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General Gutman Index of a Graph

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Abstract

For a graph G, we generalize the well-known Gutman index by introducing the general Gutman index

$$Gut_{a,b}(G) = \sum_{\{u,v\} \subseteq V(G)} [d_G(u) d_G(v)]^a [D_G(u,v)]^b,$$

where $a, b \in \mathbb{R}$, $D_G(u,v)$ is the distance between vertices u and v in G, and $d_G(u)$ and $d_G(v)$ are the degrees of u and v, respectively. We show that for some a and b, the $Gut_{a,b}$ index decreases/increases with the addition of edges. We present sharp bounds on the general Gutman index for multipartite graphs of given order, graphs of given order and chromatic number, and starlike trees of given order and maximum degree. We also state several problems open for further research.

1 Introduction

Topological indices have been used for example for chemical documentation, quantitative structure versus property/activity relationships (QSPR/QSAR), toxicology hazard assessments, isomer discrimination, drug design

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and combinatorial library design. They have been used in the process of correlating chemical structures with various characteristics such as boiling points and molar heats of formation. Topological indices provide a convenient method of translating chemical constitutions into numerical values which are applied for correlations with physical properties.

Let $V(G)$ and $E(G)$ be the vertex set and the edge set of a graph G, respectively. The order is the number of vertices of G. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of vertices adjacent to v. The distance $D_G(u,v)$ between two vertices $u,v \in V(G)$ is the number of edges in a shortest path between u and v.

The Gutman index of a connected graph G,

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u) d_G(v) D_G(u,v)$$

belongs to important topological indices. It was introduced in [8] and it has been studied due to its extensive applications, especially in chemistry.

Upper bounds on the Gutman index for graphs of prescribed order were investigated in [4] and [14]. Bounds for graphs with maximum degree and minimum degree were studied in [1] and [11]. Upper bounds for graphs of given vertex-connectivity and edge-connectivity were given in [12] and [13], respectively.

Feng [6] investigated the Gutman index of unicyclic graphs, Feng and Liu [7] studied bicyclic graphs, Chen [2] studied lower bounds for cacti. Relations between the degree distance and the Gutman index were investigated by Das, Su and Xiong [5]. Relations between the edge-Wiener index and the Gutman index were studied by Knor, Potočnik and Škrekovski [9].

We generalize the Gutman index by introducing the general Gutman index of a connected graph G as

$$Gut_{a,b}(G) = \sum_{\{u,v\} \subseteq V(G)} [d_G(u) d_G(v)]^a [D_G(u,v)]^b$$

for $a, b \in \mathbb{R}$. If $a = 1$ and $b = 1$, we get the classical Gutman index. For $a = 0$ and $b = 1$, we obtain the Wiener index. A different generalization of the Gutman index using the Steiner distance was given in [10].

We present bounds on the general Gutman index for multipartite graphs of given order, graphs of given order and chromatic number, and star-like trees of given order and maximum degree. Shortly after we introduced the general Gutman index, it also motivated other researchers to study this general index; see the work on trees by Cheng and Li [3].

2 Results

For a graph G with two non-adjacent vertices u_1, u_2, the graph $G + u_1u_2$ has vertex set $V(G)$ and edge set $E(G) \cup \{u_1u_2\}$. For $a \leq 0$ and $b \geq 0$, where at least one of a and b is not 0, we compare the $Gut_{a,b}$ indices of two graphs which differ by one edge.

Lemma 1. *Let $a \leq 0$ and $b \geq 0$, where at least one of a and b is not 0. For a connected graph G, where u_1, u_2 are any non-adjacent vertices in G, we have*

$$Gut_{a,b}(G + u_1u_2) < Gut_{a,b}(G).$$

Proof. Let $G' = G + u_1u_2$, where $u_1u_2 \notin E(G)$. Then $d_{G'}(u_i) = d_G(u_i) + 1 \geq 2$ for $i = 1, 2$. We obtain

$$d_{G'}(u_1)d_{G'}(u_2) > d_G(u_1)d_G(u_2) \geq 1.$$

Thus, for $a \leq 0$,

$$[d_{G'}(u_1)d_{G'}(u_2)]^a \leq [d_G(u_1)d_G(u_2)]^a, \tag{1}$$

with equality only if $a = 0$. We have $1 = D_{G'}(u_1, u_2) < D_G(u_1, u_2)$. For $b \geq 0$,

$$[D_{G'}(u_1, u_2)]^b \leq [D_G(u_1, u_2)]^b \tag{2}$$

with equality only if $b = 0$. By (1) and (2), if at least one of a and b is not 0, we obtain

$$0 < [d_{G'}(u_1)d_{G'}(u_2)]^a[D_{G'}(u_1, u_2)]^b < [d_G(u_1)d_G(u_2)]^a[D_G(u_1, u_2)]^b. \tag{3}$$

For $x \in V(G) \setminus \{u_1, u_2\}$, we have $d_{G'}(x) = d_G(x) \geq 1$. Let us consider

$\{y,z\} \subseteq V(G)$ where $\{y,z\} \neq \{u_1,u_2\}$. We have

$$d_{G'}(y)d_{G'}(z) \geq d_G(y)d_G(z) \geq 1.$$

Thus, for $a \leq 0$,

$$0 < [d_{G'}(y)d_{G'}(z)]^a \leq [d_G(y)d_G(z)]^a \leq 1. \tag{4}$$

By adding an edge, the distance between two vertices cannot be increased, therefore we obtain $1 \leq D_{G'}(y,z) \leq D_G(y,z)$ for $\{y,z\} \subseteq V(G)$ where $\{y,z\} \neq \{u_1,u_2\}$. Since $b \geq 0$, we get

$$1 \leq [D_{G'}(y,z)]^b \leq [D_G(y,z)]^b. \tag{5}$$

From (4) and (5), we obtain

$$0 < [d_{G'}(y)d_{G'}(z)]^a[D_{G'}(y,z)]^b \leq [d_G(y)d_G(z)]^a[D_G(y,z)]^b. \tag{6}$$

