

# Extremal General Gutman Index of Trees

Xin Cheng, Xueliang Li\*

*Center for Combinatorics and LPMC*

*Nankai University, Tianjin 300071, China*

xincheng@mail.nankai.edu.cn, lxl@nankai.edu.cn

(Received April 25, 2022)

## Abstract

The general Gutman index was introduced by Das and Vetrík very recently. For a graph  $G$ , the general Gutman index is defined by

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

where  $\alpha, \beta \in \mathbb{R}$ ,  $D_G(u, v)$  denotes the distance between  $u$  and  $v$  in  $G$ , and  $d_G(u)$  and  $d_G(v)$  denote the degrees of  $u$  and  $v$  in  $G$ , respectively. We show that for some  $\alpha$  and  $\beta$ , the general Gutman index decrease or increase with changing the adjacency of vertices. For some  $\alpha$  and  $\beta$ , we characterize trees of given order with the largest or the smallest general Gutman index.

## 1 Introduction

Topological indices provide a convenient method of translating chemical structures to numerical values, and they have been used in many fields such as chemical documentation, medicine design and so on.

We denote the vertex-set and the edge-set of a graph  $G$  by  $V(G)$  and  $E(G)$ , respectively. The order of  $G$  is the number of vertices in  $G$ . The set of neighbors of a vertex  $v \in G$  is denoted by  $N_G(v)$ , which is the set of vertices adjacent to  $v$  in  $G$ . The degree of a vertex  $v$ ,  $d_G(v)$ , is the size of

---

\*Corresponding author.

$N_G(v)$ . The distance  $D_G(u, v)$  between vertices  $u, v \in V(G)$  is the number of edges in a shortest path between  $u$  and  $v$  in  $G$ . We denote by  $P_n$  a path of order  $n$  and by  $S_n$  a star of order  $n$ .

The Gutman index,  $Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u)d_G(v)D_G(u, v)$ , is one of the most well-known distance-based topological indices and therefore has been well studied; see [6] for example. In fact, the Gutman index might be better called *ZZ-index*, for which we refer a paper [7] by Gutman that stated some facts about the history of the index. Bounds on the Gutman index for graphs with maximum degree and minimum degree were studied in [1, 9], for unicyclic graphs were studied in [4, 5]. Some methods for calculating the Gutman index were studied in [2]. In [8], the authors generalized the concept of Gutman index by Steiner distance. Some other results on the Gutman index can be found in [10, 11].

The general Gutman index was introduced by Das and Vetrík very recently in [3]. For a graph  $G$ , the general Gutman index is defined by

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

where  $\alpha, \beta \in \mathbb{R}$ ,  $D_G(u, v)$  denotes the distance between  $u$  and  $v$  in  $G$ , and  $d_G(u)$  and  $d_G(v)$  denote the degrees of  $u$  and  $v$ , respectively. In this manuscript, Das and Vetrík obtained some 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. Their results are stated as follows.

**Theorem 1.** [3] *Let  $\alpha \leq 0$  and  $\beta \geq 0$ , where at least one of  $\alpha$  and  $\beta$  is not 0. For any  $k$ -partite graph  $G$  with  $n$  vertices, where  $2 \leq k \leq n$ ,*

$$Gut_{\alpha, \beta}(G) \geq Gut_{\alpha, \beta}(K_{n_1, n_2, \dots, n_k}).$$

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

**Theorem 2.** [3] *Let  $0 \leq \alpha < \frac{1}{2}$  and  $\beta \leq 0$ , where at least one of  $\alpha$  and*

$\beta$  is not 0. For any  $k$ -partite graph  $G$  with  $n$  vertices, where  $2 \leq k \leq n$ ,

$$Gut_{\alpha,\beta}(G) \leq Gut_{\alpha,\beta}(K_{n_1,n_2,\dots,n_k}).$$

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

**Theorem 3.** [3] Let  $\alpha \leq 0$  and  $\beta \geq 0$ , where at least one of  $\alpha$  and  $\beta$  is not 0. For any connected graph  $G$  with  $n$  vertices and chromatic number  $\chi$ , where  $2 \leq \chi \leq n$ ,

$$Gut_{\alpha,\beta}(G) \geq Gut_{\alpha,\beta}(K_{n_1,n_2,\dots,n_\chi}).$$

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

**Theorem 4.** [3] Let  $0 \leq \alpha < \frac{1}{2}$  and  $\beta \leq 0$ , where at least one of  $\alpha$  and  $\beta$  is not 0. For any graph  $G$  with  $n$  vertices and chromatic number  $\chi$ , where  $2 \leq \chi \leq n$ ,

