Trees with the Minimum Wiener Number

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ABSTRACT: The Wiener number ($\mathcal{W}$) of a connected graph is the sum of distances for all pairs of vertices. As a graphical invariant, it has been found extensive application in chemistry. Considering the family of trees with n vertices and a fixed maximum vertex degree, we derive some methods that can strictly reduce $\mathcal{W}$ by shifting leaves. And then, by a process, we prove that the dendrimer on n vertices is the unique graph reaching the minimum Wiener number. Int J Quantum Chem 78: 331–340, 2000

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1. Introduction

For a (molecular) graph G, let $V(G)$ denote the set of vertices and $E(G)$ the set of edges. Sometimes, we will abuse G as $V(G)$ according the context. The *Wiener number* or *index*, $\mathcal{W}$, of a connected graph G is defined as:

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

where $d(u,v)$ is the distance between u and v. The quantity is a well-known topological index of a molecule and was introduced in 1947 by the physico-chemist Harold Wiener in his seminal article [1] where he linearly correlated $\mathcal{W}$ with the boiling points (b.p.) of high alkanes, i.e.,

$$\text{b.p.} \approx \alpha\mathcal{W} + \beta w_3 + \gamma,$$

where α, β, and γ are empirical constants, and w_3 is the "path number" (number of P_4 subgraphs in the molecular graph). In Wiener's original definition, $\mathcal{W}$ is the number of bonds (edges) between all pairs of carbon atoms (vertices) only for acyclic alkanes. Hosoya [2], in 1971, showed that $\mathcal{W}$ is equal to the half of the sum of all entries in the distance matrix of the molecular graph and basically gave the graph-theoretic definition above, which can apply on cyclic graphs.

Intuitively, $\mathcal{W}$ is a measure of how apart all pairs of vertices are in a graph, and thus a useful quantity to measure the compactness and the extent of branching in a given molecule (see [3]). Indeed, many physical and chemical properties that depend primarily on the compactness and the extent of branching are usually well correlated with $\mathcal{W}$. As summarized in [4], these properties include heats

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of formation, atomization, isomerization and vaporization, density, boiling point, critical pressure, refractive index, surface tension, etc. The applications of Wiener numbers can also be found in pharmacology and material science. The reader may refer to the survey given in [5] for more detail. The studies of $\mathcal{W}$ in mathematics have mainly focused on methods to compute it for specific types of graphs [6–15], while the most systematic study is on trees. Among them, the Merris–Mckay theorem [12, 13] is an interesting and important formula that connects $\mathcal{W}$ to eigenvalues of Laplacian matrices of trees. Let T be a tree with n vertices $v_1, v_2, \ldots, v_n$, A the adjacency matrix of T, and D a matrix such that $D_{ii} = \deg(v_i)$ and $D_{ij} = 0$ for $i \neq j$. Then

$$\mathcal{W}(T) = n \sum \frac{1}{\lambda_i},$$

where the sum is over all eigenvalues λ_i of the Laplacian matrix $L = D - A$ except the one that equals zero.

For both chemical applications and mathematics, the graphs with maximum and minimum Wiener numbers are interesting to study. The characterizations of these graphs have been identified for both connected graphs and trees with n vertices in [16] and also for connected graphs with n vertices and m edges in [17]. For trees with n vertices and a fixed maximum vertex degree, researchers are curious to know the one(s) with the minimum $\mathcal{W}$, while the dendrimer on n vertices is a conjecture. In this study, we will solve this open problem. To do so, we give two procedures (Propositions 3.1 and 3.2), which can reduce $\mathcal{W}$ by shifting leaves of a tree. In the last section, we prove that the dendrimer is the unique tree (under isomorphism) reaching the minimum $\mathcal{W}$ by a process.

2. Background

In this article, we only consider simple connected graphs. A graph is called *d subregular* if $\deg(u) \leq d$ for all its vertices u, where $\deg(\cdot)$ is the degree of a vertex, i.e., the number of edges incident to it. Let $\mathcal{T}$ be the family of $(d+1)$-subregular trees with n vertices. When $d = 1$, the path of n vertices is the only member in this family. So we set $d \geq 2$. For convenience, we always let $d = 3$, while demonstrating an example. In this study, we would like to characterize the $(d+1)$-subregular tree(s) with the minimum Wiener number in $\mathcal{T}$.

Let (T, r), or sometimes T_r if it causes no confusion, denote a rooted tree T with a root vertex r. The *level* of $u \in V(T_r)$ and the *rank* of T_r are defined as follows:

$$\ell(u) = \text{the length of the path from } r \text{ to } u,$$
$$r(T_r) = \max\{\ell(u) \mid u \in V(T_r)\}.$$

In particular, $\ell(r) = 0$. If $V(T_r) = \emptyset$, for convenience, we set $r(T_r) = -1$; in this case, r is called a *virtual* vertex and T_r a *virtual* tree. By $T_r(u)$, we denote the rooted subtree of T_r induced by u and its descendents, where u is treated as a root of $T_r(u)$.

An *S*-$(d+1)$-*subregular* tree is a rooted tree (T, r) such that each vertex has at most d children, i.e., all vertices of this tree are of degree at most $d+1$ except the root vertex r, which has degree at most d. We write $\mathcal{T}^*$ the family of all S-$(d+1)$-subregular trees with at most $n-1$ vertices. Given any $T_r \in \mathcal{T}$, we know $T_r(u) \in \mathcal{T}^*$ if vertex $u \neq r$. In this work, many notions and properties have both subregular and S-subregular versions. But it is easy to convert from one to the other.

In the following, let $|G|$ be the number of vertices in G, and $G - A$ denote the subgraph of G obtained by removing vertices or edges in A. Here we call a well-known property of trees. (See the Appendix for a proof.)

Lemma 2.1. *Given any tree T with $|T| \geq 2$, there exists a vertex t such that the connected components $T_1, T_2, \ldots, T_k$ of $T - \{t\}$ satisfying*

$$|T_i| \leq \left\lfloor \frac{|T|}{2} \right\rfloor \tag{1}$$

for each i. Furthermore, there are at most two such t in T.

