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Extremal GQ Index of Trees, Unicyclic and Bicyclic Graphs

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Abstract

The geometric quadratic (GQ) index is a recently introduced degree-based topological descriptor, and Kumar et al. observed that it is potentially a very good molecular descriptor. In this paper, we characterize the extremal graphs (chemical) and trees concerning the geometric quadratic index of a given order and size. Then, we determine the n-vertex trees, unicyclic and bicyclic graphs with the maximum, the second, the third, the fourth, the fifth, and the sixth maximum geometric quadratic indices.

1 Introduction

Let $G = (V(G), E(G))$ be a simple graph with $|V(G)| = n$ and $|E(G)| = m$. By $a \sim b$, we mean that the vertices a and b are adjacent and d_a represents the degree of the vertex a in G. A vertex of degree one is said to be a pendant vertex. A path $x_1x_2 \cdots x_l$ is said to be pendent at x_1 if $d(x_1) \geq 3$, $d(x_t) = 2$ for $i \in \{2, \cdots, l-1\}$ and $d(x_l) = 1$. An edge is

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said to be a (a,b)-edge if the vertices incident to the edge are of degrees a and b, respectively. By v_i and $E_{p,q}$, we denote the number of vertices of degree i and the number of (p,q)-edges in a graph G, respectively. A connected graph G is said to be a tree, unicyclic and bicyclic graph if and only if $m = n-1$, $m = n$ and $m = n+1$, respectively. By $\mathcal{G}_{n,m,\delta,\Delta}$, we denote the set of all connected graphs of order n, size m with maximum and minimum degrees are Δ and δ, respectively. A graph G is said to be chemical if $\Delta(G) \leq 4$. By P_n and C_n, we denote the path and cycle on the n vertices, respectively.

Quantitative structure-property relationship (QSPR) investigations apply correlation/regression models to ensure the correlation between the molecular structure of a substance and its physicochemical, thermodynamic, and quantum-theoretic properties in contemporary chemistry. Quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) are regression models that utilize statistical methods to analyze the relationship between the structure of a compound and its activity or property. These models can be either linear or nonlinear. This approach exhibits a substantial correlation with the thermodynamic, physicochemical, and biological aspects of chemical structures [20]. Statistics is very important in decision-making if it is informed by data. It assists in understanding patterns, exploring assumptions, and proving credible and significant conclusions, thus ensuring the reliability and validity of research data. This process has to be encouraged in various fields of scientific research as discussed in papers [18]. In recent times, numerous authors have employed this methodology to ascertain the relationship between the topological indices and physical characteristics of chemical compounds. The topological index of a graph G is a numerical quantity invariant under the automorphisms of the graph. Due to their application in chemistry and pharmacology, especially in QSPR/QSAR as molecular structure descriptors [7, 9, 10, 12, 22], topological indices have gained considerable popularity. Among the groups of all topological indices, one of the most investigated and widely used is the vertex degree-based topological indices [12, 17, 19]. Among the vertex degree-based topological indices, the oldest vertex degree-based topological indices, the first and the second

Zagreb indices [9, 10] were defined as

$$M_1(G) = \sum_{a\sim b}(d_a + d_b) \quad \text{and} \quad M_2(G) = \sum_{a\sim b} d_a d_b.$$

The symmetric division degree index [7] and the Sombor index [8] were defined as

$$SDD(G) = \sum_{a\sim b}\left(\frac{d_a}{d_b} + \frac{d_b}{d_a}\right) \quad \textit{and} \quad SO(G) = \sum_{a\sim b}\sqrt{d_a^2 + d_b^2}.$$

The geometrical-arithmetic index (GA) index [22] and arithmetical geometric (AG) index were defined as

$$GA(G) = \sum_{a\sim b}\frac{2\sqrt{d_a d_b}}{d_a + d_b}, \quad AG(G) = \sum_{a\sim b}\frac{d_a + d_b}{2\sqrt{d_a d_b}}.$$

In [22], Vukičević et al. observed the chemical applicability of the GA index and characterized the extremal graphs, trees and chemical trees of given size. Motivated by the advancement and success of the GA index, Kulli proposed two new indices in 2022 based on the geometric and quadratic means of degrees of end vertices of an edge and named them the Geometric–Quadratic and Quadratic–Geometric indices [14], defined as:

$$GQ(G) = \sum_{a\sim b}\sqrt{\frac{2d_a d_b}{d_a^2 + d_b^2}}, \quad QG(G) = \sum_{a\sim b}\sqrt{\frac{d_a^2 + d_b^2}{2d_a d_b}}.$$

Then, Kumar et al. [15] concentrate on this newly defined degree-based GQ and QG indices by exhibiting a comparative study with other standard degree-based topological indices. They investigated the octane, nonane and decane isomers by looking at the application of these isomers and the availability of the data of these compounds to test the usability and structural properties regarding some standard topological indices such as M_1, M_2, SDD, SO, etc. By performing quantitative structure-property relationship analysis, they observed that the acquired results of the GQ index are preferably stronger than those of the QG index for all the considered physicochemical properties, apart from the enthalpy of formation

(HFORM). They also observed that the GQ and QG indices report better prediction power for the properties HVAP and DHVAP of octane isomers in comparison to all the degree-based topological indices considered. The performed linear regression models and obtained statistical outcomes for the GQ index are better than those of the GA index. More specifically, they are stronger than the results of the GA and AG indices. This suggests that the GQ and QG indices display fine structural changes in comparison to the GA and AG indices. Therefore, the GQ index would be beneficial to the researchers working in this area. For other related works on GQ and QG indices, we refer [4–6, 16].

In chemical graph theory, one of the most famous and challenging problems is to characterize the extremal graphs with respect to different degree-based topological indices. We refer to [1–3, 13, 17] for recent advances. All these observations prompted me to consider the extremal problems with respect to the GQ indices over the trees, unicyclic graphs and bicyclic graphs.

