Harary-Albertson index of graphs

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(Received: 5 November 2021. Received in revised form: 1 December 2021. Accepted: 3 December 2021. Published online: 5 December 2021.)

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\textbf{Abstract}

The Harary-Albertson index of a connected graph $G$ is introduced in this paper. This index is defined as

$$HA(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{|d(u) - d(v)|}{d(u,v)},$$

where $d(u)$ and $d(u,v)$ are the degree of the vertex $u$ and the distance between the vertices $u$ and $v$ in $G$, respectively. This new index is useful in predicting physico-chemical properties with high accuracy compared to some classic topological indices. Mathematical relations between the Harary-Albertson index and other classic topological indices are established. The extremal values of the Harary-Albertson index for trees of given order are also determined.

\textbf{Keywords:} Harary-Albertson index; QSAR; tree.

\textbf{2020 Mathematics Subject Classification:} 05C05, 05C07, 05C09, 05C35.

1. Introduction

Let $G$ be a simple undirected connected graph with the vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, $d(v) = d_G(v)$ denotes the degree of vertex $v$ in $G$. The minimum and the maximum degree of $G$ are denoted by $\delta(G)$ and $\Delta(G)$, or simply $\delta$ and $\Delta$, respectively. A pendant vertex of $G$ is a vertex of degree one. The distance between two vertices $u,v \in V(G)$, denoted by $d(u,v) = d_G(u,v)$, is defined as the length of a shortest path between $u$ and $v$. The eccentricity of $v$, $e(v)$, is the distance between $v$ and any vertex which is furthest from $v$ in $G$. The diameter of $G$ is the maximum eccentricity in $G$, denoted by $D(G)$. Similarly, the radius of $G$ is the minimum eccentricity in $G$, denoted by $r(G)$. The join $G_1 \cup G_2$ of the graphs $G_1$ and $G_2$ is obtained from $G_1 \cup G_2$ by adding to it all edges between vertices from $V(G_1)$ and $V(G_2)$. The lexicographic product of the graphs $G_1$ and $G_2$ is denoted by $G_1[G_2]$, and it is the graph with vertex set $V(G_1) \times V(G_2)$, and two vertices $(u_1, v_1)$ and $(u_2, v_2)$ are adjacent if $u_1$ is adjacent to $u_2$ in $G_1$ or $u_1 = u_2$ and $v_1$ and $v_2$ are adjacent in $G_2$. Denote by $P_n$, $S_n$, and $C_n$ the path, the star and the complement of $G$, respectively.

In recent decades, the topological indices (graphical invariants or topological molecular descriptors) have been extensively studied in various areas of mathematics [8, 11], physics [12], informatics [16], biology [3], especially in chemical disciplines [4, 5, 14, 17], such as chemical documentation, isomer discrimination, study of molecular complexity, chirality, similarity/dissimilarity, QSAR/QSPR, drug design, database selection, lead optimization, etc. In particular, the following classic topological indices appear more frequently in the literature in the above related fields.

- Sombor index [7]: $SO = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$.
- second Zagreb index [9]: $M_2 = \sum_{uv \in E(G)} d(u)d(v)$.
- Randić index [15]: $R = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$.
- Albertson index [2]: $irr = \sum_{uv \in E(G)} |d(u) - d(v)|$.
- total irregularity index [1]: $irr_t = \sum_{\{u,v\} \subseteq V(G)} |d(u) - d(v)|$.
- atom-bond-connectivity index [6]: $ABC = \sum_{uv \in E(G)} \sqrt{\frac{2d(u) + d(v) - 2}{d(u)d(v)}}$.

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• Wiener index [18]: $W = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$.

• Harary index [10, 13]: $H = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)}$.