For an S-subregular tree, the root vertex has been assigned when the tree is given. As for a subregular tree $T \in \mathcal{T}$, we should consider it a rooted tree $(T, \overline{0})$, with a fixed root vertex t satisfying hypothesis (1) and labeled by $\overline{0}$. The character of $\overline{0}$ plays an important role in the proof of our main result.

A *dendrimer* of degree $d+1$ on n vertices, D_n, is a $(d+1)$-subregular tree defined inductively as follows. The tree D_0 is an empty set and D_1 consists of a single vertex labeled $\overline{0}$. The tree D_n has vertex set $\{\overline{0}, \overline{1}, \ldots, \overline{n-1}\}$ and is obtained by attaching a leaf $\overline{n-1}$ to the smallest numbered vertex of D_{n-1}, which has degree $<d+1$. We will consider $\overline{0}$ the root of this tree and the vertices at each level ordered left to right in increasing order of their numbering. [See Lemma A.1 in the Appendix, which shows $\overline{0}$ in D_n satisfying hypothesis (1).] A dendrimer of degree 4 on 42 vertices is given in Figure 1 as an example.

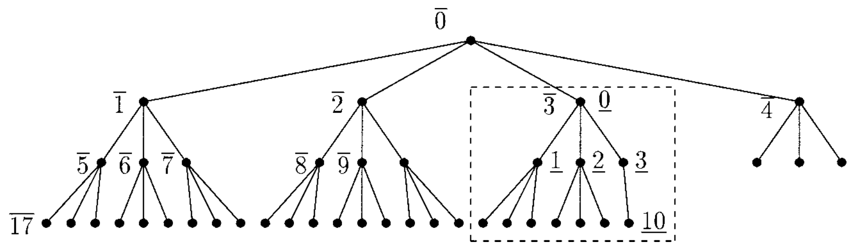


FIGURE 1. D_{42} and E_{11} in the dash box as a subgraph.

Since D_n is an extremely branched* tree in $\mathcal{T}$, the conjecture that D_n has the minimum $\mathcal{W}$ in $\mathcal{T}$ is very reasonable. Let $n_{-1} = 0$, $n_0 = 1$, and $n_k = 1 + (d+1) + (d+1)d + \cdots + (d+1)d^{k-1}$ for $k \geq 1$. A *complete* dendrimer of rank k, denoted by $D^{(k)}$, is a dendrimer on n_k vertices, i.e., $D^{(k)}$ consists of the maximum amount of vertices at each level up to k; otherwise a dendrimer is *incomplete*. The empty set is complete and is of rank -1 as a special case.

An *S dendrimer* on m vertices, denoted by E_m, and a *complete S* dendrimer of rank k, denoted by $E^{(k)}$, are S-subregular trees defined in an analogous way for regular dendrimers. Let $|E^{(k)}| = m_k$. Clearly, $m_{-1} = 0$ and $m_k = 1 + d + d^2 + \cdots + d^k$ if $k \geq 0$. To distinguish from the labeling for vertices in a regular dendrimer, we label the root of E_m by $\underline{0}$, the children of $\underline{0}$ by $\underline{1}, \ldots, \underline{d}$, etc. Note that the leading vertex at level k (i.e., the most left one) is labeled by $\underline{m_{k-1}}$. See example in Figure 1.

When discussing a subregular (resp. S subregular) tree (T, r), a vertex u is called *attachable* if $\deg(u) < d+1$ (resp. if u has less than d children). The *attachable rank* of (T, r) is defined by:

$$\rho(T_r) = \min\{\ell(u) \mid u \in V(T) \text{ is attachable}\}.$$

Again, if T_r is an empty set, we set $\rho(T_r) = -1$. Clearly, $\rho(T_r) \leq r(T_r)$ for any T_r. Using Figure 1 as an example, we have $\rho(D_{42}) = 2$ and $\rho(E_{11}) = 0$ when considering both trees subregular ones; $\rho(E_{11}) = 1$ when considering it an S-subregular tree. Also $r(D_{42}) = 3$ and $r(E_{11}) = 2$.

*A vertex is called a *branching point* in a tree if its degree is at least 3. Among all trees with n vertices, the path P_n has the maximum $\mathcal{W}$ and the star S_{n-1} has the minimum (see [16]). Note that P_n is the only n-vertex tree without branching points and S_{n-1} has only one branching point. Intuitively, branching points can decrease $\mathcal{W}$, and branching points with higher degree have stronger decreasing effect. Such property was recognized by Gutman with a nice formula (see [5]). By the construction of dendrimers, the newest branching point will not appear until the last one reaches the maximum degree, and all nonbranching points are leaves except at most one. So D_n is extremely branched.

Clearly, if $r(T_r) = -1$ or 0, then T_r is a complete dendrimer (or a complete S dendrimer). Using rank and attachable rank, we give equivalent definitions for dendrimers as well as S dendrimers. Let $(T, r) \in \mathcal{T}$ (resp. $\mathcal{T}^*$). In the following, we denote $r_1, r_2, \ldots, r_q$ the real and virtual children of r with $q = d+1$ (resp. $q = d$).

Definition 2.2. 1. *A subregular (resp. S subregular) tree (T, r) is a complete dendrimer (resp. complete S dendrimer) if $r(T_r) = \rho(T_r)$.*

2. *A subregular (resp. S subregular) tree (T, r) is an incomplete dendrimer (resp. incomplete S dendrimer) if $r(T_r) = \rho(T_r) + 1$ and $T_r(r_i)$ are complete S dendrimers for all $1 \leq i \leq q$ except at most a j such that $T_r(r_j)$ is an incomplete S dendrimer.*

3. Reducing the Wiener Number

In this section, we will develop some methods that can reduce $\mathcal{W}$. First we would like to classify vertices of $(T, \overline{0})$ into two types. The rooted $\overline{0}$ is called *standard* if $T_{\overline{0}}$ is a dendrimer, and a vertex $w \neq \overline{0}$ is called *standard* if $T_{\overline{0}}(w)$ is an S dendrimer; otherwise *nonstandard*. See example in Figure 2. By definition, all leaves and those vertices that have only leaves as descendents are standard. Also the descendents of a standard vertex must be standard. So, if $(T, \overline{0})$ is not a dendrimer, all nonstandard ver-

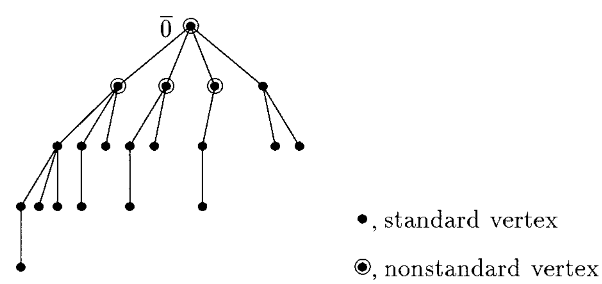


FIGURE 2. Standard and nonstandard vertices.

tices induce a proper subtree of $T_{\overline{0}}$ rooted at $\overline{0}$. We denote this subtree by $\hat{T}_{\overline{0}}$.

