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Extremal Graphs of GQ Index with Given Minimum Degree and their Comparison with ABC and Randić Index

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ABSTRACT: The Geometric-Quadratic index (GQ) of a graph G is defined as $GQ(G) = \sum_{\xi\psi\in E(G)} \sqrt{\frac{2d_\xi d_\psi}{d_\xi^2+d_\psi^2}}$ where d_ξ represents the degree of vertex ξ, is studied within the class of $G(\mu, \mho)$ of simple connected graph with $\mho$ vertices with the minimum of degree μ. The primary theoretical contribution of this article is the characterization of minimizing graphs for vast range of parameters, we provide that when either μ or even, the extremal graph that minimizes the GQ index is necessarily μ-regular. Moreover, we also determine the extremal graph G that minimize the Geometric-Quadratic value or the lower bound for all $\mu \geq \lceil \mu_0 \rceil$, with $\mu_0 = \varrho_0(\mho-1)$ and $\varrho_0 \approx 1$ is found to be the unique positive solution to the equation $(1+\varrho)\sqrt{\varrho^2+1}-2\sqrt{2\varrho} = 0$. In such cases where extremal graphs are not explicitly identified, the corresponding lower bound is established. The comparative analysis between the ABC and Randić index serves to contextualize the GQ index within the existing molecular descriptors revealing its unique structural sensitivity and validating its potential for application in chemoinformatics. Finally, we derive specialized bounds for the GQ index for chemical trees and molecular graphs.

Keywords: Geometric-Quadratic index, minimum degree, linear programming, atom-bond sum connectivity index.

Contents

1. Introduction

Let G be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The number of vertices in a graph is denoted by $\mho$ and the number of edges in a graph is denoted by m. Let d_ξ be the degree of the vertex ξ and is defined as the number of edges incident to the vertex ξ. the maximum and minimum degree of the graph G are denoted by Δ and μ respectively. The neighborhood of G denoted by $N_\xi(G) = \{\psi/\psi \in V(G) : \xi\psi \in E(G)\}$.

Chemical graph theory is a branch of discrete mathematics focused on determining the maximum or minimum possible values of various graph parameters within a given set of constraints. In chemical graph theory, extremal graphs play an important role, especially in studying topological indices—numerical values that describe the structure of chemical compounds represented as graphs where atoms correspond to vertices and chemical bonds to edges [1]. The key objective is to identify extremal graphs that either maximize or minimize a particular index under fixed constraints such as the number of vertices, edges, degree sequence, or cyclic structure.

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Topological indices capture essential information about molecule topology, such as the connectivity and arrangement of atoms.They play a significant role in chemical research, particularly in drug discovery, materials science, and other interdisciplinary fields.

In 1975 Randić [2] introduced an index named after him, the Randić index $R(G)$ which is represented as:

$$R(G) = \sum_{\xi\psi \in E(G)} \frac{1}{\sqrt{d_\xi d_\psi}}. \tag{1.1}$$

Vukičević, D. and Furtula, B. [3] introduced a new index named as geometric-arithmetic index and is defined as:

$$GA(G) = \sum_{\xi\psi \in E(G)} \frac{2\sqrt{d_\xi d_\psi}}{d_\xi + d_\psi} \tag{1.2}$$

where d_ξ symbolizes the degree of the vertex ξ.

The Quadratic-Geometric index QG is defined as

$$QG(G) = \sum_{\xi\psi \in E(G)} \sqrt{\frac{d_\xi^2 + d_\psi^2}{2\, d_\xi d_\psi}}. \tag{1.3}$$

The GA (1.2) and QG (1.3) share a common structure to analyze the relationship between the vertex degrees at the ends of the edge. However, the GA is based on the ratio of the geometric and arithmetic means, which is known to be sensitive to edges connecting vertices of different degrees. The GQ utilizes the quadratic mean, which inherently gives more weight to higher degrees and is most sensitive to the high-degree vertices in the graph.

Inspired from the definitions of GA and QG index, V.R.Kulli [4] introduced the Geometric-Quadratic index of a graph G which is defined as

$$GQ(G) = \sum_{\xi\psi \in E(G)} \sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}} \tag{1.4}$$

This GQ index bridge the perspectives of GA and QG index by employing the ratio of geometric and quadratic means. Unlike Eq. (1.2) the denominator is the quadratic mean, it reduces the large degree differences and offers a different sensitivity. Conversely, unlike the QG index the GQ captures the balance or correlation between the degrees. This suggests that the GQ captures topological futures than either GA or QG alone, making it an subject for a separate extremal analysis to understand the unique behavior and potential applications in quantifying molecular structure.

