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Research Paper

Geometric-Quadratic Index from a Mathematical Perspective

Boris Furtula[1] and Mert Sinan Oz[2*]

[1]Faculty of Science, University of Kragujevac, Kragujevac, Serbia

[2]Department of Mathematics, Faculty of Engineering and Natural Sciences, Bursa Technical University, Bursa, Turkey

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Abstract

The geometric-quadratic index (GQ) was defined in 2021 by V. R. Kulli. In a recent study, QSPR analysis for the octane isomers of GQ and some other newly defined topological indices was presented. This analysis has revealed that GQ dominates over many of the well-known topological indices in terms of chemical applicability potential, especially for the heat of vaporization. These results inspired us to investigate the mathematical properties of GQ.

In this paper, extremal graphs for GQ are investigated among connected graphs, trees, and unicyclic graphs. In addition, several mathematical relations between GQ and some well-known topological indices are presented.

1 Introduction

Topological indices are quantitative parameters that should be the product of meaningful and consistent mathematical formulae constructed on graphs. Topological indices are important tools used in QSPR/QSAR models to predict the physicochemical and biological properties and activities of compounds. Today, hundreds of topological indices are already defined, but only a few dozen have chemical applicability [1, 2]. This is one of the clearest indicators of the complexity and uncertainty in developing a useful topological index. Attempts to comply with the qualities of a proper topological index listed in [3] during the development of an index significantly reduce these problems.

Two important items of this list, often focused on in the literature when the chemical applicability potential of a topological index is investigated, are a good correlation with at least one physicochemical property and a gradual change in their structure.

*Corresponding author
E-mail addresses: furtula@uni.kg.ac.rs (B. Furtula), sinan.oz@btu.edu.tr (M. Sinan Oz)
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In [4], the correlation coefficient between the heat of vaporization values and GQ index values for octane isomers was found to be 0.9661, indicating that the most important quality of a topological index is satisfied. In the same paper, it was shown that the smoothness of the GQ is also comparable to the results of the considered well-known degree-based topological indices, indicating that it does not differ from the considered well-known topological indices (for details about smoothness that quantify the second mentioned quality (see [5]). These results suggest that GQ has good potential for chemical applicability, and encouraged us to investigate the mathematical aspects of GQ.

Let $G = (V, E)$ be a simple graph, i. e. an undirected, unweighted graph without multiple edges and self-loops. Let us denote ij, d_i, and d_j as an edge of G with end-vertices i and j, the degree of the vertex i, and the degree of the vertex j in G, respectively.

The geometric-quadratic index (GQ) was defined by V. R. Kulli in [6] as follows:

$$GQ\left(G\right) = \sum_{ij \in E} \sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} \ .$$

In addition, the following well-known topological indices will be used in the paper:

$$M_2\left(G\right) = \sum_{ij \in E} d_j \cdot d_i, \qquad GA\left(G\right) = \sum_{ij \in E} \frac{2\sqrt{d_j \cdot d_i}}{d_j + d_i},$$

$$\chi_\alpha\left(G\right) = \sum_{ij \in E} \left(d_j + d_i\right)^\alpha, \qquad R_\alpha\left(G\right) = \sum_{ij \in E} \left(d_j \cdot d_i\right)^\alpha,$$

$$SDD\left(G\right) \sum_{ij \in E} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right), \qquad SO\left(G\right) = \sum_{ij \in E} \sqrt{d_j^2 + d_i^2},$$

which are the second Zagreb index [7, 8], geometric-arithmetic index [9], the general sum-connectivity index [10], the general Randić index [11], the symmetric division deg index [12] and the Sombor index [13], respectively. In this paper, we investigate GQ from a mathematical point of view.

2 Mathematical properties of GQ

Let us denote P_n, S_n, K_n, C_n and $K_{x,y}$ $(x + y = n)$ as the path graph, star graph, complete graph, cycle graph and complete bipartite graph of order n, respectively.

Theorem 2.1. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices. Then,*

$$GQ\left(S_n\right) \leq GQ\left(G\right) \leq GQ\left(K_n\right).$$

The left and right equalities hold if and only if $G \cong S_n$ and $G \cong K_n$, respectively. Recall that $GQ(K_n) = \binom{n}{2}$ and $GQ(S_n) = \sqrt{\frac{2(n-1)^3}{n^2-2n+2}}$ for $n \geq 2$.

