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Research Paper

A Note on the General Gutman Index of Graphs

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Abstract

The general Gutman index, denoted by $G_{a,b}(H)$, is a prominent distance–degree-based topological index in chemical graph theory, defined using a combination of vertex degrees and inter-vertex distances. In this paper, we focus on bicyclic graphs as a special class of graphs and investigate the behavior of this index within that setting. In particular, we examine the case $G_{2,1}(H)$. The primary objective of this study is to establish a sharp upper bound for the general Gutman index in bicyclic graphs. By exploiting the structural properties of bicyclic graphs and employing combinatorial techniques, we derive a sharp upper bound for this index. The results obtained may provide a useful foundation for further research on distance-degree-based indices and their structural implications in mathematical chemistry.

1 Introduction

Chemical graph theory is a significant branch of applied mathematics that establishes a strong link between graph theory and mathematical chemistry. In this field, molecular structures are represented using graphs. Within this framework, topological indices play a central role in characterizing and predicting molecular properties. Among these indices, the Gutman index, which is defined as a combination of vertex degrees and inter-vertex distances, has received considerable attention. Its extension, the general Gutman index, has been extensively investigated because it captures the interplay between structural characteristics and the distance-based properties of graphs.

In recent years, researchers have devoted considerable attention to distance–degree-based indices in various classes of graphs. Within these classes, bicyclic graphs are of particular interest, since they not only possess rich structural properties but also serve as useful models

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for certain chemical compounds. Investigating the behavior of the general Gutman index in bicyclic graphs provides deeper insights into the relationship between structural characteristics and topological indices.

The main objective of this paper is to investigate the general Gutman index in bicyclic graphs for the specific parameter choice ($a = 2, b = 1$) and to establish a sharp upper bound for this index. To this end, we make use of the structural properties of bicyclic graphs along with combinatorial techniques. The results obtained not only yield an exact upper bound for the index but also provide a basis for further investigations of distance-degree-based indices in more complex classes of graphs.

A simple graph (A graph that contains no loops and has at most one edge between any two distinct vertices) H is an ordered pair $H = (V(H), E(H))$, where $V(H)$ denotes the set of vertices and $E(H)$ denotes the set of edges of H. Throughout this paper, all graphs are assumed to be simple. A simple graph in which each pair of distinct vertices is connected by an edge is called a *complete graph*. It is denoted by K_n, where n is the number of vertices.

A *bipartite graph* is a graph whose vertex set can be partitioned into two nonempty subsets V_1 and V_2 such that every edge connects a vertex in V_1 to a vertex in V_2. Equivalently, no edge exists between two vertices belonging to the same subset. The subsets V_1 and V_2 are called the parts of the graph.

A sequence of distinct vertices $v_1, v_2, \ldots, v_{n+1}$ of a simple graph H is called a *path* if, for every $i = 1, 2, \ldots, n$, the vertices v_i and v_{i+1} are adjacent in H. In this case, the length of the path is defined as n, and a path of length n is usually denoted by P_n. A graph H is said to be *connected* if there exists at least one path between every pair of distinct vertices in H; otherwise, the graph is called *disconnected*. A *cycle* is a closed path with at least three vertices. A *tree* is a connected graph with no cycles. A *unicyclic graph* is a connected graph with exactly one cycle, and a *bicyclic graph* is a connected graph containing exactly two cycles. The *distance* $d(u, v)$ between two vertices is the length of the shortest path between them. A graph is *complete* if every pair of distinct vertices is adjacent.

A *pendant vertex* (or *leaf*) is a vertex of degree one. The *open neighborhood* $N(v)$ of a vertex v is the set of all vertices adjacent to v. The *degree* $d(v)$ is the number of edges incident to vertex v.

In 2010, Feng and Liu introduced the Gutman index for connected simple graphs. In [1], they investigated this index and proved that, among all bicyclic graphs of order n, the bicyclic graph consisting of two triangles connected by a path attains the maximum Gutman index. Let $B(n)$ denote the set of all bicyclic graphs of order n. We classify these graphs into three distinct topological categories according to the arrangement of their two cycles. Specifically, for any graph $G \in B(n)$ with cycles C_p and C_q, the classification is given as follows:

Case 1: $A(p, q)$ denotes the set of graphs $G \in B(n)$ in which the cycles C_p and C_q share exactly one common vertex.

Case 2: $B(p, q)$ denotes the set of graphs $G \in B(n)$ in which the cycles C_p and C_q are vertex-disjoint.

Case 3: $C(p, q, l)$ denotes the set of graphs $G \in B(n)$ in which the cycles C_p and C_q share a common path of length l.

In 2022, the authors of [2, 3] introduced the general Gutman index as:

$$Gut_{a,b}(H) = \sum_{\{u,v\} \subseteq V(H)} [d_H(u) d_H(v)]^a [D_H(u, v)]^b.$$

They further investigated how this index is affected by the addition of an edge, establishing conditions on the parameters a and b under which the index either increases or decreases.

In this paper, we focus on the case $a = 2$ and $b = 1$, and investigate the behavior of the general Gutman index under these specific parameter values. For comparison, we also recall several related graph indices [4–8]:

- Wiener index: $W(H) = \sum_{\{u,v\}\subseteq V(H)} d(u, v)$,
- first Zagreb index: $M_1(H) = \sum_{v\in V(H)} \deg(v)^2$,
- second Zagreb index: $M_2(H) = \sum_{uv\in E(H)} \deg(u) \cdot \deg(v)$.

