MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **97** (2027) 1147–1175
ISSN: 0340–6253
doi: 10.46793/match.97-3.10326

A Novel Relationship Between Well-Known Indices: Sombor, Mostar, and Zagreb Indices

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(Received March 23, 2026)

Abstract

Graph descriptors such as normalized Laplacian energy, Sombor index, Mostar index and Zagreb index are often employed in various scientific contexts. The Sombor index is essential in chemical graph theory because it provides insights into molecule stability and reactivity by analyzing the distribution of atom degrees and distances. By measuring molecular graph topology, the Zagreb indices are vital tools in mathematical chemistry that help predict molecules' physical and chemical characteristics. This manuscript aims to broaden the characterization of extremal graphs, achieving upper sharp bounds for the Mostar and first Zagreb index with given parameters such as cut edges and girth.

Let χ_n^k be the set of all n-vertex graphs with exact chromatic number k. Das and Shang characterized graphs achieving the maximum Sombor index of graphs in χ_n^k in terms of chromatic number. This paper extends the characterized graphs, achieving the minimum Sombor of graphs in χ_n^k in terms of chromatic number. Furthermore, by employing Rayleigh's quotient principle, we present a first-ever comparison between the normalized Laplacian energy and

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the Sombor and first Zagreb indices in terms of eigenvalues. To extend our results, we suggest some open problems to contribute in the direction of extremal graph theory.

1 Introduction

Spectral graph theory offers a robust structure for a comprehensive understanding of the structural properties of graphs from the correlation of their eigenvalues and eigenvectors. Chemical graph theory, which deals with the representation of molecular structure by employing graphs, has attained significant consideration among the graph theories.

Quantitative structure-activity relationship and quantitative structure-property relationship research depend primarily on molecular descriptors, giving them an essential part of mathematical chemistry. Among those characteristics, so-called topological indices are of significant relevance. Considering that they summarize some of the characteristics of an atom in an individual term, they can quickly comprehend the fundamental thermodynamic aspects of synthetic structures. In the past decades, multiple topological indices have been developed and applied to use in the field of chemistry (for example, see references [8, 21, 22, 34]. Topological descriptors date back to the innovative research of Wiener [40] who employed the collection of all shortest paths of a (molecular) graph to characterize the physical characteristics of alkanes.

The dependency of complete π-electron energy upon the chemical graphs was discussed by Gutman and Trinajstić in 1972. The further detailed study can be read in [24]. Two well-known indices were established through this study named the first Zagreb invariant and the second Zagreb invariant, which is mathematically expressed as

$$M_1(G) = \sum_{u\sim v} \deg_G(u) + \deg_G(v),$$

$$M_2(G) = \sum_{u\sim v} \deg_G(u)\deg_G(v),$$

These well-known Zagreb indices extended the subdivision of the chemical carbon-atom structure. [4].

Motivated by this work, the Sombor index, a novel degree-based topological indicator, was introduced by Gutman [25]. For any graph G, the mathematical terminology of the Sombor descriptor is as follows,

$$SO(G) = \sum_{u \sim v} \sqrt{\deg_G(u)^2 + \deg_G(v)^2},$$

The Sombor index has acquired a large number of inquiries from mathematicians and theoretical chemists in a relatively short amount of time. For a statistical relationship of vaporization enthalpy and entropy in alkanes, Redžepović [37] examined the possible predictive power of the Sombor index. The Sombor index, well-known for its powerful prognostic capabilities, has also been applied to stimulate the physicochemical characteristics of synthetic structures. The reader interested in a rigorous mathematical explanation of the Sombor index of graphs is directed to [9, 10, 26, 31, 38].

One of the interesting properties in chemistry, which is used in complex networks, is called peripherality. The study of peripherality in a graph can be read here in detail. [5, 28–30]. In 2018, Došlić et al. [16] introduced an index named the Mostar index based on the concept of peripherality. An edge is considered to be peripheral if there are many more vertices closer to one of its end vertices than to the other one. More precisely, the absolute difference between the number of vertices closer to u than to v and the number of vertices closer to v than to u indicates a peripheral position of an edge in a graph. The mathematical representation of the Mostar index for any graph G is written as

$$M_o(G) = \sum_{uv \in E(G)} \left| n_G(u) - n_G(v) \right| ,$$

Since its introduction in 2018, the Mostar index has been exclusively studied by many researchers, particularly some of the interesting results concerning sparse graphs and trees can be read herein [2, 13], chemical graphs [14, 19], and hypercube-related graphs [17]. For detailed information regarding the Mostar index, we refer to the recent survey [1].

In 1978, Gutman [20] proposed energy of graph G based on the matrix named adjacency matrix, which is denoted by $A(G)$ such that $\lambda_1, \lambda_2, ..., \lambda_n$ its eigenvalues. The mathematical definition is illustrated as

$$E(G) = \sum_{k=1}^{n} |\lambda_k|, \tag{1}$$

The H$\ddot{u}$ckel chemical structure complete π-electron energy was one of the main reasons for establishing the energy index [35]. Graph energies or indices have an extensive range of uses. Unexpected uses for graph energies were discovered in engineering and research, including face recognition, protein sequence comparison, air travel, satellite communication, crystallography, and the processing of high-resolution satellite photos. Moreover, several experiments have been completed for medical applications. Another well-known index named Laplacian energy was proposed by Gutman and Zhou in 2006, which is defined by Laplacian matrix [23]. The Laplacian energy is expressed as

$$\mathcal{LE} = \sum_{k=1}^{n} \left| \lambda_k - \frac{2m}{n} \right|,$$

The normalized Laplacian matrix for any graph G, which is represented by $\mathcal{L}$, is mathematically written as

$$\mathcal{L} = \begin{cases} 1 & \text{if } u = v \text{ and } d_i \neq 0 \\ -\frac{1}{\sqrt{deg_G(u) deg_G(v)}} & \text{if } u \sim v \\ 0 & \text{otherwise} \end{cases}$$

$\mathcal{L} = I - D^{-\frac{1}{2}} A D^{\frac{1}{2}}$, is the relationship between adjacency and diagonal matrix for normalized Laplacian index, where D represents a diagonal matrix and A denotes the adjacency matrix for any graph.

Nikiforov [36] defined the concept of $\mathcal{M}$-energy for any graph G with a real symmetric matrix; say, $\mathcal{M}$ is defined as

$$\mathcal{E}_{\mathcal{M}}(G) = \sum_{k=1}^{n} \left| \lambda_k(\mathcal{M}) - \frac{T(\mathcal{M})}{n} \right|, \tag{2}$$

where $T(\mathcal{M})$ represents the trace of $\mathcal{M}$ and λ_k represents the eigenvalues such that $\lambda_1(\mathcal{M}) \leq \lambda_2(\mathcal{M}) \leq ... \leq \lambda_n(\mathcal{M})$. To introduce $\mathcal{L}$-energy for any graph G on normalized Laplacian matrix $\mathcal{L}$, replace normalized Laplacian matrix $\mathcal{L}$ with symmetric matrix $\mathcal{M}$ in Equation (2), which is explained as

$$\mathcal{E}_{\mathcal{L}}(G) = \sum_{k=1}^{n} |\lambda_k(\mathcal{L}) - 1| \ , \tag{3}$$

which is equivalent to

$$\mathcal{E}_{\mathcal{L}}(G) = \sum_{k=1}^{n} |\lambda_k(I - \mathcal{L})| \ , \tag{4}$$

2 Preliminaries and literature review

Consider that G is a connected graph with an edge set (resp. vertex set) symbolized as $E(G)$ (resp. $V(G)$). The collection of nodes (resp. edges) in a graph is equal to its order (resp. size), say n (resp. m). The collection of edges that are incident with a vertex j is called the degree of graph G, which is represented by $deg_G(j)$ or d_j. Assume that $G - e$ signifies the subgraph of G that is generated by deleting the edge e from $E(G)$. Adding the edge vu to $E(G)$ generates a graph denoted by $G + vu$, where v, u are nodes in $V(G)$ that are not adjacent to each other.

