On Modified and Reverse Wiener Indices of Trees

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The Wiener index is a well-known measure of graph or network structures with similarly useful variants of modified and reverse Wiener indices. The Wiener index of a tree T obeys the relation $W(T) = \sum_e n_{T,1}(e) \cdot n_{T,2}(e)$, where $n_{T,1}(e)$ and $n_{T,2}(e)$ are the number of vertices of T lying on the two sides of the edge e, and where the summation goes over all edges of T. The λ-modified Wiener index is defined as ${}^mW_\lambda(T) = \sum_e [n_{T,1}(e) \cdot n_{T,2}(e)]^\lambda$. For each $\lambda > 0$ and each integer d with $3 \le d \le n-2$, we determine the trees with minimal λ-modified Wiener indices in the class of trees with n vertices and diameter d. The reverse Wiener index of a tree T with n vertices is defined as $\Lambda(T) = \frac{1}{2}n(n-1)d(T) - W(T)$, where $d(T)$ is the diameter of T. We prove that the reverse Wiener index satisfies the basic requirement for being a branching index.

Key words: Modified Wiener Index; Reverse Wiener Index; Tree; Diameter.

1. Introduction

The Wiener index of a connected graph is the sum of distances between all unordered pairs of vertices in the graph. It is one of the oldest and most useful molecular–graph–based structure–descriptors [1 – 4] and its mathematical properties can be found in reviews [5, 6] and in the references cited therein.

Let T be a tree with the vertex set $V(T)$ and the edge set $E(T)$. For any $e \in E(T)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ denote the number of vertices of T lying on the two sides of the edge e. For a long time it has been known [1, 3] that

$$W(T) = \sum_{e \in E(T)} n_{T,1}(e) \cdot n_{T,2}(e).$$

Let P_n and S_n be, respectively, the n-vertex path and n-vertex star. Recall that a caterpillar is a tree in which removal of all pendent vertices (i. e., those of degree one) gives a path. Let $P_{n,d,i}$ be a caterpillar obtained from a path P_{d+1} by attaching $n-d-1$ pendant vertices to the i-th vertex of the path (see Fig. 1). Clearly, $P_{n,d,i}$ has the diameter d for any $1 \le i \le d-1$. Let $P_{n,d} = P_{n,d,\lfloor d/2 \rfloor}$.

In the following two sections, we investigate the modified and reverse Wiener indices, respectively. Mainly driven by theoretical physics, these variants are useful measures of graph or network structures. Further, with respect to applications in biosciences as, e. g., data mining of large molecular networks, our methods will be of future interest.

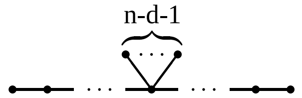

Fig. 1. The graph $P_{n,d,i}$.

2. Modified Wiener Index

Recently, Gutman et al. [7] put forward the λ-*modified Wiener index* ${}^mW_\lambda$, defined as

$${}^mW_\lambda(T) = \sum_{e \in E(T)} [n_{T,1}(e) \cdot n_{T,2}(e)]^\lambda , \qquad (1)$$

where λ is a parameter that may assume different values. Obviously, for $\lambda = 1$ the λ-modified Wiener index ${}^mW_\lambda$ reduces to the ordinary Wiener index. For all $\lambda \ne 0$, the modified Wiener indices ${}^mW_\lambda$ satisfy the basic requirement for being branching indices [7]. Some chemical properties of ${}^mW_\lambda$ were reported in [8, 9] and various mathematical properties of ${}^mW_\lambda$ were established in [10 – 13].

Note that the right–hand side of (1) may be understood as a sum of increments, each associated with an edge. The contribution of the edge e, denoted by ${}^mW_\lambda(e,T)$, is clearly equal to $[n_{T,1}(e)\cdot n_{T,2}(e)]^\lambda$.

