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Edge degree Zagreb indices of graphs and its Applications

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Abstract

Edge degree of a vertex u is defined as sum of degrees of edges which are incident to a vertex u in a graph G. In this article, we define the edge degree of first and second Zagreb indices of a graph G analogous to Zagreb index in terms of edge degree. Later, we obtain the edge degree of a vertex for some standard graphs such as path, regular graph, wheel graph, star graph, complete bipartite graph, ladder graph and friendship graph. Further linear regression analysis of the edge degree Zagreb indices with the boiling points of benzenoid hydrocarbons is carried out and analysed that the first edge degree Zagreb index has good correlation with the boiling point of benzenoid hydrocarbons.

Keywords: Edge degree of a vertex, first edge degree Zagreb index, second edge degree Zagreb index.

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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 modelled 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.

Let G be a simple, finite, connected graph with the vertex set $V(G)$ and edge set $E(G)$. 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 $d(u)$. If all the vertices of G have same degree equal to r, then G is called a regular graph of degree r. For graph fundamentals we refer the books[10].

Definition 1.1. The first and second Zagreb indices of a graph G are defined as [9]

$$Z_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

and

$$Z_2(G) = \sum_{uv \in E(G)} [d(u)d(v)].$$

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The Zagreb indices are established tools for structure-property modeling [8, 16] and their mathematical properties and chemical applications are well-documented in [3, 6, 7, 12, 13, 19]. Based on the extensive work already done in this area [3, 6, 7, 12, 13, 14, 19, 9, 8], We define the following for a simple, connected graph G: Edge degree of a vertex, first edge degree Zagreb index and second edge degree Zagreb index of a simple, connected graph G as follows:

Definition 1.2. The edge degree of a vertex u in a graph G is defined as

$$ed_G(u) = \sum_{\text{edge } e \text{ incident to } u} d_G(e) = \sum_{uv \in E(G)} [d_G(u) + d_G(v) - 2].$$

Definition 1.3. The first and second edge degree Zagreb indices of a graph G are defined as

$$EDZ_1(G) = \sum_{uv \in E(G)} [ed_G(u) + ed_G(v)]$$

and

$$EDZ_2(G) = \sum_{uv \in E(G)} [ed_G(u) ed_G(v)].$$

Definition 1.4. Fortula and Gutman in 2015 introduced Forgotten index (F-index) [5] which is defined as :

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

The paper is presented as follows. Under section 1 the edge degree of vertices of some graphs are derived and we have evaluated the linear model for predicting the boiling point of benzenoid hydrocarbons using the Zagreb indices within section 2.

2. Main Results

Theorem 2.1. Let $P_n = (v_1, v_2, ..., v_n)$ be a path with n vertices. Then,

$$ed_{P_n}(v_i) = \begin{cases} 1, & \text{for } v_i, \ i = 1 \text{ and } i = n \\ 3, & \text{for } v_i, \ i = 2 \text{ and } i = n-1 \\ 4, & \text{else} \end{cases}$$

Proof. Let $P_n = (v_1, v_2, ..., v_{n-1}, v_n)$
Let v_i is adjacent to v_{i+1}, $i = 1, 2, ..., n-1$

$$\begin{aligned} deg(v_i) &= 1 && \text{for } i = 1 \text{ and } i = n \\ deg(v_i) &= 2 && \text{for } i = 2, ..., n-1 \end{aligned}$$

v_1 is adjacent to v_2
v_n is adjacent to v_{n-1}
$deg(v_i) = 1$ and $deg(v_2) = 2$

$$\begin{aligned} ed_{P_n}(v_i) &= \sum_{e \text{ incident to } v_i} d(e) \\ &= d(v_1) + d(v_2) - 2 \\ &= 1 + 2 - 2 \\ ed_{P_n}(v_i) &= 1 && \text{for } i = 1, n \end{aligned}$$

v_2 is adjacent to v_1 and v_3

$$\begin{aligned} ed(v_2) &= \sum_{e \text{ incident to } v_2} d(e) \\ &= [d(v_1)+d(v_2)-2]+[d(v_2)+d(v_3)-2] \\ &= (1+2-2)+(2+2-2) \\ ed(v_i) &= 3 \qquad\qquad \text{for } i=1,n \end{aligned}$$

For rest,

$$\begin{aligned} ed(v_i) &= [d(v_i)+d(v_{i-1})-2]+[d(v_i)+d(v_{i+1})-2] \\ &= (2+2-2)=(2+2-2)=4 \qquad\quad \text{for } i=2,...,n-2 \end{aligned}$$