Coloring of graph G means giving each vertex a color such that no adjacent vertices possess the same color. The chromatic number of G is equal to the smallest possible number of colors in a coloring of G and is symbolized as $\chi(G)$.

Aouchiche and Hansen [3] characterized the bounds for the geometric-arithmetic index with the chromatic number of connected graphs. Ghorbani and Songhori [18] Computing multiplicative Zagreb indices with given chromatic and clique Numbers. Das and Shang [11] characterized graphs achieving the maximum chromatic number in terms of the Sombor index of graphs in χ_n^k.

Tepeh [39] characterized bicyclic graphs concerning the Mostar index. Xiao et al. [41, 42] characterized graphs achieving the first three maximal and minimum hexagonal chains for the Mostar index. Deng and Li [15] defined extremal graphs for trees with a given degree sequence with respect to the Mostar index. Li and Deng [33] characterized extremal graphs for unicyclic graphs with a given diameter. Hosamani and Basavanagoud [27] defined upper bounds for the first Zagreb index. Borovićanin and Furtula [6] characterized extremal graphs for the first Zagreb index. Motivated by existing literature related to the Mostar index and first Zagreb index [15, 33, 39, 41, 42], and [6, 27], we extend the existing literature to novel results for all $n-$ vertex graphs with given cut edges and girth and compare the characterization with the first Zagreb index with given girth.

Motivated by existing literature concerning the Sombor index [9,10,26, 31,38], we extend [11] to the sharp lower bounds for the Sombor index in terms of chromatic number. Moreover, we establish a first-ever relationship between the Sombor index and the first Zagreb index with the normalized Laplacian energy index in terms of eigenvalues by integrating Rayleigh's quotient principle.

The structure of the paper is follows as: In Sections 1 and 2, we briefly explain the introduction and some related definitions. In Section 3, we present lower bounds for the Sombor index with a given chromatic number. In Sections 4,5 and 6, we characterize extremal graphs, achieving upper bounds for the Mostar index and Zagreb index with fixed parameters such as cut edges and girth. In Sections 7 and 8, we extend the previous results towards a novel direction to establish a relationship between Sombor and Zagreb indices with normalized Laplacian energy by employing Rayleigh's quotient principle and characterizing the extremal graphs, attaining the sharp bounds.

3 Sharp lower bounds of Sombor index with given chromatic number

Here, we determine the minimum Sombor invariant in χ_n^k by implementing auxiliary results from section 3.1. Graphs attaining the lower bound have also been classified. For $n, k \geq 1$, suppose K_k is a complete graph of order k with vertex $v \in K_k$. The family K_n^k is acquired by adjoining a path

$\mathbb{P}_{n-k+1}$ with the vertex $v \in K_k$. Denote by $\mathcal{K}_k^{(n-k)}$ the graph generated by the adjoining vertex of K_k with an isolated vertex of path $\mathbb{P}_{n-k+1}$.

3.1 Auxiliary results

We begin with fundamental lemmas regarding the Sombor invariant for any graph.

Lemma 1. *[32] Consider any graph with vertices n, say G. $SO(G-uv) < SO(G)$ if $uv \in E(G)$.*

Theorem 1. *[32] Consider any connected graph with vertices n, say G. We obtain*

$$SO(P_n) \leq SO(G) \leq SO(K_n)$$

where left and right equalities are satisfied if and only if $G \cong P_n$ and $G \cong K_n$.

Lemma 2. *[23] If G is a regular graph then $LE(G) = E(G)$.*

Theorem 2. *[12] Consider that any tree T such that T is not isomorphic to P_n with $n \geq 4$. We have $SO(T) > (n-1)\sqrt{8}$.*

Lemma 3. *Let $G^{'}$ be the smallest graph in χ_n^k. Let $G^{''} \subseteq G^{'}$ with $V(G^{''}) = V(G^{'})$ and $G^{''} - E(K_k) \cong \{T_1, T_2, ..., T_k\}$, such that $|V(T_k)| = \eta_i$, $(1 \leq i \leq k)$ and $\eta_1 + \eta_2 + ... + \eta_k = n$, where, $\eta_1 \geq \eta_2 ... \geq \eta_k$.*

Case 1.

$$\sum_{u_p u_q \in E(T_i)} \sqrt{\deg G''(u_p)^2 + \deg_{G''}(u_q)^2} \geq (\eta_i - 1)\sqrt{8}, \tag{5}$$

with equality if $\eta_i = 1$ for some $4 \leq i \leq k$.

Case 2.

$$\sum_{u_p u_q \in E(T_1)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2} \geq \begin{cases} \sqrt{k^2+1}, & \eta_1 = 2, \\ \sqrt{k^2+4+(\eta_1-3)\sqrt{8}+\sqrt{5}}, & \eta_1 \geq 4. \end{cases} \tag{6}$$

where equality satisfied if and only if T_1 is isomorphic to P_{η_1} and $\deg_{T_1}(u_1) = 1$.

Proof of Case 1. Consider that

$$Z_i = \sum_{u_p u_q \in E(t_i)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2},$$

$Z_i = (\eta_i - 1)\sqrt{8} = 0$, if $\eta_i = 1$, for some $2 \leq i \leq k$. Similarly, if $\eta_i = 2$, then $Z_i = (\eta_i - 1)\sqrt{8}$, for $2 \leq i \leq k$.

Subcase 1.1 Next, the Equation (5) is satisfied for $k \geq 4$. Otherwise $\eta_i \geq 4$, consider that $T_i \cong P_{\eta_i}$. Then there are two possibilities either $\deg_{T_i}(u_i) = 1$, or $\deg_{T_i}(u_i) = 2$. If $\deg_{T_i}(u_i) = 1$, then

$$Z_i = \sqrt{k^2+4} + (\eta_i - 3)\sqrt{8} + \sqrt{5} \geq (\eta_i - 1)\sqrt{8},$$

for $k \geq 4$, then $\sqrt{20} + \sqrt{5} > 2\sqrt{8}$. If $\deg_{T_i}(u_i) = 2$, then

$$Z_i = \sqrt{k^2+4} + \sqrt{k^2+1} + (\eta_i - 4)\sqrt{8} + \sqrt{5} \geq (\eta_i - 1)\sqrt{8},$$
$$Z_i = 2\sqrt{k^2+4} + (\eta_i - 5)\sqrt{8} + 2\sqrt{5} \geq (\eta_i - 1)\sqrt{8},$$

for $k \geq 4$, then $\sqrt{20} + \sqrt{5} > 2\sqrt{8}$.

Subcase 1.2 Next, consider that $T_i \ncong P_{\eta_i}$. Then there is one possibility $\deg_{G''}(u_i) > \deg_{T_i}(u_i)$ and employing Theorem 2, we have

$$Z_i > \sum_{u_p u_q \in E(T_i)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2} \geq (\eta_i - 1)\sqrt{8},$$

By combining Subcases 1.1 and 1.2, proof is complete. ■

Proof of Case 2. Consider

$$Z_1 = \sum_{u_p u_q \in E(T_1)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2}, \tag{7}$$

As we know $k \leq n - 2$ and $n_1 \geq \eta_i (2 \leq i \leq k)$, we obtain $\eta_1 \geq 2$. The Equation (6) is satisfied for $k = 2$, so we obtain $Z_1 = \sqrt{k^2+1}$. Otherwise, $k \geq 4$. Consider that $T_1 \cong P_{\eta_1}$. Then there are two possibilities either

$\deg_{t_1}(u_1) = 1$, or $\deg_{T_1}(u_1) = 2$. Assume that $\deg_{T_1}(u_1) = 1$.

$$Z_1 = \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5},$$

the equality satisfied for Equation (6). Otherwise, $\deg_{T_1}(u_1) = 2$, there exist two possibilities.

