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Research article

Degree-weighted Wiener index of a graph

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Abstract: From geometric point of view, we introduced the Sombor-Wiener index of a graph and studied the basic properties of the new index. It was shown that the Sombor-Wiener index was useful in predicting the acentric factor of octane isomers. In addition, we proposed a degree-weighted Wiener index to generalize the Schultz index, the Gutman index, and the Sombor-Wiener index. Meanwhile, we gave the calculation formula of degree-weighted Wiener index for generalized Bethe trees.

Keywords: Sombor-Wiener index; degree-weighted Wiener index; tree

1. Introduction

In theoretical chemistry, the topological index of a graph, also called molecular structure descriptor, is a real number related to a structural graph of a molecule, and is often used to predict the physico-chemical properties and biological activities of molecules. A large number of molecular structure descriptors have been conceived and several of them have found applications in quantitative structure-activity and structure-property relationships (QSAR/QSPR) studies. In particular, degree-based topological indices and distance-based topological indices are the most important molecular structure descriptors that play an important role in QSAR/QSPR.

Throughout in this paper, G is a simple connected undirected graph with the vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, d_v is the degree of vertex v in G and $d(u, v)$ is the distance between vertices u and v in G. As a molecular descriptor, the Wiener index, introduced by Wiener [1] in 1947, is considered as one of the most used topological indexes with high correlation with many physical and chemical indices of molecular compounds. The Wiener index equals the sum of distances between all pairs of vertices of a graph G, that is,

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

In 1989, the Schultz index [2] of a chemical graph G was put forward as a topological index of alkanes. It is defined as

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} (d_u + d_v)d(u, v).$$

The proposal of this index has opened up the research on the degree-distance-type index. Plavšić et al. [3] showed that the Wiener index and the Schultz index are highly intercorrelated topological indices. For arbitrary catacondensed benzenoid graphs, Dobrynin [4] proved that the Schultz index has the same discriminating power with the Wiener index. So, it is both significant and interesting to study the Schultz index for some given class of graphs (or network), no matter whether they are molecular graphs or not.

In 1994, Gutman [5] proposed the Schultz index of the second kind, often called the Gutman index, and defined it as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} d_u d_v d(u, v).$$

Bounds of this index have been extensively studied using mathematical methods; see [6]. Moreover, for a tree T on n vertices, the Gutman index and Wiener index are closely related by

$$Gut(T) = 4W(T) - (n-1)(2n-1).$$

In 2021, from a geometric perspective (degree radius), Gutman [7] introduced a novel degree-based topological index called the Sombor index, which is defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}.$$

Note that the Sombor index is the sum of Euclidean distances of the degrees of the two vertices of each edge in the graph. This index is widely studied in mathematics and chemistry; see [8].

Inspired by the above research, we propose a new topological index called the Sombor-Wiener (SW) index , and define it as

$$SW(G) = \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2 + d_v^2}\,d(u,v).$$

The new index can be regarded as the sum of the product of degree radius and distance between any two vertices in the graph, which is a novel version of the distance-based topological index.

Naturally, we define a general topological index $DWW(G)$ of a graph G contributed by the degree weights of all vertices as

$$DWW(G) = \sum_{\{u,v\}\subseteq V(G)} f(d_u, d_v)d(u,v),$$

where $f(d_u, d_v)$ is a real function of d_u and d_v with

$$f(d_u, d_v) \geq 0 \text{ and } f(d_u, d_v) = f(d_v, d_u).$$

Clearly, the general topological index, called the degree-weighted Wiener index, is the generalization of the Schultz index, the Gutman index, and the SW index.

In this paper, we study the basic properties of the SW index, and the linear regression analysis of the SW index, with respect to acentric factor of octane isomers. In addition, we give the calculation formula of degree-weighted Wiener index for generalized Bethe trees. Our results generalize some known formulae on the Schultz index and Gutman index.