□

Corollary 2.2. Let P_n=$(v_1, v_2, ..., v_n)$ be a path with n vertices. Then for $n \geqslant 3$,
,

$$\sum ed_{P_n}(v_n) = 4(n-2).$$

Theorem 2.3. Let P_n be a path with n vertices . Then for $n \geqslant 5$,

$$EDZ_1(P_n) = 8n-18$$

$$EDZ_2(P_n) = 16n-50.$$

Proof. Consider a path P_n=$(v_1, v_2, ..., v_n)$ we know that,
for any vertex v_i,

$$ed_{P_n}(v_i) = \begin{cases} 1, & \text{for } v_i, \ i=1 \text{ and } i=n \\ 3, & \text{for } v_i, \ i=2 \text{ and } i=n-1 \\ 4, & \text{else} \end{cases}$$

$$\begin{aligned} EDZ_1(P_n) &= \sum_{u\sim v}[ed_{P_n}(u)+ed_{P_n}(v)] \\ &= [ed(v_1)+ed(v_2)]+[ed(v_{n-1})+ed(v_n)]+[ed(v_2)+ed(v_3)]+[ed(v_{n-2})+ed(v_{n-1})] \\ &+ (4+4)(n-5) \\ &= (1+3)+(3+1)+(3+4)+(4+3)+(4+4)(n-5) \\ &= 8n-18. \end{aligned}$$

$$\begin{aligned} EDZ_2(P_n) &= \sum_{u\sim v}[ed_{P_n}(u)ed_{P_n}(v)] \\ &= [ed(v_1).ed(v_2)]+[ed(v_{n-1}).ed(v_n)]+[ed(v_2).ed(v_3)]+[ed(v_{n-2}).ed(v_{n-1})] \\ &+ (4.4)(n-5) \\ &= (1\times 3)+(3\times 1)+(3\times 4)+(4\times 3)+(4\times 4)(n-5) \\ &= 16n-50. \end{aligned}$$

□

Theorem 2.4. If G is a regular graph with n vertices and degree of each vertex is r then,

$$ed_G(v) = r(2r-2).$$

Proof. Every vertex v will be adjacent to r number of edges and to each edge $e = uv$, we have $d(u) = r$ and $d(v) = r$.

$$\begin{aligned} d(e) = d(uv) &= d(u) + d(v) - 2 \\ &= r + r - 2 \\ &= 2r - 2 \end{aligned}$$

Since there will be r edges incident to v in G.

$$\begin{aligned} ed_G(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(e) + d(e) + ... + d(e)(r \text{ times}) \\ &= d(uv) + d(uv) + ... + d(uv)(r \text{ times }) \\ &= [(2r-2) + (2r-2) + ... + (2r-2)](r \text{ times}) \\ ed_G(v) &= r(2r-2). \end{aligned}$$

□

Corollary 2.5. For Cycle:
Put $r = 2$ in the above result

$$\begin{aligned} ed_G(v) &= r(2r-2) \\ &= 2(2 \times 2 - 2) \\ &= 4. \end{aligned}$$

Corollary 2.6. For Complete graph:
Put $r = n - 1$ in Theorem 2.4

$$\begin{aligned} ed_G(v) &= [2(n-1) - 2](n-1) \\ &= (2n - 2 - 2)(n-1) \\ &= 2(n-1)(n-2). \end{aligned}$$

Corollary 2.7. For Cycle C_n with n vertices:

$$\sum ed_{C_n}(v) = 4n.$$

Theorem 2.8. If G is a regular graph with n vertices and m edges, and the degree of each vertex is r then,

$$EDZ_1(G) = 2rm(2r-2)$$
$$EDZ_2(G) = (2r-2)^2 r^2 m.$$

Proof. Consider a regular graph G with n vertices and m edges, and the degree of each vertex is r then, we know that,

$$ed_G(v) = r(2r-2)$$

$$\begin{aligned} EDZ_1(G) &= \sum_{u \sim v} [ed_G(u) + ed_G(v)] \\ &= [r(2r-2) + r(2r-2)]m \\ &= 2rm(2r-2). \end{aligned}$$

$$\begin{aligned} EDZ_2(G) &= \sum_{u\sim v}[ed_G(u)ed_G(v)] \\ &= [r(2r-2)\times r(2r-2)]m \\ &= (2r-2)^2r^2m. \end{aligned}$$

□

Corollary 2.9. If C_n is a cycle with n vertices and n edges then,

$$EDZ_1(C_n) = 8n$$
$$EDZ_2(C_n) = 16n.$$

Proof. we know that,
For any vertex v_i of C_n,

$$ed_G(v_i) = 4$$

$$\begin{aligned} EDZ_1(C_n) &= \sum_{u\sim v}[ed_{C_n}(u)+ed_{C_n}(v)] \\ &= [4+4]n \qquad \because C_n \text{has } n \text{ edges} \\ &= 8n \end{aligned}$$

$$\begin{aligned} EDZ_2(C_n) &= \sum_{u\sim v}[ed_{C_n}(u)ed_{C_n}(v)] \\ &= [4\times 4]n \qquad \because C_n \text{has } n \text{ edges} \\ &= 16n \end{aligned}$$

