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Investigation of Closed Derivation Formulas for GQ and QG Indices of a Graph via M-polynomial

SHIBSANKAR DAS• AND VIRENDRA KUMAR

Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India

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ABSTRACT

A topological index is a numerical data which significantly correlates with the fundamental topology of a given chemical structure. The M-polynomial is a key mathematical tool to determine the degree-dependent topological indices. Very recently, the geometric-quadratic (GQ) and quadratic-geometric (QG) indices of a graph are introduced and computed their values by their respective mathematical formulas on some standard graphs and jagged-rectangle benzenoid system. In this research work, we propose M-polynomial based closed derivation formulas for determining the above two indices. In addition, we derive the GQ and QG indices for each of the abovementioned graphs by applying the derivation formulas, and also produce some fundamental relationships between the indices.

1. INTRODUCTION

Chemical graph theory (CGT) is a relationship between chemistry and mathematics where the atoms and bonds of a molecular structure exhibit the vertices and edges of a graph, respectively. In CGT, a topological index is a numerical representation that characterizes various physical, chemical properties, and biological activity of a molecular compound and plays a substantial role in Quantitative Structure-Property Relationships (QSPR) /

•Corresponding Author (Email address: shib.iitm@gmail.com, shibsankar@bhu.ac.in)
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Quantitative Structure-Activity Relationships (QSAR) investigation [18]. Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be an undirected, simple, and connected graph with $V(\Upsilon)$ as its vertex set and $E(\Upsilon)$ as its edge set. The total number of edges incident to a vertex $u \in V(\Upsilon)$ is known as the degree of u and is denoted as $d_\Upsilon(u)$.

In 2009, Vukičević and Furtula introduced the geometric-arithmetic index [20] which is defined as

$$GA(\Upsilon) = \sum_{uv \in E(\Upsilon)} \frac{2\sqrt{d_\Upsilon(u)d_\Upsilon(v)}}{d_\Upsilon(u)+d_\Upsilon(v)}.$$

Being inspired by the definition of geometric-arithmetic index of a graph Υ, V.R. Kulli proposed two new indices, namely, geometric-quadratic (GQ) index and quadratic-geometric (QG) index [14] based on the geometric and quadratic mean of the degrees of the end vertices of an edge $uv \in E(\Upsilon)$ and defined them as follows

$$GQ(\Upsilon) = \sum_{uv \in E(\Upsilon)} \frac{\sqrt{d_\Upsilon(u)d_\Upsilon(v)}}{\sqrt{\frac{d_\Upsilon(u)^2+d_\Upsilon(v)^2}{2}}} = \sum_{uv \in E(\Upsilon)} \frac{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}}{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}},$$

and

$$QG(\Upsilon) = \sum_{uv \in E(\Upsilon)} \frac{\sqrt{\frac{d_\Upsilon(u)^2+d_\Upsilon(v)^2}{2}}}{\sqrt{d_\Upsilon(u)d_\Upsilon(v)}} = \sum_{uv \in E(\Upsilon)} \frac{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}}{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}}.$$

Usually, topological indices are computed by using their standard mathematical definitions. Instead of calculating them separately, several algebraic polynomials have been developed, each of which generates the topological indices by differentiation, integration, or a mix of both. For example, Hosoya polynomial [12] is utilized to compute the distance-based topological indices such as the Wiener index and hyper-Wiener index and NM-polynomial [19] is used to recover the neighborhood degree sum-based topological indices. In 2015, Deutsch and Klavžar introduced the M-polynomial [11] to determine the degree-based topological indices. In [4–9,15–17], numerous degree-based topological indices of different chemical structures have been calculated with the help of their respective M-polynomials.

Definition 1. [11] The M-polynomial of a graph Υ defined as

$$M(\Upsilon; x, y) = \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon)\, x^i y^j,$$

where $\delta = \min\{\, d_\Upsilon(u) |\, u \in V(\Upsilon)\}$, $\Delta = \max\{\, d_\Upsilon(u) |\, u \in V(\Upsilon)\}$, and $\phi_{i,j}(\Upsilon)$ is the number of edges $uv \in E(\Upsilon)$ such that $d_\Upsilon(u) = i,\ d_\Upsilon(u) = j\ (i, j \ge 1)$.

As described in [10], a degree-based topological index defined on the edge set $E(\Upsilon)$ of a graph Υ can be represented as

$$I(\Upsilon) = \sum_{uv \in E(\Upsilon)} f(d_\Upsilon(u), d_\Upsilon(v)), \tag{1}$$

where $f\big(d_\Upsilon(u), d_\Upsilon(v)\big)$ is the function of $d_\Upsilon(u), d_\Upsilon(v)$ which depends on the mathematical definition of the index. By counting the edges in the graph Υ that have the same end degrees, the above definition can also be rephrased as

$$I(\Upsilon) = \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon)\, f(i,j). \quad (2)$$

