The Wiener Index for Weighted Trees

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Abstract: The Wiener index of a graph is the sum of the distances between all pairs of vertices. In fact, many mathematicians have study the property of the sum of the distances for many years. Then later, we found that these problems have a pivotal position in studying physical properties and chemical properties of chemical molecules and many other fields. Fruitful results have been achieved on the Wiener index in recent years. Most of the research focus on the extreme values and the corresponding graphs for the non-weighted simple graphs. In this paper, we consider the edge-weighted graphs. Firstly, we give the exact definition of the distances in edge-weighted graphs. Secondly, we get a useful variant formula of the Wiener index. Then, we take our attention on edge-weighted trees of order n. We get the minimum, the second minimum, the third minimum, the maximum, the second maximum values of the Wiener index, and characterize the corresponding extremal trees.

Key–Words: Weighted graph; Tree; Wiener index; Minimum value; Maximum value; Bound

1 Introduction

1.1 Background

In chemical graph theory, we use vertices to represent atoms, and use edges connecting two vertices to represent the covalence. Then the structure of each molecule can be expressed as a graph. The molecular topology is defined as the atoms and the connection between atoms in chemicals, does not include details such as bond angles. Because of some important parameters in a molecular, such as energy, key level and change density, are topology relevant essentially. It does make sense that using a graph to represent a molecular.

And nearly half a century, the development of quantum chemistry widely is largely due to the results that the concept of graph being extensive applied. One of the major topics in this field is molecular topological index. Molecular topological index is already can express the structure of molecules quantitatively, as an invariant of the graph can be used to related the relationship between the molecular structure and performance. Say simply, a topological index is a numerical quantity related to a graph that is invariant under graph isomorphism, which can reflect the physical and chemical properties and pharmacological properties of molecules, such as boiling point, water-solubility, the volume and surface area of molecular, energy levels, the election distribution, etc. Topological index of molecular graphs is one of the most widely used descriptors in quantitative structure activity relationships. Quantitative structure activity relationships ($QSAR$) is a popular computational biology paradigm in modern drug design, see [2], [7] and [18].

One of the most widely known topological descriptor is the Wiener index. The Wiener index, which named after chemist Wiener [22], is defined as the sum of the distances between all pairs of vertices of a connected graph. Namely, the Wiener index of a graph G is

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

We can omit the subscript if there are no other graphs. The Wiener index is a well-known distance-based topological index introduced as a structural descriptor for acyclic organic molecules. In fact, the property of the sum of the distances in a graph is one of the favorite problems in mathematics. Many mathematicians have done a lot of research on it. Then we found that this problem not only inspired the interest of mathematicians, but also has many application. No matter in chemistry, physics and molecular biology, the Wiener index has been highly effective applied, see [11].

The Wiener index of graphs has been extensively studied over the past years. In earlier years, the main task is to study how to calculate the value of the Wiener index for a certain graph [4],[9]. Then with the development of drug design, we need to know the extremal values and the corresponding extremal graphs in special kinds of graphs.

The earliest result is found in 1976. Mathematicians Entringer, Jackson and Snyder [5] firstly showed that the star and the path have the minimum and maximum Wiener index, respectively. At that time, they use the concept of distance in graphs, which is actually the Wiener index. Many years later, some chemists got the same results.

For non-weighted simple graphs, the property of the Wiener index have been achieved fruitful results. In 1997, Gutman et al.[10], have made a survey of them.

Recently, Mathematicians have made a lot of experiments and conjectures on calculating various kinds of graphs, see some examples in [4], [12] [20]. More importantly, there are many new results on the extremal values of the Wiener index for some special kinds of graphs, especially of trees.

For trees with bounded degrees of vertices, Jelen and Triesch [15] found a family of trees such that $W(T)$ is minimized. Fischermann et al. [6] characterized the trees which minimize the Wiener index among all trees of given order and maximum degree, and the trees which maximize the Wiener index among all trees of given order.

Moreover, the trees minimizing $W_P(T)$ among all trees T of order n and k leaves are characterized in [17], where k no less than 2 and no more than $n-1$. Hua Wang [21] characterized trees that achieve the maximum and minimum Wiener index, given the number of vertices and the degree sequence, several algorithms are presented and implemented.

At the same time, mathematicians have found a variety of sensible variations of the Wiener index, and got effective conclusions.

The tree that minimizes the Wiener index among trees of given maximal degree is studied in [16], the first two largest and first two smallest modified Wiener indices in are also identified, respectively. Bolian Liu et al. give the minimum (resp. maximum) Wiener polarity index of trees with n vertices and maximum degree are given, and the corresponding extremal trees are determined, where maximum degree no less than 2 and no more than $n-1$. Juan Rada [19] found the variation of the Wiener index under certain tree transformations, which can be described in terms of coalescence of trees. As a consequence, conditions for non-isomorphic trees having equal Wiener index are presented.

However, The angle of view of former studies are usually limited within non-weighted graph. Therefore, they only considered the connection between each atom in the molecule, and ignore the characteristics of the atom and atomic bond, such as the length of atomic bond. As well known, these factors play a decisive role in the physical and chemical properties of molecules. For instance, the length of atom bond is strongly correlated to the stability of the molecule, which is a necessary factor in examining physical and chemical properties of molecules. Therefore, it is necessary to research the molecular structure where the lengths of the bonds taken into consideration. Which more relevant to the chemical actual background. The problem can be transformed to consider the topological indices for edge-weighted graphs, where the weight of the edge represents the length of the atomic bond.

