

Exploring Bounds on Generalized Szeged Indices of Graphs

¹* K. Pattabiraman ²A. Anivarsha

¹* Assistant Professor, Department of Mathematics, Government Arts College (Autonomous), Kumbakonam, Tamil Nadu, India - 612 002.

Email: * pramank@gmail.com

²Research Scholar, Department of Mathematics, Annamalai University, Annamalai Nagar, Chidambaram, Tamil Nadu - 608 002.

Email: ² annieantony1825@gmail.com

Abstract

The *PR* index of a connected graph G is defined as $Sz_{(\alpha, \beta)}(G) = \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta$ where α, β are arbitrary real numbers. In this article, we focus the *PR*-Szeged index and establish new good upper and lower bounds for it. These bounds include terms related to the general *PI* index and Szeged index.

Keywords: Distance based Topological index, General *PI* index, General Szeged index, *PR*-Szeged index.

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1 Introduction

Topological indices are graph-based numerical descriptors that reflect key structural properties such as connectivity, branching, and distance distribution. Two classical and widely studied distance-based indices are the Szeged index and the *PI* (Peripheral) index. The Szeged index, introduced by Gutman [1], partitions vertex sets based on shortest-path distances relative to edges, providing insights into the branching nature of molecular graphs. In contrast, the general *PI* index [2] quantifies the imbalance in distances from each vertex to the endpoints of an edge, offering a complementary perspective on molecular shape. These indices have inspired several refinements to improve sensitivity and applicability. Das et al. [3] extended the Szeged index to accommodate weighted graphs, enhancing its adaptability to real-world data structures. Klavžar and Nadjafi-Arani [4] developed a decomposition-based approach to simplify the computation of the index for large-scale graphs. These advancements demonstrate the ongoing significance of Szeged-type indices in mathematical and applied graph theory.

The general first and Second Zagreb indices [5] of G are defined as

$$M_1^\alpha(G) = \sum_{xy \in E(G)} (d(x) + d(y))^\alpha$$

and

$$M_2^\alpha(G) = \sum_{xy \in E(G)} (d(x)d(y))^\alpha,$$

where the parameter $\alpha \in \mathbb{R}$.

Note that if $\alpha = -\frac{1}{2}$, then $M_1^{-\frac{1}{2}}$ is Sum-connectivity index and $M_2^{-\frac{1}{2}}$ is the Randic index.

If $\alpha = 1$, then M_1^{-1} and M_2^{-1} are the standard first and second Zagreb indices respectively.

If $\alpha = -1$, then M_1^{-1} and M_2^{-1} are the Half the harmonic and Modified Zagreb indices respectively.

Motivated by first and second Zagreb indices, we introduced a pair generalized version of graph parameters based on the n_x 's and n_y 's as follows:

For $\alpha \in \mathbb{R}$, the general *PI* index and Szeged index of a connected graph [6] G as $PI^\alpha(G) = \sum_{xy \in E(G)} (n_x + n_y)^\alpha$ and $Sz^\alpha(G) = \sum_{xy \in E(G)} (n_x n_y)^\alpha$, respectively.

In this continuation, we introduced another general version of distance-based Topological index called Pattabi-Raman Szeged index (*PR-Szeged index*), which is defined for a graph G as

$$Sz_{(\alpha, \beta)}(G) = \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta \text{ where } \alpha, \beta \in \mathbb{R}.$$

If $\alpha = 1, \beta = -1$ then $Sz_{(1, -1)}(G) = Sz_{ISI}(G)$ (Inverse sum indeg Szeged index).