We start with any nondendrimer $(T, \overline{0}) \in \mathcal{T}$. Picking out a nonstandard vertex w from the maximum level of $\hat{T}_{\overline{0}}$, we will repeat a process that only rearranges some leaves in $T_{\overline{0}}(w)$ until w turns to be standard. By reducing the size of $\hat{T}_{\overline{0}}$ as well as the value of $\mathcal{W}$, finally we will get the dendrimer on n vertice, and thus we conclude that $\mathcal{W}(D_n) < \mathcal{W}(T_{\overline{0}})$. There are two major procedures in the process: (a) if $r(T_{\overline{0}}(w)) = \rho(T_{\overline{0}}(w)) + 1$, then we will directly change $T_{\overline{0}}(w)$ to be an S dendrimer (or dendrimer if $w = \overline{0}$) by shifting leaves to the left at the maximum level; (b) if $r(T_{\overline{0}}(w)) > \rho(T_{\overline{0}}(w)) + 1$, then move some vertices from the child of w with maximum number of descendents to the one with minimum, repeatedly, until $r(T_{\overline{0}}(w)) - \rho(T_{\overline{0}}(w)) \leq 1$. The reader might consider (a) a horizontal shifting and (b) a vertical moving over levels. The reason that (a) and (b) can reduce the Wiener number of any nondendrimer $(T, \overline{0}) \in \mathcal{T}$ is based on the following two propositions, respectively.

Proposition 3.1. (I) *Let (T, r) be a subregular tree with $r(T_r) = \rho(T_r) + 1$. If (T, r) is not an dendrimer, then $\mathcal{W}(T) > \mathcal{W}(D_{|T|})$.*

(II) *The analogous property is also true for an S-subregular tree T_r. Furthermore, if $T_r = T_{\overline{0}}(r)$ for some $T_{\overline{0}} \in \mathcal{T}$, then the Wiener number of $T_{\overline{0}}$ is strictly reduced by replacing subtree T_r with $E_{|T_r|}$.*

For the second proposition, we consider a graph G constructed as follows. (Also see the graph G on the left of Fig. 3 as an example.) Let (U, u) and (V, v) be two S dendrimers with $|U| = a$, $|V| = b$, $r(U_u) = k+1$, and $\rho(V_v) = k$. (In the case $k = -1$, U has a single vertex, $V = \emptyset$, and v is a virtual vertex.) Also let $G_1, \ldots, G_p$ be any given graphs with $x_i \in V(G_i)$ for each i, with integer $p \geq 1$. We build a graph G that consists of vertices in U, V, and all G_i with its edge set

$$E(G) = E(P) \cup E(U) \cup E(V) \cup E(G_1) \cup \cdots \cup E(G_p),$$

where P is the path: $u, x_1, \ldots, x_p, v$. For convenience, we denote this graph by $(G; P, U, G_1, \ldots, G_p, V)$, or $(G; P, U, V)$ if $G_1, \ldots, G_p$ are not necessary to mention.

Let $c = \min\{a - m_k, m_{k+1} - b\}$ $(\neq 0)$. We construct a new graph H by replacing U and V with two S dendrimers, E_{a-c} and E_{b+c}, respectively. (See H on the right of Fig. 3.) And show that

$$\mathcal{W}(G; P, U, G_1, \ldots, G_p, V) < \mathcal{W}(H; P, E_{a-c}, G_1, \ldots, G_p, E_{b+c}) \quad (2)$$

under certain restrictions described in the following proposition.

Proposition 3.2. *Let $G = (G; P, U, G_1, \ldots, G_p, V)$ and $H = (H; P, E_{a-c}, G_1, \ldots, G_p, E_{b+c})$ be given as above. If*

$$|G_i| \leq |G_{p+1-i}| \qquad \text{for } i = 1, 2, \ldots, \left\lfloor \frac{p}{2} \right\rfloor, \quad (3)$$

then $\mathcal{W}(H) \leq \mathcal{W}(G)$. Furthermore, if both U and V are incomplete or if one of inequalities in (3) is strict, then $\mathcal{W}(H) < \mathcal{W}(G)$.

In the rest of this section we will prove Propositions 3.1 and 3.2. Several new notations and lemmas need to be introduced here. To avoid confusion, the reader might go to the next section for the main result and read the following verification later.

To compute the Wiener number easily, we try to count $\mathcal{W}$ in parts. Let G be the background connected graph that we are considering and let A, B be two disjoin subsets of $V(G)$ and $x \in V(G)$. We define

$$\mathcal{W}_G(x, A) = \sum_{u \in A} d(x, u),$$

$$\mathcal{W}_G(A, B) = \sum_{u \in A,\, v \in B} d(u, v),$$

$$\mathcal{W}_G(A) = \sum_{\{u,v\} \subseteq A} d(u, v).$$

For $\mathcal{W}_G(x, A)$, we allow $x \in A$ because $d(x, x) = 0$.

