Wiener–Type Invariants of Trees and Their Relation

Ivan Gutman
Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Yugoslavia;
e-mail: gutman@knez.uis.kg.ac.yu

Andrey A. Dobrynin
Sobolev Institute of Math., Russian Academy of Sciences, Siberian Branch, Novosibirsk 630090, Russia
e-mail: dobr@math.nsc.ru

Sandi Klavžar
Department of Mathematics, PeF, University of Maribor Koroška cesta 160, 2000 Maribor, Slovenia
e-mail: sandi.klavzar@uni-mb.si

Ljiljana Pavlović
Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Yugoslavia;

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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]

\[
W = W(G) = \sum_{\{u,v\} \subseteq V(G) \times V(G)} d(u, v|G) .
\]

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

\[
W = W(G) = \sum_{k \geq 1} k d(G, k) .
\]

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
\[ W(G) = W(G_1) + W(G_2) + \cdots + W(G_p) . \] (3)

An immediate generalization of the Wiener number is
\[ W_\lambda = W_\lambda(G) = \sum_{k \geq 1} d(G, k) k^\lambda \] (4)

where $\lambda$ is some real (or complex) number. For connected graphs formula (4) is tantamount to
\[ W_\lambda = W_\lambda(G) = \sum_{\{u, v\} \subseteq V(G) \times V(G)} d(u, v|G)^\lambda . \]

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 $\frac{1}{2} W_2 + \frac{1}{2} W_1$. The so-called “Tratch–Stankevich–Zefirov index” [13] was shown [9] to be equal to $\frac{1}{2} W_3 + \frac{1}{2} W_2 + \frac{1}{3} W_1$. (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
\[(n - 1 - k) d(T, k) = \sum_{e \in E(T)} d(T - e, k) \tag{5}\]
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. \qed

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
\[(n - 1 - k) d(T, k) = \sum_{u \in V(T)} d(T - u, k) \tag{5}\]
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
\[W_{\lambda+1}(T) = (n - 1) W_\lambda(T) - \sum_{e \in E(T)} W_\lambda(T - e) . \tag{6}\]

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

### 3 Applications of relation (6)

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

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

(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:

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

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

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

$$= \frac{1}{2} n (n - 1)^2 - \frac{1}{2} \sum_e [n^2 - n - 2n_1(e)n_2(e)].$$
\[ W(T) = \sum_{e} n_1(e) n_2(e) \]  

which finally yields

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

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

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

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

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

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

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

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

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

(11)
\[ W_4(P_n) = \frac{n(2n^2 - 3)}{10} \binom{n + 1}{3} \quad W_5(P_n) = \frac{(n^2 - 2)(2n^2 - 1)}{14} \binom{n + 1}{3} \]

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

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

\[ \binom{n + 1}{3}, \quad \binom{n + 2}{4}, \quad \binom{n + 3}{5} \]

respectively.

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**References**