If $\alpha = 0, \beta = 1$ then $Sz_{(0, 1)}(G) = PI_v(G)$. (Classical PI index)

If $\alpha = 1, \beta = 0$ then $Sz_{(1, 0)}(G) = Sz_v(G)$. (Classical Szeged index)

If $\alpha = 0, \beta = -1$ then $Sz_{(0, -1)}(G) = 2Sz_H(G)$. (Harmonic Szeged index)

If $\alpha = -1, \beta = 0$ then $Sz_{(-1, 0)}(G) = Sz_{M_2^*}(G)$. (Second modified Szeged index)

If $\alpha = 0, \beta = -\frac{1}{2}$ then $Sz_{(0, -\frac{1}{2})}(G) = Sz_\chi(G)$. (Sum-connectivity Szeged index)

If $\alpha = -\frac{1}{2}, \beta = 0$ then $Sz_{(-\frac{1}{2}, 0)}(G) = Sz_R(G)$. (Randic Szeged index)

If $\alpha = \beta = 1$, then $Sz_{(1, 1)}(G) = Sz_{RZ}(G)$. (Reformulated Szeged index)

Topological indices continue to provide valuable insights into the molecular structure-property relationship, particularly in theoretical chemistry and drug design. Hardy and Pólya [7] laid foundational principles in mathematical inequality theory through their seminal work *Inequalities*, which has significantly influenced the analytical methods applied in chemical graph theory and topological index optimization. Pattabiraman and Paulraja [8] made foundational contributions by analyzing Wiener and Vertex PI indices of strong product graphs, offering new perspectives on how composite graph operations affect molecular descriptors. Their work paved the way for further studies involving graph products. Building on such concepts, Vetrivel and Paulraja [9] examined edge corona graphs to analyze the variation of key topological descriptors, relevant in multi-fragment molecular models. Dhanalakshmi and Akila [10] also contributed to this domain by investigating inverse sum indeg Szeged indices in complex molecular structures. Ali and Gutman [11] expanded on these ideas through the hybridization of eccentric and Zagreb-based indices for nanostructures, aligning topological theory with practical chemical applications.

Several researchers have extended the framework of distance-based indices such as the Szeged and PI indices to capture more nuanced structural information in molecular graphs. For instance, the vertex and edge versions of these indices have been studied for various graph products and operations, enabling a more detailed quantification of molecular topology. In particular, the weighted PI index and inverse sum indeg Szeged index has been employed to model compounds with complex connectivity, as shown in works like [12]. These indices serve as vital descriptors in graph-theoretic modeling of molecular reactivity and stability.

In this article, we explore the recently proposed Pattabi–Raman Szeged index (PR-Szeged index), a flexible distance-based topological invariant that generalizes the classical Szeged index through parameterization. We establish novel upper and lower bounds for this index, demonstrating how its behavior is influenced by real-valued parameters and underlying graph structure. These bounds are expressed in relation to traditional descriptors such as the Szeged and PI indices, thereby linking the PR-Szeged index to well-known structural measures.

2 Main Results

In this section, we obtain the relation between *PR*-Szeged index with other well-known distance-based indices.

Theorem 2.1. For $\alpha, \beta \in \mathbb{R}$,

$$(i) \quad \begin{aligned} Sz_{(\alpha, \beta)}(G) &\leq \frac{PI_{(2\alpha, \beta)}(G)}{2^{2\alpha}} \text{ if } \alpha \geq 0 \text{ and} \\ Sz_{(\alpha, \beta)}(G) &\geq \frac{PI_{(2\alpha, \beta)}(G)}{2^{2\alpha}} \text{ if } \alpha < 0 \end{aligned}$$

with equality for both if and only if for some values $\alpha \neq 0$ and β if and only if $n_x = n_y$ for every $xy \in E(G)$.

(ii) $Sz_{(\alpha, \beta)}(G) \leq 2^\beta Sz_{\alpha+\beta}(G)$ if $\beta \geq 0$ and

$$Sz_{(\alpha, \beta)}(G) \leq 2^\beta Sz_{\alpha+\beta}(G) \text{ if } \beta < 0$$

with equality for both n for some values $\alpha, \beta > 0$ and β if and only if $n_x = n_y = 1$ for every $xy \in E(G)$.