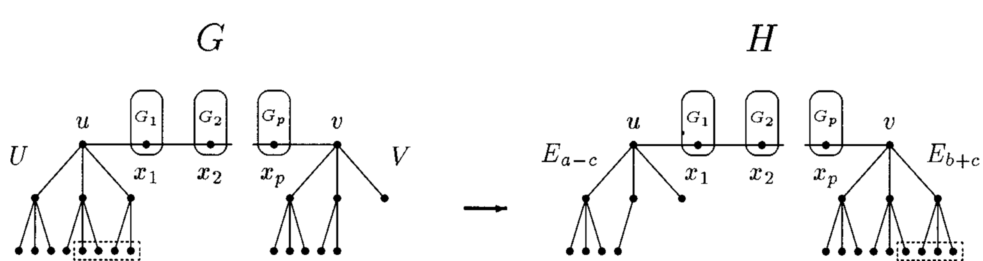


FIGURE 3. Transmission in Proposition 3.2.

Before proving the last two propositions, we need a general and useful lemma that can also reduce $\mathcal{W}$ for a graph with a bridge. Let us consider a graph $G = [G; xy, G^x, G^y]$ such that edge xy is a bridge of G and G^x, G^y are the connected components of $G - xy$ containing x and y, respectively. We can calculate $W(G)$ partially as follows:

$$\begin{aligned}\mathcal{W}(G) &= \mathcal{W}(G^x) + \mathcal{W}(G^y) + \mathcal{W}_G(G^x, G^y)\\ &= \mathcal{W}(G^x) + \mathcal{W}(G^y)\\ &\quad + \sum_{u \in G^x,\, v \in G^y} \left[d(u,x) + 1 + d(y,v)\right]\\ &= \mathcal{W}(G^x) + \mathcal{W}(G^y) + |G^y|\mathcal{W}_{G^x}(x, G^x)\\ &\quad + |G^x||G^y| + |G^x|\mathcal{W}_{G^y}(y, G^y). \qquad (4)\end{aligned}$$

An illustration of this formula is given in the Appendix. By $H = [H; xy, H^x, G^y]$, we denote the new graph obtained by replacing G^x in G with a new subgraph H^x. Directly, by the above equation, we obtain the following result.

Lemma 3.3. *If* $|H^x| = |G^x|$,

$$\mathcal{W}_{H^x}(x, H^x) \leq \mathcal{W}_{G^x}(x, G^x), \qquad (5)$$

and

$$\mathcal{W}(H^x) \leq \mathcal{W}(G^x), \qquad (6)$$

the $\mathcal{W}(H) \leq \mathcal{W}(G)$*. Furthermore, if (5) or (6) is strict then* $\mathcal{W}(H) < \mathcal{W}(G)$.

Now we start proving Propositions 3.1 and 3.2. In the following, both Lemma 3.4 and Corollary 3.6 are stepping stones for proving Proposition 3.2. And Lemma 3.5, which is modified from Lemma 3.4, is used to prove Proposition 3.1.

Recall the definition of $(G; P, U, G_1, \ldots, G_p, V)$. We should begin with a preliminary step. An example of this step is shown in Figure 4.

> [**Moving Step**] If $k = -1$, let us turn u a virtual vertex and v a real vertex. If $k > -1$, let us move the first $c = \min\{a - m_k, m_{k+1} - b\}$ leaves (from the most left) at level $k+1$ in (U, u), and attach them onto (V, v) as leaves at level $k+1$ from the most right to left.

Denote this new graph by $(G'; P, U', V')$. Note that at least one of U' and V' is an S dendrimer for the choosing of c. If U or V are complete, then $U' \cong E_{a-c} \cong V$ and $V' \cong E_{b+c} \cong U$.

Lemma 3.4. *Use the previous notation and assume that* $|G_i| = 1$ *for* $1 \leq i \leq p$.

(A) *If U or V are complete, then* $\mathcal{W}(G') = \mathcal{W}(G)$.

(B) *If both U and V are incomplete, then* $\mathcal{W}(G') < \mathcal{W}(G)$.

Proof. (A): It is obvious because $G \cong G'$. (Note that $k = -1$ belongs to this case.)

(B): Suppose both U and V are incomplete. Let A be the set of vertices moved from U and B the set of vertices attached onto V in [Moving Step]. To compute $\mathcal{W}(G)$, we separate $V(G)$ into three disjoint parts: A, S, and $R = V(G) - A - S$. First, we find

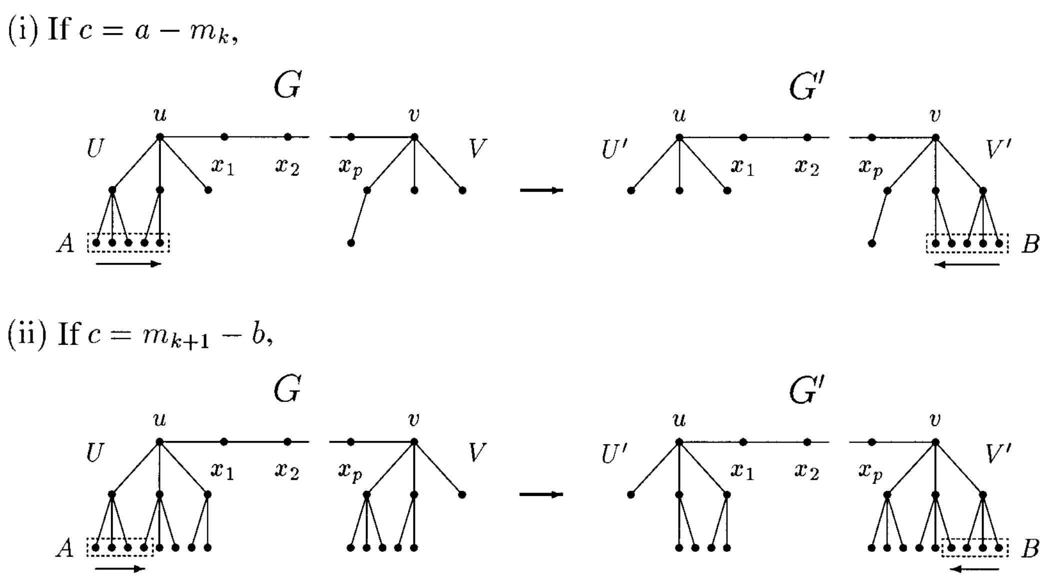
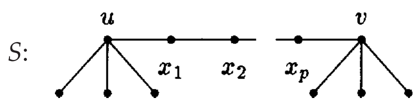