Let $\mathcal{T}_{n,d}$ be the class of trees with n vertices and diameter d, where $2 \le d \le n-1$. Obviously, if $T \in \mathcal{T}_{n,2}$ then $T = S_n$, and if $T \in \mathcal{T}_{n,n-1}$ then $T = P_n$. So we can assume in this section that $3 \le d \le n-2$. For each $\lambda > 0$ and each d, we identify the trees in $\mathcal{T}_{n,d}$ with minimal λ-modified Wiener indices.

Let $T \in \mathcal{T}_{n,d}$. For $v \in V(T), d_T(v)$ denotes the degree of v. Let $V_1(T) = \{v \in V(T) | d_T(v) \ge 3\}$. There are $d_T(v)$ components in $T - v$, each containing a vertex that is adjacent to vertex v in T. These components are called the *branches* of T at v.

It is easy to see that the function $f(t) = [t(n-t)]^\lambda$ is increasing if $\lambda > 0$ and decreasing if $\lambda < 0$ for $1 \le t \le \frac{n}{2}$. We will use this fact frequently in our proof.

Lemma 1: *Let $T \in \mathcal{T}_{n,d}$. If T is not a caterpillar, then there is a caterpillar $T^* \in \mathcal{T}_{n,d}$ such that ${}^mW_\lambda(T^*) < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(T^*) > {}^mW_\lambda(T)$ if $\lambda < 0$.*

Proof: Let $P(T) = v_0, v_1, \cdots, v_d$ be a diametrical path of T. Since T is not a caterpillar, it follows that for some i with $2 \le i \le d-2$, v_i has a neighbor w outside $P(T)$ and w is not a pendent vertex. Let n_w be the number of vertices of the branch at v_i containing w. Then $n_w \ge 2$. Let $w_1, \ldots, w_r$ be the neighbors of w in T except v_i.

Let T' denote the tree formed from T by deleting edges ww_j and adding edges v_iw_j for $j = 1, \ldots, r$. Obviously $T' \in \mathcal{T}_{n,d}$. It is easy to see that

$$\begin{aligned} &{}^mW_\lambda(T') - {}^mW_\lambda(T) \\ &= {}^mW_\lambda(v_iw, T') - {}^mW_\lambda(v_iw, T) \\ &= [1 \times (n-1)]^\lambda - [n_w(n-n_w)]^\lambda . \end{aligned} \tag{2}$$

Since $2 \le n_w \le n-d-1$, and the function $f(t) = [t(n-t)]^\lambda$ is increasing if $\lambda > 0$ and decreasing if $\lambda < 0$ for $1 \le t \le \frac{n}{2}$, we have from (2) that ${}^mW_\lambda(T') < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(T') > {}^mW_\lambda(T)$ if $\lambda < 0$. Iterating the transformation from T to T' yields the tree T^* as required.

Lemma 2: *Let $T \in \mathcal{T}_{n,d}$ be a caterpillar. If $|V_1(T)| \ge 2$, then there is an i with $1 \le i \le d-1$ such that ${}^mW_\lambda(P_{n,d,i}) < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(P_{n,d,i}) > {}^mW_\lambda(T)$ if $\lambda < 0$.*

Proof: Let $P(T) = v_0, v_1, \cdots, v_d$ be a diametrical path of T. Let $v_i, v_j \in V_1(T)$ such that the distance between v_i and v_j is as small as possible, where $1 \le i < j \le d-1$. If $j - i > 1$, then the vertices $v_{i+1}, \ldots, v_{j-1}$ have degree two. Let n_1 (respectively n_2) be the number of vertices of the branch at v_{i+1} (respectively v_{j-1}) containing v_i (respectively v_j). Then $n_1 + n_2 + (j-i-1) = n$. Assume that $n_1 \ge n_2$. Let w be a pendent vertex adjacent to v_j.

