Wiener-Type Invariants of Trees and Their Relation

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Abstract

The distance $d(u, v| G)$ between the vertices $u$ and $v$ of a (connected) graph $G$ is the length (= number of edges) of a shortest path connecting $u$ and $v$. The Wiener number $W(G)$ of $G$ is the sum of distances between all pairs of vertices of $G$. We consider a class of Wiener-type invariants $W_{\lambda}(G)$, defined as the sum of the terms $d(u, v| G)^{\lambda}$ over all pairs of vertices of $G$. Several special cases of $W_{\lambda}(G)$, namely the invariants for $\lambda = +1$ (the original Wiener number) as well as for $\lambda = -2, -1, +1/2, +2$ and $+3$, were previously studied in the chemical literature, and found applications as molecular structure descriptors. We modify the definition of $W_{\lambda}(G)$ so that it extends also to non-connected graphs and then deduce the identity $W_{\lambda+1}(T) = (n - 1) W_{\lambda}(T) - \sum W_{\lambda}(T - e)$, valid for any $n$-vertex tree $T$, with the summation embracing all edges $e$ of $T$.

1 Introduction

In this paper we are concerned with finite undirected graphs. The metric on these graphs is defined in the usual manner [1]: Let $u$ and $v$ be two vertices belonging to the same component of the graph $G$. The distance $d(u,v|G)$ between the vertices $u$ and $v$ is the length (= number of edges) of a shortest path connecting $u$ and $v$. If $u = v$, then $d(u,v|G) = 0$. If $u$ and $v$ belong to different components of $G$, then the distance between them is not determined.

Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$, and let $|V(G)| = n$ and $|E(G)| = m$.

The Wiener number (or Wiener index) of a connected graph $G$ is defined as [15]

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G) \times V(G)} d(u,v|G). \quad (1)$$

In words: the Wiener number is the sum of distances between all pairs of vertices of the respective graph. Therefore, $\binom{n}{2}^{-1} W(G)$ is just the average distance between the vertices of the graph $G$.

The graph invariant $W$ was introduced in 1947 by Wiener [15], who used it for modeling the shape of organic molecules and for calculating several of their physico-chemical properties. Mathematical research on $W$ started in 1976 [6] and since then this distance-based quantity was much studied; for details of the theory of the Wiener number and for an exhaustive list of references see the recent reviews [4, 5].

The definition (1) of the Wiener number requires that the graph $G$ be connected. As a consequence, practically the entire research on $W$, done so far [4, 5], was restricted to connected graphs. Yet, this restriction can easily be overcome.

Denote by $d(G,k)$ the number of pairs of vertices of the graph $G$ that are at distance $k$, and note that this quantity is well defined for both connected and disconnected graphs. In particular, $d(G,0) = n$ and $d(G,1) = m$. Now, evidently, the right-hand side of Eq. (1) can be rewritten as $\sum_{k \geq 1} k d(G,k)$, which hints towards the possibility to define the Wiener number of a graph $G$ as

$$W = W(G) = \sum_{k \geq 1} k d(G,k). \quad (2)$$

If $G$ is a connected graph, then Eq. (2) reduces to Eq. (1). If $G$ is disconnected, then the right-hand side of (1) is ill-determined, which is not the case with the right-hand side of Eq. (2).
From (2) follows that if $G$ is a graph consisting of components $G_1, G_2, \ldots, G_p$, then

$$W(G) = W(G_1) + W(G_2) + \cdots + W(G_p).$$  \hfill (3)

An immediate generalization of the Wiener number is

$$W_\lambda = W_\lambda(G) = \sum_{k \geq 1} d(G,k) k^\lambda$$  \hfill (4)

where $\lambda$ is some real (or complex) number. For connected graphs formula (4) is tantamount to

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

In an explicit form the Wiener–type graph invariant $W_\lambda$ was first put forward in the works [7] and [8]. However, various of its special cases have independently been considered in the chemical literature, where they found considerable applications. Thus $W_{-2}$ and $W_{-1}$, named Harary index and reciprocal Wiener index, were introduced in the papers [11] and [3], respectively, and eventually studied in numerous subsequent publications. The case $\lambda = \frac{1}{2}$ was analyzed in the article [16]. The so-called "hyper–Wiener index" [12] was shown [10] to be equal to $\frac{1}{3} W_2 + \frac{1}{2} W_1$. The so-called "Tratch–Stankevich–Zefirov index" [13] was shown [9] to be equal to $\frac{1}{3} W_3 + \frac{1}{3} W_2 + \frac{2}{3} W_1$. (Recall that the hyper–Wiener and Tratch–Stankevich–Zefirov indices were originally defined in terms completely different from the presently considered Wiener–type invariants; for details see [12, 13].) More details on the chemical applications and interconnections of various distance–based graph invariants are found in the review [2] and the book [14].