2 Main results

In this section, we examine the general Gutman index for different values of a and b and present the corresponding results.

Lemma 2.1. *Let H be a simple connected graph. For the general Gutman index with $a = b = \frac{1}{3}$, we have*

$$G_{\frac{1}{3},\frac{1}{3}}(H) \leq \frac{1}{3}M_1(H) + \frac{1}{3}W(H),$$

where $M_1(H)$ is the first Zagreb index, and $W(H)$ is the Wiener index, with equality if and only if H is K_2.

Proof. For any pair of vertices $u, v \in V(H)$, we have

$$\begin{aligned}(d(u)d(v))^{\frac{1}{3}}\, d(u,v)^{\frac{1}{3}} &= \big(d(u)d(v)d(u,v)\big)^{\frac{1}{3}} \\ &\leq \frac{1}{3}\big(d(u) + d(v) + d(u,v)\big) \\ &= \frac{1}{3}(d(u) + d(v)) + \frac{1}{3}d(u,v).\end{aligned}$$

Summing over all pairs of vertices in H, we obtain:

$$\begin{aligned}G_{\frac{1}{3},\frac{1}{3}}(H) &= \sum_{u,v\in V(H)} (d(u)d(v))^{\frac{1}{3}} d(u,v)^{\frac{1}{3}} \\ &\leq \frac{1}{3}\sum_{u,v\in V(H)} (d(u) + d(v)) + \frac{1}{3}\sum_{u,v\in V(H)} d(u,v) \\ &= \frac{1}{3}M_1(H) + \frac{1}{3}W(H).\end{aligned}$$

■

In a bigraph with independence number α, we establish a lower bound for the general Gutman index.

Lemma 2.2. *Let H be a bigraph with independence number α and $|V(H)| = n$. Then*

$$G_{a,b}(H) \;\geq\; 2^b \sum_{\{u,v\}\subseteq X} (d(u)d(v))^a \;+\; M_2(H),$$

where X denotes the independent set of size α, and $M_2(H)$ is the second Zagreb index.

Proof. Let X be the independent set in H with $|X| = \alpha$. For vertex pairs $\{u, v\} \subseteq X$, we have $d(u, v) \geq 2$. For the remaining pairs $\{u, v\} \not\subseteq X$, we have $d(u, v) \geq 1$.
Thus,

$$\begin{aligned}
G_{a,b}(H) &= \sum_{\{u,v\}\subseteq V(H)} (d(u)d(v))^a\, d(u,v)^b \\
&= \sum_{\{u,v\}\subseteq X} (d(u)d(v))^a d(u,v)^b + \sum_{\{u,v\}\not\subseteq X} (d(u)d(v))^a d(u,v)^b \\
&\geq \sum_{\{u,v\}\subseteq X} (d(u)d(v))^a \cdot 2^b + \sum_{\{u,v\}\not\subseteq X} (d(u)d(v))^a \cdot 1^b \\
&= 2^b \sum_{\{u,v\}\subseteq X} (d(u)d(v))^a + M_2(H).
\end{aligned}$$

■

Lemma 2.3. *Let H be a graph. Then,*

$$\left|G_{\frac{1}{4},\frac{1}{2}}(H)\right| \leq \sqrt{\tfrac{1}{2}\, M_1(H)\, W(H)},$$

where $M_1(H)$ is the first Zagreb index and $W(H)$ is the Wiener index.

Proof. By the definition of the general Gutman index and using the Cauchy–Schwarz and AM–GM inequalities, we obtain:

$$\begin{aligned}
\left(G_{\frac{1}{4},\frac{1}{2}}(H)\right)^2 &= \left(\sum_{u,v\in V(H)} (d(u)d(v))^{\frac{1}{4}} d(u,v)^{\frac{1}{2}}\right)^2 \\
&\leq \left(\sum_{u,v\in V(H)} (d(u)d(v))^{\frac{1}{2}}\right)\left(\sum_{u,v\in V(H)} d(u,v)\right) \\
&\leq \left(\sum_{u,v\in V(H)} \frac{d(u)+d(v)}{2}\right)\left(\sum_{u,v\in V(H)} d(u,v)\right) \\
&= \tfrac{1}{2}\, M_1(H)\, W(H).
\end{aligned}$$

Taking square roots on both sides yields:

$$\left|G_{\frac{1}{4},\frac{1}{2}}(H)\right| \leq \sqrt{\tfrac{1}{2}\, M_1(H)\, W(H)}.$$

■

Corollary 2.4. *In Lemma 2.3, equality holds if the graph H is complete.*

Proof. From the Cauchy–Schwarz inequality, we have:

$$\left(\sum (d(u)d(v))^{\frac{1}{4}} d(u,v)^{\frac{1}{2}}\right)^2 \leq \left(\sum (d(u)d(v))^{\frac{1}{2}}\right)\left(\sum d(u,v)\right).$$

Equality occurs if and only if, for some constant $k > 0$,

$$(d(u)d(v))^{\frac{1}{4}} = k\, d(u,v)^{\frac{1}{2}} \qquad \text{for all } u, v \in V(H).$$

Similarly, from the AM–GM inequality we used in Lemma 2.3,

$$\sum (d(u)d(v))^{\frac{1}{2}} \;\le\; \tfrac{1}{2} \sum (d(u) + d(v)),$$

with equality if and only if $d(u) = d(v)$ for all $u, v \in V(H)$. Hence, all vertices have the same degree, say $\deg(u) = k'$ for some constant k'.