Subcase 2.1 If $\eta_1 = 3$, then for $k \geq 4$

$$Z_1 = 2\sqrt{(k+1)^2+1} > \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5},$$

Subcase 2.2 If $\eta_1 \geq 4$, then for $k \geq 4$

$$\begin{aligned} Z_1 &= \sqrt{(k+1)^2+4} + \sqrt{(k+1)^2+1} + \sqrt{k^2+4} + (\eta_1 - 4)\sqrt{8} + \sqrt{5}, \\ &> \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5}. \end{aligned}$$

Next, Consider that $T_1 \ncong P_{\eta_1}$. If $\eta_1 = 4$, then $T_1 \cong K_{1,3}$ and $Z_1 > \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5}$. Otherwise, for $\eta_1 \geq 5$, we have two possibilities.

Subcase 2.3 If $\deg_{T_1}(u_1) = 1$. Let u_s be an adjacent vertex of $u_1 \in T_1$. Then $\deg_{T_1}(u_s) \geq 2$ as $\eta_1 \geq 5$. Assume that $T_1 - u_1 \cong P_{\eta_1 - 1}$. Then $\deg_{T_1}(u_s) = 3$

$$\begin{aligned} Z_1 &= \sum_{u_p u_q \in E(T_1 - u_p)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2} + \sqrt{(\deg_{T_1}(u_1) + k - 1)^2 + 9} \\ &= \sum_{u_p u_q \in E(T_1 - u_p)} \sqrt{\deg_{T_1}(u_p)^2 + \deg_{T_1}(u_q)^2} + \sqrt{k^2+9} \\ &> \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5} \end{aligned}$$

Now, if $T_1 - u_1 \ncong P_{\eta_1 - 1}$, then $\deg_{T_1}(u_s) \geq 2$. By employing Theorem 2 on tree $T_1 - u_1$, we derive

$$\begin{aligned} Z_1 = &\sum_{u_p u_q \in E(T_1 - u_1)} \sqrt{\deg_{G''}(u_p)^2 + \deg_{G''}(u_q)^2} \\ &+ \sqrt{(\deg_{T_1}(u_1) + k - 1)^2 + \deg_{T_1}(u_s)^2} \end{aligned}$$

$$= \sum_{u_pu_q \in E(T_1-u_1)} \sqrt{\deg_{T_1}(u_p)^2 + \deg_{T_1}(u_q)^2} + \sqrt{k^2+4}$$
$$= \sum_{u_pu_q \in E(T_1-u_1)} \sqrt{\deg_{T_1}(u_p)^2 + \deg_{T_1}(u_q)^2} + \sqrt{k^2+4}$$
$$= \sum_{u_pu_q \in E(T_1-u_1)} \sqrt{\deg_{T_1-u_1}(u_p)^2 + \deg_{T_1-u_1}(u_q)^2} + \sqrt{k^2+4}$$
$$> \sqrt{k^2+4} + (\eta_1-2)\sqrt{8} > \sqrt{k^2+4} + (\eta_1-3)\sqrt{8} + \sqrt{5}$$

Subcase 2.4 Assume that $\deg_{T_1}(u_1) \geq 2$. If $\deg_{T_1}(u_1) = \eta_1 - 1$, then $Z_1 > \sqrt{k^2+4} + (\eta_1 - 3)\sqrt{8} + \sqrt{5}$. If $\deg_{T_1}(u_1) \leq \eta_1 - 2$ for $\eta_1 \geq 5$. Consider that $T_1 - u_1 = pq + T_1^j$ with $|V(T_1^j)| = \eta_1^j$ for $1 \leq j \leq p$ where $p, q \geq 1$. Consequently, $\deg_{G''}(u_1) = \deg_{T_1}(u_1) + k - 1 = k + p + q - 1$.

Next, consider that $u_1u_s \in E(T_1)$ where u_s is a vertex of T_1^j for $1 \leq j \leq p$.

$$\sum_{u_iu_p \in E(T_1^j)} \sqrt{\deg_{T_1}(u_i)^2 + \deg_{T_1}(u_p)^2} \geq (\eta_1^j - 2)\sqrt{8} + \sqrt{5}$$

There are two possibilities, either $T_1^j \ncong P_{\eta_1^j}$ or $T_1^j \cong P_{\eta_1^j}$. Consider that $T_1^j \ncong P_{\eta_1^j}$ then there exists a tree $T_{1'}$ such that $SO(T_{1'}) > (\eta_1^j - 1)\sqrt{8}$ by employing Theorem 2. Consequently,

$$\begin{aligned}\sum_{u_iu_p \in E(T_1^j)} \sqrt{\deg_{T_1}(u_i)^2 + \deg_{T_1}(u_p)^2} &\geq \sum_{u_iu_p \in E(T_1^j)} \sqrt{\deg_{T_1^j}(u_i)^2 + \deg_{T_1^j}(u_p)^2} \\ &\geq (\eta_1^j - 1)\sqrt{8} \\ &\geq (\eta_1^j - 2)\sqrt{8} + \sqrt{5}\end{aligned}$$

Similarly, if $T_1^j \cong P_{\eta_1^j}$ then we deduce,

$$\sum_{u_iu_p \in E(T_1^j)} \sqrt{\deg_{T_1}(u_i)^2 + \deg_{T_1}(u_p)^2} = (\eta_1^j - 2)\sqrt{8} + \sqrt{5}$$

where u_s is a vertex of T_1^j for $1 \leq j \leq p$ and $\deg_{T_1^j}(u_s) = 1$, then $\deg_{T_1}(u_s) = \deg_{T_1^j}(u_s) + 1 = 2$ but for vertices $u_p \in V(T_1^j - u_s)$, we have $\deg_{T_1}(u_p) = \deg_{T_1^j}(u_p)$. Otherwise, $\deg_{T_1^j}(u_s) = 2$ and the equation

(7) satisfied for $2 \leq \eta_1^j \leq 3$. Therefore, we consider $\eta_1^j \geq 4$.

$$\begin{aligned}\sum_{u_i u_p \in E(T_1^j)} \sqrt{\deg_{T_1}(u_i)^2 + \deg_{T_1}(u_p)^2} &= 2\sqrt{13} + (\eta_1^j - 2)\sqrt{8} + 2\sqrt{5} \\ &= \sqrt{13} + \sqrt{10} + (\eta_1^j - 2)\sqrt{8} + 2\sqrt{5} \\ &> (\eta_1^j - 2)\sqrt{8} + 2\sqrt{5}\end{aligned}$$

After simplify and combining equation (7) and Subcases 2.1-2.4, we get

$$\begin{aligned}Z_1 &\geq p\sqrt{\deg_{G''}(u_1)^2 + 1} + q\sqrt{\deg_{G''}(u_1)^2 + 4} + \sum_{j=1^q} (\eta_1^j - 2)\sqrt{8} + 2\sqrt{5} \\ &= p\sqrt{(k+p+q-1)^2 + 1} + q\sqrt{(k+p+q-1)^2 + 1} \\ &\qquad + (\eta_1 - 1 - p - 2q)\sqrt{8} + q\sqrt{5} \\ &\geq \sqrt{k^2+4} + (p-1)\sqrt{(k+p+q-1)^2 + 1} + q\sqrt{(k+p+q-1)^2 + 4} \\ &\qquad + (\eta_1 - 1 - p - 2q)\sqrt{8} + q\sqrt{5} \\ &> \sqrt{k^2+4} + \sqrt{5} + (\eta_1 - 1 - 2q)\sqrt{8} + (q-1)(\sqrt{5} + \sqrt{13}) \quad for \quad p \geq 1 \\ &> \sqrt{k^2+4} + \sqrt{5} + (\eta_1 - 3)\sqrt{8}\end{aligned}$$

