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Hyper-Zagreb indices of graphs and its applications

Research Article

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.

Girish V. Rajasekharaiah (Corresponding Author); Department of Science and Humanities, PES University(EC Campus), Electronic City, Bengaluru, Karnataka, India (email: girishvr1@pes.edu, giridsi63@gmail.com).
Usha P. Murthy; Department of Mathematics, Siddaganga Institute of Technology, B.H. Road, Tumakuru, Karnataka, India (email: ushapmurhty@yahoo.com).

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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 and $v^{'}$ are adjacent in H or $v = v^{'}$ and u and $u^{'}$ are adjacent in G.

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, $W = \sum_{u,v \in V(G)} d(u,v), d(u,v)$ 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],

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)] \text{ and } M_2(G) = \sum_{uv \in E(G)} [d(u).d(v)]$$

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 of a connected graph G are defined as [1, 30]

$$\xi_1(G) = \sum_{uv \in E(G)} [e(u) + e(v)] \text{ and } \xi_2(G) = \sum_{uv \in E(G)} [e(u).e(v)].$$

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 first status connectivity index $S_1(G)$ and second status connectivity index $S_2(G)$ [27] of a connected graph G is defined as:

$$S_1(G) = \sum_{uv \in E(G)} [\sigma(u) + \sigma(v)] \text{ and } S_2(G) = \sum_{uv \in E(G)} [\sigma(u).\sigma(v)], \text{ where } \sigma(u) = \sum_{uv \in E(G)} d(u,v).$$

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

$$HM_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2 \text{ and } HM_2(G) = \sum_{uv \in E(G)} [d(u).d(v)]^2.$$

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.

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

(i) For any path P_n with n vertices,

$$HM_1(P_n) = \begin{cases} 4 & n = 2 \\ 16p + 2 & n = p + 2,\, p \geq 1 \end{cases}$$

$$HM_2(P_n) = \begin{cases} 1 & n = 2 \\ 16p - 8 & n = p + 2,\, p \geq 1 \end{cases}$$

(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,

$$HM_1(K_n) = 2n(n-1)^3$$

$$HM_2(K_n) = \frac{n(n-1)^5}{2}.$$

(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

$$\begin{aligned} HM_1(G) &\geq \sum_{uv \in E(G)} [d(u) + d(v)]^2 \\ &= \sum_{uv \in E(G)} [1+1]^2 \\ &= \sum_{uv \in E(G)} 4 = 4m. \end{aligned}$$

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

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

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

$$\begin{aligned} HM_1(G) &\geq \sum_{uv\in E(G)} [d(u).d(v)]^2 \\ &= \sum_{uv\in E(G)} [1.1]^2 \\ &= \sum_{uv\in E(G)} 1 \\ &= m. \end{aligned}$$

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

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

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 $G = P_m \square P_n, m, n \geq 3$,*

$$HM_1(G) = 128mn - 150(m+n) + 144$$

$$HM_2(G) = 512mn - 830(m+n) + 1236.$$

Proof. Let $V(G) = \{(u_i, v_j), j = 1, 2, 3, \ldots, n\}_{i=1}^{i=m}$ and $E(G) = A \cup B \cup C \cup D$, where $A = \{((u_i, v_j)(u_r, v_s))/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 2, d((u_r, v_s)) = 3\}$ with $|A| = 8$, $B = \{((u_i, v_j)(u_r, v_s))/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 3, d((u_r, v_s)) = 3\}$ with $|B| = 2[(m-3)+(n-3)]$, $C = \{((u_i, v_j)(u_r, v_s))/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 3, d((u_r, v_s)) = 4\}$ with $|C| = 2[(m-2)+(n-2)]$, $D = \{((u_i, v_j)(u_r, v_s))/(u_i, v_j), (u_r, v_s) \in V(G), d((u_i, v_j)) = 4, d((u_r, v_s)) = 4\}$ 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

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

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

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

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

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

$$= 8.5^2 + 2[(m-3) + (n-3)].6^2 + 2[(m-2) + (n-2)].7^2$$

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

$$= 128mn - 150(m + n) + 144.$$

Case 2: The second Hyper-Zagreb index is

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

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

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

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

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

$$= 8.6^2 + 2[(m-3) + (n-3)].9^2 + 2[(m-2) + (n-2)].12^2$$

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

$$= 512mn - 830(m + n) + 1236.$$ □

Theorem 3.5. *For the connected graph $G = C_m \square P_n, m, n \geq 3$,*

$$HM_1(G) = 128mn - 150m$$

$$HM_2(G) = 512mn - 830m.$$

Proof. Let $V(G) = \{(u_i, v_j), j = 1, 2, 3, \ldots, n\}_{i=1}^{i=m}$ 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