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

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

A starlike tree is a tree which consists of some paths that have a common vertex. Let  $S'_n$  be a starlike tree of order  $n$  such that all lengths of the paths except one are equal to 1, and  $S''_n$  be a tree of order  $n$  such that all paths differ in length by less than 1.

**Theorem 5.** [3] Let  $\alpha \geq 0$  and  $\beta > 0$ . For any starlike tree  $G$  with  $n$  vertices and maximum degree  $k$ , where  $3 \leq k \leq n - 1$ , we have

$$Gut_{\alpha,\beta}(S''_n) \leq Gut_{\alpha,\beta}(G) \leq Gut_{\alpha,\beta}(S'_n).$$

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

**Theorem 6.** [3] Let  $\alpha \geq 0$  and  $\beta < 0$ . For any starlike tree  $G$  with  $n$

vertices and maximum degree  $k$ , where  $3 \leq k \leq n - 1$ , we have

$$Gut_{\alpha,\beta}(S'_n) \leq Gut_{\alpha,\beta}(G) \leq Gut_{\alpha,\beta}(S''_n).$$

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

Several topological indices can be seen as special cases of the general Gutman index. For  $\alpha = 1$  and  $\beta = 1$ ,  $Gut_{\alpha,\beta}(G)$  is the classical Gutman index. For  $\alpha = 0$  and  $\beta = 1$ ,  $Gut_{\alpha,\beta}(G)$  is the Wiener index. For  $\alpha = 0$  and  $\beta = -1$ ,  $Gut_{\alpha,\beta}(G)$  is the Harary index. The results for these special indices are special cases of the general Gutman index. So, the concept of general Gutman index is very interesting and important, and thus it makes sense to study it, extensively.

In this paper, we show that for some  $\alpha$  and  $\beta$ , the general Gutman index decreases or increases with changing the adjacency of vertices, and we characterize trees of given order with the largest or the smallest general Gutman index for some values of  $\alpha$  and  $\beta$ .

The outline of this paper is as follows. In Section 2, we discuss three operations on trees. In Section 3, we show that for some values of  $\alpha$  and  $\beta$ , the trees of given order with the largest or the smallest general Gutman index is a path or a star. In Section 4, we conclude this paper with some remarks.

## 2 Three operations on trees

In this section we will introduce three kinds of operations on trees, and estimate the changes of values of the general Gutman index.

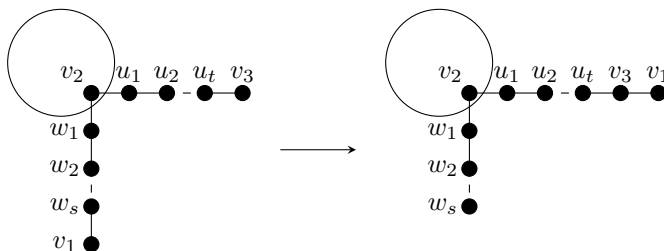
### 2.1 Operation 1 on trees

Let  $G$  be a graph with two paths  $P' = u_1 u_2 \dots u_t v_3$  and  $P'' = w_1 w_2 \dots w_s v_1$ , where  $w_1, u_1 \in N_G(v_2)$  and  $v_1, v_3$  are pendent vertices. We obtain a new graph  $G_1$  by moving  $v_1$  to  $v_3$ , i.e.,  $G_1 = G - w_s v_1 + v_3 v_1$ ; see Figure 1. We divide  $V(G)$  into four parts  $V_1 = \{v_1, v_3, w_s\}$ ,  $V_2 = \{u_1, u_2, \dots, u_t\}$ ,

$V_3 = \{w_1, w_2, \dots, w_{s-1}\}$  and  $V_4 = V(G) - V_1 - V_2 - V_3$ . Without loss of generality, let  $1 \leq s \leq t$ .

