Eccentricity-Based Topological Indices of Chain Graphs

BALKISHBANU KHAJI , SHAHISTHA HANIF* and K ARATHI BHAT

***Abstract*—This article delves into the realm of eccentricity-based topological indices, focusing particularly on a class of graphs called chain graphs. Topological indices serve as numerical descriptors derived from molecular structures, aiding in the elucidation of chemical properties and activities. Today, topological indices remain a vibrant area of research, with applications spanning various fields of chemistry, including drug design, materials science, environmental chemistry, and bioinformatics. Chain graphs are a special class of bipartite graphs having the largest spectral radius among all the bipartite graphs of prescribed order and size. Nevertheless, the high significance of chain graphs in the field of spectral graph theory, the domain of various topological indices remains unexplored. This article categorizes generalized eccentricity-based topological indices into two types and explores them. Some of the major eccentricity-based topological indices like the total eccentricity index, Zagreb eccentricity indices, ABC eccentricity index, and geometric-arithmetic eccentricity index of chain graphs are studied in detail and an inequality connecting their relationship is provided. Further, the extremities for these indices among chain graphs are presented.**

***Index Terms*—Chain, Bipartite graph, Bi-star graph, Complete bipartite graph.**

I. INTRODUCTION

Topological indices have a rich historical background, dating back to the mid-20th century when chemists and mathematicians began exploring mathematical approaches to describe molecular structures. The concept of topological indices emerged as a result of this interdisciplinary collaboration. In 1947, Harold Wiener introduced the Wiener index, which was one of the earliest topological indices. Wiener index is based on the sum of distances between all pairs of vertices in a molecular graph. He initially used this index to compare the boiling points of alkane isomers, marking the beginning of topological index applications in chemistry. Following Wiener's pioneering work, many other researchers contributed to the development of topological indices. In the subsequent decades, numerous other topological indices were proposed, each focusing on different aspects of molecular structure and properties. These indices include the Hosoya index, Zagreb index, Balaban index, and many more. With the advancement of graph theory and computational chemistry, researchers continued to refine existing indices and develop new ones to address specific challenges in chemical research.

Chain graphs are $\{2K_2, C_3, C_5\}$-free graphs, popularly known as double nested graphs. In other words, a chain graph is a bipartite graph G with $V(G) = V_1 \cup V_2$ in which each of the partite sets V_i $(i = 1, 2)$ can be partitioned into h non-empty cells $V_{11}, V_{12}, \ldots, V_{1h}$ and $V_{21}, V_{22}, \ldots, V_{2h}$ such that $N_G(u) = V_{21} \cup ... \cup V_{2(h-i+1)}$, for any $u \in V_{1i}$, $1 \leq i \leq h$. If $m_i = |V_{1i}|$ and $n_i = |V_{2i}|$, then we write $G = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$, whose order is $n = \sum_{i=1}^{h} m_i + \sum_{i=1}^{h} n_i$ (DNG stands for Double Nested Graphs) [1]. The complete bipartite graph $K_{p,q} = DNG(p, q)$ and the bi-star graph $B(p, q) = DNG(1, p-1; 1, q-1)$ (obtained by adding an edge between the two apex vertices of $K_{1,p-1}$ and $K_{1,q-1}$). When each of $m_i = n_i = 1$ for $1 \leq i \leq h$, the graph is called a half graph [2]. Figure 2 represents a chain graph, $DNG(3, 2, 5, 1; 2, 1, 3, 3)$ of order 20.

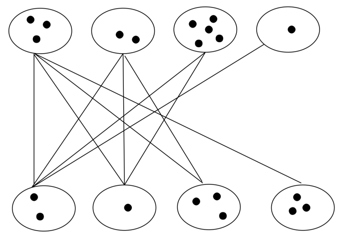

Fig. 1. Chain graph, $DNG(3, 2, 5, 1; 2, 1, 3, 3)$

Chain graphs attain the maximum spectral radius among all simple bipartite graphs of prescribed order and size ([3]), hence playing a signficant role in the field of spectral graph theory. Further results concerned with properties of chain graphs are available in the literature [4], [5], [6], [7] and [8]. A great deal of knowledge on some topological indices is accumulated in the recent literature [9], [10], [11], [12], [13], [14], [15], [16] and [17]. Some degree and distance based topological indices like Wiener index, Harary index, Zagreb indices etc. of chain graphs explored in [18], [19], [20] and [21]. They also provide algorithms for inverse topological index problems for chain graphs.

A. Eccentricity-based topological indices

Researches in the verge of refining the existing topological indices, replaced degrees by eccentricities in well known degree based topological indices. The detailed exploration of such indices and analysis of their applications are being studied in the recent years and hence currently, proved to be one of the emerging research area in Molecular chemistry and Molecular graph theory. Apparently, in this article we have

Manuscript received 17 December, 2024; revised 17 February, 2025.

Balkishbanu Khaji is a PhD scholar in the Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India-576104. (email:balkishbanu.dscmpl2023@learner.manipal.edu).

Shahistha is an Assistant Professor in the Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India-576104 (*Corresponding author to provide email: shahistha.hanif@manipal.edu).

K Arathi Bhat is an Associate Professor in the Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India-576104 (email: arathi.bhat@manipal.edu).

categorized general eccentricity-based topological indices into two types.

In the subsequent part of the article some abbreviations as well as notations are used, which are given below. A bipartite graph G with the bipartition $V(G) = V_1 \cup V_2$ is denoted by $G(V_1 \cup V_2, E)$. The adjacency and non adjacency between any two vertices u, v are denoted by $u \sim v$ and $u \nsim v$, respectively. For a vertex $v \in V(G)$ in G, $d(v)$, $e(v)$ represent degree and eccentricity of v, respectively. The distance between any two vertices $u, v \in V(G)$ is denoted by $d(u, v)$. Given a vertex v, a vertex u is said to be an eccentric vertex for v, if $d(u, v) = e(v)$. A vertex in a graph G is said to be dominating if it is adjacent to all other vertices of G. But in the context of bipartite graphs, a dominating vertex in a partite set refers to the one that is adjacent to all other vertices of the other partite set.

