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Research Article

Some Inequalities between General Randić-Type Graph Invariants

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The Randić-type graph invariants are extensively investigated vertex-degree-based topological indices and have gained much prominence in recent years. The general Randić and zeroth-order general Randić indices are Randić-type graph invariants and are defined for a graph G with vertex set V as $R_\alpha(G) = \sum_{v_i \sim v_j} (d_i d_j)^\alpha$ and $Q_\alpha(G) = \sum_{v_i \in V} d_i^\alpha$, respectively, where α is an arbitrary real number, d_i denotes the degree of a vertex v_i, and $v_i \sim v_j$ represents the adjacency of vertices v_i and v_j in G. Establishing relationships between two topological indices holds significant importance for researchers. Some implicit inequality relationships between R_α and Q_α have been derived so far. In this paper, we establish explicit inequality relationships between R_α and Q_α. Also, we determine linear inequality relationships between these graph invariants. Moreover, we obtain some new inequalities for various vertex-degree-based topological indices by the appropriate choice of α.

1. Introduction

In this paper, we consider a simple finite graph $G = (V, E)$ with the vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and the edge set E, where the quantities $n = |V|$ and $m = |E|$ are known as the order and the size of G, respectively. If $n > 1$, then G is called a nontrivial graph. The ceiling function $\lceil n/2 \rceil$ would round $n/2$ to the smallest integer greater than or equal to $n/2$, whereas the floor function $\lfloor n/2 \rfloor$ would round $n/2$ to the largest integer less than or equal to $n/2$. For a given vertex $v_i \in V$, the neighborhood of v_i is denoted by $N(v_i)$ and defined as $N(v_i) = \{v_j \in V: v_i \sim v_j\}$, where $v_i \sim v_j$ represents the adjacency of vertices v_i and v_j in G. For $v_i \in V$, the degree of the vertex is defined as $d_i = |N(v_i)|$. Among all vertices of $\mathbb{G}$, the maximum degree is given by Δ and the minimum degree is given by δ. Without loss of generality, the degree sequence $(d_i) = (d_1, d_2, \ldots, d_n)$ of the vertices in G is organized as $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. If $d_i = \delta = \Delta$ for each vertex v_i in $\mathbb{G}$, we call it a regular graph. For a vertex v_i, denote by $S_i = \sum_{v_i \sim v_j} d_j$. It is obvious that $\delta^2 = \min_{v_i \in V} \{S_i\}$ and $\Delta^2 = \max_{v_i \in V} \{S_i\}$.

A chemical (or molecular) graph can frequently be used to represent the structure of a molecule. Chemical graphs play a pivotal role in understanding and representing the structural intricacies of molecules, thereby serving as a fundamental tool in the realm of chemistry. These graphs, composed of vertices representing atoms and edges denoting chemical bonds, provide a visual abstraction that aids in deciphering the three-dimensional arrangement of atoms in a compound. The chemical importance of graphs lies in their ability to elucidate molecular properties, reactivity patterns, and overall structural characteristics critical for predicting a substance's behavior. A plethora of literature exists, delving into the development and application of various graph-based approaches in chemistry [1]. Graph theory has proven invaluable in medicinal chemistry, material science, and computational chemistry, offering insights into molecular relationships, reaction mechanisms, and the rational design of novel compounds [2].

Graph theory has contributed to the development of chemistry by providing a variety of mathematical tools such as topological indices. A graph invariant that is calculated from the parameters of a chemical graph is declared a topological index (TI) if it correlates with some molecular property. TIs are the conclusive results of a mathematical and logical procedure that maps the chemical phenomena hidden inside a molecule's symbolic representation into a useful value, and they have been shown to be useful in modelling varied physicochemical characteristics reflected by QSAR and QSPR calculations [3, 4].

