Algorithms and Extremal Problem on Wiener Polarity Index *

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Abstract

The Wiener polarity index $W_P(G)$ of a graph $G = (V, E)$ is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 3$. In this paper, we consider the index for connected graphs. In the first part, we describe a linear time algorithm **APT** for computing the index of trees, and then characterize the trees maximizing the index among all trees of given order. In the second part, we present an algorithm **APG** which computes the index $W_P(G)$ for any given connected graph G on n vertices in time $O\big(M(n)\big)$, where $M(n)$ denotes the time necessary to multiply two $n \times n$ matrices of small integers (which is currently known to be $O(n^{2.376})$).
Keywords: distance, Wiener polarity index; Wiener index, algorithm; extremal graph.

1 Introduction

We use Trinajstić [14] for terminology and notations. Let G be a connected (molecular) graph. The *distance* between two vertices u and v in G, denoted by $d_G(u, v)$, is the length of a shortest path between u and v in G. A tree is a connected acyclic graph. It is well known that for any two vertices u and v in a tree T, there exists exactly one path between u and v in T. Thus, the distance between two vertices u and v in T is the length of the path between u and v in T. The *Wiener polarity index* of a graph $G = (V, E)$, denoted by $W_P(G)$, is defined by

$$W_P(G) := \#\big\{\{u, v\} \mid d_G(u, v) = 3, u, v \in V\big\}, \tag{1}$$

which is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 3$. In organic compounds, say paraffin, this number is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. The name "Wiener polarity index" for the quantity defined in Equation

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(1) is introduced by Harold Wiener [15] in 1947. Wiener himself conceived the index only for acyclic molecules and defined it in a slightly different – yet equivalent – manner. In the same paper, Wiener also introduced another index for acyclic molecules, called *Wiener index* or *Wiener distance index* and defined by

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

Wiener [15] used a liner formula of W and W_P to calculate the boiling points t_B of the paraffins, *i.e.,*

$$t_B = aW + bW_P + c,$$

where a, b and c are constants for a given isomeric group.

The Wiener index $W(G)$ is popular in chemical literatures. In the mathematical literature, it seems to be studied firstly by Entringer *et al.*[8] in 1976. From then on, many researchers studied the Wiener index in different ways. For instance, one can see [1], [2], [3] [6], [8], [9], [11], [12] and [15] for theoretical aspects, and [4], [10] and [13] for algorithmic and computational aspects. Recently, Dobrynin *et al.* wrote a comprehensive survey [7] for the Wiener index. The reader is referred to the paper for further details.

However, it seems that less attention has been paid for the Wiener polarity index $W_P(G)$ up to now. In the present paper, we consider the index for connected graphs. By the definition of Wiener polarity index, one can readily check that $W_P(K_{1,n-1}) = 0$. Moreover, $W_P(T) > 0$ for any tree T of order $n \geq 4$. Thus, a star $K_{1,n-1}$ minimize the Wiener polarity index among all trees of given order. In Section 2, we first give a linear time algorithm **APT** for computing the index of trees, and then characterize the trees maximizing the index among all trees of given order. In Section 3, we present an algorithm **APG** which computes the index $W_P(G)$ for any given connected graph G on n vertices in time $O\big(M(n)\big)$, where $M(n)$ denotes the time necessary to multiply two $n \times n$ matrices of small integers (which is currently known to be $O(n^{2.376})$ [5]).

2 Wiener Polarity Index for Trees

In this section, we consider the Wiener polarity index W_P for trees. We first introduce a linear time algorithm **APT** for computing the index of trees, and then consider the problem of determining which trees maximize the index among all trees of given order.

2.1 A Linear Time Algorithm

According to the definition of Wiener polarity index, Equation (1), one can readily design an algorithm in $O\big(|V(T)|(\Delta(T)-1)^2\big)$ time for computing the index $W_P(T)$ of a tree T by exhausted searching. The algorithm, however, might be not linear time if the maximum degree $\Delta(T)$ of T is large. In fact, we can get a linear time algorithm **APT** for computing the index of a tree T due to a good property that for any two vertices u and v in a tree T, there exists exactly one path between u and v in T. Furthermore, we have the following result.