We now categorize eccentricity-based topological indices into two classes (type I and type II) depending on their definitions.

Definition 1.1: For a graph $G(V, E)$ of order n, a vertex eccentricity-based topological index is said to be of type I if it can be expressed as

$$\Theta_I^e = \sum_{v \in V(G)} \theta\big(e(v)\big) \tag{1}$$

Here the summation runs over all the vertices of G and θ is a function of vertex eccentricity. The class $\{\Theta_I^e\}$ comprises all the eccentricity-based topological indices of type I. When the function θ is chosen appropriately, we get some popular eccentricity-based topological indices of graphs. When $\theta(x) = x$ in Equation 1, we get the total eccentricity index given by

$$\tau(G) = \sum_{v \in V(G)} e(v)$$

Similarly, when $\theta(x) = x^2$ in Equation 1, we get the first Zagreb eccentricity index given by

$$\xi_1(G) = \sum_{v \in V(G)} e^2(v)$$

Definition 1.2: For a graph $G(V, E)$, a vertex eccentricity-based topological index is said to be of type II if it can be expressed as

$$\Theta_{II}^e = \sum_{uv \in E(G)} \theta\big(e(u), e(v)\big) \tag{2}$$

Here the summation runs over all the edges of G and θ is a symmetric function of vertex eccentricities, that is $\theta\left(e(u), e(v)\right) = \theta\big(e(v), e(u)\big)$. The class $\{\Theta_{II}^e\}$ comprises all the eccentricity-based topological indices of type II. Some of the well-known eccentricity-based topological indices belonging to the class Θ_{II}^e, namely the second Zagreb eccentricity index, eccentric connectivity index, Atom bond connectivity eccentricity index (ABC eccentricity index) and Geometric arithmetic eccentricity index (GA eccentricity index) are given in the following table.

$\theta(x,y)$	Index obtained	Expression
$\theta = xy$	The second Zagreb eccentricity index	$\xi_2(G) = \sum_{uv \in E(G)} e(v)e(u)$
$\theta = x + y$	Eccentric connectivity index	$\xi^c(G) = \sum_{uv \in E(G)} e(u) + e(v)$
$\theta = \sqrt{\frac{x+y-2}{xy}}$	Atom bond connectivity eccentricity index	$ABC^e(G) = \sum_{uv \in E(G)} \sqrt{\frac{e(u)+e(v)-2}{e(u)e(v)}}$
$\theta = \frac{2\sqrt{xy}}{x+y}$	Geometric arithmetic eccentricity index	$GA^e(G) = \sum_{uv \in E(G)} \frac{2\sqrt{e(u)e(v)}}{e(u)+e(v)}$

II. Some indices from class $\{\Theta_I^e\}$

As per the definition of chain graphs, eccentricity of any vertex is either 1, 2 or 3. Most of the indices from this class will be sum of $\theta(1)$, $\theta(2)$ and $\theta(3)$. The following is the expression.

Theorem 2.1: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Then an eccentricity-based topological index of type I $\Theta_I^e \in \{\Theta_I^e\}$ is given by

$$\Theta_I^e = (m_1 + n_1)\theta(2) + (n - m_1 - n_1)\theta(3) \tag{3}$$

Proof: Let $V_1 = V_{11} \cup V_{12} \cup \cdots \cup V_{1h}$ with $V_{1i} = m_i$ and $V_2 = V_{21} \cup V_{22} \cup \cdots \cup V_{2h}$ with $V_{2i} = n_i$ for $1 \leq i \leq h$. By definition, the vertices of V_{11} and V_{21} are dominating, for any vertex $v \in V_{11} \cup V_{21}$, $e(v) = 2$, with eccentric vertices being the ones in the same partite set. For any vertex $v \in V_1 \setminus V_{11}$, all the vertices $u \in V_{21}$ are adjacent and there exists at least one vertex $u \in V_2 \setminus V_{21}$ such that $d(u, v) = 3$ (since $p, q > 1$), hence $e(v) = 3$. The same is true for the vertices of $V_2 \setminus V_{21}$. Thus,

$$e(v) = \begin{cases} 2 & v \in V_{11} \cup V_{21} \\ 3 & else \end{cases}.$$

On enumerating the vertex eccentricities appropriately and substituting in Equation 1, we get the expression. ■

When either of p, q is one, say, $p = 1$ and $q > 1$, then $e(v) = \begin{cases} 1 & v \in V_1 \\ 2 & else \end{cases}$. Thus $\Theta_I^e = \theta(1) + q\theta(2)$. Suppose both $p = q = 1$, then $e(v) = 1 \ \forall v \in V(G)$, in which case $\Theta_I^e = 2\theta(1)$. The total eccentricity index and the first Zagreb eccentricity index can be obtained from the above theorem as the special cases.

Corollary 2.2: Let $G(V_1 \cup V_2, E)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Let $\tau(G)$ and $\xi_1(G)$ be the total eccentricity index and the first Zagreb eccentricity index of G, respectively. Then

$$\begin{aligned} \tau(G) &= 3n - k \\ \xi_1(G) &= 9n - 5k \end{aligned}$$

where k is the number of dominating vertices in G.

Half graphs are the special type of chain graphs where each of the cells contain exactly one vertex. A graph graph has even number of vertices, where the number of vertices in each partite set equlas the number of cells itself. Further, a graph graph $G(V_1 \cup V_2, E)$ has $|V_1| = |V_2|$.