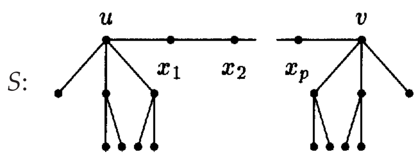
FIGURE 4. Moving step.

the symmetric counterpart of $U - A$ in V and call this counterpart C. (The existence of C needs to be checked. But we leave this work to the reader.) Now let $S = (U - A) \cup P \cup C$. It is the greatest symmetric subgraph in $G - A$ as well as in $G' - B$. To visualize S, we refer the graph G in Figure 4 and see that

(i) If $c = a - m_k$,



(ii) If $c = m_{k+1} - b$;



Here S is also abused as the vertex set of graph S. Since $|R| = |G| - |A| - |S| = -a + b + c = \min\{m_{k+1} - a, b - m_k\}$ and both U and V are incomplete, R is nonempty. It is easy to see that B, S, and R also form a partition of $V(G')$. Let us compute $\mathcal{W}(G)$ and $\mathcal{W}(G')$ partially as follows:

$$\begin{aligned}\mathcal{W}(G) &= \mathcal{W}_U(A) + \mathcal{W}(S) + \mathcal{W}_V(R) + \mathcal{W}_G(A, S) \\ &\quad + \mathcal{W}_G(S, R) + \mathcal{W}_G(A, R),\end{aligned}$$

$$\begin{aligned}\mathcal{W}(G') &= \mathcal{W}_{V'}(B) + \mathcal{W}(S) + \mathcal{W}_{V'}(R) + \mathcal{W}_{G'}(B, S) \\ &\quad + \mathcal{W}_{G'}(S, R) + \mathcal{W}_{G'}(B, R).\end{aligned}$$

By the symmetry, $\mathcal{W}(G') - \mathcal{W}(G) = \mathcal{W}_{G'}(B, R) - \mathcal{W}_G(A, R)$. Since $R \subseteq V$, the vertices in R are closer to B than A, so $\mathcal{W}_{G'}(B, R) < \mathcal{W}_G(A, R)$. Thus the proof is complete. ■

Let us consider $(G; P, U, G_1, V)$ and $(G'; P, U', G_1, V')$ while $p = 1$. Since we only move leaves at level $k + 1$ in U to the same level in V, the Wiener number affected by G_1 does not change. So, by the same reason in the proof of the previous lemma, we get the following result:

Lemma 3.5. *If $p = 1$ and G_1 is any given graph, then both results, (A) and (B), of Lemma 3.4 still hold.*

We will now use Lemmas 3.3 and 3.5(B) to prove Proposition 3.1.

Proof of Proposition 3.1. Suppose $T_r \in T^*$ is not an S dendrimer. Let r_i be a child of r and $T_i = T_r(r_i)$ for $1 \le i \le d$. Also let $r(T_r) = k + 1 = \rho(T_r) + 1$ ($k \ge 1$ otherwise T_r is an S dendrimer). We will prove (II) by induction on k.

If $k = 1$, the proposition is true by repeatedly applying Lemma 3.5(B) with (U, u) and (V, v) being two incomplete S dendrimers rooted at children of r.

Suppose $k > 1$. The equation $r(T_r) = \rho(T_r) + 1$ shows that T_i has two types: either (a) $r(T_i) = \rho(T_i)$ or (b) $r(T_i) = \rho(T_i) + 1 = k$. Recall the equivalent definition of S dendrimers; to modify T_r to be an S dendrimer we need to reduce the number of T_i of type (b). To do so, we repeat the following process containing two steps. During this process we will only shift the leaves at level $k + 1$ of T_r, so the property $r(T_r) = \rho(T_r) + 1$ preserves. Thus the classification of types (a) and (b) still works.

[Step 1] For each T_i of type (b) that is not an S dendrimer, it is clear that $\mathcal{W}(T_i) > \mathcal{W}(E_{|T_i|})$ by induction and $\mathcal{W}_{T_i}(r_i, T_i) = \mathcal{W}_{|E_{T_i}|}(\underline{0}, E_{|T_i|})$. Thus, by Lemma 3.3, we can replace $G^x = T_i$ with the incomplete S dendrimer $H^x = E_{|T_i|}$. If now T_r is an S dendrimer, then we are done; otherwise go to the next step.

[Step 2] After [Step 1], every T_i is an S dendrimer. But there are at least two T_i of type (b), since T_r is not an S dendrimer. So we apply Lemma 3.5(B) on a pair of such incomplete S dendrimers $(U, u) = T_i$ and $(V, v) = T_j$. Then back to [Step 1].

After [Step 2], T_i or T_j is a complete S dendrimer, so we reduce the number of T_i of type (b). Whenever there is no T_i of type (b) or the only such T_i is an incomplete S dendrimer, the process halts and give $E_{|T_r|}$ as output. In the whole process, we apply Lemma 3.3 or 3.5(B) at least once, so $\mathcal{W}(E_{|T_r|}) < \mathcal{W}(T_r)$.

The further result concerning $T_r = T_{\overline{0}}(r)$ in (II) directly follows from Lemma 3.3. As for Proposition 3.1 (I), it actually depends on (II) and can be done by the above two steps without involving induction. ■

Back to Lemmas 3.4 and 3.5. For (A) in both of them, we already have $U' = E_{a-c}$ and $V' = E_{b+c}$. As for (B), we want to turn both U' and V' to be S dendrimers. If U' is not an S dendrimer, then $r(U') = \rho(U') + 1$. Clearly, $\mathcal{W}(E_{|U'|}) < \mathcal{W}(U')$ by Proposition 3.1(II) and $\mathcal{W}_{E_{|U'|}}(\underline{0}, E_{|U'|}) = \mathcal{W}_{U'}(u, U')$. Therefore, by Lemma 3.3 we have

$$\mathcal{W}(G'; P, U', V') < \mathcal{W}(H; P, E_{a-c}, E_{b+c}).$$

We conclude this discussion by the following corollary.