In this paper, in Section 2, we characterize the extremal graphs (chemical) and trees concerning the GQ index with a given number of vertices. Then, we determine n-vertex trees with the second and the third for $n \geq 7$, the fourth and the fifth for $n \geq 10$ and the sixth for $n \geq 10$ maximum GQ indices. Then in Section 3, we determine the n-vertex unicyclic graphs with the maximum, the second and the third for $n \geq 5$, the fourth for $n \geq 7$, the fifth and the sixth for $n \geq 9$ maximum GQ indices. Finally, in Section 4, we determine the bicyclic graphs with the maximum for $n \geq 4$, the second and the third for $n \geq 6$ and the fourth, the fifth and the sixth for $n \geq 8$ maximum GQ indices.

2 Extremal *GQ* index of trees

Lemma 1. *Let G be a graph with l pendant paths. Then*

$$GQ(G) \leq \left(2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} - 2\right) l + m.$$

Proof. Let $e = xy$ be an edge of a graph G on n vertices. If d_x is fixed, then $f(d_y) = \sqrt{\frac{2d_x d_y}{d_x^2+d_y^2}}$ is a decreasing function for $d_x \leq d_y \leq n-1$. Then the contribution to $GQ(\mathrm{G})$ by a pendant path of length one is at most $\sqrt{\frac{2.3.1}{9+1}} = \sqrt{\frac{3}{5}} \approx 0.7745 < 2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} - 1 \approx 0.8551$. The contribution to $GQ(\mathrm{G})$ by a pendant path of length $t \geq 2$ is at most $\sqrt{\frac{2.3.2}{9+4}} + (t-2)\sqrt{\frac{2.2.2}{4+4}} + \sqrt{\frac{2.2.1}{4+1}} = 2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + t - 2$. Therefore, the contribution to $GQ(\mathrm{G})$ by the edges of a pendent path of length $t \geq 1$ is at most $2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + t - 2$. Since the graph G has l pendent paths, we have

$$GQ(G) \leq \left(2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} - 2\right) l + m. \qquad \blacksquare$$

Lemma 2. *Let* $f(x,y) = \sqrt{\frac{2xy}{x^2+y^2}}$ *and* $0 < a \leq x \leq y \leq b$ *for some real numbers* a *and* b*. Then* $\sqrt{\frac{2ab}{a^2+b^2}} \leq f(x,y) \leq 1$*, with left equality if and only if* $x = a$ *and* $y = b$*, right equality if and only if* $x = y$*.*

Proof. Since $0 < a \leq x \leq y \leq b$, we have $1 \leq \frac{y}{x} \leq \frac{b}{a}$. Let $t = \frac{y}{x}$ and $g(t) = \sqrt{\frac{2t}{1+t^2}}$. Then $g'(t) = \frac{\sqrt{1+t^2}}{2\sqrt{2t}} \frac{2-2t^2}{(1+t^2)^2} \leq 0$, since $t \geq 1$. Therefore, $g(t)$ is monotonically decreasing for $t \geq 1$. Hence

$$\sqrt{\frac{2ab}{a^2+b^2}} = g\left(\frac{b}{a}\right) \leq f(x,y) = g(t) \leq g(1) = 1,$$

with left equality if and only if $x = a$ and $y = b$ and right equality if and only if $x = y$. $\blacksquare$

Remark. Since $(x-y)^2 \geq 0$ for all real numbers x and y, we have $\sqrt{\frac{2xy}{x^2+y^2}} \leq 1$ with equality if and only if $x = y$. Therefore, $\sqrt{\frac{2d_u d_v}{d_u^2+d_v^2}} \leq 1$ for any edge uv of G. So, the maximum contribution to the GQ index by an edge is at most one. Consequently, $GQ(G) \leq m$ with equality if and only if G is a regular graph.

Theorem 1. *Let* $G \in \mathcal{G}_{n,m,\delta,\Delta}$*. Then*

$$m\sqrt{\frac{2\Delta\delta}{\Delta^2+\delta^2}} \leq GQ(G) \leq m.$$

Equality on the left holds if and only if G is regular or biregular, and on the right, equality is held if and only if G is regular.

Proof. To prove the upper bound, it suffices to note that the contribution of each edge to the GQ index is at most one (see Lemma 2). Therefore, $GQ(G) \leq m$. Moreover, equality holds if each edge contributes to $GQ(G)$ exactly one, i.e., each edge has end vertices of the same degree. This is possible only if G is regular. Now, from the definition of the GQ index and by applying Lemma 2, we have

$$GQ(G) = \sum_{uv \in E(G)} \sqrt{\frac{2d_u d_v}{d_u^2 + d_v^2}} \geq \sum_{uv \in E(G)} \sqrt{\frac{2\Delta\delta}{\Delta^2 + \delta^2}} = m\sqrt{\frac{2\Delta\delta}{\Delta^2 + \delta^2}},$$

with equality if and only if $d_u = \Delta$ and $d_v = \delta$ for all $xy \in E(G)$ i.e., G is regular or biregular. ■

Theorem 2. *For a simple connected graph G with $n \geq 3$ vertices, we have*

$$\sqrt{\frac{2(n-1)^3}{n^2 - 2n + 2}} \leq GQ(G) \leq \frac{n(n-1)}{2}.$$

Equality on the left holds if and only if G is a star graph, and on the right, the equality is held if and only if G is a complete graph.

