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Wiener Index of Trees: Theory and Applications

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Abstract. The Wiener index W is the sum of distances between all pairs of vertices of a (connected) graph. The paper outlines the results known for W of trees: methods for computation of W and combinatorial expressions for W for various classes of trees, the isomorphism–discriminating power of W, connections between W and the center and centroid of a tree, as well as between W and the Laplacian eigenvalues, results on the Wiener indices of the line graphs of trees, on trees extremal w.r.t. W, and on integers which cannot be Wiener indices of trees. A few conjectures and open problems are mentioned, as well as the applications of W in chemistry, communication theory and elsewhere.

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1. Introduction

The graph considered is G and it is assumed that G is connected. The vertex and edge sets of G are $V(G)$ and $E(G)$. The number of vertices of G is denoted by $n(G)$.

The distance between vertices u and v of G is denoted by $d_G(u, v)$. The *Wiener index* of G is denoted by $W(G)$ and is defined by

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

Consequently, the average distance between the vertices of G, denoted by $\mu(G)$, is given by $\mu(G) = W(G)/\binom{n(G)}{2}$.

The name *Wiener index* or *Wiener number* for the quantity defined in Equation (1) is usual in chemical literature, since Harold Wiener [116] in 1947 seems to be the first who considered it. Wiener himself conceived W only for acyclic molecules and defined it in a slightly different – yet equivalent – manner; the definition of the Wiener index in terms of distances between vertices of a graph, such as in Equation (1), was first given by Hosoya [73].

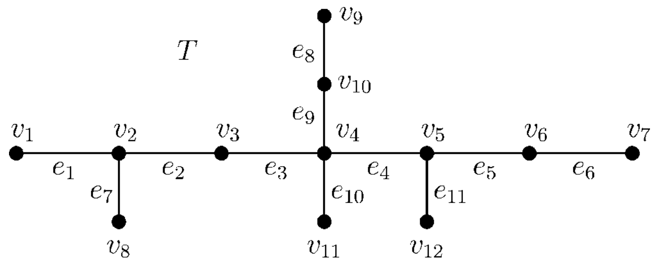

Figure 1. Acyclic molecular graph.

In the mathematical literature W seems to be first studied only in 1976 [32]; for a long time mathematicians were unaware of the (earlier) work on W done in chemistry (cf. the book [6]). The names *distance of a graph* [32] and *transmission* [102] were also used to denote W.

The *distance of a vertex* v is the sum of distances between v and all other vertices of G. This quantity is denoted by $d_G(v)$.

A tree is a connected acyclic graph. In what follows T always denotes a tree. The sets of vertices and edges of a tree T are denoted by $V(T)$ and $E(T)$, respectively; $|V(T)| = n(T)$ and $|E(T)| = n(T) - 1$. In what follows we assume that $n \geqslant 3$. Each pair of vertices of a tree is connected by a unique path.

A vertex of degree one will be called a *pendent vertex*. A tree on n vertices has at least 2 and at most $n-1$ pendent vertices. The (unique) n-vertex trees with 2 and $n-1$ pendent vertices are called the *path* and *star*, respectively, and are denoted by P_n and S_n, respectively.

Every vertex of a tree T, having degree 3 or greater, is called a *branching point* of T. The paths are the only trees without a branching point.

The vast majority of chemical applications of the Wiener index deal with acyclic organic molecules; for reviews see [64, 70, 108, 109, 110]. The molecular graphs of these are trees [63]. (For instance, the tree T from Figure 1 is the molecular graph of the hydrocarbon 2, 4, 5-trimethyl-4-ethyl heptane.) In view of this, it is not surprising that in the chemical literature there are numerous studies of properties of the Wiener indices of trees.

We mention in passing that in recent chemical studies a generalization of the Wiener-index-concept found noteworthy applications:

$$W_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^\lambda,$$

where λ is some real number. For further details and additional references see [58, 67, 84, 120].

There are two groups of closely related problems which have attracted the attention of researchers for a long time:

– how $W(T)$ depends on the structure of T;
– how $W(T)$ can be efficiently calculated, especially without the aid of a computer (by so-called 'paper-and-pencil' methods).

Investigations of the above problems mainly deal with a tree as the sole object. Other directions of investigation include studies of relations between $W(T)$ and the corresponding invariants of elements of the tree T (vertices, subtrees).

In addition to the myriad applications of the Wiener index in chemistry there are many situations in communication, facility location, cryptology, etc., that are effectively modeled by a connected graph G satisfying certain restrictions. Because of cost restraints one is often interested in finding a spanning tree of G that is optimal with respect to one or more properties. Average distance between vertices is frequently one of these properties. For example, we will consider the problem of finding a spanning tree T of G that has minimum Wiener index [75].

2. Wiener Index for Series of Trees

For a large number of trees (or more precisely: classes of trees) closed combinatorial expressions for W can be found. The best known of them are

$$W(P_n) = \binom{n+1}{3} \quad \text{and} \quad W(S_n) = (n-1)^2. \tag{2}$$

These formulas have been reported in many papers, the first time in [32]. For other expressions of this kind see [4, 69, 76, 103, 104]. Methods for systematic generation of such expressions are developed in [43, 88]. In [32] and in many subsequent works (see especially [49, 57]) it has been demonstrated that if T is any n-vertex tree different from P_n and S_n, then

$$W(S_n) < W(T) < W(P_n). \tag{3}$$

Let T_n be obtained by attaching to T_{n-1} a new pendent vertex. From Equations (2) and (3) it follows that $W(T_n)$ increases at least as a quadratic polynomial, and at most as a cubic polynomial of n. Indeed, for many reasonably chosen classes of trees such polynomials have been found [4, 43, 69, 76, 88, 103, 104].

It has been shown that the expected value of the Wiener index of certain large classes of trees is, save for a constant factor, the geometric mean of the extremes n^2 and n^3. Specifically, it was shown that the expected value of $W(T)$ over all (ordered) (rooted labeled) (or rooted binary) trees T of order n is asymptotic to $Cn^{5/2}$ where C is a constant depending only on the class of trees. Precise definitions and proofs can be found in [34].

Progress in chemical synthesis inspires great interest in new classes of trees having largely unknown properties. As an example we mention dendrimers which are extremely branched molecules (see [69, 70] and the references cited therein). Two families of regular dendrimer trees $T_{k,d}$ are shown in Figure 2 where d is the degree of a nonpendent vertex and k denotes the distance between the central vertex

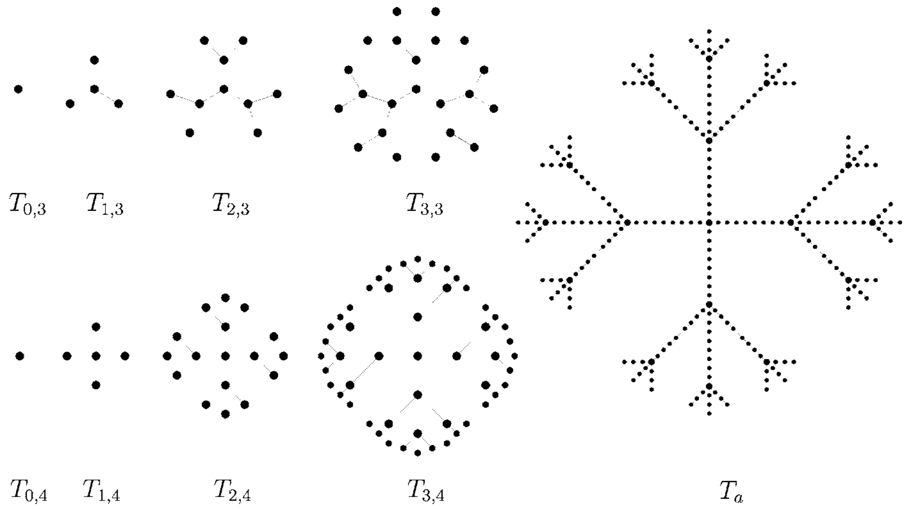

Figure 2. Molecular graphs of dendrimers.

and the pendent vertices. Arborol T_a, having 253 vertices, belongs to another kind of dendrimers (see Figure 2). For every $d \geqslant 3$, the tree $T_{k,d}$ has order

$$n(T_{k,d}) = 1 + \frac{d}{d-2}\big[(d-1)^k - 1\big]$$

and its Wiener index is

$$W(T_{k,d}) = \frac{1}{(d-2)^3}\big[(d-1)^{2k}[kd^3 - 2(k+1)d^2 + d] + + 2d^2(d-1)^k - d\big]. \quad (4)$$

For large values of k, $W \sim kn^2$ irrespective of the value of d, $d \geqslant 3$. This property may be of relevance to the understanding of the fractal nature of dendritic molecules [70].

The chemically most interesting cases of Equation (4) correspond to $d = 3, 4$:

$$W(T_{k,3}) = (9k - 15)2^{2k} + 18 \cdot 2^k - 3$$

and

$$W(T_{k,4}) = \left(4k - \frac{7}{2}\right)3^{2k} + 4 \cdot 3^k - \frac{1}{2}.$$

3. The Center and Centroid of a Tree

Before continuing our discussion of techniques and formulas for calculating the Wiener indices of trees we recall some definitions and properties of vertices that play special roles with respect to the Wiener index.

A maximal subtree containing a vertex v of a tree T as a pendent vertex will be called a *branch of T at v*. For instance, the tree T on Figure 1 has four branches at vertex v_4.

The *weight of a branch B*, denoted by $\mathrm{BW}_T(B)$ is the number of edges in it. The *branch weight of a vertex v*, denoted by $\mathrm{BW}_T(v)$ is the maximum of the weights of the branches at v. Thus, for the tree depicted in Figure 1, $\mathrm{BW}_T(v_4) = 4$. As before, we suppress some subscripts when there is no danger of ambiguity.

The centroid of a tree T, denoted by $C(T)$, is the set of vertices of T with minimum branch weight. It is easily verified that for the tree T of Figure 1, $C(T) = \{v_4\}$.

Jordan [78] has characterized the centroid of a tree.

THEOREM 1. *If $C = C(T)$ is the centroid of a tree T of order n then one of the following holds:*

(i) *$C = \{c\}$ and $\mathrm{BW}(c) \leqslant (n-1)/2$,*
(ii) *$C = \{c_1, c_2\}$ and $\mathrm{BW}(c_1) = \mathrm{BW}(c_2) = n/2$.*

In both cases, if $v \in V(T) \setminus C$ then $\mathrm{BW}(v) \geqslant n/2$.

Zelinka [119] characterized the set of vertices with minimum distance in a tree.

THEOREM 2. *The set of vertices with minimum distance in a tree T is the centroid of T.*

Combining these results we arrive at:

COROLLARY 2.1. *A vertex v of a tree has minimum distance (and, thus, is in $C(T)$) if and only if $\mathrm{BW}(v) \leqslant (n-1)/2$.*

The next result provides one way of calculating the Wiener index [32].

THEOREM 3. *Suppose $e = (x, y)$ is an edge of a connected graph G. Let $n_1(e)$ be the number of vertices of G closer to x than to y and let $n_2(e)$ be the number of vertices of G closer to y than to x. Then $d(x) - d(y) = n_2(e) - n_1(e)$.*

The following extension of Zelinka's theorem is an immediately consequence of Theorem 3.

