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A New Hyper-Wiener Index*

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If two edges e and f are deleted from a tree T, then it decomposes into three components, possessing, $n_0(e, f)$, $n_1(e, f)$, and $n_2(e, f)$ vertices. Let $n_0(e, f)$ count the vertices lying between the edges e and f. It is shown that the Wiener index W of the tree T is equal to the sum over all edges e of the products $n_1(e, e) \cdot n_2(e, e)$, and that the hyper-Wiener index WW of T is the sum over all pairs of edges e, f of the products $n_1(e, f) \cdot n_2(e, f)$. We now consider another structure-descriptor, denoted by WWW, equal to the sum over all pairs of edges of the products $n_0(e, f) \cdot n_1(e, f) \cdot n_2(e, f)$. We establish some basic properties of WWW and show how it is related to W.

INTRODUCTION

In his seminal paper[1] Wiener not only introduced the topological index W that nowadays carries his name,[2,3] but also gave an efficient method for its calculation, Eq. (1). Recall that the Wiener index W is, by definition, equal to the sum of distances between all pairs of vertices of the respective (molecular) graph. Hence, for a graph on n vertices, for the direct calculation of W a total of $n(n–1) / 2$ distances needs to be determined.[3,4] In the case of trees, Wiener showed[1] that his index can be computed by means of the formula

$$W(\mathrm{T}) = \sum_{e \in E(\mathrm{T})} n_1(e, e) \cdot n_2(e, e) \tag{1}$$

where T is a tree, E(T) is its edge set and the summation goes over all edges of T. The number of vertices of T lying on the two sides of the edge e are denoted by $n_1(e, e)$ and $n_2(e, e)$. Thus the right hand side of formula (1) consists of only $n–1$ summands, each of which is easily evaluated.

Motivated by formula (1) Randić[5] introduced the hyper-Wiener index WW. In the case of trees this structure descriptor is defined as follows. Let u and v be two vertices of a tree T and let π_{uv} be the unique path connecting u and v. Let $n_1(\pi_{uv})$ and $n_2(\pi_{uv})$ be the number of vertices of T lying on the two sides of the path π_{uv}. Then

$$WW(\mathrm{T}) = \sum_{u,v} n_1(\pi_{uv}) \cdot n_2(\pi_{uv}) \tag{2}$$

with summation going over all pairs of vertices of T. Note that if the summation in Eq. (2) would be restricted to pairs of adjacent vertices, then Eq. (2) would reduce to Eq. (1).

Formula (2) is not applicable to graphs that contain cycles. For such graphs the problem of defining WW was solved by Klein *et al.*[6]

Formula (2) can be put in a somewhat more convenient form. To do this we need some preparations.

Let T be a tree and u and v two of its vertices, see Figure 1(a). There is a unique path π_{uv}, connecting these

* Dedicated to Professor Nenad Trinajstić, my former teacher, from whom I learned much.

two vertices, see Figure 1(b). This path uniquely determines two edges e and f: We denote by e the edge of T, incident to vertex u and belonging to π_{uv}; analogously, f is the edge incident to vertex v and belonging to π_{uv}, see Figure 1(c). By deleting the edges e and f from T it decomposes into three components, T_0, T_1 and T_2, see Figure 1(d). These possess $n_0(e, f)$, $n_1(e, f)$, and $n_2(e, f)$ vertices, respectively. Note that if u and v are adjacent vertices, then the edges e and f coincide, $e \equiv f$. Then T_0 does not exist, *i.e.*, $n_0(e, e) = 0$.

The general structure of a tree T and the labeling of its components is shown in Figure 2.