Proof. To prove the upper bound, it is enough to note that for a simple connected graph of order n and size m, we have $m \leq \frac{n(n-1)}{2}$ with equality if and only if G is $(n-1)$-regular. Therefore, $GQ(G) \leq \frac{n(n-1)}{2}$ with equality if and only if G is a complete graph.
To prove the lower bound, let $d_u \leq d_v$ and $t = \frac{d_u}{d_v}$. Note that $\frac{1}{n-1} \leq t \leq 1$. Hence $\sqrt{\frac{2d_u d_v}{d_u^2 + d_v^2}} = \sqrt{\frac{2t}{1+t^2}}$. Let $f(t) = \sqrt{\frac{2t}{1+t^2}}$. Clearly $f(t)$ is ascending in the interval $[\frac{1}{n-1}, 1)$ and therefore reaches its minimum at $x = \frac{1}{n-1}$. Consequently,

$$\sqrt{\frac{2d_u d_v}{d_u^2 + d_v^2}} \geq \sqrt{\frac{\frac{2}{n-1}}{1 + (\frac{1}{n-1})^2}} = \sqrt{\frac{2(n-1)}{n^2 - 2n + 2}}.$$

Since the graph is connected, $|E(G)| \geq n-1$ and hence

$$GQ(G) \geq (n-1)\sqrt{\frac{2(n-1)}{n^2-2n+2}} = \sqrt{\frac{2(n-1)^3}{n^2-2n+2}}.$$

Moreover, the equality holds if and only if the number of $(1, n-1)$-edges is $n-1$. This happens only if G is a star graph. ■

It is well known that in a chemical graph C with $\delta(C) \geq 1$, the following relations are holds [2]:

$$v_1 + v_2 + v_3 + v_4 = n, \tag{1}$$

and

$$\begin{aligned} 2E_{1,1} + E_{1,2} + E_{1,3} + E_{1,4} &= v_1, \\ E_{1,2} + 2E_{2,2} + E_{2,3} + E_{2,4} &= 2v_2, \\ E_{1,3} + E_{2,3} + 2E_{3,3} + E_{3,4} &= 3v_3, \\ E_{1,4} + E_{2,4} + E_{3,4} + 2E_{4,4} &= 4v_4. \end{aligned} \tag{2}$$

Let $\mathbb{A} = \{(s,t) \in \mathbb{N} \times \mathbb{N} : 1 \leq s \leq t \leq 4\}$. Then from Equation 1 and 2, we have

$$n = \sum_{(a,b)\in\mathbb{A}} \frac{a+b}{ab} E_{a,b}. \tag{3}$$

Also we have

$$GQ(C) = \sum_{(a,b)\in\mathbb{A}} \sqrt{\frac{2ab}{a^2+b^2}} E_{a,b}. \tag{4}$$

Theorem 3. *In a n-vertex chemical graph C, we have*

$$GQ(C) \leq 2n,$$

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

Proof. By applying Equation 4, we have

$$\begin{aligned} GQ(C) &= \sum_{(a,b)\in\mathbb{A}} \sqrt{\frac{2ab}{a^2+b^2}} E_{a,b} \\ &= E_{4,4} + \sum_{(a,b)\in\mathbb{A}-\{(4,4)\}} \sqrt{\frac{2ab}{a^2+b^2}} E_{a,b} \\ &= 2n - \sum_{(a,b)\in\mathbb{A}-\{(4,4)\}} \frac{2a+2b}{ab} E_{a,b} + \\ &\sum_{(a,b)\in\mathbb{A}-\{(4,4)\}} \sqrt{\frac{2ab}{a^2+b^2}} E_{a,b} \\ &= 2n + \sum_{(a,b)\in\mathbb{A}-\{(4,4)\}} \left(\sqrt{\frac{2ab}{a^2+b^2}} - \frac{2a+2b}{ab} \right) E_{a,b}, \end{aligned}$$

It is easy to check that $\frac{2ab}{a^2+b^2} - \frac{2a+2b}{ab} < 0$ for all $(a,b) \in \mathbb{A} - \{(4,4)\}$. Therefore, $GQ(C) \leq 2n$. Moreover, if equality holds, then $E_{a,b} = 0$ for all $(a,b) \in \mathbb{A} - \{(4,4)\}$. Consequently, G is a regular graph.
Conversely, if G is a 4-regular graph, then $GQ(C) = E_{4,4} = \frac{4n}{2} = 2n$. ■

Theorem 4. *For a n-vertex chemical graph C, we have*

$$GQ(C) \geq \begin{cases} \frac{n}{2} & \text{if } n \text{ is even} \\ \frac{n}{2} + \frac{8-3\sqrt{5}}{2\sqrt{5}} & \text{if } n \text{ is odd.} \end{cases}$$

Equality in even case occurs if and only if $G \cong \frac{n}{2}P_2$, *and in odd case if and only if* $G \cong \frac{n-3}{2}P_2 \bigoplus P_3$.

Proof. We complete the proof by considering the following two cases:

Case (i) Let n be even. Then from Equation 4, we have

$$\begin{aligned}GQ(C) &= E_{1,1} + \sum_{(a,b)\in\mathbb{A}-\{(1,1)\}} \sqrt{\frac{2ab}{a^2+b^2}} \\ &= \frac{1}{2}\left(n - \sum_{(a,b)\in\mathbb{A}-\{(1,1)\}} \frac{a+b}{ab}E_{a,b}\right) + \sum_{(a,b)\in\mathbb{A}-\{(1,1)\}} \sqrt{\frac{2ab}{a^2+b^2}} \\ &= \frac{n}{2} + \sum_{(a,b)\in\mathbb{A}-\{(1,1)\}} \left(\sqrt{\frac{2ab}{a^2+b^2}} - \frac{a+b}{2ab}\right)E_{a,b}.\end{aligned}$$

One can easily check that

$$\sqrt{\frac{2ab}{a^2+b^2}} - \frac{a+b}{2ab} > 0, \tag{5}$$

for all $(a,b) \in \mathbb{A} - \{(1,1)\}$. Therefore

$$GQ(C) \geq \frac{n}{2}. \tag{6}$$

If $GQ(C) = \frac{n}{2}$, then $\frac{n}{2} = \frac{n}{2} + \sum_{(a,b)\in\mathbb{A}-\{(1,1)\}}\left(\sqrt{\frac{2ab}{a^2+b^2}} - \frac{a+b}{2ab}\right)E_{a,b}$. By applying relation 5, we have $E_{a,b} = 0$ for all $(a,b) \in \mathbb{A} - \{1,1)\}$. Since n is even clearly $C \cong \frac{n}{2}P_2$. Conversely, if $C \cong \frac{n}{2}P_2$ then $GQ(C) = \frac{n}{2}$.
Case (ii) Let n be odd and $\mathbb{T} = \mathbb{A} - \{(1,1),(1,2)\}$. Therefore

