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The Multiplicative Version of the Edge Wiener Index

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Abstract

The multiplicative Wiener index π, which was introduced by Ivan Gutman et al. in [5], is a molecular structure descriptor equal to the product of the distances between all pairs of vertices of the underlying molecular graph G. Also, Iranmanesh et al. in [7], introduced the edge-Wiener index of a graph. It obtains in term of the distances between all pairs of edges set of a graph. We define a new index called the multiplicative edge-Wiener index that is equal to product of distance between all pairs of edges set of a graph G. Moreover, we compute this index for some well-known graphs and we consider its relation to the edge-Wiener index in alkanes, as well.

1 Introduction

There have been considerable reports about the application of graph theory in chemistry. One of the principal areas of research in chemical graph theory is the development and application of topological indices in quantitative-property (QSPR) and quantitative structure-activity relationship (QSAR) studies. Among the topological indices reported in literature, the important ones is Wiener index. To develop new topological indices and find out their application in chemistry is an interesting program for mathematicians

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and chemists. In this paper we define a novel topological index and we recognize its relationship with the edge Wiener index in some alkanes.

Let G be a simple connected graph, with vertex and edge sets $V(G)$ and $E(G)$, respectively. The distance $d(u,v)$ or $d(u,v|G)$ between any two vertices u and v is the number of edges on the shortest path from u to v. The first topological index in mathematical chemistry was introduced by H. Wiener in 1947 [12] who realized that there are correlations between the boiling points of paraffin and the structure of the molecules. In particular, he mentions in his article that the boiling point t_B can be quite closely approximated by the formula $t_B = aw + bp + c$ where w is the Wiener index, p the polarity number and a, b and c are constants for a given isomeric group.

In our notation, it can be described as follows:

$$W_v(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y|G) \tag{1}$$

The literature on the Wiener index is vast. We refer the reader to a number of recent papers concerned with computing Wiener indices of several classes of graphs [4-6,11].

Let $f = xy$ and $g = uv$ be two edges of G. The distance between f and g is denoted by $d_e(f,g)$ or $d_e(f,g|G)$ and defined as the distance between the vertices of f and g in the line graph of G. This distance is equal to [7]:

$$\min\{d(x,u), d(x,v), d(y,u), d(y,v)\} + 1$$

Distance 1 means that the edges share a vertex; distance 2 means that at least two of the four end-vertices of two edges are adjacent. The edge Wiener index of the graph G is denoted by $W_e(G)$ and defined as the sum of distances between all pairs edges of the graph G that is

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

It is purposeful to generalize Eq. (2) in the following manner:

$$W_e{}^{\lambda} = W_e{}^{\lambda}(G) = \sum_{\{f,g\}\subseteq E(G)} d_e^{\lambda}(f,g|G) \tag{3}$$

where λ is some parameter and we name it *the edge-Wiener type index*. Evidently, if $\lambda = 1$, then $W_e{}^{\lambda}$ coincides with the ordinary edge Wiener index W_e. For $\lambda = -1$, we

name ${W_e}^{\lambda}$ *the reciprocal edge-Wiener index*. The quantity ${W_e}^{\lambda}$ for $\lambda = 2$ is closely related to the hyper-edge Wiener index, $WW_e = (W_e + W_e^2)/2$ [8-9].

The parameter λ may be assume any real value. However, if $\lambda = 0$, then, we obtain that for all (connected) graphs with m edges, ${W_e}^{0} = m\,(m-1)/2$. In view of this, the new index ${W_e}^{\lambda}$ examined only in the case of $\lambda = 0$. We now show that it is profitable to examine the behavior of ${W_e}^{\lambda}$ when λ has near-zero values. Then, somewhat surprisingly, ${W_e}^{\lambda}$ is related to the product of distances.

2 Main Results

At first we offer some properties of the edge Wiener type index.