Below we list some operators [1, 13] that will be utilized in the context of this manuscript, which are

$$D_x^{1/2}\big(h(x,y)\big) = \sqrt{x\frac{\partial h(x,y)}{\partial x}}.\sqrt{h(x,y)},$$

$$D_y^{1/2}\big(h(x,y)\big) = \sqrt{y\frac{\partial h(x,y)}{\partial y}}.\sqrt{h(x,y)},$$

$$S_x^{1/2}\big(h(x,y)\big) = \sqrt{\int_0^x \frac{h(t,y)}{t}\,dt}\,.\sqrt{h(x,y)},$$

$$S_y^{1/2}\big(h(x,y)\big) = \sqrt{\int_0^y \frac{h(x,t)}{t}\,dt}\,.\sqrt{h(x,y)},$$

and

$$J\big(h(x,y)\big) = h(x,x).$$

2. METHODOLOGY

In [14], V.R. Kulli examined the GQ and QG indices for some standard graphs, namely, complete bipartite graph, star graph, k-regular graph, cycle graph, complete graph, path, and jagged-rectangle benzenoid system $B_{m,n}$, by using the primary mathematical definition mentioned earlier in this section. In this current study, we evaluate the GQ and QG indices of a given graph with the help of the M-polynomial of the graph. At the outset, we present two closed derivation formulas for finding the GQ and QG indices of a graph via its M-polynomial, in Section 2, and then we derive the numerical values of the GQ and QG indices of the standard graphs mentioned above. Section 3 deals with the jagged-rectangle benzenoid system $B_{m,n}$, where we compute the GQ and QG indices via M-polynomial approach and illustrate them graphically. We use Maple 2020 computing environment for numerical computation and graphical depiction of the results. Additionally, Section 4 talks about some interesting relations between the GQ and QG indices for general graph, particularly for $K_{m,n}$, path, and jagged-rectangular benzenoid system $B_{m,n}$. In the end, we conclude the results in Section 5.

3. MAIN RESULTS AND DISCUSSION

Here we define some new operators which will be essential to prove the closed derivation formulas, and they are

$$P_x\left(h\big(x^{\alpha}, y^{\beta}\big)\right) = h\big(x^{\alpha^2}, y^{\beta}\big),$$

and

$$P_y\left(h\left(x^{\alpha}, y^{\beta}\right)\right) = h\left(x^{\alpha}, y^{\beta^2}\right),$$

where $\alpha, \beta \in \mathbb{N} \cup \{0\}$ and $\mathbb{N}$ is a set of natural numbers.

Next, we propose two derivation formulas for GQ and QG indices of a graph Υ with the help of the M-polynomial of the graph and above defined operators.

Theorem 1. Let $\Upsilon = \left(V(\Upsilon), E(\Upsilon)\right)$ be a graph and its geometric-quadratic index is

$$GQ(\Upsilon) = \sum_{uv \in E(\Upsilon)} f\left(d_{\Upsilon}(u), d_{\Upsilon}(v)\right), \text{ where } f(x,y) = \frac{\sqrt{2xy}}{\sqrt{x^2+y^2}},$$

then

$$GQ(\Upsilon) = \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2}\, [M(\Upsilon; x, y)]|_{x=1},$$

where $M(\Upsilon; x, y)$ is the M-polynomial of Υ.

Proof. Let $M(\Upsilon; x, y)$ be the M-polynomial of Υ as per the Definition 1, then

$$\begin{aligned}
S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}\left(M(\Upsilon; x, y)\right) &= S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2} \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon)\, x^i y^j \\
&= \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon) \cdot S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}(x^i y^j) \\
&= \sum_{\delta \le i \le j \le \Delta} \sqrt{ij}\, \phi_{i,j}(\Upsilon) \cdot S_x^{1/2} J\, P_y\, P_x\, (x^i y^j) \\
&= \sum_{\delta \le i \le j \le \Delta} \sqrt{ij}\, \phi_{i,j}(\Upsilon) \cdot S_x^{1/2} J\, (x^{i^2} y^{j^2}) \\
&= \sum_{\delta \le i \le j \le \Delta} \sqrt{ij}\, \phi_{i,j}(\Upsilon) \cdot S_x^{1/2} (x^{i^2+j^2}) \\
&= \sum_{\delta \le i \le j \le \Delta} \frac{\sqrt{ij}}{\sqrt{i^2+j^2}}\, \phi_{i,j}(\Upsilon) \cdot x^{i^2+j^2}.
\end{aligned}$$

$$\therefore \sqrt{2} S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}\left(M(\Upsilon; x, y)\right)|_{x=1} = \sum_{\delta \le i \le j \le \Delta} \frac{\sqrt{2ij}}{\sqrt{i^2+j^2}}\, \phi_{i,j}(\Upsilon)$$

$$= \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon) \cdot f(i,j). \tag{3}$$

Now, in view of Equations 1 and 2 we have

$$GQ(\Upsilon) = \sum_{uv \in E(\Upsilon)} f\left(d_{\Upsilon}(u), d_{\Upsilon}(v)\right) = \sum_{\delta \le i \le j \le \Delta} \phi_{i,j}(\Upsilon) \cdot f(i,j). \tag{4}$$

Hence, the Equations 3 and 4 complete the proof. ■

Theorem 2. Let $\Upsilon = \left(V(\Upsilon), E(\Upsilon)\right)$ be a graph and its quadratic-geometric index is

$$QG(\Upsilon) = \sum_{uv \in E(\Upsilon)} f\left(d_{\Upsilon}(u), d_{\Upsilon}(v)\right), \text{ where } f(x,y) = \frac{\sqrt{x^2+y^2}}{\sqrt{2xy}},$$

then

$$QG(\Upsilon) = \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]|_{x=1},$$

where $M(\Upsilon; x, y)$ is the M-polynomial of Υ.