$$\begin{aligned}GQ(C) &= E_{1,1} + \frac{2}{\sqrt{5}}E_{1,2} + \sum_{(a,b)\in\mathbb{T}} \sqrt{\frac{2ab}{a^2+b^2}}E_{a,b} \\ &= E_{1,1} + \frac{2}{\sqrt{5}}\left(\frac{2n}{3} - \frac{4}{3}E_{1,1} - \frac{2}{3}\sum_{(a,b)\in\mathbb{T}} \frac{a+b}{ab}E_{a,b}\right) \\ &+ \sum_{(a,b)\in\mathbb{T}} \sqrt{\frac{2ab}{a^2+b^2}} \\ &= \frac{4n}{3\sqrt{5}} + \left(1 - \frac{8}{3\sqrt{5}}\right)E_{1,1} + \sum_{(a,b)\in\mathbb{T}}\left(\sqrt{\frac{2ab}{a^2+b^2}} - \frac{4a+4b}{3\sqrt{5}ab}\right)E_{a,b}.\end{aligned}$$

Since $\delta(G) \geq 1$, we have $E_{1,1} \leq \frac{n-3}{2}$. Also, one can easily check that

$$\sqrt{\frac{2ab}{a^2+b^2}} - \frac{4a+4b}{3\sqrt{5}ab} > 0 \tag{7}$$

for all $(a,b) \in \mathbb{T}$. Hence, applying all these conditions, we have

$$\begin{aligned} GQ(C) &\geq \frac{4n}{3\sqrt{5}} + \left(1 - \frac{8}{3\sqrt{5}}\right) \\ &= \frac{n}{2} + \frac{8-3\sqrt{5}}{2\sqrt{5}}. \end{aligned}$$

If $GQ(C) = \frac{n}{2} + \frac{8-3\sqrt{5}}{2\sqrt{5}}$, we have $E_{1,1} = \frac{n-3}{2}$ and $E_{a,b} = 0$ for all $(a,b) \in \mathbb{T}$. This implies $C \cong \frac{n-3}{2} P_2 \bigoplus P_3$.
Conversely, if $C \cong \frac{n-3}{2} P_2 \bigoplus P_3$ then $GQ(C) = \frac{n-3}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{5}} = \frac{n}{2} + \frac{8-3\sqrt{5}}{2\sqrt{5}}$. ■

Theorem 5. *Let T be a tree on $n \geq 3$ vertices. Then we have*

$$\sqrt{\frac{2(n-1)^3}{n^2-2n+2}} \leq GQ(T) \leq \frac{4}{\sqrt{5}} + n - 3.$$

The equality on the left is attained if and only if T is a star graph, and on the right equality if and only if T is a path.

Proof. Let T be a tree. Then T has at least two pendant paths. The contribution to the GQ index of T by each edge incident with a pendent vertex is at most $\sqrt{\frac{2.2.1}{4+1}} = \frac{2}{\sqrt{5}}$ and by each other edge is at most 1 (see remark 2). Therefore, $GQ(G) \leq \frac{4}{\sqrt{5}} + n - 3$. Moreover, if equality holds, then G has exactly two pendant vertices, which is possible only if $T \cong P_n$. One can easily check that $GQ(P_n) = \frac{4}{\sqrt{5}} + n - 3$. The proof for the lower bound follows from Theorem 2. ■

We have already determined that the path P_n is the unique tree with the maximum geometric quadratic index in the set of n-vertex trees (see Theorem 5). Now, we are interested in determining the n-vertex trees with the second and third for $n \geq 7$, the fourth and the fifth for $n \geq 10$, and the sixth for $n \geq 11$ maximum geometric quadratic indices.

Theorem 6. *In the set of n-vertex trees,*

(a) for $n \geq 7$, the unique trees with the second maximum GQ index are the trees with exactly one vertex of maximum degree three, which is adjacent to three vertices of degree two. The value of the second maximum GQ index is $6\sqrt{\frac{3}{13}} + \frac{6}{\sqrt{5}} + n - 7$.

(b) for $n \geq 7$, the unique trees with the third maximum GQ index are the trees with exactly one vertex of the maximum degree three, which is adjacent to two vertices of degree two and one vertex of degree one. The value of the third maximum GQ index is $4\sqrt{\frac{3}{13}} + \sqrt{\frac{3}{5}} + \frac{4}{\sqrt{5}} + n - 6$.

(c) for $n \geq 10$, the unique trees with the fourth maximum GQ index are the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two. The value of the fourth maximum GQ index is $8\sqrt{\frac{3}{13}} + \frac{8}{\sqrt{5}} + n - 9$.

(d) for $n \geq 10$, the unique trees with the fifth maximum GQ index are the trees with exactly one vertex of maximum degree three, which is adjacent to one vertex of degree two and two vertices of degree one. The value of the fifth maximum GQ index is $2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + n - 5$.

(e) for $n \geq 11$, the unique trees with the sixth maximum GQ index are the trees with exactly two vertices of the maximum degree three, each adjacent to three vertices of degree two. The value of the sixth maximum GQ index is $12\sqrt{\frac{3}{13}} + \frac{8}{\sqrt{5}} + n - 11$.

Proof. Let $T \neq P_n$ be a n-vertex tree, where $n \geq 7$. Then T has at least three pendant paths.