2. Basic properties of the SW index

Theorem 2.1. *Let G be a connected graph with n vertices.*

(i) *If $G = P_n$, then*

$$SW(G) = (n-1)\left(\frac{\sqrt{2}(n^2-5n+9)}{3} + \sqrt{5}(n-2)\right).$$

(ii) *If G is r-regular, then*

$$SW(G) = \sqrt{2}rW(G).$$

Moreover, if $G = K_n$, then

$$SW(G) = \frac{\sqrt{2}n(n-1)^2}{2}.$$

If $G = C_n$, then

$$SW(G) = \begin{cases} \dfrac{\sqrt{2}n^3}{4}, & \text{if } n \text{ is even;} \\ \dfrac{\sqrt{2}n(n^2-1)}{4}, & \text{if } n \text{ is odd.} \end{cases}$$

(iii) *If $G = K_{n_1,n_2}$, then*

$$SW(G) = n_1n_2\left[\sqrt{n_1^2+n_2^2} + \sqrt{2}(n_1+n_2) - 2\sqrt{2}\right].$$

In particular, if $G = K_{1,n-1}$, then

$$SW(G) = (n-1)(\sqrt{n^2-2n+2} + \sqrt{2}n - 2\sqrt{2}).$$

Proof. (i) If $G = P_n$, then

$$\begin{aligned} SW(G) &= \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2+d_v^2}\,d(u,v) \\ &= \sqrt{5}(1+2+\cdots+n-2) + \sqrt{2}(n-1) \\ &\quad + 2\sqrt{2}(1+2+\cdots+n-3) \\ &\quad + \sqrt{5}(n-2) + \cdots + 2\sqrt{2} + 2\sqrt{5} + \sqrt{5} \\ &= \frac{\sqrt{5}(n-1)(n-2)}{2} + \sqrt{2}(n-1) \\ &\quad + 2\sqrt{2}\left(1+3+\cdots+\frac{(n-3)(n-2)}{2}\right) \\ &\quad + \sqrt{5}(1+2+\cdots+n-2) \\ &= \sqrt{2}(n-1) + \sqrt{5}(n-1)(n-2) \\ &\quad + \frac{2\sqrt{2}(n-1)(n-2)(n-3)}{6} \\ &= (n-1)\left(\frac{\sqrt{2}(n^2-5n+9)}{3} + \sqrt{5}(n-2)\right). \end{aligned}$$

(ii) If G is r-regular, then

$$SW(G) = \sum_{\{u,v\}\subseteq V(G)} \sqrt{r^2 + r^2}d(u, v) = \sqrt{2}rW(G).$$

In particular, if $G = K_n$, then

$$\begin{aligned} SW(G) &= \sqrt{2}(n-1)W(G) \\ &= \sqrt{2}(n-1)\frac{n(n-1)}{2} \\ &= \frac{\sqrt{2}n(n-1)^2}{2}. \end{aligned}$$

If G is a cycle C_n, from [9], we have

$$SW(G) = \begin{cases} \frac{\sqrt{2}n^3}{4}, & \text{if } n \text{ is even;} \\ \frac{\sqrt{2}n(n^2-1)}{4}, & \text{if } n \text{ is odd.} \end{cases}$$

(iii) If $G = K_{n_1,n_2}$, then

$$\begin{aligned} SW(G) = &\sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2 + d_v^2}d(u, v) \\ =&n_1n_2\sqrt{n_1^2 + n_2^2} + 2\binom{n_1}{2}\sqrt{n_2^2 + n_2^2} \\ &+ 2\binom{n_2}{2}\sqrt{n_1^2 + n_1^2} \\ =&n_1n_2\left[\sqrt{n_1^2 + n_2^2} + \sqrt{2}(n_1 + n_2) - 2\sqrt{2}\right]. \end{aligned}$$

Let $n_1 = 1$ and $n_2 = n - 1$, then

$$SW(K_{1,n-1}) = (n-1)(\sqrt{n^2 - 2n + 2} + \sqrt{2}n - 2\sqrt{2}).$$

This completes the proof. □

Theorem 2.2. *Let G be a connected graph with the maximum degree Δ and the minimum degree δ, then*

$$\sqrt{2}\delta W(G) \le SW(G) \le \sqrt{2}\Delta W(G)$$

with equality if, and only if, G is regular.

Proof. By definition of $SW(G)$, we have the proof. □

Corollary 2.3. *Let G be a connected graph with n vertices, then*

$$\sqrt{2}W(G) \le SW(G) \le \sqrt{2}(n-1)W(G).$$

Theorem 2.4. *Let G be a connected graph with the minimum degree δ, then*

$$\frac{1}{\sqrt{2}}S(G) \le SW(G) \le S(G) - (2 - \sqrt{2})\delta W(G) \qquad (2.1)$$

with equality (left and right) if, and only if, G is regular.