Milan Randić, a chemist, proposed a degree-based topological index, called the Randić index [5] which is useful for measuring the degree of branching in the carbon-atom skeleton of saturated hydrocarbons. This index is represented by R and is defined as follows:

$$\begin{aligned} R &= R(G) \\ &= \sum_{v_i \sim v_j} \left(d_i d_j\right)^{-1/2}. \end{aligned} \tag{1}$$

Randić proved that this index is significantly associated with a variety of physicochemical features of alkanes, including boiling points, enthalpy of formation, surface areas, and chromatographic retention times [6, 7]. Eventually R became one of the most well-known molecular descriptors, with two books [8, 9], several reviews, and a plethora of research articles devoted to it. Some bounds of this index have been studied in [10]. Bollobás and Erdös [11] extended R by substituting an arbitrary real number α for the exponent $-1/2$. This graph invariant is called the general product-connectivity index or the general Randić index [12], represented by R_α:

$$\begin{aligned} R_\alpha &= R_\alpha(G) \\ &= \sum_{v_i \sim v_j} \left(d_i d_j\right)^{\alpha}. \end{aligned} \tag{2}$$

Kier and Hall [13] put forward the zeroth-order Randić index, represented by ${}^0R$. The explicit formula of ${}^0R$ is

$$\begin{aligned} {}^0R &= {}^0R(G) \\ &= \sum_{v_i} d_i^{-1/2}. \end{aligned} \tag{3}$$

Eventually, Li and Zheng [14] proposed zeroth-order general Randić index by replacing the fraction $-1/2$ by an arbitrary real number α different from 0 and 1, denoted by Q_α:

$$\begin{aligned} Q_\alpha &= Q_\alpha(G) \\ &= \sum_{v_i} d_i^{\alpha}. \end{aligned} \tag{4}$$

This index is also studied under the name first general Zagreb index [15]. Moreover, it may be noted that Q_2 and R_2 are also studied under the names first Zagreb index M_1 [16] and second Zagreb index M_2 [17], respectively. The AutoGraphiX (conjecture-generating computer method) proposed [18] that the Zagreb indices are generally related to the inequality $M_2(G)/m \geq M_1(G)/n$ for a connected graph G with order n and size m. Though there exist graphs for which it does not hold [19], it is true for numerous classes of graphs [20–23].

The investigation of relationships between two topological indices remains an intriguing and attractive problem for researchers. Liu and Gutman [24] derived the implicit inequalities between R_α and Q_α for $\alpha > 0$ and $\alpha < 0$. Later, Zhou and Vukičević [25] established the inequalities between R_α, Q_α, $Q_{2\alpha}$, and $Q_{2\alpha+1}$. In this paper, we make a step forward by deriving the explicit relationships between R_α and Q_α for $\alpha > 0$ and $\alpha < 0$. Also, we obtain linear inequalities between R_α and Q_α for $\alpha > 0$ and $\alpha < 0$, for alpha > 0 and with some condition on the order of graph for alpha < 0. Moreover, we obtain new inequality between $M_2(G)/m$ and $M_1(G)/n$ for any graph G with order n and size m. Further, we determine new inequality between $R(G)/m$ and ${}^0R(G)/n$.

2. Some Known Results

In this section, we review some known results that will be used in our main results.

Let $p_1, p_2, \ldots, p_n$ and $q_1, q_2, \ldots, q_n$ be positive real numbers such that for $1 \leq i \leq n$, it holds that $p \leq p_i \leq P$ and $q \leq q_i \leq Q$. Then,

$$\left| n\sum_{i=1}^{n} p_i q_i - \sum_{i=1}^{n} p_i \sum_{i=1}^{n} q_i \right| \leq \tau(n)(P-p)(Q-q), \tag{5}$$

where $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$. Further, equality attains if and only if $p_1 = p_2 = \cdots = p_n$ and $q_1 = q_2 = \cdots = q_n$ [26].

Rodríguez et al. [27] established the following relationships between Q_α and $Q_{\alpha+1}$.