From (3) and (6), we get

$$\begin{aligned}
&Gut_{a,b}(G') \\
&= \sum_{\substack{\{y,z\}\subseteq V(G'),\\ \{y,z\}\neq\{u_1,u_2\}}} [d_{G'}(y)d_{G'}(z)]^a[D_{G'}(y,z)]^b + [d_{G'}(u_1)d_{G'}(u_2)]^a[D_{G'}(u_1,u_2)]^b \\
&< \sum_{\substack{\{y,z\}\subseteq V(G),\\ \{y,z\}\neq\{u_1,u_2\}}} [d_G(y)d_G(z)]^a[D_G(y,z)]^b + [d_G(u_1)d_G(u_2)]^a[D_G(u_1,u_2)]^b \\
&= Gut_{a,b}(G).
\end{aligned}$$

■

Now, we compare the $Gut_{a,b}$ indices of two graphs which differ by one edge if $a \geq 0$ and $b \leq 0$, where at least one of a and b is not 0. The proofs of Lemmas 1 and 2 are similar, therefore we omit a few steps which are the same in both proofs.

Lemma 2. *Let $a \geq 0$ and $b \leq 0$, where at least one of a and b is not 0. For a connected graph G, where u_1, u_2 are any non-adjacent vertices in G,* *we have*

$$Gut_{a,b}(G + u_1u_2) > Gut_{a,b}(G).$$

Proof. We have

$$d_{G'}(u_1)d_{G'}(u_2) > d_G(u_1)d_G(u_2) \geq 1.$$

Thus, for $a \geq 0$,

$$[d_{G'}(u_1)d_{G'}(u_2)]^a \geq [d_G(u_1)d_G(u_2)]^a, \tag{7}$$

with equality only if $a = 0$. We have $1 = D_{G'}(u_1, u_2) < D_G(u_1, u_2)$. Thus, for $b \leq 0$,

$$[D_{G'}(u_1, u_2)]^b \geq [D_G(u_1, u_2)]^b \tag{8}$$

with equality only if $b = 0$. By (7) and (8), if at least one of a and b is not 0, we obtain

$$[d_{G'}(u_1)d_{G'}(u_2)]^a[D_{G'}(u_1, u_2)]^b > [d_G(u_1)d_G(u_2)]^a[D_G(u_1, u_2)]^b > 0. \tag{9}$$

Let us consider $\{y, z\} \subseteq V(G)$ where $\{y, z\} \neq \{u_1, u_2\}$. We have

$$d_{G'}(y)d_{G'}(z) \geq d_G(y)d_G(z) \geq 1.$$

Thus, for $a \geq 0$,

$$[d_{G'}(y)d_{G'}(z)]^a \geq [d_G(y)d_G(z)]^a \geq 1. \tag{10}$$

We obtain $1 \leq D_{G'}(y, z) \leq D_G(y, z)$ for $\{y, z\} \subseteq V(G)$ where $\{y, z\} \neq \{u_1, u_2\}$. Since $b \leq 0$, we get

$$1 \geq [D_{G'}(y, z)]^b \geq [D_G(y, z)]^b > 0. \tag{11}$$

From (10) and (11), we obtain

$$[d_{G'}(y)d_{G'}(z)]^a[D_{G'}(y, z)]^b \geq [d_G(y)d_G(z)]^a[D_G(y, z)]^b > 0. \tag{12}$$

From (9) and (12), we get

$$\begin{aligned}
&Gut_{a,b}(G') \\
&= \sum_{\substack{\{y,z\}\subseteq V(G'),\\ \{y,z\}\neq\{u_1,u_2\}}} [d_{G'}(y)d_{G'}(z)]^a[D_{G'}(y,z)]^b + [d_{G'}(u_1)d_{G'}(u_2)]^a[D_{G'}(u_1,u_2)]^b \\
&> \sum_{\substack{\{y,z\}\subseteq V(G),\\ \{y,z\}\neq\{u_1,u_2\}}} [d_G(y)d_G(z)]^a[D_G(y,z)]^b + [d_G(u_1)d_G(u_2)]^a[D_G(u_1,u_2)]^b \\
&= Gut_{a,b}(G).
\end{aligned}$$

■

It is easy to use Lemmas 1 and 2 to obtain bounds on the general Gutman index for connected graphs of given order.

Proposition 1. *Let G be a connected graph with n vertices. For $a \leq 0$ and $b \geq 0$, where at least one of a and b is not 0,*

$$Gut_{a,b}(G) \geq \frac{n(n-1)^{2a+1}}{2}.$$

For $a \geq 0$ and $b \leq 0$, where at least one of a and b is not 0,

$$Gut_{a,b}(G) \leq \frac{n(n-1)^{2a+1}}{2}.$$

The equalities hold only if G is K_n.

Proof. By Lemma 1, when adding an edge to a graph, the $Gut_{a,b}$ index decreases for $a \leq 0$ and $b \geq 0$, where at least one of a and b is not 0. Thus, for graphs of order n, the only graph having the smallest $Gut_{a,b}$ index is K_n. By Lemma 2, when adding an edge to a graph, the $Gut_{a,b}$ index increases for $a \geq 0$ and $b \leq 0$, where at least one of a and b is not 0. Thus, the only graph having the largest $Gut_{a,b}$ index is K_n.