1.2 Notations

In this paper, we consider the extreme values of the Wiener index for edge-weighted trees of order n, denote by $\mathcal{T}_n$. Undefined notation and terminology can be found in [1].We show that the minimum, the second minimum, the third minimum, the maximum and the second maximum Wiener index for $\mathcal{T}_n$, respectively. And the corresponding weighted trees reach the extreme values are discussed.

Let G be a connected edge-weighted graph with vertex set $V(G)$ and edge set $E(G)$. For each edge e of G, let $\omega_G(e)$ be its weight. For clarity of exposition, we shall refer to the weight of a path p in a weighted graph as its length, denote by L_p,

$$L_p = \sum_{e\in E(p)} \omega_p(e).$$

Similarly the minimum weight of a (u, v)-path will be called the distance between u and v, denote by $d_G(u, v)$. The diameter of a graph G, denoted by $D(G)$, is the largest distance between two vertices in G. Since the Wiener index is concerned with the distance of vertices, the diameter is important for us in studying the index.The Wiener index of weighted graph G is defined as

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

We can omit the subscript if there is no other graph.

In a tree $T \in \mathcal{T}_n$, any two vertices are connected by a unique path. Consequently, the Wiener index of T can be rewritten as the sum of the lengths of $p \subseteq T$, where P is the subgraph of which is a path, i.e., $W(T) = \sum_{p\subseteq T} L_p$. Let $\mathcal{P}^i$ be the set of paths with i edges. Hence, we have a variant.

$$W = W(G) = \sum_{i=1}^{\infty} \sum_{p\in\mathcal{P}^i} L_p \tag{1}$$

Let $e_1, e_2, \cdots, e_{n-1}$ be the edge sequence in T, the corresponding edge weights sequence is $a_1, a_2, \cdots, a_{n-1}$. We denote by B the sum of all the edge weights in T. For a graph G, let $d(u)$ be the degree of a vertex u in G, and $N(u)$ be the neighbor set of u. If $d(u) = 1$, then u is said to be a pendent vertex in G, and the edge incident to u is referred to as pendent edge. The neighbor of pendent vertex is called a support vertex. Denoted by P_n and S_n , the weighted path and the weighted star on n vertex, respectively. Note that the weighted star is unique, but the weighted path is not unique for different arrangement of edge-weights. We denote by $\mathcal{T}_n^i$ ($i = 0, 1, 2, \ldots, n-3$) the set of trees with i non-pendent edges. Thus $\mathcal{T}_n$ is sorted by the number of non-pendent edges. Namely,

$$\mathcal{T}_n = \bigcup_{i=0}^{n-3} \mathcal{T}_n^i.$$

Obviously, there is only star S_n in $\mathcal{T}_n^0$, no matter what weights the edges are given . Clearly $\mathcal{T}_n^1$ is the set of the trees with two non-pendent vertices v_{i+1} and v_{i+2} adjacent to i pendent vertices and j pendent vertices, respectively, which is denoted by T_{ij}^1 ($1 \leq i, j \leq n-3, i+j = n-2$) in detail (see Figure. 1).

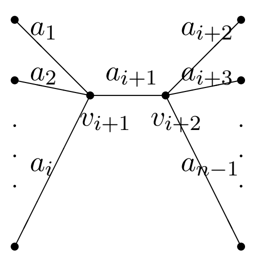

Figure 1: T_{ij}^1

2 The minimal values of the Wiener index for $\mathcal{T}_n$

Firstly, let's introduce a useful transformation. Suppose $T \in \mathcal{T}_n$ with at least one non-pendent edge, say $e = uv$. Let $Q_1 = \{w | w$ and u are in the same component of $T \backslash uv\}$, and $Q_2 = \{w | w$ and v are in the same component of $T \backslash uv\}$. By contracting uv to v and adding a pendent vertex u, with $\omega_T(uv) = \omega'_T(uv)$, and $\omega_T(f) = \omega'_T(f)$ for any $f \in E(T \backslash uv)$, we get a new tree T'. This transformation is denoted by the $f(u,v)$-transformation on T (see Fig. 2).

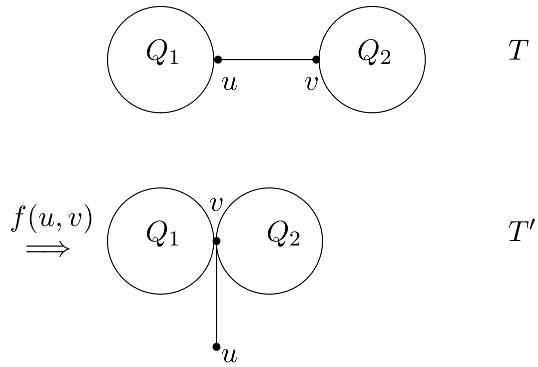

Figure 2: $f(u,v)$-transformation

The following lemma is crucial.