Now, from the first equality condition we obtain $(d(u))^{\frac{1}{2}} = k\, d(u,v)^{\frac{1}{2}}$ so, $d(u) = k'\, d(u,v)$.

Since there always exist adjacent vertices u, v with $d(u,v) = 1$, it follows that $d(u) = k'$. Thus, every vertex has the same degree k', which implies that the graph H is complete. ■

Theorem 2.5. *Let H be a semi-regular bipartite graph consisting of two parts H_1 and H_2 such that $d(x) = h$ for all $x \in V(H_1)$, and $d(x) = k$ for all $x \in V(H_2)$. Then,*

$$G_{a,b}(H) = (hk)^a\, W_b(H),$$

where

$$W_b(H) = \sum_{r,s \in V(H)} d(r,s)^b.$$

Proof. By definition of the general Gutman index, we have:

$$G_{a,b}(H) = \sum_{r,s \in V(H)} (d(r)d(s))^a\, d(r,s)^b.$$

Since H is semi-regular, for any $r \in V(H_1)$ and $s \in V(H_2)$, we have $d(r) = h$ and $d(s) = k$. Hence,

$$(d(r)d(s))^a = (hk)^a.$$

Therefore,

$$G_{a,b}(H) = (hk)^a \sum_{r,s \in V(H)} d(r,s)^b = (hk)^a\, W_b(H).$$

■

Let H be a graph. For each vertex $v \in V(H)$, we define

$$B^*_{a,b}(v) \;=\; \sum_{r \in V(H)} d(r)^a\, d(r,v)^b, \tag{1}$$

where $d(r)$ denotes the degree of vertex r and $d(r,v)$ denotes the distance between vertices r and v.

Lemma 2.6. *In the cycle graph C_k, for every $v \in V(C_k)$, we have:*

$$B^*_{2,1}(v) \;=\; \begin{cases} 4n^2, & k = 2n, \\ 4n^2 - 4n, & k = 2n-1. \end{cases} \;=\; \begin{cases} k^2, & k = 2n, \\ k^2 - 1, & k = 2n-1. \end{cases}$$

Proof. Since $\deg(v) = 2$ for every $v \in V(C_k)$, we compute $B^*_{2,1}(v)$ in the following two cases:
Case 1: $k = 2n$**:**

$$\begin{aligned} B^*_{2,1}(v) &= 4 \sum_{x \in V(C_k)} d(x,v) \\ &= 4\big([1 + 2 + \cdots + (n-1)] \times 2 + n\big) \\ &= 8 \cdot \frac{n(n-1)}{2} + 4n = 4n^2. \end{aligned}$$

Case 2: $k = 2n - 1$**:**

$$\begin{aligned} B^*_{2,1}(v) &= 4 \sum_{x \in V(C_k)} d(x,v) \\ &= 4[1 + 2 + \cdots + (n-1)] + 4[1 + 2 + \cdots + (n-2)] + 4(n-1) \\ &= 4 \cdot \frac{(n-1)n}{2} + 4 \cdot \frac{(n-2)(n-1)}{2} + 4(n-1) = 4n^2 - 4n. \end{aligned}$$

■

Lemma 2.7. *Let F be the graph consisting of a cycle C_3 and a path of length $k-3$ attached to one of the vertices of C_3 (see Figure 1). For the pendant vertex v of F, we have:*

$$B^*_{2,1}(v) = 2k^2 + 3k - 19.$$

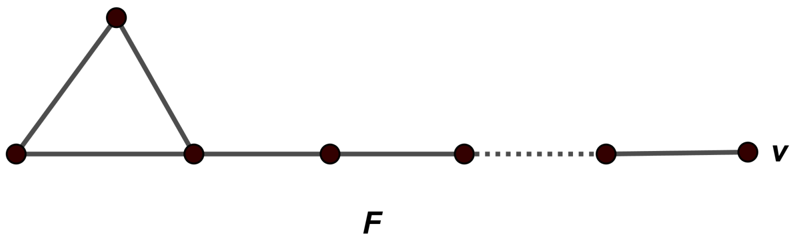

Figure 1: Unicyclic graph F with a path of length $k-3$.

Proof. By (1),

$$\begin{aligned} B^*_{2,1}(v) = 4 \cdot 1 + 4 \cdot 2 + \cdots + 4(k-4) \\ + 9(k-3) + 4(k-2) + 4(k-2). \end{aligned}$$

Therefore,

$$\begin{aligned} B^*_{2,1}(v) &= 2(k-4)(k-3) + (9k-27) + 8(k-2) \\ &= 2k^2 - 14k + 24 + 9k - 27 + 8k - 16 \\ &= 2k^2 + 3k - 19. \end{aligned}$$

■

Theorem 2.8. *Let H be a connected graph with m edges, and let v be a pendant vertex of H whose unique neighbor is w. For $a > 1$ and any $b \geq 0$ we have:*

$$G_{a,b}(H) \;\geq\; G_{a,b}\big(H \setminus \{v\}\big) \;+\; B^*_{a,b}(v_H) \;+\; B^*_{a,b}\big(w_{H\setminus\{v\}}\big) \;+\; \big(d_{H\setminus\{v\}}(w)+1\big)^a.$$

Proof.

