Research Article Harary-Albertson index of graphs

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Abstract

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

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

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.

Keywords: Harary-Albertson index; QSPR; tree.

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 δ and Δ , 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 $v, \varepsilon(v)$, 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 $G_1 \vee G_2$ 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 \overline{G} 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]: $SO = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}$.
- 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]: $irr_t = \sum_{\{u,v\} \subset V(G)} |d(u) d(v)|$.
- atom-bond-connectivity index [6]: $ABC = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$.

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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:

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

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 $HA(T_1) = 44/3$, $HA(T_2) = 43/3$.

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, 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.

$$\begin{aligned} AcenFac &= 0.4440 - 0.0064 \times HA, \\ S &= 118.3572 - 0.7602 \times HA \\ SNar &= 4.5610 - 0.0605 \times HA, \\ HNar &= 1.6838 - 0.0162 \times HA. \end{aligned}$$

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.

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Table 1: Experimental values of acentric factor (AcenFac), entropy (S), SNar, HNar and the corresponding values of									
different topological indices for octane isomers.									

Molecule	AcenFac	s	SNar	HNar	HA	SO	M_2	R	irr	irr_t	ABC	w	н
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	41.0047	27	3.8081	6	22	5.0591	76	14.2667
4-methyl-heptane	0.3715	109.32	3.871	1.5	11.9	41.0047	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	45.0791	29	3.6639	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	14.9167
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	5.4743	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
2,3,3-trimethyl-pentane	0.2932	102.06	3.178	1.315	23.3333	52.5579	36	3.504	14	34	5.4248	62	15.5
2,3,4-trimethyl-pentane	0.3174	102.39	3.296	1.333	18.6667	48.5933	33	3.5535	10	30	5.4158	65	15.1667
2,2,3,3-tetramethylbutane	0.2553	93.06	2.773	1.231	27	60.791	40	3.25	18	36	5.8085	58	16

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	irr	irr_t	ABC	w	Н
AcenFac	0.9345	0.9205	0.973	0.8176	0.8701	0.6424	0.629	0.9324	0.984
s	0.8232	0.8959	0.8868	0.8205	0.8048	0.5279	0.6727	0.7705	0.8636
SNar	0.9577	0.9688	0.894	0.9487	0.9183	0.7948	0.8216	0.8484	0.9201
HNar	0.9643	0.9251	0.8941	0.9487	0.8968	0.838	0.7912	0.8662	0.9107

3. Harary-Albertson and other degree-based indices

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

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

and

$$\frac{1}{D(G)}irr_t(G) \le HA(G) \le \frac{1}{r(G)}irr_t(G).$$

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 $n \ge 4$ vertices and m edges. Then

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

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 $n \ge 4$ 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

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

$$\leq irr(G) + \frac{1}{2} \left(\frac{1}{2}M_1 - m\right) (\Delta - \delta) + \frac{1}{3}(M_2 - M_1 + m)(\Delta - \delta)$$

$$+ \frac{1}{4} \left[\frac{n(n-1)}{2} + \frac{1}{2}M_1 - M_2 - m\right] (\Delta - \delta)$$

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

A graph is said to be self-complementary if it is isomorphic with its complement. Clearly, if G is a self-complementary graph, then $HA(G) = HA(\overline{G})$.

Theorem 3.3. Let G be an irregular connected graph with n vertices and maximum degree $\Delta(G) \leq n-2$. Then