Let $l = 3$. Then T has exactly one vertex of maximum degree 3 in T, which is adjacent to exactly one, two, or three vertices of degree two. Let u be the vertex of maximum degree three in T. Now, if

(i) u is adjacent to three vertices of degree two, then

$$\begin{aligned} GQ(G) &= 3\sqrt{\frac{2.3.2}{9+4}} + 3\sqrt{\frac{2.2.1}{4+1}} + n - 7 \\ &= 6\sqrt{\frac{3}{13}} + \frac{6}{\sqrt{5}} + n - 7 \\ &\approx n - 1.434. \end{aligned}$$

(ii) u is adjacent to two vertices of degree two and one vertex of degree one, then

$$\begin{aligned} GQ(G) &= 2\sqrt{\frac{2.3.2}{9+4}} + \sqrt{\frac{2.3.1}{9+1}} + 2\sqrt{\frac{2.2.1}{4+1}} + n - 6 \\ &= 4\sqrt{\frac{3}{13}} + \sqrt{\frac{3}{5}} + \frac{4}{\sqrt{5}} + n - 6 \\ &\approx n - 1.515. \end{aligned}$$

(iii) u is adjacent to two vertices of degree one and one vertex of degree two, then

$$\begin{aligned} GQ(T) &= 2\sqrt{\frac{2.3.1}{9+1}} + \sqrt{\frac{2.3.2}{9+4}} + \sqrt{\frac{2.2.1}{4+1}} + n - 5 \\ &= 2\sqrt{\frac{3}{5}} + 2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + n - 5 \\ &\approx n - 1.595. \end{aligned}$$

Let $l = 4$. Then we have two possibilities:
(i) T has exactly one vertex of maximum degree four, and all other vertices are of degree at most two. Then note that $\sqrt{\frac{2.4.1}{16+1}} < \sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.4}{4+16}}$ and hence

$$\begin{aligned} GQ(T) &\leq 4(\sqrt{\frac{2.1.2}{4+1}} + \sqrt{\frac{2.2.4}{4+16}} + n - 9 \\ &= \frac{16}{\sqrt{5}} + n - 9 \\ &\approx n - 1.844. \end{aligned}$$

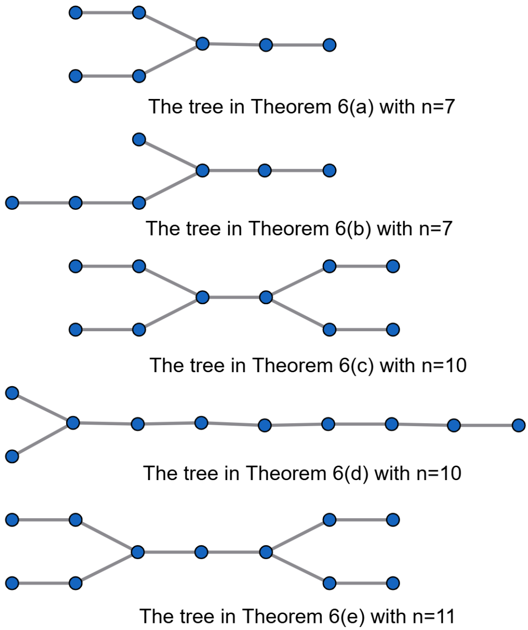

Figure 1. The trees in Theorem 6.

(ii) T has exactly two vertices of maximum degree three. Now, if T has at least one pendant path of length one, then

$$\begin{aligned} GQ(T) &\le \sqrt{\frac{2.1.3}{9+1}} + 3\left(\sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.3}{4+9}}\right) + n - 8 \\ &= \frac{6+\sqrt{3}}{\sqrt{5}} + \frac{6\sqrt{3}}{\sqrt{13}} + n - 8 \\ &\approx n - 1.659. \end{aligned}$$

Now, if each pendant path in T is of length at least two, we denote the two vertices of degree three by u and v, respectively. If u and v are adjacent, then $n \geq 10$ and

$$GQ(T) = 4\left(\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.2.1}{4+1}}\right) + n - 9$$
$$= 8\sqrt{\frac{3}{13}} + \frac{8}{\sqrt{5}} + n - 9$$
$$\approx n - 1.579.$$

If u and v are not adjacent, then $n \geq 11$ and

$$GQ(T) = 6\sqrt{\frac{2.2.3}{4+9}} + 4\sqrt{\frac{2.2.1}{4+1}} + n - 11$$
$$= 12\sqrt{\frac{3}{13}} + \frac{8}{\sqrt{5}} + n - 11$$
$$\approx n - 1.657.$$

If T has $l \geq 5$ pendant path, then

$$GQ(T) \leq \left(\sqrt{\frac{12}{13}} + \sqrt{\frac{4}{5}} - 2\right) 5 + n - 1 \approx n - 1.724. \qquad \blacksquare$$

3 *GQ* index of unicyclic graphs

In this Section, we are interested in computing the n-vertex unicyclic graphs with the maximum and the second, third, fourth, fifth, and sixth maximum GQ indices.

Theorem 7. *In the set of n-vertex unicyclic graphs,*

(a) The unique graph with the maximum GQ index is the cycle C_n, and the maximum value is n.

(b) for $n \geq 5$, the unique graphs with the second maximum GQ index are the unicyclic graphs with a single vertex of maximum degree three, adjacent to three vertices of degree two. The value of the second maximum GQ index is $6\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + n - 4$.

(c) for $n \geq 5$, the unique graphs with the third maximum GQ index are the

unicyclic graphs with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two. The value of the third maximum GQ index is $4\sqrt{\frac{3}{13}}+\sqrt{\frac{3}{5}}+n-3$.

(d) *for* $n \geq 7$*, the unique graphs with the fourth maximum GQ index are the unicyclic graphs with exactly two vertices of the maximum degree three, each adjacent to two vertices of degree two. The value of the fourth maximum GQ index is* $8\sqrt{\frac{3}{13}}+\frac{4}{\sqrt{5}}+n-6$.

(e) *for* $n \geq 9$*, the unique graphs with the fifth maximum GQ index are the unicyclic graphs obtained by attaching a path* P_t $(t \geq 2)$ *to every vertex of a triangle. The value of the fifth maximum GQ index is* $6\sqrt{\frac{3}{13}}+\frac{6}{\sqrt{5}}+n-6$.

(f) *for* $n \geq 9$*, the unique graphs with the sixth maximum GQ index are the unicyclic graphs with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two. The value of the sixth maximum GQ index is* $12\sqrt{\frac{3}{13}}+\frac{4}{\sqrt{5}}+n-8$.