Based on the Albertson index, Abdo, Brandt and Dimitrov [1] proposed the total irregularity index, which can be applied as irregularity measure when the adjacency information of the vertices is unknown, because the total irregularity index of a graph depends only on its degree sequence, see for example Figure 1. However, it is well known that there are many graphs with the same degree sequence, which makes the structure discriminating ability of the total irregularity index lower. Usually, distance-based topological indices have better structure discriminating ability than degree-based topological indices. Moreover, any interaction must decrease with the increase of the distance between the interacting particles in general situation. In order to improve the structure discriminating ability and maintain certain irregularity measuring ability, we propose the Harary-Albertson index of a connected graph $G$ as follows:

$$HA(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{|d(u) - d(v)|}{d(u,v)}.$$

In this paper, we confirm the suitability of the Harary-Albertson index in quantitative structure-property relationship (QSPR) analysis by the correlation of acentric factor (AcenFac), entropy (S), SNar and HNar with the Harary-Albertson index for octane isomers. Secondly, we obtain mathematical relations between the Harary-Albertson index and other classic topological indices. Finally, we study the extremal values of the Harary-Albertson index for trees of given order.

![Figure 1: The trees $T_1$ and $T_2$ satisfying $irr_t(T_1) = irr_t(T_2) = 22$ and $HA(T_1) = 44/3$, $HA(T_2) = 43/3$.](image)

2. The Harary-Albertson index in QSPR analysis

In this section, the chemical applicability of the Harary-Albertson index is investigated. We obtain the data related to octanes, listed in Table 1, using matlab software and the experimental data set octane isomers. We get that the correlation coefficient of the Harary-Albertson index with AcenFac, entropy (S), SNar and HNar are $-0.9667$, $-0.9073$, $-0.9786$ and $-0.9820$, respectively, for octane isomers. Thus the Harary-Albertson index can help to predict these physico-chemical properties of octane isomers. These results confirm the suitability of the Harary-Albertson index in QSPR analysis. Meanwhile, the following equations give the regression models for the Harary-Albertson index.

$$AcenFac = 0.4440 - 0.0064 \times HA,$$

$$S = 118.3572 - 0.7602 \times HA,$$

$$SNar = 4.5610 - 0.0605 \times HA,$$

$$HNar = 1.6838 - 0.0162 \times HA.$$

In order to prove that the Harary-Albertson index shows better predictive capability, we study the correlation of some classic topological indices like the second Zagreb index, Sombor index, Randić index, Albertson index, total irregularity index, atom-bond-connectivity index, Wiener index, Harary index with AcenFac, S, SNar and HNar, shown in Table 2. It is not difficult to find that sometimes the Harary-Albertson index shows better predictive capability than the existing indices.
By the definition of $n$, we have the proof.

