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THE EDGE VERSIONS OF THE WIENER INDEX

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Abstract

The Wiener index is equal to the sum of distances between all pairs of vertices of the underlying (connected) graph. The edge-Wiener index is conceived in an analogous manner as the sum of distances between all pairs of edges of the underlying (connected) graph. Several possible distances between edges of a graph are considered and, according to these, the corresponding edge-Wiener indices defined. Several of these edge-Wiener indices are mutually related, but two of them are independent novel structure descriptors. We report explicit combinatorial expressions of these two edge-Wiener indices of some familiar graphs.

INTRODUCTION

The ordinary (vertex) version of the Wiener index (or Wiener number) of a connected graph G is the sum of distances between all pairs of vertices of G, that is,

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

where $d(u,v|G)$ denotes the distance between the vertices u and v, and where the other details are explained below.

This index was introduced by the chemist Harold Wiener [19] within the study of relations between the structure of organic compounds and their properties. (In the paper [19] the boiling points of alkanes was considered). The first mathematical paper on W was published somewhat later [10]. Since then, numerous articles were published in the chemical and mathematical literature, devoted to the Wiener index and various methods for its calculation [1–9,11–18,20].

It seems that the edge version of the Wiener index has not been considered until now. In analogy with Eq. (1), the edge-Wiener index needs to be defined as

$$W_e = W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f|G) \tag{2}$$

where $d(e,f|G)$ stands for the distance between the edges e and f of the graph G. In order that formula (2) be meaningful, we have to specify what $d(e,f|G)$ actually is. In what follows we show that the "distance between edges" can be defined in several non-equivalent ways. Therefore, we will have several non-equivalent edge-Wiener indices.

BASIC DEFINITIONS

We first recall the general definition of distance.

Let $\mathbf{S}$ be any set. The distance in $\mathbf{S}$ is a mapping $\delta : \mathbf{S} \times \mathbf{S} \to \mathbf{R}$, such that for any $a,b,c \in \mathbf{S}$, 1° $\delta(a,b) \geq 0$

2° $\delta(a,b) = 0 \Longleftrightarrow a = b$

3° $\delta(a,b) = \delta(b,a)$

4° $\delta(a,b) + \delta(b,c) \geq \delta(a,c)$.

Let G be a graph, and $V(G)$, $E(G)$ be the sets of its vertices and edges, respectively. Throughout this paper we suppose that G is connected.

Definition 1. The distance between the vertices $u, v \in V(G)$ is equal to the length of (= number of edges in) a shortest path connecting u and v . This distance will be denoted by $d(u,v)$ or $d(u,v|G)$.

It is well known (and easy to verify) that d satisfies the conditions 1°–4° .

The original Wiener index of a connected graph G is equal to the sum of distances between all pairs of vertices of G , cf. Eq. (1). Because of property 2° , it is irrelevant whether the summation in (1) includes the case $u = v$.

In order to arrive at the edge version of the Wiener index, Eq. (2), we need to define the distance between edges. This can be done is several ways. Our first guess is formulated in Definition 2.

Let $L(G)$ be the line graph of G .

Definition 2a. The distance between the edges $e, f \in E(G)$ is equal to the distance between the vertices e, f in the line graph of G . We denote this distance by $d_0(e,f)$ or $d_0(e,f|G)$. Thus,

$$d_0(e,f|G) = d(e,f|L(G)) \ . \tag{3}$$

Definition 2b The edge-Wiener index pertaining to d_0 , denoted by W_{e0} , is

$$W_{e0} = W_{e0}(G) = \sum_{\{e,f\} \subseteq E(G)} d_0(e,f|G) \ . \tag{4}$$

The fact that the distance d_0 between edges satisfies the conditions 1°–4° is evident from the relation (3). From Definition 2 it immediately follows that

$$W_{e0}(G) = W(L(G)) \ .$$

ALTERNATIVE APPROACHES

Let $e, f \in E(G)$ and let $e = (u, v)$, $f = (x, y)$.

Definition 3. $d_1(e, f) = \min\{d(u, x), d(u, y), d(v, x), d(v, y)\}$.

Definition 4. $d_2(e, f) = \max\{d(u, x), d(u, y), d(v, x), d(v, y)\}$.

Based on the above two definitions we conceive the following edge-versions of the Wiener index:

$$W_{e1} = W_{e1}(G) = \sum_{\{e,f\} \subseteq E(G)} d_1(e, f|G) \tag{5}$$

and

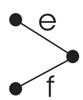
$$W_{e2} = W_{e2}(G) = \sum_{\{e,f\} \subseteq E(G)} d_2(e, f|G) \ . \tag{6}$$

The summations on the right–hand sides of (5) and (6) embrace also the terms with $e = f$. Because of $d_1(e, e) = 0$, in the case of W_{e1} this is immaterial. However, in view of $d_2(e, e) = 1$, this details is relevant in the case of W_{e2} . If preferred, instead of the W_{e2} we may consider its variant:

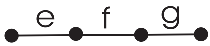
$$W^*_{e2} = W^*_{e2}(G) = \sum_{\substack{\{e,f\} \subseteq E(G) \\ e \neq f}} d_2(e, f|G) \ . \tag{7}$$

Evidently, $W^*_{e2} = W_{e2} - m$, where m stands for the number of edges of the underlying graph. In what follows we show that, from a mathematical point of view, the choice W^*_{e2} happens to be better than W_{e2} .