As defined by Estrada [5] in 1998 ,

$$ABC(G) = \sum_{\xi\psi \in E(G)} \sqrt{\frac{1}{d_\xi} + \frac{1}{d_\psi} - \frac{2}{d_\xi d_\psi}} \tag{1.5}$$

represents the atom-bond connectivity index.

Compared to other indices, Randić index is the deeply analysed and preferred index. The upper and lower bounds in terms of minimum and maximum degree is obtained in [6]. The relationship between the Randić index and many other topological indices is given in [7].Some of the other works on Randić index are given in [8,9,10,11]. Furtula et al. [12] has derived the extremal values of the ABC index for chemical trees. The upper and lower bounds of trees and graphs of ABC index is derived by Das K. C. in [13]. V.R.Kulli in [4] proposed the Geometric - Quadratic Index and has also calculated the exact values of some graphs and benzonoid systems. Shisankar et al. [14] have derived mathematical relationships between GQ and QG indices for few graph invariants such as degree sequence, size, etc. With the help of their respective M-polynomials, Shisankar et al. [15] have analysed the GQ and QG indices for silicon carbide networks.For recent studies focused on identifying extremal graphs with respect to topological indices, interested researchers may consult the following works. [16,17,18]

Currently, there is an increasing focus on investigating and comparing the connections between different topological indices. Das et al. in [19] have obtained the relationship betweeen the Randić index and sum connectivity index. The initial three extremal and maximal trees with respect to the $ABC-R$ index for both n-vertex binary and chemical trees have been identified in [20]. Building on this, the fourth, fifth, and sixth maximal chemical trees concerning the $ABC-R$ index, along with an upper bound for trees with a specified number of pendant vertices, are established in [21]. The study of the difference between the Atom-Bond Connectivity index and the Randić index, denoted as $ABS-R$, for bipartite and chemical graphs is presented in [22]. Additionally, the minimal and maximal chemical trees based on the $GA-R$ index are discussed in [23,1].

Inspired by the above findings, we now explore the geometric-quadratic index with atom-bond connectivity index and Randić index. This article primarily aims to establish the extremal values for the GQ index of the graphs that belong to the class $G(\mu,\mho)$. We also identify the extremal graphs for which the GQ index achieves the minimum value. Furthermore, the connection between the ABC index and the GQ index has been explored for both chemical trees and molecular graphs. A comparative study highlighting the relationship between the geometric-quadratic index and the Randić index for chemical graphs, along with their corresponding bounds, has also been presented.

2. Modeling the Linear Programming Framework of the Problem

We introduce some linear equalities and inequalities that must be satisfied in any graph in $G(\mu,\mho)$. The vertices of degrees ξ and ψ are joined by edges and the number of edges connecting these vertices are denoted by $x_{\xi,\psi}$. The problem P of identifying the minimum of $G(\mu,\mho)$can be mathematically formulated as $\min(\mathrm{GQ}(G)=\sum_{\mu\leqslant\xi\leqslant\psi\leqslant\mho-1}\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2+d_\psi^2}} \mid G\in G(\mu,\mho))$ and is given by:

$$\min\sum_{\mu\leqslant\xi\leqslant\psi\leqslant\mho-1}\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2+d_\psi^2}}x_{\xi,\psi}$$

subject to,

$$\begin{aligned} 2x_{\mu,\mu}+x_{\mu,\mu+1}+x_{\mu,\mu+2}+\cdots+x_{\mu,\mho-1}&=\mu\mho_\mu,\\ x_{\mu,\mu+1}+2x_{\mu+1,\mu+1}+x_{\mu+1,\mu+2}+\cdots+x_{\mu+1,\mho-1}&=(\mu+1)\mho_{\mu+1}, \qquad (2.1)\\ &\vdots\\ x_{\mu,\mho-1}+x_{\mu+1,\mho-1}+x_{\mu+2,\mho-1}+\cdots+2x_{\mho-1,\mho-1}&=(\mho-1)\mho_{\mho-1},\\ \mho_\mu+\mho_{\mu+1}+\mho_{\mu+2}+\cdots+\mho_{\mho-1}&=\mho, \qquad (2.2)\\ x_{\xi,\psi}\geq 0,\quad \mu\leq\xi\leq\psi\leq\mho-1,\quad \mho_\xi\geq 0,&\quad \mu\leq\xi\leq\mho-1. \qquad (2.3)\end{aligned}$$

Equation (2.1) represents a block of equalities, one for each degree value $\mu,\mu+1,\ldots,\mho-1$. The generic form for a fixed degree k is $2x_{\mu,\mu}+x_{\mu,\mu+1}+x_{\mu,\mu+2}+\cdots+x_{\mu,\mho-1}=\mu\,\mho_\mu$ where $x_{\mu,\mu}$ denotes the number of edges connecting two vertices, both of degree μ.