$$G_{a,b}(H) = \sum_{r,s\in V(H)} (d_H(r)d_H(s))^a\, d_H(r,s)^b.$$

Partition the sum according to whether v is involved:

$$\begin{aligned} G_{a,b}(H) = & \sum_{r,s\in V(H\setminus\{v,w\})} (d_H(r)d_H(s))^a d_H(r,s)^b \\ & + \sum_{r\in V(H\setminus\{v,w\})} (d_H(r)d_H(w))^a d_H(r,w)^b \\ & + \sum_{r\in V(H\setminus\{v,w\})} (d_H(r)d_H(v))^a d_H(r,v)^b \\ & + (d_H(w)d_H(v))^a d_H(w,v)^b. \end{aligned}$$

Since v is a pendant vertex, we have $d_H(v) = 1$ and $d_H(v,w) = 1$. Moreover, for $r, s \in V(H\setminus\{v\})$ the distances in H and in $H \setminus \{v\}$ coincide, while $d_H(w) = d_{H\setminus\{v\}}(w) + 1$. Therefore, the first large sum equals $G_{a,b}(H \setminus \{v\})$ except that each term involving w in $H \setminus \{v\}$ uses $(d_{H\setminus\{v\}}(w))^a$ instead of $(d_{H\setminus\{v\}}(w) + 1)^a$. To make this precise, add and subtract the quantity

$$\begin{aligned} & \sum_{r\in V(H\setminus\{v\})} \big(d_H(r)(d_H(w)-1)\big)^a d_H(r,w)^b \\ & \quad = \sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a d_{H\setminus\{v\}}(w)^a d_{H\setminus\{v\}}(r,w)^b. \end{aligned}$$

After rearranging the equation above, we obtain:

$$\begin{aligned} G_{a,b}(H) = G_{a,b}(H \setminus \{v\}) & + \sum_{r\in V(H\setminus\{v\})} d_H(r)^a d_H(r,v)^b \\ & + (d_{H\setminus\{v\}}(w) + 1)^a \\ & + \sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a\ \mathbf{\Omega}\ d_{H\setminus\{v\}}(r,w)^b, \end{aligned}$$

where $\mathbf{\Omega} = (d_{H\setminus\{v\}}(w) + 1)^a - d_{H\setminus\{v\}}(w)^a$.
Recognizing the second term as $B^*_{a,b}(v_H)$ and the last sum as a nonnegative multiple of $\sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a d_{H\setminus\{v\}}(r,w)^b$, we obtain:

$$\begin{aligned} G_{a,b}(H) = G_{a,b}(H \setminus \{v\}) + B^*_{a,b}(v_H) & + (d_{H\setminus\{v\}}(w) + 1)^a \\ & + \sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a\ \mathbf{\Omega}\ d_{H\setminus\{v\}}(r,w)^b. \end{aligned}$$

For $a > 1$ the function $x \mapsto x^a$ is strictly increasing and convex, so for every integer $d \geq 0$

$$(d + 1)^a - d^a \geq (0 + 1)^a - 0^a = 1.$$

Hence, $\mathbf{\Omega} = (d_{H\setminus\{v\}}(w) + 1)^a - d_{H\setminus\{v\}}(w)^a \geq 1$, and therefore

$$\sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a\ \mathbf{\Omega}\ d_{H\setminus\{v\}}(r,w)^b \geq \sum_{r\in V(H\setminus\{v\})} d_{H\setminus\{v\}}(r)^a d_{H\setminus\{v\}}(r,w)^b.$$

By (1) the right-hand side is $B^*_{a,b}(w_{H\setminus\{v\}})$. Combining the displayed inequalities yields the claimed bound

$$G_{a,b}(H) \geq G_{a,b}(H \setminus \{v\}) + B^*_{a,b}(v_H) + B^*_{a,b}(w_{H\setminus\{v\}}) + (d_{H\setminus\{v\}}(w) + 1)^a.$$

This completes the proof. ■

Remark 1. In the previous theorem, equality holds when $a = 1$.
Now, we aim to determine the exact value of $G_{a,b}(H)$ for the case $a = 2$. We have:

$$\begin{aligned} G_{2,b}(H) &= G_{2,b}(H \setminus \{v\}) + B^*_{2,b}(v_H) + \big(d_{H\setminus\{v\}}(w) + 1\big)^2 \\ &\quad + \sum_r d^2_{H\setminus\{v\}}(r) \left[\big(d_{H\setminus\{v\}}(w) + 1\big)^2 - d^2_{H\setminus\{v\}}(w)\right] d^b_{H\setminus\{v\}}(r, w). \end{aligned}$$

Simplifying the summation yields:

$$\begin{aligned} &\sum_r d^2_{H\setminus\{v\}}(r) \left[\big(d_{H\setminus\{v\}}(w) + 1\big)^2 - d^2_{H\setminus\{v\}}(w)\right] d^b_{H\setminus\{v\}}(r, w) \\ &\quad = \big(2d_{H\setminus\{v\}}(w) + 1\big) \sum_r d^2_{H\setminus\{v\}}(r) d^b_{H\setminus\{v\}}(r, w). \end{aligned}$$

Therefore, we conclude that

$$\begin{aligned} G_{2,b}(H) = G_{2,b}(H \setminus \{v\}) + B^*_{2,b}(v_H) + \big(d_{H\setminus\{v\}}(w) + 1\big)^2 \\ + \big(2d_{H\setminus\{v\}}(w) + 1\big) B^*_{2,b}(w_{H\setminus\{v\}}). \end{aligned} \tag{2}$$

Next, we will compute the general Gutman index of the graph B_n (Figure 2) for parameters $a = 2$ and $b = 1$.