For  $\{u, v\} \subseteq V_1$ ,

$$\begin{aligned}
 & \sum_{\{u,v\} \subseteq V_1} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u,v)]^\beta - \sum_{\{u,v\} \subseteq V_1} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\
 = & [d_{G_1}(v_1)d_{G_1}(v_3)]^\alpha [D_{G_1}(v_1, v_3)]^\beta - [d_G(v_1)d_G(v_3)]^\alpha [D_G(v_1, v_3)]^\beta \\
 & + [d_{G_1}(v_1)d_{G_1}(w_s)]^\alpha [D_{G_1}(v_1, w_s)]^\beta - [d_G(v_1)d_G(w_s)]^\alpha [D_G(v_1, w_s)]^\beta \\
 & + [d_{G_1}(v_3)d_{G_1}(w_s)]^\alpha [D_{G_1}(v_3, w_s)]^\beta - [d_G(v_3)d_G(w_s)]^\alpha [D_G(v_3, w_s)]^\beta \\
 = & 2^\alpha - (t+s+2)^\beta + (t+s+2)^\beta - 2^\alpha + 2^\alpha(t+s+1)^\beta - 2^\alpha(t+s+1)^\beta \\
 = & 0.
 \end{aligned} \tag{1}$$



**Figure 1.** Graph  $G$  and the resultant graph  $G_1$ .

For  $u \in V_1, v \in V_2$ ,

$$\begin{aligned}
 & \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u,v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\
 = & \sum_{v \in V_2} \{ [d_{G_1}(v_1)d_{G_1}(v)]^\alpha [D_{G_1}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \\
 & + \sum_{v \in V_2} \{ [d_{G_1}(v_3)d_{G_1}(v)]^\alpha [D_{G_1}(v_3, v)]^\beta - [d_G(v_3)d_G(v)]^\alpha [D_G(v_3, v)]^\beta \} \\
 & + \sum_{v \in V_2} \{ [d_{G_1}(w_s)d_{G_1}(v)]^\alpha [D_{G_1}(w_s, v)]^\beta - [d_G(w_s)d_G(v)]^\alpha [D_G(w_s, v)]^\beta \} \\
 = & \sum_{v \in V_2} 2^\alpha [(t+2 - D_G(v_2, v))^\beta - (s+1 + D_G(v_2, v))^\beta] \\
 & + \sum_{v \in V_2} (4^\alpha - 2^\alpha)(t+1 - D_G(v_2, v))^\beta + \sum_{v \in V_2} (2^\alpha - 4^\alpha)(s + D_G(v_2, v))^\beta
 \end{aligned}$$

$$\begin{aligned}
&= \sum_{v \in V_2} \{2^\alpha [(t+2 - D_G(v_2, v))^\beta - (s+1 + D_G(v_2, v))^\beta] \\
&\quad + (4^\alpha - 2^\alpha) [(t+1 - D_G(v_2, v))^\beta - (s + D_G(v_2, v))^\beta]\} \\
&= \sum_{D=1}^t \{2^\alpha [(t+2 - D)^\beta - (s+1 + D)^\beta] \\
&\quad + (4^\alpha - 2^\alpha) [(t+1 - D)^\beta - (s + D)^\beta]\}. \tag{2}
\end{aligned}$$