□

Corollary 2.10. If K_n is a complete graph with n vertices then,

$$EDZ_1(K_n) = 2n(n-1)^2(n-2)$$
$$EDZ_2(K_n) = 2n(n-1)^3(n-2)^2.$$

Proof. Consider a complete graph K_n with n vertices.
We know that,

$$ed_G(v) = 2(n-1)(n-2).$$

$$\begin{aligned} EDZ_1(K_n) &= \sum_{u\sim v}[ed_G(u)+ed_G(v)] \\ &= [2(n-1)(n-2)+2(n-1)(n-2)]\frac{n(n-1)}{2} \qquad \because K_n \text{ has } \tfrac{n(n-1)}{2} \text{ edges.} \\ &= 2n(n-1)^2(n-2). \end{aligned}$$

$$\begin{aligned} EDZ_2(K_n) &= \sum_{u \sim v}[ed_G(u)ed_G(v)] \\ &= [2(n-1)(n-2) \times 2(n-1)(n-2)]\frac{n(n-1)}{2} \qquad \because K_n \text{ has } \tfrac{n(n-1)}{2} \text{ edges.} \\ &= 2n(n-1)^3(n-2)^2. \end{aligned}$$

□

Theorem 2.11. Let W_n be a Wheel graph with vertices $v_1, v_2, ..., v_n$, where v_n is the central vertex. Then,

$$ed_{W_n}(v_i) = \begin{cases} n+8, & \text{for } deg(v) = 3 \\ n(n-1), & \text{for } deg(v) = n-1 \end{cases} \qquad \text{Where i=1,2,...,n.}$$

Proof. Case 1: For $deg(v) = 3$
Every v_i has 3 edges u_1v_1, u_2v_2 and u_3v_3 are incident to it.
$d(u_1) = d(v_1) = d(u_2) = d(v_2) = d(u_3) = 3$ and $d(v_3) = n-1$

$$\begin{aligned} ed_G(v_i) &= \sum_{e \text{ incident to } v_2} d(e) \\ &= [d(u_1)+d(v_1)-2]+[d(u_2)+d(v_2)-2]+[d(u_3)+d(v_3)-2] \\ &= (3+3-2)+(3+3-2)+(3+(n-1)-2) \\ ed_{W_n}(v_i) &= n+8 \end{aligned}$$

Case 2: For $deg(v) = n-1$
For vertex with $deg(v)$=$n-1$ has $n-1$ edges incident to it such that each edge $e = uv$ has $d(u) = 3$ and $d(v) = n-1$

$$\begin{aligned} ed_G(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= [d(e)+d(e)+...+d(e)](n-1 \text{ times}) \\ &= [d(e)](n-1) \\ &= [d(u)+d(v)-2](n-1) \\ &= [3+(n-1)-2](n-1) \\ ed_{W_n}(v) &= n(n-1). \end{aligned}$$

□

Corollary 2.12. Let W_n be a Wheel graph with vertices $v_1, v_2, ..., v_n$. Then,

$$\sum ed_{W_n}(v) = 2(n-1)(n+4).$$

Theorem 2.13. Let W_n be a Wheel graph with n vertices $v_1, v_2, ..., v_n$, where v_n is the central vertex. Then,

$$EDZ_1(W_n) = (n-1)(n^2+2n+24)$$
$$EDZ_2(W_n) = (n-1)(n+8)(n^2+8).$$

Proof. Consider a Wheel graph W_n with n vertices and let v_n be the central vertex.
We know that for any vertex v_i of W_n,

$$ed_{W_n}(v_i) = \begin{cases} n+8, & \text{For } deg(v) = 3 \\ n(n-1), & \text{For } deg(v) = n-1 \end{cases} \quad \text{Where i=1,2,...,n.}$$

$$\begin{aligned} EDZ_1(W_n) &= \sum_{u\sim v}[ed_G(u) + ed_G(v)] \\ &= \sum_{v_i\sim v_j,\ v_i\neq v_n,\ v_j\neq v_n}[ed(v_i) + ed(v_j)] + \sum_{v_i\sim v_n}[ed(v_i) + ed(v_n)] \\ &= [(n+8) + (n+8)](n-1) + [(n+8) + n(n-1)](n-1) \\ &= (n-1)[2(n+8) + 8 + n^2] \\ &= (n-1)(n^2 + 2n + 24). \end{aligned}$$

$$\begin{aligned} EDZ_2(W_n) &= \sum_{u\sim v}[ed_G(u).ed_G(v)] \\ &= \sum_{v_i\sim v_j,\ v_i\neq v_n,\ v_j\neq v_n}[ed(v_i).ed(v_j)] + \sum_{v_i\sim v_n}[ed(v_i).ed(v_n)] \\ &= [(n+8).(n+8)](n-1) + [(n+8).n(n-1)](n-1) \\ &= (n-1)[(n+8)^2 + n(n-1)(n+8)] \\ &= (n-1)(n+8)(n^2+8). \end{aligned}$$

