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Vertex Version of the Wiener Theorem

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Abstract

The classical theorem discovered by Wiener in 1947, shows how the Wiener index of a tree is decomposed into (easily calculable) edge–contributions. We now deduce an analogous formula, based on vertex–contributions. This result, which can be straightforwardly extended to general graphs, happens to be previously known in the theory of social networks.

1 Introduction

In his seminal paper [13] Harold Wiener not only introduced the concept of what nowadays is known as the *Wiener index* (W), but also showed how in the case of acyclic systems, W can be easily calculated from edge–contributions. In [13], this result was stated without mentioning distance, graphs, and trees, and without proof. It was then completely overseen, and was first time formulated in graph–theoretical terms and supplied by a proof almost 30 years later [11]. In what follow, we refer to this result as to the *Wiener theorem*.

In order to state the Wiener theorem, and then formulate its vertex–version, we need to introduce a convenient notation.

Let F be a forest (= acyclic, not necessarily connected graph), possessing $n(F)$ vertices. In the general case, F consists of p components, $p \geq 1$, each being a tree. We shall write this as:

$$F = T_1 \cup T_2 \cup \cdots \cup T_p \ .$$

Denote by $N_2(F)$ the sum over all pairs of components, of the product of the number of vertices of two components of F, i.e.,

$$N_2(F) = \sum_{1 \leq i < j \leq p} n(T_i)\, n(T_j) \ .$$

If $p = 1$, i.e., if F is connected, then $N_2(F) = 0$. If $p = 2$, $p = 3$, and $p = 4$, then

$$N_2(F) = n(T_1) \cdot n(T_2) \tag{1}$$

$$N_2(F) = n(T_1) \cdot n(T_2) + n(T_1) \cdot n(T_3) + n(T_2) \cdot n(T_3) \tag{2}$$

and

$$\begin{aligned} N_2(F) &= n(T_1) \cdot n(T_2) + n(T_1) \cdot n(T_3) + n(T_1) \cdot n(T_4) \\ &+ n(T_2) \cdot n(T_3) + n(T_2) \cdot n(T_4) + n(T_3) \cdot n(T_4) \end{aligned} \tag{3}$$

respectively, etc.

2 The Wiener theorem

If G is a connected graph, then its Wiener index, $W(G)$, is – by definition – equal to the sum of distances between all pairs of vertices of G. Details on this graph invariant, and on its chemical applications, can be found in some of the many surveys [4, 5, 7, 11, 12].

Let T be a tree (= acyclic connected graph), and let $E(T)$ be its edge set. Then the Wiener theorem can be stated as follows:

Theorem 1. [13]

$$W(T) = \sum_{e \in E(T)} N_2(T - e) \ . \tag{4}$$

Proof. $N_2(T-e)$ counts how many times the edge e lies on a shortest path connecting two vertices of T. Since the distance between two vertices is equal to the number of edges in the respective shortest path, the sum on the right–hand side of Eq. (4) is just the sum of distances between all pairs of vertices. □

One should note that any subgraph $T - e$ in Eq. (4) consists of exactly two components, and therefore relation (1) is always applicable.

3 The vertex Wiener theorem

Let, as before, T be a tree, and let $V(T)$ be its vertex set. In analogy to the classical Theorem 1, we have its following vertex version:

Theorem 2. *Let T be a tree on n vertices. Then,*

$$W(T) = \sum_{v \in V(T)} N_2(T - v) + \binom{n}{2} . \tag{5}$$

Proof. $N_2(T-v)$ counts how many times v is a non-terminal vertex of a shortest path connecting two vertices of T. Since the distance between two vertices is *by one greater* than the number of non-terminal vertices in the respective shortest path, the sum on the right–hand side of Eq. (5), *plus a unity for each vertex pair*, is just the sum of distances between all pairs of vertices. Of course, T has $\binom{n}{2}$ pairs of vertices. □

One should note that a subgraph $T - v$ in Eq. (5) may consist of several components (whose number is equal to the degree of the vertex v), and therefore relations (1), (2), (3), etc. are to be used. Besides, if v is a pendent vertex, then $N_2(T-v) = 0$. This fact makes the application of formula (5) significantly more complicated than that of (4).

