Hyper-Zagreb indices of graphs and its applications

Girish V. Rajasekharaiah, Usha P. Murthy

Abstract: The first and second Hyper-Zagreb index of a connected graph $G$ is defined by $HM_1(G) = \sum_{uv \in E(G)}[d(u) + d(v)]^2$ and $HM_2(G) = \sum_{uv \in E(G)}[d(u),d(v)]^2$. In this paper, the first and second Hyper-Zagreb indices of certain graphs are computed. Also the bounds for the first and second Hyper-Zagreb indices are determined. Further linear regression analysis of the degree based indices with the boiling points of benzenoid hydrocarbons is carried out. The linear model, based on the Hyper-Zagreb index, is better than the models corresponding to the other distance based indices.

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1. Introduction

In theoretical chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modeled by a graph taking vertices as atoms and edges as covalent bonds. The properties of these graph-theoretic models can be used in the study of quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) of molecules by obtaining numerical graph invariants. Many such graph invariant indices have been studied. The oldest well known parameter is the Wiener index introduced by Harold Wiener in 1947, to study the chemical properties of paraffins [32].

For a graph theoretic terminology, we refer the books [3, 16]. Let $G$ be a connected graph of order $n$ and size $m$. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of $G$. The edge joining the vertices $u$ and $v$ is denoted by $uv$. The degree of a vertex $u$ is the number of edges incident to it and is denoted by $d(u)$. As usual $P_n, K_{1,n-1}, C_n, K_n$, and $W_n$ denote path, star, cycle, complete graph and wheel graph on $n$ vertices and $F_n$ be the friendship graph with $n$ blocks, respectively.

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The Cartesian product \(G \square H\) of two graphs \(G\) and \(H\) is the graph with vertex set \(V(G) \times V(H)\) and edge set contains the edge \((u, v)(u', v')\) if and only if \(u = u'\) and \(v \neq v'\) or \(v = v'\) and \(u \neq u'\). The Wiener index \(W(G)\) of a connected graph \(G\) is defined as the sum of the distances between all pairs of vertices of \(G\) [32]. That is, \(W = \sum_{u, v \in V(G)} d(u, v)\), where \(d(u, v)\) is the shortest distance between \(u\) and \(v\). The Wiener index is also called as gross status [15] and total status [3]. For more about the Wiener index one can refer [4, 7, 14, 24–26, 31].

The first and second Zagreb indices of a graph \(G\) are defined as [13],
\[
M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} [d(u) \cdot d(v)]
\]

The Zagreb indices were used in the structure property model [12, 29]. Recent results on the Zagreb indices can be found in [5, 10, 11, 19, 22, 33]. The eccentric connectivity indices can be found in [1, 30].

Details on mathematical properties and chemical applications of eccentric connectivity indices can be found in [2, 6, 8, 9, 17, 18, 20, 21, 28, 34].

The eccentric connectivity indices of a connected graph \(G\) are defined as [1, 30]
\[
\xi_1(G) = \sum_{uv \in E(G)} [e(u) + e(v)] \quad \text{and} \quad \xi_2(G) = \sum_{uv \in E(G)} [e(u) \cdot e(v)].
\]

The first status connectivity index \(S_1(G)\) and second status connectivity index \(S_2(G)\) [27] of a connected graph \(G\) is defined as:
\[
S_1(G) = \sum_{uv \in E(G)} [\sigma(u) + \sigma(v)] \quad \text{and} \quad S_2(G) = \sum_{uv \in E(G)} [\sigma(u) \cdot \sigma(v)], \quad \text{where} \quad \sigma(u) = \sum_{uv \in E(G)} d(u, v).
\]

Harishchandra S. Ramane and Ashwini S. Yalnaik [27] had applied linear regression analysis of the distance based indices with the boiling points of benzenoid hydrocarbons and they have shown that it is better than any other distance based indices. Motivated by this, we applied linear regression analysis of the degree based indices with the boiling points of benzenoid hydrocarbons.