Otherwise, $p = 0$ and $q \geq 2$, we have

$$\begin{aligned}Z_1 &\geq q\sqrt{(k+q-1)^2 + 4} + (\eta_1 - 1 - 2q)\sqrt{8} + q\sqrt{5} \\ &> \sqrt{k^2+4} + \sqrt{5} + (\eta_1 - 3)\sqrt{8}\end{aligned}$$

The proof is complete. ■

Theorem 3. *Assume that G is a graph in χ_n^k such that $k \geq 4$. Then*

$$\begin{aligned}SO(G) \geq{}& (k-1)\sqrt{2k^2 - 2k + 1} + \sqrt{k^2+4} + (n-k-2)\sqrt{8} \\ &+ \sqrt{2}\binom{k-1}{2}(k-1) + \sqrt{5}\end{aligned}$$

where equality is satisfied if and only if $G = K_n^k$.

Proof of Theorem 3. Let $G^{'}$ be the graph chosen from χ_n^k such that $SO(G)$ $> SO(G^{'})$ for any $G \in \chi_n^k \setminus G^{'}$. Next, we shall verify that $G^{'} \cong K_n^k$. When

$k = 2$, there exists only a $\mathbb{P}_n$ graph, which achieves the least Sombor descriptor in χ_n^k by employing the result 1.

Now, assume that $4 \leq k \leq n$. Let $G^{'}$ be the smallest graph in χ_n^k. As we know, k is the chromatic number of $G^{'}$. Therefore, we suppose chromatic number $W(G^{'}) = \{u_1, u_2, ..., u_k\}$. Let $G^{''}$ be a connected subgraph with $V(G^{''}) = V(G^{'})$ and $G^{''} - E(K_k)$ is isomorphic to trees say, $t_1, t_2, ..., t_k$ such that $|V(t_k)| = \eta_i$, $(1 \leq i \leq k)$, where $\eta_1 + \eta_2 + ... + \eta_k = n$, and $\eta_1 \geq \eta_2 ... \geq \eta_k$.

Furthermore, $W(G^{'}) = W(G^{''})$. We have $SO(G^{'}) \geq SO(G^{''})$, by employing Lemma 1 and deleting edges from $G^{''}$, where equality is satisfied if $G^{'}$ isomorphic to $G^{''}$. As per the mathematical expression of the Sombor index,

$$\begin{aligned}
SO(G^{'}) &= \sum_{u_iu_j \in E(G^{'})} \sqrt{\deg_{G'}(u_i)^2 + \deg_{G'}(u_j)^2} \\
&\geq \sum_{u_iu_j \in E(G'')} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&= \sum_{\substack{u_iu_j \in E(G^{''}), u_i \in V(G^{'} - V(K_k)) \\ OR \\ u_j \in V(G^{'} - V(K_k)), u_j \in V(K_k)}} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&+ \sum_{u_iu_j \in E(K_k)} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&= \sum_{l=1}^{k} \sum_{u_iu_j \in E(t_k)} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&+ \sum_{u_iu_j \in E(K_k)} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \qquad (8)
\end{aligned}$$

By employing Lemma 3, we conclude

$$\sum_{l=1}^{k} \sum_{u_iu_j \in E(t_k)} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \geq \sqrt{k^2 + 4} + (n - k - 2)\sqrt{8} + \sqrt{5}$$

where equality satisfied if and only if $\eta_1 = \eta_2 = ... = \eta_k = 1$, and

$t_1 \cong P_{\eta_1}$ with $\deg_{t_1}(u_1) = 1$ that is $G^{'} \cong K_n^k$. As we know, $n \geq k+2$, $\deg_{G''}(u_1) \geq k$, and $\deg_{G''}(u_i) \geq k-1$ for $(4 \leq i \leq k)$, we have

$$\begin{aligned}
SO(G^{'}) &\geq \sum_{i=4}^{k} \sqrt{\deg_{G''}(u_1)^2 + \deg_{G''}(u_i)^2} \\
&+ \sum_{\substack{u_i u_j \in E(K_k) \\ 4 \leq i,j \leq k}} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&+ \sum_{l=1}^{k} \sum_{u_i u_j \in E(t_k)} \sqrt{\deg_{G''}(u_i)^2 + \deg_{G''}(u_j)^2} \\
&\geq (k-1)\sqrt{2k^2 - 2k + 1} + \sqrt{k^2+4} + (n-k-2)\sqrt{8} \\
&+ \sqrt{2}\binom{k-1}{2}(k-1) + \sqrt{5} \\
&= SO(K_n^k)
\end{aligned}$$

The proof is complete. ■

Conjecture 1. *Assume that G is a graph in χ_n^k such that $k > 4$. Then $G = \mathcal{K}_k^{(n-k)}$ graphs achieve for smallest Laplacian energy index with chromatic number.*

4 Sharp upper bounds of Mostar index with given cut-edges

In this section, we determine the maximum Mostar invariant in $G_{n,k}$ (resp. $g_{n,k}$) by implementing auxiliary results from subsection 4.1. Let $G_{n,k}$ (resp. $g_{n,k}$) be a set of all $n-$vertex graphs with exactly cut edges (resp. girth) k. Graphs attaining the upper bound have also been classified. For $n \geq 4$ and $k \geq 0$, suppose S_n is a star graph of order n with fixed pendent vertex $v \in S_n$. The family S_n^k is acquired by adjoining $n-k-2$ edges between $v \in S_n$ and the remaining $n-k-2$ pendent vertices in S_n. Consider that $k \neq n-1$. As we know S_n graph achieves maximum Mostar index over $G_n^{k=n-1}$ by employing Lemma 4. For $n \geq 4$ and $k = 3$, suppose S_n is a star graph of order n with fixed pendent vertex $v \in S_n$.

4.1 Auxiliary results

Lemma 4. *Let T be a tree graph with n vertices. Then*

$$Mo(P_n) \leq Mo(T) \leq Mo(S_n)$$

where left and right equalities are satisfied, if T isomorphic to P_n and S_n, respectively.

Lemma 5. *Let G be a simple graph such that uv is a cut edge. Then $Mo(G) \leq n-2$, where equality satisfies if and only if uv is a pendent edge.*

Lemma 6. *Consider that G is a connected graph with cut edge uv. Then $Mo(G) < M_o(G-uv)$, if uv is not a pendent edge.*

Lemma 7. *Let G_1 be a connected graph such that G_1 comprises the cycle of order 4, say $\{u_o u_1 u_2 u_3 u_o\}$. Consider that common vertices of $N_{G_1}(u_o)$ and $N_{G_1}(u_2)$ are $\{u_1, u_3\}$. Let $N_{G_1}(u_o)\backslash\{u_1,u_3\} = \{u_{o1}, u_{o2}, u_{o3}, ..., u_{o\eta_o}\}$ and $N_{G_1}(u_2)\backslash\{u_1,u_3\} = \{u_{21}, u_{22}, u_{23}, ..., u_{2\eta_2}\}$, for $\eta_o = d_{G_1}(u_o)-2 > 0$, and $\eta_2 = d_{G_1}(u_2) - 2 > 0$.*
Next, we deduce $G_2 = G_1 - \{u_o u_{o1}, ..., u_o u_{o\eta_o}\} + \{u_2 u_{21}, ..., u_2 u_{2\eta_2}\}$. Then $M_o(G_1) < M_o(G_2)$.