Any two vertices of K_n are adjacent, their degree is $n-1$, therefore

$$\begin{aligned} Gut_{a,b}(K_n) &= \sum_{\{u,v\}\subseteq V(K_n)} [(n-1)(n-1)]^a 1^b \\ &= \binom{n}{2}(n-1)^{2a} = \frac{n(n-1)^{2a+1}}{2}. \end{aligned}$$

■

Lemma 3 was presented in [15] and it is useful in the study of the general Gutman index.

Lemma 3. *Let $1 \le x < y$ and $c > 0$. For $a > 1$ and $a < 0$, we have*

$$(x+c)^a - x^a < (y+c)^a - y^a.$$

If $0 < a < 1$, then

$$(x+c)^a - x^a > (y+c)^a - y^a.$$

For $k \ge 2$, a k-partite graph (multipartite graph) is a graph whose vertices can be partitioned into k sets, such that no two vertices in the same set are adjacent. A k-partite graph with partite sets having cardinalities $n_1, n_2, \ldots, n_k$ is called complete if every two vertices from different partite sets are adjacent. It is denoted by $K_{n_1,n_2,\ldots,n_k}$. In Theorems 2 and 3, we present multipartite graphs having the minimum and maximum general Gutman index (for some intervals).

Theorem 2. *Let $a \le 0$ and $b \ge 0$, where at least one of a and b is not 0. For any k-partite graph G with n vertices, where $2 \le k \le n$,*

$$Gut_{a,b}(G) \ge Gut_{a,b}(K_{n_1,n_2,\ldots,n_k}).$$

The equality holds only if G is $K_{n_1,n_2,\ldots,n_k}$, where $|n_i - n_j| \le 1$, $1 \le i < j \le k$ and $n_1 + n_2 + \cdots + n_k = n$.

Proof. Let G' be any k-partite graph of order n having the minimum $Gut_{a,b}$ index. From Lemma 1, any two vertices of G' from distinct partite sets are adjacent. So G' is $K_{n_1,n_2,\ldots,n_k}$, where $n_1, n_2, \ldots, n_k$ are some positive integers. Let us prove that $|n_i - n_j| \le 1$, where $1 \le i < j \le k$.

Assume to the contrary that $|n_i - n_j| \ge 2$ for some i, j, where $1 \le i < j \le k$. We can assume that $n_1 \ge n_2 + 2$. Let us investigate $Gut_{a,b}(G') - Gut_{a,b}(G'')$ for $G' = K_{n_1,n_2,\ldots,n_k}$ and $G'' = K_{n_1-1,n_2+1,\ldots,n_k}$.

For any vertex $v' \in V_1'$ and any $w' \in V_2'$, we obtain $d_{G'}(v') = n - n_1$, $d_{G'}(w') = n - n_2$ and $D_{G'}(v', w') = 1$. For any vertex $v'' \in V_1''$ and any $w'' \in V_2''$, we obtain $d_{G''}(v'') = n - (n_1 - 1)$, $d_{G''}(w'') = n - (n_2 + 1)$ and $D_{G''}(v'', w'') = 1$. For any other vertex z, we have $d_{G'}(z) = d_{G''}(z)$. Therefore, we obtain $Gut_{a,b}(G') - Gut_{a,b}(G'') = A + B + C$, where

$$\begin{aligned}
A &= \sum_{v' \in V_1', w' \in V_2'} [d_{G'}(v') d_{G'}(w')]^a [D_{G'}(v', w')]^b \\
&\quad - \sum_{v'' \in V_1'', w'' \in V_2''} [d_{G''}(v'') d_{G''}(w'')]^a [D_{G''}(v'', w'')]^b \\
B &= \sum_{\{u', v'\} \subseteq V_1'} [d_{G'}(u') d_{G'}(v')]^a [D_{G'}(u', v')]^b \\
&\quad + \sum_{\{w', z'\} \subseteq V_2'} [d_{G'}(w') d_{G'}(z')]^a [D_{G'}(w', z')]^b \\
&\quad - \sum_{\{u'', v''\} \subseteq V_1''} [d_{G''}(u'') d_{G''}(v'')]^a [D_{G''}(u'', v'')]^b \\
&\quad - \sum_{\{w'', z''\} \subseteq V_2''} [d_{G''}(w'') d_{G''}(z'')]^a [D_{G''}(w'', z'')]^b \\
C &= \sum_{v' \in V_1', z' \in V(G') \setminus (V_1' \cup V_2')} [d_{G'}(v') d_{G'}(z')]^a [D_{G'}(v', z')]^b \\
&\quad + \sum_{w' \in V_2', z' \in V(G') \setminus (V_1' \cup V_2')} [d_{G'}(w') d_{G'}(z')]^a [D_{G'}(w', z')]^b \\
&\quad - \sum_{v'' \in V_1'', z'' \in V(G'') \setminus (V_1'' \cup V_2'')} [d_{G''}(v'') d_{G''}(z'')]^a [D_{G''}(v'', z'')]^b \\
&\quad - \sum_{w'' \in V_2'', z'' \in V(G'') \setminus (V_1'' \cup V_2'')} [d_{G''}(w'') d_{G''}(z'')]^a [D_{G''}(w'', z'')]^b.
\end{aligned}$$

Note that

$$\begin{aligned}(n-n_1)(n-n_2) &= n^2-n_1n-n_2n+n_1n_2\\ &< n^2-n_1n-n_2n+n_1n_2+(n_1-n_2-1)\\ &= (n-n_1+1)(n-n_2-1).\end{aligned}$$