Proof. We know from the Definition 1 that the M-polynomial of the graph Υ is given by $M(\Upsilon;x,y)=\sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\,x^iy^j$, therefore

$$\begin{aligned}
D_x^{1/2}\,J\,P_y\,P_x\,S_y^{1/2}\,S_x^{1/2}\big(M(\Upsilon;x,y)\big) &= D_x^{1/2}\,J\,P_y\,P_x\,S_y^{1/2}\,S_x^{1/2}\sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\,x^iy^j\\
&=\sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\cdot D_x^{1/2}\,J\,P_y\,P_x\,S_y^{1/2}\,S_x^{1/2}(\,x^iy^j)\\
&=\sum_{\delta\le i\le j\le\Delta}\frac{1}{\sqrt{ij}}\,\phi_{i,j}(\Upsilon)\cdot D_x^{1/2}\,J\,P_y\,P_x\,(\,x^iy^j)\\
&=\sum_{\delta\le i\le j\le\Delta}\frac{1}{\sqrt{ij}}\,\phi_{i,j}(\Upsilon)\cdot D_x^{1/2}\,J\,(\,x^{i^2}y^{j^2})\\
&=\sum_{\delta\le i\le j\le\Delta}\frac{1}{\sqrt{ij}}\,\phi_{i,j}(\Upsilon)\cdot D_x^{1/2}\,(\,x^{i^2+j^2})\\
&=\sum_{\delta\le i\le j\le\Delta}\frac{\sqrt{i^2+j^2}}{\sqrt{ij}}\,\phi_{i,j}(\Upsilon)\cdot\,x^{i^2+j^2}.
\end{aligned}$$

$$\begin{aligned}
\therefore\ \frac{1}{\sqrt{2}}D_x^{1/2}\,J\,P_y\,P_x\,S_y^{1/2}\,S_x^{1/2}\big(M(\Upsilon;x,y)\big)|_{x=1} &= \sum_{\delta\le i\le j\le\Delta}\frac{\sqrt{i^2+j^2}}{\sqrt{2ij}}\,\phi_{i,j}(\Upsilon)\\
&= \sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\cdot f(i,j). \qquad (5)
\end{aligned}$$

Now, in view of Equations 1 and 2 we have

$$QG(\Upsilon)\;=\;\sum_{uv\,\in\,E(\Upsilon)}f\big(d_\Upsilon(u),d_\Upsilon(v)\big)=\sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\cdot f(i,j). \qquad (6)$$

Hence, the Equations 5 and 6 complete the proof. ■

Now we drive the expressions of GQ and QG indices of some standard graphs (namely, complete bipartite graph, star graph, k-regular graph, cycle graph, complete graph, and path) via their respective M-polynomials based on Theorems 1 and 2.

Theorem 3. [3] Let Υ be a complete bipartite graph $K_{n,m}$ with $n+m$ vertices where $1\le n\le m$ and $m\;\ge\;2$. Then the M-polynomial of Υ is $M(\Upsilon;x,y)=\;nm\,x^ny^m$.

Proof. Here, Υ is a complete bipartite graph $K_{n,m}$ with $|V(\Upsilon)|=|V_1(\Upsilon)+V_2(\Upsilon)|=n+m$, and $|E(\Upsilon)|=nm$ where the vertex set partitions of Υ are

$$V_1(\Upsilon)=\{u\in V(\Upsilon){:}\,d_\Upsilon(u)=m\}\quad\text{and}\quad V_2(\Upsilon)=\{u\in V(\Upsilon):d_\Upsilon(u)=n\}.$$

Since every vertex of $V_1(\Upsilon)$ is incident to the vertex of $V_2(\Upsilon)$ and vice versa, therefore there is only one partition of edge set $E(\Upsilon)$ which is as follows

$$E_{\{n,m\}}=\{e=uv\in E(\Upsilon){:}\,d_\Upsilon(u)=n,d_\Upsilon(v)=m\},$$

and $|E_{\{n,m\}}|=|E(\Upsilon)|$. Therefore, the M-polynomial of Υ is

$$\begin{aligned}
M(\Upsilon;x,y)&=\sum_{\delta\le i\le j\le\Delta}\phi_{i,j}(\Upsilon)\,x^iy^j\,,\ \text{ where } i,j=\{n,m\}\\
&=\sum_{n\le m}\phi_{n,m}(\Upsilon)\,x^ny^m=|E_{\{n,m\}}|\;\;x^ny^m\;\;=nm\,x^ny^m.
\end{aligned}$$

■

Theorem 4. If Υ be a complete bipartite graph $K_{n,m}$ with $1 \le n \le m$, and $m \ge 2$. Then

(i) $GQ(\Upsilon) = \frac{nm\sqrt{2nm}}{\sqrt{n^2+m^2}}$,

(ii) $QG(\Upsilon) = \frac{1}{\sqrt{2}}\sqrt{nm(n^2+m^2)}$.

Proof. Let $M(\Upsilon; x, y) = nm\, x^n y^m$ be the M-polynomial of a complete bipartite graph $K_{n,m}$ as mentioned in Theorem 3. Then

(i) **Geometric-Quadratic Index of $\Upsilon = K_{n,m}$**

$$\begin{aligned}
GQ(\Upsilon) &= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2}\, [M(\Upsilon; x, y)]|_{x=1} \\
&= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2}\, (nm\, x^n y^m)|_{x=1} \\
&= \sqrt{2} nm\, S_x^{1/2} J\, P_y\, P_x(\sqrt{nm}\, x^n y^m)|_{x=1} \\
&= nm\sqrt{2nm}\, S_x^{1/2} J\left(x^{n^2} y^{m^2}\right)|_{x=1} \\
&= nm\sqrt{2nm}\, S_x^{1/2}\left(x^{n^2+m^2}\right)|_{x=1} \\
&= \frac{nm\sqrt{2nm}}{\sqrt{n^2+m^2}}\left(x^{n^2+m^2}\right)|_{x=1} \\
&= \frac{nm\sqrt{2nm}}{\sqrt{n^2+m^2}}.
\end{aligned}$$

(ii) **Quadratic-Geometric Index of $\Upsilon = K_{n,m}$**

$$\begin{aligned}
QG(\Upsilon) &= \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]|_{x=1} \\
&= \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} (nm\, x^n y^m)|_{x=1} \\
&= \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x \left(\frac{nm}{\sqrt{nm}}\, x^n y^m\right)|_{x=1} \\
&= \frac{\sqrt{nm}}{\sqrt{2}}\, D_x^{1/2}\, J\left(x^{n^2} y^{m^2}\right)|_{x=1} \\
&= \frac{\sqrt{nm}}{\sqrt{2}}\, D_x^{1/2}\left(x^{n^2+m^2}\right)|_{x=1} \\
&= \frac{\sqrt{nm(n^2+m^2)}}{\sqrt{2}}\left(x^{n^2+m^2}\right)|_{x=1} \\
&= \frac{1}{\sqrt{2}}\sqrt{nm(n^2+m^2)}.
\end{aligned}$$
■

The following corollaries follow immediately from the above two theorems.