Proof. Without loss of generality, let us assume that $d_j \leq d_i$. For any graph, it is clear that $\frac{1}{n-1} \leq \frac{d_j}{d_i} \leq 1$. Let us denote $\frac{d_j}{d_i}$ by x. Since we have the equation

$$\sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} = \sqrt{\frac{2}{\frac{d_j}{d_i} + \frac{d_i}{d_j}}},$$

we can rewrite the equation as the following function:

$$f(x) = \sqrt{\frac{2}{x + \frac{1}{x}}} = \sqrt{\frac{2x}{x^2+1}}.$$

One can observe that $f'(x)$ is differentiable on $\left(\frac{1}{n-1}, 1\right)$ and

$$f'(x) = \frac{1-x^2}{\left(x^2+1\right)^2} \frac{\sqrt{x^2+1}}{\sqrt{2x}} > 0,$$

on $\left(\frac{1}{n-1}, 1\right)$. Hence, $f(x)$ is an increasing function on $\left(\frac{1}{n-1}, 1\right)$ so it reaches the maximum value at $x = 1$, namely when $d_j = d_i$. In summary, the maximum value of $f(x)$ is

$$\sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} = \sqrt{\frac{2d_i^2}{2d_i^2}} = 1.$$

Furthermore, since the maximum number of edges in a simple graph is $\binom{n}{2}$, the maximum value of $GQ(G)$ is equal to

$$GQ(G) = \sum_{ij \in E} \sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} = \binom{n}{2},$$

reached for the complete graph K_n.

On the other hand, $f(x)$ reaches the minimum value at $x = \frac{1}{n-1}$. Thus, the minimum contribution of an edge to $GQ(G)$ is equal to

$$\sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} = \sqrt{\frac{\frac{2}{n-1}}{\left(\frac{1}{n-1}\right)^2 + 1}} = \sqrt{\frac{2(n-1)}{n^2 - 2n + 2}}.$$

As a result, since the contribution of each edge has the minimum,

$$GQ(S_n) = \sum_{ij \in E} \sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} = (n-1)\sqrt{\frac{2(n-1)}{n^2 - 2n + 2}} = \sqrt{\frac{2(n-1)^3}{n^2 - 2n + 2}},$$

is the minimum among all connected graphs. ■

Theorem 2.2. *Let $T = (V, E)$ be a tree with $n \geq 2$ vertices. Then,*

$$GQ(S_n) \leq GQ(T) \leq GQ(P_n).$$

The left and right equalities hold if and only if $T \cong S_n$ and $T \cong P_n$, respectively. Recall that $GQ(S_n) = \sqrt{\frac{2(n-1)^3}{n^2-2n+2}}$ for $n \geq 2$. Moreover, recall that $GQ(P_2) = 1$ and $GQ(P_n) = \frac{4}{5}\sqrt{5} + (n-3)$ for $n \geq 3$.

Proof. As a consequence of Theorem 2.1, S_n is the minimal graph among all trees with $n \geq 2$ vertices, and the minimum value is $GQ(S_n) = \sqrt{\frac{2(n-1)^3}{n^2-2n+2}}$. For the upper bound, note that $(d_i - d_j)^2 \geq 0$, so we have $d_i^2 + d_j^2 \geq 2d_i d_j$. Therefore, the maximum value

$$\sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}},$$

is 1 which occurs when $d_i = d_j$. Therefore, we need to consider trees whose edges connect vertices that are as equal in degree as possible. Let us note that there exists just one tree with $n = 2$, vertices so the result is trivial for $n = 2$. Let us continue by remembering that every tree with $n \geq 3$ vertices has at least two pendant edges. Since all edges except 2 pendant edges in P_n are edges connecting vertices of equal degrees, the maximum value of $GQ(T)$ is

$$GQ(P_n) = 2\sqrt{\frac{4}{5}} + (n-3) \cdot 1 = \frac{4}{5}\sqrt{5} + (n-3)\,.$$

■

Let us recall Radon's inequality for future use.

Lemma 2.3. *([14]). Let x_i, r be nonnegative real numbers and y_i be positive real numbers for $1 \leq i \leq k$. The following inequality holds:*

$$\sum_{i=1}^{k} \frac{x_i^{r+1}}{y_i^r} \geq \frac{\left[\sum_{i=1}^{k} x_i\right]^{r+1}}{\left[\sum_{i=1}^{k} y_i\right]^{r}}.$$

Equality holds if and only if $r = 0$ or $\frac{x_1}{y_1} = \frac{x_2}{y_2} = \cdots = \frac{x_k}{y_k}$.

More details on Radon's inequality can be found in [15] where negative values of r for Radon's inequality are also covered and Radon's inequality is applied to some general topological indices.

Theorem 2.4. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices. Then,*

$$\frac{\sqrt{2}\left(R_{\frac{1}{4}}(G)\right)^2}{SO(G)} \leq GQ(G) \leq m.$$

The left equality holds if and only if $G \cong K_{x,y}$ or G is a regular graph. The right equality holds if and only if G is a regular graph.