COROLLARY 3.1. *If $v = v_1, v_2, \ldots, v_k = w$ is a path from a centroid vertex v to a pendent vertex w of the tree T and v_2 is not in $C(T)$, then $d(v_1) < d(v_2) < \cdots < d(v_k)$.*

The above results point out the importance of centroid and pendent vertices in distance considerations. Consequently, relations among the three quantities, $W(T)$, $d_T(v)$, and $d_T(w)$, where T is a tree, $v \in C(T)$, and w is a pendent vertex of T, play an important role in the study of the Wiener index of trees.

We shall have some use, also, of the following related concepts.

The *eccentricity* of a vertex v of a connected graph G, denoted by $\mathrm{ECC}_G(v)$, is defined by $\mathrm{ECC}_G(v) = \max_{w \in V(G)} d(v, w)$. The *center* of G is the set of vertices with minimum eccentricity. As with the centroid, the center of a tree consists of a single vertex or two adjacent vertices. The *diameter* of a graph G is defined by $D = D(G) = \max_{v \in V(G)} \mathrm{ECC}_G(v)$.

4. Computing the Wiener Index of a Tree

Probably the first idea that occurs for calculating Wiener indices is to try to do this recursively. Let T be a tree, v a pendent vertex of T and u the vertex adjacent to v. Then the vertex pairs of T can be divided into two groups: those which do not contain v and those which do contain v. The sum of distances of the vertex pairs of the first type is just the Wiener index of the subgraph $T - v$. If $x \in V(T - v)$, then

$$d_T(v, x) = d_{T-v}(u, x) + 1$$

implying that the sum of distances of the vertex pairs of the second type is equal to $n(T) - 1 + d_{T-v}(u)$. Consequently,

$$W(T) = W(T - v) + d_{T-v}(u) + n(T - v), \tag{5}$$

i.e., in order to calculate $W(T)$ recursively, we must know both the Wiener index and a certain vertex distance of a pertinent subgraph of T.

Canfield *et al.* [9] elaborated a recursive approach for calculation of the Wiener index of a general tree, representing just a generalization of formula (5). We state their result as Theorem 4.

Let $m \geqslant 2$. Let $T_1, T_2, \ldots, T_m$ be trees with disjoint vertex sets and orders $n_1, n_2, \ldots, n_m$. Let for $i = 1, 2, \ldots, m$, $w_i \in V(T_i)$. In the general case, any tree T on more than two vertices can be viewed as being obtained by joining a new vertex u to each of the vertices $w_1, w_2, \ldots, w_m$ as shown in Figure 3.

THEOREM 4. *Let T be a tree on $n \geqslant 3$ vertices, whose structure is specified above. Then*

$$W(T) = \sum_{i=1}^{m} \left[W(T_i) + (n - n_i) d_{T_i}(w_i) - n_i^2 \right] + n(n - 1). \tag{6}$$

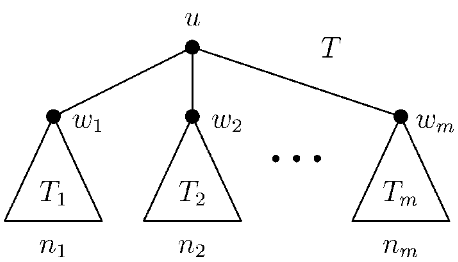

Figure 3. Branching point u of a tree T.

The application of Equation (6) in actual calculations is rather cumbersome and, from a practical point of view, Equation (6) is inferior to several other calculation methods. Indeed, Dankelmann [15] obtained the following result as a corollary to his method for computing the average distance of interval graphs.

THEOREM 5. *The average distance of a tree of order n is computable in time* $O(n)$.

Results equivalent to Theorem 5 are found also in [14, 99].

There are also nonrecurrent formulas containing distances of vertices. The following formula shows how irregularity of the distances of adjacent vertices influences W [25].

THEOREM 6. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{4}\left[n^2(n-1) - \sum_{(u,v)\in E(T)} [d_T(v) - d_T(u)]^2\right]. \tag{7}$$

For vertices of any pendent edge, $[d_T(v) - d_T(u)]^2 = (n-2)^2$ and this value is maximal among all edges. In view of Theorem 3 the minimal value of $[d_T(v) - d_T(u)]^2$, equal to zero, will be achieved if and only if $|C(T)| = 2$ and $u, v \in C(T)$.

The right-hand side of the expression $W(T) = (1/2)\sum_v d_T(v)$ may be regarded as a half-sum of vertex distances with unit weights. The next formula demonstrates how to compute the Wiener index if the weights are the vertex degrees.

THEOREM 7. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{4}\left[n(n-1) + \sum_{v\in V(T)} \deg(v) d_T(v)\right]. \tag{8}$$

Three different proofs of this formula are known [25, 46, 85]. The sum from Equation (8) is the main part of a new topological index (Schultz index) which has found interesting applications in chemistry [101].

A much more efficient calculation method is found in Wiener's first paper devoted to the quantity W [116]. It is based on the observation that $W(T)$ is equal to the number of edges in the paths between all pairs of vertices of the tree T. Consider the characteristic function for edges:

$$I_T(u, v, i) = \begin{cases} 1, & \text{if the edge } e_i \text{ belongs to the path connecting } u \text{ and } v, \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$d_T(u, v) = \sum_{e_i \in E(T)} I_T(u, v, i).$$

Now, instead of counting the edges in paths, we may count the paths going through a given edge, and then sum the result over all edges. Bearing in mind that each pair of vertices of a tree is connected by a unique path, yields:

$$W(T) = \sum_{\{u,v\}\subset V(T)} \sum_{e_i\in E(T)} I_T(u, v, i) = \sum_{e_i\in E(T)} \sum_{\{u,v\}\subset V(T)} I_T(u, v, i).$$

Let $e = (x, y)$ be an edge of T. Then, as in Theorem 3, let $n_1(e)$ be the number of vertices of T lying closer to x than to y and let $n_2(e)$ be the number of vertices of T lying closer to y than to x.

THEOREM 8. *Let T be a tree on n vertices. Then*

$$W(T) = \sum_{e\in E(T)} n_1(e)n_2(e). \tag{9}$$

Theorem 8, discovered by Wiener in 1947, happens to be the first mathematical result on the Wiener index [116]. Curiously, however, although this article of Wiener has been often quoted in the literature, Theorem 8 was overlooked until the mid 1980s, when it was re-stated in the book [63] (with due reference to [116]).

The quantities $n_1(e)$ and $n_2(e)$ can be formally defined for an edge $e = (x, y)$ as

$$\begin{aligned} n_1(e) &= |\{v \mid v \in V(T), d_T(v, x) < d_T(v, y)\}|, \\ n_2(e) &= |\{v \mid v \in V(T), d_T(v, y) < d_T(v, x)\}|, \end{aligned}$$

which straightforwardly can be generalized to all graphs. The idea to consider the right-hand side of Equation (9) for an arbitrary graph produced some quite interesting results; for a review see [52].

Another generalization of Theorem 8 was recently offered by showing how it has to be modified so as to apply to all binary Hamming graphs [82].

For practical application of Wiener's formula (9) one should observe that $n_1(e)$ and $n_2(e)$ are just the numbers of vertices lying on the two sides of the edge e. Further, because $n_1(e) + n_2(e) = n(T)$, it is sufficient to count the vertices from only one side of each edge.

For instance, in the case of the tree T in Figure 1, for the edge e_1: $n_1 = 1$ and therefore $n_2 = 11$; $n_1n_2 = 11$; the same holds for the edges $e_6, e_7, e_8, e_{10}, e_{11}$; for the edge e_2: $n_1 = 3$ and therefore $n_2 = 9$; $n_1n_2 = 27$; for the edges e_3 and e_4: $n_1 = 4$ and therefore $n_2 = 8$; $n_1n_2 = 32$; for the edges e_5 and e_9: $n_1 = 2$ and therefore $n_2 = 10$; $n_1n_2 = 20$. Therefore $W(T) = 6\cdot 11+27+2\cdot 32+2\cdot 20 = 197$.

5. Formulas for the Wiener Index Based on Branchings

Branchings and linear segments are natural characteristics of the structure of a tree. Recall that a vertex v is said to be a branching point of a tree if $\deg(v) \geqslant 3$. Every pair of neighboring branching points defines a segment in a tree. More precisely, a *segment* of a tree T is a path-subtree S whose terminal vertices are branching or pendent vertices of T (i.e., every internal vertex v of S has $\deg_T(v) = 2$). In other words, only terminal vertices of a segment may be branching (or pendent) vertices in the respective tree. The length of a segment S is equal to the number of edges in S and it is denoted by ℓ_S. For instance, arborol T_a (see Figure 2) has 36 peripheral segments of length 3, 12 segments of length 9 and 4 segments of length 9 attached to the center vertex. Denote by S^* a subpath of S containing ℓ_S vertices.

Doyle and Graver [29] discovered a result that is suitable for the calculation of the Wiener index of trees with few branching points. Consider a tree T whose structure is described in connection with Theorem 4 (see Figure 3).

THEOREM 9. *Let T be a tree on n vertices. Then*

$$W(T) = \binom{n+1}{3} - \sum_u \sum_{1 \leqslant i < j < k \leqslant m} n_i n_j n_k, \tag{10}$$

where the first summation goes over all branching points u of T.

Recall that if u is a branching point, then $m \geqslant 3$ and, consequently, for every branching point there is at least one summand of the form $n_i n_j n_k$. Recall also that the first term on the right-hand side of Equation (10) is just the Wiener index of the n-vertex path, cf. Equation (2). Every segment of a star S_n has minimal possible length; the central vertex has maximal branching and $W(S_n) = \binom{n+1}{3} - \binom{n-1}{3}$.

We illustrate the application of the Doyle–Graver formula on the example of the tree T shown in Figure 1. The three branches attached to v_2 have 1, 1 and 9 vertices. The only term $n_i n_j n_k$, originating from this branching point is $1 \cdot 1 \cdot 9 = 9$. In an analogous manner, the contribution of the branching point v_5 is $1 \cdot 2 \cdot 8 = 16$. The four branches attached to v_4 have 1, 2, 4 and 4 vertices and their contribution to the respective sum of formula (10) is $1 \cdot 2 \cdot 4 + 1 \cdot 2 \cdot 4 + 1 \cdot 4 \cdot 4 + 2 \cdot 4 \cdot 4 = 64$. This finally gives $W(T) = \binom{13}{3} - (9 + 16 + 64) = 286 - 89 = 197$.