Corollary 5. Let Υ be a complete bipartite graph $K_{s,s}$ with $s \ge 2$. Then the M-polynomial of Υ is $M(\Upsilon; x, y) = s^2 x^s y^s$.

Corollary 6. If Υ be a complete bipartite graph $K_{s,s}$ with $s \ge 2$. Then

(i) $GQ(\Upsilon) = s^2$,

(ii) $QG(\Upsilon) = s^2$.

Remark 7. If Υ be a complete bipartite graph $K_{s,s}$ with $s \geq 2$. Then

$$GQ(\Upsilon) = QG(\Upsilon) = s^2.$$

Corollary 8. [3] Let Υ be a star graph $K_{1,s-1}$ with $s \geq 2$. Then the M-polynomial of Υ is $M(\Upsilon; x, y) = (s-1)\, x^1 y^{s-1}$.

Corollary 9. If Υ be a star graph $K_{1,s-1}$ with $s \geq 2$. Then

(i) $GQ(\Upsilon) = \frac{(s-1)\sqrt{2(s-1)}}{\sqrt{(s^2-2s+2)}}$,

(ii) $QG(\Upsilon) = \frac{1}{\sqrt{2}}\sqrt{(s-1)(s^2-2s+2)}$.

Theorem 10. [2] Let Υ be a k-regular graph with n vertices and $k \geq 2$. Then the M-polynomial of Υ is given by $M(\Upsilon; x, y) = \frac{nk}{2} x^k y^k$.

Theorem 11. If Υ be a k-regular graph with n vertices and $k \geq 2$. Then

(i) $GQ(\Upsilon) = \frac{nk}{2}$,

(ii) $QG(\Upsilon) = \frac{nk}{2}$.

Proof. Let $M(\Upsilon; x, y) = \frac{nk}{2} x^k y^k$ be the M-polynomial of a k-regular graph as given in Theorem 10. Then

(i) **Geometric-Quadratic Index of Υ = k-regular graph**

$$\begin{aligned} GQ(\Upsilon) &= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2}\, [M(\Upsilon; x, y)]|_{x=1} \\ &= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2} \left(\frac{nk}{2} x^k y^k\right)|_{x=1} \\ &= \frac{nk}{\sqrt{2}}\, S_x^{1/2} J\, P_y\, P_x (k\, x^k y^k)|_{x=1} \\ &= \frac{nk^2}{\sqrt{2}}\, S_x^{1/2} J\, \left(x^{k^2} y^{k^2}\right)|_{x=1} \\ &= \frac{nk^2}{\sqrt{2}}\, S_x^{1/2} \left(x^{2k^2}\right)|_{x=1} \\ &= \frac{nk^2}{\sqrt{2}} \frac{1}{\sqrt{2k^2}} \left(x^{k^2}\right)|_{x=1} \\ &= \frac{nk}{2}. \end{aligned}$$

(ii) **Quadratic-Geometric Index of Υ = k-regular graph**

$$QG(\Upsilon) = \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]|_{x=1}$$

$$= \frac{1}{\sqrt{2}} D_x^{1/2} J P_y P_x S_y^{1/2} S_x^{1/2} \left(\frac{nk}{2} x^k y^k\right)|_{x=1}$$
$$= \frac{nk}{2\sqrt{2}} D_x^{1/2} J P_y P_x \left(\frac{1}{k} x^k y^k\right)|_{x=1}$$
$$= \frac{n}{2\sqrt{2}} D_x^{1/2} J \left(x^{k^2} y^{k^2}\right)|_{x=1}$$
$$= \frac{n}{2\sqrt{2}} D_x^{1/2} \left(x^{2k^2}\right)|_{x=1}$$
$$= \frac{n}{2\sqrt{2}} \sqrt{2k^2} \left(x^{2k^2}\right)|_{x=1}$$
$$= \frac{nk}{2}. \qquad \blacksquare$$

Some immediate corollaries of the above two theorems are given below.

Corollary 12. [3] Let Υ be a cycle C_n with $n \geq 3$ vertices, which is a 2-regular graph. Then the M-polynomial of Υ is $M(\Upsilon; x, y) = n\, x^2 y^2$.

Corollary 13. If Υ be a cycle C_n with $n \geq 3$ vertices. Then
(i) $GQ(\Upsilon) = n$,
(ii) $QG(\Upsilon) = n$.

Corollary 14. [3] Let Υ be a complete graph K_n with $n \geq 3$ vertices, which is a $(n-1)$-regular graph. Then the M-polynomial of Υ is $M(\Upsilon; x, y) = \frac{n(n-1)}{2} x^{n-1} y^{n-1}$.

Corollary 15. If Υ be a complete graph K_n with $n \geq 3$ vertices. Then
(i) $GQ(\Upsilon) = \frac{n(n-1)}{2}$,
(ii) $QG(\Upsilon) = \frac{n(n-1)}{2}$.