Proof. For the lower bound, using Lemma 2.3 we proceed as follows:

$$\begin{aligned} GQ(G) = \sum_{ij \in E} \frac{\sqrt{2d_j \cdot d_i}}{\sqrt{d_j^2 + d_i^2}} = \sum_{ij \in E} \frac{\left(\sqrt[4]{2d_j \cdot d_i}\right)^2}{\sqrt{d_j^2 + d_i^2}} \geq \frac{\left(\sum_{ij \in E} \sqrt[4]{2d_j \cdot d_i}\right)^2}{\sum_{ij \in E} \sqrt{d_j^2 + d_i^2}} \\ = \frac{\sqrt{2}\left(\sum_{ij \in E} \sqrt[4]{d_j \cdot d_i}\right)^2}{\sum_{ij \in E} \sqrt{d_j^2 + d_i^2}} = \frac{\sqrt{2}\left(R_{\frac{1}{4}}(G)\right)^2}{SO(G)}. \end{aligned}$$

Equality holds if $\frac{\sqrt[4]{2d_j \cdot d_i}}{\sqrt{d_j^2+d_i^2}}$ values are equal for all edges by Lemma 2.3. Therefore, the equality for the obtained inequality holds if and only if $G \cong K_{x,y}$ or G is a regular graph.

Let us consider the upper bound. It is known that $\frac{\sqrt{2d_j \cdot d_i}}{\sqrt{d_j^2+d_i^2}} \leq 1$ by the proof of Theorem 2.2. Namely, the possible maximum contribution of any edge of G to $GQ\left(G\right)$ is equal to 1, it occurs when $d_j = d_i$. Thus, assuming that all edges have the maximal contribution, we conclude that $GQ\left(G\right) \leq m \cdot 1 = m$. So, equality occurs when G is a regular graph. ■

Since $GQ(C_n) = m$, Theorem 2.4 leads to the next corollary.

Corollary 2.5. *Let $G = (V, E)$ be a unicyclic graph with $n \geq 3$ vertices. Then,*

$$GQ\left(G\right) \leq GQ\left(C_n\right).$$

On the other hand, a brute-force search has been performed on unicyclic graphs with 4 to 19 vertices to propose a conjecture about unicyclic graphs that reach the minimal GQ among all unicyclic graphs.

At this point, unicyclic graphs with 4 to 19 vertices are generated using nauty software developed by McKay and Piperno [16]. After that, the Python NetworkX module is used.

In order to present the result of the search, let us first introduce the special type of unicyclic graph as follows:

$U_G\left\{n, k, a, b, c\right\}$ is the unicyclic graph obtained by adding a path graph with k vertices, and b and c pendant vertices to each vertex of a C_3, respectively, where $k \cdot a + b + c = n - 3$, see Figures 1 and 2.

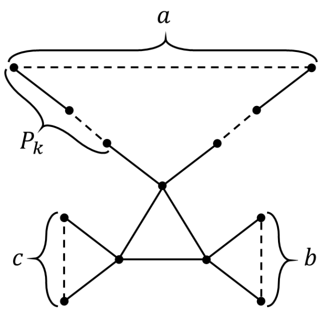

Figure 1: $U_G\left\{n, k, a, b, c\right\}$.

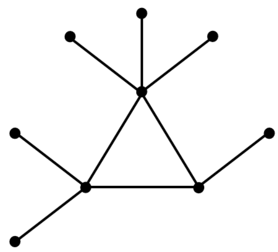

Figure 2: $U_G\left\{9, 1, 3, 1, 2\right\}$.

Conjecture 2.6. *Let $G = (V, E)$ be a unicyclic graph with $n \geq 4$ vertices. Then,*

$$GQ\left(U_G\left\{n, 1, n-3, 0, 0\right\}\right) \leq GQ\left(G\right),$$

where $GQ\left(U_G\left\{n, 1, n-3, 0, 0\right\}\right) = (n-3)\sqrt{\frac{2n-2}{n^2-2n+2}} + 4\sqrt{\frac{n-1}{n^2-2n+5}} + 1$ *for* $n \geq 4$.

Theorem 2.7. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices. Then,*

$$\frac{GA\left(G\right)}{\sqrt{2}} < GQ\left(G\right) \leq GA\left(G\right).$$

Equality holds if and only if G is a regular graph.

