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A Survey of Recent Extremal Results on the Wiener Index of Trees

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Abstract

The Wiener index of a connected graph is defined as the sum of distances between all unordered pairs of its vertices. In this paper, we survey the known extremal results about the Wiener index of trees and the roots of the Wiener polynomials of trees from 2014 together with some open problems.

1 Introduction

All graphs considered in this paper are simple and connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance of a vertex v, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G. The distance between vertices u and v of G is denoted by $d_G(u,v)$. The Wiener index of a connected graph G is defined as

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

The Wiener index belongs among the oldest graph-based structure descriptors (topological indices) which was first introduced by Wiener [42] for predicting the boiling points of paraffins. Nowadays, the Wiener index is considered as one of the most applicable topological indices. Numerous of its basic mathematical properties are well studied [4,9,34] and accumulated in the surveys [6,7,17,36].

Chemists are often interested in the Wiener index of certain trees which represent some acyclic organic molecules. Many researches are devoted to studying the extremal trees that maximize or minimize the Wiener index within certain classes of trees.

In 2001, Dobrynin, Entringer and Gutman [6] summarized a great deal of knowledge (both mathematical and chemical) on the Wiener index of trees, including many extremal results. The other extremal results on the Wiener index of trees from 2002 to 2013 were collected in the survey [36] by Xu et al..

In this review, we focus our attention to the extremal results on the Wiener index of trees appeared from 2014 to this moment. We also restrict our survey to the above defined Wiener index, and avoid to examine the related distance-based indices such as hyper-Wiener index, Harary index, Wiener polarity index, reciprocal complementary Wiener index, the terminal Wiener index and similar.

In the sequel, for convenience of discussion, we need some further terminologies and notations.

The degree $deg_G(v)$ of a vertex v in G is the number of edges of G incident with v. The *degree sequence* of a graph is the non-increasing sequence of its vertex degrees. In a tree, a vertex of degree one is called a *pendent vertex*, and a vertex of degree at least three is called a *branching vertex*.

A *segment* of a tree T is a path-subtree S whose terminal vertices are branching or pendent vertices of T. The length of a segment S is equal to the number of edges in S and it is denoted by l_S. Dobrynin, Entringer and Gutman (see Section 5 of [6]) summarized many applications of this concept to the calculation of the Wiener index of trees. If a tree T has segments S_1, S_2, ...,S_m, then the sequence $(l_{S_1}, l_{S_2}, ..., l_{S_m})$ is called the *segment sequence* of T. It is known that [6, p. 229] a sequence $(t_1, t_2, ..., t_m)$ $(m \geq 3)$ of positive integers is a segment sequence of an $n-$vertex tree if and only if

$$t_1 + t_2 + ... + t_m + 1 = n.$$

Let G be a connected graph. The eccentricity of a vertex v of G, denoted by $ecc_G(v)$, is defined by $ecc_G(v) = max_{w \in V(G)} d_G(v, w)$. The diameter of a graph G, denoted by $diam(G)$, is the maximum eccentricity in G. Similarly, the radius of G, denoted by $rad(G)$, is the minimum eccentricity in G. The *center* of G, denoted by $Cr(G)$, is the set of vertices with minimum eccentricity.

A maximal subtree containing a vertex v of a tree T as a pendent vertex will be called a *branch of T at v.* The *weight of a branch B*, denoted by $BW_T(B)$ is the number of edges in it. The *branch weight of a vertex v*, denoted by $BW_T(v)$ is the maximum of the weights of the branches at v. The *centroid* of a tree T , denoted by $Cd(T)$, is the set of vertices of T with minimum branch weight. The center and centroid play special roles with respect to the Wiener index of trees, the reader may see Section 3 of [6] for a general introduction.