Proof. Let U be a n-vertex unicyclic graphs, where $n \geq 3$. Therefore $GQ(U) \leq m = n$ (see Theorem 1). Moreover, equality holds if and only if U is a regular unicyclic graph i.e., $U \cong C_n$.

Let the number of pendant paths in U be one. Then we have two possibilities:

(i) U has exactly one vertex of maximum degree three, adjacent to three vertices of degree two. Then $n \geq 5$, and

$$\begin{aligned} GQ(G) &= 3\sqrt{\frac{2.3.2}{9+4}}+\sqrt{\frac{2.2.1}{4+1}}+n-4 \\ &= 6\sqrt{\frac{3}{13}}+\frac{2}{\sqrt{5}}+n-4 \cong n-0.2232. \end{aligned}$$

(ii) U has exactly one vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two. Then $n \geq 4$, and

$$GQ(U) = 2\sqrt{\frac{2.3.2}{9+4}} + \sqrt{\frac{2.3.1}{9+1}} + n - 3$$
$$= 4\sqrt{\frac{3}{13}} + \sqrt{\frac{3}{5}} + n - 3 \approx n - 0.3038.$$

Now, let the number of pendant paths in U be two. Then, two cases arise:

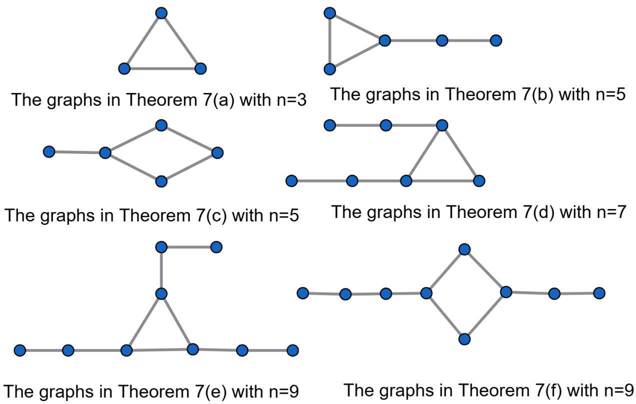

Figure 2. The unicyclic graphs in Theorem 7 with least number of vertices.

(i) U has exactly one vertex on the cycle of maximum degree four, and all other vertices of U are of degree at most two. Then note that $\sqrt{\frac{2.1.4}{16+1}} = 2\sqrt{\frac{2}{17}} < \sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.4}{4+16}} = \frac{4}{\sqrt{5}}$ and hence

$$GQ(U) \leq 4\sqrt{\frac{2.4.2}{16+4}} + 2\sqrt{\frac{2.2.1}{4+1}} + n - 6$$
$$= \frac{12}{\sqrt{5}} - 6 + n \approx n - 0.6334.$$

(ii) U has exactly two vertices of maximum degree three. Now, if both the two pendant paths are of length one in U, then

$$
\begin{aligned}
GQ(U) &\leq 2\sqrt{\frac{2.1.3}{9+1}} + n - 2 \\
&= 2\sqrt{\frac{3}{5}} + n - 2 \approx n - 0.4508.
\end{aligned}
$$

If U has exactly one pendant path of length one, then

$$
\begin{aligned}
GQ(U) &\leq 3\sqrt{\frac{2.3.2}{9+4}} + \sqrt{\frac{2.3.1}{9+1}} + \sqrt{\frac{2.2.1}{4+1}} + n - 5 \\
&= 6\sqrt{\frac{3}{13}} + \sqrt{\frac{3}{5}} + \frac{2}{\sqrt{5}} + n - 5 \approx n - 0.4486.
\end{aligned}
$$

If the length of both pendent paths in U is greater equal to two, denote the two vertices of degree three by x and y. If x and y are adjacent, then $n \geq 7$ and

$$
\begin{aligned}
GQ(U) &= 4\sqrt{\frac{2.3.2}{9+4}} + 2\sqrt{\frac{2.1.2}{4+1}} + n - 6 \\
&= 8\sqrt{\frac{3}{13}} + \frac{4}{\sqrt{5}} + n - 6 \approx n - 0.3680.
\end{aligned}
$$

If x and y are not adjacent, then $n \geq 8$ and hence

$$
\begin{aligned}
GQ(G) &= 6\sqrt{\frac{2.3.2}{9+4}} + 2\sqrt{\frac{2.2.1}{4+1}} + n - 8 \\
&= 12\sqrt{\frac{3}{13}} + \frac{4}{\sqrt{5}} + n - 8 \approx n - 0.4465.
\end{aligned}
$$

Let us consider that U has exactly three pendant paths. If U has at least one pendant path of length one, then

$$
\begin{aligned}
GQ(U) &\leq \sqrt{\frac{2.1.3}{9+1}} + 2\left(\sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.3}{4+9}}\right) + n - 5 \\
&= \frac{4}{\sqrt{5}} + \sqrt{\frac{3}{5}} + 4\sqrt{\frac{3}{13}} + n - 5 \approx n - 0.5150.
\end{aligned}
$$

Let all three pendant paths be of length greater than or equal to two. Now, if U has a pendent path at the vertex , say x, such that $d(x) \geq 4$, then

$$GQ(U) \leq \sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.4}{4+16}} + 2\left(\sqrt{\frac{2.1.2}{4+1}} + \sqrt{\frac{2.2.3}{4+9}}\right) + n - 6$$
$$= \frac{8}{\sqrt{5}} + 4\sqrt{\frac{3}{13}} + n - 6 \approx n - 0.5007.$$

Suppose that the three pendant paths in U are all at the vertices u, v, w, of degree three. If at most two pairs of vertices are adjacent, then

$$GQ(U) \leq 5\sqrt{\frac{2.2.3}{4+9}} + 3\sqrt{\frac{2.1.2}{1+4}} + n - 8$$
$$= 10\sqrt{\frac{3}{13}} + \frac{6}{\sqrt{5}} + n - 8 \approx n - 0.5128.$$