The first and second Hyper-Zagreb index of a connected graph \(G\) [19] is defined by
\[
HM_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2 \quad \text{and} \quad HM_2(G) = \sum_{uv \in E(G)} [d(u) \cdot d(v)]^2.
\]

In this paper, the first and second Hyper-Zagreb indices of certain graphs are computed. Also the bounds for the first and second Hyper-Zagreb indices are determined. Further linear regression analysis of the degree based indices with the boiling points of benzenoid hydrocarbons is carried out. The linear model, based on the Hyper-Zagreb index, is better than the models corresponding to the other distance based indices.

2. Computation of first and second Hyper-Zagreb indices of standard graphs

(i) For any path \(P_n\) with \(n\) vertices,
\[
HM_1(P_n) = \begin{cases} 
\frac{4}{16p + 2} & n = 2 \\
\frac{1}{16p - 8} & n = p + 2, p \geq 1 
\end{cases}
\]
\[
HM_2(P_n) = \begin{cases} 
1 & n = 2 \\
\frac{1}{16p - 8} & n = p + 2, p \geq 1 
\end{cases}
\]
(ii) For any cycle \( C_n \),
\[ HM_1(C_n) = 16n = HM_2(C_n). \]

(iii) For any star graph \( K_{1,n-1} \),
\[ HM_1(K_{1,n-1}) = n^2(n-1) \]
\[ HM_2(K_{1,n-1}) = (n-1)^3. \]

(iv) For any complete graph \( K_n \),
\[ HM_1(K_n) = 2n(n-1)^3 \]
\[ HM_2(K_n) = \frac{n(n-1)^4}{2}. \]

(v) For any wheel graph \( W_n \),
\[ HM_1(W_n) = (n-1)[(n+2)^2 + 6^2] \]
\[ HM_2(W_n) = 9(n-1)[(n-1)^2 + 3^2]. \]

(vi) For any friendship graph \( F_n \) with \( n \) blocks,
\[ HM_1(F_n) = 8n^3 + 16n^2 + 24n. \]
\[ HM_2(F_n) = 32n^3 + 16n. \]

3. Bounds for first and second Hyper-Zagreb indices

**Theorem 3.1.** Let \( G \) be the connected graph with \( n \) vertices and \( m \) edges, then
\[ 4m \leq HM_1(G) \leq 4m(n-1)^2. \]

Equality holds for \( K_2 \).

**Proof.** For the lower bound, since for the connected graph \( G \), the degree of each vertex is greater than or equal 1. Hence
\[ HM_1(G) \geq \sum_{uv \in E(G)} [d(u) + d(v)]^2 \]
\[ = \sum_{uv \in E(G)} [1 + 1]^2 \]
\[ = \sum_{uv \in E(G)} 4 = 4m. \]

For the upper bound, since for the connected graph \( G \), the degree of each of vertex is less than or
equal to $n - 1$. Hence

\[ HM_1(G) \leq \sum_{uv \in E(G)} [d(u) + d(v)]^2 \]
\[ = \sum_{uv \in E(G)} [n - 1 + n - 1]^2 \]
\[ = \sum_{uv \in E(G)} 4(n - 1)^2 \]
\[ = 4m(n - 1)^2. \]

Equality: For $K_2$, $m = 1$, $n = 2$, the result follows from 2(i) and 2(iv).

**Theorem 3.2.** Let $G$ be the connected graph with $n$ vertices and $m$ edges, then

\[ m \leq HM_2(G) \leq m(n - 1)^4. \]

Equality holds for $K_2$.