$\mho_\mu$ in Equation (2.2) denotes the summing of all possible degree which gives the total number of vertices μ.

Equation (2.3) represents the non-negativity integrality where the variables $x_{\xi,\psi}$ and $\mho_\xi$ are integers. The linear programming optimization problem are defined in Eqs. (2.1) - (2.3).

3. Main Theorem

In this section, in order to find a lower bound for the geometric-quadratic index and extremal graphs we used a linear programming approach. By this approach, GQ index attains its minimum value $GQ(G) \geq \frac{\mu\mho}{2}$.

Theorem 3.1 *If $\mu \geq \lceil \mu_0 \rceil$ where $\mu_0 = \varrho_0(\mho - 1)$ and $\varrho_0 \approx 1$ is the unique positive root of the equation $(1+\varrho)\sqrt{\varrho^2+1} - 2\sqrt{2\varrho} = 0$ and if $G \in G(\mu, \mho)$ then*

$$GQ(G) \geq \frac{\mu\mho}{2}$$

If μ or $\mho$ is an even number, then regular graphs with degree μ can achieve this value.

Proof: The problem considered here is

$$\min \sum_{\mu\leqslant\xi\leqslant\psi\leqslant\mho-1} \sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}}\, x_{\xi,\psi},$$

subject to the Eqs. (2.1) - (2.3). This is a linear programming problem where $\mho_\xi$, $x_{\mu\mu}$, $\mu \leqslant \xi \leqslant \mho - 1$ are the basic variables. The inequalities (2.1) and (2.2) can be derived with $x_{\mu\mu}$ and $\mho_\xi$. We have

$$\mho_\xi = \frac{x_{\mu,\xi} + x_{\mu+1,\xi} + \dots\dots\dots + 2x_{\xi,\xi} + \dots\dots + x_{\xi,\mho-1}}{\xi}, \qquad \mu+1 \leqslant \xi \leqslant \mho - 1 \tag{3.1}$$

From equation (2.2),

$$\mho_\mu = \mho - \sum_{\xi=\mu+1}^{\mho-1} \mho_\xi = \mho - \sum_{\xi=\mu+1}^{\mho-1} \frac{1}{\xi} x_{\mu,\xi} - \sum_{\mu+1\leqslant\xi\leqslant\psi\leqslant\mho-1} \left(\frac{1}{\xi} + \frac{1}{\psi}\right) x_{\xi,\psi} \tag{3.2}$$

From the first equation (2.1), we have

$$x_{\mu,\mu} = \frac{1}{2}\mu\mho_\mu - \frac{1}{2}\sum_{\xi=\mu+1}^{\mho-1} x_{\mu,\xi} \tag{3.3}$$

After substitution of $\mho_\mu$ from (3.2) and (3.3), we get

$$x_{\mu,\mu} = \frac{\mu\mho}{2} - \frac{1}{2}\sum_{\xi=\mu+1}^{\mho-1} \left(1 + \frac{\mu}{\xi}\right) x_{\mu,\xi} - \sum_{\mu+1\leqslant\xi\leqslant\psi\leqslant\mho-1} \left(\frac{\mu}{\xi} + \frac{\mu}{\psi}\right) x_{\xi,\psi}$$

Then

$$GQ(G) = \sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}}$$

$$= \sqrt{\frac{2\mu\mu}{\mu^2+\mu^2}} \left[\frac{\mu\mho}{2} - \frac{1}{2}\sum_{\xi=\mu+1}^{\mho-1}\left(1+\frac{\mu}{\xi}\right) x_{\mu\xi} - \frac{1}{2}\sum_{\mu+1\leq\xi\leq\psi\leq\mho-1}\left(\frac{\mu}{\xi}+\frac{\mu}{\psi}\right) x_{\xi\psi}\right] + \sum_{\xi=\mu+1}^{\mho-1}\sqrt{\frac{2\mu\xi}{\mu^2+\xi^2}}\, x_{\mu,\xi} + \sum_{\mu+1\leq\xi\leq\psi\leq\mho-1}\sqrt{\frac{2\xi\psi}{\xi^2+\psi^2}}\, x_{\xi\psi}$$

$$= \frac{\mu\mho}{2} + \sum_{\xi=\mu+1}^{\mho-1}\left[\sqrt{\frac{2\mu\xi}{\mu^2+\xi^2}} - \frac{\mu}{2}\left(\frac{1}{\mu}+\frac{1}{\xi}\right)\right] x_{\mu,\xi} + \sum_{\mu+1\leq\xi\leq\psi\leq\mho-1}\left[\sqrt{\frac{2\xi\psi}{\xi^2+\psi^2}} - \frac{\mu}{2}\left(\frac{1}{\xi}+\frac{1}{\psi}\right)\right] x_{\xi\psi}$$