Theorem 16. [3] Let Υ be a path P_n with $n \geq 3$ vertices. Then the M-polynomial of Υ is given by $M(\Upsilon; x, y) = 2\, x^1 y^2 + (n-3)\, x^2 y^2$.

Theorem 17. If Υ be a path P_n with $n \geq 3$ vertices. Then
(i) $GQ(\Upsilon) = n - 3 + \frac{4}{\sqrt{5}}$,
(ii) $QG(\Upsilon) = n - 3 + \sqrt{5}$.

Proof. Let $M(\Upsilon; x, y) = 2x^1 y^2 + (n-3)x^2 y^2$ be the expression of the M-polynomial of a path P_n as mentioned in Theorem 16. Then

(i) **Geometric-Quadratic Index of $\boldsymbol{\Upsilon = P_n}$**

$$GQ(\Upsilon) = \sqrt{2}\, S_x^{1/2} J P_y P_x D_y^{1/2} D_x^{1/2} [M(\Upsilon; x, y)]|_{x=1}$$

$$= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2}\, D_x^{1/2}\, (2\, x^1 y^2 + (n-3)\, x^2 y^2)|_{x=1}$$
$$= \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x \big(2\sqrt{2}\, x^1 y^2 + 2(n-3)\, x^2 y^2\big)|_{x=1}$$
$$= \sqrt{2}\, S_x^{1/2} J\, \big(2\sqrt{2}\, x^1 y^4 + 2(n-3)\, x^4 y^4\big)|_{x=1}$$
$$= \sqrt{2}\, S_x^{1/2}\, \big(2\sqrt{2}\, x^5 + 2(n-3)\, x^8\big)|_{x=1}$$
$$= \sqrt{2}\left(\tfrac{2\sqrt{2}}{\sqrt{5}}\, x^5 + \tfrac{2(n-3)}{\sqrt{8}}\, x^8\right)|_{x=1}$$
$$= n - 3 + \tfrac{4}{\sqrt{5}}.$$

(ii) **Quadratic-Geometric Index of $\boldsymbol{\Upsilon = P_n}$**

$$QG(\Upsilon) = \tfrac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]|_{x=1}$$
$$= \tfrac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} (2\, x^1 y^2 + (n-3)\, x^2 y^2)|_{x=1}$$
$$= \tfrac{1}{\sqrt{2}}\, D_x^{1/2} J\, P_y\, P_x \left(\sqrt{2}\, x^1 y^2 + \tfrac{(n-3)}{2}\, x^2 y^2\right)|_{x=1}$$
$$= \tfrac{1}{\sqrt{2}}\, D_x^{1/2} J\, \left(\sqrt{2}\, x^1 y^4 + \tfrac{(n-3)}{2}\, x^4 y^4\right)|_{x=1}$$
$$= \tfrac{1}{\sqrt{2}}\, D_x^{1/2}\, \left(\sqrt{2}\, x^5 + \tfrac{(n-3)}{2}\, x^8\right)|_{x=1}$$
$$= \tfrac{1}{\sqrt{2}}\left(\sqrt{10}\, x^5 + \tfrac{(n-3)\sqrt{8}}{2}\, x^8\right)|_{x=1}$$
$$= n - 3 + \sqrt{5}. \qquad \blacksquare$$

Remark 18. One can observe that the M-polynomial based closed derivation formulas (as proposed in Theorems 1 and 2) for calculating the GQ and QG indices of complete bipartite graph, star graph, *k*-regular graph, cycle graph, complete graph and path are producing the same results as determined in [14].

4. GQ AND QG INDICES OF JAGGED–RECTANGLE BENZENOID SYSTEM $\boldsymbol{B_{m,n}}$

The molecular structure of the jagged-rectangular benzenoid system $B_{m,n}$, where $m \in \mathbb{N}\backslash\{1\}$ and $n \in \mathbb{N}$ is shown in Figure 1. One can see that the degree of any vertex of $B_{m,n}$ is either 2 or 3. Also, note that the total number of vertices and edges of $B_{m,n}$ are $4mn + 4m + 2n - 2$ and $6mn + 5m + n - 4$, respectively.