Lemma 1 *Suppose $T \in \mathcal{T}_n$ with at least one non-pendent edge $e = uv$. T' is the tree get from T by $f(u,v)$-transformation. Then we have $W(T) > W(T')$.*

Proof: Let w_1 be a vertex in Q_1 and w_2 be a vertex in Q_2. Since

$$\begin{aligned} W(T) &= \sum_{w_1 \in Q_1} d(w_1, u) + \sum_{w_2 \in Q_2} d(w_2, u) \\ &+ \sum_{w_1 \in Q_1} d(w_1, v) + \sum_{w_2 \in Q_2} d(w_2, v) \\ &+ \sum_{w_1 \in Q_1, w_2 \in Q_2} d(w_1, w_2) + d(v, u) \\ &+ \sum_{\{x,y\} \subseteq Q_1} d(x,y) + \sum_{\{x,y\} \subseteq Q_2} d(x,y). \end{aligned}$$

Assume that $\omega(uv) = a$ ($a > 0$). Then by straightforward observation, we have that the distance between w_1 and w_2 decreases by $f(u,v)$-transformation. There are altogether $|Q_1| \cdot |Q_2|$ such pairs. So the total reduction is $|Q_1| \cdot |Q_2| \cdot a$. The distance between w_1 and u increases a by $f(u,v)$-transformation. The total is $|Q_1| \cdot a$. The distance between w_1 and v decreases a. The total is $|Q_1| \cdot a$. Therefore the sum of $d(w_1, u) + d(w_1, v)$ does not change. Similarly, the sum of $d(w_2, u) + d(w_2, v)$ does not change, too. And the distances between all pairs of the remaining vertices do not change. Consequently,

$$W(T) - W(T') = |Q_1| \cdot |Q_2| \cdot a,$$

By the definition of Q_1 and Q_2, we have $|Q_1| \geq 1$ and $|Q_2| \geq 1$. Hence we get $W(T) > W(T')$. $\square$

The following theorem shows the sharp lower bound of $W(T)$ in weighted trees.

Theorem 2 *The weighted star S_n has the minimum value of the Wiener index in weighted trees of order n, and $W(S_n) = (n-1)B$, where $B = \sum_{i=1}^{n-1} a_i$.*

Proof: By contradiction, we assume that weighted tree $T \neq S_n$ has the minimum Wiener index. Then T has at least a non-pendent edge. By $f(u,v)$-transformation, we get a new tree T'. From Lemma1, we have $W(T) > W(T')$, a contradiction. We conclude that $T = S_n$.

Now let's compute the Wiener index of weighted star S_n. Since the diameter of S_n is 2. Let p be a path in S_n, then either $p \in \mathcal{P}^1$ or $p \in \mathcal{P}^2$. According to variant formula Eq.(1), we have

$$W(S_n) = \sum_{p\in\mathcal{P}^1} L_p + \sum_{p\in\mathcal{P}^2} L_p$$

Obviously,

$$\sum_{p\in\mathcal{P}^1} L_p = \sum_{i=1}^{n-1} a_i = B$$

Now we compute $\sum_{p\in\mathcal{P}^2} L_p$. Since for any edge $e \in E(S_n)$, there are $n-2$ paths covering e in $\mathcal{P}^2$. So that $\omega(e)$ will accumulate $n-2$ times in computing $\sum_{P\in\mathcal{P}^2} L_p$.Therefore, $\sum_{p\in\mathcal{P}^2} L_p = (n-2)B$.

From the above, $W(S_n) = (n-1)B$.

The following two theorems consider the second minimum value and the third minimum value of $W(T)$ for weighted trees. Firstly, Let's introduce some notations. Denote by $S_{i,j}^{min}$, the weighted tree belongs to T_{ij}^1 and the weight of the unique non-pendent edge is $a_{min} = \min_{1\le i\le n-1}\{a_i\}$. Let a_{sec} be the second minimum number of $a_1, a_2, \cdots, a_{n-1}$. Similarly, denote by $S_{i,j}^{sec}(S_{i,j}^{third})$, the tree with the unique non-pendent edge weights the second (third) minimum number of $a_1, a_2, \cdots, a_{n-1}$.

Theorem 3 *The weighted tree $S_{1,n-3}^{min}$ has the second minimum value of the Wiener index for weighted trees of order n, and $W(S_{1,n-3}^{min}) = (n-1)B + (n-3)a_{min}$, where $a_{min} = \min_{1\le i\le n-1}\{a_i\}$*

Proof: Suppose $T \in \mathcal{T}_n$ has the second minimum value of Wiener index. By Theorem 2, we have $T \neq S_n$. Thus, T has at least one non-pendent edge. If T has at least two non-pendent edges. By $f(u,v)$-transformation on T, we get T', and $T' \neq S_n$. By Lemma 1, we have $W(T) > W(T')$, contradicting to the choice of T. So there is only one non-pendent edge in T, i.e., $T \in \mathcal{T}_n^1 = T_{ij}^1$, $(1 \le i, j \le n-3, i + j = n-2)$. We shall compute the Wiener index of T_{ij}^1. For the sake of convenience, we regard T_{ij}^1 as two stars joining together (see Figure. 3).