Thus

$$[(n-n_1)(n-n_2)]^a \geq [(n-n_1+1)(n-n_2-1)]^a$$

for $a \leq 0$ and

$$\begin{aligned}A &= n_1n_2(n-n_1)^a(n-n_2)^a\\ &\quad -(n_1-1)(n_2+1)[n-(n_1-1)]^a[n-(n_2+1)]^a\\ &= (n_1n_2+n_1-n_2-1)([(n-n_1)(n-n_2)]^a\\ &\quad -[(n-n_1+1)(n-n_2-1)]^a)-(n_1-n_2-1)(n-n_1)^a(n-n_2)^a\\ &\geq -(n_1-n_2-1)(n-n_1)^a(n-n_2)^a.\end{aligned}$$

We have

$$\begin{aligned}B &= \binom{n_1}{2}(n-n_1)^a(n-n_1)^a2^b+\binom{n_2}{2}(n-n_2)^a(n-n_2)^a2^b\\ &\quad -\binom{n_1-1}{2}[n-(n_1-1)]^a[n-(n_1-1)]^a2^b\\ &\quad -\binom{n_2+1}{2}[n-(n_2+1)]^a[n-(n_2+1)]^a2^b\\ &= \Big[\frac{n_1(n_1-1)}{2}(n-n_1)^{2a}+\frac{n_2(n_2-1)}{2}(n-n_2)^{2a}\\ &\quad -\frac{(n_1-1)(n_1-2)}{2}(n-n_1+1)^{2a}-\frac{(n_2+1)n_2}{2}(n-n_2-1)^{2a}\Big]2^b\\ &= \Big[\frac{(n_1-1)(n_1-2)}{2}[(n-n_1)^{2a}-(n-n_1+1)^{2a}]\\ &\quad -\frac{(n_2+1)n_2}{2}[(n-n_2-1)^{2a}-(n-n_2)^{2a}]\\ &\quad +(n_1-1)(n-n_1)^{2a}-n_2(n-n_2)^{2a}\Big]2^b\\ &\geq [(n_1-1)(n-n_1)^{2a}-n_2(n-n_2)^{2a}]2^b\\ &\geq (n_1-1)(n-n_1)^{2a}-n_2(n-n_2)^{2a}.\end{aligned}$$

If $b > 0$, then the last inequality is strict since $2^b > 1$. If $a < 0$, then the first inequality is strict since $\frac{(n_1-1)(n_1-2)}{2} \geq \frac{(n_2+1)n_2}{2}$ and by Lemma 3,

$$(n-n_1)^{2a} - (n-n_1+1)^{2a} > (n-n_2-1)^{2a} - (n-n_2)^{2a}$$

which is greater than 0. Thus, if at least one of a and b is not 0, we have

$$B > (n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a}$$

and

$$\begin{aligned} A+B &> (n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a} \\ &\quad - (n_1-n_2-1)(n-n_1)^a(n-n_2)^a \\ &= (n_1-1)(n-n_1)^a[(n-n_1)^a - (n-n_2)^a] \\ &\quad - n_2(n-n_2)^a[(n-n_2)^a - (n-n_1)^a] \\ &= [(n_1-1)(n-n_1)^a + n_2(n-n_2)^a][(n-n_1)^a - (n-n_2)^a] \\ &\geq 0, \end{aligned}$$

since $(n-n_1)^a \geq (n-n_2)^a$ for $a \leq 0$. We get

$$\begin{aligned} C &= n_1(n-n_1)^a + n_2(n-n_2)^a \\ &\quad - (n_1-1)(n-n_1+1)^a - (n_2+1)(n-n_2-1)^a \\ &= (n_1-1)[(n-n_1)^a - (n-n_1+1)^a] \\ &\quad - (n_2+1)[(n-n_2-1)^a - (n-n_2)^a] + (n-n_1)^a - (n-n_2)^a \\ &\geq 0, \end{aligned}$$

since $(n-n_1)^a - (n-n_2)^a \geq 0$ for $a \leq 0$, $n_1 - 1 \geq n_2 + 1$ and by Lemma 3, for $a < 0$,

$$(n-n_1)^a - (n-n_1+1)^a > (n-n_2-1)^a - (n-n_2)^a$$

which is greater than 0. Clearly, for $a = 0$, we have $(n-n_1)^a - (n-n_1+1)^a = (n-n_2-1)^a - (n-n_2)^a = 0$.

Since $A+B > 0$ and $C \geq 0$, we have $Gut_{a,b}(G') - Gut_{a,b}(G'') > 0$, so $Gut_{a,b}(G') > Gut_{a,b}(G'')$. Thus, G' does not have the minimum $Gut_{a,b}$ index which is a contradiction. Hence, $|n_i - n_j| \leq 1$. ∎

The proof of Theorem 3 is similar to the proof of Theorem 2, therefore we omit some steps which are the same in both proofs.

Theorem 3. *Let $0 \leq a < \frac{1}{2}$ and $b \leq 0$, where at least one of a and b is not 0. For any k-partite graph G with n vertices, where $2 \leq k \leq n$,*

$$Gut_{a,b}(G) \leq Gut_{a,b}(K_{n_1,n_2,\ldots,n_k}).$$

The equality holds only if G is $K_{n_1,n_2,\ldots,n_k}$, where $|n_i - n_j| \leq 1$, $1 \leq i < j \leq k$ and $n_1 + n_2 + \cdots + n_k = n$.

Proof. Let G' be a k-partite graph of order n having the maximum $Gut_{a,b}$ index. By Lemma 2, G' is the complete k-partite graph.