**Proof.** For the lower bound, since for the connected graph $G$, the degree of each vertex is greater than or equal 1. Hence

\[ HM_1(G) \geq \sum_{uv \in E(G)} [d(u)d(v)]^2 \]
\[ = \sum_{uv \in E(G)} [1]^2 \]
\[ = \sum_{uv \in E(G)} 1 \]
\[ = m. \]

For the upper bound, since for the connected graph $G$, the degree of each of vertex is less than or equal to $n - 1$. Hence

\[ HM_1(G) \leq \sum_{uv \in E(G)} [d(u) + d(v)]^2 \]
\[ = \sum_{uv \in E(G)} [(n - 1)(n - 1)]^2 \]
\[ = \sum_{uv \in E(G)} (n - 1)^4 \]
\[ = m(n - 1)^4. \]

Equality: For $K_2$, $m = 1$, $n = 2$, the result follows from 2(i) and 2(iv).

**Corollary 3.3.** Let $G$ be a connected graph with $n$ vertices, the

\[ 2n \leq HM_1(G) \leq 2n(n - 1)^3 \]
\[ n - 1 \leq HM_2(G) \leq \frac{n(n - 1)^5}{2}. \]

**Theorem 3.4.** For the connected graph $G = P_m \square P_n$, $m, n \geq 3$,

\[ HM_1(G) = 128mn - 150(m + n) + 144 \]
\[ HM_2(G) = 512mn - 830(m + n) + 1236. \]
Theorem 3.5. For the connected graph \( G = C_m \square P_n, m, n \geq 3, \)

\[
HM_1(G) = 128mn - 150(m + n) + 144.
\]

\[
HM_2(G) = 512mn - 830(m + n) + 1236.
\]

Proof. Let \( V(G) = \{(u_i, v_j) : i = 1, 2, 3, \ldots, n\} \) and \( E(G) = A \cup B \cup C \cup D, \) where \( A = \{(u_i, v_j)(u_i, v_k) : (u_i, v_j), (u_i, v_k) \in V(G), d((u_i, v_j)) = 2, d((u_i, v_k)) = 3\} \) with \( |A| = 8, \)

\( B = \{(u_i, v_j)(u_i, v_k) : (u_i, v_j), (u_i, v_k) \in V(G), d((u_i, v_j)) = 3, d((u_i, v_k)) = 3\} \) with \( |B| = 2\left[(m - 3) + (n - 3)\right], \)

\( C = \{(u_i, v_j)(u_i, v_k) : (u_i, v_j), (u_i, v_k) \in V(G), d((u_i, v_j)) = 3, d((u_i, v_k)) = 4\} \) with \( |C| = 2\left[(m - 2) + (n - 2)\right], \)

\( D = \{(u_i, v_j)(u_i, v_k) : (u_i, v_j), (u_i, v_k) \in V(G), d((u_i, v_j)) = 4, d((u_i, v_k)) = 4\} \) with \( |D| = (m - 3)(n - 2) + (n - 3)(m - 2) \) such that \( |A| + |B| + |C| + |D| = |E(G)| = n(m - 1) + (n - 1)m. \)

Case 1: The first Hyper-Zagreb index is

\[
HM_1(G) = \sum_{(u_i, v_j)(u_i, v_k) \in E(G)}[d((u_i, v_j)) + d((u_i, v_k))]^2.
\]

\[
= \sum_{(u_i, v_j)(u_i, v_k) \in A}[d((u_i, v_j)) + d((u_i, v_k))]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in B}[d((u_i, v_j)) + d((u_i, v_k))]^2 +
\]

\[
\sum_{(u_i, v_j)(u_i, v_k) \in C}[d((u_i, v_j)) + d((u_i, v_k))]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in D}[d((u_i, v_j)) + d((u_i, v_k))]^2.
\]

\[
= \sum_{(u_i, v_j)(u_i, v_k) \in A}[2 + 3]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in B}[3 + 3]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in C}[3 + 4]^2 +
\]

\[
\sum_{(u_i, v_j)(u_i, v_k) \in D}[4 + 4]^2.
\]

\[
= 8.5^2 + 2\left[(m - 3) + (n - 3)\right], 6^2 + 2\left[(m - 2) + (n - 2)\right], 7^2
\]

\[
+ [m - 3](n - 2) + (n - 3)(m - 2)], 8^2.
\]

\[
= 128mn - 150(m + n) + 144.
\]