Lemma 2.1. *Let G be a connected graph of order n. Then $W_e^{\lambda}(G) \geq (n-1)(n-2)/2$ when $\lambda \geq 0$ and $W_e^{\lambda}(G) \leq (n-1)(n-2)/2$ when $\lambda < 0$. Equality hold if and only if G is a star.*

Proof. The graph G has at least $n-1$ edges, and the distance between any two edges is at least 1. Hence for $\lambda \geq 0$,

$$W_e^{\lambda}(G) = \sum_{\{f,g\} \subseteq E(G)} d_e^{\lambda}(f,g\,|G) \geq \binom{|E(G)|}{2} \geq \binom{n-1}{2}$$

and similarly for $\lambda < 0$, we obtain the desired result. If we had the above equality, then G must had $n-1$ edges, so is a tree. Moreover, the line graph of G is the complete graph, since the distance between any two edges is 1. Hence G is a star. □

Corollary 2.2. *Let G be a connected graph of order n. Then $W_e(G) \leq (n-1)(n-2)/2$. Equality hold if and only if G is a star.*

In continue, we bring some definitions [1,10]. Let G be a connected graph and ω be a real valued weight function on the vertices of G (a *vertex–weighted graph* (G,ω)). Then the Wiener number $W(G,\omega)$ of a weighted graph (G,ω) is defined as:

$$W(G,\omega) = \frac{1}{2} \sum_{u,v \in V(G)} \omega(u)\,\omega(v)\,d(u,v) \tag{4}$$

We note that for $\omega \equiv 1$ this yields the usual Wiener index, while for $\omega(u) = deg(u)$ we obtain the Gutman index where is defined as:

$$\mathrm{Gut}(G) = \frac{1}{2} \sum_{u,v \in V(G)} \deg(u)\,\deg(v)\,d(u,v) \tag{5}$$

Also we define the Wiener type number $W^{\lambda}(G,\omega)$ of a weighted graph (G,ω) as follows:

$$W^{\lambda}(G,\omega)=\frac{1}{2}\sum_{u,v\in V(G)}\omega(u)\,\omega(v)\,d^{\lambda}(u,v) \tag{6}$$

where λ is some parameter. We have *the Gutman type index*, as well:

$$\mathrm{Gut}^{\lambda}(G)=\frac{1}{2}\sum_{u,v\in V(G)}\deg(u)\,\deg(v)\,d^{\lambda}(u,v) \tag{7}$$

Evidently, if $\lambda=1$, then $\mathrm{Gut}^{\lambda}(G)$ coincides with the ordinary Gutman index $\mathrm{Gut}(G)$.

The edge-Wiener type index of a graph is connected to its Gutman type index by the following inequality.

Theorem 2.3. *Let G be a connected graph of order n and $\lambda\geq 0$. Then*

$$\left|W_e^{\lambda}(G)-\frac{1}{4}\mathrm{Gut}^{\lambda}(G)\right|\leq\frac{n^4}{8}.$$

Proof. Consider the graph $S(G)$ obtained from G by subdividing each edge once. Consider the following functions α and β on $V(S(G))$ which defined as follows:

$$\alpha(v)=\begin{cases}\deg(v) & v\in V(G)\\ 0 & v\in V(S(G))\backslash V(G)\end{cases},\quad \beta(v)=\begin{cases}0 & v\in V(G)\\ 2 & v\in V(S(G))\backslash V(G)\end{cases}$$

Now for any two vertices u and v of G, we have $d(u,v|S(G))=2\,d(u,v|G)$. So we have

$$\begin{aligned}W^{\lambda}(S(G),\alpha) &= \frac{1}{2}\sum_{u,v\in V(S(G))}\alpha(u)\,\alpha(v)\,d^{\lambda}(u,v\,|S(G))\\ &= \frac{1}{2}\sum_{u,v\in V(G)}2^{\lambda}\deg(u)\,\deg(v)\,d^{\lambda}(u,v\,|G)\\ &= 2^{\lambda}\,\mathrm{Gut}^{\lambda}(G)\end{aligned}$$

Denote the vertex of degree 2 in $V(S(G))\backslash V(G)$ that subdivides the edge $f\in E(G)$ by v_f. Then $\beta(x)\neq 0$ only if $x=v_f$ for some edge f in G. For every $f,\,g\in E(G)$, we have $d(v_e,v_f\,|S(G))=2d_e(f,g\,|G)$, and so

$$\begin{aligned}W^{\lambda}(S(G),\beta) &= \frac{1}{2}\sum_{u,v\in V(S(G))\backslash V(G)}\beta(u)\,\beta(v)\,d^{\lambda}(u,v\,|S(G))\\ &= \frac{1}{2}\sum_{f,g\in E(G)}2^{\lambda+2}\,d_e^{\lambda}(f,g\,|G)\\ &= 2^{\lambda+2}\,\mathrm{W}_e^{\lambda}(G)\end{aligned}$$