\begin{table}
\centering
\begin{tabular}{llllllllllllllllll}
\hline
Molecule & AcenFac & $S$ & SNar & HNar & HA & SO & $M_2$ & R & $\sigma r$ & $\sigma r_1$ & ABC & W & H \\
\hline
Octane & 0.3979 & 111.67 & 4.159 & 1.6 & 4.9 & 37.2285 & 24 & 3.9142 & 2 & 12 & 4.9497 & 84 & 13.7429 \\
2-methyl-heptane & 0.3779 & 109.84 & 3.871 & 1.5 & 11.1333 & 41.3029 & 26 & 3.7701 & 6 & 22 & 5.1685 & 79 & 14.1 \\
3-methyl-heptane & 0.3710 & 111.26 & 3.871 & 1.5 & 11.7333 & 41.8045 & 27 & 3.8081 & 6 & 22 & 5.0591 & 76 & 14.2667 \\
4-methyl-heptane & 0.3715 & 109.32 & 3.871 & 1.5 & 11.9 & 41.8047 & 27 & 3.8081 & 6 & 22 & 5.0591 & 75 & 14.3167 \\
3-ethyl-hexane & 0.3625 & 109.43 & 3.871 & 1.5 & 12 & 40.7066 & 28 & 3.8461 & 6 & 22 & 4.9497 & 72 & 14.4833 \\
2,2-dimethyl-hexane & 0.3394 & 103.42 & 3.466 & 1.391 & 18.5 & 49.4668 & 30 & 3.5607 & 12 & 30 & 5.4265 & 71 & 14.7667 \\
2,3-dimethyl-hexane & 0.3482 & 108.02 & 3.584 & 1.412 & 16 & 44.799 & 30 & 3.6807 & 8 & 28 & 5.2375 & 70 & 14.7333 \\
2,4-dimethyl-hexane & 0.3442 & 106.98 & 3.584 & 1.412 & 16.6667 & 45.6791 & 29 & 3.6393 & 10 & 28 & 5.2779 & 71 & 14.65 \\
2,5-dimethyl-hexane & 0.3568 & 105.72 & 3.584 & 1.412 & 16.3333 & 45.3773 & 28 & 3.6259 & 10 & 28 & 5.3873 & 74 & 14.4667 \\
3,3-dimethyl-hexane & 0.3226 & 104.74 & 3.466 & 1.391 & 19.5 & 48.9821 & 32 & 3.6213 & 12 & 30 & 5.2676 & 67 & 15.0333 \\
3,4-dimethyl-hexane & 0.3403 & 106.59 & 3.584 & 1.412 & 16.5 & 44.5009 & 31 & 3.7187 & 8 & 28 & 5.1281 & 68 & 14.8667 \\
2-methyl-3-ethyl-pentane & 0.3324 & 106.06 & 3.584 & 1.412 & 16.3333 & 44.5009 & 31 & 3.7187 & 8 & 28 & 5.1281 & 67 & 14.9117 \\
3-methyl-3-ethyl-pentane & 0.3069 & 101.48 & 3.466 & 1.391 & 20 & 48.4954 & 34 & 3.682 & 12 & 20 & 5.1087 & 64 & 15.25 \\
2,2,3-trimethyl-pentane & 0.3008 & 101.31 & 3.178 & 1.315 & 23 & 52.7464 & 35 & 3.4814 & 14 & 34 & 5.4734 & 63 & 15.4167 \\
2,2,4-trimethyl-pentane & 0.3054 & 104.09 & 3.178 & 1.315 & 23 & 53.5431 & 32 & 3.4165 & 16 & 34 & 5.6453 & 66 & 15.1667 \\
2,2,3-trimethyl-pentane & 0.2932 & 102.06 & 3.178 & 1.315 & 23.3333 & 52.5579 & 36 & 3.504 & 14 & 34 & 5.4248 & 62 & 15.5 \\
2,3,3-trimethyl-pentane & 0.3174 & 102.39 & 3.296 & 1.333 & 18.6667 & 48.4933 & 33 & 3.5335 & 10 & 30 & 5.4158 & 65 & 15.1667 \\
2,2,2,3,3-pentamethyl-butane & 0.2553 & 93.06 & 2.773 & 1.231 & 27 & 60.7911 & 40 & 3.25 & 18 & 36 & 5.8085 & 58 & 16 \\
\hline
\end{tabular}
\end{table}

3. Harary-Albertson and other degree-based indices

**Theorem 3.1.** Let $G$ be an irregular connected graph with $n$ vertices. Then

$$HA(G) \leq (\Delta - \delta)H(G)$$

and

$$\frac{1}{D(G)} \text{irr}_t(G) \leq HA(G) \leq \frac{1}{r(G)} \text{irr}_t(G).$$

**Proof.** By the definition of $HA(G)$, we have the proof.

**Theorem 3.2.** Let $G$ be a triangle- and quadrangle-free irregular connected graph with $n \geq 4$ vertices and $m$ edges. Then

$$HA(G) \leq \text{irr}(G) + \frac{1}{24} [3n(n - 1) + M_1 + 2M_2 - 10m](\Delta - \delta),$$

where $M_1 = \sum_{v \in V(G)} d^2(v)$.

**Proof.** Let $d(G, k)$ be the number of vertex pairs of the graph $G$ that are at distance $k$. If $G$ be a triangle- and quadrangle-free irregular connected graph with $n \geq 4$ vertices and $m$ edges, from [20], we have

$$d(G, 1) = m, \quad d(G, 2) = \frac{1}{2} M_1 - m, \quad d(G, 3) = M_2 - M_1 + m, \quad \sum_{k=1}^{D(G)} d(G, k) = \frac{n(n - 1)}{2}.$$ 

By the definition of $HA(G)$, we have

$$HA(G) = \sum_{u,v \subseteq V(G)} \frac{|d(u) - d(v)|}{d(u,v)} \leq \text{irr}(G) + \frac{1}{2} \left( \frac{1}{2} M_1 - m \right)(\Delta - \delta) + \frac{1}{3} \left( M_2 - M_1 + m \right)(\Delta - \delta) + \frac{1}{4} \left( \frac{n(n - 1)}{2} + \frac{1}{2} M_1 - M_2 - m \right)(\Delta - \delta).$$