Assume that $G' = K_{n_1,n_2,\ldots,n_k}$, where $|n_i - n_j| \geq 2$, say $n_1 \geq n_2 + 2$. Let $G'' = K_{n_1-1,n_2+1,\ldots,n_k}$. Since $(n-n_1)(n-n_2) < (n-n_1+1)(n-n_2-1)$, we have

$$[(n-n_1)(n-n_2)]^a \leq [(n-n_1+1)(n-n_2-1)]^a$$

for $a > 0$ and

$$\begin{aligned} A &= (n_1n_2 + n_1 - n_2 - 1)([(n-n_1)(n-n_2)]^a \\ &\quad - [(n-n_1+1)(n-n_2-1)]^a) - (n_1 - n_2 - 1)(n-n_1)^a(n-n_2)^a \\ &\leq -(n_1 - n_2 - 1)(n-n_1)^a(n-n_2)^a. \end{aligned}$$

We have

$$\begin{aligned} B &= \Big[\frac{(n_1-1)(n_1-2)}{2}[(n-n_1)^{2a} - (n-n_1+1)^{2a}] \\ &\quad - \frac{(n_2+1)n_2}{2}[(n-n_2-1)^{2a} - (n-n_2)^{2a}] \\ &\quad + (n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a}\Big]2^b \\ &= \Big[\frac{(n_2+1)n_2}{2}[(n-n_2)^{2a} - (n-n_2-1)^{2a}] \end{aligned}$$

$$
\begin{aligned}
& - \frac{(n_1-1)(n_1-2)}{2}[(n-n_1+1)^{2a}-(n-n_1)^{2a}] \\
& + (n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a}\Big]2^b \\
\le\ & [(n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a}]2^b \\
\le\ & (n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a},
\end{aligned}
$$

If $b<0$, then the last inequality is strict since $0<2^b<1$. If $0<a<\frac{1}{2}$, then the first inequality is strict since $\frac{(n_2+1)n_2}{2} \le \frac{(n_1-1)(n_1-2)}{2}$ and by Lemma 3,

$$(n-n_2)^{2a}-(n-n_2-1)^{2a} < (n-n_1+1)^{2a}-(n-n_1)^{2a}.$$

Thus, if at least one of a and b is not 0, we have $B<(n_1-1)(n-n_1)^{2a} - n_2(n-n_2)^{2a}$. Then

$$A+B < [(n_1-1)(n-n_1)^a + n_2(n-n_2)^a][(n-n_1)^a-(n-n_2)^a] \le 0,$$

since $(n-n_1)^a \le (n-n_2)^a$ for $a \ge 0$. We get

$$
\begin{aligned}
C &= (n_2+1)[(n-n_2)^a-(n-n_2-1)^a] \\
&\quad - (n_1-1)[(n-n_1+1)^a-(n-n_1)^a] + (n-n_1)^a-(n-n_2)^a \\
&\le 0,
\end{aligned}
$$

since $(n-n_1)^a-(n-n_2)^a \le 0$ for $a\ge 0$, $n_2+1\le n_1-1$ and by Lemma 3,

$$(n-n_2)^a-(n-n_2-1)^a < (n-n_1+1)^a-(n-n_1)^a$$

for $0<a<\frac{1}{2}$.

Since $A+B<0$ and $C\le 0$, we have $Gut_{a,b}(G') < Gut_{a,b}(G'')$. So G' does not have the maximum $Gut_{a,b}$ index which is a contradiction. ■

The chromatic number of a graph G is the smallest number of colors needed to color the vertices of G such that no two adjacent vertices have the same color. We use Theorem 2 to obtain the following theorem for graphs with given chromatic number.

Theorem 4. *Let $a \leq 0$ and $b \geq 0$, where at least one of a and b is not 0. For any connected graph G with n vertices and chromatic number χ, where $2 \leq \chi \leq n$,*

$$Gut_{a,b}(G) \geq Gut_{a,b}(K_{n_1,n_2,\ldots,n_\chi}).$$

The equality holds only if G is $K_{n_1,n_2,\ldots,n_\chi}$, where $|n_i - n_j| \leq 1$, $1 \leq i < j \leq \chi$ and $n_1 + n_2 + \cdots + n_\chi = n$.

Proof. Let G' be any graph of order n and chromatic number χ having the minimum $Gut_{a,b}$ index. The graph G' contains no edges connecting the vertices in the same color class, thus G' is a χ-partite graph. Hence, by Theorem 2, G' is $K_{n_1,n_2,\ldots,n_\chi}$, where $|n_i - n_j| \leq 1$ and $1 \leq i < j \leq \chi$. ■

Similarly, Theorem 5 follows from Theorem 3.

Theorem 5. *Let $0 \leq a < \frac{1}{2}$ and $b \leq 0$, where at least one of a and b is not 0. For any graph G with n vertices and chromatic number χ, where $2 \leq \chi \leq n$,*

$$Gut_{a,b}(G) \leq Gut_{a,b}(K_{n_1,n_2,\ldots,n_\chi}).$$

The equality holds only if G is $K_{n_1,n_2,\ldots,n_\chi}$, where $|n_i - n_j| \leq 1$, $1 \leq i < j \leq \chi$ and $n_1 + n_2 + \cdots + n_\chi = n$.

It seems complicated to obtain sharp bounds on the general Gutman index for trees. Thus we consider a special class of trees called starlike trees. A starlike tree is a tree having exactly one vertex of degree greater than 2. For the starlike tree $S(n_1, n_2, \ldots, n_k)$ with a vertex v_0 of degree $k \geq 3$, we have

$$S(n_1, n_2, \ldots, n_k) - v_0 = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k},$$

where P_{n_i} is the path of order n_i $(1 \leq i \leq k)$; see Figure 1. This tree has $n_1 + n_2 + \cdots + n_k + 1 = n$ vertices. In particular, $S(n_1, n_2, \ldots, n_k)$ is the star S_n for $n_1 = n_2 = \cdots = n_k = 1$. Let S'_n be a starlike tree $S(n_1, n_2, \ldots, n_k)$ of order n such that all $n_1, n_2, \ldots, n_k$ except for one are equal to 1. We denote by S''_n a tree $S(n_1, n_2, \ldots, n_k)$ of order n such that

$|n_i - n_j| \le 1$ for any $1 \le i < j \le k$. Let us compare the $Gut_{a,b}$ index of two starlike trees.