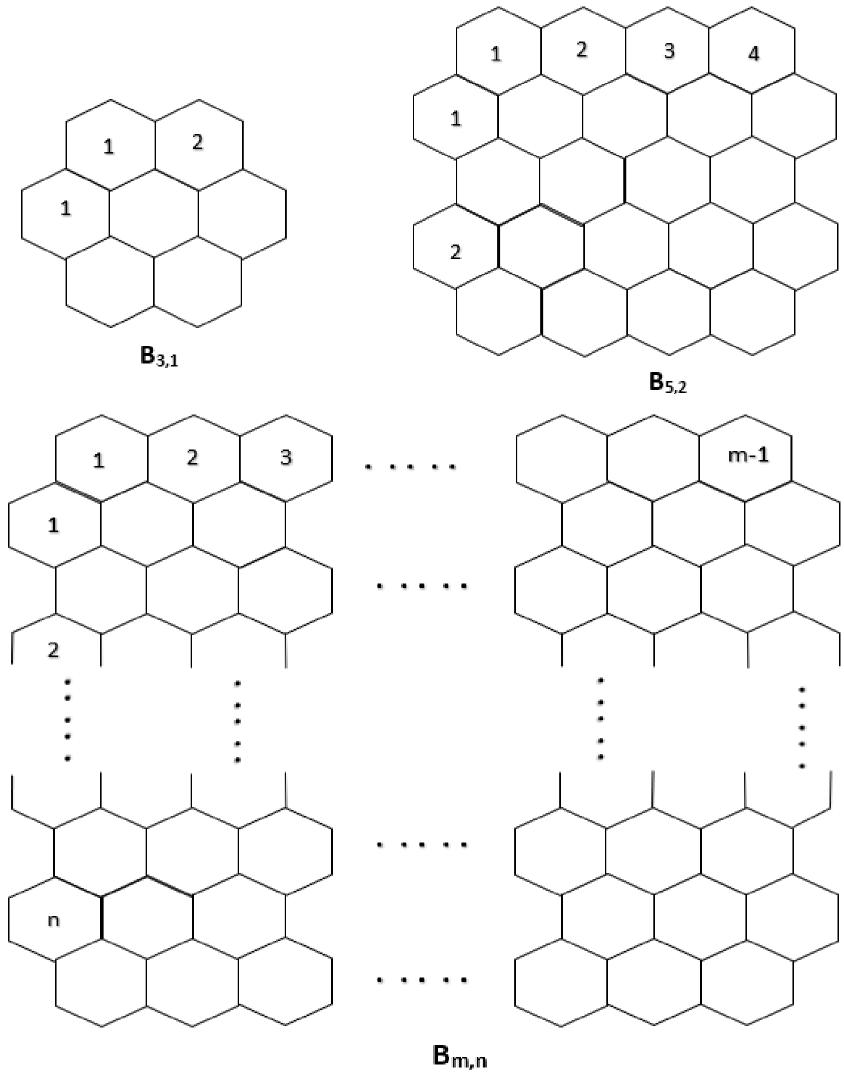


Figure 1. Molecular structure of the jagged-rectangular benzenoid system $B_{m,n}$.

Theorem 19. [21] Let us consider Υ be the family of jagged-rectangle benzenoid system $B_{m,n}$ with $m \in \mathbb{N}\backslash\{1\}$ and $n \in \mathbb{N}$. Then,

$$M(\Upsilon; x, y) = (2n+4)x^2y^2 + (4m+4n-4)x^2y^3 + (6mn+m-5n-4)x^3y^3.$$

We now utilize Theorems 1, 2, and 19 to determine the geometric-quadratic and quadratic-geometric indices of $B_{m,n}$.

Theorem 20. Let Υ be the jagged-rectangle benzenoid system $B_{m,n}$ with $m \in \mathbb{N}\backslash\{1\}$ and $n \in \mathbb{N}$. Then its GQ and QG indices are given by

(i) $GQ(\Upsilon) = 6mn + \left(1 + \frac{8\sqrt{3}}{\sqrt{13}}\right)m + \left(\frac{8\sqrt{3}}{\sqrt{13}} - 3\right)n - \frac{8\sqrt{3}}{\sqrt{13}},$

(ii) $QG(\Upsilon) = 6mn + \left(1 + \frac{2\sqrt{13}}{\sqrt{3}}\right)m + \left(\frac{2\sqrt{13}}{\sqrt{3}} - 3\right)n - \frac{2\sqrt{13}}{\sqrt{3}}$.

Proof. We know that the M-polynomial of $B_{m,n}$ is

$$M(\Upsilon; x, y) = (2n+4)x^2y^2 + (4m+4n-4)x^2y^3 + (6mn+m-5n-4)x^3y^3.$$

as given in Theorem 19. Then

- $S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}\, [M(\Upsilon; x, y)]$

$$= S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}\, [(2n+4)x^2y^2 + (4m+4n-4)x^2y^3 + (6mn+m-5n-4)x^3y^3]$$

$$= S_x^{1/2} J\, P_y\, P_x \big[2(2n+4)x^2y^2 + \sqrt{6}(4m+4n-4)x^2y^3 + 3(6mn+m-5n-4)x^3y^3\big]$$

$$= S_x^{1/2} J\, [2(2n+4)x^4y^4 + \sqrt{6}(4m+4n-4)x^4y^9 + 3(6mn+m-5n-4)x^9y^9]$$

$$= S_x^{1/2}\, [2(2n+4)x^8 + \sqrt{6}(4m+4n-4)x^{13} + 3(6mn+m-5n-4)x^{18}]$$

$$= \frac{2}{\sqrt{8}}(2n+4)x^8 + \frac{\sqrt{6}}{\sqrt{13}}(4m+4n-4)x^{13} + \frac{3}{\sqrt{18}}(6mn+m-5n-4)x^{18}.$$

- $D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]$

$$= D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [(2n+4)x^2y^2 + (4m+4n-4)x^2y^3 + (6mn+m-5n-4)x^3y^3]$$

$$= D_x^{1/2}\, J\, P_y P_x [\tfrac{1}{2}(2n+4)x^2y^2 + \tfrac{1}{\sqrt{6}}(4m+4n-4)x^2y^3 + \tfrac{1}{3}(6mn+m-5n-4)x^3y^3]$$

$$= D_x^{1/2}\, J\, [\tfrac{1}{2}(2n+4)x^4y^4 + \tfrac{1}{\sqrt{6}}(4m+4n-4)x^4y^9 + \tfrac{1}{3}(6mn+m-5n-4)x^9y^9]$$

$$= D_x^{1/2}\, [\tfrac{1}{2}(2n+4)x^8 + \tfrac{1}{\sqrt{6}}(4m+4n-4)x^{13} + \tfrac{1}{3}(6mn+m-5n-4)x^{18}]$$

$$= \frac{\sqrt{8}}{2}(2n+4)x^8 + \frac{\sqrt{13}}{\sqrt{6}}(4m+4n-4)x^{13} + \frac{\sqrt{18}}{3}(6mn+m-5n-4)x^{18}.$$