For a tree T, we remark that $Cr(T)$ may not coincide with $Cd(T)$. Let T be the tree as shown in Figure 1, then $Cr(T) = \{c_1, c_2\}$. A direct calculation gives that $d_T(u) = 22$, $d_T(c_1) = 24$, $d_T(c_2) = 28$, $d_T(v_1) = 40$, $d_T(v_2) = 30$, $d_T(v_3) = d_T(v_4) = d_T(v_5) = d_T(v_6) = 26$, $d_T(v_7) = 34$, $d_T(v_8) = 42$ and $d_T(v_9) = 52$. Thus, $Cd(T) = \{u\}$ and $Cd(T) \cap Cr(T) = \emptyset$.

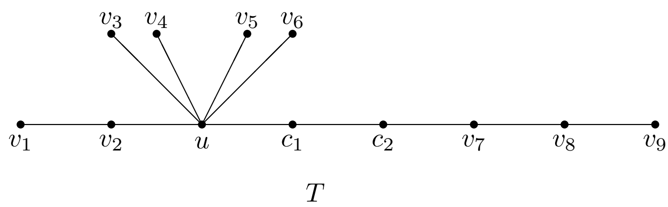


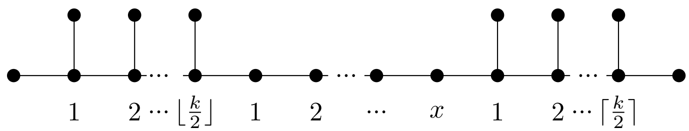
Figure 1. The tree T

We now introduce some special trees which will frequently appeared in several extremal results.

The unique n-vertex trees with 2 and $n-1$ pendent vertices are called the *path* and *star* and denoted by P_n and S_n, respectively. A tree T is called a *caterpillar* if the tree obtained from T by removing all pendent vertices is a path.

The *dumbbell* $D(n, a, b)$ consists of the path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P and b independent vertices adjacent to the other pendent vertex.

For a real number x, the symbols $\lfloor x \rfloor$ and $\lceil x \rceil$ denote the greatest integer not exceeding the real number x and the smallest integer not less than x, respectively. The following $n-$vertex tree $M(n,k)$ depicted in Figure 2 will appear in several extremal results.



$M(n,k)$

$x = n - 2k - 2$

Figure 2. The tree $M(n,k)$

2 On the minimum and maximum Wiener index of trees with some fixed parameters

In this section, we give a survey of lower and upper bounds for the Wiener index of trees of given order with some fixed parameters.

The trees with a given diameter that minimise the Wiener index were characterized in [27, 41]. There have been many attempts to overcome the corresponding maximisation problem [27, 28, 37, 41]. In 2019, Sun et al. [35] investigated the question that which graphs with a given diameter attains the maximum value with respect to the Wiener index. One result (see Theorem 6 of [35]) implied the following.

Theorem 1 ([35]). If T is a tree on n vertices with diameter $n-c$, where c is a constant and n is large enough relative to c, then

$$W(T) \le W(D(n, \lfloor \tfrac{c+1}{2} \rfloor, \lceil \tfrac{c+1}{2} \rceil)),$$

the equality holds if and only if $T = D(n, \lfloor \frac{c+1}{2} \rfloor, \lceil \frac{c+1}{2} \rceil)$.

Sun et al. [35] pointed out that for the general case $c \geq 3$, Theorem 1 holds for $n \geq \frac{1}{6}(7c^3 - 18c^2 + 23c - 6)$.

Recently, Das et al. [5] obtained the trees with the maximal Wiener index among all trees with given order and radius (see Theorem 3.1 of [5]).

Theorem 2 ([5]). Let T be a tree on n vertices with radius r. Then

$$W(T) \leq r(n-r)[n - r + \frac{r(r-1)}{n-1}]$$

with the equality holding if and only if $T = S_n$.

Now we turn our attention to trees with some degree restrictions. Many researches are devoted to this topics, we refer the reader to two surveys [6, 36] for extremal trees with respect to the Wiener index with specific degree condition, such as trees with given number of pendent vertices.