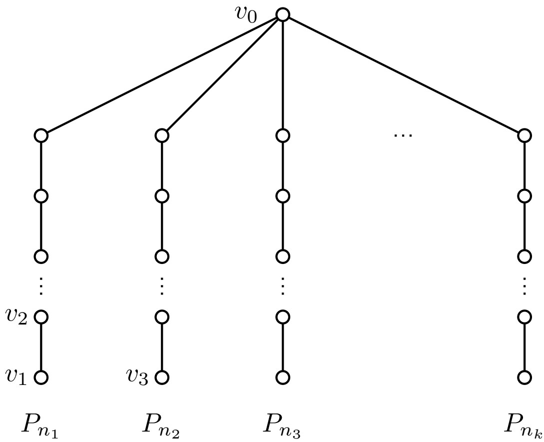

Figure 1. Starlike tree $S(n_1, n_2, \ldots, n_k)$.

Lemma 4. *Let $a \ge 0$ and $b > 0$. For $n_1 \ge n_2 + 2$, we have*

$$Gut_{a,b}(S(n_1, n_2, \ldots, n_k)) > Gut_{a,b}(S(n_1 - 1, n_2 + 1, \ldots, n_k)).$$

Proof. Let $n_1 \ge n_2 + 2$. In $H_1 = S(n_1, n_2, \ldots, n_k)$, let v_1 and v_2 be adjacent vertices of $V(P_{n_1})$ such that $d_{H_1}(v_1) = 1 < 2 = d_{H_1}(v_2)$, and let $v_3 \in V(P_{n_2})$ such that $d_{H_1}(v_3) = 1$ (see Figure 1).

Let $H_2 = S(n_1 - 1, n_2 + 1, \ldots, n_k) = S(n_1, n_2, \ldots, n_k) - v_1v_2 + v_1v_3$. Let $Z = \{v_1, v_2, v_3\}$. Then

$$\sum_{\{u,v\} \subseteq Z} [d_{H_1}(u) d_{H_1}(v)]^a [D_{H_1}(u,v)]^b = (n_1 + n_2)^b + 2^a (n_1 + n_2 - 1)^b + 2^a$$
$$= \sum_{\{u,v\} \subseteq Z} [d_{H_2}(u) d_{H_2}(v)]^a [D_{H_2}(u,v)]^b$$

and

$$\sum_{\{u,v\}\subseteq V(H_1)\setminus Z}[d_{H_1}(u)d_{H_1}(v)]^a[D_{H_1}(u,v)]^b$$
$$=\sum_{\{u,v\}\subseteq V(H_2)\setminus Z}[d_{H_2}(u)d_{H_2}(v)]^a[D_{H_2}(u,v)]^b.$$

Let $F=\{v_0\}\cup V(P_{n_1})\cup V(P_{n_2})$. Then

$$\begin{aligned}
&Gut_{a,b}(H_1)-Gut_{a,b}(H_2)\\
&=\sum_{\{u,v\}\subseteq Z}([d_{H_1}(u)d_{H_1}(v)]^a[D_{H_1}(u,v)]^b-[d_{H_2}(u)d_{H_2}(v)]^a[D_{H_2}(u,v)]^b)\\
&\quad+\sum_{\{u,v\}\subseteq V(H_1)\setminus Z}([d_{H_1}(u)d_{H_1}(v)]^a[D_{H_1}(u,v)]^b-[d_{H_2}(u)d_{H_2}(v)]^a[D_{H_2}(u,v)]^b)\\
&\quad+\sum_{u\in Z,v\in V(H_1)\setminus Z}([d_{H_1}(u)d_{H_1}(v)]^a[D_{H_1}(u,v)]^b-[d_{H_2}(u)d_{H_2}(v)]^a[D_{H_2}(u,v)]^b)\\
&=\sum_{u\in Z,v\in V(H_1)\setminus Z}([d_{H_1}(u)d_{H_1}(v)]^a[D_{H_1}(u,v)]^b-[d_{H_2}(u)d_{H_2}(v)]^a[D_{H_2}(u,v)]^b)\\
&=\sum_{v\in V(H_1)\setminus Z}[d_{H_1}(v)]^a[D_{H_1}(v_1,v)]^b-\sum_{v\in V(H_1)\setminus Z}[d_{H_2}(v)]^a[D_{H_2}(v_1,v)]^b\\
&\quad+2^a\sum_{v\in V(H_1)\setminus Z}[d_{H_1}(v)]^a[D_{H_1}(v_2,v)]^b-\sum_{v\in V(H_1)\setminus Z}[d_{H_2}(v)]^a[D_{H_2}(v_2,v)]^b\\
&\quad+\sum_{v\in V(H_1)\setminus Z}[d_{H_1}(v)]^a[D_{H_1}(v_3,v)]^b-2^a\sum_{v\in V(H_1)\setminus Z}[d_{H_2}(v)]^a[D_{H_2}(v_3,v)]^b\\
&=\sum_{v\in V(H_1)\setminus Z}[d_{H_1}(v)]^a([D_{H_1}(v_1,v)]^b-[D_{H_2}(v_1,v)]^b)\\
&\quad+(2^a-1)\sum_{v\in V(H_1)\setminus Z}[d_{H_1}(v)]^a([D_{H_1}(v_2,v)]^b-[D_{H_1}(v_3,v)]^b).
\end{aligned}$$