Lemma 1. *Let $T = (V, E)$ be a tree. Then*

$$W_P(T) = \sum_{uv \in E} \big(d_T(u) - 1\big)\big(d_T(v) - 1\big). \tag{1}$$

Proof. We first define a set $D_3(T)$ as follows:

$$D_3(T) := \big\{\{u, v\} \mid d_T(u, v) = 3, u, v \in V\big\}.$$

Clearly, $W_P(T) = |D_3(T)|$ by the definition of Wiener polarity index. Next, we introduce another set $S_E(T)$ as follows:

$$S_E(T) := \big\{\{u, v\} \mid \exists\ xy \in E \textit{ such that } ux \text{ and } vy \in E\big\}.$$

One can readily see that

$$|S_E(T)| = \sum_{xy \in E} \big(d_T(x) - 1\big)\big(d_T(y) - 1\big).$$

Let $\varphi : D_3(T) \to S_E(T)$ be a mapping such that $\varphi\big(\{u, v\}\big) = \{u, v\}$ for any $\{u, v\} \in D_3(T)$. One can easily check that the mapping φ is a bijection. Thus, $|D_3(T)| = |S_E(T)|$, and then Equation (1) follows. □

Let T be a tree of order n. In the sequel, we use a list $li(T)$ concerning edges of T and degrees of $V(T)$ to represent T. Formally, we define

$$li(T) := \{e_1 = x_1y_1, e_2 = x_2y_2, \ldots, e_{n-1} = x_{n-1}y_{n-1}, d_T(v_1), \ldots, d_T(v_n)\}.$$

The following is a linear time algorithm for computing the Wiener polarity index $W_P(T)$ of a tree T represented by a list $li(T)$ of T.

APT

```
Input:  A tree T of order n represented by a list li(T) of T.
Output:  Wiener polarity index WP(T) of T.
   begin
     WP(T):=0
     for all edges u[i]v[i] of T, i:=1 to (n-1) do
   end  WP(T) = WP(T) + (d(u[i])-1)(d(v[i])-1)
```

According to Lemma 1, the algorithm **APT** correctly computes the Wiener polarity index $W_P(T)$ of T. Obviously, the algorithm **APT** can be done in $O(n)$ time. Hence, we have the following result.

Theorem 1. *Let T be a tree of order n. Then the algorithm* **APT** *correctly computes the Wiener polarity index $W_P(T)$ of T in $O(n)$ time.*

2.2 Extremal Trees

As we mentioned in the introduction, a star $K_{1,n-1}$ minimizes the Wiener polarity index among all trees of order n. The goal of this part is to characterize the trees maximizing the index among all trees of given order. For this purpose, we first consider a simple case.

The *diameter* of a connected graph G, denoted by $diam(G)$, is the maximum distance between two vertices of G. Since there exists exactly one path between any two vertices of a tree, the diameter of a tree is the length of a longest path in the tree. In what follows, we use $\mathcal{T}(n)$ to denote the set of trees on n vertices. Let $T \in \mathcal{T}(n)$ with $diam(T) = 3$, and let $P_L(T) = v_0v_1v_2v_3$ be a longest path in T. It follows from Equation (1) that

$$W_P(T) = \big(d_T(v_1) - 1\big)\big(d_T(v_2) - 1\big).$$

Thus,

$$W_P(T) \le \left(\left\lceil \frac{n}{2} \right\rceil - 1\right)\left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right) = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor. \tag{2}$$

On the other hand, if $T \in \mathcal{T}(n)$, $n \ge 4$, and $P_L(T) = v_0v_1v_2v_3$ is a longest path of T with $d_T(v_1) = \lceil \frac{n}{2} \rceil$ and $d_T(v_2) = \lfloor \frac{n}{2} \rfloor$ then $W_P(T) = \lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor$. Hence, the following set

$$\mathcal{T}_3(n) := \{T \in \mathcal{T}(n) \mid diam(T) = 3 \text{ and } W_P(T) = \lceil \tfrac{n-2}{2} \rceil \lfloor \tfrac{n-2}{2} \rfloor\}$$

is not empty. In the following, we will see that the above value $\lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor$ is the maximum value of W_P for trees of order n. Hence, $\mathcal{T}_3(n)$ is one of the classes of extremal trees maximizing the Wiener polarity index W_P.

To characterize extremal trees with diameter larger than 3, we introduce an operation on trees. Let $T \in \mathcal{T}(n)$ be a tree with $diam(T) = k$ where $k \ge 4$ is an integer. We suppose that $P_L(T) = v_0v_1v_2v_3v_4 \dots v_k$ is a longest path of T. Let $T \circledast v_0$ denote the tree obtained from T by deleting the edge v_0v_1 and adding a new edge v_0v_3 as shown in *Figure 1.*

$P_L(T)$

The corresponding subgraph of $P_L(T)$ in $T \circledast v_0$

Figure 1. Maximization operation of a tree T with $diam(T) \ge 4$.