For  $u \in V_1, v \in V_3$ ,

$$\begin{aligned}
&\sum_{\substack{u \in V_1 \\ v \in V_3}} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
&= \sum_{v \in V_3} \{[d_{G_1}(v_1)d_{G_1}(v)]^\alpha [D_{G_1}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta\} \\
&\quad + \sum_{v \in V_3} \{[d_{G_1}(v_3)d_{G_1}(v)]^\alpha [D_{G_1}(v_3, v)]^\beta - [d_G(v_3)d_G(v)]^\alpha [D_G(v_3, v)]^\beta\} \\
&\quad + \sum_{v \in V_3} \{[d_{G_1}(w_s)d_{G_1}(v)]^\alpha [D_{G_1}(w_s, v)]^\beta - [d_G(w_s)d_G(v)]^\alpha [D_G(w_s, v)]^\beta\} \\
&= \sum_{v \in V_3} 2^\alpha [(t+2 + D_G(v_2, v))^\beta - (s+1 - D_G(v_2, v))^\beta] \\
&\quad + \sum_{v \in V_3} (4^\alpha - 2^\alpha)(t+1 + D_G(v_2, v))^\beta + \sum_{v \in V_3} (2^\alpha - 4^\alpha)(s - D_G(v_2, v))^\beta \\
&= \sum_{v \in V_3} \{2^\alpha [(t+2 + D_G(v_2, v))^\beta - (s+1 - D_G(v_2, v))^\beta] \\
&\quad + (4^\alpha - 2^\alpha) [(t+1 + D_G(v_2, v))^\beta - (s - D_G(v_2, v))^\beta]\} \\
&= \sum_{D=1}^{s-1} \{2^\alpha [(t+2 + D)^\beta - (s+1 - D)^\beta] \\
&\quad + (4^\alpha - 2^\alpha) [(t+1 + D)^\beta - (s - D)^\beta]\}. \tag{3}
\end{aligned}$$

By adding Equation 2 to Equation 3, we get

$$\sum_{\substack{u \in V_1 \\ v \in V_2}} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta$$

$$\begin{aligned}
& + \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
& = 2^\alpha \left\{ \left[ \sum_{D=2}^{s+t+1} D^\beta - (t+2)^\beta \right] - \left[ \sum_{D=2}^{s+t+1} D^\beta - (s+1)^\beta \right] \right\} \\
& \quad + (4^\alpha - 2^\alpha) \left\{ \left[ \sum_{D=1}^{s+t} D^\beta - (t+1)^\beta \right] - \left[ \sum_{D=1}^{s+t} D^\beta - s^\beta \right] \right\} \\
& = 2^\alpha [(s+1)^\beta - (t+2)^\beta] + (4^\alpha - 2^\alpha) [s^\beta - (t+1)^\beta]. \tag{4}
\end{aligned}$$

For  $u \in V_1, v \in V_4$ ,

$$\begin{aligned}
& \sum_{\substack{u \in V_1 \\ v \in V_4}} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_4}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
& = \sum_{v \in V_4} \{ [d_{G_1}(v_1)d_{G_1}(v)]^\alpha [D_{G_1}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \\
& \quad + \sum_{v \in V_4} \{ [d_{G_1}(v_3)d_{G_1}(v)]^\alpha [D_{G_1}(v_3, v)]^\beta - [d_G(v_3)d_G(v)]^\alpha [D_G(v_3, v)]^\beta \} \\
& \quad + \sum_{v \in V_4} \{ [d_{G_1}(w_s)d_{G_1}(v)]^\alpha [D_{G_1}(w_s, v)]^\beta - [d_G(w_s)d_G(v)]^\alpha [D_G(w_s, v)]^\beta \} \\
& = \sum_{v \in V_4} d_G(v)^\alpha [(t+2 + D_G(v_2, v))^\beta - (s+1 + D_G(v_2, v))^\beta] \\
& \quad + \sum_{v \in V_4} d_G(v)^\alpha (2^\alpha - 1)(t+1 + D_G(v_2, v))^\beta \\
& \quad + \sum_{v \in V_4} d_G(v)^\alpha (1 - 2^\alpha)(s + D_G(v_2, v))^\beta \\
& = \sum_{v \in V_4} d_G(v)^\alpha \{ [(t+2 + D_G(v_2, v))^\beta - (s+1 + D_G(v_2, v))^\beta] \\
& \quad + (2^\alpha - 1)[(t+1 + D_G(v_2, v))^\beta - (s + D_G(v_2, v))^\beta] \}. \tag{5}
\end{aligned}$$

For  $\{u, v\} \subseteq V(G) - V_1$ , it is obvious that

$$\sum_{\{u, v\} \not\subseteq V_1} [d_{G_1}(u)d_{G_1}(v)]^\alpha [D_{G_1}(u, v)]^\beta = \sum_{\{u, v\} \not\subseteq V_1} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta,$$

since the degrees and distance between  $u$  and  $v$  are not change.

We begin with a lemma that is frequently used in subsequent proofs.