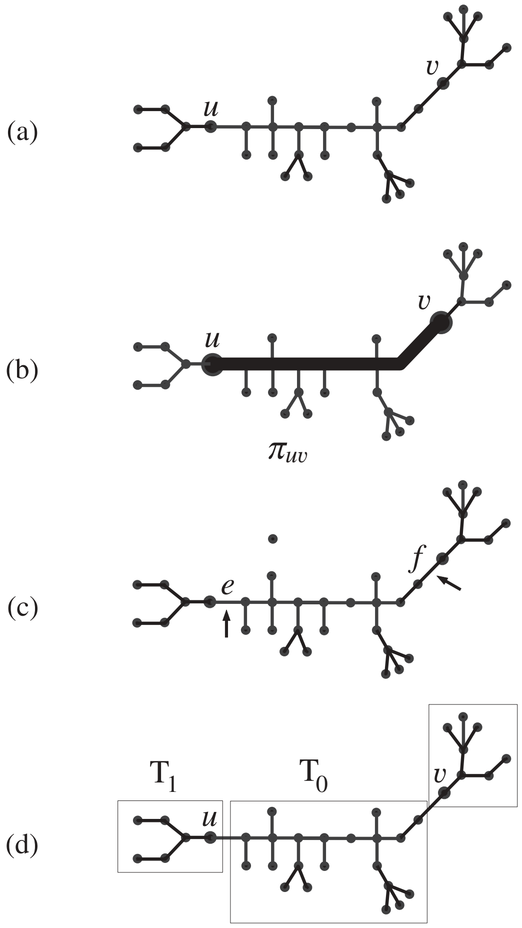

Figure 1. (a) A tree with a pair of its vertices (u, v) indicated. (b) The unique path π_{uv} connecting the vertices u and v. (c) The path π_{uv} uniquely determines the edges e and f. (d) The components T_0, T_1, and T_2 of T obtained by deleting the edges e and f.

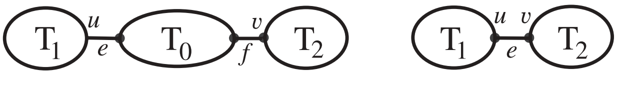

Figure 2. The structure of a tree T and the labeling of its components pertaining to the vertex pair u, v. Eqs. (1), (3), (5) and (6) refer to such a tree. Left: the case when the vertices u and v are not adjacent; right: the case of adjacent u, v. The components T_0, T_1, and T_2 of T have $n_0(e, f)$, $n_1(e, f)$, and $n_2(e, f)$ vertices, respectively. If u and v are adjacent, then the edges e and f coincide, and then $n_0(e, f) = 0$.

If the tree T has n vertices, then evidently

$$n_0(e, f) + n_1(e, f) + n_2(e, f) = n$$

holds for any choice of the edges e and f, *i.e.*, for any two vertices u and v of T.

Bearing the above in mind, we see that the quantities $n_1(\pi_{uv})$ and $n_2(\pi_{uv})$, occurring in Eq. (2), coincide with $n_1(e, f)$ and $n_2(e, f)$, and that Eq. (2) may be rewritten as

$$WW(\mathrm{T}) = \sum_{e,f} n_1(e, f) \cdot n_2(e, f) \tag{3}$$

where the summation goes over all pairs of edges, including those in which $e \equiv f$.

In view of Eq. (1), formula (3) is transformed into

$$WW(\mathrm{T}) = W(\mathrm{T}) + \sum_{e \neq f} n_1(e, f) \cdot n_2(e, f) \tag{4}$$

with $\sum_{e \neq f}$ indicating summation only over pairs of different edges.

A MODIFICATION OF THE HYPER-WIENER INDEX

Already Eq. (4) implies that there must be some relation between the Wiener and hyper-Wiener indices. However, only a short time ago[7] it was discovered that WW is bounded from both below and from above by linear functions of W:

$$\frac{3n}{4} W(\mathrm{T}) - \frac{1}{12} n(n-1)^2 (n+1) \leq$$
$$WW(\mathrm{T}) \leq (\frac{n}{2} + 1)\, W(\mathrm{T}) - \frac{1}{2} (n^2 - 2n + 2)(n-1)\,.$$

Quite recently these estimates were improved as[8]

$$\frac{3}{2} W(\mathrm{T}) - \frac{1}{2} (n-1) \leq WW(\mathrm{T}) \leq$$
$$(\frac{n}{4} + 2)\, W(\mathrm{T}) - \frac{1}{4} n(n-1)(n+1)\,.$$

The above relations suggest that W and WW must be highly correlated quantities, what eventually was confirmed by extensive numerical testing.[8]

In order to eliminate the effect on the hyper-Wiener index, Eq. (3), of terms pertaining to $e \equiv f$, we arrived at a new structure-descriptor WWW, defined as follows.

Let T be a tree whose structure is depicted in Figure 2. Then the new hyper-Wiener index is equal to:

$$WWW(\mathrm{T}) = \sum_{e,f} n_0(e,f) \cdot n_1(e,f) \cdot n_2(e,f)\,. \tag{5}$$

Because of $n_0(e, e) = 0$, formula (5) is tantamount to

$$WWW(\mathrm{T}) = \sum_{e \neq f} n_0(e, f) \cdot n_1(e, f) \cdot n_2(e, f)\,. \tag{6}$$

Consequently, the terms that contribute to the Wiener index, Eq. (1), have no effect on *WWW*. As a result, the correlation between *WWW* and *W* is significantly weaker than the correlation between *WW* and *W*. An illustrative example is given in Table I and Figure 3.