Table 2: The square of correlation coefficient of different topological indices with AcenFac, S, SNar and HNar.

| Physico-chemical property | HA | SO | $M_2$ | R | $\sigma r$ | $\sigma r_1$ | ABC | W | H |
|---------------------------|----|----|-------|---|-----------|-----------|-----|---|---|
| AcenFac                   | 0.9345 | 0.9205 | 0.9733 | 0.8176 | 0.8701 | 0.6424 | 0.629 | 0.9224 | 0.984 |
| S                         | 0.8232 | 0.8959 | 0.8868 | 0.8205 | 0.8048 | 0.5279 | 0.6727 | 0.7710 | 0.8636 |
| SNar                      | 0.9577 | 0.9688 | 0.894 | 0.9183 | 0.7948 | 0.9216 | 0.8404 | 0.9201 |
| HNar                      | 0.9643 | 0.9251 | 0.8941 | 0.9487 | 0.9868 | 0.838 | 0.7912 | 0.8662 | 0.9107 |
Let $G$ be an irregular connected graph with $n$ vertices and maximum degree $\Delta(G) \leq n - 2$. Then

$$HA(\overline{G}) \leq \text{irr}_1(G) - \frac{1}{2} \text{irr}(G).$$

In particular, if $D(G) \geq 3$, then

$$HA(\overline{G}) \geq \frac{1}{3} \text{irr}_1(G).$$

Furthermore, if $D(G) \geq 4$, then

$$HA(\overline{G}) \geq \frac{1}{2} \text{irr}_1(G).$$

Proof. Let $d(u) + d(u') = n - 1$ and $d(v) + d(v') = n - 1$ for $u, v \in V(G)$. Since $G$ is a connected graph with maximum degree $\Delta(G) \leq n - 2$, we know that $\overline{G}$ is a connected graph with $r(\overline{G}) \geq 2$. By the definition of the Harary-Albertson index, we have

$$HA(\overline{G}) = \sum_{\{u', v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{d(u', v')}$$

$$= \sum_{\{u, v\} \subseteq V(G), d(u, v) \geq 2} \frac{|n - 1 - d(u) - (n - 1 - d(v))|}{d(u', v')}
+ \sum_{\{u, v\} \subseteq V(G), d(u, v) = 1} \frac{|n - 1 - d(u) - (n - 1 - d(v))|}{d(u', v')}$$

$$= \text{irr}_1(G) - \sum_{\{u, v\} \subseteq V(G), d(u, v) = 1} \frac{|d(u) - d(v)|}{d(u', v')}
+ \sum_{\{u, v\} \subseteq V(G), d(u, v) = 1} \frac{|d(u) - d(v)|}{d(u', v')}$$

$$\leq \text{irr}_1(G) - \text{irr}(G) + \sum_{\{u, v\} \subseteq V(G), d(u, v) = 1} \frac{|d(u) - d(v)|}{r(\overline{G})}
\leq \text{irr}_1(G) - \text{irr}(G) + \sum_{\{u, v\} \subseteq V(G), d(u, v) = 1} \frac{|d(u) - d(v)|}{2}$$

$$= \text{irr}_1(G) - \frac{1}{2} \text{irr}(G).$$

If $D(G) \geq 3$, then $D(\overline{G}) \leq 3$. Thus, we have

$$HA(\overline{G}) = \sum_{\{u', v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{d(u', v')}$$

$$\geq \sum_{\{u', v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{D(\overline{G})}
\geq \sum_{\{u, v\} \subseteq V(G)} \frac{|n - 1 - d(u) - (n - 1 - d(v))|}{3}
= \frac{1}{3} \sum_{\{u, v\} \subseteq V(G)} |d(u) - d(v)|
= \frac{1}{3} \text{irr}_1(G).$$