Note that

$$D_{H_1}(v_2,v)=D_{H_2}(v_2,v)>D_{H_1}(v_3,v)=D_{H_2}(v_3,v)$$

for $v \in V(H_1)\backslash F$. We obtain

$$
\begin{aligned}
R &= \sum_{v \in V(H_1)\backslash Z} [d_{H_1}(v)]^a([D_{1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\
&= \sum_{v \in V(H_1)\backslash F} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\
&\quad + \sum_{v \in F\backslash Z} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\
&> \sum_{v \in F\backslash Z} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\
&= 2^a[1 + 2^b + \cdots + (n_1 - 2)^b + n_1^b + \cdots + (n_1 + n_2 - 2)^b] \\
&\quad - 2^a[1 + 2^b + \cdots + (n_2 - 1)^b + (n_2 + 1)^b + \cdots + (n_1 + n_2 - 2)^b] \\
&\quad + k^a(n_1 - 1)^b - k^a\, n_2^b \\
&= k^a(n_1 - 1)^b - 2^a(n_1 - 1)^b + 2^a\, n_2^b - k^a\, n_2^b \\
&= (k^a - 2^a)[(n_1 - 1)^b - n_2^b] \\
&\geq 0,
\end{aligned}
$$

since $k^a - 2^a \geq 0$ for $k \geq 3$ and $a \geq 0$, and $(n_1 - 1)^b - n_2^b > 0$ for $n_1 - 1 > n_2$ and $b > 0$. For $v \in V(H_1)\backslash F$, we have $D_{H_1}(v_1, v) > D_{H_2}(v_1, v)$. Thus

$$
\begin{aligned}
P &= \sum_{v \in V(H_1)\backslash Z} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)]^b - [D_{H_2}(v_1, v)]^b) \\
&= \sum_{v \in V(H_1)\backslash F} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)]^b - [D_{H_2}(v_1, v)]^b) \\
&\quad + \sum_{v \in F\backslash Z} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)^b] - [D_{H_2}(v_1, v)]^b) \\
&> \sum_{v \in F\backslash Z} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)]^b - [D_{H_2}(v_1, v)]^b) \\
&= 2^a[2^b + \cdots + (n_1 - 1)^b + (n_1 + 1)^b + \cdots + (n_1 + n_2 - 1)^b] \\
&\quad - 2^a[2^b + \cdots + n_2^b + (n_2 + 2)^b + \cdots + (n_1 + n_2 - 1)^b] \\
&\quad + k^a n_1^b - k^a(n_2 + 1)^b \\
&= k^a n_1^b - 2^a n_1^b + 2^a(n_2 + 1)^b - k^a(n_2 + 1)^b \\
&= (k^a - 2^a)[n_1^b - (n_2 + 1)^b] \geq 0,
\end{aligned}
$$

since $n_1^b - (n_2+1)^b > 0$ for $n_1 > n_2+1$ and $b > 0$. We have $R > 0$, $P > 0$ and $2^a \geq 1$ for $a \geq 0$, thus

$$Gut_{a,b}(H_1) - Gut_{a,b}(H_2) = P + (2^a - 1)R > 0.$$

Hence $Gut_{a,b}(H_1) > Gut_{a,b}(H_2)$. ■

We obtain a similar lemma for $a \geq 0$ and $b < 0$.

Lemma 5. *Let $a \geq 0$ and $b < 0$. For $n_1 \geq n_2 + 2$, we have*

$$Gut_{a,b}(S(n_1, n_2, \ldots, n_k)) < Gut_{a,b}(S(n_1 - 1, n_2 + 1, \ldots, n_k)).$$

Proof. We present those parts of the proof of Lemma 5 that differ from the proof of Lemma 4.

Let $H_1 = S(n_1, n_2, \ldots, n_k)$ and $H_2 = S(n_1 - 1, n_2 + 1, \ldots, n_k) = S(n_1, n_2, \ldots, n_k) - v_1v_2 + v_1v_3$. We have $D_{H_1}(v_2, v) > D_{H_1}(v_3, v)$, thus $[D_{H_1}(v_2, v)]^b < [D_{H_1}(v_3, v)]^b$ since $b < 0$. Then

$$\begin{aligned} R &= \sum_{v \in V(H_1)\setminus F} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\ &\quad + \sum_{v \in F\setminus Z} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\ &< \sum_{v \in F\setminus Z} [d_{H_1}(v)]^a([D_{H_1}(v_2, v)]^b - [D_{H_1}(v_3, v)]^b) \\ &= (k^a - 2^a)[(n_1 - 1)^b - n_2^b] \leq 0, \end{aligned}$$

since $(n_1 - 1)^b - n_2^b < 0$ for $n_1 - 1 > n_2$ and $b < 0$. For $v \in V(H_1)\setminus F$, we have $D_{H_1}(v_1, v) > D_{H_2}(v_1, v)$, thus $[D_{H_1}(v_1, v)]^b < [D_{H_2}(v_1, v)]^b$, since $b < 0$. Then

$$\begin{aligned} P &= \sum_{v \in V(H_1)\setminus F} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)]^b - [D_{H_2}(v_1, v)]^b) \\ &\quad + \sum_{v \in F\setminus Z} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)^b] - [D_{H_2}(v_1, v)]^b) \\ &< \sum_{v \in F\setminus Z} [d_{H_1}(v)]^a([D_{H_1}(v_1, v)]^b - [D_{H_2}(v_1, v)]^b) \end{aligned}$$

$$= \quad (k^a - 2^a)[n_1^b - (n_2+1)^b] \leq 0,$$

since $n_1^b - (n_2+1)^b < 0$ for $n_1 > n_2 + 1$ and $b < 0$. We have $R < 0$, $P < 0$ and $2^a \geq 1$ for $a \geq 0$, thus

$$Gut_{a,b}(H_1) - Gut_{a,b}(H_2) = P + (2^a - 1)R < 0.$$

Hence $Gut_{a,b}(H_1) < Gut_{a,b}(H_2)$. ■

In Theorems 6 and 7, we obtain bounds on the $Gut_{a,b}$ index of starlike trees for $a \geq 0$ and $b > 0$.