Proof. First, we prove the left-hand side of (2.1). By Cauchy-Schwarz's inequality, we have

$$\begin{aligned} SW(G) &= \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2 + d_v^2}d(u, v) \\ &\ge \sum_{\{u,v\}\subseteq V(G)} \frac{1}{\sqrt{2}}(d_u + d_v)d(u, v) \\ &= \frac{1}{\sqrt{2}}S(G) \end{aligned}$$

with equality if, and only if, $d_u = d_v$ for $u, v \in V(G)$, that is, G is regular.

Second, we prove the righthand side of (2.1). For any $u, v \in V(G)$ $(d_u \ge d_v)$, we have

$$\sqrt{d_u^2 + d_v^2} \le d_u + (\sqrt{2} - 1)d_v$$

with equality if, and only if, $d_u = d_v$. Thus,

$$\begin{aligned} SW(G) &= \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2 + d_v^2}d(u, v) \\ &\le \sum_{\{u,v\}\subseteq V(G)} [d_u + (\sqrt{2} - 1)d_v]d(u, v) \\ &\le \sum_{\{u,v\}\subseteq V(G)} (d_u + d_v)d(u, v) - \sum_{\{u,v\}\subseteq V(G)} (2 - \sqrt{2})\delta d(u, v) \\ &\le S(G) - (2 - \sqrt{2})\delta W(G) \end{aligned}$$

with equality if, and only if, G is regular.

This completes the proof. □

Theorem 2.5. *Let G be a connected graph with the maximum degree Δ and the minimum degree δ, then*

$$\frac{\sqrt{2}}{\Delta}Gut(G) \le SW(G) \le \frac{\sqrt{2}}{\delta}Gut(G)$$

with equality (left and right) if, and only if, G is regular.

Proof. Note that

$$\sqrt{d_u^2 + d_v^2} = d_ud_v\sqrt{\frac{1}{d_u^2} + \frac{1}{d_v^2}},$$

then we have

$$
\begin{aligned}
SW(G) &= \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2+d_v^2}\,d(u,v)\\
&\le \sum_{\{u,v\}\subseteq V(G)} d_ud_v\sqrt{\frac{1}{\delta^2}+\frac{1}{\delta^2}}\,d(u,v)\\
&= \frac{\sqrt{2}}{\delta}\sum_{\{u,v\}\subseteq V(G)} d_ud_vd(u,v)\\
&= \frac{\sqrt{2}}{\delta}Gut(G)
\end{aligned}
$$

and

$$
\begin{aligned}
SW(G) &= \sum_{\{u,v\}\subseteq V(G)} \sqrt{d_u^2+d_v^2}\,d(u,v)\\
&\ge \sum_{\{u,v\}\subseteq V(G)} d_ud_v\sqrt{\frac{1}{\Delta^2}+\frac{1}{\Delta^2}}\,d(u,v)\\
&= \frac{\sqrt{2}}{\Delta}\sum_{\{u,v\}\subseteq V(G)} d_ud_vd(u,v)\\
&= \frac{\sqrt{2}}{\Delta}Gut(G).
\end{aligned}
$$

This completes the proof. □

3. Degree-weighted Wiener index of generalized Bethe trees

The generalized Bethe tree is an important graph structure that has wide applications in many fields. The investigation on topological indices of generalized Bethe trees and dendrimer trees frequently appeared in various journals. A Bethe tree $B_{k,d}$ is a rooted tree at k levels whose root is on level 1 and has degree equal to d, the vertices of levels from 2 to $k-1$ have degrees equal to $d+1$, and the vertices on the level k have degree equal to 1; see [10]. In 2007, Rojo [11] generalized the notion of a Bethe tree as follows: A generalized Bethe tree B_k is a rooted tree whose vertices at the same level have equal degrees. Moreover, a regular dendrimer tree $T_{k,d}$ is a generalized Bethe tree of $k+1$ levels with each non-pendent vertex having degree d.