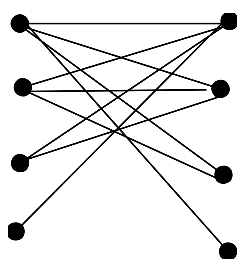

Fig. 2. A Half graph, $DNG(1, 1, 1, 1; 1, 1, 1, 1)$

Corollary 2.3: Let $G(V_1 \cup V_2, E)$ be a half graph of order $n \geq 2$. Then an eccentricity-based topological index of type I $\Theta_I^e \in \{\Theta_I^e\}$ is given by

$$\Theta_I^e = 2\theta(2) + (n-2)\theta(3) \tag{4}$$

Proof: The above result follows by substituting $m_1 = n_1 = 1$. ■

Next we have the theorem giving bounds for these indices.

Theorem 2.4: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Let $\tau(G), \xi_1(G)$ be the total eccentricity index and the first Zagreb eccentricity index of G, respectively. Then

$$2n \leq \tau(G) \leq 3n - 2$$
$$4n \leq \xi_1(G) \leq 9n - 10$$

Proof: From Corollary 2.2, both $\tau(G), \xi_1(G)$ are minimum when k is maximum, that is the number of dominating vertices are the maximum. Since $|V_1| = p$ and $|V_2| = q$, the number of dominating vertices is at most $p + q$. The graph G has the minimum total eccentricity index/the first Zagreb eccentricity index when all the vertices are dominating, that is $G = K_{p,q}$ and $k = p + q = n$. Thus $\tau(G) \geq 2n$ and $\xi_1(G) \geq 4n$. Similarly, they attain the maxima when k is as minimum as possible. That is when the number of dominating vertices is the minimum. This happens only when each of V_1, V_2 has exactly one dominating vertex due to the property that both the partite sets of a chain graph have at least one dominating vertex. Thus the total eccentricity index/ the first Zagreb eccentricity index is the maximum when $k = 2$ and $G = B(p, q)$, which implies $\tau(G) \leq 3n-2$ and $\xi_1(G) \leq 9n - 10$. ■

We next move to the class of eccentricity-based indices of type II.

III. Some indices from class $\{\Theta_{II}^e\}$

The four specific eccentricity-based indices namely, the second Zagreb eccentricity index, eccentric connectivity index, ABC eccentricity index and GA eccentricity index (defined in the table given in the introduction part) are discussed in this section in detail. The first theorem here gives the general expression for any eccentricity-based topological index of type II.

Theorem 3.1: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Suppose $\Theta_{II}^e = \sum\limits_{uv \in E(G)} \theta\big(e(u), e(v)\big)$ be an eccentricity-based topological index of type II. Then

$$\Theta_{II}^e = m_1 n_1 \theta(2,2) + \left(m_1 \sum_{j=2}^{h} n_j + n_1 \sum_{i=2}^{h} m_i \right) \theta(2,3) + \left(\sum_{j=2}^{h-1} \sum_{i=2}^{h-j+1} n_j m_i \right) \theta(3,3) \tag{5}$$

Proof: Let $V_1 = V_{11} \cup V_{12} \cup ... \cup V_{1h}$ and $V_2 = V_{21} \cup V_{22} \cup ... \cup V_{2h}$. Since $p, q > 1$, it is true that $G \neq K_{1,n-1}$. As discussed in the earlier proofs, for any vertex v in G, $e(v) = 2$, if $v \in V_{11}$ or $v \in V_{21}$ and $e(v) = 3$, otherwise. Further, any vertex $u \in V_{1i}$ is adjacent with all the vertices of $V_{21} \cup V_{22} \cup ... \cup V_{2(h-i+1)}$. Since the summation runs over only those pairs of vertices which are adjacent with each other, the possible adjacent vertex pairs (u, v) with respective eccentricities, contributing nonzero terms in the summation are given below:

i. $u \in V_{11}$ and $v \in V_{21}$ such that $e(u) = e(v) = 2$.
ii. $u \in V_{11}$ and $v \in V_2 \setminus V_{21}$ such that $e(u) = 2, e(v) = 3$.
iii. $u \in V_1 \setminus V_{11}$ and $v \in V_{21}$ such that $e(u) = 3, e(v) = 2$.
iv. $u \in V_1 \setminus V_{11}$ and $v \in V_2 \setminus V_{21}$ such that $e(u) = e(v) = 3$.

Thus, $\Theta_{II}^e = T_1\theta(2,2) + T_2\theta(2,3) + T_3\theta(3,3)$, where T_1, T_2 and T_3 are the number of pairs of adjacent vertices both of which have eccentricity 2, the number of pairs of adjacent vertices in which one of them has eccentricity 2 and the other has eccentricity 3, and the number of pairs of adjacent vertices both of which have eccentricity 3, respectively. On enumerating T_1, T_2, T_3, using the definition of chain graphs, we get $T_1 = m_1 n_1$, $T_2 = m_1 \sum\limits_{j=2}^{h} n_j + n_1 \sum\limits_{i=2}^{h} m_i$ and $T_3 = \sum\limits_{j=2}^{h-1} \sum\limits_{i=2}^{h-j+1} n_j m_i$. ■

In the proof discussed above, one can note that the number of dominating vertices plays a significant role as they are the only vertices of eccentricity 2. The other non-dominating vertices play the same role irrespective of the cell V_{1i} or V_{2i} for $2 \leq i \leq h$ to which it belongs. Thus, we simplify the above expression and obtain a new one in terms of the number of dominating vertices and the number of edges.