The Doyle–Graver formula holds not only for trees, but for all geodetic graphs [6]. Applications of Equation (10), and its comparison with Equations (6) and (9) were reported in [42]. Numerous special cases of Equation (10) were worked out in [43]. Applications of the Doyle–Graver method to highly branched, but symmetrical, trees were elaborated in [69]. Of all these special cases we mention only one. If a tree T has a single branching point of degree 3, such that its branches possess a, b and c vertices, $a + b + c = n - 1$, then

$$W(T) = \binom{n+1}{3} - abc. \tag{11}$$

We apply this formula to find trees of this class having the same Wiener index. Let T, T' be trees having a unique branching vertex of degree 3. Suppose that branches of T and T' have a, b, c and a', b', c' vertices, respectively. Because of

Equation (11), $W(T) = W(T')$ if and only if $abc = a'b'c'$ and $a + b + c = a' + b' + c' = n - 1$. Among trees of this kind on $n \leqslant 30$ vertices, there are 29 pairs satisfying $W(T) = W(T')$. The smallest such trees have branches of sizes 1, 6, 6 and 2, 2, 9. A triplet of such trees with equal Wiener indices first occurs at $n = 40$ and pertains to branches with 4, 15, 20; 5, 10, 24 and 6, 8, 25 vertices.

We now mention modifications of formulas (7)–(9) based on a tree's branchings [24]. If every segment of T is an edge (i.e., $\ell_S = 1$ for any S), then Equations (7)–(9) coincide with their modifications. If all internal vertices and all edges of a segment are deleted from a tree, we have two nontrivial connected components. Denote by $n_1(S)$ and $n_2(S)$ the number of vertices of these components, $n_1(S) + n_2(S) = n(T) - \ell_S + 1$.

THEOREM 10. *Let T be a tree on n vertices. Then*

$$W(T) = \sum_S n_1(S) n_2(S) \ell_S + \frac{1}{6} \sum_S \ell_S(\ell_S - 1)(3n - 2\ell_S + 1), \tag{12}$$

where the summations go over all segments S of T.

The above result and the next theorems of this section will be also reformulated using W for segments of a tree.

COROLLARY 10.1. *Let T be a tree on n vertices. Then*

$$W(T) = \sum_S n_1(S) n_2(S) \ell_S + (n+1) \sum_S W(S) - (n+3) \sum_S W(S^*),$$

where the summations go over all segments S of T.

If T has a unique segment (i.e., T is a path), the first sum of (12) is equal to $n - 1$. Equation (12) is more convenient for the calculation of W than (9). For the arborol T_a shown in Figure 2, we have

$$\begin{aligned} W(T_a) &= 36[1 \cdot (253 - 3) \cdot 3] + 12[10 \cdot (253 - 18) \cdot 9] + \\ &\quad + 4[55 \cdot (253 - 63) \cdot 9] + \\ &\quad + [36 \cdot 6 \cdot (3 \cdot 253 - 6 + 1) + 16 \cdot 72 \cdot (3 \cdot 253 - 18 + 1)]/6 \\ &= 826,608. \end{aligned}$$

Every edge of a tree makes a contribution to the sum in formula (7). The following result demonstrates how Equation (7) may be rewritten in terms of segments of a tree.

THEOREM 11. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{12}\left[(3n^2 + 1)(n - 1) - 3 \sum_S \frac{1}{\ell_S}[d_T(u) - d_T(v)]^2 - \sum_S \ell_S^3\right], \tag{13}$$

where the summations go over all segments of T.

COROLLARY 11.1. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{4}\left[n^2(n-1) - \sum_S \frac{1}{\ell_S}[d(v) - d(u)]^2 - 2\sum_S W(S^*)\right],$$

where the summations go over all segments of T.

Since $d_T(u) - d_T(v) = [n_1(S) - n_2(S)]\ell_S$ for every segment S with terminal vertices v and u, for computational purposes it is more convenient to use the right-hand side of the above equality. Applying formula (13) to the arborol T_a, we have

$$\begin{aligned} W(T_a) &= [(3 \cdot 253^2 + 1)(253 - 1) - 3[36 \cdot (250 - 1)^2 \cdot 3 + \\ &\quad + 12 \cdot (235 - 10)^2 \cdot 9 + 4 \cdot (190 - 55)^2 \cdot 9)] - \\ &\quad - (36 \cdot 3^3 + 12 \cdot 9^3 + 4 \cdot 9^3)]/12 \\ &= 826,608. \end{aligned}$$

Recall that the degree of a vertex v is the number of edges in a star with center at v. A *generalized star* associated with a vertex v consists of this vertex, now called its branching point, and all segments beginning at v. The number of edges in a generalized star is denoted by q_v. The set of such stars covers every edge of a tree twice, i.e., $\sum_v q_v = 2(n(T) - 1)$. Denote by BP $=$ BP(T) the set of all branching points and pendent vertices of a tree T.

The next formula shows that for calculating the Wiener index it is sufficient to consider only generalized stars corresponding to the vertices of BP.

THEOREM 12. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{12}\left[(3n+1)(n-1) + 3\sum_{v \in \mathrm{BP}} q_v d_T(v) - \sum_S \ell_S^3\right], \tag{14}$$

where the second summation goes over all segments of T.

COROLLARY 12.1. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{4}\left[n(n-1) + \sum_{v \in \mathrm{BP}} q_v d_T(v) - \sum_S W(S^*)\right],$$

where the second summation goes over all segments of T.

Arborol T_a has 17 branching points and 36 pendent vertices. Because of symmetry, we need to know the distances of four vertices in T_a. Applying Equation (14), we have

$$\begin{aligned} W(T_a) &= [(3\cdot 253+1)(253-1)+3(36\cdot 3\cdot 7839+12\cdot 18\cdot 7092+ \\ &\quad +4\cdot 36\cdot 5067+1\cdot 36\cdot 3852)-(36\cdot 3^3+12\cdot 9^3+4\cdot 9^3)]/12 \\ &= 826,608. \end{aligned}$$

Theorem 13 shows how to compute the Wiener index of T through weighted distances between vertices of BP.

Consider two distinct generalized stars of T with branching points v and u. These stars and the path between v and u form a *double* (*generalized*) *star* of the respective tree. Let $q_{vu} = q_u - \ell$, where ℓ is the length of the unique segment coming from the vertex u and belonging to the path between v and u. The theorem is based on the fact that the distance of an arbitrary vertex v in a tree T may be expressed through the distances from v to all branching points of T [24]. Let T be a tree on n vertices and v be the ith vertex of an arbitrary segment S_m, $1 \leqslant i \leqslant \ell_{S_m} + 1$. Then

$$d_T(v) = \sum_u d(v,u)q_{vu} + \frac{1}{2}\left(\sum_S \ell_S^2 + n - 1\right) - (i-1)(\ell_{S_m} + 1 - i),$$

where the first summation goes over all branching points of T and the second summation goes over all segments of T. For all vertices of BP the last term of the above expression is equal to zero.

For the double star, define $Q_{uv} = [q_v - \deg(v) + 2]q_{vu} + [q_u - \deg(u) + 2]q_{uv}$. It is clear that $Q_{uv} = Q_{vu}$. If u is a pendent vertex and v is a branching point in a tree then $q_{vu} = 0$ and $Q_{uv} = (q_u + 1)q_{uv}$. If the vertices u and v are both pendent then $q_{vu} = q_{uv} = 0$ and, therefore, $Q_{uv} = 0$.

THEOREM 13. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{12}\left[(3n+1)(n-1) + 3\sum_{\{u,v\}\subseteq \mathrm{BP}} d(u,v)Q_{uv} + \sum_S \ell_S^2(3n - \ell_S)\right],$$

where the second summation goes over all segments of T.

Note that the expression under the first sum is the product of characteristics of the respective double star in the tree.

COROLLARY 13.1. *Let T be a tree on n vertices. Then*

$$W(T) = \frac{1}{4}\left[\sum_{\{u,v\}\subseteq \mathrm{BP}} d(u,v)Q_{uv} + 2n\sum_S W(S) - 2(n+1)\sum_S W(S^*)\right],$$

where the second and the third summations go over all segments of T.

6. Laplacian Eigenvalues and the Wiener Index

Let G be a graph on n vertices $v_1, v_2, \ldots, v_n$. The diagonal matrix, whose ith diagonal entry is $\deg(v_i)$, is denoted by Δ. Then the Laplacian matrix of G is defined as $L = \Delta - A$, where A is the adjacency matrix. The eigenvalues of L, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, form the Laplacian graph spectrum. If these eigenvalues are labelled so that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, then for all graphs $\lambda_n = 0$ whereas for all connected graphs $\lambda_{n-1} > 0$. The theory of Laplacian spectra of graphs has been extensively studied (for a review see [95, 96]).

The following peculiar result was communicated around 1990 independently in several papers [93, 94, 96, 97].

THEOREM 14. *Let T be a tree on n vertices. If $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ are the Laplacian eigenvalues of T, then*

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i}. \tag{15}$$

Theorem 14 is an unexpected result, because it connects the Wiener index (a quantity defined on the basis of graph distances) and matrix eigenvalues. The possible chemical implications of Equation (15) were discussed in [56, 98]. It was hoped that via Equation (15) the powerful apparatus of linear algebra would become applicable in the theory of the Wiener index. Until now no noteworthy such application could be found.

Quite recently, Chan, Lam and Merris arrived at a related result, namely they expressed $W(T)$ as a linear function of a hook immanant of $L(T)$ [13]. This (algebraic!) result was used to show that $W(T)$ is formally related to several other graph invariants of interest in chemistry [12].

The right-hand side of Equation (15) is a well defined quantity for all connected graphs. Attempts to extend the applicability of Equation (15) to graphs other than trees led to the introduction of the Kirchhoff [86] and quasi-Wiener indices [60, 98]. Eventually the two indices were shown to coincide [61], and to be both equal to the right-hand side of Equation (15).

7. Wiener Index for Line Graph of Trees

The line graph, $L(G)$, of a graph G has the vertex set $V(L(G)) = E(G)$ and two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G share a common endvertex. The concept of line graph has found various applications in chemical research [2, 35, 53]. The iterated line graph, $L^k(G)$, of G is defined as $L^k(G) = L(L^{k-1}(G))$, where $k \geqslant 1$ and $L^0(G) \equiv G$. In this section we are concerned with trees satisfying

$$W(T) = W(L^k(T)). \tag{16}$$

Table I. Numbers of n-vertex trees for which $W(T) = W(L^2(T))$.

n	9	10	11	12	13	14	15	16	17
N_n	47	106	235	551	1301	3159	7741	19320	48629
N_W	1	1	1	0	7	8	22	25	66

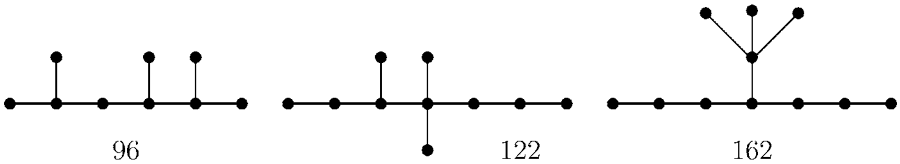

Figure 4. Smallest trees with $W(T) = W(L^2(T))$.

As early as in 1981 Buckley investigated the relation between the Wiener index of a tree and of its line graph and established a quite simple result [5].

THEOREM 15. *Let T be a tree on n vertices. Then*

$$W(L(T)) = W(T) - \binom{n}{2}.$$

Theorem 15 implies that there are no trees having the property $W(T) = W(L(T))$. This theorem was eventually rediscovered [53] and, recently, generalized to both cycle-containing graphs [48] and to other distance-based invariants of trees [50]. If a cycle-containing graph, different than C_n, satisfies (16) for $k = 1$, then it has at least two cycles [27, 55, 62]. The following question naturally arises: does there exist a tree T having the property (16) for $k = 2$? A positive answer to this question has been reported in [23].