The above operation is called *maximization operation.* One can easily see that $diam(T \circledast v_0) \le diam(T)$. To establish the main theorem of this subsection, we first prove the following lemma concerning the relation between $W_P(T)$ and $W_P(T \circledast v_0)$.

Lemma 2. *Let $T = (V, E)$ be a tree, and let $P_L(T) = v_0v_1 \dots v_k$ be a longest path of T, where $k \ge 4$ is an integer. Then*

i) $W_P(T) < W_P(T \circledast v_0)$ *if $diam(T) \ge 5$,*

ii) $W_P(T) \le W_P(T \circledast v_0)$ *if $diam(T) = 4$.*

Proof. We only prove the first assertion, and suppose that T is a tree with $diam(T) \geq 5$. Let

$$D_3(T) = \big\{\{u, v\} \mid d_T(u, v) = 3, u, v \in V\big\}.$$

Obviously, $W_P(T) = |D_3(T)|$. Thus, to show the first assertion, it is sufficient to show that

$$|D_3(T)| < |D_3(T \circledast v_0)|.$$

In order to establish the above inequality, we introduce a notion concerning a subset of $D_3(T)$. Let

$$D_3(T, u) = \big\{\{u, v\} \mid \{u, v\} \in D_3(T)\big\}.$$

Obviously, $D_3(T, u) \subseteq D_3(T)$ for any vertex $u \in V$, and $|D_3(T)| = \frac{1}{2}\sum_{u\in V} \big|D_3(T, u)\big|$. In fact, one can readily verify that

$$|D_3(T, v_0)| < |D_3(T \circledast v_0, v_0)|, \ |D_3(T, v_1)| = |D_3(T \circledast v_0, v_1)| - 1,$$

and

$$|D_3(T, v_3)| = |D_3(T \circledast v_0, v_3)| + 1.$$

Furthermore, one can also verify that if $u \in V \setminus \{v_0, v_1, v_3\}$ then

$$|D_3(T, u)| \leq |D_3(T \circledast v_0, u)|.$$

Thus, $|D_3(T)| < |D_3(T \circledast v_0)|$ and then the first assertion holds.

Using a similar method, one can readily prove the second assertion. □

By the second assertion of Lemma 2, if T is a tree with $diam(T) \geq 4$ then we can construct another tree $T \circledast v_0$ by the maximization operation such that

$$W_P(T) \leq W_P(T \circledast v_0),$$

where v_0 is one end of a longest path in T. Since $W_P(T) \leq \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$ for any tree $T \in \mathcal{T}(n)$ with $diam(T) = 3$, we have the following result.

Theorem 2. *For any tree T of order n we have that $0 \leq W_P(T) \leq \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$.*

By the first assertion of Lemma 2, if T is a tree with $diam(T) \geq 5$ then we can construct another tree $T \circledast v_0$ by the maximization operation such that

$$W_P(T) < W_P(T \circledast v_0),$$

where v_0 is one end of a longest path in T. Moreover, by Theorem 2, one can readily see that if T is a tree with $|V(T)| = n$ and $W_P(T) = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$ then $diam(T) \leq 4$. In the following, we characterize trees T of order n with $diam(T) = 4$ and $W_P(T) = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$.

Lemma 3. *There exists a tree T of order n such that $diam(T) = 4$ and $W_P(T) = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor$.*

Proof. Let T be a tree with $|V(T)| = n$ and $diam(T) = 4$. It is not difficult to see that T can be represented by $m+3$ integers (see *Figure 2*) $k_1, k_2, k_3, l_1, \ldots, l_m$ satisfying that $k_i \geq 0$ ($i = 1, 2, 3$), $m \geq 0$, $l_j \geq 1$ when $m \geq 1$ and $1 \leq j \leq m$, and

$$k_1 + k_2 + k_3 + l_1 + \cdots + l_m = n - 5 - m. \tag{3}$$

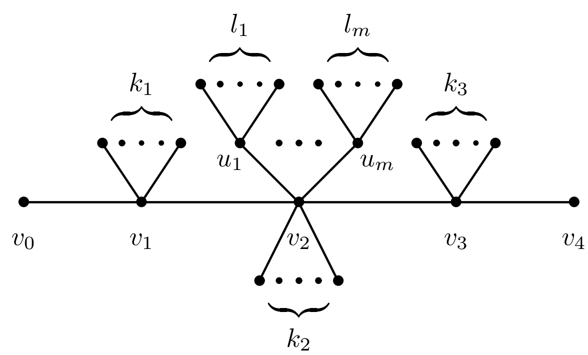

Figure 2. The structure of $T(k_1, k_2, k_3, l_1, \ldots, l_m)$.