In particular, as for trees with given degree sequence, Wang [40] and Zhang et al. [43] independently determined the tree that minimizes the Wiener index among trees of given degree sequence. But the following problem from [16, 31, 44] is still open, although it is known for longer time that extremal graphs are caterpillars [30].

Problem 1([16, 31, 44]). Which trees maximize the Wiener index among trees of given degree sequence?

In [10, 11, 19], the trees extremal with respect to the Wiener index as well as the trees with the first few smallest and first few greatest Wiener indices were determined in the class of trees of order $2n$ whose all vertices have odd degrees.

Let $\mathbb{ET}_{n,r}$ be the set of all $n-$vertex trees with exactly $r(\geq 1)$ vertices of even degree and let $S(n, m)$ be an $n-$vertex tree obtained from m disjoint paths (each has $\lceil \frac{n-1}{m} \rceil$ or $\lfloor \frac{n-1}{m} \rfloor$ vertices) by attaching one endvertex of each path to a new vertex a.

In [22], the trees which minimize and maximize the Wiener index among all trees with given number of vertices of even degree were characterized respectively by the author of present paper.

Theorem 3 ([22]). Let $T \in \mathbb{ET}_{n,r}$, where $1 \leq r < n - 2$ and $n \equiv r$

(mod 2). Then

$$W(S(n,n-r)) \leq W(T) \leq W(M(n, \frac{n-r-2}{2}))\,,$$

with the left equality if and only if $T = S(n,n-r)$ and right equality if and only if $T = M(n, \frac{n-r-2}{2})$.

Branchings are natural characteristics of the structure of a tree. In [21], the lower bound and the upper bound of the Wiener index of an $n-$vertex tree with given number of branching vertices were obtained respectively by the author of present paper.

Let $\mathbb{BT}_{n,r}$ be the set of all $n-$vertex trees having exactly r branching vertices and let $B(n,r)$ be the tree shown in Figure 3.

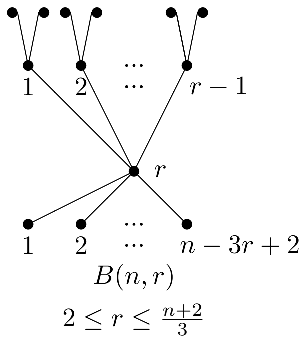


Figure 3. The tree $B(n,r)$

Theorem 4 ([21]). Let $T \in \mathbb{BT}_{n,r}$, where $1 \leq r \leq \frac{n}{2} - 1$, then the following holds.
(a) $W(T) \leq W(M(n,r))$,
with equality if and only if $T = M(n,r)$.
(b) If $r = 1$, then

$$W(T) \geq W(S_n),$$

with equality if and only if $T = S_n$,
if $2 \leq r \leq \frac{n}{2} - 1$, then

$$W(T) \geq (n-r)(n-1) + 3(r-1)(n-3),$$

moreover, if n and r satisfy one of the following conditions:

$$\text{(b-1) } r = 2,\ n \geq 6,$$

$$\text{(b-2) } r = 3,\ n \geq 8,$$

$$\text{(b-3) } 4 \leq r \leq \tfrac{n+2}{3},$$

then the above bound is sharp and $B(n, r)$ is the unique tree realizing this bound.

Let $\mathbb{MT}_{n,k}$ be the set of trees of order n with exactly $k(\leq n-2)$ vertices of maximum degree. Note that the path P_n is the unique element in $\mathbb{MT}_{n,n-2}$. In [23], the trees with the maximal Wiener index in $\mathbb{MT}_{n,k}$ were characterized by the author of present paper.

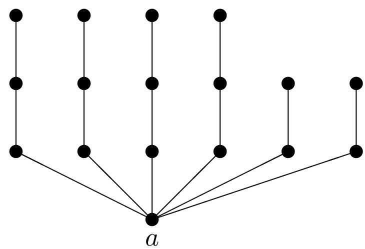
Theorem 5 ([23]). Let $T \in \mathbb{MT}_{n,k}$, where $1 \leq k \leq n-3$. Then

$$W(T) \leq W(M(n,k)),$$

with equality if and only if $T = M(n, k)$.