The results obtained are presented in Table I. Here N_n is the number of all trees on n vertices; N_W denotes the number of n-vertex trees satisfying equality (16) for $k = 2$. Diagrams of the three smallest trees of this kind and their Wiener indices are shown in Figure 4.

The size of $L^k(T)$ rapidly increases when k tends to infinity. Therefore for sufficiently large k the inequality $W(T) < W(L^k(T))$ holds for any tree T except for simple paths and $K_{1,3}$.

PROBLEM 1. *Does there exist a tree satisfying equality* (16) *for $k \geqslant 3$?*

8. The Wiener Index for Growing Trees

The growth of a tree may be regarded as increasing segment lengths, the number of branching points, and/or their degrees. In this section several operations of this kind will be considered.

Let a tree T' be obtained by k-subdivision of a tree T, i.e., k new vertices are added to every edge of the tree T. Then the length of every segment in T increases $k+1$ times. In order to establish a relation between the Wiener indices of T and T', the Doyle–Graver formula may be applied. Let the subtree T_i, having n_i vertices, be attached to some branching point (see Figure 3). Then the corresponding subtree in T' has $n_i + (n_i - 1)k + k = (k+1)n_i$ vertices and T' has $n' = k(n-1) + n$ vertices. Therefore $W(T')$ may be computed as follows [26]:

THEOREM 16. *Let T be a tree and T' be its k-subdivision. Then*

$$W(T') = (k+1)^3 W(T) + \binom{n'+1}{3} - (k+1)^3 \binom{n+1}{3}. \tag{17}$$

For the minimal subdivision ($k = 1$) of a tree, $W(T') = 8W(T) - 2n(n-1)$. If $k = n$, where n is the number of vertices of T, then formula (17) gives

$$W(T') = (n+1)^3 W(T) - (3n^2 + 2n + 1)\binom{n+1}{3}.$$

If not all edges of a tree are subdivided then W depends on the distances of the tree's vertices. For example, let T_1 be obtained by subdivision of an edge $e = (u, v)$ in a tree T. Then $W(T_1)$ depends on the distance characteristics of the endpoints of e [103]:

$$W(T_1) = W(T) + \frac{1}{2}[d_T(u) + d_T(v)] + \frac{1}{2}[n_u(e) + n_v(e) + 2n_u(e)n_v(e)].$$

The next graph operation leads to increasing the number of branching points in a tree. Let a tree T^* be obtained by attaching n_i new vertices of degree one to the vertex v_i of a tree T, $i = 1, 2, \ldots, n$. The tree T^* is called the *thorn tree* of T and has $n^* = \sum_{i=1}^{n}(n_i + 1)$ vertices. The degree of every vertex increases by n_i; if $n_i \geqslant 2$ then every vertex of T becomes a branching point in T^*; every segment of T^* consists of a single edge. Then the Wiener indices of T and T^* satisfy [51]:

THEOREM 17. *Let T be a tree and T^* be its thorn tree. Then*

$$\begin{aligned} W(T^*) \;=\; & W(T) + \sum_{1 \leqslant i < j \leqslant n} (n_i + n_j) d_T(v_i, v_j) + \sum_{1 \leqslant i < j \leqslant n} n_i n_j d_T(v_i, v_j) + \\ & + \left(\sum_{i=1}^{n} n_i\right)^2 + (n-1)\sum_{i=1}^{n} n_i \end{aligned}$$

or

$$W(T^*) = \sum_{1 \leqslant i < j \leqslant n} (n_i + 1)(n_j + 1) d_T(v_i, v_j) + \left(\sum_{i=1}^{n} n_i\right)^2 + (n-1)\sum_{i=1}^{n} n_i.$$

The above result allows the derivation of relations between $W(T)$ and $W(T^*)$ for special cases. In the first case the growth of a tree is uniform [48].

COROLLARY 17.1. *If T^* is the thorn tree of the tree T and $n_i = k$, $i = 1, 2, \dots, n$, then*

$$W(T^*) = (k+1)^2 W(T) + nk(nk + n - 1).$$

The minimal growth of T ($k = 1$) leads to $W(T^*) = 4W(T) + 2n(n-1)$; if $k = n$ then $W(T^*) = (n+1)^2 W(T) + n^2(n^2 + n - 1)$.

The most interesting cases arise when the number of attached vertices depends on the structure of the initial tree [48].

COROLLARY 17.2. *If T^* is the thorn tree of the tree T and $n_i = \deg(v_i)$, $i = 1, 2, \dots, n$, then*

$$W(T^*) = 9W(T) + (n-1)(3n-5).$$

Let m be an integer with the property $m \geqslant \deg(v_i)$ for all $i = 1, 2, \dots, n$ [48].

COROLLARY 17.3. *If T^* is the thorn tree of the tree T and $n_i = m - \deg(v_i)$, $i = 1, 2, \dots, n$, then*

$$W(T^*) = (m-1)^2 W(T) + [(m-1)n + 1]^2. \tag{18}$$

If $m = 4$ then the thorn tree T^* is just what Cayley [11] calls a 'prelogram' and Pólya a 'C–H graph' [105] (the parent tree T would then be referred to as a 'kenogram' or 'C-graph'). These notions have their origins in the attempts to represent molecular structure by means of graphs [63]; for work along these lines, involving Equation (18), see [67]. It is also worth mentioning that so-called 'caterpillars' [71] are thorn trees whose parent tree is a path.

Recall that the growth of a tree may also be realized in an irregular way. The simplest case is described by formula (5). The following formulas may be also used:

THEOREM 18. *Let T be obtained from arbitrary trees T_1 and T_2 of orders n_1 and n_2, respectively, and $v_1 \in V(T_1)$, $v_2 \in V(T_2)$.*

(a) *If v_1 and v_2 are linked by a path on k vertices, then*

$$\begin{aligned} W(T) = {} & W(T_1) + W(T_2) + (n_1 + k - 2)d_{T_2}(v_2) + \\ & + (n_2 + k - 2)d_{T_1}(v_1) + (k-1)n_1 n_2 + \\ & + \frac{1}{2}(k-1)(k-2)(n_1 + n_2) + \frac{1}{6}(k-1)(k-2)(k-3). \end{aligned}$$

(b) *Let* $p_1 = (v_1, \dots, u_1)$ *and* $p_2 = (v_2, \dots, u_2)$ *be paths on* k *vertices without branching points in trees* T_1 *and* T_2*, respectively. If the tree* T *is constructed by identifying* p_1 *with* p_2 (v_1 *is identified with* v_2*, etc.), then*

$$\begin{aligned} W(T) \;=\; & W(T_1) + W(T_2) + (n_1 - k)d_{T_2}(v_2) + (n_2 - k)d_{T_1}(v_1) + \\ & + 2(k-1)[n_{u_1}(p_1) + n_{u_2}(p_2) - n_{u_1}(p_1)n_{u_2}(p_2)] - \\ & - \frac{1}{2}k(k-1)(n_1 + n_2) + \frac{1}{6}(k-1)(5k^2 - k - 12), \end{aligned}$$

where $n_{u_1}(p_1)$ *is the number of vertices in the connected component of* $T_1 - p_1$ *containing* u_1*, etc.*

The formula of case (a) can be applied to arbitrary graphs while the equality (b) is valid only for some classes of bipartite graphs. The well-known simplest formulas, that are frequently used in applications, are just the special cases of the above expressions [112, 20, 103]:

COROLLARY 18.1. *Let* T *be obtained from arbitrary trees* T_1 *and* T_2 *of orders* n_1 *and* n_2*, respectively, and* $v_1 \in V(T_1)$*,* $v_2 \in V(T_2)$.

(a) *If* v_1 *and* v_2 *are linked by an edge, then*

$$W(T) = W(T_1) + W(T_2) + n_1 d_{T_2}(v_2) + n_2 d_{T_1}(v_1) + n_1 n_2.$$

(b) *If* v_1 *and* v_2 *are identified, then*

$$W(T) = W(T_1) + W(T_2) + (n_1 - 1)d_{T_2}(v_2) + (n_2 - 1)d_{T_1}(v_1).$$

(c) *Let* $e_1 = (v_1, u_1) \in E(T_1)$ *and* $e_2 = (v_2, u_2) \in E(T_2)$*. If the tree* T *is constructed by identifying* e_1 *with* e_2 (v_1 *is identified with* v_2*), then*

$$\begin{aligned} W(T) \;=\; & W(T_1) + W(T_2) + (n_1 - 2)d_{T_2}(v_2) + (n_2 - 2)d_{T_1}(v_1) + \\ & + 2[n_{u_1}(e_1) + n_{u_2}(e_2) - n_{u_1}(e_1)n_{u_2}(e_2)] - (n_1 + n_2) + 1, \end{aligned}$$

where $n_{u_1}(e_1)$ *is the number of vertices of* T_1*, lying closer to* u_1 *than to* v_1*, etc.*

Important examples of growing trees are polygraphs that model the structure of polymers. Formulas of the previous corollary are convenient for calculating the Wiener index of the class of polygraphs called fasciagraphs. The structure of the simplest fasciagraph F is uniquely specified by the structure of the monomer unit G and the numbers of monomer units. Monomer units are linked regularly to each other by a single edge (u, v), such that the vertex u of one copy of G is linked to the vertex v of the next copy of G. Every unit of F is adjacent with two other units, except the terminal units (see Figure 5). Then the Wiener index of F may be computed through the distance characteristics of G as follows [103].

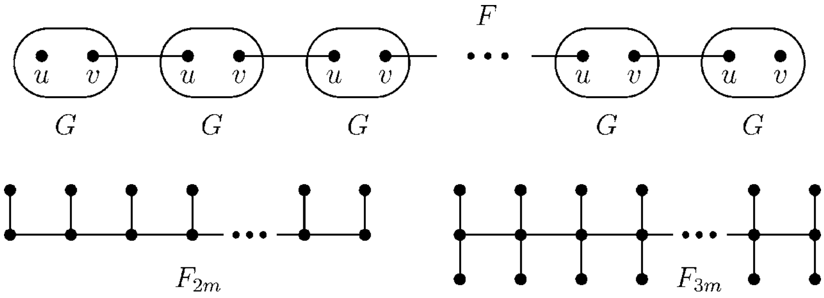

Figure 5. A fasciagraph F and chemical polytrees.

COROLLARY 18.2. *Let F be a fasciagraph composed of m copies of a graph G on n vertices. Then*

$$\begin{aligned}W(F) &= mW(G) + \frac{1}{2}nm(m-1)[d_G(u) + d_G(v)] + \\ &\quad + \frac{1}{6}n^2m(m-1)[(m-2)d_G(u,v) + m + 1].\end{aligned}$$

As an illustration consider a polytree F_{nm} consisting of m copies of the star S_n such that $u \in C(S_n)$ and the vertex v coincides with u. Applying the above formula, we obtain

$$W(F_{nm}) = m\left[(n-1)(nm-1) + \frac{1}{6}n^2(m^2-1)\right].$$

Chemically relevant fasciagraphs F_{nm} correspond to the cases $n = 2$ (monomer unit S_2) and $n = 3$ (monomer unit S_3) (see Figure 5). For these simple polytrees, $W(F_{2m}) = \frac{1}{3}m(2m^2 + 6m - 5)$ and $W(F_{3m}) = \frac{1}{2}m(3m^2 + 12m - 7)$. Note that the path P_{2m} may also be regarded as a polytree with the monomer S_2, where the vertices u and v are distinct. For other results concerning the Wiener index of compound graphs and of molecular graphs as well as for additional references see [39, 47, 76, 79, 80, 83, 92, 102, 118].