Let G be a nontrivial graph having the parameters n and m. Then, for $\alpha > 0$,

$$Q_{\alpha+1}(G) \geq \frac{2m}{n} Q_\alpha(G), \tag{6}$$

and for $\alpha < 0$,

$$Q_{\alpha+1}(G) \leq \frac{2m}{n} Q_\alpha(G). \tag{7}$$

Equality attains in each case if and only if G is regular.

Also, Rodríguez et al. [27] derived the following relation between Q_α and $Q_{2\alpha}$.

If G is a nontrivial graph with the parameters n, δ, and Δ, then for $\alpha < 0$,

$$Q_{2\alpha}(G) \leq \frac{1}{4n}\left[\left(\frac{\Delta}{\delta}\right)^{\alpha} + \left(\frac{\delta}{\Delta}\right)^{\alpha} + 2\right] Q_\alpha^2(G). \tag{8}$$

Further, equality attains if and only if G is regular.

Liu and Gutman [24] derived the following implicit quadratic inequality between R_α and Q_α.

If G is a nontrivial graph with the parameters n, δ, and Δ, then for $\alpha > 0$,

$$R_\alpha(G) \leq \frac{1}{2} Q_\alpha(G)\left[\left(1 - \frac{1}{n}\right) Q_\alpha(G) + (\Delta - n + 1)\delta^{\alpha}\right], \tag{9}$$

and the equality is achieved if and only if G is regular.

Also, Liu and Gutman [24] established the following inequality between R_α, Q_α, $Q_{\alpha+1}$, and $Q_{2\alpha}$.

$$R_\alpha(G) \geq \frac{1}{2}\left[Q_\alpha^2(G) - (n-1)\delta^\alpha Q_\alpha(G) + \delta^\alpha Q_{\alpha+1}(G) - Q_{2\alpha}(G)\right]. \quad (10)$$

Further, equality attains if and only if G is regular.

3. Main Results

Lemma 1. *Let G be a nontrivial graph; then, for any real number α,*

$$Q_{\alpha+1}(G) = \sum_{i=1}^{n} S_i(\alpha), \quad (11)$$

where $S_i(\alpha) = \sum_{v_j \in N(v_i)} d_j^\alpha$.

Proof

$$\begin{aligned} Q_{\alpha+1}(G) &= \sum_{i=1}^{n} d_i^{\alpha+1} \\ &= \sum_{i=1}^{n} d_i d_i^\alpha = d_1 d_1^\alpha + d_2 d_2^\alpha + \cdots + d_n d_n^\alpha \\ &= \underbrace{d_1^\alpha + d_1^\alpha + \cdots + d_1^\alpha}_{d_1 \text{times}} + \underbrace{d_2^\alpha + d_2^\alpha + \cdots + d_2^\alpha}_{d_2 \text{times}} + \cdots + \underbrace{d_n^\alpha + d_n^\alpha + \cdots + d_n^\alpha}_{d_n \text{times}}. \end{aligned} \quad (12)$$

By rearranging with respect to the sum of degrees of neighbor vertices of each vertex v_i, we have

$$Q_{\alpha+1}(G) = \sum_{i=1}^{n} \sum_{v_j \in N(v_i)} d_j^\alpha. \quad (13)$$

By setting $S_i(\alpha) = \sum_{v_j \in N(v_i)} d_j^\alpha$, the required result follows. □

If G is a nontrivial graph having the parameters n and δ, then for $\alpha < 0$,

Lemma 2. *Let G be a nontrivial graph; then, for any real number α,*

$$R_\alpha(G) = \frac{1}{2}\sum_{i=1}^{n} d_i^\alpha S_i(\alpha), \quad (14)$$

where $S_i(\alpha) = \sum_{v_j \in N(v_i)} d_j^\alpha$.