If $D(G) \geq 4$, then $D(\overline{G}) = 2$. By a similar reasoning as the above, we have the proof.
Theorem 3.4. Let \( G_1 \) and \( G_2 \) be connected graphs with \( |V(G_1)| = n_1 \) and \( |V(G_2)| = n_2 \) such that \( n_1 \geq n_2 \geq 2 \). Then

\[
HA(G_1 \cup G_2) \leq \frac{1}{2}[\text{irr}_t(G_1) + \text{irr}_t(G_2)] + \frac{1}{2}[\text{irr}(G_1) + \text{irr}(G_2)]
\]

\[
+ n_1 n_2 \max\{|n_2 - n_1 + \Delta(G_1) - \delta(G_2)|, |n_2 - n_1 - \Delta(G_1) + \delta(G_2)|\}.
\]

Proof. By the definition of \( G_1 \cup G_2 \), we have \( |G_1 \cup G_2| = n_1 + n_2 \), \( d_{G_1 \cup G_2}(u) = d(u) + n_2 \) and \( d_{G_1 \cup G_2}(v) = d(v) + n_1 \) for \( u \in V(G_1) \) and \( v \in V(G_2) \). Moreover, \( d_{V(G_1 \cup G_2)}(u, v) = 1 \) for \( uv \in E(G_1) \) or \( uv \in E(G_2) \) or \( u \in V(G_1) \) and \( v \in V(G_2) \), \( d_{V(G_1 \cup G_2)}(u, v) = 2 \) otherwise. Thus,

\[
HA(G_1 \cup G_2) = \sum_{\{u,v\} \subseteq V(G_1 \cup G_2)} \frac{|d_{G_1 \cup G_2}(u) - d_{G_1 \cup G_2}(v)|}{d_{G_1 \cup G_2}(u, v)}
\]

\[
= \sum_{uv \in E(G_1)} |d(u) - d(v)| + \sum_{uv \in E(G_2)} |d(u) - d(v)|
\]

\[
+ \sum_{u \in V(G_1) \cap v \in V(G_2)} \sum_{d(u,v) \geq 2} |(n_2 - d(v)) - (n_1 - d(u))|
\]

\[
+ \sum_{\{u,v\} \subseteq V(G_1) \cap d(u,v) \geq 2} \frac{|d(u) - d(v)|}{2} + \sum_{\{u,v\} \subseteq V(G_2) \cap d(u,v) \geq 2} \frac{|d(u) - d(v)|}{2}
\]

\[
= \text{irr}(G_1) + \text{irr}(G_2) + \sum_{uv \in E(G_1) \cap v \in V(G_2)} |(n_2 - d(v)) - (n_1 - d(u))|
\]

\[
+ \frac{1}{2}[\text{irr}_t(G_1) - \text{irr}(G_1)] + \frac{1}{2}[\text{irr}_t(G_2) - \text{irr}(G_2)]
\]

\[
= \frac{1}{2}[\text{irr}_t(G_1) + \text{irr}_t(G_2)] + \frac{1}{2}[\text{irr}(G_1) + \text{irr}(G_2)]
\]

\[
+ \sum_{u \in V(G_1) \cap v \in V(G_2)} \sum_{d(u,v) \geq 2} |(n_2 - d(v)) - (n_1 - d(u))|
\]

\[
\leq \frac{1}{2}[\text{irr}_t(G_1) + \text{irr}_t(G_2)] + \frac{1}{2}[\text{irr}(G_1) + \text{irr}(G_2)]
\]

\[
+ n_1 n_2 \max\{|n_2 - n_1 + \Delta(G_1) - \delta(G_2)|, |n_2 - n_1 - \Delta(G_1) + \delta(G_2)|\}.
\]

\[\square\]

Theorem 3.5. Let \( G_1 \) and \( G_2 \) be connected graphs with \( |V(G_1)| = n_1 \), \( |V(G_2)| = n_2 \) and \( |E(G_2)| = m_2 \). Then

\[
HA(G_1[G_2]) \leq n_2^2 HA(G_1) + \frac{n_2}{4} \left[ \frac{n_2(n_2 - 1)}{2} - m_2 \right] \text{irr}_t(G_1) + \frac{n_1(n_1 - 1)}{8} \text{irr}(G_2) + \frac{3n_1^2 + n_1}{8} \text{irr}(G_2).
\]