Corollary 3.6. *Let* $G = (G; P, U, G_1, \ldots, G_p, V)$ *and* $H = (H; P, E_{a-c}, G_1, \ldots, G_p, E_{b+c})$ *be described as before with (i)* $|G_i| = 1$ *for* $1 \leq i \leq p$ *or (ii)* $p = 1$ *and* G_1 *is any given graph.*

(A) *If U or V are complete, then* $\mathcal{W}(H) = \mathcal{W}(G)$.

(B) *If both U and V are incomplete, then* $\mathcal{W}(H) < \mathcal{W}(G)$.

Now we can prove Proposition 3.2 by the above corollary.

Proof of Proposition 3.2. First, let us consider just moving one vertex, say y, from level $k+1$ of U onto the same level of V. Write the new vertex attached onto V by y' and the new graph by H. For any $1 \leq i \leq p$, since

$$\mathcal{W}_G(y, G_i) = (k+1+i)|G_i| + \mathcal{W}_{G_i}(x_i, G_i)$$

and

$$\mathcal{W}_H(y', G_i) = (k+p+2-i)|G_i| + \mathcal{W}_{G_i}(x_i, G_i),$$

the change of $\mathcal{W}$ affected by the pair (G_i, G_{p+1-i}) after moving y is

$$\mathcal{W}_H(y', G_i) + \mathcal{W}_H(y', G_{p+1-i}) - \mathcal{W}_G(y, G_i) - \mathcal{W}_G(y, G_{p+1-i}) = (p+1-2i)\big(|G_i| - |G_{p+1-i}|\big).$$

So moving $c = \min\{a - m_k, m_{k+1} - b\}$ vertices will just cause a multiple change. Now combining the above argument with Corollary 3.6, we learn that

$$|G_i| \leq |G_{p+1-i}| \qquad \text{for } i = 1, 2, \ldots, \left\lfloor \frac{p}{2} \right\rfloor$$

is a sufficient condition to show $\mathcal{W}(H) \leq \mathcal{W}(G)$.

To get $\mathcal{W}(H) < \mathcal{W}(G)$, the hypothesis $|G_i| < |G_{p+1-i}|$ for some i is direct from the above discussion; the alternative hypothesis that requires both U and V be incomplete follows from Corollary 3.6(B). ■

4. Main Result

Theorem 4.1. *The dendrimer on n vertices is the unique graph reaching the minimum Wiener numbers of all subregular trees in* $\mathcal{T}$.

Proof. We will prove this theorem by a process described as follows. Given a nondendrimer $(T, \bar{0}) \in \mathcal{T}$ as an input, the process will turn $w \in \hat{T}_{\bar{0}}$ standard one by one and finally give $D_{|T|}$ as an output. An example of this process is shown in Figure 5.

while $\hat{T}_{\bar{0}} \neq \emptyset$ **do**
  Pick out $w \in \hat{T}_{\bar{0}}$ with the maximum level
  while $r(T_{\bar{0}}(w)) > \rho(T_{\bar{0}}(w)) + 1$ **do**
    if $w = \bar{0}$ **then call** [P$\bar{0}$]
    call [PV]
  endwhile
  if $r(T_{\bar{0}}(w)) = \rho(T_{\bar{0}}(w)) + 1$ **then call** [PH]
  renew $\hat{T}_{\bar{0}}$
endwhile

There are three subprocedures in this process. Roughly speaking, [PV] is a vertical moving of leaves, [PH] is a horizontal shifting, and [P$\bar{0}$] only works for a special case. We will describe procedures [P$\bar{0}$] and [PV] in detail later. Given that w is nonstandard, we have $r(T_{\bar{0}}(w)) > \rho(T_{\bar{0}}(w))$. Repeating [PV] (and [P$\bar{0}$] when $w = \bar{0}$) with sufficient times, we can drop $r(T_{\bar{0}}(w)) - \rho(T_{\bar{0}}(w))$ to either 0 or 1 in the second loop. The former case has just turned w standard and the latter one will initiate [PH] described as follows.

Procedure [PH] Turn w standard if it is not by Proposition 3.1.

Hence the first loop of the process reduce $|\hat{T}_{\bar{0}}|$ strictly.

Before describing the other two procedures, we need some notations. Let w_i be the children of w and $T_i = T_{\bar{0}}(w_i)$ for $i = 1, \ldots, q$, where $q = d+1$ or d depending on $w = \bar{0}$ or not. Note that each T_i is an S dendrimer for the choosing of w and $T_i = \emptyset$ if w_i is a virtual child. For convenience, we require the indexing satisfies

$$|T_1| \geq |T_2| \geq \cdots \geq |T_q|. \tag{7}$$

With this ordering and also because all T_i are S dendrimers, we have a useful property:

$$r\big(T_{\bar{0}}(w)\big) = r(T_1) + 1 \quad \text{and} \quad \rho\big(T_{\bar{0}}(w)\big) = \rho(T_q) + 1. \tag{8}$$

So at any stage of the process, the children of w should be reordered to keep (7). Also the fixed root vertex $\bar{0}$ should satisfy hypothesis (1), but only the change in [P$\bar{0}$] need to worry about this. We want to turn w standard, so there should be no descendents of w turn to be nonstandard after any procedure.

Procedure [P$\bar{0}$] If (C): both T_{q-1} and T_q are incomplete and $r(T_{q-1}) = r(T_q)$, then repeatedly apply Proposition 3.2 on $(T_{\bar{0}}; P\colon w_q - \bar{0} -$