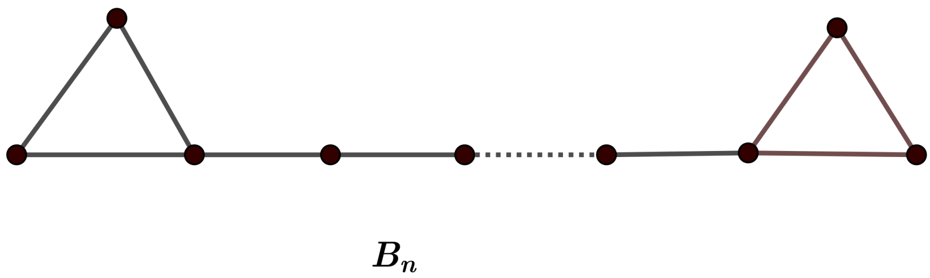

Figure 2: Bicyclic graph B_n of order n.

Lemma 2.9. *For the graph B_n, the following holds:*

$$G_{2,1}(B_n) = \frac{8}{3}n^3 + 20n^2 - \frac{329}{3}n + 99.$$

Proof. Starting from the definition, we have

$$\begin{aligned}
G_{2,1}(B_n) = & 4^2\left[\frac{(n-5)(n-4)}{2}+2n-6\right]+6^2(n-3)\\
&+4^2\left[\frac{(n-5)(n-4)}{2}+2n-7\right]+6^2(n-3)\\
&+6^2\left[\frac{(n-6)(n-5)}{2}+2n-8\right]+9^2(n-5)\\
&+2\times 6^2+4^2\\
&+4^2\left(\frac{1}{6}n^3+\frac{1}{4}n^2+\frac{1}{12}n-70-\frac{13(n+8)(n-7)}{4}+21(n-7)\right)\\
&+4^2\big((n-5)(n-4)-2\big)+6^2\frac{(n-6)(n-5)}{2}.
\end{aligned}$$

Expanding and simplifying terms inside the brackets step-by-step:

$$\begin{aligned}
&4^2\Bigg[n^2-9n+20+4n-13+1+\frac{1}{6}n^3+\frac{1}{4}n^2+\frac{1}{12}n-70\\
&-\frac{13}{4}n^2-\frac{13}{4}n+\frac{13}{4}\times 56+21n-147+n^2-9n+18\Bigg]\\
&+6^2\left[2n-6+\frac{1}{2}n^2-\frac{11}{2}n+15+2n-8+2+\frac{1}{2}n^2-\frac{11}{2}n+15\right]\\
&+9^2(n-5).
\end{aligned}$$

After careful simplification, the expression reduces to

$$G_{2,1}(B_n)=\frac{8}{3}n^3+20n^2-\frac{329}{3}n+99.$$

This completes the proof. ■

Theorem 2.10. *Let H be a connected graph with a cut vertex v, and let H_1 and H_2 be two connected subgraphs of H such that $H_1 \cap H_2 = \{v\}$ and $H_1 \cup H_2 = H$. Then, the general Gutman index of H satisfies:*

$$\begin{aligned}
G_{a,b}(H) =& G_{a,b}(H_1)+G_{a,b}(H_2)\\
&+\sum_{r\in H_1\setminus\{v\}}\left([d_{H_1}(r)d_H(v)]^a-[d_{H_1}(r)d_{H_1}(v)]^a\right)d^b_{H_1}(r,v)\\
&+\sum_{r\in H_2\setminus\{v\}}\left([d_{H_2}(r)d_H(v)]^a-[d_{H_2}(r)d_{H_2}(v)]^a\right)d^b_{H_2}(r,v)\\
&+\sum_{r\in H_1\setminus\{v\} s\in H_2\setminus\{v\}}[d_H(r)d_H(s)]^a d^b_H(r,s).
\end{aligned}$$

Proof. To compute the general Gutman index $G_{a,b}(H)$, we classify the pairs of vertices into the following cases:

1. Both $r, s \in V(H_1)$ with $r, s \neq v$,
2. Both $r, s \in V(H_2)$ with $r, s \neq v$,

3. $r, v \in V(H_1)$,
4. $r, v \in V(H_2)$,
5. $r \in V(H_1)$ and $s \in V(H_2)$.

Thus, we have:

$$\begin{aligned} G_{a,b}(H) = & \sum_{r,s \in H_1 \setminus \{v\}} [d_H(r) d_H(s)]^a d_H^b(r,s) \\ & + \sum_{r,s \in H_2 \setminus \{v\}} [d_H(r) d_H(s)]^a d_H^b(r,s) \\ & + \sum_{r \in H_1 \setminus \{v\}} [d_H(r) d_H(v)]^a d_H^b(r,v) \\ & + \sum_{r \in H_2 \setminus \{v\}} [d_H(r) d_H(v)]^a d_H^b(r,v) \\ & + \sum_{\substack{r \in H_1 \setminus \{v\} \\ s \in H_2 \setminus \{v\}}} [d_H(r) d_H(s)]^a d_H^b(r,s). \end{aligned}$$

