 and the upper bound given in Theorem 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 $k \ge 2$, 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.

Proposition 1 *The following statements are equivalent for a 2-tree G :*

1. *G has diameter at most 2.*
2. *G does not contain P_6^2.*
3. *G is $T + K_1$ for any tree T, or any graph formed by adding any number of vertices adjacent to pairs of vertices of K_3. See Fig. 1.*

Proof (3 ⇒ 1) The graphs described all have diameter at most 2.

(1 ⇒ 2) (contrapositive) We see P_6^2 is a 2-tree with diameter 3. Adding a new degree 2 vertex v to a 2-tree cannot decrease its diameter, since v's neighbors are adjacent. Thus a 2-tree containing P_6^2 has diameter at least 3.

(2 ⇒ 3) Assume G does not contain P_6^2. The 2-trees with orders 4 and 5 ($K_4 - e$, $P_4 + K_1$, and $K_2 + \overline{K}_3$) don't contain P_6^2 and can be described as $T + K_1$. Any 2-tree not containing $P_4 + K_1$ is $K_1 + K_{1,r}$, because any additional vertices must be rooted

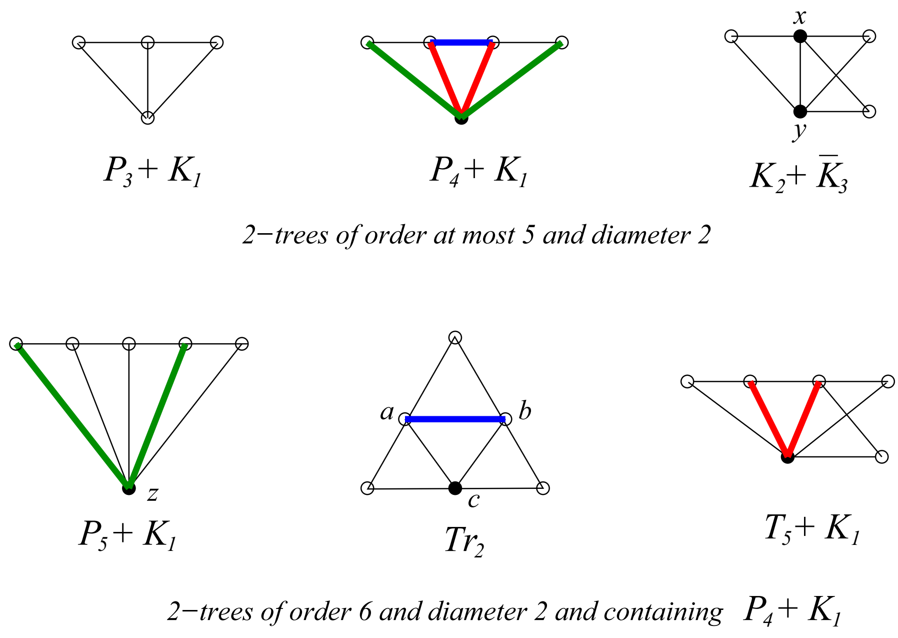

Fig. 1 Examples of 2-trees

at the edge xy of $K_2 + \overline{K}_3$, see Fig. 1. Assume G has order at least 6. Since it does not contain P_6^2, there are 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 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 outerplanar graphs are exactly the 2-trees that are outerplanar [15]. A graph is outerplanar if and only if it does not contain a subdivision of K_4 or $K_{2,3}$ [5]. Thus we have the following corollary.

Corollary 2 *The maximal outerplanar graphs with diameter at most* 2 *are fans* $P_{n-1} + K_1$ *and the triangular grid* Tr_2.

A characterization of all maximal 2-degenerate graphs with diameter 2, generalizing Proposition 1, has been proved in [3].

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 3 *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 definition, a k-tree 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 starting clique. Thus the smallest order of a k-tree with diameter 3 is $n = 2k+2$. To achieve this, there is a unique choice (up to isomorphism) for the neighborhood of each newly added vertex. Since P_{2k+2}^k has diameter 3, this is the k-tree that is constructed. Thus the result holds for the base case of $n = 2k+2$.

Let G be a k-tree of order $n \geq 2k+3$ that maximizes $W(G)$, and assume that the result holds for all k-trees of order $n-1$. By the definition of a k-tree, G has a vertex v of degree k such that $G - v$ is a k-tree. By Lemma 1(ii), $W(G) \leq W(G-v) + \sigma_G(v)$. We will show that G simultaneously achieves the maximum possible values of $W(G-v)$ and $\sigma_G(v)$, which means that no extremal graph exists that does not do so.

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 $N_G(v) = \{1, 2, \ldots, k\}$ (or $N_G(v) = \{n-k, \ldots, n-1\}$) since it achieves the bound in Lemma 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 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 2 when $k \leq n \leq k+2$ or $n \geq 2k+2$, but not when $k+3 \leq n \leq 2k+1$.

By Theorems 1, 2 and Corollary 1, we have the following sharp bounds on Wiener indices of maximal k-degenerate graphs for $1 \leq k \leq 3$.

Corollary 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 [10].*
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 1; the extremal graphs for the upper bound are P_n^2 and $K_2 + \overline{K}_3$ (of order 5), see Theorem 3.
   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 $n^2 - 4n + 6 \leq W(G) \leq \lfloor \frac{n^3}{18} + \frac{n^2}{6} \rfloor$.*
   For 3-trees, it is easily checked that the extremal graphs for the upper bound

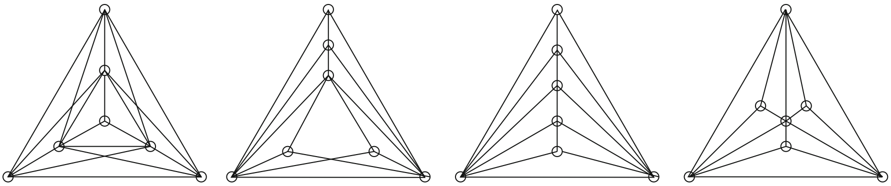

Fig. 2 Examples of 3-trees of order 7

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 Fig.* 2.

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

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