Proof. Let $C_4 = u_o u_1 u_2 u_3 u_o$ be a cycle with 4 vertices in a graph, say G_1. Consider that $N_{G_1}(u_o) \setminus \{u_1,u_3\} = \{u_{o1}, u_{o2}, u_{o3}, ..., u_{o\eta_o}\} + 2 = n_{G_1}(u_o)$, and $N_{G_1}(u_2) \setminus \{u_1,u_3\} = \{u_{21}, u_{22}, u_{23}, ..., u_{2\eta_2}\} + 2 = n_{G_1}(u_2)$. Similarly, $N_{G_2}(u_o) \setminus \{u_1,u_3\} = 2 = n_{G_2}(u_o)$, and $N_{G_2}(u_2) \setminus \{u_1,u_3\} = \{u_{21}, u_{22}, u_{23}, ..., u_{2\eta_2}\} + \{u_{o1}, u_{o2}, u_{o3}, ..., u_{o\eta_o}\} + 2 = n_{G_2}(u_2)$. Next, we derive $G_2 = G_1 - \{u_o u_{o1}, ..., u_o u_{o\eta_o}\} + \{u_2 u_{21}, ..., u_2 u_{2\eta_2}\}$. This shifting of edges require the following relationship between $M_o(G_1)$ and $M_o(G_2)$,

$$\begin{aligned} M_o(G_1) - M_o(G_2) = &\sum_{i=1}^{\eta_o} |n_{G_1}(u_o) - n_{G_1}(u_{oi})| + \sum_{uv \in E(C_4)} |n_{G_1}(u) - n_{G_1}(v)| \\ &+ \sum_{j=1}^{\eta_2} |n_{G_1}(u_2) - n_{G_1}(u_{2j})| - \sum_{uv \in E(C_4)} |n_{G_2}(u) - n_{G_2}(v)| \end{aligned}$$

$$-\sum_{i=1}^{\eta_o}|n_{G_2}(u_2)-n_{G_2}(u_{2i})|-\sum_{j=1}^{\eta_2}|n_{G_2}(u_2)-n_{G_2}(u_{2j})|,$$

As we know $n_{G_1}(u)=n_{G_1}(v)$, for all $uv\in C_4$, and $n_{G_2}(u)>n_{G_2}(v)$, for all $uv\in C_4$. Similarly, $n_{G_1}(u_o)\geq n_{G_1}(u_{oi})$ and $n_{G_2}(u_2)\geq n_{G_2}(u_{2i})$, and $n_{G_2}(u_2)\geq n_{G_2}(u_{2j})$. In other words, $n_{G_1}(u_o)=n_{G_2}(u_2)$, and $n_{G_1}(u_{oi})=n_{G_2}(u_{2i})$, and $n_{G_1}(u_{oi})=n_{G_2}(u_{2j})$. By combining these we obtain,

$$M_o(G_1)-M_o(G_2)<0\Rightarrow M_o(G_1)<M_o(G_2) \qquad \blacksquare$$

Lemma 8. *Consider that G_1 is a connected graph with the cycle of order 3, say $\{u_ou_1u_2u_o\}$. Consider that the common vertex of $N_{G_1}(u_o)$ and $N_{G_1}(u_1)$ is $\{u_2\}$. Consider that $N_{G_1}(u_o)\setminus\{u_1,u_2\}=\{u_{o1},u_{o2},u_{o3},...,u_{o\eta_o}\}$ and $N_{G_1}(u_1)\setminus\{u_o,u_2\}=\{u_{11},u_{12},u_{13},...,u_{1\eta_1}\}$, for $\eta_o=d_{G_1}(u_o)-2>0$, and $\eta_1=d_{G_1}(u_1)-2>0$.*
Next, we deduce $G_2=G_1-\{u_ou_{o1},...,u_ou_{o\eta_o}\}+\{u_1u_{11},...,u_1u_{1\eta_1}\}$. Then $M_o(G_1)<M_o(G_2)$.

Proof. Let $C_3=u_ou_1u_2u_o$ be a cycle with 3 vertices in a graph, say G_1. Consider that $N_{G_1}(u_o)\setminus\{u_1,u_2\}=\{u_{o1},u_{o2},u_{o3},...,u_{o\eta_o}\}=n_{G_1}(u_o)$, and $N_{G_1}(u_1)\setminus\{u_o,u_2\}=\{u_{11},u_{12},u_{13},...,u_{1\eta_1}\}=n_{G_1}(u_1)$. Similarly, $N_{G_2}(u_o)\setminus\{u_1,u_2\}=0=n_{G_2}(u_o)$, and $N_{G_2}(u_1)\setminus\{u_o,u_2\}=\{u_{11},u_{12},u_{13},...,u_{1\eta_1}\}+\{u_{o1},u_{o2},u_{o3},...,u_{o\eta_o}\}=n_{G_2}(u_1)$.
Next, we derive $G_2=G_1-\{u_ou_{o1},...,u_ou_{o\eta_o}\}+\{u_1u_{11},...,u_1u_{1\eta_1}\}$. This shifting of edges require the following relationship between $M_o(G_1)$ and $M_o(G_2)$,

$$\begin{aligned}M_o(G_1)-M_o(G_2)=&\sum_{i=1}^{\eta_o}|n_{G_1}(u_o)-n_{G_1}(u_{oi})|+\sum_{uv\in E(C_3)}|n_{G_1}(u)-n_{G_1}(v)|\\&+\sum_{j=1}^{\eta_1}|n_{G_1}(u_1)-n_{G_1}(u_{1j})|-\sum_{uv\in E(C_3)}|n_{G_2}(u)-n_{G_2}(v)|\\&-\sum_{i=1}^{\eta_o}|n_{G_2}(u_1)-n_{G_2}(u_{1i})|-\sum_{j=1}^{\eta_1}|n_{G_2}(u_1)-n_{G_2}(u_{1j})|.\end{aligned}$$

By employing the definition of Mostar index, we have $n_{G_1}(u) = n_{G_1}(v)$ and $n_{G_2}(u) > n_{G_2}(v)$, for all $uv \in C_3$. Similarly, $n_{G_1}(u_o) \geq n_{G_1}(u_{oi})$ and $n_{G_2}(u_1) \geq n_{G_2}(u_{1i})$, and $n_{G_2}(u_1) \geq n_{G_2}(u_{1j})$. In other words, $n_{G_1}(u_o) = n_{G_2}(u_1)$, and $n_{G_1}(u_{oi}) = n_{G_2}(u_{1i})$, and $n_{G_1}(u_{oi}) = n_{G_2}(u_{1j})$. After considering these, we obtain

$$M_o(G_1) - M_o(G_2) < 0 \Rightarrow M_o(G_1) < M_o(G_2) \qquad \blacksquare$$

Theorem 4. *Let G be a graph in $G_{n,k}$ with $n \geq 4$ and $0 \leq k \leq n-3$. Then*

$$M_o(G) \leq (n-k-2)(n-k-3) + (n-k-2)(n-3) + k(n-2),$$

where equality satisfies if and only if $G = S_n^k$.

Proof of Theorem 4. Consider that $G \in G_{n,k}$ is a connected graph achieving maximum Mostar index, and every cut edge is a pendent in G by employing Lemma 5. Next, we show the following claims.

Claim 1. The length of every cycle is 3 or 4 in G.