The following problem proposed in [23] is still open to the present moment.

Problem 2 ([23]). Characterize the tree(s) with the minimal Wiener index in $\mathbb{MT}_{n,k}$.



$ST(17, 6)$

Figure 4. The tree $ST(17, 6)$

Let $\mathbb{ST}_{n,t}$ be the set of all $n-$vertex trees with exactly t segments. Note that the path P_n is the unique element in $\mathbb{ST}_{n,1}$, the star S_n is the unique element in $\mathbb{ST}_{n,n-1}$ and the set $\mathbb{ST}_{n,2}$ is empty. So in the following we only consider the class $\mathbb{ST}_{n,t}$ with $3 \le t \le n-2$. Let $ST(n,m)$ be an $n-$vertex tree obtained from m disjoint paths (each has $\lceil \frac{n-1}{m} \rceil$ or $\lfloor \frac{n-1}{m} \rfloor$ vertices) by attaching one endvertex of each path to a new vertex a, see Figure 4 for an example.

In [24], the trees with the minimal Wiener index in the class $\mathbb{ST}_{n,t}$ were characterized by Song and one author of present paper.

Theorem 6 ([24]). For any tree $T \in \mathbb{ST}_{n,t}$, where $3 \le t \le n-2$, it holds that

$$W(T) \ge W(ST(n,t)),$$

with equality if and only if $T = ST(n,t)$.

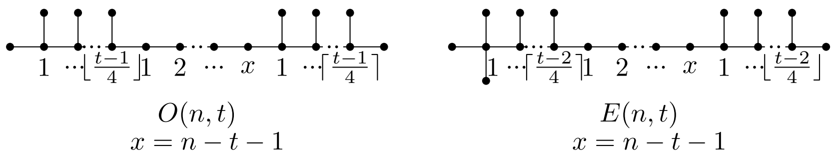


Figure 5. Two trees $O(n,t)$ and $E(n,t)$

Let $O(n,t)$ and $E(n,t)$ be the trees depicted in Figure 5.

In [1], the tree with the maximal Wiener index in the class $\mathbb{ST}_{n,t}$ was obtained by Andriantiana et al., which is a conjecture presented in [24].

Theorem 7 ([1]). Among all trees in $\mathbb{ST}_{n,t}$, $O(n,t)$ (resp. $E(n,t)$) attains the maximum value of the Wiener index for odd (resp. even) t.

For more detailed results on this topic, we refer the reader to the monograph by Wagner and Wang [38].

3 Extremal Wiener index of trees with some special structures

3.1 Trees with a P_r-factor

A subgraph F of a graph G is called a *factor* of G if F is a spanning subgraph of G. A *path factor* of a graph G is a factor of G such that each component of the factor is a path, in particular, if each component of the factor is required to be a path with exactly r vertices, such a factor is called a P_r*-factor* of G. In this sense, the well-known perfect matchings (or 1-factor) is a P_2-factor. In [12], Gutman and Rouvray proved that if T and T' are two trees with perfect matchings on equal number of vertices. then $W(T) \equiv W(T') \pmod 4$. This result was generalized by the author of present paper [20] to trees with P_r-factor and further generalized by Gutman, Xu and Liu [13] to even much larger class of graphs. In [15], K. Hriňáková, M. Konr, R. Škrekovski and A. Tepeh continued to generalized it to a large families of graphs with a tree-like structure.