$$HA(\overline{G}) \le irr_t(G) - \frac{1}{2}irr(G)$$

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

$$HA(\overline{G}) \ge \frac{1}{3}irr_t(G)$$

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

$$HA(\overline{G}) \ge \frac{1}{2}irr_t(G).$$

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

$$\begin{split} HA(\overline{G}) &= \sum_{\{u',v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{d(u',v')} \\ &= \sum_{\{u,v\} \subseteq V(G), d(u,v) \geq 2} \frac{|n - 1 - d(u) - (n - 1 - d(v))||}{d(u',v')} \\ &+ \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} \frac{|n - 1 - d(u) - (n - 1 - d(v))||}{d(u',v')} \\ &= \sum_{\{u,v\} \subseteq V(G), d(u,v) \geq 2} |d(u) - d(v)| + \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} \frac{|d(u) - d(v)|}{d(u',v')} \\ &= irr_t(G) - \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} |d(u) - d(v)| + \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} \frac{|d(u) - d(v)|}{d(u',v')} \\ &\leq irr_t(G) - irr(G) + \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} \frac{|d(u) - d(v)|}{r(\overline{G})} \\ &\leq irr_t(G) - irr(G) + \sum_{\{u,v\} \subseteq V(G), d(u,v) = 1} \frac{|d(u) - d(v)|}{2} \\ &= irr_t(G) - \frac{1}{2}irr(G). \end{split}$$

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

$$\begin{split} HA(\overline{G}) &= \sum_{\{u',v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{d(u',v')} \\ &\geq \sum_{\{u',v'\} \subseteq V(\overline{G})} \frac{|d(u') - d(v')|}{D(\overline{G})} \\ &\geq \sum_{\{u,v\} \subseteq V(G)} \frac{|n - 1 - d(u) - (n - 1 - d(v))|}{3} \\ &= \frac{1}{3} \sum_{\{u,v\} \subseteq V(G)} |d(u) - d(v)| \\ &= \frac{1}{3} \operatorname{irr}_{t}(G). \end{split}$$

If $D(G) \ge 4$, 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 $n_1 \ge n_2 \ge 2$. Then

$$HA(G_1 \lor G_2) \leq \frac{1}{2} [irr_t(G_1) + irr_t(G_2)] + \frac{1}{2} [irr(G_1) + irr(G_2)] + n_1 n_2 \max\{|n_2 - n_1 + \Delta(G_1) - \delta(G_2)|, |n_2 - n_1 - \Delta(G_2) + \delta(G_1)|\}$$

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

$$\begin{split} HA(G_1 \lor G_2) &= \sum_{\{u,v\} \subseteq V(G_1 \lor G_2)} \frac{|d_{G_1 \lor G_2}(u) - d_{G_1 \lor G_2}(v)|}{d_{G_1 \lor G_2}(u,v)} \\ &= \sum_{uv \in E(G_1)} |d(u) - d(v)| + \sum_{uv \in E(G_2)} |d(u) - d(v)| \\ &+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} |(n_2 - d(v)) - (n_1 - d(u))| \\ &+ \sum_{u \in V(G_1)} \frac{|d(u) - d(v)|}{2} + \sum_{\{u,v\} \subseteq V(G_2)} \frac{|d(u) - d(v)|}{2} \\ &= irr(G_1) + irr(G_2) + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} |(n_2 - d(v)) - (n_1 - d(u))| \\ &+ \frac{1}{2} [irr_t(G_1) - irr(G_1)] + \frac{1}{2} [irr_t(G_2) - irr(G_2)] \\ &= \frac{1}{2} [irr_t(G_1) + irr_t(G_2)] + \frac{1}{2} [irr(G_1) + irr(G_2)] \\ &+ \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} |(n_2 - d(v)) - (n_1 - d(u))| \\ &\leq \frac{1}{2} [irr_t(G_1) + irr_t(G_2)] + \frac{1}{2} [irr(G_1) + irr(G_2)] \\ &+ n_1 n_2 \max\{|n_2 - n_1 + \Delta(G_1) - \delta(G_2)|, |n_2 - n_1 + \delta(G_1) - \Delta(G_2)|\}. \end{split}$$