9. Forbidden Values for the Wiener Index of Trees

A group of results deals with the question of which numbers can be Wiener indices of trees. (Such questions were, of course, also considered for other classes of graphs.)

Lukovits examined the parity of distances between vertices of trees [89]. The rule pertaining to the parity of $W(T)$ is quite simple [45]. Each tree is a connected bipartite graph. If a connected bipartite graph G has n_1 vertices of one class and n_2 vertices of the other class, then $W(G)$ is odd if and only if both n_1 and n_2 are odd. In particular, all trees on an odd number of vertices have an even Wiener index.

For trees with a perfect matching the following result was deduced [65].

THEOREM 19. *Let T, T' be trees on n vertices. If both T and T' have perfect matchings, then $W(T) \equiv W(T') \pmod 4$.*

Theorem 19 implies that the Wiener index of a tree T with a perfect matching is even if and only if $n(T)$ is divisible by 4.

We now use the Doyle–Graver formula and the concept of segments to find further congruence relations for the Wiener index.

Consider the class of *k-proportional trees*. Trees of this class have the same order and the lengths of all segments are proportional to the coefficient k, $k \geqslant 1$. More precisely, if $\ell_1, \ell_2, \ldots, \ell_m$ and $\ell'_1, \ell'_2, \ldots, \ell'_{m'}$ are the lengths of the segments of the trees T and T', respectively, then $\ell_i = kr_i$, $i = 1, 2, \ldots, m$ and $\ell'_j = kr'_j$, $j = 1, 2, \ldots, m'$, where r_i and r'_j are some positive integers.

Let T_1 and T_2 be k_1- and k_2-proportional trees having the same order. Then they are also k-proportional trees where k is the common divisor of k_1 and k_2.

Recall that $n(T) = \ell_1 + \ell_2 + \cdots + \ell_m + 1$. This fact and the Doyle–Graver formula (10) result in:

THEOREM 20. *Let T and T' be k-proportional trees. Then*

$$W(T) \equiv W(T') \pmod{k^3}.$$

COROLLARY 20.1. *Let T and T' be k-proportional trees of odd order. If k is also odd, then*

$$W(T) \equiv W(T') \pmod{2k^3}.$$

COROLLARY 20.2. *Let T and T' be k-proportional trees having perfect matchings. If k is odd then*

$$W(T) \equiv W(T') \pmod{4k^3}.$$

Any two trees of equal order become k-proportional trees after $(k-1)$-subdivision of their edges. In this case, Theorem 20 may be directly obtained from Equation (17).

The question which positive integers can be Wiener numbers of graphs or of bipartite graphs has been solved [68]. The natural next question is which positive integers can be Wiener numbers of trees. This problem is at the moment unsolved. In [68] the following conjecture is given:

CONJECTURE 1. *There is a finite number of positive integers that are not Wiener indices of some trees.*

Recently an extensive computer search has been performed [87], which showed that the following numbers are not Wiener indices of trees: 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147 and 159.

Furthermore, if there is any other such 'forbidden' integer, its value must exceed 1206. This result justifies a somewhat stronger hypothesis [87]:

CONJECTURE 2. *There are exactly* 49 *positive integers that are not Wiener indices of some trees. These are just the above listed numbers.*

Now let us consider the average distance, $\mu(T)$, of a tree T. Hendry [72] proved the following by considering trees obtained by identifying a pendent vertex of a path with the central vertex of a star.

THEOREM 21. *Let* $t \geqslant 2$ *and* ϵ *be real numbers. Then there exists a tree* T *such that* $|\mu(T) - t| < \epsilon$.

We shall have much further use for these particular trees in Section 11.

Solving a problem posed by Hendry, Winkler obtained [117]:

THEOREM 22. *Let a rational number* r *be given. If* $r > 2$*, then there is a* (*countably*) *infinite number of nonisomorphic trees whose mean distance is exactly* r. *If* $r < 2$*, then there is a tree whose mean distance is* r *just when* r *can be written in the form* $2 - 2/k$*, where* k *is an integer greater than* 1*; if* $k = \binom{m}{2}$ *for some integer* $m > 3$ *or if* $k = 30$*, then there are exactly two such trees, otherwise only one. Finally, there are two trees whose mean distance is* 2.

10. Trees Preserving the Wiener Index of a Graph

In this section we deal with the following problem: given a graph G, does there exist a connected subtree T such that $W(G) = W(T)$? The graph G may be regarded as a result of growing of T. It is clear that G must contain cycles and T must not be a spanning tree of G. The Wiener index of G must not belong to the list of forbidden values for trees from Section 9.

In the simplest case G is a monocyclic graph, i.e., $T = G - v$ for some vertex $v \in V(G)$. If G has even order then an odd number is a forbidden value for $W(G - v)$ and, therefore, for $W(G)$. Table II reports the number of monocyclic graphs of order $n \leqslant 14$ with subtrees preserving their Wiener indices (N_1). Here m denotes the total number of monocyclic graphs on n vertices; t_1 is the number of nonisomorphic subtrees.

Diagrams of the minimal monocyclic graphs G_1, G_2 and the minimal graph G_3 having two nonisomorphic subtrees are depicted in Figure 6 (deleted vertices are marked by heavy dots). Note that the cycle C_{11} is the unique known graph for which the equality $W(G) = W(G - v)$ holds for every vertex $v \in V(G)$ [114].

The second part of Table II contains the numbers of preserving trees for bicyclic graphs of order $n \leqslant 12$ (N_2). Here b is the total number of bicyclic graphs on

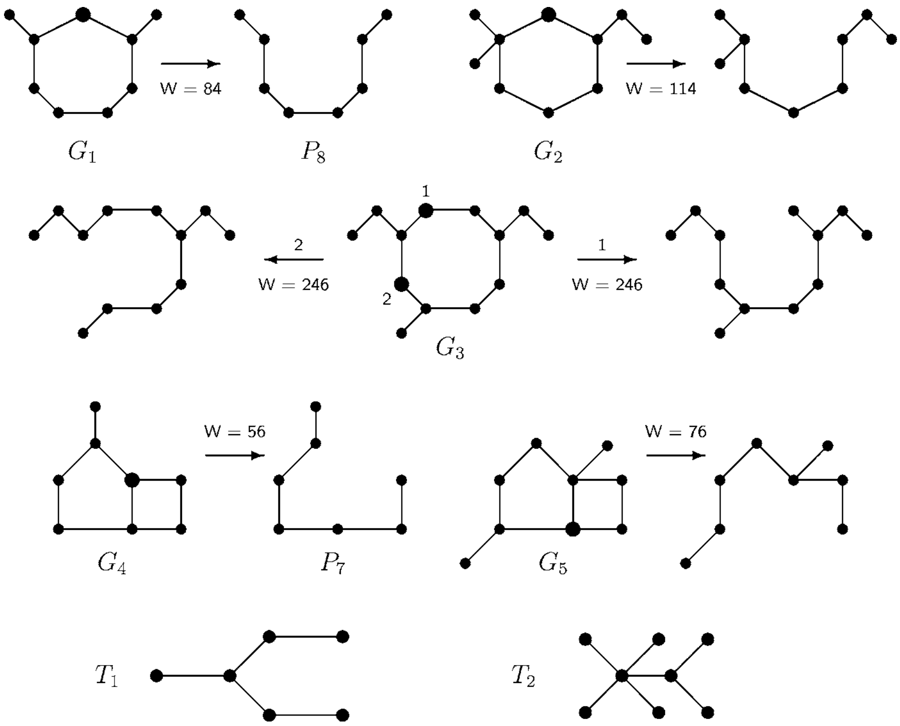

Figure 6. Examples of graphs with subtrees preserving W.

Table II. Subtrees preserving the Wiener index for mono- and bicyclic graphs.

n	4	5	6	7	8	9	10	11	12	13	14
m	2	5	13	33	89	240	657	1806	5026	13999	39260
N_1	0	0	0	0	0	1	2	7	32	78	242
t_1	0	0	0	0	0	1	1	5	22	58	195
b	1	5	19	67	236	797	2678	8833	28908	–	–
N_2	0	0	0	0	1	8	33	90	256	–	–
t_2	0	0	0	0	1	3	14	38	101	–	–

n vertices and t_2 is the number of nonisomorphic subtrees. Examples of bicyclic graphs G_4 and G_5 and their subtrees are depicted in Figure 6.

Consider now graphs with several cycles. Namely, let $G = T \cdot v$, where T is a tree and every vertex of T is connected to a new vertex v. There are only two graphs of this class having the property $W(G) = W(T)$. Denote by n the order of a tree T. Since G has diameter $D = 2$, $W(G) = |V(G)|^2 - |V(G)| - |E(G)| = n(n-1)+1$.

For $n \leqslant 5$ and $n = 7, 9, 10$, the Wiener index of G belongs to the list of forbidden values for $W(T)$. For $n = 6, 8$, there are exactly two trees for which $W(T) = W(T \cdot v)$ (see the trees T_1 and T_2 in Figure 6). For $n \geqslant 11$, the inequalities $W_2 < W(G) < W_3$ hold, where $W_2 = n(n-1) - 2$ and $W_3 = n^2 - 7$ are the second and the third smallest values of the Wiener index for n-vertex trees.

The next examples show that a subtree preserving W may be constructed by deleting several elements of a graph.

Consider the wheel $G \cong C_5 \cdot v$ on 6 vertices and delete the vertex v and an edge e of C_5. Then $(G - v) - e \cong P_5$ and $W(G) = W(P_5) = 20$.

For the wheel $G \cong C_8 \cdot v$ on 9 vertices, we delete two vertices. In this case $(G - v) - u \cong P_7$ and $W(G) = W(P_7) = 56$, where u is a vertex of C_8.

Let $\mathcal{G} = \{(((T+u)\cdot v_1)\cdot v_2)\cdot v_3\}$, where T is an n-vertex tree and $T+u$ goes over all monocyclic graphs. For $G \in \mathcal{G}$, $W(G) = n^2 + 3n + 5$. There are many graphs with the considered property, pertaining to various values of n. For example, there are exactly 289 graphs $G \in \mathcal{G}$ of order 16 ($n = 12$) having a subtrees T such that $W(T) = W(G - \{v_1, v_2, v_3, u\}) = 185$, where u belongs to the corresponding monocyclic graph.