Clearly, the above representation is unique for a given tree $T \in \mathcal{T}(n)$ with diameter 4. In what follows, we use $T(k_1, k_2, k_3, l_1, \ldots, l_m)$ to denote a tree which can be represented by integers $k_1, k_2, k_3, l_1, \ldots, l_m$. By Equation (1), we have

$$\begin{aligned} W_P\big(T(k_1, k_2, k_3, l_1, \ldots, l_m)\big) &= (m + k_2 + 1)(k_1 + 1) + (m + k_2 + 1)(k_3 + 1) \\ &\quad + (m + k_2 + 1)l_1 + \cdots + (m + k_2 + 1)l_m \\ &= (m + k_2 + 1)(k_1 + k_3 + l_1 + \cdots + l_m + 2). \end{aligned}$$

Using Equation (3), we have

$$W_P\big(T(k_1, k_2, k_3, l_1, \ldots, l_m)\big) = \big(m + k_2 + 1\big)\big(n - 2 - (m + k_2 + 1)\big).$$

One can readily check that $n-2-(m+k_2+1) = \lfloor \frac{n-2}{2} \rfloor$ if $m+k_2+1 = \lceil \frac{n-2}{2} \rceil$, and $n-2-(m+k_2+1) = \lceil \frac{n-2}{2} \rceil$ if $m + k_2 + 1 = \lfloor \frac{n-2}{2} \rfloor$. Thus, for a tree $T(k_1, k_2, k_3, l_1, \ldots, l_m)$ with $m + k_2 + 1 = \lceil \frac{n-2}{2} \rceil$ or $\lfloor \frac{n-2}{2} \rfloor$, we have

$$W_P\big(T(k_1, k_2, k_3, l_1, \ldots, l_m)\big) = \left\lceil \frac{n-2}{2} \right\rceil \left\lfloor \frac{n-2}{2} \right\rfloor,$$

and then the lemma follows. □

Let

$$\mathcal{T}_4(n) = \{T(k_1, k_2, k_3, l_1, \ldots, l_m) \in \mathcal{T}(n) \mid m + k_2 + 1 = \lceil \tfrac{n-2}{2} \rceil \text{ or } \lfloor \tfrac{n-2}{2} \rfloor\}.$$

By the proof of the above lemma, one can easily see that $W_P(T) = \lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor$ if $T \in \mathcal{T}_4(n)$. According to our analysis above, we can obtain the main result of this subsection.

Theorem 3. *Among all trees of order n, a tree T has the maximal Wiener polarity index if and only if T belongs to $\mathcal{T}_3(n) \cup \mathcal{T}_4(n)$, and $W_P(T) = \lceil \frac{n-2}{2} \rceil \lfloor \frac{n-2}{2} \rfloor$.*

3 An Algorithm for Connected Graphs

Let G be a graph with ω components $C_1, \ldots, C_\omega$. Obviously,

$$W_P(G) = \sum_{i=1}^{\omega} W_P(C_i).$$

Thus, to calculate the Wiener polarity index for general graphs, it is sufficient to study how to calculate the index for connected graphs. In this section, we present an algorithm **APG** which computes the index $W_P(G)$ for any given connected graph G on n vertices in time $O\big(M(n)\big)$, where $M(n)$ denotes the time necessary to multiply two $n \times n$ matrices of small integers (which is currently known to be $O(n^{2.376})$ [5]).

To any graph $G = (V, E)$ with the vertex set $V = \{v_1, \ldots, v_n\}$ there corresponds an $n \times n$ matrix, called the *adjacency matrix of* G and denoted by $A(G)$ or A, in which $a_{ij} = 1$ if and only if $v_i v_j \in E$. We use $A^k = \big(a_{ij}^{(k)}\big)_{n\times n}$ to denote the k-th repeated product of A where k is a positive integer. To establish our main result of this section, we first introduce some lemmas.

Lemma 4. *Let G be a connected graph, and let $A = (a_{ij})_{n\times n}$ be the adjacency matrix of G. If G has a path of length k between two vertices v_i and v_j, then $a_{ij}^{(k)} > 0$ where $\big(a_{ij}^{(k)}\big)_{n\times n} = A^k$ and k is a positive integer.*

Lemma 5. *Let G be a connected graph, and let $A = (a_{ij})_{n\times n}$ be the adjacency matrix of G. If v_i and v_j are two vertices of G, and $a_{ij}^{(k)} > 0$ then $d_G(v_i, v_j) \le k$ where $\big(a_{ij}^{(k)}\big)_{n\times n} = A^k$ and k is a positive integer.*

The above two lemmas are well-known results. In fact, one can readily prove them by induction on k.