Proof of Claim 1. Suppose on the contrary that G comprises the cycle with length $r > 4$ say, $C = \{u_1u_2, ..., u_ru_1\}$. Consider that $n_G(u_1) = max\{n_G(u_i)| \ 1 \leq i \leq r\}$. Next, we deduce G_1 from G such that $G_1 = G - \{u_3u_4\} + \{u_1u_3, u_1u_4\}$.

$$\begin{aligned} M_o(G_1) - M_o(G) &= \sum_{uv \in E(G)} |n_G(u) - n_G(v)|, \\ &= \sum_{j=3}^{4} |n_{G_1}(u_1) - n_{G_1}(u_j)| - |n_G(u_3) - n_G(u_4)| \geq 0. \end{aligned}$$

As we know, $n_G(u_3) = n_G(u_4)$, $n_{G_1}(u_1) \geq 0$, and $n_{G_1}(u_j) \geq 0$. Consequently, $M_o(G_1) - M_o(G) \geq 0$ leads to a contradiction to our choice of G. Hence, G comprises a cycle of length 3 or 4. $\blacksquare$

Claim 2. Every $C_4 \in G$ comprises at most 2 vertices of degree greater than 2.

Proof of Claim 2. Let C_4 be a cycle of length 4, say, $u_1u_2u_3u_4u_1$ comprises at least 2 vertices with a degree greater than 2. As G achieves the maximum Mostar index and by employing Lemma 3, every two vertices of degree greater than 2 is adjacent in the cycle. Consequently, the other 2 vertices in the cycle have degree 2. Consider that $n_G(u_1) = \eta_1 + 2$, $n_G(u_2) = \eta_2 + 2$ and similarly, $n_G(u_3) = n_G(u_4) = 2$. Assume that $N_G(u_1) \setminus \{u_2, u_4\} = \{u_{11}, u_{12}, u_{13}, ..., u_{1\eta_1}\}$ and $N_G(u_2) \setminus \{u_1, u_3\} = \{u_{21}, u_{22}, u_{23}, ..., u_{2\eta_2}\}$.
Next, we construct G_2 from G such that $G_2 = G - \{u_2u_{21}, u_2u_{22}, ..., u_2u_{2\eta_2}\} + \{u_1u_{21}, u_1u_{22}, ..., u_1u_{2\eta_2}\}$. This shifting of edges requires the following relationship between $M_o(G)$ and $M_o(G_2)$.

$$\begin{aligned} M_o(G) - M_o(G_2) = &\sum_{i=1}^{\eta_1} |n_G(u_1) - n_G(u_{1i})| + \sum_{uv \in E(C_4)} |n_G(u) - n_G(v)| \\ &+ \sum_{j=1}^{\eta_2} |n_G(u_2) - n_G(u_{2j})| - \sum_{uv \in E(C_4)} |n_{G_2}(u) - n_{G_2}(v)| \\ &- \sum_{i=1}^{\eta_1} |n_{G_2}(u_1) - n_{G_2}(u_{1i})| - \sum_{j=1}^{\eta_2} |n_{G_2}(u_1) - n_{G_2}(u_{2j})|. \end{aligned}$$

As we know $n_G(u) = n_G(v)$, for all $uv \in C_4$, and $n_{G_2}(u) > n_{G_2}(v)$, for all $uv \in C_4$. Similarly, $n_{G_2}(u_1) = n_G(u_2)$, and $n_{G_2}(u_{1i}) = n_G(u_{2i})$, and $n_{G_2}(u_{1i}) = n_G(u_{2j})$. By combining these, we obtain,

$$M_o(G) - M_o(G_2) < 0 \Rightarrow M_o(G) < M_o(G_2)$$

which is again a contradiction to our choice of G. ■

Similarly, by employing Lemma 8, every cycle of length 3 has at most 2 vertices of degree greater than 2. The graph G is generated by adjoining $n - k - 2$ edges at fixed pendent vertex $v \in S_n$, which represent different copies of C_3 and C_4 by employing the Claims 4 and 5. The proof is complete. ■

5 Sharp upper bounds of Mostar index with given girth

Moreover, the family H_n^k is acquired by adjoining $n-k+1$ edges between $v \in S_n$ and the remaining $n-k+1$ pendent vertices in S_n. Similarly, For $n \geq 4$ and $k > 4$, the family C_n^{*k} is acquired by adjoining $n-k$ pendent vertices at vertex $v \in C_k$, where C_k is a cycle of order k.

Theorem 5. *Let G be a graph in $g_{n,k}$ with $n \geq 4$ and $k = 3$. Then*

$$M_o(G) \leq 2(n-2)(n-k),$$

where equality satisfies if and only if $G = H_n^k$.

By Lemma 7 and 8, the proof is obvious.

Theorem 6. *Let G be a graph in $g_{n,k}$ with $n \geq 4$ and $k > 4$. Then*

$$M_o(G) \leq k(k-1) + n(n-1),$$

where equality satisfies if and only if $G = C_n^{*k}$.

Proof of Theorem 6. We prove the result by mathematical induction on n. The result is satisfied for $n = k$, and we have to prove for $n > k+2$. Consider that G has a maximum Mostar index for graphs in $g_{n,k}$.

Let $rs \in E(G)$ be an isolated edge and s be an isolated vertex. Then $n_G(r) = t \geq 2$. Since $G \in g_{n,k}$, consequently, $t \leq n-k$. Assume that $N(r) = \{s, r_1, r_2, ..., r_{t-1}\}$ with $n_G(r_i) = t_i$, where $1 \leq i \leq q-1$.

Claim 3. We claim there exists at least one vertex of degree 2 in $\{r_1, r_2, ...$ $, r_{t-2}, r_{t-1}\}$.

Proof of claim 3. Let $X = \{r_1, r_2, ..., r_{t-1}\}$ be a set of neighbors of vertex r. Suppose, on the contrary, there is exactly one of degree at least 2 in X. By employing Lemma 6, there is a graph $G_1 \in g_{n,k}$ such that $M_o(G_1) > M_o(G)$, which is a contradiction to our choice of G. ■

Next, we consider that there exist at least two vertices of degree at least 2 in X. Consider that $G_2 = G - s$, then $G_2 \in g_{n,k}$.

$$
\begin{aligned}
M_o(G) = M_o(G-s) + M_o(s) + \sum_{i=1}^{t} \Big[|n_G(r) - n_G(r_i)| - |n_{G_2}(r) \\
&- n_{G_2}(r_i)| \Big] = M_o(G_2) + |t-1| + \sum_{i=1}^{t} \Big[|t - t_i| - |(t-1) - t_i| \Big], \\
&\leq M_o(G_2) + (t-2) + 2\Big[|t-2| - |(t-1)-2| \Big] + (t-3) \\
&\cdot \Big[|t-1| - |t-2| \Big] = k|n-k| + (n-k)|n-2| + |n-k-1| + \\
&+ 2\Big[|n-k| - |n-k| \Big] + (t-3)\Big[|n-1| - |n-1| \Big] \\
&\leq k(k-1) + n(n-1),
\end{aligned}
$$

with inequality if and only if $G = C^{*k}_{n-1}$ and $n_G(r) = t = n-k$, exactly 2 vertices of degree 2 in X and $(t-3)$ vertices of degree 1 in X, that is $G = C^{*k}_{n}$. The proof is complete. ■

Conjecture 2. *Assume that G is a graph in $G_{n,k}$. There are some open problems for readers to derive the result minimum Mostar index with cut edges and maximum Mostar index with girth $k = 4$.*

6 Sharp bounds on the first Zagreb index with given girth

Let $g_{n,k}$ be a set of all graphs of order n with exactly girth k. Let C_k be a cycle graph of order k with a central vertex $p \in C_k$. Obtaining the family C^k_n by attaching a path P_{n-k} to the vertex $p \in C_n$ for $\forall\, n, k \geq 1$. Denote by $C_{n,1}$ the graph generated by adjoining one pendant edge to a vertex of C_{n-1} and U_2 be a unicyclic graph with precisely one pendant path of minimum length 2.