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

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

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

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

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

$$= 512mn - 830m.$$

□

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

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

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

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

Case 1: The first Hyper-Zagreb index is

$$HM_1(G) = \sum_{(u_i,v_j)(u_r,v_s)\in E(G)}[d((u_i,v_j)) + d((u_r,v_s))]^2$$
$$= \sum_{(u_i,v_j)(u_r,v_s)\in E(G)}[4+4]^2$$
$$= [(m-1)n + m(n-1) + mn]8^2 = 192mn - 64(m+n).$$

Case 2: The second Hyper-Zagreb index is

$$HM_2(G) = \sum_{(u_i,v_j)(u_r,v_s)\in E(G)}[d((u_i,v_j)) + d((u_r,v_s))]^2$$
$$= \sum_{(u_i,v_j)(u_r,v_s)\in E(G)}[4+4]^2$$
$$= [(m-1)n + m(n-1) + mn]16^2 = 768mn - 256(m+n).$$

□

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.

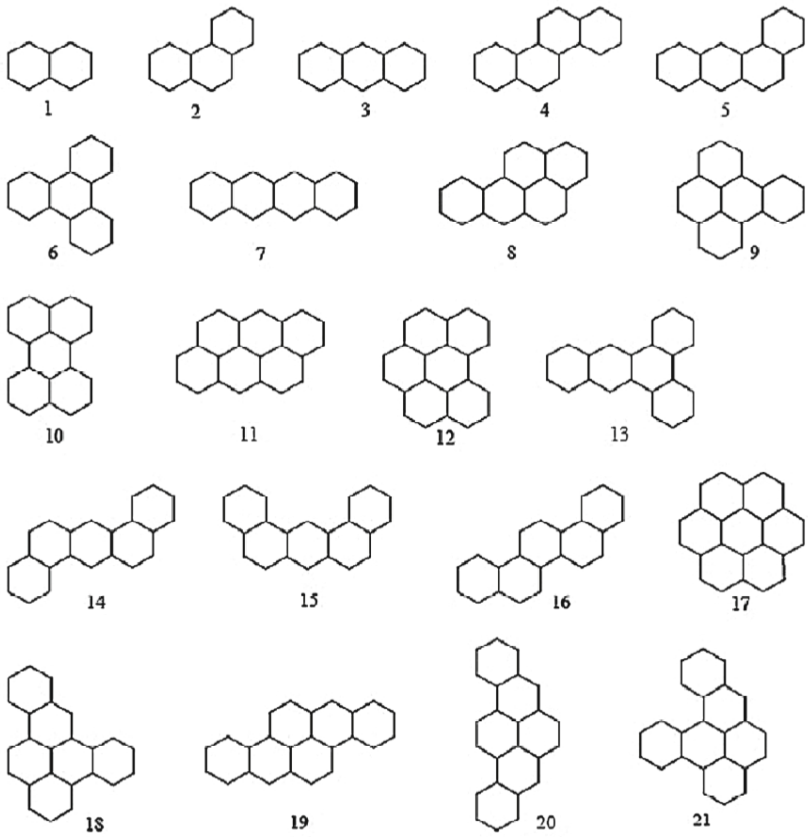

Figure 1. Molecular graphs of benzenoid hydrocarbons under consideration

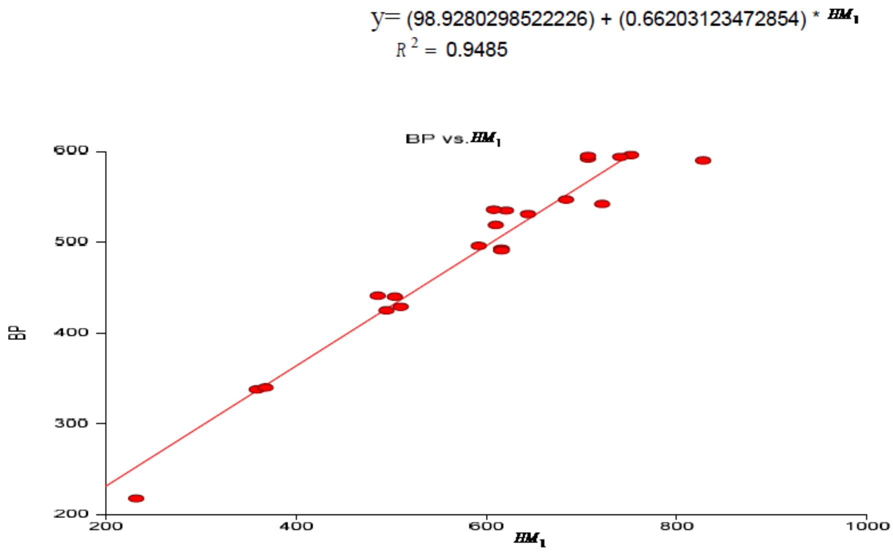

Figure 2. Scatter plot between the boiling point (BP) and the first Hyper-Zagreb index (HM_1)