Corollary 3.2: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Let M be the number of edges in G. Then

$$\Theta_{II}^e = m_1 n_1 \theta(2,2) + (m_1 q + n_1 p - 2 m_1 n_1)\,\theta(2,3) + (M + m_1 n_1 - m_1 q - n_1 p)\,\theta(3,3) \tag{6}$$

Proof: It is true that $\sum\limits_{i=2}^{h} m_i = p - m_1$ and $\sum\limits_{j=2}^{h} n_j = q - n_1$. The terms T_1 and T_2 enumerates all the edges of G which is incident on at least one of V_{11} or V_{21}. Specifically, T_1 enumerates the edges whose end vertices are in V_{11} and V_{22}.The term T_2 enumerates all the edges whose end vertices are in $V_{11}, V_2 \setminus V_{22}$ and $V_{22}, V_1 \setminus V_{11}$. Thus $T_1 = m_1 n_1$ and $T_2 = m_1(q - n_1) + n_1(p - m_1)$. The term T_3 is the number of edges in G which are not included in both T_1 and T_2, that is $T_3 = M - T_1 - T_2 = M + m_1 n_1 - m_1 q - n_1 p$. ■

Corollary 3.3: Let $G(V_1 \cup V_2, E)$ be a half graph of order $n \geq 2$. Then

$$\Theta_{II}^e = \theta(2,2) + (n-2)\theta(2,3) + \left(\frac{n^2 - 6n + 8}{8} \right) \theta(3,3) \tag{7}$$

Proof: By definition of ahalf graph $|V_1| = |V_2| = \frac{n}{2}$. Further, the $\frac{n}{2}$ vertices in $|V_1|$ have degree given by $\frac{n}{2}, \frac{n}{2} - 1, \frac{n}{2}, \ldots, 2, 1$. Thus, the number o edges in G is $\frac{n^2+2n}{8}$. On substituting $m_1 = n_1 = 1$ and $M = \frac{n^2+2n}{8}$ in Corollary 3.2, we get the result. ■

We refer the three terms of the Corollary 3.2 as T_1, T_2 and T_3 further, that is $T_1 = m_1 n_1$, $T_2 = m_1(q - n_1) + n_1(p - m_1)$ and $T_3 = M + m_1 n_1 - m_1 q - n_1 p$. On substituting appropriate θ, one can get any eccentricity-based topological index of type II from the class Θ_{II}^e. The second Zagreb index $\xi_2(G)$, the eccentric connectivity index $\xi^c(G)$, the ABC eccentricity index $ABC^e(G)$, the GA eccentricity index $GA^e(G)$ can be obtained as follows.

$$\xi_2(G) = 4T_1 + 6T_2 + 9T_3 = 9M - 3\,(m_1q + n_1p) + m_1n_1 \tag{8}$$

$$\xi^c(G) = 4T_1 + 5T_2 + 6T_3 = 6M - m_1q - n_1p \tag{9}$$

$$\begin{aligned} ABC^e(G) &= \frac{1}{\sqrt{2}}\,(T_1 + T_2) + \frac{2}{3}T_3 \\ &= \frac{3 - 2\sqrt{2}}{3\sqrt{2}}\,(m_1q + n_1p - m_1n_1) + \frac{2M}{3} \end{aligned} \tag{10}$$

$$\begin{aligned} GA^e(G) &= T_1 + \frac{2\sqrt{6}}{5}T_2 + T_3 \\ &= \frac{2\sqrt{6} - 5}{5}\,(m_1q + n_1p - 2m_1n_1) + M \end{aligned} \tag{11}$$

It is natural to consider whether or not there is a relationship between several topological indices of the same kind when they are defined. Upon computing these several numerical descriptors for a given graph, it could be discovered that they have some relationship, which is described in the next theorem.

Theorem 3.4: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Let $\xi_2(G), \xi^c(G), ABC^e(G)$ and $GA^e(G)$ be the second Zagreb eccentricity index, Eccentric connectivity index, ABC eccentricity index and GA eccentricity index of G, respectively. Then

$$ABC^e(G) < GA^e(G) < \xi^c(G) \leq \xi_2(G)$$

Proof: From Equations 10 and 11, we have

$$\begin{aligned} GA^e(G) - ABC^e(G) &= T_1 + \frac{2\sqrt{6}}{5}T_2 + T_3 - \\ &\qquad \frac{1}{\sqrt{2}}(T_1 + T_2) - \frac{2}{3}T_3 \\ &= \left(1 - \frac{1}{\sqrt{2}}\right)T_1 + \\ &\qquad \left(\frac{2\sqrt{6}}{5} - \frac{1}{\sqrt{2}}\right)T_2 + \frac{1}{3}T_3 \end{aligned}$$

where $T_1 = m_1n_1$, $T_2 = m_1(q - n_1) + n_1(p - m_1)$ and $T_3 = M - T_2 - T_1 = M + m_1n_1 - m_1q - n_1p$. Since each of V_i for $i = 1, 2$ has at least one dominating vertex, $m_1, n_1 > 0$, it is true that $T_1 > 0$. Also, since $p \geq m_1, q \geq n_1$ and $M > 0$, it follows that $T_2 \geq 0$. Similarly, $T_3 = M - T_1 - T_2 \geq 0$. Thus $(\frac{\sqrt{2}-1}{\sqrt{2}})T_1 > 0$, $\left(\frac{2\sqrt{12}-5}{5\sqrt{2}}\right)T_2 \geq 0$ and $\frac{1}{3}T_3 \geq 0$ and hence $GA^e(G) - ABC^e(G) > 0$. This implies $ABC^e(G) < GA^e(G)$.
Similarly, consider

$$\begin{aligned} \xi^c(G) - GA^e(G) &= 4T_1 + 5T_2 + 6T_3 - T_1 - \tfrac{2\sqrt{6}}{5}T_2 - T_3 \\ &= 3T_1 + \left(\tfrac{25 - 2\sqrt{6}}{5}\right)T_2 + 5T_3 > 0 \end{aligned}$$