Define $a_{\xi\psi} = \sqrt{\frac{2\xi\psi}{\xi^2+\psi^2}} - \frac{\mu}{2}\left(\frac{1}{\xi}+\frac{1}{\psi}\right)$ for $\mu \le \xi \le \psi \le \mho - 1$
we show $a_{\xi\psi} \ge 0$ for $\mu \le \xi \le \psi \le \mho - 1$. We have

$$a_{\xi\xi} = 1 - \frac{\mu}{\xi} \ge 1 - \frac{\mu}{\mu} = 0 \text{ for } \mu \le \xi \le \mho - 1$$

Since,

$$\frac{\partial a_{\xi\psi}}{\partial \xi} = \frac{\xi}{\sqrt{2\xi\psi}\sqrt{\xi^2+\psi^2}} - \frac{\xi\sqrt{2\xi\psi}}{(\xi^2+\psi^2)^{3/2}} + \frac{\mu}{2\xi^2} > 0$$

for $\psi \ge \xi$, we have $a_{\xi\psi} > a_{\mu\psi}$, $\mu \le \xi \le \psi \le \mho - 1$. Further

$$\begin{aligned}
a_{\xi\psi} &= \sqrt{\frac{2\mu\psi}{\mu^2+\psi^2}} - \frac{1}{2}\left(\frac{\mu}{\mu}+\frac{\mu}{\psi}\right) \\
&= \sqrt{\frac{2\mu\psi}{\mu^2+\psi^2}} - \frac{1}{2}\left(1+\frac{\mu}{\psi}\right) = \sqrt{1 - \frac{(\mu-\psi)^2}{\mu^2+\psi^2}} - \frac{1}{2} - \frac{\mu}{2\psi} \\
&= \sqrt{\frac{\mu^2+\psi^2-(\mu-\psi)^2}{\mu^2+\psi^2}} + \frac{(-\psi-\mu)}{2\psi} = \sqrt{\frac{\mu^2+\psi^2-(\mu-\psi)^2}{\mu^2+\psi^2}} + \frac{-\psi-\mu}{2\psi} \\
&= \sqrt{\frac{\mu^2+\psi^2-(\mu^2+\psi^2-2\mu\psi)}{\mu^2+\psi^2}} + \frac{-\psi-\mu}{2\psi} = \sqrt{\frac{2\mu\psi}{\mu^2+\psi^2}} + \frac{-\psi-\mu}{2\psi} \\
&= \frac{1}{2\psi\sqrt{\mu^2+\psi^2}}\left[2\psi\sqrt{2\mu\psi} + \sqrt{\mu^2+\psi^2}(-\psi-\mu)\right] \\
&= \frac{1}{2\psi\sqrt{\mu^2+\psi^2}}\left[\tilde{a}_{\mu\psi}\right]
\end{aligned}$$

where

$$\tilde{a}_{\mu\psi} = 2\psi\sqrt{2\mu\psi} + \sqrt{\mu^2+\psi^2}(-\psi-\mu)$$

$$\frac{\partial^2 a_{\mu\psi}}{\partial \psi} = \frac{3\mu}{\sqrt{2\mu\psi}} - \frac{3\psi+\mu}{\sqrt{\mu^2+\psi^2}} + \frac{\psi^2(\psi+\mu)}{(\psi^2+\mu^2)^{3/2}} < 0$$

We establish that the function $\tilde{a}_{\mu\psi}$ is concave for the range $\mu \le \psi \le \mho - 1$. The function evaluates to

$$\tilde{a}_{\mu\mu} = \sqrt{2\mu^2}(2\mu - 2\mu) = 0.$$

Additionally, $\tilde{a}_{\mu\psi}$ remains non-negative provided that the expression

$$\tilde{a}_{\mu,\mho-1} = 2(\mho-1)\sqrt{2\mu(\mho-1)} + \sqrt{\mu^2+(\mho-1)^2}(-(\mho-1)-\mu)$$

is greater than or equal to zero. This condition is equivalent to the inequality:

$$2(\mho-1)\sqrt{2\mu(\mho-1)} - \mu\sqrt{\mu^2+(\mho-1)^2} - \sqrt{\mu^2+(\mho-1)^2}(\mho-1) \ge 0,$$

which simplifies to:

$$(1+\varrho)\sqrt{\varrho^2+1} - 2\sqrt{2\varrho} \ge 0,$$

where $\varrho = \frac{\mu}{\mho-1}$. It can be verified that the only positive root of the equation

$$(1+\varrho)\sqrt{\varrho^2+1} - 2\sqrt{2\varrho} = 0$$

occurs at approximately $\varrho_0 \approx 1$. Hence, the inequality holds for all $\varrho \ge \varrho_0$, implying that $\tilde{a}_{\mu,\mho-1} \ge 0$ (and consequently $a_{\mu,\mho-1} \ge 0$) when $\mu \ge \varrho_0(\mho-1)$.