**Lemma 1.** *Let  $0 < x_1 < x_2, y > 0$  and  $f(x) = x^a$ . Then for  $a > 1$  or  $a < 0$ , we have  $f(x_1 + y) - f(x_1) < f(x_2 + y) - f(x_2)$ . For  $0 < a < 1$ , we have  $f(x_1 + y) - f(x_1) > f(x_2 + y) - f(x_2)$ .*

The proof of this lemma is simple and we omit it.

**Lemma 2.** *Let  $\alpha \geq 0$  and  $\beta > 0$ , we have*

$$Gut_{\alpha,\beta}(G_1) > Gut_{\alpha,\beta}(G).$$

*Proof.* For Equation 5, it is easy to obtain that  $[(t+2+D_G(v_2, v))^\beta - (s+1+D_G(v_2, v))^\beta] + (2^\alpha - 1)[(t+1+D_G(v_2, v))^\beta - (s+D_G(v_2, v))^\beta] > 0$  for  $\alpha \geq 0$  and  $\beta > 0$ , since  $s \leq t$ . In particular, if  $v$  is  $v_2$  in Equation 5, we have that

$$\begin{aligned} & d_G(v_2)^\alpha \{[(t+2+D_G(v_2, v))^\beta - (s+1+D_G(v_2, v))^\beta] \\ & + (2^\alpha - 1)[(t+1+D_G(v_2, v))^\beta - (s+D_G(v_2, v))^\beta]\} \\ = & d_G(v_2)^\alpha \{[(t+2)^\beta - (s+1)^\beta] + (2^\alpha - 1)[(t+1)^\beta - s^\beta]\} \\ \geq & 2^\alpha \{[(t+2)^\beta - (s+1)^\beta] + (2^\alpha - 1)[(t+1)^\beta - s^\beta]\}. \end{aligned}$$

Thus, the sum of Equations 4 and 5 greater than 0. So,  $Gut_{\alpha,\beta}(G_1) > Gut_{\alpha,\beta}(G)$ . The proof is thus complete.  $\blacksquare$

**Lemma 3.** *For  $\alpha \geq 0$  and  $\beta < 0$ , we have*

$$Gut_{\alpha,\beta}(G_1) < Gut_{\alpha,\beta}(G).$$

The proof is similar to that of Lemma 2 and we omit it.

## 2.2 Operation 2 on trees

Let  $G$  be a graph with pendent vertex  $v_1$  and path  $P' = u_1u_2 \dots u_tv_3$ , where  $v_1, u_1 \in N_G(v_2)$  and  $v_3$  is a pendent vertex. We obtain a new graph  $G_2$  by moving  $v_1$  to  $v_3$ , i.e.,  $G_2 = G - v_2v_1 + v_3v_1$ ; see Figure 2. We divide  $V(G)$  into three parts  $V_1 = \{v_1, v_2, v_3\}$ ,  $V_2 = \{u_1, u_2, \dots, u_t\}$  and  $V_3 = V(G) - V_1 - V_2$ .



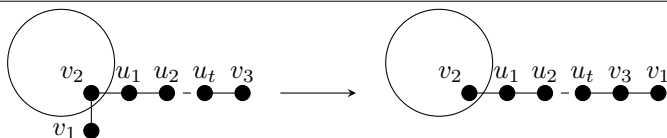


Figure 2. Graph  $G$  and the resultant graph  $G_2$ .

For  $\{u, v\} \subseteq V_1$ ,

$$\begin{aligned}
 & \sum_{\{u,v\} \subseteq V_1} [d_{G_2}(u)d_{G_2}(v)]^\alpha [D_{G_2}(u,v)]^\beta - \sum_{\{u,v\} \subseteq V_1} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\
 = & [d_{G_2}(v_1)d_{G_2}(v_2)]^\alpha [D_{G_2}(v_1, v_2)]^\beta - [d_G(v_1)d_G(v_2)]^\alpha [D_G(v_1, v_2)]^\beta \\
 & + [d_{G_2}(v_1)d_{G_2}(v_3)]^\alpha [D_{G_2}(v_1, v_3)]^\beta - [d_G(v_1)d_G(v_3)]^\alpha [D_G(v_1, v_3)]^\beta \\
 & + [d_{G_2}(v_2)d_{G_2}(v_3)]^\alpha [D_{G_2}(v_2, v_3)]^\beta - [d_G(v_2)d_G(v_3)]^\alpha [D_G(v_2, v_3)]^\beta \\
 = & (d_G(v_2) - 1)^\alpha (t + 2)^\beta - d_G(v_2)^\alpha + 2^\alpha - (t + 2)^\beta \\
 & + [2^\alpha (d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] (t + 1)^\beta. \tag{6}
 \end{aligned}$$