We now compare $W^{\lambda}(S(G),\alpha)$ and $W^{\lambda}(S(G),\beta)$. Clearly, the weight function α is obtained from the weight function β by moving one weight unit of a vertex v_{uw} to vertex

u and the other weight unit to vertex w for all $uw \in E(G)$. Hence no weight has been changed unless that weights with the same distance 1, and the distances between them has changed by at most 2. Since in total, we have $2|E(G)|$ weight units, the sum of the distances between the weight units has changed by at most $2^{\lambda}\binom{2|E(G)|}{2}$. Hence

$$\left|W^{\lambda}(S(G),\alpha) - W^{\lambda}(S(G),\beta)\right| \leq 2^{\lambda}\binom{2|E(G)|}{2} \leq 2^{\lambda-1}n^4$$

and so we have $\left|\,\mathrm{W}_e^{\lambda}(G) - \frac{1}{4}\,\mathrm{Gut}^{\lambda}(G)\right| \leq \frac{n^4}{8}$. □

Corollary 2.4. *Let G be a connected graph of order n. Then*

$$\left|\mathrm{W}_e(G) - \frac{1}{4}\,\mathrm{Gut}(G)\right| \leq \frac{n^4}{8}.$$

In follow, we introduce a new topological index.

We know that:

$$e^x = \sum_{i=0}^{\infty}\frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots; \quad -\infty < x < \infty$$

implying that for near-zero values of x, as a good approximation, $e^x \simeq 1 + x$. For any positive number a, we have $a^x = e^{x\ln a}$, therefore we can conclude $d_e^{\lambda}(e, f\,|G) \simeq 1 + \lambda\ln(d_e(f, g\,|G))$, for near-zero values of λ. Substitution back into Eq. (3) readily yields

$$\begin{aligned} W_e^{\lambda}(G) &\simeq \sum_{\{f,g\}\subseteq E(G)} 1 + \lambda\ln(d_e(f, g\,|G)) \qquad (8)\\ &= \binom{|E(G)|}{2} + \lambda\ln\left(\prod_{\{f,g\}\subseteq E(G)} d_e(f, g\,|G)\right) \end{aligned}$$

Formula (8) suggests a novel distance-based topological index, which in fact is *the multiplicative edge-Wiener index*:

$$\pi_e(G) = \prod_{\{f,g\}\subseteq E(G)} d_e(f, g) \qquad (9)$$

Then it is easy to see that $\pi_e(G)^2 = \prod_{f\in E(G)} \pi_e(f)$, where $\pi_e(f) = \prod_{f\neq g\in E(G)} d_e(f, g)$.

The most remarkable difference between W_e and π_e is that edge pairs at distance 1, do not at all contribute to π_e (whereas their contribution to W_e is not negligible).

Examples

1. Let K_n be the n-vertex complete graph. By considering any two edges of K_n at distance 2, for all values of n, we have

$$\pi_e(K_n) = 2^{\frac{n(n-1)(n-2)(n-3)}{2}}.$$

2. All edge pairs in the star S_n with n vertices are at distance 1 and consequently $\pi_e(S_n) = 1$. This simple result illustrates the earlier mentioned fact that the π_e index is insensitive to adjacent edge pairs.

3. A proper generalization of the latter formula is

$$\pi_e(K_{m,n}) = 2^{\frac{mn(m-1)(n-1)}{2}}.$$

   where $K_{m,n}$ denotes the complete bipartite graph with m vertices in one class and n vertices in the other class. Recall that $S_n = K_{1,n-1}$.

4. Let P_n be the n-vertex path. Then

$$\pi_e(P_n) = \prod_{k=1}^{n-2} k!$$

5. Let C_n be the cycle with n vertices. Then

$$\pi_e(C_n) = \begin{cases} \left(\left(\frac{n}{2}-1\right)!\right)^n \frac{n}{2}^{\frac{n}{2}} & n \text{ even} \\ \left(\left(\frac{n-1}{2}\right)!\right)^n & n \text{ odd} \end{cases}$$

A tree is a connected acyclic graph. Any tree with n vertices possesses $n-1$ edges, and this is the minimal number of edges in connected n-vertex graphs. Since the majority of the chemical applications of the Wiener number deal with chemical compounds that have acyclic organic molecules, whose molecular graphs are trees and, actually, most of the prior work on Wiener numbers deals with trees. When the graph is restricted to trees, the problem is more complicated. In view of this, it is not surprising that in the chemical literature there are numerous studies of properties of the Wiener numbers of trees. Therefore, in the following, we give a theorem about multiplicative index of trees. Recall that the star S_n and the path P_n are n-vertex trees.