Proof. We can set the following inequality:

$$GQ(G) = \sum_{ij\in E} \frac{\sqrt{2d_j \cdot d_i}}{\sqrt{d_j^2 + d_i^2}} > \sum_{ij\in E} \frac{\sqrt{2d_j \cdot d_i}}{\sqrt{d_j^2 + 2d_j \cdot d_i + d_i^2}} = \sum_{ij\in E} \frac{\sqrt{2d_j \cdot d_i}}{d_j + d_i} = \frac{GA(G)}{\sqrt{2}}.$$

As a result, we obtain that $\frac{GA(G)}{\sqrt{2}} < GQ(G)$.

Since $(d_i - d_j)^2 \geq 0$, it is obtained that $\frac{d_j + d_i}{\sqrt{2}} \leq \sqrt{d_j^2 + d_i^2}$ with equality in the case of $d_j = d_i$. Hence, the following inequality is obtained:

$$GQ(G) = \sum_{ij\in E} \frac{\sqrt{2d_j \cdot d_i}}{\sqrt{d_j^2 + d_i^2}} \leq \sum_{ij\in E} \frac{2\sqrt{d_j \cdot d_i}}{d_j + d_i} = GA(G).$$

Since equality in the inequality $\frac{d_j + d_i}{\sqrt{2}} \leq \sqrt{d_j^2 + d_i^2}$ holds if and only if $d_j = d_i$, equality holds if and only if G is a regular graph. ■

Theorem 2.8. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices. Then,*

$$\frac{\sqrt{2}m^2}{SDD(G)} < GQ(G) < M_2(G) + \frac{1}{2}\chi_{-1}(G).$$

Proof. For the lower bound, first note that we can rewrite $GQ(G)$ as

$$GQ(G) = \sum_{ij\in E} \frac{\sqrt{2}}{\sqrt{\frac{d_i}{d_j} + \frac{d_j}{d_i}}}.$$

This leads to the following inequality by using Lemma 2.3:

$$\sum_{ij\in E} \frac{\sqrt{2}}{\sqrt{\frac{d_i}{d_j} + \frac{d_j}{d_i}}} = \sum_{ij\in E} \frac{\left(\sqrt[4]{2}\right)^2}{\sqrt{\frac{d_i}{d_j} + \frac{d_j}{d_i}}} \geq \frac{\left(\sum_{ij\in E} \sqrt[4]{2}\right)^2}{\sum_{ij\in E} \sqrt{\frac{d_i}{d_j} + \frac{d_j}{d_i}}} > \frac{\left(\sum_{ij\in E} \sqrt[4]{2}\right)^2}{\sum_{ij\in E} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)} = \frac{\sqrt{2}m^2}{SDD(G)}.$$

For the upper bound, using the inequality between the geometric mean and the arithmetic mean, the following is reached:

$$\begin{aligned} GQ(G) = \sum_{ij\in E} \sqrt{\frac{2d_j \cdot d_i}{d_j^2 + d_i^2}} &< \sum_{ij\in E} \frac{2d_j \cdot d_i + \frac{1}{d_j^2 + d_i^2}}{2} \\ &= \sum_{ij\in E} d_j \cdot d_i + \frac{1}{2}\sum_{ij\in E} \frac{1}{d_j^2 + d_i^2} \\ &< \sum_{ij\in E} d_j \cdot d_i + \frac{1}{2}\sum_{ij\in E} \frac{1}{d_j + d_i} \\ &= M_2(G) + \frac{1}{2}\chi_{-1}(G). \end{aligned}$$

■

Table 1: The correlation coefficients between $GQ(G)$ and stated well-known topological indices.

	$M_2(G)$	$GA(G)$	$\chi_{-1}(G)$	$R_{\frac{1}{4}}(G)$	$\chi_{\frac{1}{4}}(G)$	$R_{\frac{1}{2}}(G)$	$SDD(G)$	$SO(G)$
$GQ(G)$	0.95401	0.99895	0.57808	0.98603	0.98781	0.97679	0.87562	0.96178

The table below presents the correlation coefficients of $GQ(G)$ with stated well-known topological indices by using all connected graphs with 10 vertices.

Results from Table 1 show that the geometric-quadratic index is highly correlated with the general Randić and the general sum-connectivity index when $\alpha = 1/4$. However, the highest correlation coefficient was noted when GQ is correlated with the geometric-arithmetic index. This is rationalized by the fact that the formulas of these indices are quite similar. So, the geometric-quadratic index could be seen as a descendant of the well-known geometric-arithmetic index.

3 Concluding remarks

Connected graphs and trees that reach upper and lower bounds for GQ have been determined. In addition, unicyclic graphs that reach the upper bound for GQ have been determined. Furthermore, a conjecture for unicyclic graphs that reach the lower bound has been presented and has been left as an open problem. Finally, mathematical relations between GQ and several well-known topological indices have been established. As inferred from Theorem 2.7 and confirmed in Table 1, there is a strong relationship between GQ and GA.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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