Therefore, from Theorems 1 and 2, we have

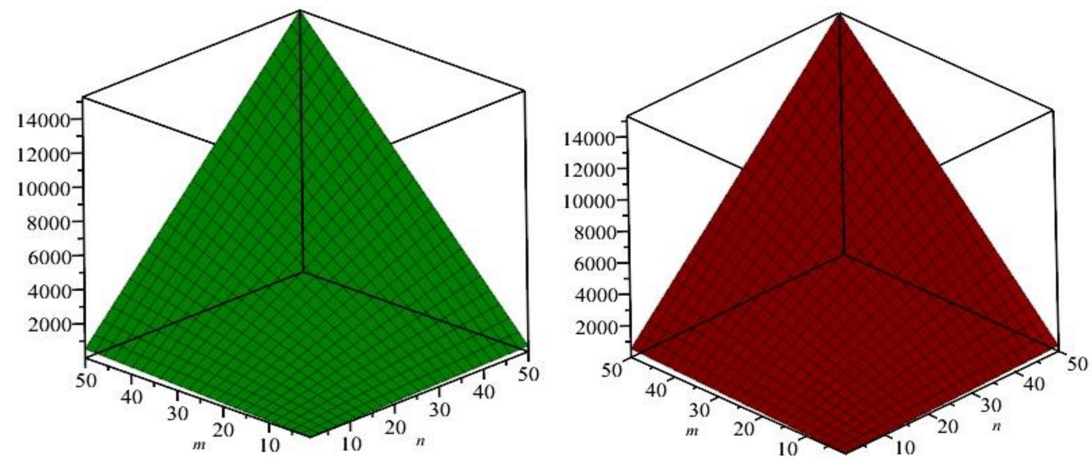
(i) $GQ(\Upsilon) = \sqrt{2}\, S_x^{1/2} J\, P_y\, P_x\, D_y^{1/2} D_x^{1/2}\, [M(\Upsilon; x, y)]|_{x=1}$

$$= 6mn + \left(1 + \frac{8\sqrt{3}}{\sqrt{13}}\right)m + \left(\frac{8\sqrt{3}}{\sqrt{13}} - 3\right)n - \frac{8\sqrt{3}}{\sqrt{13}},$$

(ii) $QG(\Upsilon) = \frac{1}{\sqrt{2}}\, D_x^{1/2}\, J\, P_y P_x S_y^{1/2} S_x^{1/2} [M(\Upsilon; x, y)]|_{x=1}$

$$= 6mn + \left(1 + \frac{2\sqrt{13}}{\sqrt{3}}\right)m + \left(\frac{2\sqrt{13}}{\sqrt{3}} - 3\right)n - \frac{2\sqrt{13}}{\sqrt{3}}$$

Next, we present the numerical computation of GQ and QG indices of $B_{m,n}$ for different values of m, n and give their graphical interpretations with the help of Maple 2020 software.



(a) $GQ(\Upsilon)$ indices **(b)** $QG(\Upsilon)$ indices

Figure 2. Graphical depiction of GQ and QG indices of $\Upsilon = B_{m,n}$ with $2 \leq m \leq 50$ and $1 \leq n \leq 50$.

Table 1. Numerical computation of GQ and QG indices of $\Upsilon = B_{m,n}$ where $m = n$.

$[m,n]$	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]	[8,8]	[9,9]	[10,10]
$GQ(\Upsilon)$	31.5292	67.2154	114.9015	174.5877	246.2738	329.9599	425.6461	533.3323	653.0184
$QG(\Upsilon)$	32.4899	68.8166	117.1433	177.4699	249.7966	334.1233	430.4499	538.7766	659.1033

Table 2. Numerical computation of GQ and QG indices of $\Upsilon = B_{m,n}$, where $2 \leq m \leq 10$ and $n = 5$.

$[m,n]$	[2,5]	[3,5]	[4,5]	[5,5]	[6,5]	[7,5]	[8,5]	[9,5]	[10,5]
$GQ(\Upsilon)$	70.0584	104.9015	139.7446	174.5877	209.4307	244.2738	279.1169	313.9599	348.8030
$QG(\Upsilon)$	71.9799	107.1433	142.3066	177.4699	212.6333	247.7966	282.9599	318.1233	353.2866

Table 3. Numerical computation of GQ and QG indices of $\Upsilon = B_{m,n}$, where $m = 5$ and $1 \leq n \leq 10$.

$[m,n]$	[5,1]	[5,2]	[5,3]	[5,4]	[5,5]	[5,6]	[5,7]	[5,8]	[5,9]	[5,10]
$GQ(\Upsilon)$	51.2154	82.0584	112.9015	143.7446	174.5877	205.4307	236.2738	267.1169	297.9599	328.8030
$QG(\Upsilon)$	52.8166	83.9799	115.1433	146.3066	177.4699	208.6333	239.7966	270.9599	302.1233	333.2866

Remark 21. From Tables 1, 2, and 3 and Figure 2, one can conclude that the geometric-quadratic and quadratic-geometric indices of $B_{m,n}$ increase with the values of m and n.

Remark 22. Note that the M-polynomial based closed derivation formulas (as given in Theorems 1 and 2) for computing the GQ and QG indices of $B_{m,n}$ are producing the same results as evaluated in [14].

5. RELATION BETWEEN GQ AND QG INDICES

Let us now discuss some relations between GQ and QG indices for a general graph and in particular for $K_{n,m}$, path and jagged-rectangular benzenoid system $B_{m,n}$.