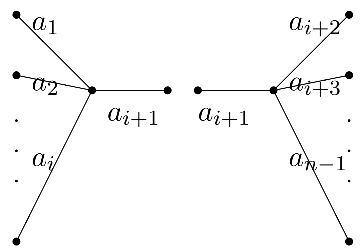

Figure 3:

According to formula of $W(S_n)$, for any $T \in T_{ij}^1$,

$$\begin{aligned} W(T) &= \sum_{i=1}^{3}\sum_{p\in\mathcal{P}^i} L_p \\ &= \sum_{p\in\mathcal{P}^1} L_p + \sum_{p\in\mathcal{P}^2} L_p + \sum_{p\in\mathcal{P}^3} L_p \\ &= B + i\cdot(a_1 + a_2 + \cdots + a_{i+1}) \\ &\quad +(n-i-2)\cdot(a_{i+1} + a_{i+2} + \cdots + a_{n-1}) \\ &\quad +j\cdot(a_1 + a_2 + \cdots + a_i) + i\cdot j\cdot a_{i+1} \\ &\quad +i\cdot(a_{i+2} + a_{i+3} + \cdots + a_{n-1}) \\ &= (n-1)B + i\cdot j\cdot a_{i+1} \end{aligned} \quad (2)$$

Since $(n-1)B$ is a constant, then $W(T)$ is decided by the value of $i\cdot j\cdot a_{i+1}$. Now we discuss the value of $i\cdot j\cdot a_{i+1}$. Since $1 \le i, j \le n-3, i+j = n-2$. Then according to the principle of rearrangement inequality, we may conclude that

$$(n-3)\cdot a_{min} \le i\cdot j\cdot a_{i+1}$$

with equality if and only if $i = 1, j = n-3$, $a_{i+1} = a_{min} = \min_{1\le i\le n-1}\{a_i\}$, namely $T = S_{1,n-3}^{min}$. The proof is completed. □

Theorem 4 *If $a_{sec} \ge \frac{2(n-4)}{n-3}a_{min}$, then the the weighted tree $S_{2,n-4}^{min}$ has the third minimum value of the Wiener index for weighted trees of order n; and if $a_{sec} \le \frac{2(n-4)}{n-3}a_{min}$, then the weighted tree $S_{1,n-3}^{sec}$ has the third minimum value of the Wiener index for weighted trees of order n.*

Proof: Suppose $T \in \mathcal{T}_n$ has the third minimum value of Wiener index. By Theorem2, we have $T \neq S_n$.

Thus, T has at least one non-pendent edge. Let m be the number of the non-pendent edges in T.

If $m \geq 3$, by $f(u, v)$-transformation on T, we get a new tree T', $T' \neq S_n$ and $T \neq S^{min}_{1,n-3}$. From Lemma1, we have $W(T) > W(T')$, contradicting to the choice of T.

If $m = 2$, i.e., $T \in \mathcal{T}^2_n$. Then T(see Figure.4) has three non-pendent vertices, says u ,v and w, adjacent to r, s and t pendent vertices, where $s \leq 0, r, t \leq 1$, $r + s + t = n - 3$.

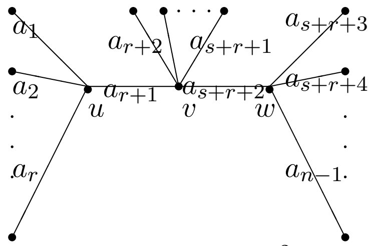

Figure 4: $T \in \mathcal{T}^2_n$

Now let's compute the Wiener index of weighted tree T.

$$\begin{aligned} W(T) &= \sum_{i=1}^{4} \sum_{p \in \mathcal{P}^i} L_p \\ &= \sum_{p \in \mathcal{P}^1} L_p + \sum_{p \in \mathcal{P}^2} L_p + \sum_{p \in \mathcal{P}^3} L_p + \sum_{p \in \mathcal{P}^4} L_p \end{aligned}$$

It is obvious that $\sum\limits_{p \in \mathcal{P}^1} L_p = B$

And we have

$$\begin{aligned} & \sum_{p \in \mathcal{P}^2} L_p \\ = \; & r \cdot (a_1 + a_2 + \cdots + a_{r+1}) \\ & +(s + 1) \cdot (a_{r+1} + \cdots + a_{r+s+2}) \\ & +t \cdot (a_{r+s+2} + \cdots + a_{n-1}) \end{aligned}$$

$$\begin{aligned} & \sum_{p \in \mathcal{P}^3} L_p \\ = \; & (s + 1) \cdot (a_1 + a_2 + \cdots + a_r) \\ & +a_{r+1} r(s + 1) \\ & +(s + 1) \cdot (a_{r+s+3} + \cdots + a_{n-1} \\ & +t \cdot (a_{r+1} + \cdots + a_{r+s+1}) \\ & +(s + 1) \cdot t \cdot a_{r+s+2} \end{aligned}$$

$$\begin{aligned} & \sum_{p \in \mathcal{P}^4} L_p \\ = \; & t \cdot (a_1 + a_2 + \cdots + a_r) \\ & +r \cdot (a_{r+s+3} + \cdots + a_{n-1}) \\ & +r \cdot t \cdot (a_{r+1} + \cdots + a_{r+s+2}) \end{aligned}$$

By simplification, we have

$$W(T) = (n-1)B + r(n-2-r)a_{r+1} + t(n-2-t)a_{r+s+2}.$$

Since $S^{min}_{2,n-4} \in T^1_{ij}$, according to Eq. (2), we have

$$W(S^{min}_{2,n-4}) = (n - 1)B + 2(n - 4)a_{min}.$$

As we know that $S^{min}_{2,n-4} \neq S_n, S^{min}_{2,n-4} \neq S^{min}_{1,n-3}$.

$$\begin{aligned} & W(T) - W(S^{min}_{2,n-4}) \\ \geq \; & [r(n - 2 - r) + t(n - 2 - t)]a_{min} - 2(n - 4)a_{min} \\ \geq \; & 2(n - 3)a_{min} - 2(n - 4)a_{min} > 0 \end{aligned}$$

Namely, for any $T \in \mathcal{T}^2_n$, we have

$$W(T) > W(S^{min}_{2,n-4}).$$

It contradicts to the choice of T.