Lemma 9. *Suppose that two pendant paths in a connected graph G say, U and V identify at vertices u and v, respectively. Suppose that p (resp.*

q) is neighbour vertex of u (resp. v), which exists on pendant paths U and V, respectively. Given that $G^* = G - up + pq$. Consequently, $M_1(G^*) < M_1(G)$.

Proof. Consider that $u \neq v$, and r is a neighbor vertex of q. By employing the mathematical concept of the first Zagreb index, we have

$$\begin{aligned} M_1(G) - M_1(G^*) = &\sum_{w \in N_G(u)\setminus p} \Big[(deg_G(u) + deg_G(w)) + (deg_G(u) + deg_G(p)) \\ &+ (1 + deg_G(r)) - ((deg_G(u) - 1)\Big] + \sum_{w \in N_G(u)\setminus p} \Big[deg_G(w)) \\ &- (2 + deg_G(p)) - (2 + deg_G(r)) > (deg_G(u) + deg_G(p)) \\ &+ (1 + deg_G(r)) - (2 + deg_G(p)) - (2 + deg_G(r))\Big] \end{aligned} \tag{9}$$

Now, consider that $u = v$, and $|V| = 1$. Consequently, $u = r$. According to the mathematical concept of the first Zagreb index, we have

$$\begin{aligned} M_1(G) - M_1(G^*) = &\sum_{w \in N_G(u)\setminus\{p,y\}} \Big[(deg_G(u) + deg_G(w)) + (deg_G(u) \\ &+ deg_G(p)) + (1 + deg_G(r))\Big] - \sum_{w \in N_G(u)\setminus\{p,y\}} \Big[((deg_G(u) - 1) \\ &+ deg_G(w)) - (2 + deg_G(p)) - (2 + (deg_G(u) - 1))\Big] \\ &> (deg_G(u) + deg_G(p)) - (2 + deg_G(p)) \geq 0 \end{aligned}$$

Since, $deg_G(u) \geq 2$. If $|V| \geq 1$. Suppose that a neighbour vertex of u on the pendant path V, say p'. Consequently, by employing the mathematical concept of the first Zagreb index, we have

$$\begin{aligned} M(G) - M(G^*) = &\sum_{w \in N_G(u)\setminus\{p,p'\}} \Big[(deg_G(u) + deg_G(w)) + (deg_G(u) \\ &+ deg_G(p')) + (deg_G(u) + deg_G(p)) + (1 + deg_G(r)) \\ &- ((deg_G(u) - 1) + deg_G(w)) - (2 + deg_G(p)) \\ &- (2 + (deg_G(r))) - ((deg_G(u) - 1) + deg_G(p'))\Big] \end{aligned}$$

$$> (deg_G(u) + deg_G(p)) + (1 + deg_G(r) \geq 0 \tag{10}$$

Consequently, by (9) and (6) inequalities, we get

$$M_1(G) - M_1(G^*) > (3 + deg_G(p)) - (2 + deg_G(p)) - \beta(2) \tag{11}$$

As we know, $deg_G(u) \geq 3$, $deg_G(r) \geq 2$, and $\beta(t)$ is not increasing. Hence, $deg_G(p) \leq 2$. If $deg_G(p) = 1$. Consequently, we get $M_1(G) > M_1(G^*)$ by employing inequality (11). Otherwise, if $deg_G(p) = 2$. So, we have $M_1(G) - M_1(G^*) > 5 - 4 - \beta(2) > 0$ by employing inequality (11). ■

Theorem 7. *Suppose that $G \in g_{n,k}$ is a connected graph such that $n \geq 4$ and $k \geq 1$, then we have*

$$M_1(G) \leq 4(k-2) + 4(n-k-2) + 18,$$

where equality unless $G = C_n^k$.

Proof. Let C_n be a cycle graph with n vertices such that uv is not a cut edge in G because $uv \notin C_n$. Therefore, $M_1(G) > M_1(G - uv)$ and it conforms to G is a unicyclic graph. Consequently, if G is $k = n-1$ then $G \cong C_{n,1}$, which is the required result. Otherwise, if $k \leq n-2$, then $G \ncong U_2$. By employing repeatedly Lemma 9, the proof is complete. ■

7 Correlation between Sombor index and normalized Laplacian index

Theorem 8. *Let G be a connected graph with n vertices and m edges. Let $\lambda_1, \lambda_2, ..., \lambda_n$ be a eigenvalues of G such that*

$$\lambda_2 \leq 1 + \frac{2}{m} M \leq \lambda_n,$$

where left and right equalities hold if G is a union of regular complete graphs.

Proof of theorem 8. Let G be a connected graph with n vertices and m edges. Let $\lambda_1, \lambda_2, ..., \lambda_n$ be an eigenvalue of G such that $0 = \lambda_1 \leq \lambda_2 \leq$

... $\leq \lambda_n$ and $\overline{x}$ be an eigenvector such that $\mathcal{L}(\overline{x}) = 0$. Consider that any vector,

$$y_k^{ij} = \begin{cases} \sqrt{d_i} & k = i \\ -\sqrt{d_j} & k = j \\ 0 & k \neq i, j \end{cases} \tag{12}$$

such that $y_k^{ij} \perp \overline{x}$. Since G is a connected graph. Therefore, $\lambda_2 > 0$. Using the min-max theorem, we have $\lambda_2 = \min\limits_{x \perp 1} R_{\mathcal{L}}(x) \leq \min\limits_{i \sim j} R_{\mathcal{L}}(\vec{y}^{ij})$ and $\lambda_n = \max\limits_{x \perp 1} R_{\mathcal{L}}(x) \geq \max\limits_{i \sim j} R_{\mathcal{L}}(\vec{y}^{ij})$. Consequently,

$$\lambda_2 \leq R_{\mathcal{L}}(\vec{y}^{ij}) \leq \lambda_n \text{ for any } \{i, j\} \in E. \tag{13}$$

As we know, $\lambda_2 = \min\limits_{y_k^{ij} \perp \overline{x}} R_{\mathcal{L}}(y_k^{ij})$ and $\lambda_n = \max\limits_{y_k^{ij} \perp \overline{x}} R_{\mathcal{L}}(y_k^{ij})$. Consequently, $\lambda_2 \leq R_{\mathcal{L}}(y_k^{ij}) \leq \lambda_n$.

$$\lambda_2 \leq \frac{1}{m} \sum_{\{i,j\} \in E(G)} R_{\mathcal{L}}(y_k^{ij}) \leq \lambda_n, \tag{14}$$

To prove the required result, we have to prove the following claim.

Claim 4. $\sum\limits_{\{i,j\} \in E(G)} R_{\mathcal{L}}(y_k^{ij}) = m + 2 \sum\limits_{\{i,j\} \in E(G)} \dfrac{1}{d_i + d_j}$.

Proof of Claim 4: Let G be a complete graph with size m. Let y_k^{ij} be a vector given in Equation (12). By employing the definition of Rayleigh's quotient and Laplacian normalized matrix, we have

$$\begin{aligned} \sum_{\{i,j\} \in E(G)} R_{\mathcal{L}}(y_k^{ij}) &= \sum_{\{i,j\} \in E(G)} \frac{L_{uv} y_u^{ij} y_v^{ij}}{d_i + d_j}, \\ &= \sum_{\{i,j\} \in E(G)} \frac{(d_i + d_j) + 2(-\frac{1}{d_i d_j})(-d_i d_j)}{d_i + d_j}, \\ &= \sum_{\{i,j\} \in E(G)} (1 + \frac{2}{d_i + d_j}) \end{aligned}$$

$$= m + 2 \sum_{\{i,j\}\in E(G)} \frac{1}{d_i + d_j},$$

$$\lambda_2 \le \frac{1}{m}(m + 2 \sum_{i,j\in E(G)} \frac{1}{d_i + d_j}) \le \lambda_n$$

$$\lambda_2 \le 1 + \frac{2}{m}(\sum_{i,j\in E(G)} \frac{1}{d_i + d_j}) \le \lambda_n$$

By combining the Equation (14) and Claim 4, where $\sum_{\{i,j\}\in E(G)} \frac{1}{d_i + d_j} = \frac{1}{M_1} = M$, if G is a union of regular complete graphs. Moreover, $\lambda_2 = 1 + \frac{2}{m}M$ if and only if $\lambda_n = 1 + \frac{2}{m}M$ if and only if G is a complete graph. To prove this, we have the following Claims.