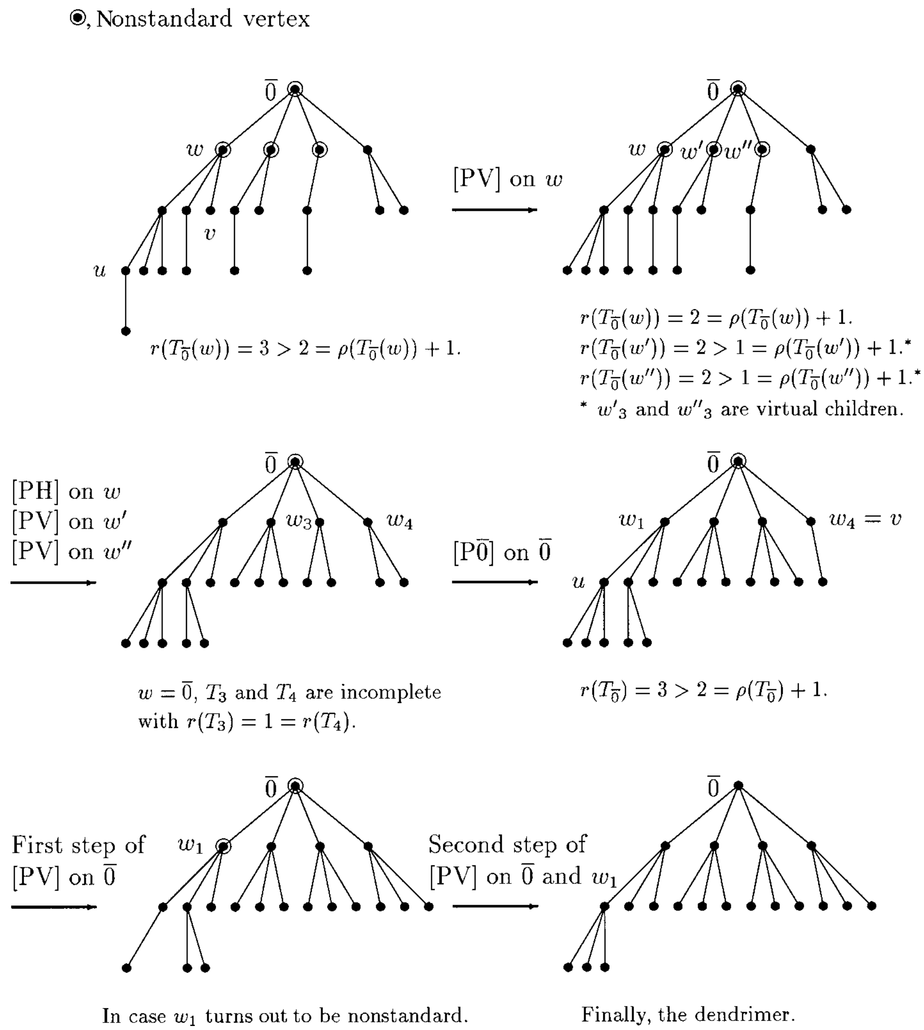


FIGURE 5. Example for the process.

$w_{q-1}, T_q, T_{q-1})$ until condition (C) fails, i.e., until T_{q-1} or T_q is a complete S dendrimer. (We need to reorder $w_1, \ldots, w_{q-1}$ but not w_q if necessary.)

As mention before, we have to check hypothesis (1). Note that $w = \bar{0}$ and $r(T_{\bar{0}}) > \rho(T_{\bar{0}}) + 1$ are given. After moving some vertices from T_q to T_{q-1}, it might happen that $|T_{q-1}| > |T_1|$ ($q-1 \neq 1$ for $w = \bar{0}$) and then $|T_1|$ is increasing after reordering of w_i. But in this case, we must have $r(T_1) = r(T_{q-1}) = \rho(T_q)+1$ before change as well as after. So, by (8), $r(T_{\bar{0}}) = \rho(T_{\bar{0}}) + 1$ before change. This contradicts the given condition. Thus $|T_1|$ never increases, and $\bar{0}$ still satisfies hypothesis (1) after [P$\bar{0}$].

Before describing the next procedure, let us have a look at the input. Note that [P$\bar{0}$] does not alter the given condition $r(T_{\bar{0}}(w)) > \rho(T_{\bar{0}}(w)) + 1$. By (8), this inequality implies $r(T_1) > \rho(T_q) + 1$. Let $h = r(T_1)$, $k = \rho(T_q)$, $p = h - k$ (≥ 2), and $(V, v) = (T_q, w_q)$. We need to find a suitable (U, u) in T_1 with $r(U_u) = k + 1$. Clearly, we can let u be the leading vertex at level $p - 1$ of T_1, i.e., let $(U, u) = T_1(\underline{m_{p-2}})$. (Here the numbering is labeled for $T_1 \in T^*$. The reader should recall that the leading vertex at level $p - 1$ is labeled by $\underline{m_{p-2}}$.) So the input of [PV] can be written as $(T; P, U, G_i, \ldots, G_p, V)$ where path P: $u = \underline{m_{p-2}}$, $x_1 = \underline{m_{p-3}}$, $\ldots$, $x_{p-1} = \underline{m_{-1}} = w_1$, $x_p = w$, $v = w_q$.

Procedure [PV] Apply Proposition 3.2 on the graph $(T; P, U, V)$ and get $(H; P, E_{a-c}, E_{b+c})$. Reset $T_{\bar{0}} := H_{\bar{0}}$ and turn $T_{\bar{0}}(w_1)$ an S dendrimer if it is not.

In this procedure, the second step follows from Proposition 3.1(II) and avoids any descendent of w turn to be nonstandard. Given that $r(T_{\bar{0}}(w)) > \rho(T_{\bar{0}}(w))+1$, we analyze why [PV] together with [P$\bar{0}$] can drop $r(T_{\bar{0}}(w)) - \rho(T_{\bar{0}}(w)) = r(T_1) - \rho(T_q)$ to 0 or 1. Clearly, $\rho(T_q)$ is weakly increasing, even though [P$\bar{0}$] might move out vertices from T_q. On the other hand, $|T_1|$ does not change after [P$\bar{0}$], and it does decrease strictly after running [PV] a few times. Therefore in finite many steps $\rho(T_1)$ increases or $r(T_1)$ decreases.

In order to show [PV] reducing $\mathcal{W}$, we check the hypotheses of Proposition 3.2. Note that $G_i \subseteq T_1$ for $i = 1, 2, \ldots, p-1$. Since T_1 is an S dendrimer, it is clear that $|G_i| \leq |G_{i+1}|$ for any $1 \leq i \leq p-2$. Thus $|G_i| \leq |G_{p+1-i}|$ holds for $i = 2, 3, \ldots, \lfloor p/2 \rfloor$. In the following three cases, we will show that $|G_1| < |G_p|$, where $G_1 = T_{\bar{0}}(x_1) - U$ and $G_p = T_{\bar{0}} - T_1 - T_q$.