□

Theorem 2.14. Let S_n be a Star graph with n vertices $v_1, v_2, ..., v_n$. Then,

$$ed_{S_n}(v) = \begin{cases} (n-1)(n-2), & \text{For } deg(v) = n-1 \\ (n-2), & \text{For } deg(v) = 1 \end{cases}$$

Proof. Case 1: For $deg(v) = 1$
Every v has 1 edge $e = uv$ incident to it.
$d(u) = n-1$ and $d(v) = 1$

$$\begin{aligned} ed_{S_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(e) \\ &= [d(u) + d(v) - 2] \\ &= 1 + (n-1) - 2 \\ ed_{S_n}(v) &= n-2. \end{aligned}$$

Case 2: For $deg(v) = n-1$
For vertex with $deg(v)$=$n-1$ has $n-1$ edges incident to it such that each edge $e = uv$ has $d(u) = 1$ and $d(v) = n-1$

$$\begin{aligned} ed_G(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= [d(e) + d(e) + ... + d(e)](n-1 \text{ times}) \\ &= [d(e)](n-1) \\ &= [d(u) + d(v) - 2](n-1) \\ &= [1 + (n-1) - 2](n-1) \\ ed_G(v) &= (n-1)(n-2). \end{aligned}$$

□

Corollary 2.15. Let S_n be a Star graph with n vertices $v_1, v_2, ..., v_n$. Then,

$$\sum ed_{S_n}(v) = 2(n-1)(n-2).$$

Theorem 2.16. Let S_n be a Star graph with n vertices $v_1, v_2, ..., v_n$ Then,

$$EDZ_1(S_n) = n(n-1)(n-2)$$

$$EDZ_2(S_n) = (n-1)^2(n-2)^2.$$

Proof. Consider a Star graph S_n with n vertices.
We know that,

$$d_e(v) = \begin{cases} (n-1)(n-2), & \text{For } deg(v) = n-1 \\ (n-2), & \text{For } deg(v) = 1 \end{cases}$$

$$\begin{aligned} EDZ_1(S_n) &= \sum_{u\sim v} [d_e(u) + d_e(v)] \\ &= [(n-2) + (n-1)(n-2)](n-1) \\ &= (n-1)(n-2)[1 + (n-1)] \\ &= n(n-1)(n-2). \end{aligned}$$

$$\begin{aligned} EDZ_2(S_n) &= \sum_{u\sim v} [d_e(u).d_e(v)] \\ &= [(n-2).(n-1)(n-2)](n-1) \\ &= (n-1)^2(n-2)^2. \end{aligned}$$

□

Theorem 2.17. Let $K_{m,n}$ be a complete bipartite graph. Let the vertices of $K_{m,n}$ be partitioned into two sets,
$V_1 = \{v_1, v_2, ..., v_m\}$ and
$V_2 = \{v_1', v_2', ..., v_n'\}$, then

$$ed_{K_{m,n}}(v) = \begin{cases} (m+n-2)n, & \text{if } v \in V_1 \\ (m+n-2)m, & \text{if } v \in V_2 \end{cases}$$

Proof. Case 1: For $v_i \in V_1$
Every v_i has n edges $e = uv$ incident to it. Each edge $e = uv$ has $d(u) = m$ and $d(v) = n$
$d(e) = d(uv) = d(u) + d(v) - 2 = m + n - 2$

$$\begin{aligned} ed_{K_{m,n}}(v) &= \sum_{e \text{ incident to } v_i} d(e) \\ &= [d(e) + d(e) + ... + d(e)](n \text{ times}) \\ &= d(e) \times n \\ ed_{K_{m,n}}(v) &= (m+n-2)n. \end{aligned}$$

Case 2: For $v_i' \in V_2$
Every v_i' has m edges $e = uv$ incident to it. Each edge $e = uv$ has $d(u) = m$ and $d(v) = n$

$d(e) = d(uv) = d(u) + d(v) - 2 = m + n - 2.$

$$\begin{aligned} ed_{K_{m,n}}(v) &= \sum_{e \text{ incident to } v_i} d(e) \\ &= [d(e) + d(e) + ... + d(e)](m \text{ times}) \\ &= d(e) \times m \\ ed_{K_{m,n}}(v) &= (m+n-2)m. \end{aligned}$$

□

Corollary 2.18. Let $K_{m,n}$ be a Complete Bipartite graph. Then,

$$\sum ed_{K_{m,n}}(v) = 2mn(m+n-2).$$

Theorem 2.19. Let $K_{m,n}$ be a Complete Bipartite graph. Then,

$$\begin{aligned} EDZ_1(K_{m,n}) &= mn(m+n)(m+n-2) \\ EDZ_2(K_{m,n}) &= m^2n^2(m+n-2)^2. \end{aligned}$$