Next, we add and subtract the terms $\sum_{r \in H_1 \setminus \{v\}} [d_{H_1}(r) d_{H_1}(v)]^a d_{H_1}^b(r,v)$ and $\sum_{r \in H_2 \setminus \{v\}} [d_{H_2}(r) d_{H_2}(v)]^a d_{H_2}^b(r,v)$.
Rearranging, we get:

$$\begin{aligned} G_{a,b}(H) = & \sum_{r,s \in H_1 \setminus \{v\}} [d_H(r) d_H(s)]^a d_H^b(r,s) + \sum_{r \in H_1 \setminus \{v\}} [d_{H_1}(r) d_{H_1}(v)]^a d_{H_1}^b(r,v) \\ & + \sum_{r,s \in H_2 \setminus \{v\}} [d_H(r) d_H(s)]^a d_H^b(r,s) + \sum_{r \in H_2 \setminus \{v\}} [d_{H_2}(r) d_{H_2}(v)]^a d_{H_2}^b(r,v) \\ & + \sum_{r \in H_1 \setminus \{v\}} \left([d_H(r) d_H(v)]^a - [d_{H_1}(r) d_{H_1}(v)]^a \right) d_{H_1}^b(r,v) \\ & + \sum_{r \in H_2 \setminus \{v\}} \left([d_H(r) d_H(v)]^a - [d_{H_2}(r) d_{H_2}(v)]^a \right) d_{H_2}^b(r,v) \\ & + \sum_{\substack{r \in H_1 \setminus \{v\} \\ s \in H_2 \setminus \{v\}}} [d_H(r) d_H(s)]^a d_H^b(r,s) - \sum_{r \in H_1 \setminus \{v\}} [d_{H_1}(r) d_{H_1}(v)]^a d_{H_1}^b(r,v) \\ & - \sum_{r \in H_2 \setminus \{v\}} [d_{H_2}(r) d_{H_2}(v)]^a d_{H_2}^b(r,v). \end{aligned}$$

Simplifying, this yields:

$$\begin{aligned} G_{a,b}(H) = & G_{a,b}(H_1) + G_{a,b}(H_2) \\ & + \sum_{r \in H_1 \setminus \{v\}} \left([d_{H_1}(r) d_H(v)]^a - [d_{H_1}(r) d_{H_1}(v)]^a \right) d_{H_1}^b(r,v) \\ & + \sum_{r \in H_2 \setminus \{v\}} \left([d_{H_2}(r) d_H(v)]^a - [d_{H_2}(r) d_{H_2}(v)]^a \right) d_{H_2}^b(r,v) \\ & + \sum_{\substack{r \in H_1 \setminus \{v\} \\ s \in H_2 \setminus \{v\}}} [d_H(r) d_H(s)]^a d_H^b(r,s). \end{aligned}$$

Table 1: Values of general Gutman index for small cycles.

Graph C_k	$G_{2,1}(C_k)$
C_4	$G_{2,1}(C_4) = 4(16 \times 1) + 2(16 \times 2)$
C_5	$G_{2,1}(C_5) = 5(16 \times 1 + 16 \times 2)$
C_6	$G_{2,1}(C_6) = 6(16 \times 1 + 16 \times 2) + 3(16 \times 3)$
C_7	$G_{2,1}(C_7) = 7(16 \times 1 + 16 \times 2 + 16 \times 3)$
C_8	$G_{2,1}(C_8) = 8(16 \times 1 + 16 \times 2 + 16 \times 3) + 4(16 \times 4)$

■

Remark 2. In the above theorem, by setting $a = 2$ and $b = 1$, we obtain:

$$\begin{aligned} G_{2,1}(H) =& G_{2,1}(H_1) + G_{2,1}(H_2) + \big(d_H^2(v) - d_{H_1}^2(v)\big) B^*_{2,1}(v_{H_1}) \\ &+ \big(d_H^2(v) - d_{H_2}^2(v)\big) B^*_{2,1}(v_{H_2}) + \sum_{\substack{r \in H_1 \setminus \{v\} \\ s \in H_2 \setminus \{v\}}} d_H^2(r) d_H^2(s) d_H(r,s). \end{aligned}$$

Consider a bicyclic graph H with $|V(H)| = n$ where $n \geq 4$. Our goal is to find an upper bound for $B^*_{2,1}(v_H)$.

Lemma 2.11. *Consider the bicyclic graph H with $|V(H)| = k$ and $k \geqslant 5$. If v is a pendant vertex, then*

1) *If $k = 2n$, then $B^*_{2,1}(v_H) \leqslant k^2 + 7k - 4$.*

2) *If $k = 2n - 1$, then $B^*_{2,1}(v_H) \leqslant k^2 + 7k - 3$.*

If graph H has no pendant vertex, then for some $v_H \in V(H)$ we have:

1) *If $k = 2n$, then $B^*_{2,1}(v_H) \leqslant k^2 + 5k - 10$.*

2) *If $k = 2n - 1$, then $B^*_{2,1}(v_H) \leqslant k^2 + 5k - 11$.*

If graph H has a pendant vertex v and w is the neighbor vertex of v, then

1) *If $k = 2n$, then $B^*_{2,1}(v_H) \leqslant k^2 + 3k - 14$.*

2) *If $k = 2n - 1$, then $B^*_{2,1}(v_H) \leqslant k^2 + 3k - 13$.*

3) *If $k = 2n$, then $B^*_{2,1}(w_{H\setminus\{v\}}) \leqslant k^2 + 5k - 10$.*

4) *If $k = 2n - 1$, then $B^*_{2,1}(w_{H\setminus\{v\}}) \leqslant k^2 + 5k - 11$.*