Theorem 2.5. *Let T_n be any n-vertex tree, different from S_n and P_n. Then*

$$\pi_e(S_n) < \pi_e(T_n) < \pi_e(P_n).$$

Proof. S_n is the only graph having no edge pairs at a distance greater than one. So $\pi_e(S_n) < \pi_e(T_n)$. Now let G be an arbitrary (connected) graph and x be its arbitrary vertex. It is required that G possesses at least one more vertex in addition to x. Let a and b be two integers such that $0 \leq a < b$. Construct the graph H by attaching two paths P_{a+1} and P_b to the vertex x of graph G. The other terminal vertex of path P_{a+1} is located on the edge f of P_{a+1} (see Figure 1).

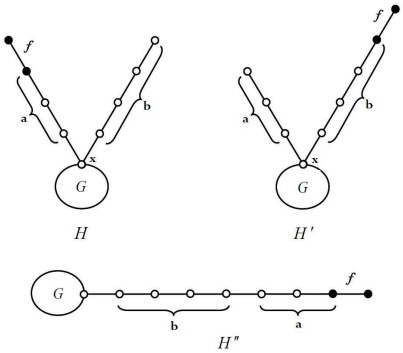

Figure 1: Construction of the graph H, H' and H''.

Construct the graph H' by attaching two paths P_a and P_{b+1} to the vertex x of graph G. This time we denote the terminal edge of P_{b+1} by f. It is seen that H' is obtained from H (and vice versa) by moving the edge f from one position to the other. All structural details of the graphs H and H', except the position of the edge f, are identical. All edges distances in H and H', except those involving the edge f are equal. The distances between the edge f and the edges in two branches attached to vertex x are also equal and does not need to be considered. All that remains are the distances between edge f and the edges of the subgraph of G. Now, let $g = wz$ be an edge of G and let $D(x, g) = \min\{d(x, w), d(u, z)\}$. Since $0 \leq a < b$, we have:

$$\pi'_e(f\,|H) = \prod_{g \in E(G)} (D(x, g\,|G) + a + 1) < \pi'_e(f\,|H') = \prod_{g \in E(G)} (D(x, g\,|G) + b + 1)\,.$$

That is in π'_e, we ignore the equal distances in H and H'. Therefore, by adding these distances, we have $\pi_e(H) < \pi_e(H')$. This manner show that if edges are moved from a shorter branch to a longer branch (attached to the same vertex), then the product edge-Wiener index will necessarily increase. Repeating the construction $H \to H'$ a sufficient number of times we conclude that π'_e will achieve its maximum value when the shorter

branch is completely removed (this is graph H'' in Figure 1). Applying this argument to all branching points of an n-vertex tree we immediately conclude that the path graph P_n (which has no branching points at all) has maximal product edge-Wiener index. Since all trees except the path graph have at least one branching point, we also see that any n-vertex tree different from P_n has product edge-Wiener index strictly smaller than $\pi_e(P_n)$. □

Relation between the π_e-index and the edge-Wiener index

Alkanes are chemical compounds that consist only of hydrogen and carbon atoms and are bonded exclusively by single bonds (i.e., they are saturated compounds) without any cycles (or loops; i.e., cyclic structure). Alkanes belong to a homologous series of organic compounds in which the members differ by a constant relative molecular mass of 14. Each carbon atom has 4 bonds (either C-H or C-C bonds), and each hydrogen atom is joined to a carbon atom (H-C bonds). The number of carbon atoms is used to define the size of the alkane. There are many different alkanes. We first focus our attention to normal alkanes $CH_3(CH_2)_{n-2}CH_3$ whose molecular graph is the path graph P_n [2], see Figure 2.