11. Wiener Index for Distance Palindromic Trees

Let $a(G) = (a_0, a_1, \dots, a_m)$ be a sequence of integers or symbols associated with a graph G. The graph G is said to be palindromic with respect $a(G)$ if the equality $a_k = a_{m-k}$ holds for all $k = 0, 1, \dots, m$. Graphs palindromic with respect to a sequence of coefficients of graph polynomials have recently attracted much attention and have been duly studied. The systematic study of such palindromic graphs started with the work of Kennedy [81] and was initially focused on the characteristic and matching polynomials [36, 37, 41, 81]. Eventually, other graph polynomials were also examined, in particular the independence [40] and the Hosoya (Wiener) polynomial [21, 22, 44, 54]. The Hosoya polynomial was put forward by Hosoya in 1988 [74]. If G is a connected graph, then its Hosoya polynomial is given by $H(G, \lambda) = \sum_{k=0}^{D} d_k \lambda^k$, where D denotes the diameter of G and d_k is the number of pairs of vertices in G that are at distance k apart; d_0 coincides with the number of vertices of G.

Data on Hosoya polynomials of all trees with up to 10 vertices are available [115].

The sequence $(d_1, d_2, \dots, d_D)$ is also known (since 1981) as the *distance distribution* of a graph [7]. It is easy to see that $W(G) = \sum_{k=1}^{D} k d_k$.

A graph G with diameter D is said to be *distance palindromic* (or H-palindromic) if the equality $d_k = d_{D-k}$ is satisfied for all $k = 0, 1, \dots, \lfloor D/2 \rfloor$.

Families of distance palindromic cyclic graphs have been constructed in [21, 22]. The following conjecture was stated by Gutman in 1993 [44] and (after performing an extensive computer-aided search) restated in [54]:

CONJECTURE 3. *There are no distance palindromic trees.*

Table III. Distance palindromic trees.

T	n	D	$(d_0, d_1, \ldots, d_D)$	$W(T)$
T_1	21	8	(21, 20, 34, 25, 31, 25, 34, 20, 21)	924
T_2	22	6	(22, 21, 52, 63, 52, 21, 22)	759
T_3	22	6	(22, 21, 52, 63, 52, 21, 22)	759
T_4	24	8	(24, 23, 39, 41, 46, 41, 39, 23, 24)	1200
T_5	24	8	(24, 23, 37, 41, 50, 41, 37, 23, 24)	1200

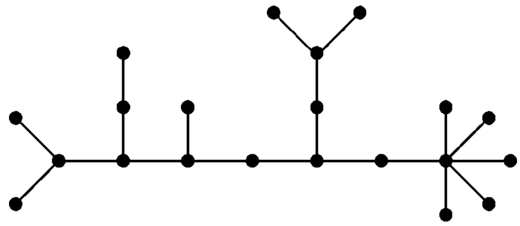

Figure 7. Smallest distance palindromic tree.

This conjecture has been disproved in [10]:

THEOREM 23. *There exist only five distance palindromic trees among all trees on* $3 \leqslant n \leqslant 27$ *vertices.*

Parameters of these trees are collected in Table III. The smallest such tree is shown in Figure 7.

The Wiener index of a palindromic tree depends only on its diameter and the number of vertices [10]:

THEOREM 24. *If T is a distance palindromic tree on n vertices and with diameter D, then*

$$W(T) = D\frac{n(n+1)}{4}.$$

It should be noted that all trees in Table III have even diameters. Distance palindromic trees with odd diameter (if such exist) satisfy [10]:

THEOREM 25. *If T is a distance palindromic tree on n vertices and with odd diameter D, then*

(a) *either* $n \equiv 0 (\mathrm{mod}\, 4)$*, in which case $W(T)$ is divisible by D,*
(b) *or* $n \equiv 7 (\mathrm{mod}\, 8)$*, in which case $W(T)$ is divisible by $2D$.*

In addition to this,

(c) *n cannot be a prime number.*

Attempts to find such trees lead to a new conjecture.

CONJECTURE 4. *There are no distance palindromic trees with odd diameter.*

12. Wiener Index and Extremal Graphs

Two particular classes of trees will appear in several of the extremal results. The first tree, $T(n,r)$, is the tree of order n consisting of a path P of length $r-1$ together with $n-r$ independent vertices all adjacent to the same pendent vertex of P. The second, 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. Theorem 8 can be used to show that

$$W(D(n,a,b)) = \frac{1}{6}\big[n^3 - [3a(a-1) + 3b(b-1) + 1]n + {} + a(a-1)(2a+5) + b(b-1)(2b+5)\big]$$

and that, because $T(n,r) = D(n,0,n-r)$,

$$W(T(n,r)) = \frac{1}{6}\big[6n^2 + 3(r^2 - 3r - 2)n - r(r+1)(2r-5)\big].$$

12.1. CENTROID VERTICES AND PENDENT VERTICES

Recalling that the centroid of a tree T is denoted by $C(T)$ we note that $v \in C(K_{1,n-1})$ implies $d(v) = n-1$ and no tree of order n, different from $K_{1,n-1}$, has a centroid vertex with distance as small. Similar remarks with respect to $K_{1,n-1}$ hold for pendent vertices. It is clear that if we wish to maximize $d(u)$, where u is a pendent vertex of a tree T of order n, then $T = P_n$. Likewise, the maximum of $d(v)$, where v is a centroid vertex of a tree T of order n, occurs only when $T = P_n$.

The next three results, obtained by Barefoot *et al.* [1], give extremal values for several ratios.

THEOREM 26. *If w and u are end vertices of the tree T and the integers $k \geqslant 1$ and s are defined by $2n = k^2 + s$, $0 \leqslant s \leqslant 2k$, then*

$$\frac{d_T(w)}{d_T(u)} \leqslant 2\frac{(n-2)r + 2(n-1)}{r^2 - 3r + 4(n-1)} - 1,$$

where

$$r = \begin{cases} \lfloor 2\sqrt{n} \rfloor - 2, & 0 \leqslant s \leqslant k-6, \\ \lfloor 2\sqrt{n} \rfloor - 1, & k-5 \leqslant s \leqslant 2k. \end{cases}$$

For $n \geqslant 5$ equality is achieved if and only if $T = T(n,r)$.

If $n = 4$, then both P_4 and $K_{1,3}$ are extremal graphs in Theorem 26.

Perhaps the following bounds for the ratio in Theorem 26 provide a better perspective on its magnitude:

$$\frac{1}{4}\lfloor 2\sqrt{n}\rfloor - \frac{1}{8} \leqslant \frac{d_T(w)}{d_T(u)} \leqslant \frac{1}{4}\lfloor 2\sqrt{n}\rfloor + \frac{1}{4}.$$

THEOREM 27. *If T is a tree of order n, w is an end vertex of T, $v \in C(T)$, and $k \geqslant 1$ and s are defined by $2n = k^2 + s$, $0 \leqslant s \leqslant 2k$, then*

$$1 + \frac{4(n-2)}{n^2 - 2n + \epsilon} \leqslant \frac{d_T(w)}{d_T(v)} \leqslant \frac{2rn - r^2 - r}{r^2 + 2n - 3r},$$

where ϵ is 8 if n is even, 5 if n is odd, and

$$r = \begin{cases} \lfloor\sqrt{2n}\rfloor - 1, & 0 \leqslant s \leqslant k-4, \\ \lfloor\sqrt{2n}\rfloor, & k-3 \leqslant s \leqslant 2k. \end{cases}$$

For $n \geqslant 3$ the lower bound is achieved if and only if T consists of a path $u_1, u_2, \ldots, u_{n-1}$ together with an additional vertex w adjacent to $u_{\lfloor(n-1)/2\rfloor}$. The upper bound is obtained if and only if $T = T(n, r)$.

Thus if T is a tree of order n for which $d_T(w)/d_T(v)$ is maximized, elementary calculations show that

$$\frac{1}{2}\lfloor\sqrt{2n}\rfloor + \frac{1}{48} \leqslant \frac{d_T(w)}{d_T(v)} \leqslant \frac{1}{2}\lfloor\sqrt{2n}\rfloor + \frac{3}{4}.$$

THEOREM 28. *If the tree T has order $n = k^2 + s$, $0 \leqslant s \leqslant 2k$, and $v \in C(T)$ then*

$$\frac{1}{3}\frac{r^3 - 3r^2 - (3n^2 - 12n + 10)r - 9n^2 + 12n}{r^2 - 2(n-1)r - 2n + \epsilon} \leqslant \frac{W(T)}{d_T(v)} \leqslant n - 1,$$

where $\epsilon = 0$ if n is even and $\epsilon = 1$ if n is odd and

$$r = \begin{cases} 2k-1 & \text{if } 0 \leqslant s \leqslant k/3 - 1 \text{ and } n \text{ is odd}, \\ 2k+1 & \text{if } k/3 \leqslant s \leqslant 2k \text{ and } n \text{ is odd}, \\ 2k & \text{if } 0 \leqslant s \leqslant 4k/3 - 1 \text{ and } n \text{ is even}, \\ 2k+2 & \text{if } 4k/3 \leqslant s \leqslant 2k \text{ and } n \text{ is even}. \end{cases}$$

The lower bound is achieved if and only if $T = D(n, (n-r)/2, (n-r)/2)$ and the upper if and only if $T = K_{1,n-1}$.

Porter [106] also determined a lower bound for the Wiener index-centroid distance ratio but in terms of the branch weight of a centroid vertex.

THEOREM 29. *If T is a tree of order n, and $v \in C(T)$, then*

$$\frac{W(T)}{d_T(v)} \geqslant n - \mathrm{BW}(v).$$

Although a sharp upper bound for the ratio $W(T)/d_T(w)$, where w is a pendent vertex of the tree T of order n, is not known, Barefoot *et al.* [1] did show the following. Here the graph $S(n, m)$, $3 \leqslant m \leqslant n-1$, is the tree of order n with just one centroid vertex, say v, and each of the m branches of T at v is a path of length $\lfloor (n-1)/m \rfloor$ or $\lceil (n-1)/m \rceil$. We set $S(n, 2) = P_n$. The tree $S'(n, m)$ consists of the tree $S(n-1, m)$ together with an additional pendent vertex adjacent to a centroid vertex of $S(n-1, m)$.

THEOREM 30. *If the tree T has order n and w is a pendent vertex of T then, defining k and s by $2n-2 = k^2 + s$ with $0 \leqslant s \leqslant 2k$,*

$$\frac{1}{3}\left\lfloor \frac{r^3 - 3nr^2 + (12n-13)r - 24n^2 + 39n - 12}{r^2 - 4(n-1)r - 4n - 3} \right\rfloor \leqslant \frac{W(T)}{d_T(w)} \leqslant [1 + \mathrm{o}(1)]n,$$

where

$$r = \begin{cases} 2k-1 & \text{if } 0 \leqslant s \leqslant k/3 - 1, \\ 2k+1 & \text{if } k/3 \leqslant s \leqslant 2k. \end{cases}$$

The lower bound is achieved if and only if $T = T(n, (r-1)/2)$ and the upper bound if $T = S'(n, \lfloor (n-2)\lceil \sqrt{3n} \rceil \rfloor)$.

The bounds of Theorems 28–30 are useful for the estimation of the subgraph invariant defined by the formula $\sum_{v \in H} d_G(v)/W(G)$ for $H \subset G$. The ratios of this kind are applied for the numerical characterization of the location of a fragment H in molecular graphs [28, 91, 113].