2 Two identities for distances in trees

A tree is a connected acyclic graph. Any two vertices of a tree are connected by a unique path; the number of edges of this unique path is the distance between the respective two vertices.

Let $T$ be a tree on $n$ vertices and let $e$ be one of its edges. The subgraph $T - e$ is obtained by deleting from $T$ the edge $e$. Thus, $V(T - e) = V(T)$.

The subgraph $T - e$ is disconnected, possessing two components. Denote them by $T_1(e)$ and $T_2(e)$, and let the number of their vertices be $n_1(e)$ and $n_2(e)$, respectively, $n_1(e) + n_2(e) = |V(T - e)| = n$. 

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Lemma 1. Let $T$ be a tree on $n$ vertices. Then

$$ (n - 1 - k) d(T, k) = \sum_{e \in E(T)} d(T - e, k) $$

holds for all $k = 0, 1, 2, \ldots$.

Proof. Consider the difference $d(T, k) - d(T - e, k)$. In view of the uniqueness of the path connecting any given pair of vertices of a tree, any two vertices of $T$, connected by a path that contains the edge $e$, belong to different components of $T - e$. Consequently, the difference $d(T, k) - d(T - e, k)$ counts the pairs of vertices of $T$ that are at distance $k$ and whose connecting path contains the edge $e$. By summing this difference over all edges of $T$ we will count any pair of vertices of $T$ at distance $k$. Furthermore, every such pair will be counted exactly $k$ times, because there are exactly $k$ edges in the path connecting them. Hence,

$$ \sum_{e \in E(T)} [d(T, k) - d(T - e, k)] = k d(T, k). $$

Formula (5) follows now by taking into account that $T$ has $n - 1$ edges. □

Lemma 2 is deduced in a fully analogous manner. Here $u$ stands for a vertex of the tree $T$ and $T - u$ is the subgraph obtained by deleting $u$ (together with its incident edges) from $T$.

Lemma 2. Let $T$ be a tree on $n$ vertices. Then

$$ (n - 1 - k) d(T, k) = \sum_{u \in V(T)} d(T - u, k) $$

holds for all $k = 0, 1, 2, \ldots$.

Theorem 3. Let $T$ be a tree on $n$ vertices. Let $\lambda$ be a real (or complex) number. Then

$$ W_{\lambda + 1}(T) = (n - 1) W_\lambda(T) - \sum_{e \in E(T)} W_\lambda(T - e). $$

Proof. By multiplying Eq. (5) by $k^\lambda$ one obtains

$$ d(T, k) k^{\lambda + 1} = (n - 1) d(T, k) k^\lambda - \sum_{e \in E(T)} d(T - e, k) k^\lambda $$

which summed over all $k \geq 1$ and in view of Eq. (4) yields (6). □
In an analogous manner, from Lemma 2 follows:

**Theorem 4.** Let $T$ be a tree on $n$ vertices. Let $\lambda$ be a real (or complex) number. Then

$$W_{\lambda+1}(T) = (n-1)W_\lambda(T) - \sum_{u \in V(T)} W_\lambda(T-u).$$

**Remark.** The identity (5) can be rewritten as

$$(m-k)d(F,k) = \sum_{e \in E(F)} d(F-e,k),$$

in which case it holds for any forest $F$ (= acyclic graph, not necessarily connected), with $m \leq n-1$ edges. Analogously, relation (6) then becomes

$$W_{\lambda+1}(F) = mW_\lambda(F) - \sum_{e \in E(F)} W_\lambda(F-e).$$

### 3 Applications of relation (6)

First of all, using Eq. (3) and the notation defined above, Eq. (6) can be rewritten as

$$W_{\lambda+1}(T) = (n-1)W_\lambda(T) - \sum_{e \in E(T)} [W_\lambda(T_1(e)) + W_\lambda(T_2(e))]. \quad (7)$$

Note that all graphs occurring in formula (7) are connected.

For any connected $n$-vertex graph $G$, $W_0(G) = \binom{n}{2}$.