(iii) If $\beta \geq 0$ and G has only vertex for every $xy \in E(G)$ with $n_x \geq 2$ for every $x \in V(G)$, then

$$Sz_{(\alpha, \beta)}(G) \leq Sz_{(\alpha+\beta)}(G) \text{ if } \beta \geq 0 \text{ and}$$

$$Sz_{(\alpha, \beta)}(G) \geq Sz_{(\alpha+\beta)}(G) \text{ if } \beta < 0.$$

with equality for both for some values $\alpha, \beta \neq 0$ if and only if $n_x = n_y = 2$ for every $xy \in E(G)$.

(i) **Proof.** One can see that $2\sqrt{ab} \leq a + b$ with equality if and only if $a = b$.

If $\alpha \geq 0$, then

$$\begin{aligned} (n_x n_y)^\alpha (n_x + n_y)^\beta &= (\sqrt{n_x n_y})^{2\alpha} (n_x + n_y)^\beta \\ &\leq \left(\frac{n_x + n_y}{2}\right)^{2\alpha} (n_x + n_y)^\beta. \end{aligned}$$

For every $xy \in E(G)$,

$$(n_x n_y)^\alpha (n_x + n_y)^\beta \leq \frac{(n_x + n_y)^{2\alpha + \beta}}{2^{2\alpha}} \tag{2.1}$$

Taking summation over all edges xy of G , we have

$$\begin{aligned} \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta &\leq \sum_{xy \in E(G)} \frac{(n_x n_y)^{2\alpha + \beta}}{2^{2\alpha}} \\ Sz_{(\alpha, \beta)}(G) &= \frac{PI_{(2\alpha + \beta)}(G)}{2^{2\alpha}}. \end{aligned}$$

The equality attained in Equation (2.1) for some values of $\alpha > 0$ and β if and only if $n_x = n_y$ for every $xy \in E(G)$. If $\alpha \geq 0$, then

$$(n_x n_y)^\alpha (n_x + n_y)^\beta \geq \left(\frac{n_x + n_y}{2}\right)^{2\alpha} (n_x + n_y)^\beta.$$

This gives

$$Sz_{(\alpha, \beta)}(G) \geq \frac{PI_{(2\alpha + \beta)}(G)}{2^{2\alpha}}.$$

Equality holds if and only if $n_x = n_y$ for every $xy \in E(G)$.

(ii) **Proof.** Note that $x + y \leq 2xy$ for every $x, y \geq 1$ with equality if and only if $x = y = 1$.

$$\begin{aligned} (n_x n_y)^\alpha (n_x + n_y)^\beta &\leq (n_x n_y)^\alpha (2n_x n_y)^\beta \\ &= 2^\beta (n_x + n_y)^{\alpha+\beta}. \end{aligned}$$

Taking summation over all edges xy of G , we obtain

$$Sz_{(\alpha,\beta)}(G) \leq 2^\beta Sz_{(\alpha+\beta)}(G).$$

Equality holds for some values of $\alpha, \beta > 0$ if and only if $n_x = n_y = 1$ for every $xy \in E(G)$.

Likewise, if $\beta < 0$, then we have to obtain the converse inequality.

(iii) **Proof.** Let G be a graph with $n_x \geq 2$ for every $x \in V(G)$. We know that $x + y \leq xy$ for every $x, y \geq 2$ with equality if and only if $x = y = 2$. Then

$$\begin{aligned} (n_x n_y)^\alpha (n_x + n_y)^\beta &\leq (n_x n_y)^\alpha (n_x n_y)^\beta \\ &\leq (n_x n_y)^\alpha (n_x n_y)^\beta \\ &= (n_x + n_y)^{\alpha+\beta}. \end{aligned}$$

Taking summation over all edges of G , we get

$$Sz_{(\alpha,\beta)}(G) \leq Sz_{\alpha+\beta}(G).$$

Equality holds if and only if $n_x = n_y = 2$ for every $xy \in E(G)$.