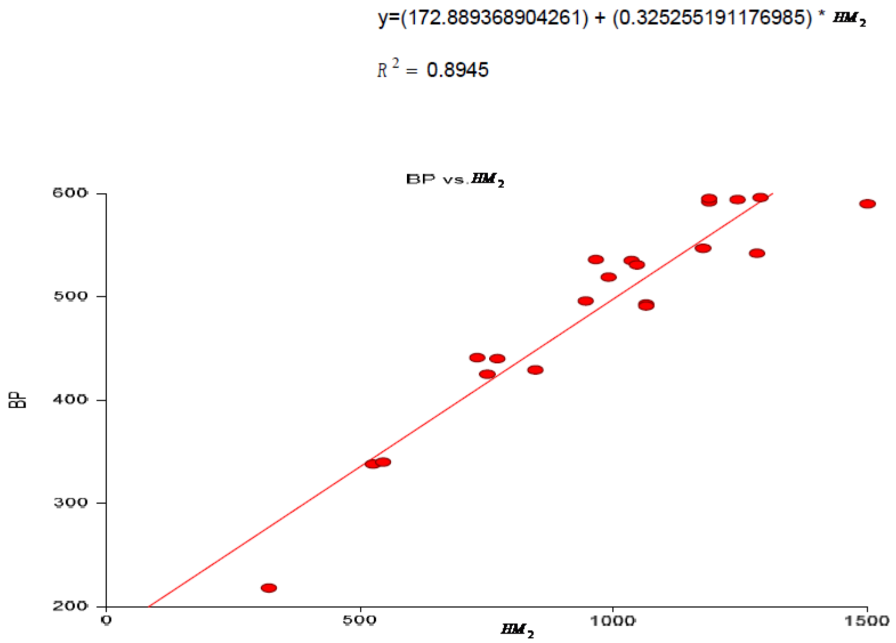

Figure 3. Scatter plot between the boiling point (BP) and the second Hyper-Zagreb index (HM_2)

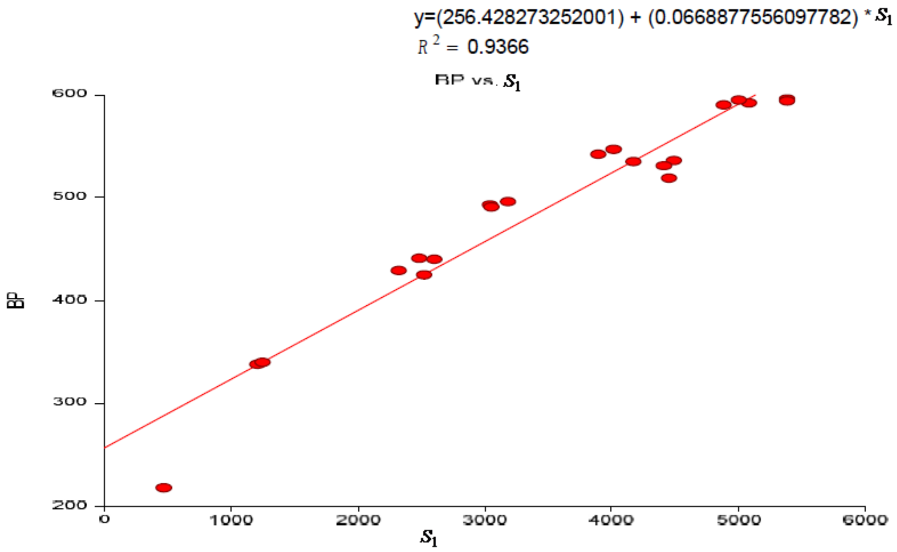

Figure 4. **Scatter plot between the boiling point (BP) and the first status connectivity index (S_1)**