From above discussion, we have $m = 1$, i.e.,$T \in \mathcal{T}^1_n$. According to Eq. (1), we have

$$W(S^{min}_{1,n-3}) < W(S^{min}_{2,n-4}) < \cdots < W(S^{min}_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}).$$

Moreover, it is clear that

$$W(S^{min}_{1,n-3}) < W(S^{sec}_{1,n-3}) < W(S^{third}_{1,n-3}).$$

We can make the conclusion that the weighted tree with the third minimum value of the Wiener index is $S^{sec}_{1,n-3}$ or $S^{min}_{2,n-4}$. Furthermore, since

$$W(S^{sec}_{1,n-3}) - w(S^{min}_{2,n-4}) = (n-3)a_{sec} - 2(n-4)a_{min}.$$

Then if $a_{sec} > \frac{2(n-4)}{n-3} a_{min}$, $S^{min}_{2,n-4}$ has the third minimum value of the Wiener index; if $a_{sec} < \frac{2(n-4)}{n-3} a_{min}$, $S^{sec}_{1,n-3}$ has the third minimum value of the Wiener index.

3 The maximal values of the Wiener index for $\mathcal{T}_n$

Let $\mathcal{P}^{n-1} = e_1 e_2 \cdots e_{n-1}$ be the classes of the weighted paths with edge weight $a_1, a_2, \cdots, a_{n-1}$. respectively. We denote by P^*_n the weighted path, which the distribution of the weights is unimodal, namely,

$$a_1 \leq a_2 \leq \cdots \leq a_{\lceil \frac{n}{2} \rceil - 1} \leq a_{\lceil \frac{n}{2} \rceil}$$

and

$$a_{\lceil \frac{n}{2} \rceil} \geq a_{\lceil \frac{n}{2} \rceil + 1} \geq \cdots a_{n-2} \geq a_{n-1}.$$

Firstly, let's introduce a useful transformation. Suppose $T \in \mathcal{T}_n$. Let $v_0 v_1 v_2 \cdots v_d$ be the longest path in T , and v_i be the first vertex with degree more than 2. Suppose $N(v_i) \setminus \{v_{i-1}, v_{i+1}\} = \{u_1, u_2, \cdots, u_j\}$.

By deleting the edge $v_i u_k$ and adding the edge $v_0 u_k (k = 1, 2, \cdots, j)$, we get a new tree T'. Then let $\omega_T(v_i u_k) = \omega_{T'}(v_0 u_k)$ for $k = 1, 2, \cdots, j$, and $\omega_T(f) = \omega_{T'}(f)$, for any $f \in E(T \backslash v_i u_k)$. This transformation is denoted by the g-transformation on T(see Fig.5).

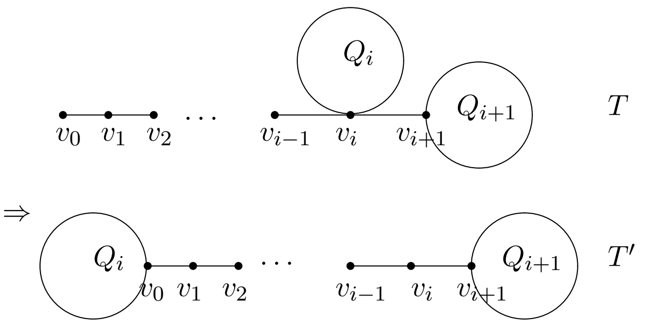

Figure 5: g-transformation

Lemma 5 *Let T be a weighted tree of order n. If $T \notin \mathcal{P}^{n-1}$ by g-transformation on T, we get T'. Then $W(T) < W(T')$.*

Proof: Let $v_0 v_1 v_2 \cdots v_d$ be the longest path in $T \in \mathcal{T}_n$, and v_i be the first vertex with degree more than 2, since $T \notin \mathcal{P}^{n-1}$. Let $Q_1 = \{w | w$ and v_i are in the same component of $T \backslash \{v_{i-1}v_i, v_i v_{i+1}\}\}$, and $Q_2 = \{w | w$ and v_{i+1} are in the same component of $T \backslash \{v_i v_{i+1}\}\}$.

Since

$$W(T) = \sum_{k=0}^{i} \sum_{j=k+1}^{i+1} d(v_k, v_j) + \sum_{j=0}^{i+1} \sum_{w_1 \in Q_i} d(w_1, v_j)$$
$$+ \sum_{j=0}^{i+1} \sum_{w_2 \in Q_{i+1}} d(w_2, v_j) + \sum_{\{x,y\} \subseteq Q_i} d(x, y)$$
$$+ \sum_{w_1 \in Q_i, w_2 \in Q_{i+1}} d(w_1, w_2) + \sum_{\{x,y\} \subseteq Q_{i+1}} d(x, y).$$

We consider the change of the distances between all pairs of vertices after g-transformation on T. If $w_1 \in Q_1$, $w_2 \in Q_2$, then the value of $d(w_1, w_2)$ increases. Note that the value of $\sum_{j=0}^{i} d(w_1, v_j)$ does not change, and the distances between remaining pairs of vertices do not change.

Consequently, $W(T) < W(T')$. The proof is completed. □

The following theorem shows the maximum value of $W(T)$ for weighted trees.