For  $u \in V_1, v \in V_2$ ,

$$\begin{aligned}
 & \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_{G_2}(u)d_{G_2}(v)]^\alpha [D_{G_2}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
 = & \sum_{v \in V_2} \{ [d_{G_2}(v_1)d_{G_2}(v)]^\alpha [D_{G_2}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \\
 & + \sum_{v \in V_2} \{ [d_{G_2}(v_2)d_{G_2}(v)]^\alpha [D_{G_2}(v_2, v)]^\beta - [d_G(v_2)d_G(v)]^\alpha [D_G(v_2, v)]^\beta \} \\
 & + \sum_{v \in V_2} \{ [d_{G_2}(v_3)d_{G_2}(v)]^\alpha [D_{G_2}(v_3, v)]^\beta - [d_G(v_3)d_G(v)]^\alpha [D_G(v_3, v)]^\beta \} \\
 = & \sum_{v \in V_2} 2^\alpha [(t + 2 - D_G(v_2, v))^\beta - (D_G(v_2, v) + 1)^\beta] \\
 & + \sum_{v \in V_2} 2^\alpha [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D_G(v_2, v)^\beta \\
 & + \sum_{v \in V_2} (4^\alpha - 2^\alpha) (t + 1 - D_G(v_2, v))^\beta \\
 = & 2^\alpha \sum_{D=1}^t \{ [(t + 2 - D)^\beta - (D + 1)^\beta] + [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D^\beta \}
 \end{aligned}$$

$$\begin{aligned}
& + [(2^\alpha - 1)(t + 1 - D)^\beta] \} \\
= & 2^\alpha [2^\alpha - 1 + (d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] \sum_{D=1}^t D^\beta. \tag{7}
\end{aligned}$$

For  $u \in V_1, v \in V_3$ ,

$$\begin{aligned}
& \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_{G_2}(u)d_{G_2}(v)]^\alpha [D_{G_2}(u, v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
= & \sum_{v \in V_3} \{ [d_{G_2}(v_1)d_{G_2}(v)]^\alpha [D_{G_2}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \\
& + \sum_{v \in V_3} \{ [d_{G_2}(v_2)d_{G_2}(v)]^\alpha [D_{G_2}(v_2, v)]^\beta - [d_G(v_2)d_G(v)]^\alpha [D_G(v_2, v)]^\beta \} \\
& + \sum_{v \in V_3} \{ [d_{G_2}(v_3)d_{G_2}(v)]^\alpha [D_{G_2}(v_3, v)]^\beta - [d_G(v_3)d_G(v)]^\alpha [D_G(v_3, v)]^\beta \} \\
= & \sum_{v \in V_3} d_G(v)^\alpha [(D_G(v_2, v) + t + 2)^\beta - (D_G(v_2, v) + 1)^\beta] \\
& + \sum_{v \in V_3} d_G(v)^\alpha [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D_G(v_2, v)^\beta \\
& + \sum_{v \in V_3} d_G(v)^\alpha (2^\alpha - 1)(t + 1 + D_G(v_2, v))^\beta \\
= & \sum_{v \in V_3} d_G(v)^\alpha \{ [(D_G(v_2, v) + t + 2)^\beta - (D_G(v_2, v) + 1)^\beta] \\
& + [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D_G(v_2, v)^\beta + (2^\alpha - 1)(t + 1 + D_G(v_2, v))^\beta \}. \tag{8}
\end{aligned}$$

For  $\{u, v\} \subseteq V_2 \cup V_3$ , it is obvious that

$$\sum_{\{u, v\} \not\subseteq V_1} [d_{G_2}(u)d_{G_2}(v)]^\alpha [D_{G_2}(u, v)]^\beta = \sum_{\{u, v\} \not\subseteq V_1} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta,$$

since the degrees and distance between  $u$  and  $v$  are not change.