Using Theorem 35 (stated below) Shi [111] obtained the upper bound in the following result. This bound was later obtained independently [31]. The lower bound was obtained by Burns and Entringer [8].

THEOREM 31. *If T is a tree of order n with k pendent vertices, $2 \leqslant k \leqslant n$, then*

$$W(S(n,k)) \leqslant W(T) \leqslant W(D(n, \lfloor k/2 \rfloor, \lceil k/2 \rceil)).$$

The lower bound is realized if and only if $T = S(n, k)$ and the upper if and only if $T = D(n, \lfloor k/2 \rfloor, \lceil k/2 \rceil)$.

The next result, although not an extremal result *per se*, arose in the study of optimal distributed processing in networks. Using it Gerstel and Zaks [38] showed that, given a network with a tree topology, choosing a centroid vertex and then routing all the information through it is the best possible strategy, in terms of worst-case number of messages sent during any execution of any distributed sorting algorithm.

THEOREM 32. *If T is a tree of order n then $v \in C(T)$ if and only if $V(T)$ (or $V(T) \setminus v$ if n is odd) can be partitioned into pairs (u_i, v_i) such that each u_i–v_i path contains v. Furthermore, $\sum_{i=1}^{\lfloor n/2 \rfloor} d(u_i, v_i)$ is largest among all such partitions.*

If we modify the proof of Gerstel and Zaks appropriately we obtain one that, in summary form, reads as follows.

We note that, by the concluding statement in Jordan's theorem, if v is not a centroid vertex of the tree T then by the pigeonhole principle the desired partition into pairs cannot exist. On the other hand, if $v \in C(T)$ and two pendent vertices u and w are chosen, one from each of the two branches of T at v with greatest weight, then $V(T)$ has the desired partition into pairs. One of the pairs is $\{u, w\}$ and the remaining can be obtained from $T - \{u, w\}$ by induction since it follows from Jordan's theorem that $C(T - \{u, w\}) = C(T)$. Furthermore, if $v \in C(T)$ and $\{w_i, w_i'\}$ is any pairing of the vertices of $V(T)$ (or $V(T) \setminus \{v\}$ if n is odd), then

$$\sum_{i \geqslant 1} d(w_i, w_i') \leqslant \sum_{i \geqslant 1} [d(w_i, v) + d(v, w_i')] + d(v),$$

so that the sum of the distances between members of pairs is maximized if and only if the pairing is one of the desired partitions into pairs.

12.2. INDEPENDENCE AND MATCHING NUMBERS

The *independence number* of a graph G is the maximum size of an independent (pair-wise nonadjacent) set of vertices of G and will be denoted by $\alpha(G)$. The corresponding invariant for edges involves the concept of matching. Thus the *matching number* of a graph G is the maximum size of an independent (pair-wise nonincident) set of edges of G and will be denoted by $\beta(G)$.

Dankelmann [16] obtained:

THEOREM 33. *If the graph G has independence number α, $n/2 < \alpha \leqslant n - 1$ then*

$$\mu(G) \leqslant \mu(D(n, \alpha - \lfloor (n-1)/2 \rfloor, \alpha - \lceil (n-1)/2 \rceil)).$$

Equality holds if and only if $G = D(n, \alpha - \lfloor (n-1)/2 \rfloor, \alpha - \lceil (n-1)/2 \rceil)$.

Dankelmann also considered the case $2 \leqslant \alpha \leqslant n/2$ but in this case the extremal graph is not a tree [16].

THEOREM 34. *If the graph G has order $n > 4$ and matching number $\beta > 1$, then*

$$\mu(G) \leqslant \mu(D(n, \lfloor (n+1)/2 - \beta \rfloor, \lceil (n+1)/2 - \beta \rceil)).$$

Equality holds if and only if $G = D(n, \lfloor (n+1)/2 - \beta \rfloor, \lceil (n+1)/2 - \beta \rceil)$.

12.3. DEGREE SEQUENCES AND INVERSE DEGREES

A sequence of positive integers $d_1, d_2, \ldots, d_n$ is the sequence of degrees of the vertices of some tree if and only if $\sum_{i=1}^{n} d_i = 2(n-1)$. Among other results, Shi [111] obtained:

THEOREM 35. *Of those trees having a given degree sequence, if T is one with maximum average distance then the tree obtained from T by removing all pendent vertices is a path.*

The widely known GRAFFITI program of Fajtlowicz has generated several conjectures involving average distance and related invariants. Shi [111] provided counterexamples to the following two.

GRAFFITI CONJECTURE 583. *If T is a tree of order n then $\beta(T)+\mathrm{ID}(T)+2 \geqslant n$.*

Here $\mathrm{ID}(T) = \sum_{v \in V(T)} 1/\deg(v)$; as before, $\deg(v)$ is the degree of the vertex v. The same invariant appears again in the third conjecture.

The *deficiency* of a vertex v of a graph G is the number of nonadjacent pairs of vertices adjacent to v or, in other words, the number of nonedges in the graph induced by the neighborhood of v in G. This number is denoted by $\mathrm{DF}(v)$. The *mean deficiency of* G, denoted by $\mathrm{MDF}(G)$, thus is defined by $\mathrm{MDF}(G) = \sum_{v \in V(G)} \mathrm{DF}(v)/n$.

GRAFFITI CONJECTURE 587. *If T is a tree of order n then $\mathrm{MDF}(T) \cdot \mu(T) \leqslant n$.*

A third conjecture was shown by Shi [111] to be true.

THEOREM 36 (GRAFFITI Conjecture 592). *If T is a tree of order n then $\mu(T) \cdot \mathrm{ID}(T) \geqslant n$.*

In Theorem 37 a stronger lower bound is stated. Both the lower and upper bounds of Theorem 37 were obtained by Entringer [31], but the lower bound had been proven earlier by Moon [100].

THEOREM 37. *If T is a tree of order n then*

$$2n - 4 + \frac{4}{n} \leqslant \mu(T) \cdot \mathrm{ID}(T) \leqslant \frac{3 + \alpha - 3\alpha^2}{16} n^2 [1 + o(1)],$$

where $\alpha = 0.5 + \sqrt{3}\cos((\phi + 4\pi)/3) \approx 0.27244788$ and $\cos\phi = 2/(3\sqrt{3})$. The lower bound is achieved only by $K_{1,n-1}$ whereas the upper bound is achieved by the dumbbell $D(n, d_1, d_2)$ with $|d_1 - d_2| \leqslant 1$ and $d_1 \sim \alpha n$.

If the tree T has order n, maximum degree $\Delta = 2$, and $v \in C(T)$, then obviously $T = P_n$ and an easy calculation gives $d_T(v) = \lfloor n^2/4 \rfloor$. For $\Delta > 2$ we have [30]:

THEOREM 38. *If T is a tree of order n, maximum degree $\Delta > 2$, $v \in C(T)$, and the integers r and s are defined by*

$$n = 1 + \frac{\Delta}{\Delta - 2}[(\Delta - 1)^r - 1] + s; \quad 0 \leqslant s < \Delta(\Delta - 1)^r,$$

then

$$s(r+1) + \frac{\Delta}{(\Delta - 2)^2}\left\{[(\delta - 2)(r+1) - 1](\Delta - 1)^{r+1} + 1\right\}$$
$$\leqslant d(v) \leqslant \begin{cases} \lfloor \frac{n^2}{4} \rfloor - \frac{(\Delta-1)(\Delta-2)}{2} & \text{if } \Delta \leqslant n/2, \\ \binom{n-\Delta+1}{2} + \Delta - 1 & \text{if } \Delta \geqslant n/2. \end{cases}$$

The lower bound is achieved if and only if $T \in \mathcal{T}$ and the upper bound is achieved if and only if $T = T(n, n - \Delta + 1)$.

In Theorem 38 the class $\mathcal{T}$ consists of the rooted trees with root v and maximum degree Δ defined further as follows. If n is the order of such a tree we write $n - 1 = \Delta[(\Delta - 1)^r - 1]/(\Delta - 2) + s$ where $0 \leqslant s \leqslant \Delta(\Delta - 1)^r$ and require there to be exactly $\Delta(\Delta - 1)^{i-1}$ vertices distance i from v for $1 \leqslant i \leqslant r$ and s vertices distance $r + 1$ from v. Such a tree is well-defined except for the neighborhoods of the pendent vertices.

12.4. SPANNING TREES WITH MINIMUM WIENER INDEX

Every connected graph G contains a spanning tree T, i.e., a subgraph of G that is a tree and contains all the vertices of G. Among all such trees we are interested in finding those (or at least one) with smallest Wiener index. Such trees are of great practical importance in the design of economical networks. Let us state the problem formally.

PROBLEM 2. *Given a connected graph G, find a spanning tree of G with minimum Wiener index.*

Burns and Entringer [8] found such a tree for complete r-partite graphs.

THEOREM 39. *Let $G = K_{n_1,n_2,\ldots,n_r}$ be a complete r-partite graph of order n with r-partition $\{V_1, V_2, \ldots, V_r\}$, $r \geqslant 2$, satisfying $|V_i| = n_i$, $1 \leqslant i \leqslant r$, and $n_1 \leqslant n_2 \leqslant \cdots \leqslant n_r$. A spanning tree of G is a spanning tree with minimum Wiener index if and only if $n_1 = 1$ and $T = K_{1,n-1}$ or $n_1 > 1$ and T is the spanning tree with exactly two nonpendent vertices, one with degree $n - n_1$ and the other with degree n_1. This tree has Wiener index equal to $n^2 - 3n + 2 + nn_1 - {n_1}^2$.*

Given a nontrivial connected graph G define $s(G) = \min_T W(T)/W(G)$ where T is a spanning tree of G. Letting T be the tree defined in Theorem 39 for the case $r = 2$ and $n_1 = n_2 = m$ gives

$$s(K_{m,m}) = \frac{W(T)}{W(K_{m,m})} = \frac{5m^2 - 6m + 2}{3m^2 - 2m} \sim \frac{5}{3}.$$

Dankelmann and Entringer [19] obtained the following four results. Here C_k denotes a cycle of length k and the *girth* of the graph G is the length of the smallest cycle of G.