Proof

$$\begin{aligned} R_\alpha(G) &= \frac{1}{2}\sum_{v_i \sim v_j} 2 d_i^\alpha d_j^\alpha \\ &= \frac{1}{2}\left[d_1^\alpha \sum_{v_j \in N(v_1)} d_j^\alpha + d_2^\alpha \sum_{v_j \in N(v_2)} d_j^\alpha + \cdots + d_n^\alpha \sum_{v_j \in N(v_n)} d_j^\alpha\right] \\ &= \frac{1}{2}\sum_{i=1}^{n} d_i^\alpha \sum_{v_j \in N(v_n)} d_j^\alpha. \end{aligned} \quad (15)$$

By taking $S_i(\alpha) = \sum_{v_j \in N(v_i)} d_j^\alpha$, the desired result follows.

In the following theorem, we derive the left and right explicit inequalities between R_α and Q_α for $\alpha > 0$ and $\alpha < 0$, respectively. □

Theorem 3. *Let G be a nontrivial graph with order n, size m, minimum vertex-degree δ, and maximum vertex-degree Δ. Then, the following left and right inequalities hold for $\alpha > 0$ and $\alpha < 0$, respectively:*

$$-\phi(m,n,\alpha)+\left(\frac{Q_\alpha(G)}{n}\right)^2\le\frac{R_\alpha(G)}{m}\le\left(\frac{Q_\alpha(G)}{n}\right)^2+\phi(m,n,\alpha), \tag{16}$$

where $\phi(m,n,\alpha)=\tau(n)/2\mathrm{mn}(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha)$ *and* $\tau(n)=n\lceil n/2\rceil(1-1/n\lceil n/2\rceil)$. *Further, each equality holds if and only if G is a regular graph.*

Proof. We choose $p_i=d_i^\alpha$ and $q_i=S_i(\alpha)$ in inequality (1); then, for $\alpha\ge 0$, $\delta^\alpha\le d_i^\alpha\le\Delta^\alpha$ and $\delta^{2\alpha}\le S_i(\alpha)\le\Delta^{2\alpha}$ and for $\alpha\le 0$, $\Delta^\alpha\le d_i^\alpha\le\delta^\alpha$ and $\Delta^{2\alpha}\le S_i(\alpha)\le\delta^{2\alpha}$, where $i=1,2,\ldots,n$. Note that for any real number α, $(\Delta^\alpha-\delta^\alpha)(\Delta^{2\alpha}-\delta^{2\alpha})=(\delta^\alpha-\Delta^\alpha)(\delta^{2\alpha}-\Delta^{2\alpha})$. Then, for any real number α, inequality (1) takes the form

$$\left|n\sum_{i=1}^n d_i^\alpha S_i(\alpha)-\sum_{i=1}^n d_i^\alpha\sum_{i=1}^n S_i(\alpha)\right|\le\tau(n)(\Delta^\alpha-\delta^\alpha)\left(\Delta^{2\alpha}-\delta^{2\alpha}\right), \tag{17}$$

where $\tau(n)=n\lceil n/2\rceil(1-1/n\lceil n/2\rceil)$.

From (11) and (14), we have

$$\left|2nR_\alpha(G)-Q_\alpha(G)Q_{\alpha+1}(G)\right|\le\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha). \tag{18}$$

This implies that

$$-\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha)\le 2nR_\alpha(G)-Q_\alpha(G)Q_{\alpha+1}(G)\le\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha). \tag{19}$$

This gives

$$\begin{aligned}-\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha)+Q_\alpha(G)Q_{\alpha+1}(G)&\le 2nR_\alpha(G)\\&\le Q_\alpha(G)Q_{\alpha+1}(G)+\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha).\end{aligned} \tag{20}$$

By using (6) with $\alpha>0$ and (7) with $\alpha<0$ in the left and right inequalities, respectively, we have

$$\begin{aligned}-\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha)+\frac{2m}{n}(Q_\alpha(G))^2&\le 2nR_\alpha(G)\\&\le\frac{2m}{n}(Q_\alpha(G))^2+\tau(n)(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha).\end{aligned} \tag{21}$$

By taking $\phi(m,n,\alpha)=\tau(n)/2\mathrm{mn}(\Delta^\alpha-\delta^\alpha)^2(\Delta^\alpha+\delta^\alpha)$, the required inequality (16) follows.