Let T' denote the tree formed from T by deleting edge v_jw and adding edge v_iw. Obviously $T' \in \mathcal{T}_{n,d}$. It is easy to see that

$$\begin{aligned} &{}^mW_\lambda(T') - {}^mW_\lambda(T) \\ &= {}^mW_\lambda(v_{j-1}v_j, T') - {}^mW_\lambda(v_iv_{i+1}, T) \\ &= [(n_2-1)(n-n_2+1)]^\lambda - [n_1(n-n_1)]^\lambda . \end{aligned}$$

Since $n_2 - 1 < \min\{n_1, n-n_1\} \le \frac{n}{2}$, we have ${}^mW_\lambda(T') < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(T') > {}^mW_\lambda(T)$ if $\lambda < 0$. Iterating the transformation from T to T' yields the tree T^* as required.

Lemma 3: *Let $T = P_{n,d,i}$ with $1 \le i \le d-1$. If $i \ne \lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil$, then ${}^mW_\lambda(P_{n,d}) < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(P_{n,d}) > {}^mW_\lambda(T)$ if $\lambda < 0$.*

Proof: Since $T = P_{n,d,i}$ with $1 \le i \le d-1$ and $i \ne \lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil$, we may assume that $1 \le i < \lfloor \frac{d}{2} \rfloor$. It is easy to see that

$$\begin{aligned} &{}^mW_\lambda(P_{n,d,i+1}) - {}^mW_\lambda(P_{n,d,i}) \\ &= [(i+1)(n-i-1)]^\lambda - [(i+n-d)(d-i)]^\lambda . \end{aligned}$$

Note that $i+1 < \min\{i+n-d, d-i\} \le \frac{n}{2}$. We have ${}^mW_\lambda(P_{n,d,i+1}) < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(P_{n,d,i+1}) > {}^mW_\lambda(T)$ if $\lambda < 0$. Iterating the procedure, we prove the lemma.

Theorem 4: *Let $T \in \mathcal{T}_{n,d}$ and $T \ne P_{n,d}$, where $3 \le d \le n-2$. Then*

$$\begin{aligned} &{}^mW_\lambda(T) > {}^mW_\lambda(P_{n,d}) \text{ if } \lambda > 0, \\ &{}^mW_\lambda(T) < {}^mW_\lambda(P_{n,d}) \text{ if } \lambda < 0. \end{aligned}$$

Proof: If T is not a caterpillar, we have by Lemma 1 that there is a caterpillar $T' \in \mathcal{T}_{n,d}$ such that ${}^mW_\lambda(T') < {}^mW_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(T') > {}^mW_\lambda(T)$ if $\lambda < 0$.

If $|V_1(T')| \geq 2$, we have by Lemma 2 that for some i with $1 \leq i \leq d-1$, ${}^mW_\lambda(P_{n,d,i}) <^m W_\lambda(T)$ if $\lambda > 0$ and ${}^mW_\lambda(P_{n,d,i}) >^m W_\lambda(T)$ if $\lambda < 0$.

Now the result follows from Lemma 3.

For given n and d, the λ-modified Wiener index of $P_{n,d}$ are given by

$$
\begin{aligned}
{}^mW_\lambda(P_{n,d}) &= (n-d-1)(n-1)^\lambda \\
&\quad + \sum_{i=1}^{\lfloor d/2 \rfloor} [i(n-i)]^\lambda + \sum_{i=1}^{\lceil d/2 \rceil} [i(n-i)]^\lambda .
\end{aligned}
$$

Remark: Vukičević and Žerovnik [14] initiated the study of the variable Wiener indices, defined as

$$
\lambda W(T) = \frac{1}{2} \sum_{e \in E(T)} \left[|V(T)|^\lambda - n_{T,1}(e)^\lambda - n_{T,2}(e)^\lambda \right].
$$

Let $T \in \mathcal{T}_{n,d}$ and $T \neq P_{n,d}$, where $3 \leq d \leq n-2$. Using the fact that the function $g(t) = t^\lambda + (n-t)^\lambda$ is decreasing if $\lambda > 1$ and increasing if $\lambda < 1$ for $1 \leq t \leq \frac{n}{2}$ and similar arguments as above, we have

$$
\begin{aligned}
&{}_\lambda W(T) > {}_\lambda W(P_{n,d}) \text{ if } \lambda > 1, \\
&{}_\lambda W(T) < {}_\lambda W(P_{n,d}) \text{ if } \lambda < 1.
\end{aligned}
$$