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

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

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 $u_i \in V(G_1)$ $(1 \le i \le n_1)$ and $v_j \in V(G_2)$ $(1 \le j \le n_2)$. 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 $v_k v_l \in E(G_2)$, $d_{G_1[G_2]}((u_i, v_k), (u_j, v_l)) = 2$ otherwise. Thus

$$\begin{split} HA(G_{1}[G_{2}]) &= \frac{1}{2} \sum_{\substack{(u_{i},v_{k}) \in V(G_{1}[G_{2}])\\(u_{j},v_{l}) \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_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{d((u_{i},v_{k}),(u_{j},v_{l}))} \\ &= \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\v_{k} = v_{l}}} \frac{n_{2}|d(u_{i}) - d(u_{j})|}{d(u_{i},u_{j})} + \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} = u_{j},v_{k}v_{l} \in E(G_{2})}} |d(v_{k}) - d(v_{l})| \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j}))|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in V(G_{2})\\u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{l} \in E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{k} \in E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})) + d(v_{k}) - d(v_{l})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{k} \in E(G_{2})}} \frac{|n_{2}(d(u_{i}) - d(u_{j})|}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{k} \in E(G_{2})}} \frac{|n_{2}(u_{i}) + u_{i},v_{k} \in E(G_{2})}}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{k} \in E(G_{2})}} \frac{|n_{2}(u_{i}) + u_{i},v_{k} \in E(G_{2})}}{2} \\ &+ \frac{1}{2} \sum_{\substack{u_{i},u_{j} \in V(G_{1})\\v_{k},v_{k} \in E(G$$

$$\leq n_{2}^{3}HA(G_{1}) + \frac{1}{2}n_{1}^{2}irr(G_{2}) + \frac{1}{4} \sum_{\substack{u_{i},u_{j} \in V(G_{1}) \\ v_{k},v_{l} \in V(G_{2}) \\ u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} n_{2}|d(u_{i}) - d(u_{j})|$$

$$+ \frac{1}{4} \sum_{\substack{u_{i},u_{j} \in V(G_{1}) \\ v_{k},v_{l} \in V(G_{2}) \\ u_{i} \neq u_{j},v_{k} \neq v_{l},v_{k}v_{l} \notin E(G_{2})}} |d(v_{k}) - d(v_{l})|$$

$$= n_{2}^{3}HA(G_{1}) + \frac{1}{2}n_{1}^{2}irr(G_{2}) + \frac{1}{4}n_{2} \left[\binom{n_{2}}{2} - m_{2} \right] irr_{t}(G_{1})$$

$$+ \frac{1}{4} \binom{n_{1}}{2} [irr_{t}(G_{2}) - irr(G_{2})]$$

$$= n_{2}^{3}HA(G_{1}) + \frac{n_{2}}{4} \left[\frac{n_{2}(n_{2} - 1)}{2} - m_{2} \right] irr_{t}(G_{1}) + \frac{n_{1}(n_{1} - 1)}{8}irr_{t}(G_{2})$$

$$+ \frac{3n_{1}^{2} + n_{1}}{8}irr(G_{2}).$$

4. The Harary-Albertson index of trees

Theorem 4.1. Let T_n be a tree with *n* vertices. Then

$$2\left(1 + \frac{1}{2} + \dots + \frac{1}{n-2}\right) \le HA(T_n) \le (n-1)(n-2),$$

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

$$HA(T_n) \le irr_t(T_n) \le irr_t(S_n) = (n-1)(n-2)$$

with equality if and only if $T_n = S_n$.

If the maximum degree $\Delta(T_n) \ge 3$, then the number of pendant vertices $p \ge 3$. Let v_1, v_2, \ldots, v_n 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

$$HA(T_n) > p + \sum_{i=1}^{p} \sum_{j=p+1}^{n} \frac{d(v_j) - 1}{d(v_i, v_j)}$$

> $2\left(1 + \frac{1}{2} + \dots + \frac{1}{n-2}\right)$
= $HA(P_n).$

Thus, $HA(T_n) \ge HA(P_n)$ 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.

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