Theorem 6 *The weighted path P_n^* has the maximum value of the Wiener index for weighted trees of order n. Moreover, $W(P_n^*) = \sum_{k=1}^{n-1} k(n-k)a_k$.*

Proof: By contradiction, we assume that $T \in \mathcal{T}_n$ has the maximum Wiener index. If $T \notin \mathcal{P}^{n-1}$, by g-transformation on T, we get a new tree T'. By Lemma 5, we have $W(T) < W(T')$, a contradiction. So $T \in \mathcal{P}^{n-1}$ (see Figure.6).

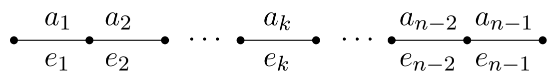

Figure 6: $T \in \mathcal{P}_{n-1}$

We now compute the Wiener index of T. Let p be a path covering the edge $e_k (k = 1, 2, \cdots, n-1)$. There are k different choices on the left of e_k in p, while $n-k$ on the right. So there are $k(n-k)$ paths covering the edge e_k. So the accumulation times of the weight of e_k is $k(n-k)$. when calculating the Wiener index of T. Therefore,

$$W(T) = \sum_{k=1}^{n-1} k(n-k)a_k.$$

Now we consider the maximum value of $W(T)$. Let $\emptyset(k) = k(n-k), k = 1, 2, \cdots, n-1$, we have

$$\emptyset(1) \leq \emptyset(2) \leq \cdots \leq \emptyset(\lceil \frac{n}{2} \rceil),$$

$$\emptyset(\lceil \frac{n}{2} \rceil) \geq \emptyset(\lceil \frac{n}{2} + 1 \rceil) \geq \cdots \geq \emptyset(n-1).$$

According to the principle of rearrangement inequality, we may conclude that the value of $W(T)$ reaches its maximum when the edge weights sequence satisfies

$$a_1 \leq a_2 \leq \cdots \leq a_{\lceil \frac{n}{2} \rceil - 1} \leq a_{\lceil \frac{n}{2} \rceil}$$

and

$$a_{\lceil \frac{n}{2} \rceil} \geq a_{\lceil \frac{n}{2} \rceil + 1} \geq \cdots a_{n-2} \geq a_{n-1}.$$

i.e., $T = P_n^*$. And $W(P_n^*) = \sum_{k=1}^{n-1} k(n-k)a_k$. □

Before considering the second maximum value of the wiener index, we introduce a special kind of weighted trees. We denote by $\mathcal{T}_n^*$, the set of the weighted trees of order n, with only one 3-degree vertex (which also called branching vertex), three 1-degree vertices and the other vertices are of degree 2. The diameter of T, denote by $D(T)$, is the maximum distance in T. Let

$$\mathcal{T}_n^{*1} = \{T : T \in \mathcal{T}_n^*, D(T) = n-2\},$$

$$\mathcal{T}_n^{*2} = \{T : T \in \mathcal{T}_n^*, D(T) < n-2\}.$$

Then $\mathcal{T}_n^* = \mathcal{T}_n^{*1} \bigcup \mathcal{T}_n^{*2}$.

Suppose the weighted tree $H \in \mathcal{T}_n^{*2}$, let $P = v_0v_1v_2, \cdots, v_{D(H)}$, the longest path in H, and $d_H(v_i) = 3$. Let $Q = \{u_1, u_2, \cdots, u_j\} = \{w \in V(H) | w$ and v_i are in the same component of $H \backslash \{v_{i-1}v_i, v_iv_{i+1}\}\}$, where $2 \le j \le \min\{i, D(H) - i\}$. By deleting the edge u_1u_2 and adding the edge v_0u_1, we get a new tree H'. Let $\omega_H(u_1u_2) = \omega_{H'}(v_0u_1)$, and $\omega_H(f) = \omega_{H'}(f)$ for any $f \in E(H \backslash u_1u_2)$. The transformation from H to H' is denoted the h-transformation on H (see Fig.7).

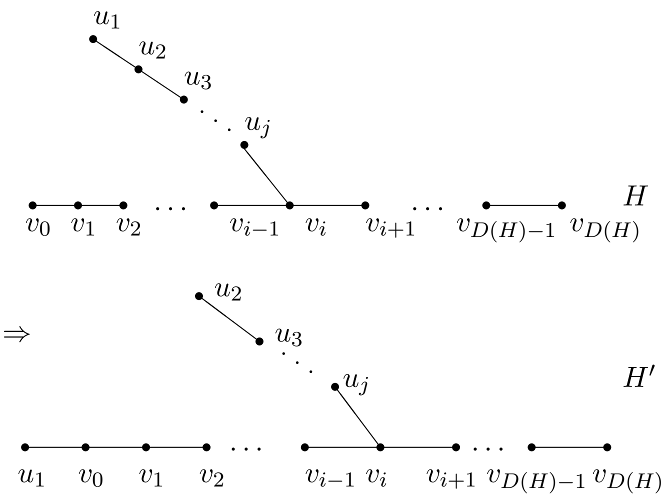

Figure 7: h-transformation

Lemma 7 *Suppose $H \in \mathcal{T}_n^{*2}$. By h-transformation on H, we get H'. Then we have $W(H) < W(H')$.*

Proof: Since

$$\begin{aligned} W(T) &= \sum_{k=0}^{D(H)-1} \sum_{r=k+1}^{D(H)} d(v_k, v_r) + \sum_{k=2}^{j} \sum_{r=0}^{D(H)} d(u_k, v_r) \\ &+ \sum_{k=2}^{j} d(u_1, u_k) + \sum_{k=0}^{i} d(u_1, v_k) \\ &+ \sum_{k=i+1}^{D(H)} d(u_1, v_k) + \sum_{k=2}^{j-1} \sum_{r=k+1}^{j} d(u_k, u_r) \end{aligned}$$

We consider the change of the distances between all pairs of vertices after h-transformation on H.