Given that all coefficients $a_{\xi\psi} \geq 0$ for $\mu \leq \xi \leq \psi \leq \mho - 1$, it follows that the geometric-quadratic index achieves its minimum value of $\frac{\mu\mho}{2}$ when $x_{\xi,\psi} = 0$ for all $\mu \leq \xi \leq \psi \leq \mho - 1$, except for $x_{\mu,\mu}$. Thus we have proved that

$$GQ(G) \geq \frac{\mu\mho}{2}$$

The geometric-quadratic index achieves its minimum value $\dfrac{\mu\mho}{2}$ if μ or $\mho$ is even, on graphs for $x_{\mu,\mu} = \dfrac{\mu\mho}{2}$, $\mho_\mu = \mho$ and with all other $x_{\xi,\psi} = 0$ and $\mho_\xi = 0$

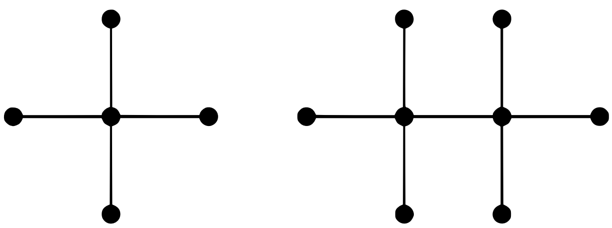
□

4. Comparison Between GQ Index and ABC Index

We compare the GQ index and ABC index and analyse $GQ(T) > ABC(T)$ for any chemical tree T. We present a counter example that $T = K_{1,4}$, $GQ(K_{1,4}) = 2.7 < 3.4 = ABC(K_{1,4})$. Also, $GQ(T^*) = 5.1 < 5.8 = ABC(T^*)$. But we have the following theorem.

Table 1: Values of $F_1(d_\xi, d_\psi)$ for different edges $v_\xi v_\psi \in E(G)$

$d_\xi d_\psi$	(4,1)	(4,2)	(4,3)	(4,4)	(3,1)	(3,2)	(3,3)	(2,1)	(2,2)
$\sqrt{\frac{2\xi\psi}{\xi^2+\psi^2}}$	$\sqrt{\frac{8}{17}}$	$\frac{2}{\sqrt{5}}$	$\frac{2\sqrt{6}}{5}$	1	$\sqrt{\frac{3}{5}}$	$\frac{2\sqrt{3}}{\sqrt{13}}$	1	$\frac{2}{\sqrt{5}}$	1
$\sqrt{\frac{1}{\xi}+\frac{1}{\psi}-\frac{2}{\xi\psi}}$	$\sqrt{\frac{3}{4}}$	$\frac{1}{\sqrt{2}}$	$\sqrt{\frac{5}{12}}$	$\sqrt{\frac{3}{8}}$	$\sqrt{\frac{2}{3}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{3}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$



$K_{1,4}$ T^*

Figure 1: Chemical Trees $K_{1,4}$ and T^*

Theorem 4.1 *Let T be a chemical tree with $\mho$ vertices. Then, for all trees T except $K_{1,4}$ and T^*, the geometric-quadratic index satisfies $GQ(T) > ABC(T)$.*

Proof: If $\mho = 2$, then the tree T is isomorphic to $K_{1,1}$, which implies that $GQ(T) > ABC(T)$. Since T is a chemical tree, the degrees of its vertices must satisfy $1 \leq d(\xi) \leq d(\psi) \leq 4$. Therefore, the possible edge types based on vertex degrees are: $(4,1)$, $(4,2)$, $(4,3)$, $(4,4)$, $(3,1)$, $(3,2)$, $(3,3)$, $(2,1)$, $(2,2)$.