Proof. By the definition of \( G_1[G_2] \), we know that \( d_{G_1[G_2]}((u_i, v_j)) = n_2 d(u_i) + d(v_j) \) for \( u_i \in V(G_1) \) (1 \( \leq i \leq n_1 \)) and \( v_j \in V(G_2) \) (1 \( \leq j \leq n_2 \)). Moreover, we have \( d_{G_1[G_2]}((u_i, v_k), (u_j, v_l)) = d(u_i, u_j) \) for \( v_k = v_l \), \( d_{G_1[G_2]}((u_i, v_k), (u_j, v_l)) = 1 \) for \( u_i = u_j \) and \( v_k \neq v_l \). Thus,

\[
HA(G_1[G_2]) = \frac{1}{2} \sum_{(u_i, v_k) \in V(G_1[G_2])} \frac{|d((u_i, v_k)) - d((u_j, v_l))|}{d((u_i, v_k), (u_j, v_l))}
\]

\[
= \frac{1}{2} \sum_{u_i, u_j \in V(G_1) \cap v_k, v_l \in V(G_2)} |n_2 d(u_i) - d(u_j)| + d(v_k) - d(v_l)|
\]

\[
= \frac{1}{2} \sum_{u_i, u_j \in V(G_1) \cap v_k, v_l \in V(G_2)} n_2 |d(u_i) - d(u_j)| + \frac{1}{2} \sum_{u_i, u_j \in V(G_1) \cap v_k, v_l \in V(G_2)} |d(v_k) - d(v_l)|
\]

\[
+ \frac{1}{2} \sum_{u_i, u_j \in V(G_1) \cap v_k, v_l \in V(G_2) \cap u_i \neq u_j, v_k \neq v_l} |n_2 d(u_i) - d(u_j)| + d(v_k) - d(v_l)|
\]

\[\square\]
\[\begin{align*}
&\leq n_1^2 HA(G_1) + \frac{1}{2} n_1^2 irr(G_2) + \frac{1}{4} \sum_{u_i, u_j \in V(G_1)} n_2 |d(u_i) - d(u_j)| \\
&\quad + \frac{1}{4} \sum_{v_k, v_l \in V(G_2)} |d(v_k) - d(v_l)| \\
&\quad + \frac{1}{4} \sum_{u_i, u_j \in V(G_1) \setminus \{v_k, v_l\} \in E(G_2)} |d(v_k) - d(v_l)| \\
&= n_1^2 HA(G_1) + \frac{1}{2} n_1^2 irr(G_2) + \frac{1}{4} n_2 \left[ \binom{n_2}{2} - m_2 \right] irr_t(G_1) \\
&\quad + \frac{1}{4} \left( \sum_{t=1}^{n_1} \binom{n_1}{2} \right) [irr_t(G_2) - irr(G_2)] \\
&= n_1^2 HA(G_1) + \frac{n_2}{4} \left[ \frac{n_2(n_2 - 1)}{2} - m_2 \right] irr_t(G_1) + \frac{n_1(n_1 - 1)}{8} irr_t(G_2) \\
&\quad + 3n_1^2 + n_1 irr(G_2).
\end{align*}\]

4. The Harary-Albertson index of trees

**Theorem 4.1.** Let \(T_n\) be a tree with \(n\) vertices. Then
\[2 \left( 1 + \frac{1}{2} + \cdots + \frac{1}{n-2} \right) \leq HA(T_n) \leq (n-1)(n-2),\]
where the left (right) equality holds if and only if \(T_n = P_n\) (\(T_n = S_n\)).

**Proof:** Abdo et al. [1] proved that the star has the maximum total irregularity among all trees with \(n\) vertices. Note that \(HA(S_n) = irr_t(S_n) = (n-1)(n-2)\). Thus we have
\[HA(T_n) \leq irr_t(T_n) \leq irr_t(S_n) = (n-1)(n-2)\]
with equality if and only if \(T_n = S_n\).