Proof. Let $K_{m,n}$ be a Complete Bipartite graph. Let the vertices of $K_{m,n}$ be partitioned into two sets,
$V_1 = \{v_1, v_2, ..., v_m\}$ and
$V_2 = \{v_1', v_2', ..., v_n'\}$
We know that,

$$ed_{K_{m,n}}(v) = \begin{cases} (m+n-2)n, & \text{if } v \in V_1 \\ (m+n-2)m, & \text{if } v \in V_2 \end{cases}$$

$$\begin{aligned} EDZ_1(K_{m,n}) &= \sum_{v_i \sim v_j'} [ed_{K_{m,n}}(v_i) + ed_{K_{m,n}}(v_j')] \qquad \text{Where } i = 1,2,...,m \text{ and } j = 1,2,...,n \\ &= [(m+n-2)n + (m+n-2)m]mn \\ &= (m+n-2)(m+n)mn \\ &= mn(m+n)(m+n-2). \end{aligned}$$

$$\begin{aligned} EDZ_2(K_{m,n}) &= \sum_{v_i \sim v_j'} [ed_{K_{m,n}}(v_i).ed_{K_{m,n}}(v_j')] \qquad \text{Where } i = 1,2,...,m \text{ and } j = 1,2,...,n \\ &= [(m+n-2)n.(m+n-2)m]mn \\ &= m^2n^2(m+n-2)^2. \end{aligned}$$

□

Theorem 2.20. Let L_n be a Ladder graph with $2n$ vertices and n rungs. Then,

$$ed_{L_n}(v) = \begin{cases} 5, & \text{for vertex } v \text{ on 1st and } n\text{th rung} \\ 11, & \text{for vertex } v \text{ on 2nd and } (n-1)\text{th rung} \\ 12, & \text{for rest} \end{cases}$$

Proof. Case 1: For vertices v on the 1st and nth rung, v have two edges u_1v_1 and u_2v_2 incident to it, such that
$d(u_1) = 2,\ d(u_2) = 2,\ d(v_1) = 3,\ d(v_2) = 2$

$$\begin{aligned} ed_{L_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(u_1v_1) + d_(u_2v_2) \\ &= d(u_1) + d(v_1) - 2 + d(u_2) + d(v_2) - 2 \\ &= 2 + 3 - 2 + 2 + 2 - 2 \\ ed_{L_n}(v) &= 5. \end{aligned}$$

Case 2: For vertices v on the 2nd and $(n-1)$th rung, v has three edges u_1v_1, u_2v_2 and u_3v_3 incident to it, such that
$d(u_1) = 2,\ d(u_2) = 3,\ d(u_3) = 3,\ d(v_1) = 3,\ d(v_2) = 3,\ d(v_3) = 3$

$$\begin{aligned} ed_{L_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(u_1v_1) + d(u_2v_2) + d(u_3v_3) \\ &= d(u_1) + d(v_1) - 2 + d(u_2) + d(v_2) - 2 + d(u_3) + d(v_3) - 2 \\ &= 2 + 3 - 2 + 3 + 3 - 2 + 3 + 3 - 2 \\ ed_{L_n}(v) &= 11. \end{aligned}$$

Case 3: For vertices v on the other rungs, v has three edges u_1v_1, u_2v_2 and u_3v_3 incident to it, such that
$d(u_1) = 3,\ d(u_2) = 3,\ d(u_3) = 3,\ d(v_1) = 3,\ d(v_2) = 3,\ d(v_3) = 3$

$$\begin{aligned} ed_{L_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(u_1v_1) + d(u_2v_2) + d(u_3v_3) \\ &= d(u_1) + d(v_1) - 2 + d(u_2) + d(v_2) - 2 + d(u_3) + d(v_3) - 2 \\ &= 3 + 3 - 2 + 3 + 3 - 2 + 3 + 3 - 2 \\ ed_{L_n}(v) &= 12. \end{aligned}$$

□

Corollary 2.21. Let L_n be a Ladder graph with $2n$ vertices and n rungs. Then,

$$\sum ed_{L_n}(v) = 8(3n - 4).$$

Theorem 2.22. Let L_n be a Ladder graph with $2n$ vertices and n rungs and $E(L_n)$ is the edge set of L_n. Then,

$$\begin{aligned} EDZ_1(L_n) &= 72n - 116 \\ EDZ_2(L_n) &= 432n - 976. \end{aligned}$$

Proof. Let L_n be a Ladder graph. We know that,

$$ed_{L_n}(v) = \begin{cases} 5, & \text{for vertex } v \text{ on 1st and } n\text{th rung} \\ 11, & \text{for vertex } v \text{ on 2nd and } (n-1)\text{th rung} \\ 12, & \text{for rest} \end{cases}$$