Thus, $GA^e(G) < \xi^c(G)$.
Similarly, $\xi_2(G) - \xi^c(G) = T_2 + 3T_3 \geq 0$ and $\xi^c(G) \leq \xi_2(G)$ ∎

IV. Bounds for indices from the class $\{\Theta^e_{II}\}$

The bounds for some eccentricity-based topological indices from the class $\{\Theta^e_{II}\}$ are obtained in this section. In an attempt to do the same, we began with the study of variation of respective indices on addition of edges, for graphs of prescribed order. Before moving to the bounds, the results concerned with change in indices on addition of edges is given. Since the expression for the indices is prominently depending only on m_1, n_1, the variation of m_1, n_1 on adding the edges play crucial role, rather than the other values m_i, n_j for $i, j > 1$. These variations are given in detail in the following theorems separately for the cases $h > 2$ and $h = 2$.

Theorem 4.1: Let $G(m_1, m_2; n_1, n_2)$ be a chain graph of order n on M edges with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$. Let $u \in V_{12}$ and $v \in V_{22}$ where $u \nsim v$. Let $\Theta^e_{II} \in \{\Theta^e_{II}\}$. Then $\Theta^e_{II}(G + e)$ is

$$\begin{cases} \Theta^e_{II}(G) + (m_1 + n_1 + 1) & \\ \theta(2,2) + (n - 2m_1 - 2n_1 & \\ -2)\theta(2,3) & if \;\; |V_{12}| = |V_{22}| = 1 \\ \Theta^e_{II}(G) + n_1\theta(2,2) + & \\ (q - 2n_1)\theta(2,3) + & \\ (n_1 - q + 1)\theta(3,3) & if \;\; |V_{22}| = 1, |V_{12}| > 1 \\ \Theta^e_{II}(G) + m_1\theta(2,2) + & \\ (p - 2m_1)\theta(2,3) + & \\ (m_1 - p + 1)\theta(3,3) & if \;\; |V_{22}| > 1, |V_{12}| = 1 \\ \Theta^e_{II}(G) + \theta(3,3) & else \end{cases} \tag{12}$$

Proof: Let $G + e = DNG(m'_1, m'_2; n'_1, n'_2)$, where $m'_1 = |V'_{11}|, m'_2 = |V'_{12}|$ and $n'_1 = |V'_{21}|, n'_2 = |V'_{22}|$. Then $m'_1 \geq m_1$ and $n'_1 \geq n_1$. Clearly, $u \in V_{12}$ and $v \in V_{22}$ as V_{11}, V_{21} contain dominating vertices and no more edges can be added to the vertices of V_{11}, V_{21}. Then the following cases are considered.

- Case i: $|V_{12}| = |V_{22}| = 1$: Then on adding an edge e in G, we get $V'_{11} = V_{11} \cup \{u\}$ and $V'_{21} = V_{21} \cup \{v\}$ and $G = DNG(m_1 + 1; n_1 + 1)$. Thus $m'_1 = m_1 + 1$, $n'_1 = n_1 + 1$. On substituting m'_1, n'_1 in Equation 7, we get $\Theta^e_{II}(G + e)$. One can note that the coefficient of $\theta(3,3)$, T'_3 in $\Theta^e_{II}(G+e)$ is same as that of T_3, the coefficient of $\theta(3,3)$ in $\Theta^e_{II}(G)$.
- Case ii: $|V_{12}| > 1$ and $|V_{22}| = 1$: Then on adding the edge $e = uv$ in G, we get $V'_{11} = V_{11} \cup \{u\}$ and $V'_{22} = V_{22} = \{v\}$. Thus $m'_1 = m_1 + 1$, $n'_1 = n_1$.
- Case iii: $|V_{12}| = 1$ and $|V_{22}| > 1$: Results in $m'_1 = m_1$ and $n'_1 = n_1 + 1$
- Case iv: $|V_{12}| > 1$ and $|V_{22}| > 1$: Results in $m'_1 = m_1$, $n'_1 = n_1$.

∎

Theorem 4.2: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph with $|V_1| = p$ and $|V_2| = q$, where $p, q > 1$ and $h > 2$. Let

$u \in V_1$ and $v \in V_2$ such that $u \nsim v$ and $e = uv$. Then

$$\Theta^e_{II}(G{+}e) = \begin{cases} \Theta^e_{II}(G) + n_1\theta(2,2) + (q - 2n_1) \\ \theta(2,3) + (n_1 - q + 1)\theta(3,3) & if \;\; u \in V_{12}, \\ & v \in V_{2h}, \\ & |V_{2h}| = 1 \\ \Theta^e_{II}(G) + \theta(3,3) & else \end{cases} \quad (13)$$

Proof: Let $G + e = DNG(m'_1, m'_2, ..., m'_h; n'_1, n'_2, ..., n'_h)$, where $m'_i = |V'_{1i}|$ and $n'_j = |V'_{2j}|$ for $1 \le i \le h$ and $1 \le j \le h$. Since $h > 2$, if $u \in V_{1i}$ and $v \in V_{2j}$ for $i, j > 2$, then on adding the edge $e = uv$, either a new cell is created or the vertices u, v are added to the previous cells $V_{1(i-1)}$ or $V_{2(j-1)}$. In all these cases, neither m_1 and n_1 are affected. Thus $m'_1 = m_1$ and $n'_1 = n_1$. On substituting in 7, we get $\Theta^e_{II}(G + e) = \Theta^e_{II}(G) + \theta(3, 3)$.
Now, we consider the instance of $u \in V_{1i}$ and $v \in V_{2j}$ for $i = j = 2$ and look into all the possible cases. When $|V_{12}| = |V_{2h}| = 1$, since $h > 2$, on adding the edge $e = uv$, only V_{11}, V_{12}, V_{2h}, $V_{2(h-1)}$ are affected. That is, $V'_{11} = V_{11} \cup \{u\}$, $V'_{12} = \emptyset$,$V'_{2(h-1)} = V_{2(h-1)} \cup \{v\}$ and $V'_{2h} = \emptyset$. This results in $m'_1 = m_1 + 1$ and $n'_1 = n_1$. Similarly, all the other cases are listed in below.