Theorem 3.1. *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. If d_1 denotes the degree of rooted vertex and d_i+1 denotes the degree of vertices on the i-th level of B_{k+1} for $i<1\le k$, then*

$$DWW(B_{k+1}) = \sum_{l=1}^{k+1} A_l,$$

where n_j is the number of vertices on the j-th level of B_{k+1}, and

$$n_1 = 1 \ \ and \ \ n_{j+1} = d_1d_2\cdots d_j$$

for $1\le j\le k$, and

$$
\begin{aligned}
A_1 =& \sum_{j=2}^{k} n_j(j-1)f(d_1,d_j+1) + kn_{k+1}f(d_1,1),\\
A_l =& \Big[2\binom{d_{l-1}}{2} + 4\binom{d_{l-1}}{1}\binom{d_{l-1}d_{l-2}-d_{l-1}}{1} + \cdots\\
&+ 2(l-1)\binom{d_{l-1}\cdots d_2}{1}\binom{n_l-d_{l-1}\cdots d_2}{1}\Big]f(d_l+1,d_l+1)\\
&+ \sum_{j=l+1}^{k} n_j(j-l)f(d_l+1,d_j+1)\\
&+ (k-l+1)n_{k+1}f(d_l+1,1)\\
&+ (d_{l-1}-1)\Big[\sum_{j=l+1}^{k} n_j(j-l+2)f(d_l+1,d_j+1)\\
&+ (k-l+3)n_{k+1}f(d_l+1,1)\Big]\\
&+ (d_{l-1}d_{l-2}-d_{l-1})\Big[\sum_{j=l+1}^{k} n_j(j-l+4)f(d_l+1,d_j+1)\\
&+ (k-l+5)n_{k+1}f(d_l+1,1)\Big] + \cdots\\
&+ (n_l-d_{l-1}\cdots d_2)\Big[\sum_{j=l+1}^{k} n_j(j+l-2)f(d_l+1,d_j+1)\\
&+ (k+l-1)n_{k+1}f(d_l+1,1)\Big],\\
A_{k+1} =& f(1,1)\Big[2\binom{d_k}{2} + 4\binom{d_k}{1}\binom{d_kd_{k-1}-d_k}{1} + \cdots\\
&+ 2k\binom{d_k\cdots d_2}{1}\binom{n_{k+1}-d_k\cdots d_2}{1}\Big].
\end{aligned}
$$

Proof. Let A_i be the value of degree-weighted Wiener index of vertices on the i-th level of B_{k+1}, then

$$DWW(B_{k+1}) = \sum_{i=1}^{k+1} A_i.$$

By definition of B_{k+1}, we have

$$
\begin{aligned}
A_1 =& n_2f(d_1,d_2+1) + 2n_3f(d_1,d_3+1) + \cdots\\
&+ (k-1)n_kf(d_1,d_k+1) + kn_{k+1}f(d_1,1)\\
=& \sum_{j=2}^{k} n_j(j-1)f(d_1,d_j+1) + kn_{k+1}f(d_1,1),\\
A_2 =& 2\binom{d_1}{2}f(d_2+1,d_2+1) + n_2\Big[d_2f(d_2+1,d_3+1)\\
&+ 2d_2d_3f(d_2+1,d_4+1) + \cdots
\end{aligned}
$$