If u, v, w are pairwise adjacent, then $U \cong C_3(1)(2)$ and hence

$$GQ(U) \leq 3\sqrt{\frac{2.2.3}{4+9}} + 1 + 1 + 1 + 3\sqrt{\frac{2.1.2}{1+4}} + n - 9$$
$$= 6\sqrt{\frac{3}{13}} + \frac{6}{\sqrt{5}} + n - 6 \approx n - 0.4344.$$

If U has $l \geq 4$ pendant paths, then by Lemma 1, we have

$$GQ(U) \leq \left(\sqrt{\frac{12}{13}} + \sqrt{\frac{4}{5}} - 2\right) l + m$$
$$\leq \left(\sqrt{\frac{12}{13}} + \sqrt{\frac{4}{5}} - 2\right) 4 + n \approx n - 0.5792.$$

Therefore, combining all the above cases, we have the desired results. ■

4 *GQ* index of bicyclic graphs

In this section, we determine the family of n-vertex bicyclic graphs with the maximum, second, third, fourth, fifth, and sixth maximum GQ index. By $\beta_1^1(n)$, we denote the family of bicyclic graphs obtained from C_n by adding an edge, where $n \geq 4$. Let $\beta_1^2(n)$ be the family of bicyclic graphs obtained by joining two vertex-disjoint cycles C_s and C_t with $s+t=n$ by an edge, where $n \geq 6$. Let $\beta_2(n)$ be the family of bicyclic graphs obtained from $C_s = v_0v_1 \cdots v_{s-1}$ with $4 \leq s \leq n-2$ by joining v_0 and v_2 by an edge and attaching a path on the $n-a$ vertices to v_1. Also, by $\beta_3^1(n)$, we denote the family of bicyclic graphs obtained by joining two non-adjacent vertices of C_s with $4 \leq s \leq n-1$ by a path of length $n-s+1$, where $n \geq 5$. Let $\beta_3^2(n)$ be the family of bicyclic graphs obtained by joining two vertex-disjoint cycles C_s and C_t with $s+t<n$ by a path of length $n-s-t+1$, where $n \geq 7$. By $\beta_4(n)$, we denote the family of bicyclic graphs obtained by attaching a path on at least two vertices to the two vertices of degree two of the unique 4-vertex bicyclic graph, where $n \geq 8$. Let $\beta_5^1(n)$ be the bicyclic graphs obtained from a graph $\beta_1^1(t)$ with $t \geq 5$ or $\beta_1^2(t)$ with $t \geq 6$ by attaching a path of length $n-t \geq 2$ to a vertex of degree two, whose two neighbors are of degree two and three, where $n \geq 7$. Let $\beta_5^2(n)$ denotes the bicyclic graphs obtained from a graph $\beta_3^1(t)$ with $t \geq 5$ or $\beta_3^2(t)$ with $t \geq 7$ by attaching a path on $n-t \geq 2$ vertices to a vertex of degree two, whose two neighbors are both of degree three, where $n \geq 7$. Let $\beta_6(n)$ denote the bicyclic graph obtained from $C_{n-1} = v_0v_1 \cdots v_{n-2}$ by joining v_0 and v_2 by an edge and attaching a vertex of degree one to v_1, where $n \geq 5$. By $\beta_I(n)$, we denote the n vertex bicyclic graph obtained by identifying one vertex of two cycles.

Theorem 8. *In the set of n-vertex bicyclic graphs*

(a) The unique graphs with the maximum GQ index are the graphs in $\beta_1^1(n)$ for $n \geq 4$ and the graphs in $\beta_1^2(n)$ for $n \geq 6$. The maximum value of the GQ index is $8\sqrt{\frac{3}{13}} + n - 3$.

(b) The unique graphs with the second maximum GQ index are the graphs in $\beta_2(n)$ for $n \geq 6$. The value of the second maximum GQ index is $6\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + n - 3$.

(c) The unique graphs with the third maximum GQ index are the graphs in $\beta_3^1(n)$ for $n \geq 5$ and $\beta_3^2(n)$ for $n \geq 7$. The value of the third maximum GQ index is $12\sqrt{\frac{3}{13}} + n - 5$.

(d) The unique graphs with the fourth maximum GQ index are the graphs

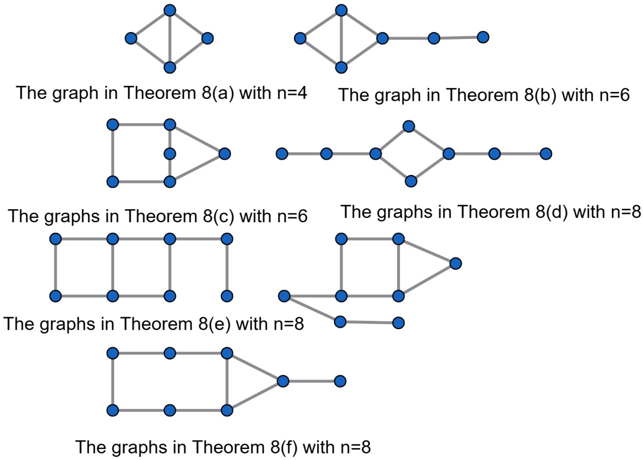

Figure 3. The bicyclic graphs in Theorem 8 with least number of vertices.

in $\beta_4(n)$ *for* $n \geq 8$. *The value of the fourth maximum GQ index is* $4\sqrt{\frac{3}{13}} + \frac{4}{\sqrt{5}} + n - 3$.

(e) *The unique graphs with the fifth maximum GQ index are the graphs in* $\beta_5^1(n)$ *or* $\beta_5^2(n)$ *for* $n \geq 8$. *The value of the fifth maximum GQ index is* $10\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} + n - 5$.

(f) *The unique graphs with the sixth maximum GQ index are the graphs in* $\beta_6(n)$ *for* $n \geq 8$. *The value of the sixth maximum GQ index is* $4\sqrt{\frac{3}{13}} + \sqrt{\frac{3}{5}} + n - 2$.