It should be pointed out that the distance–like quantities d_1 and d_2 are not true distances, i. e., they do not satisfy the conditions 1°–4° . To see this, consider the following.



$d_1(e, f) = 0$, $e \neq f$. Condition 2° is violated.



$d_1(e,f) = 0$, $d_1(f,g) = 0$, but $d_1(e,g) = 1$. Therefore, $d_1(e,f) + d_1(f,g) = 0 < d_1(e,g)$. Condition 4° is violated.

If $e = f$, then $d_2(e,f) = 1$, and condition 2° is violated.

We now proceed to amend the above difficulties.

Definition 5.

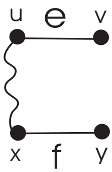
$$d_3(e,f) = \begin{cases} d_1(e,f) + 1 & \text{if } \ e \neq f \\ d_1(e,f) & \text{if } \ e = f \ . \end{cases}$$

Lemma 6. *For all* $e, f \in E(G)$ *,* $d_3(e,f) = d_0(e,f)$ *.*

Proof. *Case 1*: $e = f$. Then $d_3(e,f) = d_1(e,f) = 0$ and also $d_0(e,f) = 0$.

Case 2: e is incident to f . Then $d_3(e,f) = d_1(e,f) + 1 = 0 + 1 = 1$. The edges e and f correspond to adjacent vertices in $L(G)$. Therefore, $d(e,f|L(G)) = 1$ i. e., $d_0(e,f|G) = 1$ and the equality in Lemma 6 holds.

Case 3: e and f are independent edges:



Let $d_1(e,f) = k$ and therefore $d_3(e,f) = k+1$. This means that the minimal distance between the vertex pairs (u,x) , (u,y) , (v,x) , and (v,y) is k . Without loss of generality, we assume that $d(u,x) = k$. If $d(u,x) = k$, then the (shortest) path starting at u and ending at x possesses k edges. Then the (shortest) path starting at edge e and ending at the edge f possesses $k+2$ edges. The respective path in $L(G)$ possesses $k+2$ vertices. Thus the length of this path (in $L(G)$) is $k+1$. Thus, $d(e,f|L(G)) = k+1$, i. e., $d_0(f,g|G) = k+1$. The equality in Lemma 6 holds. ■

Corollary 7. The quantity d_3 , defined via Definition 5, satisfies conditions 1°–4° and is thus a true distance.

Corollary 8. Let m be the number of edges of the graph G. Then,

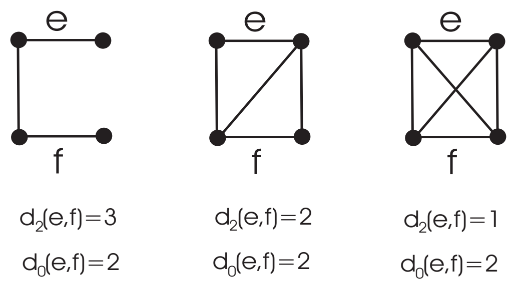
$$W_{e1}(G) = W_{e0}(G) - \frac{1}{2}\, m(m-1)\ .$$

Proof.

$$\begin{aligned}
W_{e1}(G) &= \sum_{\{e,f\}\subseteq E(G)} d_1(e,f|G) \\
&= \sum_{\substack{\{e,f\}\subseteq E(G)\\ e=f}} d_3(e,f|G) + \sum_{\substack{\{e,f\}\subseteq E(G)\\ e\neq f}} [d_3(e,f|G)-1] \\
&= \sum_{\substack{\{e,f\}\subseteq E(G)\\ e=f}} d_0(e,f|G) + \sum_{\substack{\{e,f\}\subseteq E(G)\\ e\neq f}} d_0(e,f|G) - \binom{m}{2} \\
&= \sum_{\{e,f\}\subseteq E(G)} d_0(e,f|G) - \binom{m}{2} = W_{e0} - \frac{1}{2}\, m(m-1)\ . \quad \blacksquare
\end{aligned}$$

Corollary 9. $W_{e1}(G) = W(L(G)) - m(m-1)/2$.

It seems that it is not possible to "improve" the distance-like quantity d_2 in a manner similar to what we did with d_1. This is seen from the following examples:



However, fortunately, there is a simple way out of the problem.