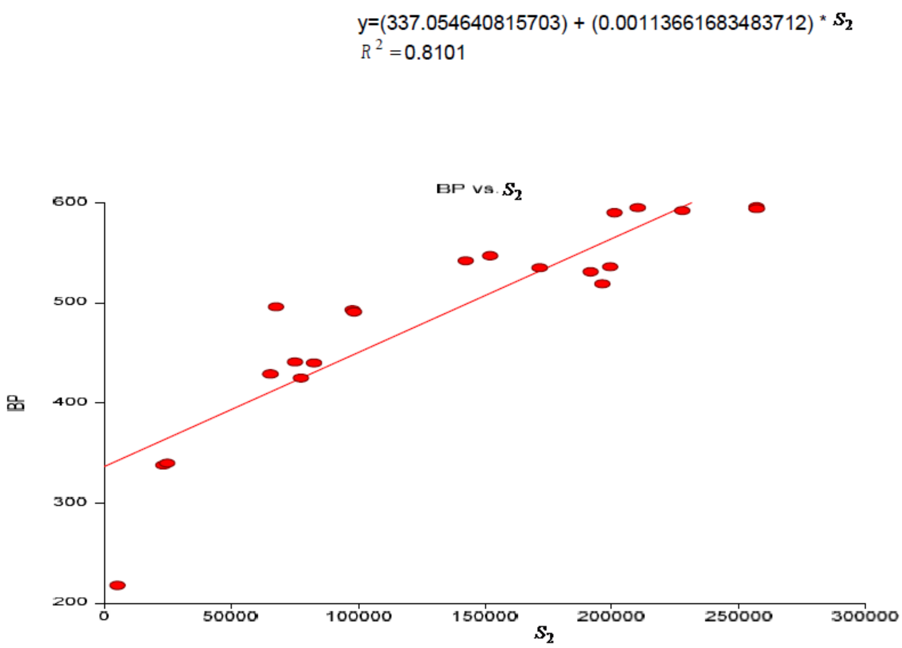

Figure 5. **Scatter plot between the boiling point (BP) and the second status connectivity index (S_2)**

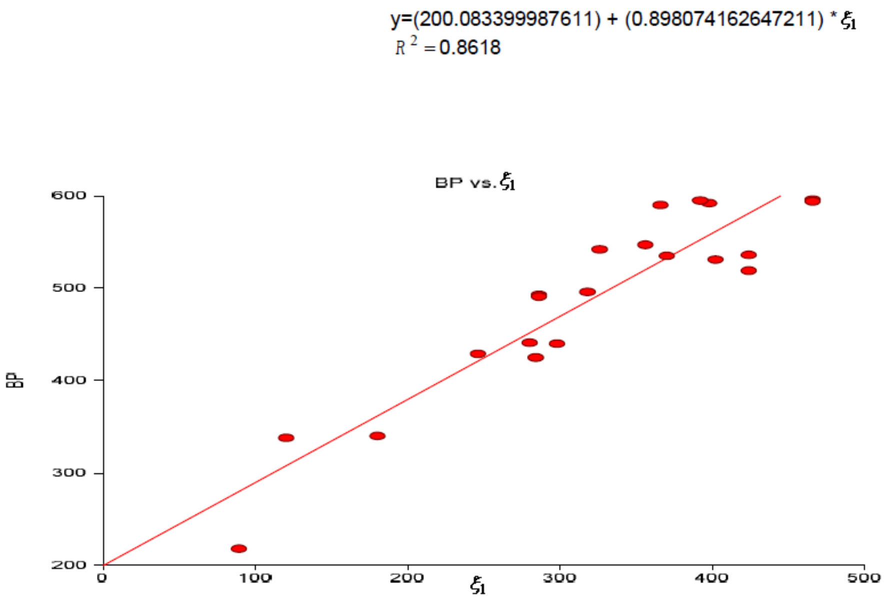

Figure 6. **Scatter plot between the boiling point (BP) and the first eccentricity index (S_2)**