Formulas (6) holds for any value of $\lambda$. By setting $\lambda = 0$ and by taking into account that $n_1(e) - n_2(e) = n$, we obtain:

$$W_1(T) = (n-1)W_0(T) - \sum_e [W_0(T_1(e)) + W_0(T_2(e))]$$

$$= (n-1) \binom{n}{2} - \sum_e \left[ \binom{n_1(e)}{2} + \binom{n_2(e)}{2} \right]$$

$$= \frac{1}{2} n(n-1)^2 - \frac{1}{2} \sum_e \left[ n_1(e)^2 + n_2(e)^2 - (n_1(e) + n_2(e)) \right]$$

$$= \frac{1}{2} n(n-1)^2 - \frac{1}{2} \sum_e \left[ n^2 - n - 2n_1(e)n_2(e) \right]$$
\[
= \frac{1}{2} n (n - 1)^2 - \frac{1}{2} (n - 1)(n^2 - n) + \sum_{e} n_1(e) n_2(e)
\]

which finally yields

\[
W(T) = \sum_{e} n_1(e) n_2(e) \quad (8)
\]

a result first reported by Wiener himself [15]. Thus, the relation (6) may be viewed as a generalization of the Wiener formula (8).

The \( n \)-vertex tree possessing a maximum number (= \( n - 1 \)) vertices of degree 1 is called the star \( (S_n) \). The \( n \)-vertex tree possessing a minimum number (= 2) vertices of degree 1 is the path graph \( (P_n) \). In the set of all \( n \)-vertex trees, \( S_n \) and \( P_n \) usually have extremal properties. It has been shown elsewhere [7] that for \( T_n \) being any \( n \)-vertex tree different from \( S_n \) and \( P_n \), and for any \( \lambda > 0 \),

\[
W_\lambda(S_n) < W_\lambda(T_n) < W_\lambda(P_n).
\]

If \( \lambda < 0 \), then in the above inequalities "less than" has to be exchanged into "greater than".

Because \( d(S_n, k) = 0 \) for \( k \geq 3 \), one directly gets

\[
W_\lambda(S_n) = n - 1 + \binom{n - 1}{2} 2^\lambda.
\]

The calculation of the Wiener-type invariants of \( P_n \) is less easy.

By means of formulas (6) or (7) the Wiener-type invariants of a tree can be computed recursively. This is especially efficient if the respective tree possesses some structural regularity. For instance, for \( P_n \), formula (7) reduces to

\[
W_{\lambda+1}(P_n) = (n - 1) W_\lambda(P_n) - 2 \sum_{i=1}^{n-1} W_\lambda(P_i) \quad (9)
\]

We start with \( \lambda = 0 \) and the obvious relation \( W_0(P_n) = \binom{n}{2} \). Then, by applying (9),

\[
W_1(P_n) = \binom{n}{2} - 2 \sum_{i=1}^{n-1} \frac{i}{2} = \binom{n+1}{3} \quad (10)
\]

For \( \lambda = 1, 2, \ldots, 5 \) analogous calculations yield

\[
W_2(P_n) = \frac{n}{2} \binom{n+1}{3} \quad W_3(P_n) = \frac{3n^2 - 2}{10} \binom{n+1}{3} \quad (11)
\]

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\[ W_4(P_n) = \frac{n(2n^2 - 3)}{10} \binom{n+1}{3} \]
\[ W_5(P_n) = \frac{(n^2 - 2)(2n^2 - 1)}{14} \binom{n+1}{3} \]
\[ W_6(P_n) = \frac{n(n^2 - 2)(3n^2 - 5)}{28} \binom{n+1}{3}. \]

By induction it can be shown that for \( \lambda \) being a positive integer, \( W_\lambda(P_n) \) has the following properties:
- \( W_\lambda(P_n) \) is a polynomial in the variable \( \lambda \), of degree \( n+2 \);
- if \( n \) is even/odd, the coefficients at odd/even terms are 0;
- the nonzero coefficients alternate in sign.

Using expressions (10) and (11) one can immediately check that
\[ \frac{1}{2} W_2(P_n) + \frac{1}{2} W_1(P_n) = \binom{n+2}{4} \]
and
\[ \frac{1}{6} W_3(P_n) + \frac{1}{2} W_2(P_n) + \frac{1}{3} W_1(P_n) = \binom{n+3}{5} \]
Thus we arrive at the remarkable result that the Wiener number [15], the hyper-Wiener index [12] and the Tratch-Stankevich-Zefirov index [13] of the \( n \)-vertex path graph are given by
\[ \binom{n+1}{3}, \binom{n+2}{4}, \binom{n+3}{5} \]
respectively.

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References