□

Table 1: Edge degree of L_n

Edge degree, $(ed_{L_n}(u), ed_{L_n}(v))$, $uv \in E(L_n)$	(5,5)	(11,11)	(12,12)	(5,11)	(11,12)
No. of Edges	2	2	$(n-4)+2(n-5)$	4	4

By using the following Table 1, we compute the $EDZ_1(L_n)$ and $EDZ_2(L_n)$,

$$\begin{aligned} EDZ_1(L_n) &= \sum_{u\sim v}[ed_{L_n}(u)+ed_{L_n}(v)] \\ &= 2(5+5)+2(11+11)+(3n-14)(12+12)+4(5+11)+4(11+12) \\ &= 20+44+72n-336+64+92 \\ &= 72n-116. \\ EDZ_2(L_n) &= \sum_{u\sim v}[ed_{L_n}(u)ed_{L_n}(v)] \\ &= 2(5\times 5)+2(11\times 11)+(3n-14)(12\times 12)+4(5\times 11)+4(11\times 12) \\ &= 50+242+432n-2016+220+528 \\ &= 432n-976. \end{aligned}$$

Theorem 2.23. Let F_n be the Friendship graph with n triangles and $2n+1$ vertices. Then,
$$ed_{F_n}(v) = \begin{cases} 2(n+1), & \text{for } deg(v)=2 \\ 4n^2, & \text{for } deg(v)=2n \end{cases}$$

Proof. Case 1: For $deg(v)=2$
Every v has 2 edges u_1v_1 and u_2v_2 incident to it.
$d(u_1)=2$, $d(v_1)=2n$, $d(u_2)=2$, $d(v_2)=2$,

$$\begin{aligned} ed_{F_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(u_1v_1)+d(u_2v_2) \\ &= [d(u_1)+d(v_1)-2+d(u_2)+d(v_2)-2] \\ &= (2+2n-2+2+2-2) \\ ed_{F_n}(v) &= 2n+1. \end{aligned}$$

Case 2: For $deg(v)=2n$
For vertex with $deg(v)$=$2n$ has $2n$ edges incident to it such that each edge $e=uv$ has $d(u)=2n$ and $d(v)=2$

$$\begin{aligned} ed_{F_n}(v) &= \sum_{e \text{ incident to } v} d(e) \\ &= d(uv)\times 2n \\ &= [d(u)+d(v)-2](2n) \\ &= [2n+2-2](2n) \\ ed_{F_n}(v) &= 4n^2. \end{aligned}$$

□

Corollary 2.24. Let F_n be the Friendship graph with n triangles and $2n+1$ vertices. Then,

$$\sum ed_{F_n}(v) = 4n(2n+1).$$

Theorem 2.25. If F_n is the Friendship graph with n triangles and $2n+1$ vertices then,

$$\begin{aligned} EDZ_1(F_n) &= 8n(n^2+n+1) \\ EDZ_2(F_n) &= 4n(n+1)(4n^2+n+1). \end{aligned}$$

Proof. Let F_n be the Friendship graph with n triangles and $2n+1$ vertices.

We know that, $ed_{F_n}(v) = \begin{cases} 2(n+1), & \text{for } deg(v) = 2 \\ 4n^2, & \text{for } deg(v) = 2n \end{cases}$

$$\begin{aligned} EDZ_1(F_n) &= \sum_{u\sim v}[ed_{F_n}(u) + ed_{F_n}(v)] \\ &= \sum_{v_i\sim v_j,\ v_i\neq v_n,\ v_j\neq v_n}[ed_{F_n}(v_i) + ed_{F_n}(v_j)] + \sum_{v_i\sim v_n}[ed_{F_n}(v_i) + ed_{F_n}(v_n)] \\ &= [2(n+1)+2(n+1)]n + [2(n+1)+4n^2]2n \\ &= 8n(n+1)+8n^3 \\ &= 8n(n^2+n+1). \\ EDZ_1(F_n) &= \sum_{u\sim v}[ed_{F_n}(u)ed_{F_n}(v)] \\ &= \sum_{v_i\sim v_j,\ v_i\neq v_n,\ v_j\neq v_n}[ed_{F_n}(v_i)\times ed_{F_n}(v_j)] + \sum_{v_i\sim v_n}[ed_{F_n}(v_i)\times ed_{F_n}(v_n)] \\ &= [2(n+1)\times 2(n+1)]n + [2(n+1)\times 4n^2]2n \\ &= 4n(n+1)^2 + 16n^3(n+1) \\ &= 4n(n+1)(4n^2+n+1). \end{aligned}$$

□

Lemma 2.26. In any graph G,

$$ed_G(u) = du^2 - 2du + N(u), \quad \text{where } N(u) \text{ is neighborhood degree sum of a vertex } u.$$

Proof.

$$\begin{aligned} ed_G(u) &= \sum_{u\sim v}(du+dv-2) && 1.2 \\ &= \sum_{u\sim v}(du-2) + \sum_{u\sim v} dv \\ &= du(du-2)+N(u) && N(u) \text{ is Neighborhood degree sum of a vertex } u \\ &= du^2-2du+N(u). \end{aligned}$$