Since equality attains in (5) if and only if $p_1=p_2=\cdots=p_n$ and $q_1=q_2=\cdots=q_n$, this gives that equality attains in (16) if and only if $d_1^\alpha=d_2^\alpha=\cdots=d_n^\alpha$ and $S_1(\alpha)=S_2(\alpha)=\cdots=S_n(\alpha)$. Also, $d_1^\alpha=d_2^\alpha=\cdots=d_n^\alpha$ and $S_1(\alpha)=S_2(\alpha)=\cdots=S_n(\alpha)$ imply that $d_1=d_2=\cdots=d_n$ and $S_1=S_2=\cdots=S_n$. This recommends that each equality in (16) attains if and only if G is a regular graph.

In the following corollary, we derive the linear inequality between Q_α and R_α for any positive real number α. □

Corollary 4. *Let G be a nontrivial graph having order n, size m, minimum vertex-degree δ, and maximum vertex-degree Δ with* $n(n-1)\ne 2m$. *Then, for* $\alpha>0$, *we have*

$$R_\alpha(G)\ge\frac{m}{n(n-1)-2m}\left[(n-\Delta-1)\delta^\alpha Q_\alpha(G)-n(n-1)\phi(m,n,\alpha)\right], \tag{22}$$

where $\phi(m,n,\alpha) = \tau(n)/2mn(\Delta^{\alpha} - \delta^{\alpha})^2(\Delta^{\alpha} + \delta^{\alpha})$ *and* $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$. *Moreover, equality attains if and only if G is a regular graph.*

Proof. From inequality (9) with $\alpha > 0$, we have

$$R_{\alpha}(G) \leq \frac{n(n-1)}{2}\left(\frac{Q_{\alpha}(G)}{n}\right)^2 + \frac{1}{2}(\Delta - n + 1)\delta^{\alpha}Q_{\alpha}(G). \tag{23}$$

Also, from left inequality (16), we get

$$\left(\frac{Q_{\alpha}(G)}{n}\right)^2 \leq \frac{R_{\alpha}(G)}{m} + \phi(m,n,\alpha), \tag{24}$$

where $\phi(m,n,\alpha) = \tau(n)/2mn(\Delta^{\alpha} - \delta^{\alpha})^2(\Delta^{\alpha} + \delta^{\alpha})$ and $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$.

By using inequality (24) in inequality (23), we have

$$R_{\alpha}(G) \leq \frac{n(n-1)}{2}\left[\frac{R_{\alpha}(G)}{m} + \phi(m,n,\alpha)\right] + \frac{1}{2}(\Delta - n + 1)\delta^{\alpha}Q_{\alpha}(G). \tag{25}$$

After simplifying (25) and then rearranging, we get the desired inequality (22).

Since the equality attains in both inequality (9) and left inequality (16) if and only if G is a regular graph, equality in (22) holds if and only if G is a regular graph. □

Lemma 5. *For* $\alpha < 0$, *it is easy to observe that*

$$Q_{\alpha+1}(G) \geq \delta Q_{\alpha}, \tag{26}$$

where equality attains if and only if G is a regular graph.

In the upcoming corollary, we derive the linear inequality between R_{α} and Q_{α} for any negative real number α which satisfies some condition on the order of graph G.

Corollary 6. *Let G be a nontrivial graph having order n, size m, minimum vertex-degree δ, and maximum vertex-degree Δ. Then, for* $\alpha < 0$ *and* $n > \lambda/4$,

$$R_{\alpha}(G) \leq \frac{m}{n(4n-\lambda) - 8m}\left[4\delta^{\alpha}(n - \delta - 1)Q_{\alpha}(G) + n(4n-\lambda)\psi(m,n,\alpha)\right], \tag{27}$$

where $\lambda = \lambda(\alpha) = (\Delta/\delta)^{\alpha} + (\delta/\Delta)^{\alpha} + 2, \phi(m,n,\alpha) = \tau(n)/2mn(\Delta^{\alpha} - \delta^{\alpha})^2(\Delta^{\alpha} + \delta^{\alpha})$ *and* $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$. *Further, equality attains if and only if G is a regular graph.*