THEOREM 40. *Let G be a connected graph with n vertices and minimum degree δ. Then G has a spanning tree with $\mu(T) \leqslant n/\delta + 5$. Apart from the additive constant, this inequality is best possible.*

THEOREM 41. *Let G be a connected C_3-free graph with n vertices and minimum degree δ. Then G has a spanning tree T with $\mu(T) \leqslant (2n/3)\delta + 25/3$. Apart from the additive constant, this inequality is best possible.*

THEOREM 42. *Let G be a connected C_4-free graph with n vertices and minimum degree δ. Then G has a spanning tree T with*

$$\mu(T) \leqslant \frac{5}{3} \cdot \frac{n}{\delta^2 - 2\lfloor \delta/2 \rfloor + 1 + 29/3}.$$

There exists an infinite number of C_4-free graphs with minimum degree δ and order n, such that for every spanning tree T of G

$$\mu(T) \geqslant \frac{5}{3} \cdot \frac{n}{\delta^2 + 3\delta + 2} + \mathrm{O}(1).$$

THEOREM 43. *Let G be a connected graph with n vertices, minimum degree $\delta \geqslant 3$ and girth g.*

(a) *If g is odd then G has a spanning tree T with*

$$\mu(T) \leqslant \frac{gn}{3K} + \frac{7g}{3} - 2,$$

where

$$K = 1 + \frac{\delta}{\delta - 2}\left[(\delta - 1)^{(g-1)/2} - 1\right].$$

(b) *If g is even then G has a spanning tree T with*

$$\mu(T) \leqslant \frac{gn}{3L} + \frac{7g}{3} - 2,$$

where

$$L = \frac{2}{\delta - 2}\left[(\delta - 1)^{g/2} - 1\right].$$

Because Johnson, Lenstra, and Rinnooy–Kan [77] have shown that Problem 2 is NP-complete, finding nearly optimal spanning trees is of interest. If T is any spanning tree of the connected graph G then it is obvious that $W(T) \geqslant W(G)$. On the other hand Entringer, Kleitman, and Székely [33] have deduced:

THEOREM 44. *A connected graph G of order n contains a spanning tree T satisfying $W(T) \leqslant 2(1 - 1/n)W(G)$. Equality is achieved if and only if $G = K_n$ and $T = K_{1,n-1}$.*

Two proofs were given for Theorem 44; each suggested an algorithm guaranteed to find a spanning tree satisfying the inequality of the theorem. They both involve distance preserving spanning trees. A spanning tree T of a connected graph G is said to be *distance preserving* if there is a vertex $v \in V(G)$ such that $d_T(u, v) = d_G(u, v)$ for all $u \in V(G)$. We will refer to v as the *root* of T and say T is *distance preserving from* v. For example, every breadth-first search tree is distance preserving from its root.

ALGORITHM 1. For every vertex v of G construct a distance preserving spanning tree T_v and compute $W(T_v)$. Select the tree which yields the smallest value.

ALGORITHM 2. Compute $d_G(v)$ for each $v \in V(G)$ and then construct a distance preserving spanning tree T_v rooted at the vertex v for which $d_G(v)$ is minimum.

These algorithms suggested two questions posed in [30]. Thinking in terms of average distance rather than Wiener index, following Dankelmann [18] we will call a spanning tree with smallest Wiener index a MAD tree.

PROBLEM 3. *Does every connected graph G have a MAD tree that is also distance preserving?*

PROBLEM 4. *If a graph has a MAD tree that is distance preserving, is it distance preserving from a vertex v for which $d_G(v)$ is minimum?*

Dankelmann [18] answered these in the negative by means of counterexamples.

In view of Theorem 44 we know that $1 \leqslant s(G) < 2$ for every connected graph. If it is known a priori that $s(G)$ is nearly 2 for some graph G there may be no need to find a spanning tree with smallest Wiener index since any spanning tree found using Algorithms 1 or 2 will have approximately the same distance.

PROBLEM 5. *Find graphs G for which $s(G) > 2(1 - \epsilon)$.*

Because $K_{1,n-1}$ is the MAD tree of order n,

$$s(K_n) = \frac{(n-1)^2}{\binom{n}{2}} = 2\left(1 - \frac{1}{n}\right).$$

Consequently $s(K_n) \sim 2$. On the other hand, we have

$$s(C_n) = \frac{W(P_n)}{W(C_n)} = \frac{\binom{n+1}{3}}{(n/2)\lfloor n^2/4 \rfloor} = \frac{4}{3}$$

for odd n.

It is not clear from these three examples (including Theorem 39) how the value of $s(G)$ depends on the density of G. Although we do not know of any class of sparse graphs G_n satisfying $s(G_n) \sim 2$, we are inclined to speculate that the hypercubes, Q_n form such a class. So let us focus on the following.

PROBLEM 6. *Find a MAD spanning tree of Q_n.*

Recognizing that $Q_n = K_2 \times Q_{n-1}$ we first consider the more general problem of constructing a MAD spanning tree T^* of $G = K_2 \times H$ from a MAD spanning tree T of the connected graph H of order n. Two techniques suggest themselves.

Type 1. Suppose $G = K_2 \times H$ and T is a MAD spanning tree of H. To form a Type 1 spanning tree $T^{*,1}$ of G simply append one pendent vertex to each vertex of T. Calculations give $W(T^{*,1}) = 4W(T) + 2n^2 - n$.

Type 2. Suppose $G = K_2 \times H$ and T is a MAD spanning tree of H. To form a Type 2 spanning tree $T^{*,2}$ of G take two disjoint copies of T, say T and T', choose centroid vertices v and v' in T and T', respectively, and join these vertices with an edge. Calculations give $W(T^{*,2}) = 2W(T) + 2nd_T(v) + n^2$.

As shown in [30] neither the Type 1 tree nor the Type 2 tree has smaller distance than the other in all cases. Equality is possible as we shall show.

Let $H = Q_n$ (so that H has order 2^n). Solving the recurrence relation for the Wiener index of the Type 1 spanning tree $T_n^{*,1}$ of Q_n results in

$$W(T_n^{*,1}) = \frac{n-1}{2}4^n + 2^{n-1}.$$

Now let $T_n^{*,2}$ be a Type 2 spanning tree of Q_n and denote a centroid vertex of it by v_n. Then $d(v_n) = n2^{n-1}$ since it satisfies the recurrence relation $d(v_{n+1}) = 2d(v_n) + 2^n$. Next, the recurrence relation $W(T_{n+1}^{*,2}) = 2W(T_n^{*,2}) + 4^n(n+1)$ gives:

$$W(T_n^{*,2}) = \frac{n-1}{2}4^n + 2^{n-1}.$$

Thus the Type 1 and Type 2 trees have equal Wiener indices when $G = Q_n$. In fact, as McCanna [90] has shown, more is true.

THEOREM 45. *The Type* 1 *and Type* 2 *spanning trees are the identical for Q_n.*

Empirical results for small n suggest:

CONJECTURE 5. *The tree defined above is a MAD spanning tree of Q_n, $n \geqslant 1$.*

If this conjecture is true, we would have

$$s(Q_n) = 2\left(1 - \frac{1}{n}\right) + \frac{1}{n2^{n-1}} \sim 2.$$

13. Tree-Distinguishing Properties of the Wiener Index

Given a class of graphs $\mathcal{G}_n$ of order n let $N = N(\mathcal{G}_n)$ be the number of graphs in the class and denote by $t = t(\mathcal{G}_n)$ the number of distinct values assumed by $W(G)$ for $G \in \mathcal{G}_n$. The *isomorphism-discriminating power*, $\mathrm{IDP} = \mathrm{IDP}(\mathcal{G}_n) = t/N$ has been studied in the case when $\mathcal{G}_n$ is the class of trees of order n and when it is the class of chemical trees of order n, i.e., trees with maximum vertex degree at most 4. These latter classes are denoted by $\mathcal{T}_n$ and $\mathcal{T}_n^{\mathrm{ch}}$, respectively.

According to the definition, $\mathrm{IDP} = 1$ means that among the elements of the set considered, no two nonisomorphic graphs have the same Wiener index. If $\mathrm{IDP} = 1/N$ then all graphs (from the set considered) have equal Wiener indices.

The fact that the isomorphism-discriminating power of the Wiener index is very low was first explicitly pointed out by Razinger, Chretien and Dubois [107]. In particular, it was demonstrated by Gutman and Šoltés [66] that for the set of all connected graphs with n vertices and m edges (m having a fixed, but otherwise arbitrary value), IDP tends to zero when $n \to \infty$. Numerical values of IDP for 6- and 7-vertex graphs were reported by Gutman, Luo, and Lee [59].

The Wiener index (W) has been calculated for all trees (and thus for all chemical trees) with 20 and fewer vertices. Corroborating an earlier observation [107], Lepović and Gutman [87] showed that the ability of W to distinguish between nonisomorphic n-vertex trees (chemical trees) depends on n in an alternating manner for $n \leqslant 11$ ($n \leqslant 15$, respectively): it increases for even values of n and decreases for odd values of n.

In Table IV we give the IDP-values of n-vertex trees and chemical trees, $4 \leqslant n \leqslant 20$, together with the respective values of N and t. As it can be seen, the $\mathrm{IDP}(\mathcal{T}_n^{\mathrm{ch}})$-values alternate until $n = 15$, and monotonically decrease for $n \geqslant 16$. However, a closer inspection of the actual numerical values of $\mathrm{IDP}(\mathcal{T}_n^{\mathrm{ch}})$ shows that the violation of the Razinger–Chretien–Dubois rule (occurring for $n \geqslant 16$) is very small and its cause is easily recognized (see below).

In the set $\mathcal{T}_n$ the trees with minimal and maximal Wiener index are the star and the path graph, having $W = (n-1)^2$ and $W = n(n^2-1)/6$, respectively. Therefore, if T is an n-vertex tree, then $W(T)$ belongs to the interval $[(n-1)^2\,,\ n(n^2-1)/6]$ implying $t(\mathcal{T}_n) \leqslant n(n^2-1)/6 - (n-1)^2 + 1 = (n^3 - 6n^2 + 11n)/6$. Thus the number of distinct values which the Wiener index can assume in $\mathcal{T}_n$ increases with

Table IV. The isomorphism-discriminating powers (IDP) of the n-vertex trees and chemical trees.

n	$N(\mathcal{T}_n)$	$t(\mathcal{T}_n)$	IDP$(\mathcal{T}_n)$	$N(\mathcal{T}_n^{\text{ch}})$	$t(\mathcal{T}_n^{\text{ch}})$	IDP$(\mathcal{T}_n^{\text{ch}})$
4	2	2	1.0000	2	2	1.0000
5	3	3	1.0000	2	3	1.0000
6	6	6	1.0000	5	5	1.0000
7	11	9	0.8182	9	7	0.7778
8	23	20	0.8696	18	16	1.8889
9	47	21	0.4468	35	16	0.4571
10	106	53	0.5000	75	40	0.5333
11	235	51	0.2170	159	37	0.2327
12	551	113	0.2051	355	87	0.2451
13	1301	92	0.0707	802	69	0.0860
14	3159	217	0.0687	1858	163	0.0877
15	7741	151	0.0195	4347	116	0.0267
16	19320	355	0.0184	10359	276	0.0266
17	48629	230	0.0047	24894	185	0.0074
18	123867	538	0.0043	60523	431	0.0071
19	317955	331	0.0010	148284	277	0.0019
20	823065	760	0.0009	366319	632	0.0017

n relatively slowly, at most as a cubic polynomial in n. On the other hand, the number of trees of order n grows exponentially with n.

If the number of vertices n of a tree T is odd, then the Wiener index of this graph must be an even number since, by Theorem 8, it is the sum of even numbers, a result first communicated in [3]. As a consequence, for even n we can expect, heuristically, the t-values pertaining to $\mathcal{T}_n$ and $\mathcal{T}_n^{\text{ch}}$ to be roughly two times greater than the t-values pertaining to, respectively, $\mathcal{T}_{n-1}$ and $\mathcal{T}_{n-1}^{\text{ch}}$. The quality of this estimation can be seen from the data given in Table IV.

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