Formula (5) describes a decomposition of the Wiener index into vertex–contributions. It's practical applicability for calculation of $W(T)$ is much less convenient that of Eq. (4), which may be the reason why this simple modification of original Wiener's theorem was hardly ever mentioned in mathematical chemistry (see, however, [2]).

On the other hand, formula (5) can be extended to general (cycle–containing graphs) as it is stated in Theorem 4. This extended version of Theorem 2 seems to have been first mentioned in Silvia Gago's Ph.D. thesis [9] (see also [3,10]) as identity

$$\overline{B}(G) = \frac{(n-1)(\overline{\ell}(G) - 1)}{2}. \tag{6}$$

where $\overline{B}(G)$ is the average betweenness (defined later) of a vertex and $\overline{\ell}(G)$ is the average distance in a graph G.

4 The Doyle–Graver formula

In connection with Theorem 2, a formula discovered by Doyle and Graver [6] deserves to be mentioned.

Using the same notation as in *Introduction*, denote by $N_3(F)$ the sum over all triplets of components, of the product of the number of vertices of three components of F, i.e.,

$$N_3(F) = \sum_{1 \le i < j < k \le p} n(T_i)\, n(T_j)\, n(T_k) \ .$$

If $p = 1$ or $p = 2$, then $N_3(F) = 0$. If $p = 3$ and $p = 4$, then

$$N_3(F) = n(T_1) \cdot n(T_2) \cdot n(T_3)$$

and

$$\begin{aligned} N_3(F) &= n(T_1) \cdot n(T_2) \cdot n(T_3) + n(T_1) \cdot n(T_2) \cdot n(T_4) \\ &+ n(T_1) \cdot n(T_3) \cdot n(T_4) + n(T_2) \cdot n(T_3) \cdot n(T_4) \end{aligned}$$

respectively, etc.

Theorem 3. [6] *Let T be a tree on n vertices. Then,*

$$W(T) = \binom{n+1}{3} - \sum_{v \in V(T)} N_3(T - v) \ .$$

5 Vertex Wiener theorem for general graphs

In order to extend Theorem 2 to general (connected) graphs, one needs to take into account that such graphs may possess several shortest paths connecting the same pair of vertices. In addition, $G - v$ needs not be disconnected.

The *betweenness centrality* $B(x)$ of a vertex $x \in V(G)$ is the sum of the fraction of all-pairs shortest paths that pass through x:

$$B(x) = \sum_{\substack{u,v \in V(G) \setminus \{x\} \\ u \neq v}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}}$$

where $\sigma_{u,v}$ denotes the total number of shortest (u,v)-paths in G and $\sigma_{u,v}(x)$ represents the number of shortest (u,v)-paths passing through the vertex x. It is one of the most important centrality indices and it was introduced by Anthonisse [1], and popularized by Freeman [8] (see also [2]).

Now, we state the extension of Theorem 2. Notice before that for a vertex v in a tree T, it holds $B(v) = N_2(T - v)$.

Theorem 4. *Let G be a graph on n vertices. Then,*

$$W(G) = \sum_{v \in V(G)} B(v) + \binom{n}{2} . \tag{7}$$

Proof. The proof follows easily by the fact that the contribution of a pair u, v to the sum of the betweenness of all vertices is precisely $d(u,v) - 1$. So,

$$\begin{aligned} \sum_{x \in V(G)} B(x) &= \sum_{x \in V(G)} \sum_{\substack{u,v \in V(G) \setminus \{x\} \\ u \neq v}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} = \sum_{\substack{u,v \in V(G) \\ u \neq v}} \sum_{x \in V(G) \setminus \{u,v\}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} \\ &= \sum_{\substack{u,v \in V(G) \\ u \neq v}} \big[d(u,v) - 1 \big] = W(G) - \binom{n}{2} \end{aligned}$$

which establishes the equality. □

For a graph G on n vertices,

$$\overline{B}(G) = \frac{1}{n} \sum_{v \in V(G)} B(v) \qquad \text{and} \qquad \overline{\ell}(G) = \frac{1}{\binom{n}{2}} W(G)$$

which implies that equations (6) and (7) are equivalent.

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