First of all, the value of $\sum_{k=2}^{j} d(u_1, u_k) + \sum_{k=0}^{i} d(u_1, v_k)$ does not change.

The distance between u_1 and v_k ($k = i+1, i+2, \ldots, D(H)$) increases, since $p = v_0v_1v_2, \cdots, v_{D(H)}$ is the longest path. The distances between all pairs of the remaining vertices do not change. Consequently, we have $W(H) < W(H')$. The proof is thus completed. □

Now let's introduce another useful transformation. Suppose the weighted tree $H \in \mathcal{T}_n^{*1}$, let $p = v_1v_2, \cdots, v_{n-1}$ be the path in H. Let v_i be the branching vertex, i.e., $d(v_i) = 3$. Without lose of generality, we can assume $2 \le i \le \lceil \frac{n-1}{2} \rceil$. By deleting edge v_iv_n and adding the edge $v_{i-1}v_n$, we get a new tree H'. Let $\omega_H(v_iv_n) = \omega_{H'}(v_{i-1}v_n)$, and $\omega_H(f) = \omega_{H'}(f)$ for any $f \in E(H \backslash v_iv_n)$. The transformation is denoted by the ψ-transformation on (see Fig. 8).

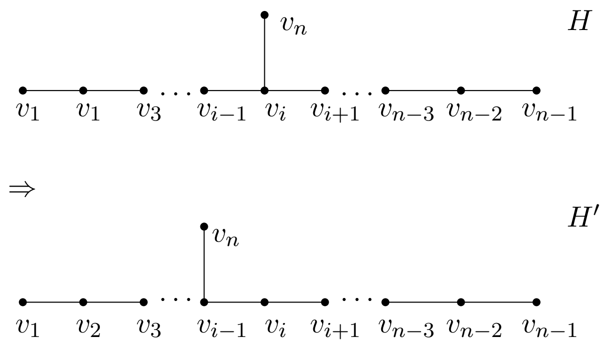

Figure 8: ψ-transformation

Lemma 8 *Suppose $H \in \mathcal{T}_n^{*1}$. By ψ-transformation on H, we get a new tree H'. Then we have $W(H) < W(H')$.*

Proof: Let a $(a > 0)$ be the weight of edge $v_{i-1}v_i$. Since

$$W(T) = \sum_{k=1}^{n-2} \sum_{r=k+1}^{n-1} d(v_k, v_r) + \sum_{j=1}^{i-1} d(v_j, v_n)$$

$$+ \quad \sum_{j=i}^{n-1} d(v_j, v_n)$$

Now we consider the change of the distances between all pairs of vertices. The distance between the vertex v_j and v_n decreases a, for $j = 1, 2, \ldots, i-1$. There are altogether $i-1$ such pairs. So the total decrease is $(i-1)a$. The distance between the vertex v_j and v_n increases a, for $j = i, i+1, \ldots, n-1$. There are altogether $n-i$ such pairs. So the total increase is $(n-i)a$. The distances between all pairs of the remaining vertices do not change. Consequently,

$$\begin{aligned} W(H) - W(H') &= (i-1)a - (n-i)a \\ &= (2i - n - 1)a \end{aligned}$$

Since $2 \leq i \leq \lceil \frac{n-1}{2} \rceil$ and $a > 0$, then we have $W(H) < W(H')$. □

Denote by H^* the weighted tree in $\mathcal{T}_n^{*1}$ with two pendent vertices adjacent to the unique branching vertex. Let $p = v_1 v_2, \cdots, v_{n-1}$ be the path with $D(H^*)$ edges in H^* with the corresponding weights are $a_1, a_3, \cdots, a_{n-1}$, and the edge $v_2 v_n$ weights a_2 (see Fig. 9). The weights $a_1, a_2, \cdots, a_{n-1}$ meet the following conditions:

$$a_1 \leq a_2 \leq \cdots \leq a_{\lceil \frac{n}{2} \rceil - 1} \leq a_{\lceil \frac{n}{2} \rceil},$$

and

$$a_{\lceil \frac{n}{2} \rceil} \geq a_{\lceil \frac{n}{2} \rceil + 1} \geq \cdots \geq a_{n-2} \geq a_{n-1}.$$

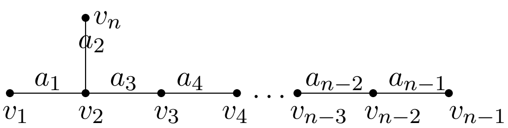

Figure 9: H^*

Theorem 9 *The weighted tree H^* has the maximum value of the Wiener index in $\mathcal{T}_n^*$.*

Proof: Suppose $H \in \mathcal{T}_n^*$ have the maximum Wiener index in $\mathcal{T}_n^*$. Then either $H \in \mathcal{T}_n^{*1}$ or $H \in \mathcal{T}_n^{*2}$.

If $H \in \mathcal{T}_n^{*2}$. By h-transformation on H, we get a new tree H'. By Lemma7, we have $W(H) < W(H')$. It contrary to the hypothesis.