We formulate the values of $\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2+d_\psi^2}}$ and $\sqrt{\frac{1}{d_\xi}+\frac{1}{d_\psi}-\frac{2}{d_\xi d_\psi}}$ for all above degree pairs in Table 1. From Table 1, we see that

$$\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2+d_\psi^2}} - \sqrt{\frac{1}{d_\xi}+\frac{1}{d_\psi}-\frac{2}{d_\xi d_\psi}} = \begin{cases} \geq \frac{4\sqrt{2}-\sqrt{51}}{2\sqrt{17}} \approx -0.18003 \text{ for } (d_\xi, d_\psi) = \{(4,1),(3,1)\} \\ \geq \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{2}} \approx 0.1873 \text{ for } (d_\xi, d_\psi) = \{(4,2),(4,3),(4,4), \\ \qquad (3,2),(3,3),(2,1),(2,2)\} \end{cases}$$

Let a denote the number of non-pendent edges in the tree T. Then, the tree contains $a+1$ non-pendent vertices and $\mho - 1 - a$ pendent vertices. Therefore, we obtain:

$$2(\mho - 1) = \sum_{d_\xi=1}^{\mho} d_\xi \leq (\mho - 1 - a) + (a+1)4, \quad (i.e)\ a \geq \frac{\mho - 5}{3}$$

$$\begin{aligned}
GQ(T) - ABC(T) &= \sum_{\xi\psi\in E} \left[\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}} - \sqrt{\frac{1}{d_\xi} + \frac{1}{d_\psi} - \frac{2}{d_\xi d_\psi}}\right] \\
&= \sum_{\xi\psi\in E,\ d_\psi=1} \left[\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}} - \sqrt{\frac{1}{d_\xi} + \frac{1}{d_\psi} - \frac{2}{d_\xi d_\psi}}\right] \\
&+ \sum_{\xi\psi\in E,\ d_\psi\neq 1} \left[\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}} - \sqrt{\frac{1}{d_\xi} + \frac{1}{d_\psi} - \frac{2}{d_\xi d_\psi}}\right] \\
&\geq (n-1-a)\left[\sqrt{\frac{8}{17}} - \frac{\sqrt{3}}{2}\right] + a\left[\frac{2\sqrt{2}-\sqrt{5}}{\sqrt{10}}\right] \\
&\geq \left[\sqrt{\frac{8}{17}} - \frac{\sqrt{3}}{2}\right](a+1) + (\mho - 5)\left[\frac{2\sqrt{2}-\sqrt{5}}{\sqrt{10}}\right] \\
&\text{as } a \geq \frac{\mho - 5}{3} \\
&\geq 0
\end{aligned}$$

Hence the theorem. □

Theorem 4.2 *Let G be a molecular graph with $\mho$ vertices. Then $GQ(G) > ABC(G)$ holds for all graphs G except when $G \cong K_{1,4}$ or $G \cong T^*$.*

Proof: The desired result follows directly when G is a chemical tree, from Theorem 4.1. Otherwise, if G contains a cycle, it must include at least three non-pendent edges. Moreover, if the number of pendent edges in G does not exceed nine, then by Theorem 4.1, it follows that $GQ(G) > ABC(G)$. In the remaining case, we must have $\mho \geq 11$. By applying a similar method as used in Theorem 4.1, the required result can be established. This completes the pf.

□

Now the GQ index and ABC index is compared for general graphs. For star $K_{1,\mho-1}, (\mho > 4)$ we have

$$GQ(K_{1,\mho-1}) = \sqrt{\frac{2(\mho-1)}{\mho^2 - 2\mho + 2}} < \sqrt{(\mho-1)(\mho-2)} = ABC(K_{1,\mho-1})$$

Let H be the graph obtained by modifying the star graph $K_{1,\mho-1}$ such that an edge is added between two of its pendent vertices. Assume further that $\mho > 6$.

$$\begin{aligned}
GQ(H) &= (\mho - 3)\sqrt{\frac{2(\mho-1)}{\mho^2 - 2\mho + 2}} + 4\sqrt{\frac{(\mho-1)}{\mho^2 - 2\mho + 5}} + 1 \\
&< (\mho - 3)\sqrt{\frac{\mho - 2}{\mho - 1}} + \frac{3}{\sqrt{2}} = ABC(H)
\end{aligned}$$

Theorem 4.3 *Let G be a simple graph with maximum degree Δ and minimum degree μ. If the degree difference satisfies $\Delta - \mu \leq 3$ and $G \ncong K_{1,4}$, T^*, then the inequality $GQ(G) > ABC(G)$ holds.*

Proof: If $\mu = 1$, then $\Delta \leq 4$. Since $G \neq K_{1,4}$, T^*, we have $GQ(G) > ABC(G)$, by Theorem 4.2. Otherwise $\mu \geq 2$

$$\sqrt{\frac{2d_\xi d_\psi}{d_\xi^2 + d_\psi^2}} \geq \sqrt{\frac{d_\xi + d_\psi - 2}{d_\xi d_\psi}} \text{ for every edge } d_\xi d_\psi \in E(G)$$

(i.e),

$$2(d_\xi^2 d_\psi^2) \geq (d_\xi^2 + d_\psi^2)(d_\xi + d_\psi - 2) \text{ for every edge } \xi\psi \in E(G) \tag{4.1}$$

Given that $2 \leq \mu \leq \Delta \leq \mu + 3$, the degree difference between the endpoints of any edge in G satisfies $|d_\xi - d_\psi| \leq 3$, where $d_\xi, d_\psi \geq 2$. Without loss of generality, we may assume $d_\xi \geq d_\psi$. Therefore, it follows that $2 \leq d_\psi \leq d_\xi \leq d_\psi + 3$.