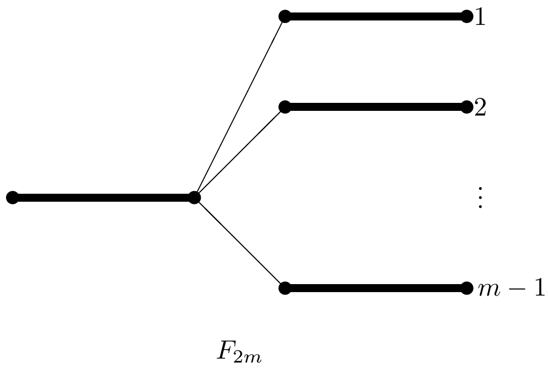


Figure 6. The tree F_{2m}

Let $\mathbb{T}_{2m}$ be the set of $2m-$vertex trees with perfect matchings and let F_{2m} be the tree shown in Figure 6. The following result was independently obtained by Du et al. [8] and Lin et al. [26].

Theorem 8 ([8, 26]). Let $T \in \mathbb{T}_{2m}$, where $m \geq 2$. Then

$$W(T) \geq W(F_{2m}),$$

with equality if and only if $T = F_{2m}$.

Let $\mathbb{F}_{P_r,k}$ be the set of trees of order kr with a P_r-factor, $k \geq 2$, $r \geq 2$. Let T^*_{kr} be the tree (depicted Figure 7) obtained from k vertex disjoint $r-$vertex paths L_1, L_2, ..., L_k by joining u_1 to each of the vertices u_2, u_3,

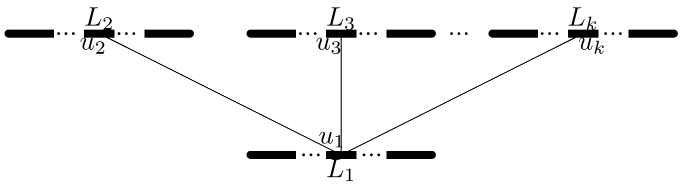


Figure 7. The tree T^*_{kr}

..., u_k, where $u_i \in Cr(L_i)$ for each $i = 1, 2, ..., k$. Clearly, $T^*_{kr} \in \mathbb{F}_{P_r,k}$. The following result was obtained by the author of present paper [25].

Theorem 9 ([25]). Let $T \in \mathbb{F}_{P_r,k}$ where $r \geq 2$ and $k \geq 2$. Then

$$W(T^*_{kr}) \leq W(T) \leq \binom{kr+1}{3},$$

with left equality if and only if $T = T^*_{kr}$ and with right equality if and only if $T = P_{kr}$.

Remark. By the definition of the P_r−factor, the perfect matching is a P_2−factor. Note that any vertex of the path P_2 belongs to $Cr(P_2)$, namely $V(P_2) = Cr(P_2)$, thus the set $\mathbb{T}_{2m}$ is just the set $\mathbb{F}_{P_2,m}$, and hence Theorem 9 is a natural generalization of Theorem 8.

It is interesting that Theorem 9 might be generalized to a even much large class of trees. Let R be the forest consisting of k disjoint trees T_1, T_2, ..., T_k. Let $\mathbb{F}_{T_1,T_2,...,T_k}$ $(k \geq 2)$ be the set of trees with R as a factor. Clearly, if for each $i = 1, 2, ..., k$, $T_i = P_r$, then $\mathbb{F}_{T_1,T_2,...,T_k} = \mathbb{F}_{P_r,k}$.

The following problem proposed in [25] by the author of present paper is still open up to now.

Problem 3 ([25]). Characterize the tree(s) with the minimal and maximal Wiener index in $\mathbb{F}_{T_1,T_2,...,T_k}$, $k \geq 2$, respectively.

3.2 Trees containing a prescribed subtree

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A graph H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.

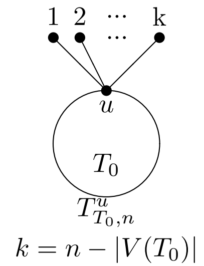


Figure 8. The tree $T^u_{T_0,n}$

Given a tree T_0 and an integer $n > |V(T_0)|$, let $\mathbb{S}_{T_0,n}$ be the set of trees of order n that contain T_0 as a subtree and let $T^u_{T_0,n}$ be the tree (see Figure 8) obtained by attaching $n - |V(T_0)|$ new vertices of degree one to one vertex, say u, in the centroid of T_0.