Case i: When $|V_{12}| = 1$, $|V_{2h}| = 1$: The cells affected are $V'_{11} = V_{11} \cup \{u\}$, $V'_{12} = \emptyset$, $V'_{2(h-1)} = V_{2(h-1)} \cup \{v\}$, $V'_{2h} = \emptyset$ and hence $m'_1 = m_1 + 1$, $n'_1 = n_1$.

Case ii: When $|V_{12}| > 1$
$|V_{2h}| = 1$: $V'_{11} = V_{11} \cup \{u\}$, $V'_{12} = V_{12} \setminus \{u\}$, $V'_{2(h-1)} = V_{2(h-1)} \cup \{v\}$, $V'_{2h} = \emptyset$. Hence $m'_1 = m_1 + 1$ and $n'_1 = n_1$.

Case iii: When $|V_{12}| = 1$
$|V_{2h}| > 1$: $V'_{11} = V_{11}$, $V'_{12} = V_{12}$, $V'_{2(h-1)} = V_{2(h-1)}$, $V'_{2h} = V_{2h}$. Hence $m'_1 = m_1$ and $n'_1 = n_1$

Case iv: When $|V_{12}| > 1$
$|V_{2h}| > 1$: $V'_{11} = V_{11}$, $V'_{12} = \{u\}$, $V'_{2(h-1)} = \{v\}$, $V'_{2h} = V_{2h}$. Hence $m'_1 = m_1$ and $n'_1 = n_1$

On substituting these variations of m_1, n_1 in Equation 7 one can get $\Theta^e_{II}(G + e)$ in terms of $\Theta^e_{II}(G)$. ■

Now, on substituting the suitable function $\theta(x, y)$, we obtain variations for the second Zagreb eccentricity index, eccentric connectivity index, ABC eccentricity index, GA eccentricity index. The cases when the end vertices of the edge $e = uv$ join the vertices of the cells V_{12}, V_{2h} have different subcases. The remaining possibilities of connecting vertices of other cells do not make any difference(as mentioned in the proof of Theorem 4.2). For the sake of simplicity, for the edge $e = uv$ satisfying the condition $C : u \in V_{12}, v \in V_{2h}$, we write $e \sim C$.

The second Zagreb eccentricity index $\xi_2(G + e) =$:

$$\begin{cases} \xi_2(G) - 2n + 8 & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, \\ & h = 2 \\ \xi_2(G) + n_1 - 3q + 9 & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, \\ & h > 2 \text{ or } e \sim C, |V_{12}| > 1, \\ & |V_{2h}| = 1, h \ge 2 \\ \xi_2(G) + m_1 - 3p + 9 & \text{if } e \sim C, |V_{12}| = 1, |V_{2h}| > 1, \\ & h = 2 \\ \xi_2(G) + 9 & else \end{cases} \quad (14)$$

The eccentric connectivity index: $\xi^c(G + e) =$

$$\begin{cases} \xi^c(G) + 6 - n & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, \\ & h = 2 \\ \xi^c(G) - q + 6 & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, \\ & h > 2 \text{ or } e \sim C, |V_{12}| > 1, \\ & |V_{2h}| = 1, h \ge 2 \\ \xi^c(G) - p + 6 & \text{if } e \sim C, |V_{12}| = 1, |V_{2h}| > 1, \\ & h = 2 \\ \xi^c(G) + 6 & else \end{cases} \quad (15)$$

ABC eccentricity index : $ABC^e(G + e) =$

$$= \begin{cases} ABC^e(G) + \frac{1}{\sqrt{2}} & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1 \text{ or} \\ & e \sim C, |V_{12}| > 1, |V_{2h}| = 1 \text{ or} \\ & e \sim C, |V_{12}| = 1, |V_{2h}| > 1, h = 2 \\ ABC^e(G) + \frac{2}{3} & else \end{cases} \quad (16)$$

GA eccentricity index: $GA^e(G + e) =$

$$\begin{cases} GA^e(G) + c_1 n + c_2 & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, h = 2 \\ GA^e(G) + c_1 q + c_2 & \text{if } e \sim C, |V_{12}| = |V_{2h}| = 1, h > 2 \\ & \text{ or } e \sim C, |V_{12}| > 1, |V_{2h}| = 1, \\ & h \ge 2 \\ GA^e(G) + c_1 p + c_2 & \text{if } e \sim C, |V_{12}| = 1, |V_{2h}| > 1, \\ & h = 2 \\ GA^e(G) + 1 & else \end{cases} \quad (17)$$

where c_1, c_2 are constants given by $c_1 = \left(\frac{5-2\sqrt{6}}{5}\right)$ and $c_2 = \left(\frac{4\sqrt{6}-5}{5}\right)$.

From Equations 16 and 17, one can note that these indices increase all the time whenever an edge is added irrespective of where it is added. Unlike these, the second Zagreb eccentricity index and the eccentric connectivity index may increase or decrease. This is an important observation, very helpful in giving the extremities for these indices.