Similarly, to apply the previous argument if $\alpha < 0$, we obtain the converse equality. \square

Lemma 2.1. (Jensen inequality) [7] If f is a convex function on an interval I and $x_1, x_2, \dots, x_k \in I$, then

$$f\left(\frac{x_1 + x_2 + \dots + x_k}{k}\right) \leq \frac{f(x_1) + f(x_2) + \dots + f(x_k)}{k}$$

Equality holds if and only if $x_1 = x_2 = \dots = x_k$.

Theorem 2.2. Let G be a graph with m edges and $\alpha, \beta, r \in \mathbb{R}$. Then $(Sz_{(\alpha,\beta)}(G))^r \leq s^{r-1} Sz_{(\alpha r, \beta r)}(G)$ if $r \geq 1$ or $r \leq 0$ and $(Sz_{(\alpha,\beta)}(G))^r \geq s^{r-1} Sz_{(\alpha r, \beta r)}(G)$ if $0 < r < 1$.

Proof. Since $f(x) = x$ is a convex function on \mathbb{R}_+ for every $r \geq 1$ or $r \leq 0$, by Lemma 1, we have

$$\begin{aligned} \left(\sum_{xy \in E(G)} \frac{(n_x n_y)^\alpha (n_x + n_y)^\beta}{s} \right)^r &\leq \frac{1}{s} \sum_{xy \in E(G)} ((n_x n_y)^\alpha (n_x + n_y)^\beta)^r \\ &\leq \frac{1}{s} \sum_{xy \in E(G)} (n_x n_y)^{\alpha r} (n_x + n_y)^{\beta r} \\ \frac{(SZ_{(\alpha, \beta)}(G))^r}{s^r} &\leq \frac{1}{s} SZ_{(\alpha r, \beta r)}(G) \\ (SZ_{(\alpha, \beta)}(G))^r &\leq s^{r-1} SZ_{(\alpha r, \beta r)}(G). \end{aligned}$$

If $0 < r < 1$, then we take the convex function $f(x) = -x^r$ and the previous argument gives the converse inequality. □

Theorem 2.3. For $\alpha, \beta, r \in \mathbb{R}$ with $r > 1$,

$$SZ_{(\alpha, \beta)}(G) \leq (SZ_{\alpha r}(G))^{\frac{1}{r}} \left(PI_{\left(\frac{\beta r}{r-1}\right)}(G) \right)^{\frac{r-1}{r}}.$$

Proof. By Holder inequality, we have

$$\begin{aligned} \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta &\leq \left(\sum_{xy \in E(G)} (n_x n_y)^{\alpha r} \right)^{\frac{1}{r}} \left(\sum_{xy \in E(G)} (n_x + n_y)^{\frac{\beta r}{r-1}} \right)^{\frac{r-1}{r}} \\ SZ_{(\alpha, \beta)}(G) &\leq (SZ_{\alpha r}(G))^{\frac{1}{r}} \left(PI_{\left(\frac{\beta r}{r-1}\right)}(G) \right)^{\frac{r-1}{r}}. \end{aligned}$$

□

Lemma 2.2. For real numbers $r > 0$ and $s_1, s_2, \dots, s_n, x_1, x_2, \dots, x_n > 0$,

$$\sum_{i=1}^n \frac{x_i^{r+1}}{s_i^r} \geq \frac{(\sum_{i=1}^n x_i)^{r+1}}{(\sum_{i=1}^n s_i)^r}$$

Theorem 4. For $\alpha, \beta, r \in \mathbb{R}$, $SZ_{(\alpha, \beta)}(G) \geq \left(SZ_{-\frac{\alpha}{r}}(G) \right)^r \left(PI_{\left(\frac{\beta}{r+1}\right)}(G) \right)^{r+1}$ and $SZ_{(\alpha, \beta)}(G) \geq \left(SZ_{\left(\frac{\alpha}{r+1}\right)}(G) \right)^r \left(PI_{\left(-\frac{\beta}{r+1}\right)}(G) \right)^{r+1}$.