□

Lemma 2.27. Let G be a connected graph. Let $Z_1(G)$ be a first Zagreb index and $F(G)$ be the forgotten index of a graph G. Then,

$$EDZ_1(G) = F(G) - 2Z_1(G) + N(G)$$

and

$$EDZ_2(G) = \sum_{uv \in E(G)} \left[du^2dv^2 - 2du^2dv + du^2N(u) - 2du^2dv^2 + 4dudv - 2duN(u) + N(u)dv^2 - 2N(u)dv + N(u)N(v)\right],$$

where $N(G)$ is the neighborhood degree of a graph G.

Proof.

$$\begin{aligned} \text{Let} \quad EDZ_1(G) &= \sum_{u \sim v} [ed_G(u) + ed_G(v)] \\ &= \sum [du^2 - 2du + N(u)] + [dv^2 - 2dv + N(v)] \quad 2.27 \\ &= \sum (du^2 + dv^2) - 2\sum (du + dv) + \sum (N(u) + N(v)) \\ &= F(G) - 2Z_1(G) + N(G). \end{aligned}$$

and

$$\begin{aligned} EDZ_2(G) &= \sum_{u \sim v} [ed_G(u)ed_G(v)] \\ &= \sum [du^2 - 2du + N(u)][dv^2 - 2dv + N(v)] \quad 2.27 \\ &= \sum [du^2dv^2 - 2du^2dv + du^2N(u) - 2du^2dv^2 + 4dudv \\ -2 & \quad duN(u) + N(u)dv^2 - 2N(u)dv + N(u)N(v)]. \end{aligned}$$

□

3. Regression analysis for boiling point

In this section, We analyze the connection between the boiling point of benzenoid hydrocarbons and edge degree Zagreb indices. We used experimental boiling point values for the hydrocarbons in figure 1, sourced from reference [14]. Figures 2 and 3 show graphs plotting the boiling point against the degree based indices EDZ_1 and EDZ_2.

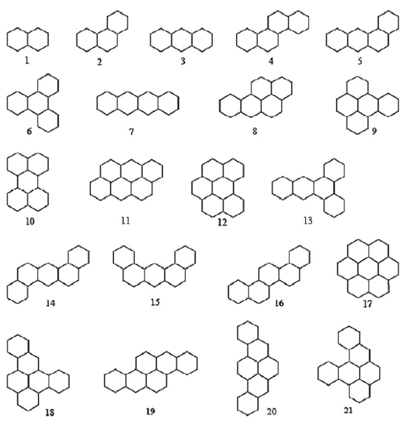

Figure 1: Molecular graphs of benzenoid hydrocarbons under consideration[14]

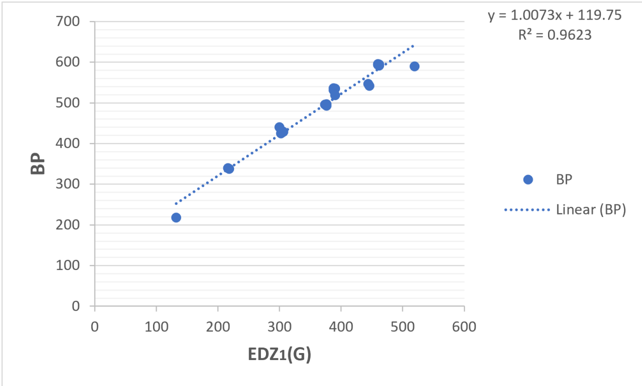

Figure 2: Scatter plot between boiling point(BP) and First edge degree Zagreb index

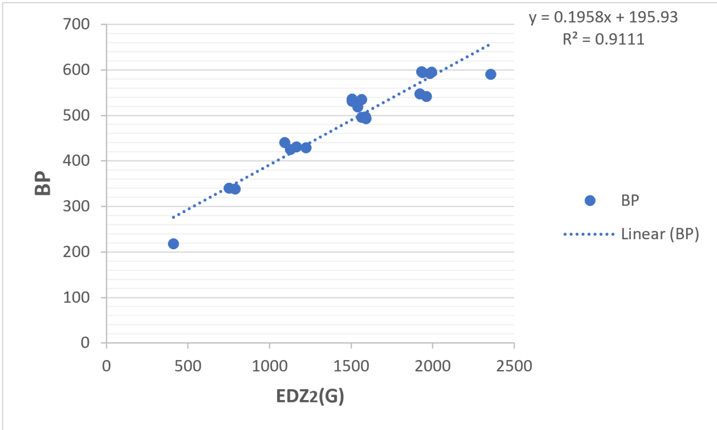

Figure 3: Scatter plot between boiling point(BP) and Second edge degree Zagreb index

The linear regression models for the boiling point (BP)using the data of Table 2 are obtained using the least square fitting procedure as implemented in SPSS Statistics programme, and they are

$$\mathsf{BP} = 119.7(\pm 17.35) + 1.007(\pm 0.04573)\mathsf{EDZ}_1$$
$$\mathsf{BP} = 195.9(\pm 22.09) + 0.1958(\pm 0.01403)\mathsf{EDZ}_2.$$

The above equations shows that the correlation of the experimental boiling point of benzenoid hydrocarbons with first edge degree Zagreb index(R=0.9809) and second edge degree Zagreb index(R=0.9545).