$$+ d_2d_3\cdots d_{k-1}(k-2)f(d_2+1,d_k+1)$$
$$+ d_2d_3\cdots d_k(k-1)f(d_2+1,1)$$
$$+ (n_2-1)(3d_2f(d_2+1,d_3+1)$$
$$+ 4d_2d_3f(d_2+1,d_4+1)+\cdots$$
$$+ d_2d_3\cdots d_{k-1}kf(d_2+1,d_k+1)$$
$$+ d_2d_3\cdots d_k(k+1)f(d_2+1,1))\Big]$$
$$=d_1(d_1-1)f(d_2+1,d_2+1)$$
$$+ n_2\Big[n_3/d_1f(d_2+1,d_3+1)$$
$$+ 2n_4/d_1f(d_2+1,d_4+1)+\cdots$$
$$+ n_k/d_1(k-2)f(d_2+1,d_k+1)$$
$$+ n_{k+1}/d_1(k-1)f(d_2+1,1)$$
$$+ (n_2-1)(3n_3/d_1f(d_2+1,d_3+1)$$
$$+ 4n_4/d_1f(d_2+1,d_4+1)+\cdots$$
$$+ kn_k/d_1f(d_2+1,d_k+1)$$
$$+ n_{k+1}/d_1(k+1)f(d_2+1,1))\Big]$$
$$=d_1(d_1-1)f(d_2+1,d_2+1)$$
$$+ n_2/d_1\Big[\sum_{j=3}^{k}(j-2)n_jf(d_2+1,d_j+1)$$
$$+ (k-1)n_{k+1}f(d_2+1,1)$$
$$+ (n_2-1)(\sum_{j=3}^{k}jn_jf(d_2+1,d_j+1)$$
$$+ (k+1)n_{k+1}f(d_2+1,1))\Big]$$
$$=d_1(d_1-1)f(d_2+1,d_2+1)$$
$$+ \sum_{j=3}^{k}(j-2)n_jf(d_2+1,d_j+1)$$
$$+ (k-1)n_{k+1}f(d_2+1,1)$$
$$+ (n_2-1)\Big[\sum_{j=3}^{k}jn_jf(d_2+1,d_j+1)$$
$$+ (k+1)n_{k+1}f(d_2+1,1)\Big],$$
$$A_3=\Big[2\binom{d_2}{2}+4\binom{d_2}{1}\binom{n_3-d_2}{1}\Big]f(d_3+1,d_3+1)$$
$$+ n_3\Big[d_3f(d_3+1,d_4+1)$$
$$+ 2d_3d_4f(d_3+1,d_5+1)+\cdots$$
$$+ (k-3)d_3d_4\cdots d_{k-1}f(d_3+1,d_k+1)$$
$$+ (k-2)d_3d_4\cdots d_kf(d_3+1,1)$$
$$+ (d_2-1)(3d_3f(d_3+1,d_4+1)$$
$$+ 4d_3d_4f(d_3+1,d_5+1)+\cdots$$
$$+ (k-1)d_3d_4\cdots d_{k-1}f(d_3+1,d_k+1)$$
$$+ kd_3d_4\cdots d_kf(d_3+1,1))$$
$$+ (n_3-d_2)(5d_3f(d_3+1,d_4+1)$$
$$+ 6d_3d_4f(d_3+1,d_5+1)+\cdots$$
$$+ (k+1)d_3d_4\cdots d_{k-1}f(d_3+1,d_k+1)$$
$$+ (k+2)d_3d_4\cdots d_kf(d_3+1,1))\Big]$$
$$=\Big[2\binom{d_2}{2}+4\binom{d_2}{1}\binom{n_3-d_2}{1}\Big])f(d_3+1,d_3+1)$$
$$+ \sum_{j=4}^{k}n_j(j-3)f(d_3+1,d_j+1)$$
$$+ (k-2)n_{k+1}f(d_3+1,1)$$
$$+ (d_2-1)\Big[\sum_{j=4}^{k}n_j(j-1)f(d_3+1,d_j+1)$$
$$+ kn_{k+1}f(d_3+1,1)\Big]$$
$$+ (n_3-d_2)\Big[\sum_{j=4}^{k}n_j(j+1)f(d_3+1,d_j+1)$$
$$+ n_{k+1}(k+2)f(d_3+1,1)\Big].$$

By calculating similarly to the above, for any $2\le l\le k$, we have

$$A_l=\Big[2\binom{d_{l-1}}{2}+4\binom{d_{l-1}}{1}\binom{d_{l-1}d_{l-2}-d_{l-1}}{1}+\cdots$$
$$+ 2(l-1)\binom{d_{l-1}\cdots d_2}{1}\binom{n_l-d_{l-1}\cdots d_2}{1}\Big]f(d_l+1,d_l+1)$$
$$+ \sum_{j=l+1}^{k}n_j(j-l)f(d_l+1,d_j+1)$$
$$+ (k-l+1)n_{k+1}f(d_l+1,1)$$
$$+ (d_{l-1}-1)\Big[\sum_{j=l+1}^{k}n_j(j-l+2)f(d_l+1,d_j+1)$$
$$+ (k-l+3)n_{k+1}f(d_l+1,1)\Big]$$
$$+ (d_{l-1}d_{l-2}-d_{l-1})\Big[\sum_{j=l+1}^{k}n_j(j-l+4)f(d_l+1,d_j+1)$$
$$+ (k-l+5)n_{k+1}f(d_l+1,1)\Big]+\cdots$$
$$+ (n_l-d_{l-1}\cdots d_2)\Big[\sum_{j=l+1}^{k}n_j(j+l-2)f(d_l+1,d_j+1)$$
$$+ (k+l-1)n_{k+1}f(d_l+1,1)\Big].$$