Proof. From inequalities (4) and (14) with $\alpha < 0$, inequality (6) becomes

$$R_{\alpha}(G) \geq \frac{1}{2}\left[\left[1 - \frac{1}{4n}\left(\left(\frac{\Delta}{\delta}\right)^{\alpha} + \left(\frac{\delta}{\Delta}\right)^{\alpha} + 2\right)\right]Q_{\alpha}^2(G) - (n - \delta - 1)\delta^{\alpha}Q_{\alpha}(G)\right]. \tag{28}$$

By taking $\lambda = \lambda(\alpha) = (\Delta/\delta)^{\alpha} + (\delta/\Delta)^{\alpha} + 2$ and rearranging, we have

$$R_{\alpha}(G) \geq \frac{1}{2}\left[n\left(n - \frac{\lambda}{4}\right)\left(\frac{Q_{\alpha}(G)}{n}\right)^2 - (n - \delta - 1)\delta^{\alpha}Q_{\alpha}(G)\right]. \tag{29}$$

Also, from right inequality (9) with $\alpha < 0$ and $n > \lambda/4$, we get

$$R_{\alpha}(G) \geq \frac{n(4n-\lambda)}{8}\left[\frac{R_{\alpha}(G)}{m} - \phi(m,n,\alpha)\right] - \frac{(n - \delta - 1)}{2}\delta^{\alpha}Q_{\alpha}(G), \tag{30}$$

where $\phi(m,n,\alpha) = \tau(n)/2mn(\Delta^{\alpha} - \delta^{\alpha})^2(\Delta^{\alpha} + \delta^{\alpha})$ and $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$.

After simplifying (30), we achieve the desired inequality (27).

Since equality attains in right inequality (16) and each of the inequalities (4), (14), and (6) if and only if G is a regular graph, this implies that equality in (27) attains if and only if G is a regular graph.

In the following corollary, we get a new inequality between $M_2(G)/m$ and $M_1(G)/n$ for any graph G with order n and size m by taking $\alpha = 2$ in the left inequality (16). □

Corollary 7. *Let G be a nontrivial graph with order n and size m; then,*

$$\frac{M_2(G)}{m} \geq \left(\frac{M_1(G)}{n}\right)^2 - \phi(m,n), \tag{31}$$

where $\phi(m,n) = \tau(n)/2mn(\Delta^4 - \delta^4)(\Delta^2 - \delta^2)$ *and* $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$. *Further, each equality holds if and only if G is a regular graph.*

In the following corollary, we obtain a new inequality between $R(G)/m$ and ${}^0R(G)/n$ for any graph G with order n and size m by setting $\alpha = -1/2$ in the right inequality (16).

Corollary 8. *Let G be a nontrivial graph having order n and size m; then,*

$$\frac{R(G)}{m} \leq \left(\frac{{}^0R(G)}{n}\right)^2 + \psi(m,n), \tag{32}$$

where $\psi(m,n) = \tau(n)(\Delta - \delta)(\sqrt{\Delta} - \sqrt{\delta})/2mn(\Delta\delta)^{3/2}$ *and* $\tau(n) = n\lceil n/2\rceil(1 - 1/n\lceil n/2\rceil)$. *Moreover, each equality holds if and only if G is a regular graph.*

4. Conclusions

A major contribution of this paper lies in the derivation of explicit inequality relationships between the general Randić and zeroth-order general Randić indices. Furthermore, the paper goes beyond the implicit relationships and determines linear inequality relationships between the general Randić and zeroth-order general Randić indices, providing a more comprehensive framework for their comparison. We would like to conclude this paper by proposing the following open problem.

Open Problem 9. Drive the linear inequality between the general Randić index R_α and zeroth-order general Randić index Q_α for any negative real number α.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

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