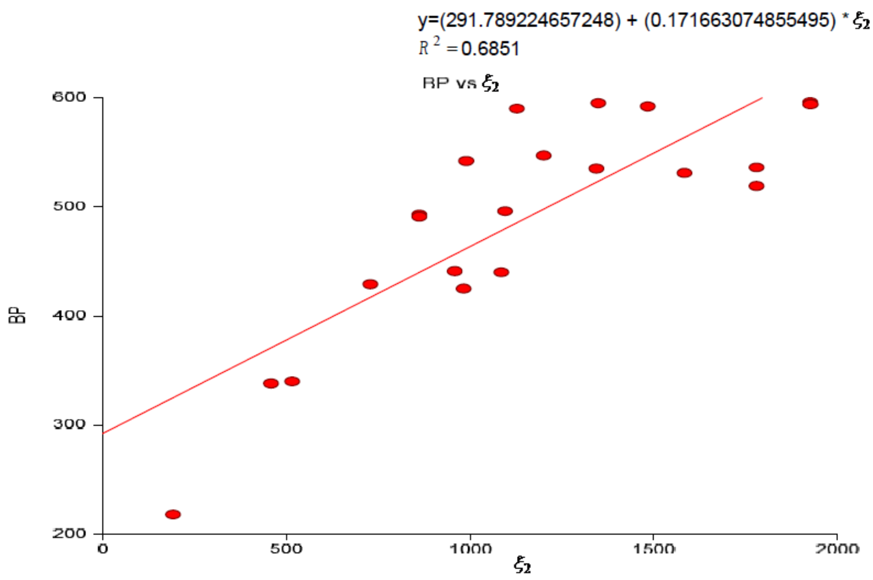

Figure 7. **Scatter plot between the boiling point (BP) and the second eccentricity index (S_2)**

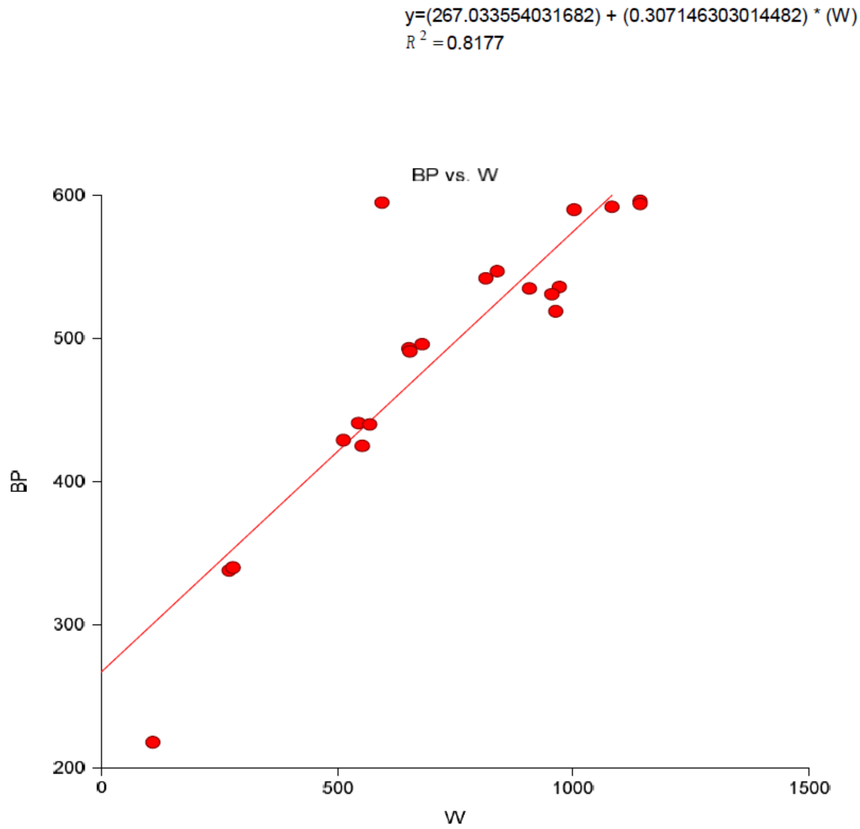

Figure 8. Scatter plot between the boiling point (BP) and index (W)

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.

Benzenoid hydrocarbon	$BP(^0C)$	HM_1	HM_2	S_1	S_2	ξ_1	ξ_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 1. **The values of experimental boiling points, degree and distance based indices of 21 benzenoid hydrocarbons**

Index	Correlation coefficient (R) with boiling point	Standard error of the estimate
HM_1	0.974	23.2112
HM_2	0.9458	33.2095
S_1	0.968	25.73552
S_2	0.9001	44.54677
ξ_1	0.928	38.00616
ξ_2	0.8277	57.364
W	0.9043	43.646

$BP = 98.928 + 0.662\ HM_1$ -----------(1)

$BP = 172.8894 + 0.3253\ HM_2$ --------(2)

$BP = 256.4283 + 0.0669\ S_1$ ------------(3)

$BP = 337.05 + 0.0011\ S_2$ ------------(4)

$BP = 200.08 + 0.8980\ \xi_1$ ---------------(5)

$BP = 291.549 + 0.172\ \xi_2$ ----------------(6)

$BP = 267.003 + 0.3071\ W$ -------------(7)

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

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