In particular, we have

$$\begin{aligned} A_{k+1} =& f(1,1)\Big[2\binom{d_k}{2}+4\binom{d_k}{1}\binom{d_kd_{k-1}-d_k}{1}+\cdots \\ &+2k\binom{d_k\cdots d_2}{1}\binom{n_{k+1}-d_k\cdots d_2}{1}\Big]. \end{aligned}$$

This completes the proof. □

Corollary 3.2. *The degree-weighted Wiener index of a Bethe tree $B_{k,d}$ is*

$$DWW(B_{k,d})=\sum_{l=1}^{k}A_l,$$

where

$$\begin{aligned} A_1 =& \sum_{j=2}^{k-1} d(d+1)^{j-2}(j-1)f(d,d+1)+(k-1)d(d+1)^{k-2}f(d,1), \\ A_l =& \Big[2\binom{d+1}{2}+4\binom{d+1}{1}\binom{(d+1)^2-(d+1)}{1}+\cdots \\ &+2(l-1)\binom{d^{l-2}}{1}\binom{n_l-d^{l-2}}{1}\Big]f(d+1,d+1) \\ &+\sum_{j=l+1}^{k-1} n_j(j-l)f(d+1,d+1)+(k-l)n_kf(d+1,1) \\ &+(d_{l-1}-1)\Big[\sum_{j=l+1}^{k-1} f(d+1,d+1)n_j(j-l+2) \\ &+(k-l+2)n_kf(d+1,1)\Big] \\ &+(d_{l-1}d_{l-2}-d_{l-1})\Big[\sum_{j=l+1}^{k-1} n_j(j-l+4)f(d+1,d+1) \\ &+(k-l+4)n_kf(d+1,1)\Big]+\cdots \\ &+(n_l-d_{l-1}\cdots d_2)\Big[\sum_{j=l+1}^{k-1} n_j(j+l-2)f(d+1,d+1) \\ &+(k+l-2)n_kf(d+1,1)\Big], \\ A_k =& f(1,1)\Big[2\binom{d}{2}+4\binom{d}{1}\binom{d(d-1)}{1}+\cdots \\ &+2(k-1)\binom{d^{k-2}}{1}\binom{(d-1)d^{k-2}}{1}\Big]. \end{aligned}$$

Corollary 3.3. *The degree-weighted Wiener index of a regular dendrimer tree $T_{k,d}$ is*

$$DWW(T_{k,d})=\sum_{l=1}^{k+1}A_l,$$

where

$$\begin{aligned} A_1 =& \sum_{j=2}^{k} n_j(j-1)f(d,d)+kd(d-1)^{k-1}f(d,1), \\ A_l =& \Big[2\binom{d-1}{2}+4\binom{d-1}{1}\binom{(d-1)(d-2)}{1}+\cdots \\ &+2(l-1)\binom{(d-1)^{l-2}}{1}\binom{n_l-(d-1)^{l-2}}{1}\Big]f(d,d) \\ &+\sum_{j=l+1}^{k} n_j(j-l)f(d,d)+(k-l+1)n_{k+1}f(d,1) \\ &+(d-2)\Big[\sum_{j=l+1}^{k} n_j(j-l+2)f(d,d) \\ &+(k-l+3)n_{k+1}f(d,1)\Big] \\ &+(d-1)(d-2)\Big[\sum_{j=l+1}^{k} n_j(j-l+4)f(d,d) \\ &+(k-l+5)n_{k+1}f(d,1)\Big]+\cdots \\ &+(n_l-(d-1)^{l-2})\Big[\sum_{j=l+1}^{k} n_j(j+l-2)f(d,d) \\ &+(k+l-1)n_{k+1}f(d,1)\Big], \\ A_{k+1} =& f(1,1)\Big[2\binom{d-1}{2}+4\binom{d-1}{1}\binom{(d-1)(d-2)}{1}+\cdots \\ &+2k\binom{(d-1)^{k-1}}{1}\binom{(d-1)^k}{1}\Big]. \end{aligned}$$

4. Applications of SW indices to the acentric factor of octane isomers

In this section, the chemical applicability of the SW index is investigated. The acentric factor (AcenFac) is a measure of the non-sphericity of molecules. We consider the correlation between acentric factors of octane isomers and the respective SW indices. The experimental values of acentric factors of octane isomers were taken from http://www.moleculardescriptors.eu/dataset/dataset.htm.