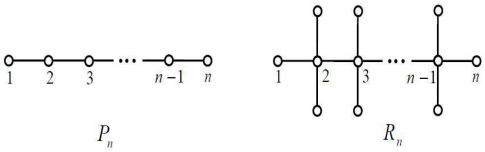

Figure 2: The molecular graphs of the normal alkanes (P_n) and of a class of highly branched alkanes (R_n).

We can show that

$$W_e(P_n) = \binom{n}{3} = \frac{(n-2)(n-1)n}{6} \tag{10}$$

and by example 4

$$\pi_e(P_n) = \prod_{k=1}^{n-2} k! \tag{11}$$

If $f_1(x)$ and $f_2(x)$ are two functions, and if $\lim\limits_{x\to\infty} \frac{f_1(x)}{f_2(x)} = 1$, then we say that for $x \to \infty$ the functions $f_1(x)$ and $f_2(x)$ are asymptotically equal and denoted by $f_1(x) \sim f_2(x)$. Suppose that the parameter n sufficiently large and let us examine the asymptotic behavior of $W_e(P_n)$ and $\ln \pi_e(P_n)$. From Eq. (10) immediately follows that $W_e(P_n) \sim \frac{n^3}{6}$, i.e.,

$$n \sim \sqrt[3]{6\ W_e(P_n)} \tag{12}$$

Series expansion of $\ln k!$ at ∞ is equal to

$$k(\ln k - 1) + \frac{1}{2}(\ln 2\pi - \ln(\frac{1}{x})) + \frac{1}{12x} + \frac{1}{360x^3} + \frac{1}{1260x^5} + O((\frac{1}{x})^{11/2}).$$

Therefore $\ln k! \sim (k \ln k - k)$ and for the asymptotic behavior of the π_e-index, we have

$$\begin{aligned} \ln \pi_e(P_n) &= \ln \prod_{k=1}^{n-2} k! = \sum_{k=1}^{n-2} \ln k! \sim \sum_{k=1}^{n-2} (k \ln k - k) \sim \sum_{k=1}^{n} (k \ln k - k) \\ &\sim \int_1^n (x \ln x - x)\, \mathrm{d}x = \frac{1}{2}x^2 \ln x - \frac{3}{4}x^2 \Big|_1^n \sim \frac{1}{2}n^2 \ln n - \frac{3}{4}n^2. \end{aligned}$$

Finally, we have the following results:

$$\ln \pi_e(P_n) \sim \frac{1}{2}n^2 \ln n \tag{13}$$

Substituting Eq. (12) into Eq. (13), we arrive at

$$\ln \pi_e(P_n) \sim \frac{1}{\sqrt[3]{6}} W_e(P_n)^{2/3} \ln W_e(P_n) \tag{14}$$

The molecular graph R_n (see Figure 2) corresponds to the highly branched alkanes $CH_3(CH_2)_{n-2}CH_3$. Since $W_e(R_n) \sim \frac{3}{2}n^3$, we obtain

$$n \sim \sqrt[3]{\frac{2}{3} W_e(R_n)} \tag{15}$$

Also, $\pi_e(R_n) = \pi_e(P_n)^9 = \left(\ln \prod_{k=1}^{n-2} k!\right)^9$. Now we have

$$\ln \pi_e(R_n) = \ln \left(\prod_{k=1}^{n-2} k!\right)^9 = 9 \ln \prod_{k=1}^{n-2} k!$$

and therefore

$$\ln \pi_e(R_n) \sim \frac{9}{2}n^2 \ln n \tag{16}$$

From Eqs. (15) and (16), we obtain

$$\ln \pi_e(R_n) \sim \sqrt[3]{\frac{3}{2}} W_e(R_n)^{2/3} \ln W_e(R_n) \tag{17}$$

Both Eq. (14) and (17) have the same mathematical form and differ only in the value of the constant C. Since P_n and R_n are two trees with the minimal and maximal branches respectively, we conclude that Eq. (18) holds for other homologous series as well (at least for alkanes).

$$\ln \pi_e = C\, W_e^{\frac{2}{3}} \ln W_e. \tag{18}$$

3 Conclusion

The novel topological index (π_e) proposed in this work is based on the distances between two edges of a graph and constructed easily from the edge Wiener type index in particular case. This index is well related with the edge Wiener index and for alkanes we conclude that $\ln \pi_e = C\, W_e^{\frac{2}{3}} \ln W_e$ for a constant C.

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