Next, we obtain the general Guttman index for the graph C_k. According to Table 1, in general, we have:

$$\begin{aligned} G_{2,1}(C_k) &= \begin{cases} 16(2n-1)(1 + 2 + \cdots + (n-1)), & k = 2n - 1, \\ 16(2n)(1 + 2 + \cdots + (n-1)) + 16n^2, & k = 2n. \end{cases} \\ &= \begin{cases} 16n^3 - 24n^2 + 8n, & k = 2n - 1, \\ 16n^3, & k = 2n. \end{cases} \end{aligned}$$

$$= \begin{cases} 2k^3 - 2k, & k = 2n-1, \\ 2k^3, & k = 2n. \end{cases}$$

Now, we compute the general Gutman index of graph F of order k:
$G_{2,1}(F) = 16 \times 1 + 36 \times 1 + 36 \times 1 +$
$16 \times 2 + 16 \times 3 + \cdots + 16(k-3) + 4(k-2)$
$16 \times 2 + 16 \times 3 + \cdots + 16(k-3) + 4(k-2)$
$36 \times 1 + 36 \times 2 + \cdots + 36(k-4) + 9(k-4) +$
$16 \times 2 + 16 \times 3 + \cdots + 16(k-5) + 4(k-4)$
$16 \times 2 + 16 \times 3 + \cdots + 16(k-6) + 4(k-5) + \cdots$
$16 \times 1 + 16 \times 2 + 4 \times 3 + 16 \times 1 + 4 \times 2 + 4 \times 1$
$= \frac{8}{3}k^3 + 4k^2 - \frac{233}{3}k + 189.$
Remark 3. Comparing $G_{2,1}(C_k)$ and $G_{2,1}(F)$, we obtain:
$\forall k \geqslant 6 : G_{2,1}(C_k) < G_{2,1}(F)$.

Lemma 2.12. *Let H be a monocyclic graph of order $k \geqslant 6$. Then,*

$$G_{2,1}(H) \leqslant \frac{8}{3}k^3 + 4k^2 - \frac{233}{3}k + 189.$$

Equality holds if and only if H is the graph obtained by attaching a path of order $k-3$ to one vertex of a triangle C_3; this graph is denoted by F.

Proof. We proceed by induction on k. The base case $k = 6$ is verified. Now assume $k \geqslant 7$. We consider two cases:

Case 1: $H = C_k$. By Remark 3, we have $G_{2,1}(C_k) < G_{2,1}(F)$.

Case 2: H has a pendant vertex v with neighbor w. Then $H \setminus \{v\}$ is a monocyclic graph of order $k-1$, and by the induction hypothesis:

$$G_{2,1}(H \setminus \{v\}) \leqslant \frac{8}{3}(k-1)^3 + 4(k-1)^2 - \frac{233}{3}(k-1) + 189.$$

Using Equation (2), we have:

$$\begin{aligned} G_{2,1}(H) &= G_{2,1}(H \setminus \{v\}) + B^*_{2,1}(v_H) + (d_{H\setminus\{v\}}(w)+1)^2 \\ &\quad + (2d_{H\setminus\{v\}}(w)+1)B^*_{2,1}(w_{H\setminus\{v\}}) \\ &= G_{2,1}(H \setminus \{v\}) + (2k^2 + 3k - 19) + 4 \\ &\quad + 3\left(2(k-1)^2 + 3(k-1) - 19\right) \\ &= G_{2,1}(H \setminus \{v\}) + 8k^2 - 75 \\ &< \left[\frac{8}{3}(k-1)^3 + 4(k-1)^2 - \frac{233}{3}(k-1) + 189\right] + (8k^2 - 75) \\ &= \frac{8}{3}k^3 + 4k^2 - \frac{233}{3}k + 189. \end{aligned}$$

This completes the induction step.

■

Theorem 2.13. *Let H be a connected graph with $n \geqslant 2$ vertices and m edges, C_k be a cycle of order $k \geqslant 4$, and F be a graph of order k consisting of C_3 with a path of order $k-3$ attached to one vertex of C_3. Let H_1 be the graph obtained by merging a vertex of H and a vertex of C_k, and H_2 be the graph obtained by merging a vertex of H and the pendant vertex of F. Then,*

$$G_{2,1}(H_1) < G_{2,1}(H_2).$$

Proof. Suppose $H \cap C_k = H \cap F = \{v\}$. By Theorem 2.10, we have:

$$\begin{aligned} G_{2,1}(H_1) - G_{2,1}(H_2) = {} & G_{2,1}(C_k) + G_{2,1}(H) - G_{2,1}(F) - G_{2,1}(H) \\ & + \left(d^2_{H_1}(v) - d^2_{C_k}(v)\right) B^*_{2,1}(v_{C_k}) - \left(d^2_{H_2}(v) - d^2_F(v)\right) B^*_{2,1}(v_F) \\ & + \left(d^2_{H_1}(v) - d^2_H(v)\right) B^*_{2,1}(v_H) - \left(d^2_{H_2}(v) - d^2_H(v)\right) B^*_{2,1}(v_H) \\ & + \sum_{\substack{r \in C_k \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_1}(r) d^2_{H_1}(s) d_{H_1}(r,s) - \sum_{\substack{r \in F \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_2}(r) d^2_{H_2}(s) d_{H_2}(r,s). \end{aligned}$$