Using the data from Table 1, we find the correlation of AcenFac with the value of SW index for octane isomers; see Figure 1. The following equations give the regression models for the SW index:

$$AcenFac = 0.00198\times SW+0.008141.$$

Thus, the SW index can also help to predict the properties of octane isomers.

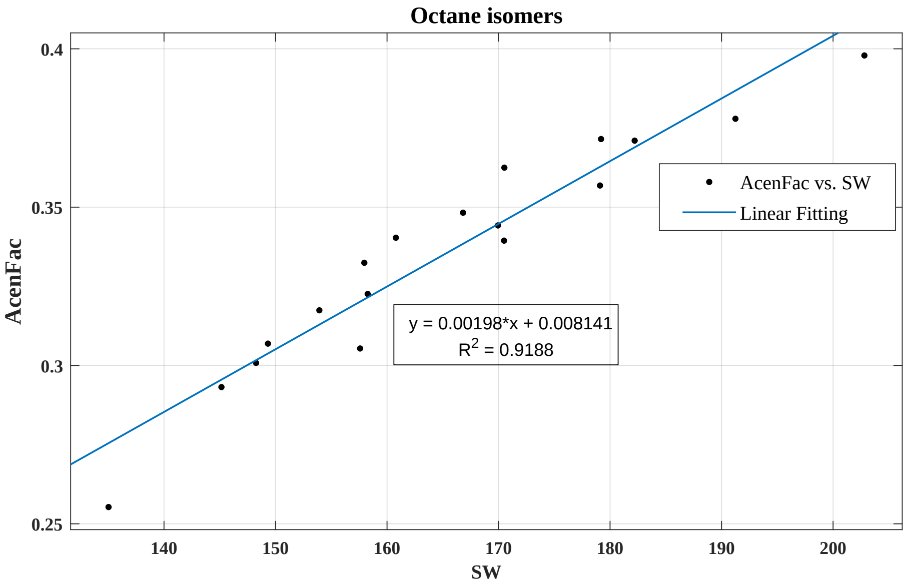

Figure 1. Scatter plot between acentric factor of Octane isomers and their SW index.

Table 1. Experimental values of AcenFac and SW index for octane isomers.

Molecule	AcenFac	SW
Octane	0.397898	202.8093
2-methyl-heptane	0.377916	191.2453
3-methyl-heptane	0.371002	182.2057
4-methyl-heptane	0.371504	179.1925
3-ethyl-hexane	0.362472	170.5225
2,2-dimethyl-hexane	0.339426	170.4970
2,3-dimethyl-hexane	0.348247	166.8181
2,4-dimethyl-hexane	0.344223	169.9447
2,5-dimethyl-hexane	0.35683	179.0977
3,3-dimethyl-hexane	0.322596	158.2653
3,4-dimethyl-hexane	0.340345	160.7917
2-methyl-3-ethyl-pentane	0.332433	157.9633
3-methyl-3-ethyl-pentane	0.306899	149.3210
2,2,3-trimethyl-pentane	0.300816	148.2544
2,2,4-trimethyl-pentane	0.30537	157.5862
2,3,3-trimethyl-pentane	0.293177	145.1517
2,3,4-trimethyl-pentane	0.317422	153.9314
2,2,3,3-tetramethylbutane	0.255294	135.0271

5. Conclusions

In this paper, we propose the SW index, and establish some mathematical relations between the Harary-Sombor index and other classic topological indices. Morover, we obtain the calculation formula of degree-weighted Wiener index for generalized Bethe trees. In addition, some numerical results are discussed. We calculate the SW index of octane isomers. The regression models show that the AcenFac and SW index of octane isomers are highly correlated.

In 1993, Klein and Randić [12] introduced the notion of resistance distance. Naturally, from the perspective of distance, we similarly propose the degree-weighted resistance-distance index of a graph G and define it as

$$DWR(G) = \sum_{\{u,v\}\subseteq V(G)} f(d_u, d_v) r(u, v),$$

where $r(u, v)$ is the resistance distance between u and v. It would be interesting to explore chemical and mathematical properties and possible predictive potential of this index.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare no conflicts of interest to this work.

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