If the maximum degree \(\Delta(T_n) \geq 3\), then the number of pendant vertices \(p \geq 3\). Let \(v_1, v_2, \ldots, v_p\) be the vertices of \(T_n\), and let \(v_1, v_2, \ldots, v_p\) be the pendant vertices. Since any two vertices are connected by exactly one path in a tree, we have
\[HA(T_n) > p + \sum_{i=1}^{p} \sum_{j=p+1}^{n} \frac{d(v_j) - 1}{d(v_i, v_j)}\]
\[> 2 \left( 1 + \frac{1}{2} + \cdots + \frac{1}{n-2} \right)\]
\[= HA(P_n).\]
Thus, \(HA(T_n) \geq HA(P_n)\) with equality if and only if \(T_n = P_n\).

5. Conclusion

In this paper, we propose the Harary-Albertson index, which can be successfully applied to quantitative structure-property relationship (QSPR) analysis. Some mathematical relations between the Harary-Albertson index and other classic topological indices are established. Additionally, the Harary-Albertson index of trees is studied. For measuring the non-self-centrality of a graph \(G\), the non-self-centrality number of \(G\) was introduced in [19] as \(N(G) = \sum_{\{u, v\} \subseteq V(G)} |\varepsilon(u) - \varepsilon(v)|\). Based on this, one can propose the Harary non-self-centrality number of a connected graph \(G\) as follows:
\[HN(G) = \sum_{\{u, v\} \subseteq V(G)} \frac{|\varepsilon(u) - \varepsilon(v)|}{d(u, v)} = \frac{1}{2} \sum_{u, v \in V(G)} \frac{|\varepsilon(u) - \varepsilon(v)|}{d(u, v)}.\]
The following four problems related to the present study will be considered in the future:

1. Determine the extremal (minimum and maximum) values of the Harary-Albertson index among all connected graphs with $n$ vertices and $m$ edges.

2. Determine the extremal values of the Harary-Albertson index among all molecular graphs with $n$ vertices.

3. Study the properties of the Harary non-self-centrality number of connected graphs.

4. Establish relations between the Harary-Albertson index and the Harary non-self-centrality number of connected graphs.

Acknowledgments

This research was supported by NSFC (through grant no. 11661068) and NSFQH (through grant no. 2021-ZJ-703). The author is grateful to the anonymous referees for careful reading and valuable comments which improved the original manuscript.

References

[1] H. Abdo, S. Brandt, D. Dimitrov, The total irregularity of a graph, *Discrete Math. Theoret. Comput. Sci.* **16** (2014) 201–206.

[2] M. O. Albertson, The irregularity of a graph, *Ars Combin.* **46** (1997) 219–225.

[3] J. Bajorath, *Chemoinformatics and Computational Chemical Biology*, Humana Press, Totowa, 2011.

[4] J. Devillers, A. T. Balaban, *Topological Indices and Related Descriptors in QSAR and QSIPR*, Gordon & Breach, Amsterdam, 1999.

[5] M. V. Diudea, *QSIPR/QSIPR Studies by Molecular Descriptors*, Nova, Huntington, 2001.

[6] E. Estrada, L. Torres, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem. Sec. A* **37** (1998) 849–855.

[7] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[8] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[9] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[10] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Design of topological indices. IV. Reciprocal distance matrix, related local vertex invariants and topological indices. Applied graph theory and discrete mathematics in chemistry, *J. Math. Chem.* **12** (1993) 309–318.

[11] D. Janežič, A. Milčević, S. Nikolić, N. Trinajstić, *Graph-Theoretical Matrices in Chemistry*, CRC Press, Boca Raton, 2015.

[12] N. K. Labanowski, I. Motec, R. A. Dammkoehler, The physical meaning of topological indices, *Comput. Chem.* **15** (1991) 47–53.

[13] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.

[14] T. Puzyn, J. Leszczynski, M. T. Cronin, *Recent Advances in QSIPR Studies: Methods and Applications*, Springer, Dordrecht, 2010.

[15] M. Randić, Characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.

[16] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.

[17] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[18] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[19] K. Xu, K. C. Das, A. D. Maden, On a novel eccentricity-based invariant of a graph, *Acta Math. Sin. (Engl. Ser.)* **32** (2016) 1477–1493.

[20] B. Zhou, I. Gutman, Relationships between Wiener, hyper-Wiener and Zagreb indices, *Chem. Phys. Lett.* **394** (2004) 93–95.