Theorem 4.3: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n. Let $ABC^e(G)$ be the atom bond connectivity eccentricity index of G. Then

$$ABC^e(G) \leq \begin{cases} \dfrac{n^2}{4\sqrt{2}} & \text{if n is even} \\ \dfrac{n^2-1}{4\sqrt{2}} & \text{else} \end{cases}$$

$$ABC^e(G) \geq \frac{n-1}{\sqrt{2}}$$

Proof: From Equation 10, $ABC^e(G) = \frac{3-2\sqrt{2}}{3\sqrt{2}}(m_1q + n_1p - m_1n_1) + \frac{2M}{3}$. Further as $ABC^e(G+e) > ABC^e(G)$, it reaches the maximum (minimum) when the number of edges M in G is the maximum (minimum). A chain graph $G(V_1 \cup V_2, E)$ has the maximum number of edges when it is a complete bipartite graph with $|V_1| = |V_2|$, if $|V_1| + |V_2|$ is even and $|V_1| - |V_2| = 1$ when $|V_1| + |V_2|$ is odd. That is, $M = \frac{n^2}{4}$, if n is even and $M = \frac{n^2-1}{4}$, if n is odd. If n is even, then for the extremal graph $G = DNG(\frac{n}{2}; \frac{n}{2})$ (the complete bipartite graph), on substituting $p = q = \frac{n}{2}, m_1 = n_1 = \frac{n}{2}$ and $M = \frac{n^2}{4}$, we get $ABC^e(G) \leq \frac{n^2}{4\sqrt{2}}$. If n is odd, the extremal graph $G = DNG(\frac{n+1}{2}; \frac{n-1}{2})$ has $p = m_1 = \frac{n+1}{2}$ and $q = n_1 = \frac{n-1}{2}$. On substituting in Equation 10, we get $ABC^e(G) \leq \frac{n^2-1}{4\sqrt{2}}$. Similarly, for a chain graph, $ABC^e(G)$ is the minimum when G is a bi-star graph $DNG(1, p-1; 1, q-1)$ as it is a tree with the minimum number of edges $M = n-1$. Thus, from Equation 10, $ABC^e(G) = \frac{n-1}{\sqrt{2}}$. ∎

Since $GA^e(G+e) > GA^e(G)$, similarly, one can obtain the bounds for the GA eccentricity index of a chain graph G, which is stated in the theorem below.

Theorem 4.4: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n. Let $GA^e(G)$ be the geometric arithmetic eccentricity index of G. Then

$$GA^e(G) \leq \begin{cases} \dfrac{n^2}{4} & \text{if n is even} \\ \dfrac{n^2-1}{4} & \text{else} \end{cases}$$

$$GA^e(G) \geq \frac{2\sqrt{6}}{5}(n-2) + 1$$

Unlike ABC eccentricity index and GA eccentricity index, the second Zagreb eccentricity index and the eccentric connectivity index does not always increase with edge addition. Now, we have the theorems giving the upper and the lower bound for these two indices.

Theorem 4.5: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p + q = n$. Let $\xi^c(G)$ be the eccentric connectivity index of G. Then

$$\xi^c(G) \leq \begin{cases} 4pq & \text{if } n \leq 6 \\ 4pq + n - 6 & \text{else} \end{cases}$$

$$\xi^c(G) \geq 5n - 6$$

Proof: By Equation 9, one can note that $\xi^c(G)$ attains the maximum when the number of edges in graph is as maximum as possible, that is, when G has the maximum number of dominating vertices. One of the best possibilities is that when all the vertices in G are dominating, that is $G = DNG(p; q)$ with $M = pq$. The next better option is when $M = pq - 1$ and $G = DNG(p-1, 1; q-1, 1)$. Also one can note that the graph $DNG(p; q)$ is obtained from $DNG(p-1, 1; q-1, 1)$ by adding an edge. That is, $DNG(p; q) = DNG(p-1, 1; q-1, 1) + e$, where e is an edge joining the two non-dominating vertices of $DNG(p-1, 1; q-1, 1)$. But from Equation 15, on adding the edge e, the index increases only when $n = p+q > 6$ (refer to the case 1 of Equation 15). Thus $DNG(p-1, 1; q-1, 1) < DNG(p; q)$, whenever $n > 6$. Thus

$$\xi^c(G) \leq \xi^c(DNG(p-1, 1; q-1, 1)) \leq 4pq + n - 6 \text{ when } n > 6$$

When $n \leq 6$,

$$\xi^c(G) \leq \xi^c(DNG(p; q)) \leq 4pq$$

Similarly, $\xi^c(G)$ is the minimum when $m_1 = n_1 = 1$ and $G = DNG(1, p-1; 1, q-1)$. Thus $\xi^c(G) \geq 5n - 6$. ∎

Lastly, we have the second Zagreb eccentricity index.

Theorem 4.6: Let $G(V_1 \cup V_2, E) = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$ be a chain graph of order n with $|V_1| = p$ and $|V_2| = q$, where $p+q = n$. Let $\xi_2(G)$ be the second Zagreb eccentricity index of G. Then

$$\xi_2(G) \leq \begin{cases} 4pq & \text{if } n \leq 4 \\ 4pq + 2n - 8 & \text{else} \end{cases}$$

$$\xi_2(G) \geq 6n - 8$$

V. Concluding remarks

The eccentricity-based topological indices are that domain of molecular chemistry which is currently being explored extensively by various chemists and mathematicians. This article categorizes the eccentricity-based indices into two classes $\{\Theta_I^e\}$ and $\{\Theta_{II}^e\}$. A detailed study of the same is done for a special class of graphs called chain graphs. There are numerous eccentricity-based topological indices that are unexplored, especially belonging to the second class $\{\Theta_{II}^e\}$, a study of which can be a good direction for future work. Further, one can study extended matrices of chain graphs corresponding to these topological indices.