(I) If $w \neq \bar{0}$, then $w, \bar{0} \in G_p$ and $T_{\bar{0}}(\bar{i}) \subseteq G_p$ for all children $\bar{i}$ of $\bar{0}$ except a $\bar{j}$ such that $T_{\bar{0}}(\bar{j})$ properly contains G_1 and w. Therefore $|G_p| \geq 2 + \sum_{\bar{i} \neq \bar{j}} |T_{\bar{0}}(\bar{i})| > \lfloor |T|/2 \rfloor \geq |T_{\bar{0}}(\bar{j})| > |G_1|$.

(II) If $w = \bar{0}$ and V is incomplete, then T_{q-1} is either an S dendrimer of rank $>k+1$ or a complete S dendrimer of rank $k+1$ due to [P$\bar{0}$]. So $|T_i| \geq m_{k+1}$ for $i \leq q-1$ and hence $|G_p|$ is at least $(d-1)m_{k+1}+1$. On the other hand $|G_1|$ is at most $(d-1)m_{k+1}+1$. But the extrema of them cannot be achieved in the same time. If they were, the fact that $|G_1| = (d-1)m_{k+1}+1$ implies that U is complete of rank $k+1$, so $|T_1| \geq |T_{\bar{0}}(x_1)| = |G_1| + |U| = dm_{k+1} + 1$. Also $|T - T_1| = |G_p| + |T_q| = (d-1)m_{k+1} + 1 + |V| < dm_{k+1} + 1$ since V is incomplete with $\rho(V) = k$. But this contradicts that $\lfloor |T|/2 \rfloor \geq |T_1|$.

(III) If $w = \bar{0}$ and V is complete, then $r(V) = \rho(V) = k < r(U)$; so $|V| < |U|$. We have $|G_1| \leq |T_1 - U| \leq \lfloor |T|/2 \rfloor - |U|$ and $|G_p| = |T - T_1| - |T_q| \geq \lfloor |T|/2 \rfloor - |V|$. Thus $|G_1| < |G_p|$.

Given a nondendrimer $T_{\bar{0}} \in \mathcal{T}$ as an input, $D_{|T|}$ is the only output and the process at least call [P$\bar{0}$], [PV], or [PH] once, so $\mathcal{W}$ is reduced strictly. Thus we conclude that the dendrimer on n vertices is the only tree reaching the minimum Wiener number in $\mathcal{T}$. ■

We now quote the formula of $\mathcal{W}$ for complete dendrimers of degree $d+1$ given by Gutman et al. [8]:

$$\mathcal{W}\big(D^{(k)}\big) = \big\{d^{2k}\big[kd^3 + (k-2)d^2 - (k+3)d - (k+1)\big] + 2d^k(d+1)^2 - (d+1)\big\}\big/(d-1)^3.$$

There also exists a generalized formula for a dendrimer on n vertices given by Sagan and Yeh [14].

Appendix

Proof of Lemma 2.1. Pick out any leaf w in T to be a root and orient each edge from parent to child. Since T is a tree, every edge is a bridge, so we can label an oriented edge uv by

$$\text{number of vertices on } v\text{'s side} - \text{number of vertices on } u\text{'s side}.$$

Thus, the edge incident to w is labeled $|T| - 2$, and the edges incident to other leaves are all labeled $2 - |T|$. Let P be the subgraph induced by the edges labeled with non-negative integers. It is clear that, along the path from w to any other leaf, the labels of edges are strictly decreasing. So P is a connected subtree. We claim that P is actually a path starting from w. If it is not, then there exists a Y-shaped subgraph in P. Let u be the center of Y. By the way we orient edges, only one neighbor of u could point into it. So u points into at least two end vertices of Y. Call these two end vertices v and w. Since the label of uv non-negative, the number of vertices on v's side $\geq \lceil |T|/2 \rceil$. The argument is the same for w. Now we get a contradiction that $|T| \geq 2 +$ number of vertices on v's side $+$ number of vertices on w's side $\geq 2 + 2\lceil |T|/2 \rceil > |T|$.

No doubt, the vertex at the other end of path P is the one wanted. If the last edge of this path is labeled by zero, we actually have two such t.

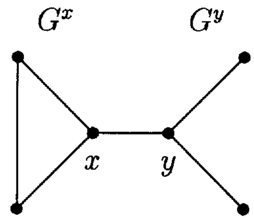
If we replace w with another leaf w', the orientation will only change direction on those edges along the w'–w path. So the labeling does not change except the sign along the w'–w path. Therefore the position(s) of t independs on the choice of w. ■

Lemma A.1. *Given any $(T, t) \in \mathcal{T}$. If $r(T_t) \leq \rho(T_t)+1$, then t satisfies hypothesis (1) in Lemma 2.1.*

Proof. It is trivial when $r(T_t) = \rho(T_t)$. Suppose $r(T_t) = \rho(T_t) + 1 = k + 1$. Let t' be a child of t with maximum number of descendents. Also let $T_t^* = (T - T_t(t'), t)$. Both $T_t(t')$ and T_t^* are S subregular and $r(T_t(t')) = k$ and $\rho(T_t^*) = k$; so $|T_t(t')| \leq |E^{(k)}| \leq |T_t^*|$. Thus $|T_t(t')| \leq \lfloor |T|/2 \rfloor$ and the proof is complete. ■

Recall Definition 2.2, we know that $\bar{0}$ in any dendrimer satisfies hypothesis (1).

An illustration of formula (4):



$$G = [G; xy, G^x, G^y] \quad \text{and} \quad |G^x| = |G^y| = 3,$$
$$\mathcal{W}(G^x) = 3, \qquad \mathcal{W}(G^y) = 4,$$
$$\mathcal{W}_{G^x}(x, G^x) = \mathcal{W}_{G^y}(y, G^y) = 2.$$

By (4), we have

$$\begin{aligned}\mathcal{W}(G) &= \mathcal{W}(G^x) + \mathcal{W}(G^y) + |G^y|\mathcal{W}_{G^x}(x, G^x) \\ &\quad + |G^x||G^y| + |G^x|\mathcal{W}_{G^y}(y, G^y) \\ &= 3 + 4 + 3 \times 2 + 3 \times 3 + 3 \times 2 \\ &= 28.\end{aligned}$$

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