Case 2: The second Hyper-Zagreb index is

\[
HM_2(G) = \sum_{(u_i, v_j)(u_i, v_k) \in E(G)}[d((u_i, v_j)).d((u_i, v_k))]^2.
\]

\[
= \sum_{(u_i, v_j)(u_i, v_k) \in A}[d((u_i, v_j)).d((u_i, v_k))]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in B}[d((u_i, v_j)).d((u_i, v_k))]^2 +
\]

\[
\sum_{(u_i, v_j)(u_i, v_k) \in C}[d((u_i, v_j)).d((u_i, v_k))]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in D}[d((u_i, v_j)).d((u_i, v_k))]^2.
\]

\[
= \sum_{(u_i, v_j)(u_i, v_k) \in A}[2.3]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in B}[3.3]^2 + \sum_{(u_i, v_j)(u_i, v_k) \in C}[3.4]^2 +
\]

\[
\sum_{(u_i, v_j)(u_i, v_k) \in D}[4.4]^2.
\]

\[
= 8.6^2 + 2\left[(m - 3) + (n - 3)\right], 9^2 + 2\left[(m - 2) + (n - 2)\right], 12^2
\]

\[
+ [m - 3](n - 2) + (n - 3)(m - 2)], 16^2.
\]

\[
= 512mn - 830(m + n) + 1236.
\]
Proof. Let $V(G) = \{(u_i, v_j), j = 1, 2, 3, \ldots, n\}_{i=1}^m$ and $E(G) = A \cup B \cup C$, where $A = \{(u_i, v_j)(u_r, v_s)\}/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 3, d((u_r, v_s)) = 3\}$ with $|A| = 2(m - 1) + 2$, $B = \{(u_i, v_j)(u_r, v_s)\}/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 3, d((u_r, v_s)) = 4\}$ with $|B| = 2m$, $C = \{(u_i, v_j)(u_r, v_s)\}/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 4$ with $|C| = [(m - 1)(n - 2) + m(n - 3) + (n - 2)]$ such that $|A| + |B| + |C| = |E(G)| = n(m - 1) + (n - 1)m + n$.

Case 1: The first Hyper-Zagreb index is

$$HM_1(G) = \sum_{(u_i, v_j)(u_r, v_s) \in E(G)}[d((u_i, v_j)) + d((u_r, v_s))]^2.$$ 

$$= \sum_{(u_i, v_j)(u_r, v_s) \in A}[d((u_i, v_j)) + d((u_r, v_s))]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in B}[d((u_i, v_j)) + d((u_r, v_s))]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in C}[d((u_i, v_j)) + d((u_r, v_s))]^2.$$

$$= \sum_{(u_i, v_j)(u_r, v_s) \in A}[3 + 3]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in B}[3 + 4]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in C}[4 + 4]^2$$

$$= [2(m - 1) + 2].6^2 + 2m.7^2 + [(m - 1)(n - 2) + m(n - 3) + (n - 2)].8^2$$

$$= 128mn - 150m.$$ 

Case 2: The second Hyper-Zagreb index is

$$HM_2(G) = \sum_{(u_i, v_j)(u_r, v_s) \in E(G)}[d((u_i, v_j)).d((u_r, v_s))]^2.$$ 

$$= \sum_{(u_i, v_j)(u_r, v_s) \in A}[d((u_i, v_j)).d((u_r, v_s))]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in B}[d((u_i, v_j)).d((u_r, v_s))]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in C}[d((u_i, v_j)).d((u_r, v_s))]^2.$$

$$= \sum_{(u_i, v_j)(u_r, v_s) \in A}[3.3]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in B}[3.4]^2 + \sum_{(u_i, v_j)(u_r, v_s) \in C}[4.4]^2 +$$

$$= [2(m - 1) + 2].9^2 + 2m.12^2 + [(m - 1)(n - 2) + m(n - 3) + (n - 2)].16^2$$

$$= 512mn - 830m.$$ 

\[\square\]