In [32], the trees with the minimal Wiener index in the class $\mathbb{S}_{T_0,n}$ were characterized by Song and the author of present paper.

Theorem 10 ([32]). Given a tree T_0 and an integer $n > |V(T_0)|$, then for any tree $T \in \mathbb{S}_{T_0,n}$ it holds that

$$W(T) \geq W(T^u_{T_0,n}),$$

where u is a vertex in the centroid of T_0.

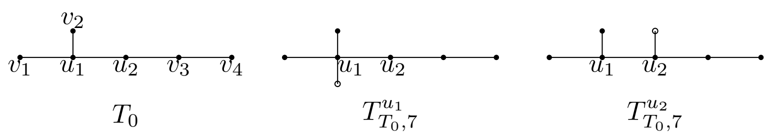


Figure 9. The trees T_0, $T^{u_1}_{T_0,7}$ and $T^{u_2}_{T_0,7}$

We remark that the set of extremal trees attain the minimum Wiener index in $\mathbb{S}_{T_0,n}$ may not consist of a single tree. Consider the 6-vertex tree T_0 in Figure 9 and the set $\mathbb{S}_{T_0,7}$. A direct calculation gives that $d_{T_0}(u_1) = d_{T_0}(u_2) = 8$, $d_{T_0}(v_1) = d_{T_0}(v_2) = 12$, $d_{T_0}(v_3) = 10$, $d_{T_0}(v_4) = 14$, thus

$Cd(T_0) = \{u_1, u_2\}$. Note that the tree $T^{u_1}_{T_0,7}$ is not isomorphic to $T^{u_2}_{T_0,7}$ (see Figure 9) and $W(T^{u_1}_{T_0,7}) = W(T^{u_2}_{T_0,7}) = 46$. Thus both $T^{u_1}_{T_0,7}$ and $T^{u_2}_{T_0,7}$ are extremal trees in Theorem 10.

The following problem proposed in [32] is still open up to now.

Problem 4 ([32]). Characterize the trees with the maximal Wiener index in $\mathbb{S}_{T_0,n}$, $n > |V(T_0)|$.

3.3 Trees with a prescribed segment sequence

Given a sequence $(l_1, l_2, ..., l_m)$ of positive integers, denote by $\mathbb{S}_{l_1,l_2,...,l_m}$ the set of all trees with the segment sequence $(l_1, l_2, ..., l_m)$, and by $S(l_1, l_2, ..., l_m)$ the tree obtained from m disjoint paths P_{l_1}, P_{l_2}, ..., P_{l_m} by adding a new vertex u and joining u to each of the vertices w_1, w_2, ..., w_m, where w_i is a terminal vertex of the path P_{l_i} for $i = 1, 2, ..., m$.

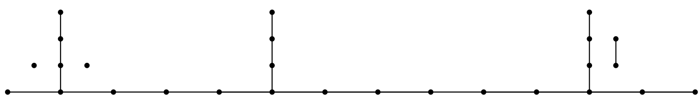
In [24], the tree with the minimal Wiener index in the class $\mathbb{S}_{l_1,l_2,...,l_m}$ was characterized by Song and the author of present paper.

Theorem 11 ([24]). For any tree $T \in \mathbb{S}_{l_1,l_2,...,l_m}$, $m \geq 3$, it holds that

$$W(T) \geq W(S(l_1, l_2, ..., l_m)),$$

with equality if and only if $T = S(l_1, l_2, ..., l_m)$.

This leaves the natural question which trees with segment sequence $(l_1, l_2, ..., l_m)$ maximize the Wiener index. The answer to this question seems to be much more complicated,



R

Figure 10. A quasi caterpillar R

Define a *quasi-caterpillar* to be a tree with the property that all its branching vertices lie on a path, see Figure 10 for an example. Let the longest path of a quasi-caterpillar containing all the branching vertices be called the *backbone*, all segments that do not lie on the backbone (and thus connect a pendent vertex with a branching vertex) are called *pendant segments*.