Theorem 23. Let Υ be a simple, connected and undirected graph. Then we have

$$0 < GQ(\Upsilon) \leq QG(\Upsilon)\,.$$

Proof. From the mathematical definitions of GQ and QG indices of a graph Υ, we have

$$\begin{aligned} QG(\Upsilon) - GQ(\Upsilon) &= \sum_{uv\,\in\,E(\Upsilon)} \frac{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}}{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}} - \sum_{uv\,\in\,E(\Upsilon)} \frac{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}}{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}} \\ &= \sum_{uv\,\in\,E(\Upsilon)} \left(\frac{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}}{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}} - \frac{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)}}{\sqrt{d_\Upsilon(u)^2+d_\Upsilon(v)^2}} \right) \\ &= \sum_{uv\,\in\,E(\Upsilon)} \frac{d_\Upsilon(u)^2+d_\Upsilon(v)^2-2d_\Upsilon(u)d_\Upsilon(v)}{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)\{d_\Upsilon(u)^2+d_\Upsilon(v)^2\}}} \\ &= \sum_{uv\,\in\,E(\Upsilon)} \frac{\{d_\Upsilon(u)-d_\Upsilon(v)\}^2}{\sqrt{2d_\Upsilon(u)d_\Upsilon(v)\{d_\Upsilon(u)^2+d_\Upsilon(v)^2\}}}. \end{aligned}$$

Since, for every pair of vertices $u, v \in V(\Upsilon)$

$$\{d_\Upsilon(u) - d_\Upsilon(v)\}^2 \geq 0 \text{ and } \sqrt{2d_\Upsilon(u)d_\Upsilon(v)\{d_\Upsilon(u)^2 + d_\Upsilon(v)^2\}} > 0\,.$$

Therefore,

$$QG(\Upsilon) - GQ(\Upsilon) \geq 0$$
$$\Rightarrow\; QG(\Upsilon) \geq GQ(\Upsilon)\,.$$

Also, from the definition of GQ index, we have $GQ(\Upsilon) > 0$. Hence, $0 < GQ(\Upsilon) \leq QG(\Upsilon)$. ∎

Theorem 24. Let Υ be a complete bipartite graph $K_{n,m}$ with $1 \leq n \leq m$ and $m \geq 2$. Then

$$QG(\Upsilon) - GQ(\Upsilon) = \frac{\sqrt{nm}(n-m)^2}{\sqrt{2(n^2+m^2)}}\,.$$

Proof. From Theorem 4, we have

$$QG(\Upsilon) - GQ(\Upsilon) = \frac{1}{\sqrt{2}}\sqrt{nm(n^2+m^2)} - \frac{nm\sqrt{2nm}}{\sqrt{(n^2+m^2)}}$$

$$= \frac{\sqrt{nm}(n^2+m^2)-2nm\sqrt{nm}}{\sqrt{2(n^2+m^2)}}$$
$$= \frac{\sqrt{nm}(n-m)^2}{\sqrt{2(n^2+m^2)}}. \qquad \blacksquare$$

Theorem 25. Let Υ be a path P_n with $n \geq 3$ vertices. Then $QG(\Upsilon) - GQ(\Upsilon) = \frac{1}{\sqrt{5}}$, which is a constant.

Proof. From Theorem 17, we have $QG(\Upsilon) - GQ(\Upsilon) = \left(n - 3 + \sqrt{5}\right) - \left(n - 3 + \frac{4}{\sqrt{5}}\right) = \frac{1}{\sqrt{5}}$, which is a constant.

Theorem 26. Let Υ be the jagged-rectangle benzenoid system $B_{m,n}$ with $m \in \mathbb{N}\backslash\{1\}$ and $n \in \mathbb{N}$. Then $QG(\Upsilon) - GQ(\Upsilon) = \frac{2}{\sqrt{39}}(m + n - 1)$.

Proof. From Theorem 20, we have

$$\begin{aligned} QG(\Upsilon) - GQ(\Upsilon) &= \left\{6mn + \left(1 + \frac{2\sqrt{13}}{\sqrt{3}}\right)m + \left(\frac{2\sqrt{13}}{\sqrt{3}} - 3\right)n - \frac{2\sqrt{13}}{\sqrt{3}}\right\} \\ &\quad - \left\{6mn + \left(1 + \frac{8\sqrt{3}}{\sqrt{13}}\right)m + \left(\frac{8\sqrt{3}}{\sqrt{13}} - 3\right)n - \frac{8\sqrt{3}}{\sqrt{13}}\right\} \\ &= m\left(\frac{2\sqrt{13}}{\sqrt{3}} - \frac{8\sqrt{3}}{\sqrt{13}}\right) + n\left(\frac{2\sqrt{13}}{\sqrt{3}} - \frac{8\sqrt{3}}{\sqrt{13}}\right) - \left(\frac{2\sqrt{13}}{\sqrt{3}} - \frac{8\sqrt{3}}{\sqrt{13}}\right) \\ &= \left(\frac{2\sqrt{13}}{\sqrt{3}} - \frac{8\sqrt{3}}{\sqrt{13}}\right)(m + n - 1) \\ &= \frac{2}{\sqrt{39}}(m + n - 1). \qquad \blacksquare \end{aligned}$$

6. CONCLUSION

In this present study, we have come up with two closed derivation formulas to evaluate the geometric-quadratic and quadratic-geometric indices of a graph with the help of its M-polynomial, which can be helpful in investigating the GQ and QG indices of various chemical structures. Furthermore, we have calculated the indices of some standard graphs and the jagged-rectangular benzenoid system by using proposed derivation formulas. Note that the values of the GQ and QG indices of all our considered graphs derived from their respective M-polynomials produced the identical values as computed by V.R. Kulli in [14]. Also, we have proposed some key relationships, in general, between the indices of the graphs. The results obtained may be helpful to describe the structural characteristics of the standard graphs as well as jagged-rectangular benzenoid system $B_{m,n}$.

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