Claim 5. G be a d-regular graph.

Proof of Claim 5: Let G be a union of connected graphs with order n. Since, $d_i = d_j$, $\forall\{ij\} \in E(G)$, then G is a d-regular graph. [7] By employing the result, y^{ij} must be an eigenvector of normalized Laplacian corresponding to eigenvalue $\lambda = \frac{d}{d-1}$.

Claim 6. If G is connected, then G is complete.

Proof of Claim 6: Let G be a connected graph with order n. Let y_k^{ij} (resp. λ) be an eigenvector (resp. eigenvalues) of G. Assume that $\mathcal{L}(y_k^{ij}) = \lambda(y_k^{ij})$.

Case 3. Consider that $k \sim i, j$.

Let $k \sim i$. $\mathcal{L}(y^{ij})_i = y_i^{ij} - \sum_{k\sim i} y_k^{ij}(\frac{1}{\sqrt{d} - \sqrt{d}}) = \sqrt{d} + \frac{\sqrt{d}}{d} = \lambda\sqrt{d} \Rightarrow \lambda = 1 + \frac{1}{d} = \frac{d+1}{d} = \mathcal{L}(y^{ij})_j = k \sim j$.

Case 4. Consider that $k \nsim i, j$.

Let $k \sim i$. $\mathcal{L}(y^{ij})_k = 0 - \frac{1}{d} \sum_{k'\sim k} (y^{ij})_{k'} = \lambda \cdot 0 \Rightarrow \sum_{k'\sim k} (y^{ij})_{k'} = 0 \Rightarrow k \sim j$.

Case 5. If $k \sim i$, then $k \sim j$. If $k \nsim i$, then $k \nsim j$. Similarly, if $k \sim j$, then $k \sim i$, and if $k \nsim j$ then $k \nsim i$.

Consider that $k \nsim i, j$. By employing 3 and 4 cases, we get $\sum_{k\sim v}(y^{ij})_v = 0$, which is the required result. Denote $N(i, j) = \{k \in V(G)|k \sim i, j\}$.

Since $k_2 \sim i$. By employing case 5 on y^{ik_1}, we have $k_2 \sim k_1$, for all $k_1, k_2 \in N(i,j)$.

Case 6. $K_1 \sim k_2$, for all $k_1, k_2 \in N(i,j)$.

Since $k \in |N(i,j)|$, $k \sim i, j$.

$$\begin{cases} N_1(i,j) = \{u \in V(G) | u \sim s\} & s \in N(i,j) \\ N_2(i,j) = \{u \in V(G) | u \sim s\} & s \in N_1(i,j) \\ N_3(i,j) = \{u \in V(G) | u \sim s\} & s \in N_2(i,j) \\ ... \end{cases} \tag{15}$$

As we know $\forall u \in N_2(i,j)$, $u \sim s$ and $s \sim i, j$. By employing case 5 on us, we get $u \sim i, j$. By mathematical induction, $\forall u \in N_k(i,j) \Rightarrow u \sim i, j$. Consequently, G is completed by combining all of the above cases. If G is not connected graph then $G = G_1 \cup G_2 \cup ... \cup G_p$, each G_i is connected graph. By employing case 6 on each G_i, we have $|G_1| = |G_2| = ... = |G_p|$ and now by case 5, we have $d+1$ vectors. The proof is complete. ■

Corollary. *Let G be a connected graph with vertices n and $\lambda_1, \lambda_2, ..., \lambda_n$ be its eigenvalues. Then*

$$\lambda_n \geq 1 + \frac{\sqrt{2}m}{SO(G)},$$

with equality satisfied if G is the union of complete graphs with the same degrees.

Proof. Let G be a connected graph with n vertices. By employing the Theorem 8, we have $\lambda_n \geq 1 + \frac{2}{m} \sum\limits_{i,j \in E(G)} \frac{1}{d_i + d_j}$. Since,

$$\sum_{i,j \in E(G)} \frac{2}{d_i + d_j} \geq \sum_{i,j \in E(G)} \sqrt{\frac{2}{d_i^2 + d_j^2}}.$$

Consequently,

$$
\begin{aligned}
\lambda_n &\geq 1 + \frac{1}{m} \sum_{i,j \in E(G)} \sqrt{\frac{2}{d_i^2 + d_j^2}}, \\
&\geq 1 + \frac{\sqrt{2}}{m} \frac{m^2}{\sum\limits_{i,j \in E(G)} \sqrt{d_i^2 + d_j^2}}, \quad \textit{where, } d_i = d_j = d \in N^+ \\
&= 1 + \frac{\sqrt{2}m}{SO(G)},
\end{aligned}
$$

where equality is satisfied if G is the union of the complete graph with the same degrees. ■

8 Correlation between first Zagreb index and normalized Laplacian index

Note that

$$\frac{2\Delta}{d_i + d_j} \geq \frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{\sqrt{d_i d_j}}{\Delta}$$

for any $\{i, j\} \in E$, where Δ represents the maximum degree of the graph.

Theorem 9. *Let G be a connected graph with n vertices and $\lambda_1, \lambda_2, ..., \lambda_n$ be its eigenvalues such that we have*

$$\frac{2m}{\lambda_2 - 1} \leq M_1(G) \leq \Delta m(\lambda_n - 1)$$

with left and right equalities satisfies if and only if G is complete graphs or union of complete graphs or G is d- regular graphs.

Proof. It is easy to see

$$\frac{2\Delta}{d_i + d_j} \geq \frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{2d}{d_i + d_j}$$

with the left equality holds if and only if $d_i = d_j = \Delta$, and the right equality holds if and only if $d_i = d_j = d$.

$$M_1(G) \geq m^2 \geq \frac{m^2}{\sum \frac{1}{d_i+d_j}} \geq \frac{m^2}{\frac{m}{2}(\lambda_2 - 1)} = \frac{2m}{(\lambda_2 - 1)} \geq \frac{m^2}{\frac{m}{2}(\lambda_2 - 1)}$$

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} \leq \frac{2\Delta}{d_i + d_j} = 2\Delta \sum \frac{1}{d_i + d_j} \leq 2\Delta . \frac{m}{2}(\lambda_n - 1) = \Delta m(\lambda_n - 1)$$

with left and right equalities satisfies if and only if G are complete graphs or G is d- regular graphs. ■

9 Conclusion

In this article, we achieved the least Sombor index with a given chromatic number in χ_n^k by extending the innovative results of Das and Shang for the Sombor index to characterize the extremal graphs. We extend the characterization of extremals graphs to get upper limits for the Mostar and first Zagreb index with fixed cut edges and girth, allowing characterizations for other indices to be compared. The two families H_n^k and C_n^{*k} are characterized, where C_n^k is characterized by the Zagreb index with given girth and the Mostar index with fixed girth yielding extremal graphs. Additionally, we present a new approach that uses Rayleigh's quotient principle to compare the Sombor index and the first Zagreb index with the normalized Laplacian index.

***Acknowledgment*:** The author thanks the anonymous reviewers for their valuable comments, which helped to improve the manuscript.

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