Theorem 3.6. For the connected graph $G = C_n \square C_n$,

$$HM_1(G) = 192mn - 64(m + n)$$

$$HM_2(G) = 768mn - 256(m + n).$$ 

Proof. Let $V(G) = \{(u_i, v_j), j = 1, 2, 3, \ldots, n\}_{i=1}^m$. For the graph $G = C_n \square C_n$, the degree of each vertex is 4.
Case 1: The first Hyper-Zagreb index is

\[ HM_1(G) = \sum_{(u_i, v_j) \in E(G)} [d((u_i, v_j)) + d((u_r, v_s))]^2 \]
\[ = \sum_{(u_i, v_j) \in E(G)} [4 + 4]^2 \]
\[ = [(m - 1)n + m(n - 1) + mn]^2 = 192mn - 64(m + n). \]

Case 2: The second Hyper-Zagreb index is

\[ HM_2(G) = \sum_{(u_i, v_j) \in E(G)} [d((u_i, v_j)) + d((u_r, v_s))]^2 \]
\[ = \sum_{(u_i, v_j) \in E(G)} [4 + 4]^2 \]
\[ = [(m - 1)n + m(n - 1) + mn]^2 = 768mn - 256(m + n). \]

4. Regression model for boiling point

Here we investigate the correlation between the boiling point (BP) of benzenoid hydrocarbons and the distance based indices of the corresponding molecular graphs. Experimental values of boiling points of benzenoid hydrocarbons represented in Fig. 1 are taken from [23]. The scatter plot between BP and indices \( HM_1(G), HM_2(G), S_1, S_2, \xi_1, \xi_2 \) and \( W \) are shown in Figs. 2, 3, 4, 5, 6, 7 and 8.

Figure 1. Molecular graphs of benzenoid hydrocarbons under consideration
Figure 2. Scatter plot between the boiling point (BP) and the first Hyper-Zagreb index ($HM_1$)

\[ y = (98.9280298522226) + (0.66203123472854) \cdot BM_1 \]
\[ R^2 = 0.9485 \]

Figure 3. Scatter plot between the boiling point (BP) and the second Hyper-Zagreb index ($HM_2$)

\[ y = (172.88938904261) + (0.32525619117685) \cdot BM_2 \]
\[ R^2 = 0.8945 \]
Figure 4. Scatter plot between the boiling point (BP) and the first status connectivity index ($S_1$)

Figure 5. Scatter plot between the boiling point (BP) and the second status connectivity index ($S_2$)
Figure 6. Scatter plot between the boiling point (BP) and the first eccentricity index ($S_2$)

Figure 7. Scatter plot between the boiling point (BP) and the second eccentricity index ($S_2$)
The linear regression models for the boiling point (BP) using the data of Table 1 are obtained using the least square fitting procedure as implemented in NCSS Statistics programme.

In Table 2, the model (1), shows that the correlation of the experimental boiling point of benzenoid hydrocarbons with first hyper zagreb index is better \( R = 0.974 \) than the correlation with other distance based indices considered in this paper. The linear model (2) is also good \( R = 0.945 \) compared to the models (4), (5), (6) and (7).

5. Conclusion

For the degree based topological indices namely first and second Hyper-Zagreb index of graphs, we computed these indices for some specific graphs. Also the bounds for these indices are reported. Further a regression analysis of the boiling points of benzenoid hydrocarbons with the degree based indices have been carried out and compared the linear models. The linear model obtained, based on the status index, is better than the corresponding model based on the other distance indices. Among the distance based topological indices considered in this paper, the first Hyper-Zagreb index has good correlation with the boiling point of benzenoid hydrocarbons.
### Table 1. The values of experimental boiling points, degree and distance based indices of 21 benzenoid hydrocarbons