Moreover, we verify that the degree combinations $d_\xi = d_\psi$, $d_\xi = d_\psi + 1$, $d_\xi = d_\psi + 2$, and $d_\xi = d_\psi + 3$ all satisfy inequality (4.1), given that $d_\psi \geq 2$. This completes the proof.

□

5. Comparison Between GQ Index and Randić Index

This section focuses on investigating $GQ - R$ for the connected chemical graphs. From the equations (1.1) and (1.4), we can formulate as

$$GQ(G) - R(G) = \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2 + \psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2 + \psi^2}}$$

Now we consider the following function

$$F_2(d_\xi, d_\psi) = \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2 + \psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2 + \psi^2}}$$

Then we have

$$GQ(G) - R(G) = \sum_{v_\xi v_\psi \in E(G)} F_2(d_\xi, d_\psi)$$

Theorem 5.1 *Let G be a chemical graph with $\mho$ vertices. Then the following inequality holds:*

$$GQ(G) - R(G) \leq \frac{3\mho}{2}, \tag{5.1}$$

with equality if and only if G is isomorphic to a 4-regular graph.

Proof: The graph G considered here is a chemical graph, we have

$$2m = \sum_{\xi=1}^{\mho} d_\xi \leq 4\mho \ \Rightarrow m \leq 2\mho$$

The following equality is true if and only if $d_\xi = 4$ for any vertex $v_\xi \in V(G)$. From Table. 2 we get

$$GQ(G) - R(G) = \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2 + \psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2 + \psi^2}} \leq \frac{3m}{4} \leq \frac{3\mho}{2}$$

The equality holds in Eq. (5.1) if and only if

$$\frac{\sqrt{2}\xi\psi - \sqrt{\xi^2 + \psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2 + \psi^2}} = \frac{3}{4} \text{ for any edge } v_\xi v_\psi \in E(G)$$

And graph G is isomorphic to a 4-regular graph if and only if every vertex $v_\xi \in V(G)$ has degree $d_\xi = 4$. □

For instance, consider a 4-regular graph with $\mho = 5$. Then,

$$GQ(G) - R(G) = \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2+\psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2+\psi^2}} = 10\left[\frac{\sqrt{2}(4.4) - \sqrt{4^2+4^2}}{\sqrt{4.4}.\sqrt{4^2+4^2}}\right] = \frac{3\,(5)}{2} = \frac{3\,(\mho)}{2}$$

Hence the numerical calculation of Theorem 5.1 for $d_\xi = 4$.

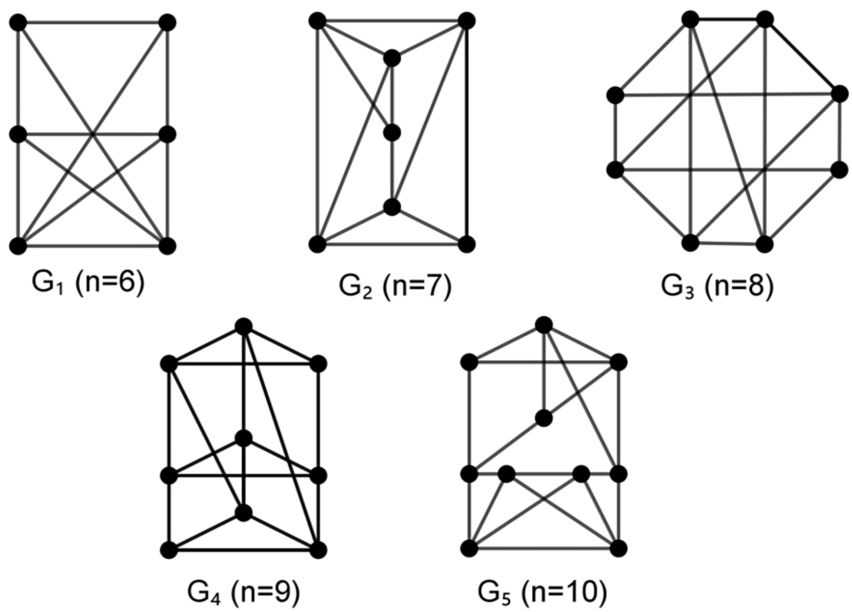


Figure 2: Chemical Graphs $G_i, (i = 6, 7, 8, 9, 10)$

Table 2: Values of $F_2(d_\xi, d_\psi)$ for different edges $v_\xi v_\psi \in E(G)$