3. Reverse Wiener Index

Balaban et al. [15] proposed a novel topological index, the reverse Wiener index. Let G be a graph with n vertices. Then the *reverse Wiener index* Λ is defined as

$$
\Lambda(G) = \frac{1}{2} n(n-1)d - W(G),
$$

where d is the diameter of G. In [15], analytical forms were presented for the values of Λ of several classes of graphs, including complete graph, star, path, cycle and linear polyacenes, relationships with other topological indices were discussed, and it was tested in a large number of QSPR relationship models, demonstrating the usefulness of this index.

Let $\mathcal{T}_n$ be the class of trees with n vertices. Using Theorem 4, in the following we prove that the reverse Wiener index also satisfies the basic requirement for being a branching index, that is

$$
\Lambda(P_n) > \Lambda(T) > \Lambda(S_n), \tag{3}
$$

where T is any tree in $\mathcal{T}_n \setminus \{P_n, S_n\}$ and n is any integer greater than 4.

Theorem 5: *Let $T \in \mathcal{T}_n \setminus \{P_n\}$ with $n \geq 4$. Then $\Lambda(T) < \Lambda(P_n)$.*

Proof: Let d be the diameter of T. Then $2 \leq d \leq n-2$. By Theorem 4, $W(T) \geq W(P_{n,d})$, which implies that $\Lambda(T) \leq \Lambda(P_{n,d})$. On the other hand, since

$$
\begin{aligned}
&\Lambda(P_{n,d+1,\lfloor d/2 \rfloor}) - \Lambda(P_{n,d}) \\
&= \frac{n(n-1)}{2} - W(P_{n,d+1,\lfloor d/2 \rfloor}) + W(P_{n,d,\lfloor d/2 \rfloor}) \\
&= \frac{n(n-1)}{2} - \left(\lceil \frac{d}{2} \rceil + 1 \right) \left(n - \lceil \frac{d}{2} \rceil - 1 \right) + (n-1) \\
&\geq \frac{n(n-1)}{2} - \frac{n}{2} \times \frac{n}{2} + (n-1) = \frac{(n+1)^2 - 5}{4}
\end{aligned}
$$

and $n \geq 4$, we have $\Lambda(P_{n,d}) < \Lambda(P_{n,d+1,\lfloor d/2 \rfloor})$. It follows that $\Lambda(T) \leq \Lambda(P_{n,d,\lfloor d/2 \rfloor}) < \Lambda(P_{n,d+1,\lfloor d/2 \rfloor}) < \cdots < \Lambda(P_n)$.

Let $\mathcal{CPT}_n$ be the class of trees T in $\mathcal{T}_n$ such that one center of T is adjacent to at least one pendent vertex.

Lemma 6: *Let $T \in \mathcal{CPT}_n$ with diameter at least 4. Then there is a tree $T^* \in \mathcal{T}_n \setminus CPT_n$ such that $\Lambda(T^*) < \Lambda(T)$.*

Proof: Let v be a center of T such that it is adjacent to a pendent vertex, say w. We know that at least one branch not containing the vertex w at v, say T_1 has $n_1 \leq \frac{n}{2} - 1$ vertices. Suppose that v is adjacent to v_1 in T_1. Let T' denote the tree formed from T by deleting edge vw and adding edge wv_1. Since

$$
\begin{aligned}
&W(T') - W(T) = W(T', vv_1) - W(T, vv_1) \\
&= (n_1 + 1)(n - n_1 - 1) - n_1(n - n_1)
\end{aligned}
$$

and $n_1 \leq \frac{n}{2} - 1$, we have $W(T') > W(T)$. Note that T' and T have the same diameter. We have $\Lambda(T') < \Lambda(T)$. Iterating the transformation from T to T' yields the tree T^* as required.