Proof. Choose $s_i = (n_x n_y)^{\frac{-\alpha}{r}}$ and $x_i = (n_x + n_y)^{\frac{\beta}{r+1}}$ in Lemma 2, we obtain

$$\begin{aligned} \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta &\geq \frac{\left(\sum_{xy \in E(G)} (n_x + n_y)^{\frac{\beta}{r+1}}\right)^{r+1}}{\left(\sum_{xy \in E(G)} (n_x n_y)^{\frac{-\alpha}{r}}\right)^r} \\ &= \frac{\left(PI_{\left(\frac{\beta}{r+1}\right)}(G)\right)^{r+1}}{\left(SZ_{\frac{-\alpha}{r}}(G)\right)^r} \\ SZ_{(\alpha, \beta)}(G) &= \left(PI_{\left(\frac{\beta}{r+1}\right)}(G)\right)^{r+1} \left(SZ_{\frac{-\alpha}{r}}(G)\right)^r. \end{aligned}$$

Likewise $s_i = (n_u + n_v)^{\frac{-\beta}{r}}$ and $x_i = (n_u n_v)^{\frac{\alpha}{r+1}}$ in Lemma 2, we have

$$\sum_{xy \in E(G)} (n_u n_v)^\alpha (n_u + n_v)^\beta \geq \frac{\left(\sum_{xy \in E(G)} (n_u n_v)^{\frac{\alpha}{r+1}}\right)^{r+1}}{\left(\sum_{xy \in E(G)} (n_u + n_v)^{\frac{-\beta}{r}}\right)^r}.$$

This gives

$$SZ_{(\alpha, \beta)}(G) \geq \left(SZ_{\left(\frac{\alpha}{r+1}\right)}(G)\right)^r \left(PI_{\left(-\frac{\beta}{r+1}\right)}(G)\right)^{r+1}. \quad \square$$

Proof. Note that $(n_x - n_y)^2 + (n_x - r)^2 + (n_y - r)^2 \geq 0$. This implies that

$$\begin{aligned} n_x^2 + n_y^2 - 2n_x n_y + r^2 - 2rn_x + n_y^2 + r^2 - 2n_y r &\geq 0 \\ \Rightarrow n_x^2 + n_y^2 + r^2 &\geq r(n_x + n_y) + n_x + n_y \\ \Rightarrow (n_x + n_y)^2 + r^2 &\geq r(n_x + n_y) + 3n_x n_y \end{aligned}$$

multiple by $(n_x + n_y)^\beta (n_x n_y)^\alpha$ on both sides, we have

$$\begin{aligned} &(n_x + n_y)^{\beta+2} (n_x n_y)^\alpha + (n_x + n_y)^\beta (n_x n_y)^\alpha r^2 \\ &\geq r(n_x + n_y)^{\beta+1} (n_x n_y)^\alpha + 3(n_x + n_y)^\beta (n_x n_y)^{\alpha+1}. \end{aligned}$$

Taking summation over all edges of G , we obtain

$$\begin{aligned} \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^{\beta+2} + r^2 \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^\beta &\geq t \sum_{xy \in E(G)} (n_x n_y)^\alpha (n_x + n_y)^{\beta+1} \\ &+ 3 \sum_{xy \in E(G)} (n_x n_y)^{\alpha+1} (n_x + n_y)^\beta. \end{aligned}$$

This gives that

$$SZ_{(\alpha, \beta+2)}(G) + r^2 SZ_{(\alpha, \beta)}(G) \geq rSZ_{(\alpha, \beta+1)}(G) + 3SZ_{(\alpha+1, \beta)}(G). \quad \square$$

3 Conclusion

In this paper, inspired by the classical Zagreb indices, we introduced a pair-generalized distance-based topological index called the Pattabi-Raman Szeged index (*PR*-Szeged index). This index incorporates vertex partition counts and extends the traditional Szeged index with adjustable parameters α , β , and r . We established several new inequalities involving *PR*-Szeged indices, providing both upper and lower bounds depending on the range of r . These results offer a deeper understanding of the structural behavior of graphs and reveal connections between the *PR*-Szeged index and other well-known topological indices. Our findings pave the way for further studies in both theoretical graph analysis and applications in network modeling.

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