Proof. Let B be a n-vertex bicyclic graph, where $n \geq 4$. If B has no pendant path, then either (i) $B \in \beta_1^1(n)$ or $B \in \beta_1^2(n)$ with $n \geq 6$ or (ii) $B \in \beta_3^1(n)$ with $n \geq 5$ or $B \in \beta_3^2(n)$ with $n \geq 7$ or (iii) $B \in \beta_I(n)$. If (i) holds, then $GQ(B) = 8\sqrt{\frac{3}{13}} + (n + 1 - 4) \approx n + 0.8430$. If (ii) holds, then $GQ(B) = 6\sqrt{\frac{2.2.3}{4+9}} + n - 5 \approx n + 0.7646$. If (iii) holds, then $GQ(B) = 4\sqrt{\frac{2.1.2}{5}} + n - 3 \approx n + 0.5777$.

Now, suppose that B has exactly one pendant path. Clearly $\Delta(B) \in \{3, 4, 5\}$. Now we have two possibilities: (i) The pendant path is of length one. If $\Delta(B) \in \{4,5\}$, then we have

$$\begin{aligned} GQ(B) &\leq 2\sqrt{\frac{2.2.\Delta}{4+\Delta^2}} + \sqrt{\frac{2.1.3}{1+9}} + n - 2 \\ &\leq 2\sqrt{\frac{2.2.4}{4+16}} + \sqrt{\frac{2.1.3}{1+9}} + n - 2 \approx n + 0.5634. \end{aligned}$$

Let $\Delta(B) = 3$. Then B has exactly three vertices, say x,y, z, of degree three in B. If at most two pairs of vertices x, y, z are adjacent, then

$$GQ(G) \leq 4\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.1.3}{1+9}} + n - 4 \approx n + 0.6176.$$

If x, y, z are pairwise adjacent, then $B \in \beta_6(n)$ with $n \geq 5$ and $GQ(B) = 2\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.3.1}{9+1}} + 6 + n + 1 - 9 \approx n + 0.6961$.
(ii) The length of the pendant path is at least two. If $\Delta(B) \in \{4,5\}$, then

$$\begin{aligned} GQ(B) &\leq 3\sqrt{\frac{2.2.\Delta}{4+\Delta^2}} + \sqrt{\frac{2.1.2}{1+4}} + n + 1 - 4 \\ &\leq 3\sqrt{\frac{2.2.4}{4+16}} + \sqrt{\frac{2.1.2}{1+4}} + n + 1 - 4 \approx n + 0.57770. \end{aligned}$$

If $\Delta(B) = 3$, then B has exactly three vertices, say x_1, x_2 and x_3. If at most one pair of vertices x_1, x_2, x_3 is adjacent, then

$$GQ(B) \leq 7\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.1.2}{1+4}} + n + 1 - 8 \approx n + 0.6198.$$

If there are exactly two pairs of vertices x_1, x_2, x_3 are adjacent, then $B \in \beta_5^1(n)$ or $B \in \beta_5^2(n)$ with $n \geq 7$, and $GQ(B) = 5\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.2.1}{1+4}} + n + 1 - 6 \approx n + 0.69827$. If x_1, x_2, x_3 are pairwise adjacent, then $B \in \beta_2(n)$ with $n \geq 6$, and $GA(B) = 3\sqrt{\frac{2.2.3}{4+9}} + \sqrt{\frac{2.2.1}{1+4}} + n + 1 - 4 \cong n + 0.7767$.
Let the number of pendant paths in B be exactly two. Then $\Delta(B) \in$

$\{3,4,5,6\}$. If $\Delta(B) \in \{4,5,6\}$, then

$$GQ(B) \leq 2\sqrt{\frac{2.2.\Delta}{4+\Delta^2}} + 2\left\{\sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.3}{4+9}}\right\} + n + 1 - 6$$
$$\leq 2\sqrt{\frac{2.2.4}{4+16}} + 2\left\{\sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.3}{4+9}}\right\} + n + 1 - 6 \approx n + 0.4992.$$

Suppose $\Delta(B) = 3$. The B has exactly four vertices , say x_1, x_2, x_3, x_4, of degree three. If there is at least one pendant path of length one, then

$$GQ(B) \leq \sqrt{\frac{2.1.3}{1+9}} + \sqrt{\frac{2.1.2}{1+4}} + \sqrt{\frac{2.2.3}{4+9}} + n + 1 - 3 \approx n + 0.6297.$$

Suppose both the pendant paths are at least two in length. Since B is bicyclic, at most five pairs of vertices x_1, x_2, x_3, x_4 are adjacent. If at most four pairs of x_1, x_2, x_3, x_4 are adjacent, then

$$GQ(B) \leq 4\sqrt{\frac{2.2.3}{4+9}} + 2\sqrt{\frac{2.1.2}{1+4}} + n + 1 - 6 \approx n + 0.6319.$$

If there are exactly five pairs of vertices x_1, x_2, x_3, x_4 are adjacent, then $B \in \beta_4(n)$ with $n \geq 8$, and $GQ(B) = 2\sqrt{\frac{2.2.3}{4+9}} + 2\sqrt{\frac{2.2.1}{1+4}} + n - 3 \approx n + 0.7103$. If there are $l \geq 3$ pendant paths in B, then by Lemma 1, we have

$$GQ(B) \leq \left(2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} - 2\right) l + m$$
$$\leq \left(2\sqrt{\frac{3}{13}} + \frac{2}{\sqrt{5}} - 2\right) 3 + n + 1 \approx n + 0.5655.$$

Combining all the above arguments, we have the desired result. ■

Conclusion

In this paper, we have analyzed the GQ index of a simple graph G defined as $GQ(G) = \sum_{a\sim b} \sqrt{\frac{2d_a d_b}{d_a^2 + d_b^2}}$. We have determined the extremal values and extremal graphs with respect to the GQ indices over simple connected graphs, chemical graphs and trees with the given number of vertices. In addition, we have studied the first six maximum values and the corresponding n-vertex trees with respect to the GQ index. In addition, we have determined the n-vertex unicyclic and bicyclic graphs with the first six maximum values with respect to the GQ index.

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