References

[1] Abdullah Alazemi, Milica Andelic, Tamara Koledin, Zoran Stanic, "Eigenvalue-free intervals of distance matrices of threshold and chain graphs." *Linear and Multilinear Algebra*, vol. 69, no. 16, pp. 2959–2975, 2019.
[2] Ebrahim Ghorbani, "Some spectral properties of chain graphs," *arXiv:1703.03581v1[math.CO]*, 2017.
[3] Amitava Bhattacharya, Shumel Friedland, Uri N. Peled, On the First Eigenvalues of Bipartite Graphs, *The electronic journal of combinatorics*, vol. 15, 2008.
[4] Shahistha Hanif, K. Arathi Bhat and Sudhakara G, "Some Properties of Chain and Threshold Graphs," *Journal of the Indian Mathematical Society*, vol. 90, no. 1-2, pp.75–84, 2023.
[5] M.Anelica, E.Andradea, D.M.Cardosoa, C.M.da Fonsecab, S.K.Simic, D.V.Tosice, Some new considerations about double nested graphs, *Linear Algebra and Applications*, vol. 483, pp. 323–341, 2015.
[6] Francis K. Bell, Drago Cvetkovic, Peter Rowlinson, Slobodan K. Simic, "Graphs for which the least Eigen value is minimal," *Linear Algebra and its Applications*, vol. 429, pp. 2168—2179, 2008.
[7] Milica Andelic, Carlos M. da Fonseca, Slobodan K. Simic, Dejan V. Tosic, "Connected graphs of fixed order and size with maximal Q-index: Some spectral bounds," *Discrete Applied Mathermatics*, vol. 60, no. 4-5, pp. 448–459, 2011.
[8] Fernando Tura, "Counting Spanning trees in Double nested graphs," *arXiv:1605.04760v1 [math.CO]*, 2016.

[9] L. Li, X. Li, W. Liu, ”Note on the product of Wiener and Harary indices,” *MATCH Commun. Math. Comput. Chem*, vol. 91, pp. 299—305, 2024.
[10] Babujee, J. Baskar, and S. Ramakrishnan, ”Topological indices and new graph structures,” *Applied Mathematical Sciences*, vol. 6, no. 108, pp. 5383–5401, 2012.
[11] Alaeiyan, M., Sardar, M.S., Zafar, S., Zahid, Z. and Farahani, M.R., ”Computation of topological indices of line graph of Jahangir Graph,” *International Journal of Applied Mathematics*, vol. 18, pp. 91–107, 2018.
[12] Ali, A., Bhatti, A. A., and Raza, Z. ”Further inequalities between vertex-degree-based topological indices,” *International Journal of Applied and Computational Mathematics*, vol. 3, pp. 1921–1930, 2017.
[13] Mondal, S., De, N. and Pal, A., ”Topological properties of Graphene using some novel neighborhood degree-based topological indices,” *International Journal of Mathematics for Industry*, vol. 11, no. 01, pp. 1950006, 2019.
[14] Cruz, R., Perez, T. and Rada, J., ”Extremal values of vertex-degree-based topological indices over graphs,” *Journal of Applied Mathematics and Computing*, vol. 48, pp. 395-406, 2015.
[15] Jose Luis Palacios, More on topological indices and their reciprocals, *MATCH Commun. Math. Comput. Chem*, vol. 92, no. 1, pp. 53-63, 2024.
[16] V Kumar, S Das, ”On structure sensitivity and chemical applicability of some novel degree based topologoical indices,” *MATCH Commun. Math. Comput. Chem*, vol. 92, no. 1, pp. 165-203, 2024, .
[17] Ivan Gutman, ”Geometric Approach to Degree–Based Topological Indices: Sombor Indices,” *MATCH Commun. Math. Comput. Chem*, vol. 86, pp. 11–16, 2021.
[18] K. Arathi Bhat, Shahistha Hanif and Sudhakara G, ”Metric dimension and its variations of Chain Graphs,” *Proceedings of Jangjeon Mathematical Society*, vol. 24, no. 3, pp. 309–321, 2021.
[19] Shahistha, K. Arathi Bhat and Sudhakara G, ”Wiener Index of Chain Graphs,” *IAENG International Journal of Applied Mathematics*, vol. 50, no. 4, pp. 783–790, 2020.
[20] K. Arathi Bhat and Shahistha Hanif, ”Forbidden Values for Wiener Indices of Chain /Threshold Graphs,” *Engineering Letters*, vol. 31, no. 1, pp. 180–185, 2023.
[21] Shahistha Hanif, ”Inverse Harary Index Problem for Chain Graphs,” *Engineering Letters*, vol. 32, no. 4, pp. 812–817, 2024.

Balkishbanu Khaji received her B. Sc. Degree from Karnataka University, Dharwad, Karnataka India, in 2021. and M. Sc. degree from from the same university in 2011. At present she is persuing PhD in the Department of Mathematics at Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal. Her research interests include Algebraic graph theory, Network theory and Combinatorics.

Shahistha received her B. Sc. Degree from Mangalore University, Mangalore, in 2012 and M. Sc. degree from Manipal Academy of Higher Education, Manipal, in 2014. She then received her Ph.D. from Manipal Academy of Higher Education, Manipal, in 2022. At present she is working as an Assistant Professor in the Department of Mathematics at Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal. Her research interests include Graph theory and Network theory.

K Arathi Bhat received her B. Sc. Degree from Mangalore University, Mangalore, India, in 2000. and M. Sc. degree from Manipal Academy of Higher Education, Manipal, in 2011. She then received her Ph.D. from Manipal Academy of Higher Education, Manipal, in 2018. At present she is working as an Associate Professor in the Department of Mathematics at Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal. Her research interests include Algebraic graph theory, Network theory and Combinatorics.