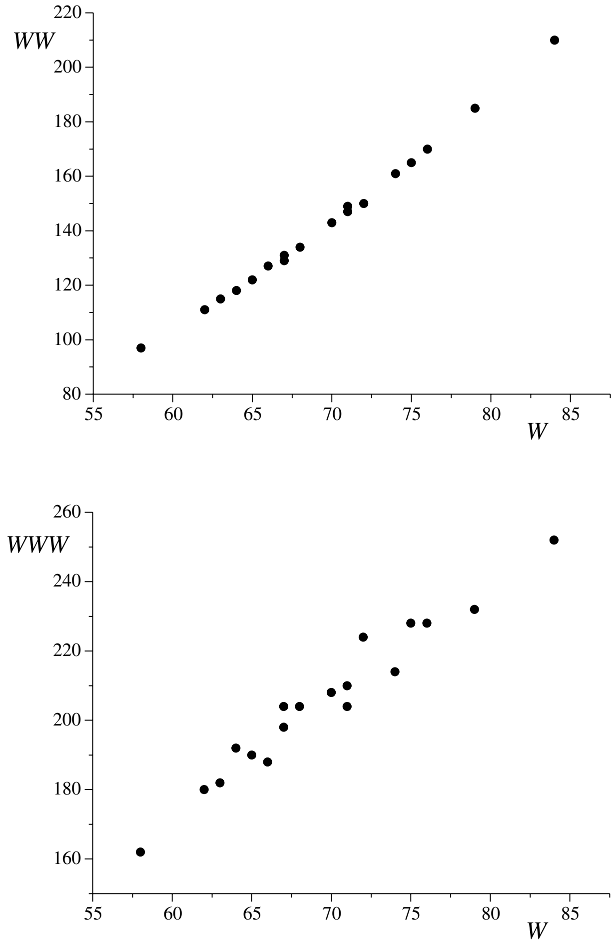

Figure 3. Correlation between the Wiener index (*W*), the hyper-Wiener index (*WW*) and the new hyper-Wiener index (*WWW*) for isomeric octanes, *cf.* Table 1. The respective correlation coefficients are 0.997 (for *WW vs. W*) and 0.976 (for *WWW vs. W*).

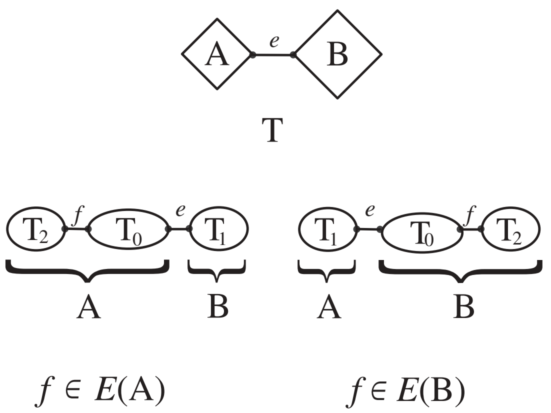

Figure 4. The notation used in the proof of Eq. (8). It is in agreement with, and refers to, the notation specified in Figure 2.

TABLE I. Wiener indices (*W*), hyper-Wiener indices (*WW*) and the new hyper-Wiener indices (*WWW*) for the isomeric octanes, *cf.* Figure 3

Compound	*W*	*WW*	*WWW*
octane	84	210	252
2-methylheptane	79	185	232
3-methylheptane	76	170	228
4-methylheptane	75	165	228
3-ethylhexane	72	150	224
2,2-dimethylhexane	71	149	204
2,3-dimethylhexane	70	143	208
2,4-dimethylhexane	71	147	210
2,5-dimethylhexane	74	161	214
3,3-dimethylhexane	67	131	198
3,4-dimethylhexane	68	134	204
3-ethyl-2-methylpentane	67	129	204
3-ethyl-3-methylpentane	64	118	192
2,2,3-trimethylpentane	63	115	182
2,2,4-trimethylpentane	66	127	188
2,3,3-trimethylpentane	62	111	180
2,3,4-trimethylpentane	65	122	190
2,2,3,3-tetramethylbutane	58	97	162

The consequence of the good correlation between *WW* and *W* is that the structure-property and structure-activity relations, based on the ordinary hyper-Wiener index, are of exactly same quality as the corresponding relations based on the Wiener index.[8] Because of the much weaker correlation between *WWW* and *W* (and also between *WWW* and *WW*), the efficiency of the new hyper-Wiener index in QSPR and QSAR studies is different, sometimes better, than the efficiency of *W* and *WW*. Details on this matter will be reported elsewhere.[9]

A RELATION BETWEEN THE NEW HYPER-WIENER INDEX AND THE WIENER INDEX

In this section we report a relation between the *WWW*-index of a tree T and the Wiener indices of some fragments of T. In order to formulate and prove this relation we shall use the following notation (illustrated in Figure 4).