Since $d_{C_k}(v) = 2$ and $d_F(v) = 1$, we obtain:

$$\begin{aligned} G_{2,1}(H_1) - G_{2,1}(H_2) = {} & G_{2,1}(C_k) - G_{2,1}(F) \\ & + \left(d^2_{H_1}(v) - 4\right) B^*_{2,1}(v_{C_k}) \\ & - \left(d^2_{H_2}(v) - 1\right) B^*_{2,1}(v_F) \\ & + d^2_{H_2}(v) B^*_{2,1}(v_H) - d^2_{H_1}(v) B^*_{2,1}(v_H) \\ & + \sum_{\substack{r \in C_k \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_1}(r) d^2_{H_1}(s) d_{H_1}(r,s) \\ & - \sum_{\substack{r \in F \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_2}(r) d^2_{H_2}(s) d_{H_2}(r,s). \end{aligned}$$

By the definitions of H_1 and H_2, if $d_{H_2}(v) = a$, then $d_{H_1}(v) = a + 1$. By Lemmas 2.6 and 2.7, we have $B^*_{2,1}(v_{C_k}) < B^*_{2,1}(v_F)$. Therefore,

$$\begin{aligned} & \left(d^2_{H_1}(v) - 4\right) B^*_{2,1}(v_{C_k}) - \left(d^2_{H_2}(v) - 1\right) B^*_{2,1}(v_F) \\ & \quad = (d_{H_1}(v) - 2)\,(d_{H_1}(v) + 2)\, B^*_{2,1}(v_{C_k}) \\ & \qquad - (d_{H_2}(v) - 1)\,(d_{H_2}(v) + 1)\, B^*_{2,1}(v_F) \\ & \quad = (a-1)(a+3) B^*_{2,1}(v_{C_k}) - (a-1)(a+1) B^*_{2,1}(v_F) \\ & \quad = (a-1)\left[(a+3)k^2) - (a+1) \times 2k^2)\right] < 0. \end{aligned}$$

Moreover,

$$d^2_{H_2}(v) B^*_{2,1}(v_H) - d^2_{H_1}(v) B^*_{2,1}(v_H) = B^*_{2,1}(v_H)\left(d^2_{H_2}(v) - d^2_{H_1}(v)\right) < 0.$$

For $s \in H \setminus \{v\}$, let $d_{H_1}(s) = d_{H_2}(s) = b$. Then,

$$\begin{aligned} & \sum_{\substack{r \in C_k \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_1}(r) d^2_{H_1}(s) d_{H_1}(r,s) - \sum_{\substack{r \in F \setminus \{v\} \\ s \in H \setminus \{v\}}} d^2_{H_2}(r) d^2_{H_2}(s) d_{H_2}(r,s) \\ & = 4b^2 \sum d_{H_1}(r,s) - 4b^2 \sum d_{H_2}(r,s) - 9b^2 \sum d_{H_2}(r,s) < 0. \end{aligned}$$

Therefore, all terms are negative, and we conclude that $G_{2,1}(H_1) < G_{2,1}(H_2)$. ■

Theorem 2.14. *Suppose H is a bicyclic graph of order $n \geqslant 6$. Then,*

$$G_{2,1}(H) \leqslant \frac{8}{3}n^3 + 20n^2 - \frac{329}{3}n + 99,$$

with equality if and only if $H \cong B_n$.

Proof. We proceed by induction on n. The result holds for $n = 6$ by direct verification. Suppose $n \geqslant 7$. We consider the four possible cases for a bicyclic graph:
Case 1: Let H consist of two disjoint cycles, each with minimum degree 2. The statement holds by using Theorem 2.13.
Case 2: H contains a pendant vertex v with neighbor w. By the induction hypothesis,

$$G_{2,1}(H \setminus \{v\}) \leqslant \frac{8}{3}(n-1)^3 + 20(n-1)^2 - \frac{329}{3}(n-1) + 99.$$

Using Lemmas 2.11 and 2.12, we get:

$$\begin{aligned}
G_{2,1}(H) &= G_{2,1}(H \setminus \{v\}) + B^*_{2,1}(v_H) + (d_{H\setminus\{v\}}(w) + 1)^2 \\
&\quad + (2d_{H\setminus\{v\}}(w) + 1)B^*_{2,1}(w_{H\setminus\{v\}}) \\
&\leqslant \frac{8}{3}(n-1)^3 + 20(n-1)^2 - \frac{329}{3}(n-1) + 99 \\
&\quad + (n^2 + 7n - 3) + 3^2 + 5(n^2 + 5n - 10) \\
&= \frac{8}{3}n^3 + 18n^2 - \frac{329}{3}n + 182.
\end{aligned}$$

Since $\frac{8}{3}n^3 + 18n^2 - \frac{329}{3}n + 182 \leqslant \frac{8}{3}n^3 + 20n^2 - \frac{329}{3}n + 99$ for $n \geqslant 7$, the inequality follows.
Case 3: H is 2-connected. The result follows by an argument similar to Case 3 of Theorem 2.7 in [1].
Case 4: H consists of two cycles intersecting at exactly one vertex. This case can be handled by combining the methods used in Case 1 and Theorem 2.13. In all cases, the inequality holds, and equality is attained only when $H \cong B_n$. ■

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