(d_ξ, d_ψ)	$F(d_\xi, d_\psi)$	(d_ξ, d_ψ)	$F(d_\xi, d_\psi)$	(d_ξ, d_ψ)	$F(d_\xi, d_\psi)$
(2,1)	0.187	(2,2)	$\frac{1}{2} \approx 0.5$	(3,1)	0.197
(3,2)	0.552	(3,3)	$\frac{2}{3} \approx 0.667$	(4,1)	0.185
(4,2)	0.540	(4,3)	0.691	(4,4)	$\frac{3}{4} \approx 0.75$

Theorem 5.2 *Let G be a chemical graph of order $\mho$ that is not isomorphic to a 4-regular graph. Then,*

$$GQ(G) - R(G) \leq \frac{3(2\mho - 7)}{4} + 4.147$$

Proof: Let the number of edges in G be m. Since G is not isomorphic to 4-regular graph it follows that $m < 2\mho$. (ie) $m \leq 2\mho - 1$
If $m \leq 2\mho - 2$ then

$$\begin{aligned} GQ(G) - R(G) &= \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2+\psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2+\psi^2}} \\ &\leq \frac{3m}{4} \leq \frac{3(\mho - 1)}{2} < \frac{3(2\mho - 7)}{4} + 4.147 \end{aligned}$$

by Table. 2.
Otherwise $m = 2\mho - 1$.Let δ_ϖ represent the minimum degree of the graph G. Since G is a chemical graph.

$$2m = \sum_{\xi=1}^{\mho} d_\xi = 4\mho - 2$$

where $\mu = 2$ or $\mu = 3$.
For $\mu = 2$, the graph consists of vertices of degree 4 except for one vertex of degree 2.

For the case when $\mu = 2$, we examine the following scenario:

Case 1: Let v_α be the vertex of degree 2 in G.
Here we have two edges with $(d_\xi, d_\psi) = (4,2)$ and all other edges with $(d_\xi, d_\psi) = (4,4)$, thus we get

$$\begin{aligned} GQ(G) - R(G) &= \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2+\psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2+\psi^2}} \\ &\leq \frac{3(2\mho-3)}{4} + 1.0817 < \frac{3(2\mho-7)}{4} + 4.147 \end{aligned}$$

If $\mu = 3$, we examine the following cases:

Case 2: Let v_α and v_β be two vertices of degree 3 in G. Let $v_\alpha v_\beta \in E(G)$ be any edge in G. For $\mho = 6$ we have four edge with $(d_\xi d_\psi) = (4,3)$, one edge with $(d_\xi d_\psi) = (3,3)$, and all other edges with $(d_\xi d_\psi) = (4,4)$,
Thus we get

$$\begin{aligned} GQ(G) - R(G) &= \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2+\psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2+\psi^2}} \\ &= \frac{3(\mho-2)}{2} + \left(4\left(\frac{2\sqrt{6}}{5} - \frac{1}{\sqrt{12}}\right)\right) + \frac{2}{3} < \frac{3(2\mho-7)}{4} + 4.147. \end{aligned}$$

Case 3: For $\mu = 3$, let $v_\alpha v_\beta \notin E(G)$. Then we have six edges with $(d_\xi d_\psi) = (4,3)$ and all the remaining edges with $(d_\xi d_\psi) = (4,4)$. Thus we have

$$\begin{aligned} GQ(G) - R(G) &= \sum_{v_\xi v_\psi \in E(G)} \frac{\sqrt{2}\xi\psi - \sqrt{\xi^2+\psi^2}}{\sqrt{\xi\psi}\sqrt{\xi^2+\psi^2}} \\ &= \frac{3(2\mho-7)}{4} + 4.147. \end{aligned}$$

Hence the theorem. □

6. Conclusion

The extremal graph and the lower bound of GQ index is found for $\mu \geq \lceil \mu_0 \rceil$. The relationship between the GQ index and the ABC index has been investigated for both chemical trees and molecular graphs. In addition, an analysis on general graphs reveals that the GQ index exceeds the ABC index when the difference between the maximum and minimum vertex degrees is less than or equal to three. Furthermore, a comparative study between the GQ index and the Randić index has also been conducted for chemical graphs.The present work can be further extended to unicyclic, bicyclic, and, in general, c-cyclic graphs. Moreover, the relationship between the GQ index and other degree-based topological indices may be explored in greater depth. Future investigations may also focus on deriving sharp bounds for the GQ index within specific chemical graph classes, examining its behavior under common graph operations, and studying its correlation with physicochemical properties.

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