So $H \in \mathcal{T}_n^{*1}$. Let $p = v_1 v_2, \cdots, v_{n-1}$ be the longest path in H, and $d(v_i) = 3$. Without lose of generality, we can assume $2 \leq i \leq \lceil \frac{n-1}{2} \rceil$. From Lemma 8, we can conclude that the branching vertex in H is v_2.

We shall calculate the Wiener index of H. For the sake of convenience, we look H as two paths joining together (see Fig. 10).

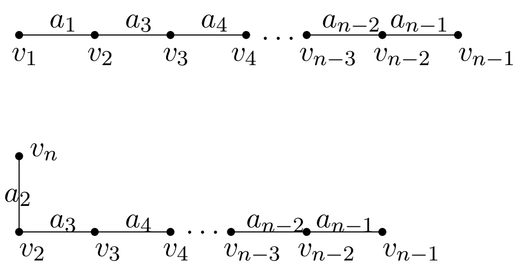

Figure 10:

According to Wiener index formula of P_n,

$$\begin{aligned} & W(H) = (n-2)\left(a_1 + \sum_{k=3}^{n-1} a_k\right) \\ & + \sum_{k=2}^{n-3} [(n-1) - k - 1](k-1) a_{k+1} \\ & + (n-2) \sum_{k=2}^{n-1} a_k \\ & + \sum_{k=2}^{n-3} [(n-1) - k - 1](k-1) a_{k+1} \\ & - (n-2) \sum_{k=3}^{n-1} a_k + a_1 + a_2 \\ & + \sum_{k=2}^{n-4} [(n-1) - k - 1](k-1) a_{k+2} \\ = \; & (n-1)B + \sum_{k=2}^{n-3} 2(n-k-2)(k-1) a_{k+1} \\ & - \sum_{k=3}^{n-3} (n-k-2)(k-1) a_{k+1} \\ = \; & (n-1)B + (2n-4) a_3 \\ & + \sum_{k=3}^{n-3} (n-k-2) k \cdot a_{k+1} \\ = \; & (n-1)B + (2n-4) a_3 \\ & + \sum_{k=4}^{n-2} (n-k-1)(k-1) a_k \end{aligned}$$

$$= \quad (n-1)B + \sum_{k=3}^{n-2}(n-k-1)(k-1)a_k$$

According to the principle of rearrangement inequality, we may conclude that $W(H)$ will reach its maximum value while the edge weights sequence satisfies

$$a_1 \le a_2 \le \cdots \le a_{\lceil \frac{n}{2} \rceil - 1} \le a_{\lceil \frac{n}{2} \rceil}$$

and

$$a_{\lceil \frac{n}{2} \rceil} \ge a_{\lceil \frac{n}{2} \rceil + 1} \ge \cdots \ge a_{n-2} \ge a_{n-1}.$$

i.e., $H = H^*$. Moreover,

$$W(H^*) = (n-1)B + \sum_{k=3}^{n-2}(n-k-1)(k-1)a_k$$

The proof is completed. □

The following theorem shows the second maximum value of $W(T)$ for weighted trees.

Theorem 10 *Suppose $T \in \mathcal{T}_n$ has the second maximum value of the wiener index, then $T \in \mathcal{P}^{n-1}$ or $T = H^*$.*

Proof: Suppose $T \in \mathcal{T}_n, T \neq P_n^*$ have the second maximum Wiener index. If $T \notin \mathcal{P}_{n-1}$ and $T \notin \mathcal{T}_n^*$, by g-transformation, we can get weighted tree H'. By Lemma5, we have

$$W(H) < W(H'),$$

a contradiction. So we have either $T \in \mathcal{P}_{n-1}$ or $T \in \mathcal{T}_n^*$. By Theorem9, the weighted tree H^* has maximum Wiener index in $\mathcal{T}_n^*$.Therefore, if $T \in \mathcal{T}_n$ has the second maximum value of the Wiener index. Then $T \in \mathcal{P}_{n-1}$ or $T = H^*$. □

4 Conclusion

We explore a new class of trees for computing Wiener indices that have not been studied before to the best of our knowledge.We introduced tree operations and derived formulas for the Wiener indices under these operations. Our main results are listed as follows.

1. The weighted star S_n has the minimum value of the Wiener index in weighted trees of order n, and $W(S_n) = (n-1)B$, where $B = \sum_{i=1}^{n-1} a_i$;

2. The weighted tree $S_{1,n-3}^{min}$ has the second minimum value of the Wiener index for weighted trees of order n, and $W(S_{1,n-3}^{min}) = (n-1)B + (n-3)a_{min}$, where $a_{min} = \min_{1 \le i \le n-1}\{a_i\}$

3. If $a_{sec} > \frac{2(n-4)}{n-3}a_{min}$, then the the weighted tree $S_{2,n-4}^{min}$ has the third minimum value of the Wiener index for weighted trees of order n; and if $a_{sec} < \frac{2(n-4)}{n-3}a_{min}$, then the weighted tree $S_{1,n-3}^{sec}$ has the third minimum value of the Wiener index for weighted trees of order n.

4. The weighted path P_n^* has the maximum value of the Wiener index for weighted trees of order n. Moreover, $W(P_n^*) = \sum_{k=1}^{n-1} k(n-k)a_k$.

5. Suppose $T \in \mathcal{T}_n$ has the second maximum value of the wiener index, then $T \in \mathcal{P}^{n-1}$ or $T = H^*$.

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