In [1], Andriantiana et al. obtained the following result which is a conjecture presented in [24] proposed by Song and the author of present paper.

Theorem 12 ([1]). Let T_{max} be the tree with the maximum Wiener index among all trees with segment sequence $(l_1, l_2, ..., l_m)$, then T_{max} is a quasi-caterpillar.

In [1], Andriantiana et al. also presented some further characteristics of extremal quasi-caterpillars.

Theorem 13 ([1]). A quasi-caterpillar that maximizes the Wiener index among trees with segment sequence $(l_1, l_2, ..., l_m)$ must satisfy the following:

1. If the number of segments is odd, all branching vertices have degree exactly 3. If the number of segments is even, all but one of the branching vertices have degree 3. The only exception must be a branching vertex of degree 4, which must be the first (or last) branching vertex on the backbone. This also means that the number of segments on the backbone is $k = \lfloor \frac{m+1}{2} \rfloor$, the number of pendant segments is $k' = \lceil \frac{m-1}{2} \rceil$,

2. The lengths of the segments on the backbone, listed from one end to the other, form a unimodal sequence r_1, r_2, ..., r_k, i.e.,

$$r_1 \leq r_2 \leq ... \leq r_j \geq ... \geq r_k$$

for some $j \in \{1, 2, ..., k\}$,

3. The lengths of the pendant segments, starting from one end of the backbone towards the other, form a sequence of values s_1, s_2, ..., $s_{k'}$ such that

$$s_1 \geq s_2 \geq ... \geq s_{j'} \leq ... \leq s_{k'}$$

for some $j' \in \{1, 2, ..., k'\}$.

The following problem from [1, 24] is still open.

Problem 5 ([1,24]). Which trees maximize the Wiener index among trees of given segment sequence $(l_1, l_2, ..., l_m)$?

4 Extremal results of the roots of the Wiener polynomials of trees

The Wiener polynomial (Hosoya polynomial) of a connected graph G is

$$W(G,x) = \sum_{i=1}^{diam(G)} d_i(G)x^i,$$

where $diam(G)$ is the diameter of G, and $d_i(G)$ is the number of unordered pairs of vertices of G at distance i.

The Wiener polynomial was introduced in [14] and independently in [29]. It is easy to see that the Wiener index of a graph is equal to the derivative of its Wiener polynomial evaluated at $x = 1$. Data on Wiener polynomials of all trees with up to 10 vertices are available [33]. Some basic properties of the Wiener polynomial of trees can be found in [3], we also refer the reader to [6] for details.

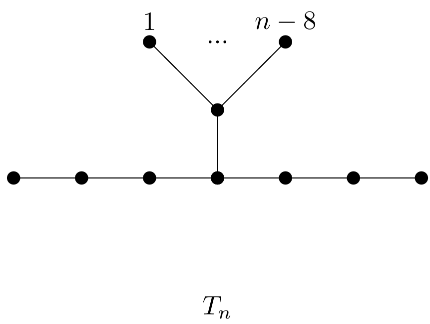


Figure 11. The tree T_n

In 2018, Brown et al. investigated the roots of the Wiener polynomials of graphs [2]. In 2020, Wang proved the following theorem ([39], Theorem 1.4]) which solved a problem of [2]. Let T_n be the tree depicted in Figure 11.

Theorem 14 ([39]). Among all trees on $n > 31$ vertices, the tree T_n uniquely attains the maximum modulus among all the roots of its Wiener polynomial.

In [2], Brown et al. also proved that there are connected graphs (even trees) with roots of their Wiener polynomials having arbitrarily large imaginary part and there are connected graphs (even trees) with roots of their Wiener polynomials having arbitrarily large positive real part ([2], Proposition 4.1 and Proposition 4.2).

5 Conclusion

This survey gathers all the extremal results on the Wiener index of trees from 2014 to this moment and presents some open problems in order to inspire readers to obtained new extremal results on this topic.

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