Theorem 6. *Let $a \geq 0$ and $b > 0$. For any starlike tree G with n vertices and maximum degree k, where $3 \leq k \leq n-1$, we have*

$$Gut_{a,b}(G) \geq Gut_{a,b}(S_n'').$$

The equality holds only if G is S_n''.

Proof. Let G' be any starlike tree of order n and maximum degree k with the smallest $Gut_{a,b}$ index. Let us show that G' is S_n''.

Assume to the contrary that G' is not S_n''. So G' is $S(n_1, n_2, \ldots, n_k)$ and there exist i and j, where $1 \leq i < j \leq k$, such that $|n_i - n_j| \geq 2$. Without loss of generality, assume that $n_1 - n_2 \geq 2$. By Lemma 4

$$Gut_{a,b}(S(n_1, n_2, \ldots, n_k)) > Gut_{a,b}(S(n_1 - 1, n_2 + 1, \ldots, n_k)).$$

Hence, $S(n_1, n_2, \ldots, n_k)$ does not have the smallest $Gut_{a,b}$ index, which is a contradiction. ■

Theorem 7. *Let $a \geq 0$ and $b > 0$. For any starlike tree G with n vertices and maximum degree k, where $3 \leq k \leq n-1$, we have*

$$Gut_{a,b}(G) \leq Gut_{a,b}(S_n').$$

The equality holds only if G is S_n'.

Proof. Let G' be any starlike tree with n vertices and maximum degree k having the largest $Gut_{a,b}$ index. We prove that G' is S_n'.

Assume to the contrary that G' is not S''_n. So, G' is $S(n_1, n_2, \ldots, n_k)$ and there exist i and j, where $1 \leq i < j \leq k$, such that $n_i, n_j \geq 2$. Without loss of generality, we can assume that $n_1 \geq n_2 \geq 2$. From Lemma 4

$$Gut_{a,b}(S(n_1 + 1, n_2 - 1, \ldots, n_k)) > Gut_{a,b}(S(n_1, n_2, \ldots, n_k)).$$

Hence, $S(n_1, n_2, \ldots, n_k)$ does not have the largest $Gut_{a,b}$ index, which is a contradiction. ■

Lemma 4 was used to obtain bounds for the $Gut_{a,b}$ index of starlike trees if $a \geq 0$ and $b > 0$. Similarly, Lemma 5 can be used to obtain bounds on the $Gut_{a,b}$ index for starlike trees if $a \geq 0$ and $b < 0$.

Theorem 8. *Let $a \geq 0$ and $b < 0$. For any starlike tree G with n vertices and maximum degree k, where $3 \leq k \leq n - 1$, we have*

$$Gut_{a,b}(S'_n) \leq Gut_{a,b}(G) \leq Gut_{a,b}(S''_n).$$

The first equality holds only if G is S'_n and the second equality holds only if G is S''_n.

3 Conclusion

In this paper, we generalized the Gutman index and presented some first results on the general Gutman index. Let us state several problems open for future research.

Problem 9. *Find a tree with the smallest or a tree having the largest $Gut_{a,b}$ index among trees with given order for some a and b.*

Problem 10. *Find bounds on the $Gut_{a,b}$ index for unicyclic graphs and bicyclic graphs graphs with given order for some a and b.*

Problem 11. *Find a sharp lower bound or an upper bound on the $Gut_{a,b}$ index for graphs with given order and vertex connectivity for some a and b.*

Problem 12. *Find bounds on the general Gutman index for graphs with given order and number of pendant vertices.*

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References

[1] V. Andova, D. Dimitrov, J. Fink, R. Škrekovski, Bounds on Gutman index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 515–524.

[2] S. Chen, Cacti with the smallest, second smallest, and third smallest Gutman index, *J. Comb. Optim.* **31** (2016) 327–332.

[3] X. Cheng, X. Li, Extremal general Gutman index of trees, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 567–582.

[4] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, The edge-Wiener index of a graph, *Discr. Math.* **309** (2009) 3452–3457.

[5] K. C. Das, G. Su, L. Xiong, Relation between degree distance and Gutman index of graphs, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 221–232.

[6] L. Feng, The Gutman index of unicyclic graphs, *Discr. Math. Algor. Appl.* **4** (2012) 669–708.

[7] L. Feng, W. Liu, The maximal Gutman index of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 699–708.

[8] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[9] M. Knor, P. Potočnik, R. Škrekovski, Relationship between the edge-Wiener index and the Gutman index of a graph, *Discr. Appl. Math.* **167** (2014) 197–201.

[10] Y. Mao, K. C. Das, Steiner Gutman index, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 779–794.

[11] J. P. Mazorodze, S. Mukwembi, T. Vetrík, On the Gutman index and minimum degree, *Discr. Appl. Math.* **173** (2014) 77–82.

[12] J. P. Mazorodze, S. Mukwembi, T. Vetrík, The Gutman index and the edge-Wiener index of graphs with given vertex-connectivity, *Discuss. Math. Graph Theory* **36** (2016) 867–876.

[13] J. P. Mazorodze, S. Mukwembi, T. Vetrík, Gutman index, edge-Wiener index and edge-connectivity, *Trans. Comb.* **9** (2020) 231–242.

[14] S. Mukwembi, On the upper bound of Gutman index of graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 343–348.

[15] T. Vetrík, M. Masre, Generalized eccentric connectivity index of trees and unicyclic graphs, *Discr. Appl. Math.* **284** (2020) 301–315.