| Benzenoid hydrocarbon | BP (°C) | RM$_1$ | RM$_2$ | $s_1$ | $s_2$ | $s_1'$ | $s_2'$ | $w$   |
|-----------------------|---------|--------|--------|--------|--------|--------|--------|-------|
| 1                     | 218     | 2323   | 321    | 470    | 5067   | 89     | 192    | 109   |
| 2                     | 338     | 359    | 526    | 1208   | 23176  | 120    | 459    | 271   |
| 3                     | 340     | 368    | 546    | 1248   | 24784  | 180    | 516    | 279   |
| 4                     | 441     | 486    | 731    | 2482   | 75085  | 280    | 959    | 545   |
| 5                     | 425     | 495    | 751    | 2522   | 77477  | 284    | 983    | 553   |
| 6                     | 429     | 510    | 846    | 2322   | 65471  | 246    | 729    | 513   |
| 7                     | 440     | 504    | 771    | 2602   | 82581  | 298    | 1085   | 569   |
| 8                     | 496     | 592    | 945    | 3182   | 67676  | 318    | 1096   | 680   |
| 9                     | 493     | 616    | 1064   | 3040   | 97776  | 286    | 862    | 652   |
| 10                    | 491     | 616    | 1064   | 3052   | 98416  | 286    | 862    | 654   |
| 11                    | 547     | 684    | 1176   | 4016   | 152039 | 356    | 1201   | 839   |
| 12                    | 542     | 722    | 1282   | 3894   | 142365 | 326    | 990    | 815   |
| 13                    | 535     | 621    | 1035   | 4172   | 171570 | 370    | 1344   | 907   |
| 14                    | 536     | 608    | 965    | 4492   | 199410 | 424    | 1780   | 971   |
| 15                    | 531     | 644    | 1046   | 4412   | 161586 | 402    | 1584   | 955   |
| 16                    | 519     | 610    | 990    | 4452   | 196234 | 424    | 1780   | 963   |
| 17                    | 590     | 828    | 1500   | 4884   | 201032 | 366    | 1128   | 1002  |
| 18                    | 592     | 707    | 1188   | 5082   | 227848 | 398    | 1484   | 1082  |
| 19                    | 596     | 752    | 1289   | 5384   | 257084 | 466    | 1926   | 1142  |
| 20                    | 594     | 741    | 1244   | 5384   | 257148 | 466    | 1927   | 1142  |
| 21                    | 595     | 707    | 1188   | 5002   | 210223 | 392    | 1349   | 595   |

### Table 2. Correlation coefficient and standard error of the estimation

| Index | Correlation coefficient ($R$) with boiling point | Standard error of the estimate |
|-------|-----------------------------------------------|-------------------------------|
| RM$_1$| 0.974                                        | 23.2112                       |
| RM$_2$| 0.9458                                       | 33.2095                       |
| $s_1$ | 0.968                                        | 25.73552                      |
| $s_2$ | 0.9001                                       | 44.54677                      |
| $s'_1$| 0.928                                        | 38.00616                      |
| $s'_2$| 0.827                                        | 57.364                        |
| $w$   | 0.9043                                       | 43.646                        |

\[
BP = 98.928 + 0.662 \text{RM}_1, \quad \text{(1)}
\]
\[
BP = 172.8894 + 0.3253 \text{RM}_2, \quad \text{(2)}
\]
\[
BP = 256.4283 + 0.0669 \text{RM}_1 + 0.0669 \text{RM}_2, \quad \text{(3)}
\]
\[
BP = 337.65 + 0.0011 \text{RM}_1 + 0.0011 \text{RM}_2, \quad \text{(4)}
\]
\[
BP = 200.68 + 0.8980 \text{s}_1, \quad \text{(5)}
\]
\[
BP = 291.54 + 0.172 \text{s}'_1, \quad \text{(6)}
\]
\[
BP = 267.003 + 0.3071w, \quad \text{(7)}
\]
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