We use B to denote an $n \times n$ matrix, called the distance-2 matrix of G, in which $b_{ij} = 1 (i \neq j)$ if and only if $a_{ij} = 1$ or $a_{ij}^{(2)} > 0$, and $b_{ii} = 0$. Furthermore, we use C to denote another $n \times n$ matrix, called the distance-3 matrix of G, in which $c_{ij} = 1 (i \neq j)$ if and only if $b_{ij} = 1$ or $a_{ij}^{(3)} > 0$, and $c_{ii} = 0$. Using the above notations, we can characterize the distance between two vertices of a connected graph G by the distance-2 matrix and distance-3 matrix of G as follows.

Lemma 6. *Let G be a connected graph of order n, and let $B = (b_{ij})_{n\times n}$ and $C = (c_{ij})_{n\times n}$ be the distance-2 matrix and distance-3 matrix of G, respectively. If v_i and v_j are two distinct vertices of G, then*

i) $b_{ij} = 1$ *if and only if* $d_G(v_i, v_j) \le 2$,

ii) $c_{ij} = 1$ *if and only if* $d_G(v_i, v_j) \le 3$.

Proof. We only show the first assertion. If $d_G(v_i, v_j) = 2$ then $a_{ij}^{(2)} > 0$ by Lemma 4. Clearly, $a_{ij} = 1$ if $v_i v_j$ is an edge of G. Thus $b_{ij} = 1$ by the definition the distance-2 matrix. Conversely, if $b_{ij} = 1$ then $a_{ij} = 1$ or $a_{ij}^{(2)} > 0$ by the definition the distance-2 matrix. Thus $d_G(v_i, v_j) \le 2$ by Lemma 5.

One can easily prove the second assertion by a similar manner. □

Using above lemmas, we can prove the main theorem in this section.

Theorem 4. *Let G be a connected graph of order n, and let B and C be the distance-2 matrix and distance-3 matrix of G, respectively. If $Z := C - B$ then*

$$W_P(G) = \sum_{i=1}^{n} \sum_{j>i} z_{ij},$$

where $(z_{ij})_{n\times n} = Z$.

Proof. Let v_i and v_j be two distinct vertices of G. By Lemma 6, $z_{ij} = 1$ if and only if $d_G(v_i, v_j) = 3$. Thus,

$$\sum_{i=1}^{n} \sum_{j>i} z_{ij} = \#\big\{\{u, v\} \mid d_G(u, v) = 3, u, v \in V\big\}.$$

Therefore, $W_P(G) = \sum_{i=1}^{n} \sum_{j>i} z_{ij}$ due to the definition of the Wiener polarity index. □

According to the above theorem, we can design the following algorithm **APG** to compute the Wiener polarity index $W_P(G)$ for any connected graph G represented by the adjacency matrix A of G.

APG

```
Input:  A connected graph G with vertex set V := {v[1], ··· , v[n]}
         represented by the adjacency matrix A := (a[i][j]) of G.
Output:  Wiener polarity index WP(G) of G.
   begin
     X := A · A and B := (b[i][j])
     for i:=1 to n do
        for j:=1 to n do
           if i=j then b[i][j]:=0.
           if i ≠ j and (a[i][j] = 1 or x[i][j] > 0) then b[i][j]:=1, else
           b[i][j]:=0.
     Y := X · A and C := (c[i][j])
     for i:=1 to n do
        for j:=1 to n do
           if i=j then c[i][j]:=0.
           if i ≠ j and (b[i][j] = 1 or y[i][j] > 0) then c[i][j]:=1, else
           c[i][j]:=0.
     Z:=C-B and WP(G):=0
     for i:=1 to n do
        for j:=i+1 to n do
   end     WP(T) = WP(T) + z[i][j]
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The correctness of the algorithm **APG** follows from Theorem 4. It is not difficult to see that the algorithm **APG** can be done in $O\big(M(n)\big)$ time, where $M(n)$ denotes the time necessary to multiply two $n \times n$ matrices of small integers. Up to now, the complexity of the known fast matrix multiplication algorithm $M(n)$ by Coppersmith and Winograd [5] is $O(n^{2.376})$. Thus we have the following result.

Theorem 5. *Let G be a connected graph of order n. Then the algorithm* **APG** *correctly computes Wiener polarity index $W_P(G)$ of G in $O\big(M(n)\big)$ time.*

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