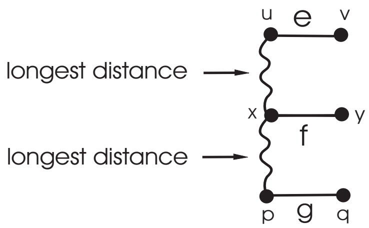
Definition 10.

$$d_4(e,f) = \begin{cases} d_2(e,f) & \text{if } \ e \neq f \\ 0 & \text{if } \ e = f\ . \end{cases}$$

Lemma 11. *The quantity d_4 satisfies the conditions 1°–4° and is thus a true distance.*

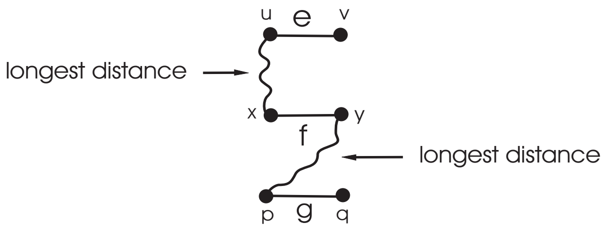
Proof. The fact that conditions 1°–3° are obeyed is evident. In order to verify that also 4° holds, we have to consider two cases. Let $e = (u, v)$, $f = (x, y)$, and $g = (p, q)$.

Case 1.



$d_2(e, f) = d(u, x)$ and $d_2(f, g) = d(x, p)$. Then, evidently, the longest distance between the vertices u, v and p, q is either $d(u, x) + d(x, p)$ or smaller. Condition 4° holds.

Case 2.



$d_2(e, f) = d(u, x)$ and $d_2(f, g) = d(y, p)$. The path going through p, y, x, u has length $d(u, x) + d(y, p) + 1$, but this is not the shortest path between u and p . For instance, (u, x, p) is shorter, of length at most $d(u, x)+d(y, p)$. Therefore the distance between u and p is less than or equal to $d(u, x) + d(y, p)$. Condition 4° holds. ■

CONCLUSIONS

We found two mathematically consistent ways to define the edge-Wiener index: either as W_{e0} , Eq. (4), or as W_{e4} , Eq. (8),

$$W_{e4} = W_{e4}(G) = \sum_{\{e,f\} \subseteq E(G)} d_4(e, f|G) \ . \tag{8}$$

As already pointed out, the edge-Wiener index W_{e1}, Eq. (6), is not based on a correct edge–distance concept and therefore should be abandoned. However, by adding to it the simple (and, in most applications, constant) term $m(m-1)/2$ it becomes equal to the well-defined W_{e0}:

$$W_{e1}(G) + \frac{1}{2}\, m(m-1) = W_{e0}(G) \ . \tag{9}$$

Analogously, the usage of the edge-Wiener index W_{e2}, Eq. (6), should also be avoided, and preference given to W_{e4}. However, it is sufficient to subtract from W_{e2} the simple (and, in most applications, constant) term m, and then it coincides with its well-defined congener W_{e4}:

$$W_{e2}(G) - m = W_{e4}(G) \ . \tag{10}$$

On the other hand, $W_{e2} - m$ is just the edge-Wiener index W_{e2}^*, Eq. (7). In other words, the quantities $W_{e4}(G)$ and $W_{e2}^*(G)$ coincide for all graphs G.

Bearing in mind the relations (9) and (10), the difference between W_{e1} and W_{e0} as well as between W_{e2} and W_{e4} is, from a practitioner's point of view, insignificant. Consequently, in practical (especially QSPR and QSAR) applications W_{e1} and W_{e2} would perform equally well as W_{e0} and W_{e4}, respectively. Yet, we prefer W_{e0} and W_{e4} (or, what is the same, W_{e2}^*) over W_{e1} and W_{e2}, and recommend their usage in the future.

THE EDGE-WIENER INDICES OF SOME FAMILIAR GRAPHS

Let, as usual, P_n, S_n, C_n, and K_n, denote, respectively, the n-vertex path, star, cycle, and complete graph. Let $K_{a,b}$ be the complete bipartite graph on $a+b$ vertices. Then by means of simple combinatorial considerations (the details of which will be omitted) we arrive at the following formulas for the edge-Wiener indices W_{e0} and W_{e4}, Eqs. (4) and (8). The other edge-Wiener indices can then be computed by using the relations (9) and (10) and by bearing in mind that P_n, S_n, C_n, K_n, and $K_{a,b}$ have $n-1$, $n-1$, n, $n(n-1)/2$, and ab edges, respectively.

$W_{e0}(P_n) = \frac{1}{6}\, n(n-1)(n-2)$; $W_{e4}(P_n) = \frac{1}{6}(n-1)(n-2)(n+3)$

$W_{e0}(S_n) = \frac{1}{2}(n-1)(n-2)$; $W_{e4}(S_n) = (n-1)(n-2)$

$W_{e0}(C_n) = \frac{1}{8}\, n^3$ if n is even

$W_{e0}(C_n) = \frac{1}{8}\, n(n^2-1)$ if n is odd

$W_{e4}(C_n) = \frac{1}{8}\, n(n^2+4n-8)$ if n is even

$W_{e4}(C_n) = \frac{1}{8}\, n(n-1)(n+5)$ if n is odd

$W_{e0}(K_n) = \frac{1}{4}\, n(n-1)^2\,(n-2)$; $W_{e4}(K_n) = \frac{1}{8}\, n(n+1)(n-1)(n-2)$

$W_{e0}(K_{a,b}) = \frac{1}{2}\, ab(2ab-a-b)$; $W_{e4}(K_{a,b}) = ab(ab-1)$.

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