Let T be a tree and e its edge. The subtrees obtained by deleting e from T are denoted by A and B. Clearly, A and B depend on the choice of the edge e.

The edge sets of T, A, and B are denoted by $E(\mathrm{T})$, $E(\mathrm{A})$ and $E(\mathrm{B})$, respectively. The trees A and B have n_A and n_B vertices. Evidently, $n_\mathrm{A} + n_\mathrm{B}$ = number of vertices of T and $E(\mathrm{T}) = E(\mathrm{A}) \cup E(\mathrm{B}) \cup \{e\}$.

With this notation, Wiener's formula (1) reads

$$W(\mathrm{T}) = \sum_{e \in E(T)} n_\mathrm{A} \cdot n_\mathrm{B} \,. \tag{7}$$

From the definition of the *WWW*-index, Eq. (5), and the fact that $n_0(e, e) = 0$ we have

$$WWW(\mathrm{T}) = \sum_{e,f} n_0(e,f)\cdot n_1(e,f)\cdot n_2(e,f)$$
$$= \frac{1}{2}\sum_{e\in E(\mathrm{T})}\sum_{f\in E(\mathrm{T})} n_0(e,f)\cdot n_1(e,f)\cdot n_2(e,f)$$
$$= \frac{1}{2}\sum_{e\in E(\mathrm{T})}\left(\sum_{f\in E(\mathrm{A})} n_0(e,f)\cdot n_1(e,f)\cdot n_2(e,f) + \sum_{f\in E(\mathrm{B})} n_0(e,f)\cdot n_1(e,f)\cdot n_2(e,f)\right)$$

because the edge f lies either in A or in B, see Figure 4.

Now, using the notation explained in Figure 4, if $f\in E(\mathrm{A})$, then $n_1(e,f) = n_\mathrm{B}$, whereas if $f\in E(\mathrm{B})$, then $n_1(e,f) = n_\mathrm{A}$. Therefore,

$$WWW(\mathrm{T}) = \frac{1}{2}\sum_{e\in E(\mathrm{T})}\left(n_\mathrm{B}\sum_{f\in E(\mathrm{A})} n_0(e,f)\cdot n_2(e,f) + n_B\sum_{f\in E(\mathrm{B})} n_0(e,f)\cdot n_2(e,f)\right).$$

In accordance with Eq. (1), for any fixed edge e,

$$\sum_{f\in E(\mathrm{A})} n_0(e,f)\cdot n_2(e,f) = W(\mathrm{A})$$

and

$$\sum_{f\in E(\mathrm{B})} n_0(e,f)\cdot n_2(e,f) = W(\mathrm{B})$$

which results in the following remarkable identity:

$$WWW(\mathrm{T}) = \frac{1}{2}\sum_{e\in E(\mathrm{T})} [n_\mathrm{B} W(\mathrm{A}) + n_\mathrm{A} W(\mathrm{B})]\ . \qquad (8)$$

It is worth comparing relation (8) with Wiener's formula (7) as well as with an analogous, recently obtained,[7] expression for the ordinary hyper-Wiener index:

$$WW(\mathrm{T}) = \frac{n}{2} W(\mathrm{T}) - \frac{1}{2}\sum_{e\in E(\mathrm{T})} [W(\mathrm{A}) + W(\mathrm{B})]\ .$$

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SAŽETAK

Novi hiper-Wienerov indeks

Ivan Gutman

Ako se iz stabla T izbace dva brida e i f, onda se ono razlaže na tri komponente, koje posjeduju $n_0(e,f)$, $n_1(e,f)$, i $n_2(e,f)$ vrhova. Neka $n_0(e,f)$ broji one vrhove koji leže između e i f. Pokazuje se da je Wienerov indeks W stabla T jednak zbroju preko svih bridova e produkta $n_1(e,e)\cdot n_2(e,e)$, a da je hiper-Wienerov indeks WW istog stabla jednak zbroju preko svih parova bridova e, f produkta $n_1(e,f)\cdot n_2(e,f)$. U radu se razmatra i jedan novi strukturni deskriptor, označen s WWW, jednak zbroju preko svih parova bridova produkta $n_0(e,f)\cdot n_1(e,f)\cdot n_2(e,f)$. Utvrđena su neka temeljna svojstva indeksa WWW i pokazano je kako je on povezan s W.