Lemma 7: *Let $T \in \mathcal{T}_n \setminus CPT_n$ with diameter $d \geq 4$. Then there is a tree $T^* \in CPT_n$ with diameter $d-2$ such that $\Lambda(T^*) < \Lambda(T)$.*

Proof: Let v be a center of T with neighbors $v_1,\ldots,v_p$. Then there are p branches $T_1,\ldots,T_p$ at v. Let r_i denote the number of vertices of T_i. Assume that $r_1 = \min_{1\le i\le p} r_i$. Let $v_{i1},\ldots,v_{ir_i}$ be the neighbors of v_i in T_i, $1 \le i \le p$. Let T^* be the tree formed from T by deleting edges v_iv_{ij} and adding edges vv_{ij} for all $i = 1,\ldots,p$ and $j = 1,\ldots,r_i$. Clearly,

$$\begin{aligned}
\Lambda(T^*) - \Lambda(T) &= -\frac{n(n-1)}{2} \times 2 + W(T) - W(T^*)\\
&= -n(n-1) + \sum_{i=1}^{p} r_i(n-r_i) - p(n-1)\\
&\le -n\times(n-1) + (n-r_1)\sum_{i=1}^{p} r_i - p(n-1)\\
&= -n(n-1) + (n-1)(n-r_1) - p(n-1)\\
&= -(n-1)(r_1+p) < 0.
\end{aligned}$$

This proves the lemma.

Theorem 8: *Let $T \in \mathcal{T}_n \setminus \{S_n\}$ with $n \ge 4$. Then $\Lambda(S_n) < \Lambda(T)$.*

Proof: The case for $n = 4$ is trivial. Suppose that $n \ge 5$. If the diameter of T is at least 4, then by using Lemmas 6 and 7 alternately as possible as we can, we obtain a tree T' with n vertices and diameter 2 or 3 such that $\Lambda(T') < \Lambda(T)$. If the diameter T' is 2, we are done. Suppose that the diameter of T' or T is 3. Then T' is formed by attaching $p, n-2-p$ pendent vertices to the two vertices of P_2, respectively, for some p with $1 \le p \le \frac{n}{2} - 1$. It is easy to see that

$$\begin{aligned}
&\Lambda(S_n) - \Lambda(T)\\
&\le -\frac{n(n-1)}{2} + (p+1)(n-p-1) - (n-1)\\
&= -(n-1)\left(\frac{n}{2}+1\right) + (p+1)(n-p-1) < 0.
\end{aligned}$$

So we have $\Lambda(S_n) < \Lambda(T')$.

By Theorems 5 and 8, the reverse Wiener index obeys the inequalities (3) and can therefore be viewed as a branch index.

Remark: Let $T \in \mathcal{T}_n \setminus \{P_n, S_n\}$ where $n > 4$. Then $W(P_n) > W(T) > W(S_n)$, as (3) is [16]. Suppose that $n \ge 6$ and that the diameter of T is d. By Theorem 4, $\Lambda(T) \le \Lambda(P_{n,d,\lfloor d/2\rfloor})$. It is easy to see that $\Lambda(P_{n,d,\lfloor d/2\rfloor}) \le \Lambda(P_{n,d+1,\lfloor (d+1)/2\rfloor})$. Thus we have $\Lambda(T) \le \Lambda(P_{n,n-2,\lfloor (n-2)/2\rfloor})$. However, it can be easily checked that $W(T) \le W(P_{n,n-2,1})$.

4. Outlook

The Wiener index is a well-known measure of graph or network structures, with similarly useful variants of modified and reverse Wiener indices. For each $\lambda > 0$ and each integer d with $3 \le d \le n-2$, we determined the trees with minimal λ-modified Wiener indices in the class of trees with n vertices and diameter d. We also proved that the reverse Wiener index can be used as a branching index.

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