4. Conclusion

We have introduced the Edge degree of a vertex and the first edge degree Zagreb index and second edge degree Zagreb index of graphs and computed these indices for some specific graphs. Furthermore, We performed a regression analysis to compare linear models relating these degree based indices to the boiling points of benzenoid hydrocarbons. Our results, presented in Table 3, show that the First edge degree Zagreb index has a strong correlation with the boiling point of these compounds.

References

[1] A. R. Ashrafi, T. Doslic, A. Hamzeha, The Zagreb coindices of graph operations, Discrete Appl. Math., 158 (2010), 1571-1578.

Table 2: The values of experimental boiling points and degree based indices of 21 benzenoid hydrocarbons

Benzenoid Hydrocarbons	BP(°C)	$EDZ_1(G)$	$EDZ_2(G)$
1	218	132	412
2	338	218	788
3	340	216	752
4	431	304	1165
5	425	302	1129
6	429	306	1224
7	440	300	1092
8	496	374	1565
9	493	376	1592
10	497	376	1590
11	547	444	1922
12	542	446	1962
13	535	390	1566
14	536	388	1506
15	531	388	1506
16	519	390	1542
17	590	519	2356
18	592	462	1982
19	596	460	1932
20	594	460	1937
21	595	462	1993

Table 3: Correlation coefficient (R) with boilng point (BP) of benzenoid hydrocarbons

Index	Correlation coefficient (R)
EDZ_1	0.9809
EDZ_2	0.9545

[2] K. C. Das, I. Gutman, Estimating the Wiener index by means of number of vertices, number of edges and diameter, MATCH Commun. Math. Comput. Chem., 64 (2010), 647-660.

[3] K. C. Das, K. Xu, J. Nam, Zagreb indices of graphs, Font. Math. China, 10 (2015), 567-582. 1

[4] N. De, S. M. A. Nayeem, A. Pal, The F-coindex of some graph operations, Springer Plus, 5(2016), 221.

[5] B. Furtula, I. Gutman, A forgotten topological index, J. Math. Chem., 53 (2015), 1184-1190. 1.4

[6] I. Gutman, K. C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem., 50 (2004) , 83-92. 1

[7] I. Gutman, B. Furtula, Z. Kovijanic Vukicevic, G. Popivoda, On Zagreb indices and coindices, MATCH Commun. Math. Comput. Chem., 74 (2015), 5-16. 1

[8] I. Gutman, B. Ruscic, N. Trinajstic, C. F. Wilcox, Graph theory and molecular orbitals, XII, Acyclic polyenes, J. Chem. Phys., 62 (1975), 3399-3405. 1

[9] I. Gutman, N. Trinajstic, Graph theory and molecular orbitals, total pi-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972), 535-538. 1.1, 1

[10] F. Harary, Graph Theory, Addison-Wesley Publishing Company, Reading, 1969. 1

[11] H. Hua, K. C. Das, The relationship between the eccentric connectivity index and Zagreb indices, Discrete Appl. Math., 161(2013) , 2480-2491.

[12] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, The first and second Zagreb indices of some graph operations, Discrete Appl. Math., 157(2009), 804-811. 1

[13] S. Nikolic, G. Kovacevic, A. Milicevic, N. Trinajstic, The Zagreb indices 30 years after, Croat. Chem. Acta, 76 (2003), 113-124. 1

[14] S. Nikolic, A. Milicevic, N. Trinajstic, A. Juric, On use of the variable Zagreb (${}^{\nu}M_2$) index in QSPR: boiling points of benzenoid hydrocarbons, Molecules 9 (2004), 1208-1221. 1, 3

[15] H. S. Ramane, A. S. Yalnaik, Status connectivity indices of graphs and its applications to the boiling point of benzenoid hydrocarbons, J. Appl. Math. Comput., 55 (2017), 609-627.

[16] R. Todeschini, V. Consonni, handbook of Molecular Descriptors, Wiley, Weinheim (2000). 1
[17] K. Xu, K. C. Das, On Harary index of graphs, Discrete Appl. Math.,159(2011), 1631-1640.
[18] B. Zhou, Z. Du, On eccentric connectivity index. MATCH Commun. Math. Comput. Chem., 63 (2010), 181-198.
[19] B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem., 54 (2005), 233-239. 1