**Lemma 4.** *Let  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0. Then we have*

$$Gut_{\alpha, \beta}(G_2) > Gut_{\alpha, \beta}(G).$$

*Proof.* In fact, for  $\alpha \geq 0, \beta \geq 0$ , Equation 6 not less than 0, since

$$\begin{aligned} & (d_G(v_2) - 1)^\alpha (t + 2)^\beta - d_G(v_2)^\alpha + 2^\alpha - (t + 2)^\beta \\ & + [2^\alpha (d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] (t + 1)^\beta \\ & \geq 2^\alpha (d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha + (d_G(v_2) - 1)^\alpha - 1 + 2^\alpha - d_G(v_2)^\alpha \\ & \geq 0, \end{aligned}$$

the last equality obtained by Lemma 1 and at least one of the two inequalities strictly holds.

We can obtain that Equation 7 is not less than 0 for  $0 \leq \alpha \leq 1$  by Lemma 1.

For Equation 8, we have

$$\begin{aligned} & [(D_G(v_2, v) + t + 2)^\beta - (D_G(v_2, v) + 1)^\beta] \\ & + [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D_G(v_2, v)^\beta + [(2^\alpha - 1)(t + 1 + D_G(v_2, v))^\beta] \\ & \geq [(d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha] D_G(v_2, v)^\beta + [(2^\alpha - 1)(t + 1 + D_G(v_2, v))^\beta] \\ & \geq (d_G(v_2) - 1)^\alpha - d_G(v_2)^\alpha + (2^\alpha - 1) \\ & \geq 0, \end{aligned}$$

the last equality obtained by Lemma 1.

Thus, for  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$ , and at least one of  $\alpha$  and  $\beta$  is not 0, we have that  $Gut_{\alpha, \beta}(G_2) > Gut_{\alpha, \beta}(G)$  holds. The proof is this complete. ■

**Lemma 5.** *Let  $\alpha \leq 0$  and  $\beta \leq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0. Then we have*

$$Gut_{\alpha, \beta}(G_2) < Gut_{\alpha, \beta}(G).$$

The proof is similar to that of Lemma 4 and we omit it.

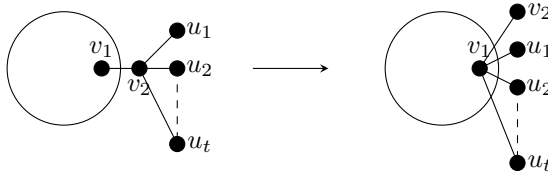
## 2.3 Operation 3 on trees

Let  $G$  be a graph with  $t \geq 1$  pendent vertices  $\{u_1, u_2, \dots, u_t\}$  which are adjacent to  $v_2$ , and  $v_1$  is adjacent to  $v_2$  too. We obtain a new graph  $G_3$  by moving  $\{u_1, u_2, \dots, u_t\}$  to  $v_1$ , i.e.,  $G_3 = G - \{v_2 u_1, v_2 u_2, \dots, v_2 u_t\} +$

$\{v_1u_1, v_1u_2, \dots, v_1u_t\}$ ; see Figure 3. We divide  $V(G)$  into three parts  $V_1 = \{v_1, v_2\}$ ,  $V_2 = \{u_1, u_2, \dots, u_t\}$  and  $V_3 = V(G) - V_1 - V_2$ .

For  $\{u, v\} \subseteq V_1$ ,

$$\begin{aligned} & \sum_{\{u,v\} \subseteq V_1} [d_{G_3}(u)d_{G_3}(v)]^\alpha [D_{G_3}(u,v)]^\beta - \sum_{\{u,v\} \subseteq V_1} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\ &= [d_{G_3}(v_1)d_{G_3}(v_2)]^\alpha [D_{G_3}(v_1, v_2)]^\beta - [d_G(v_1)d_G(v_2)]^\alpha [D_G(v_1, v_2)]^\beta \\ &= (t + d_G(v_1))^\alpha - (t + 1)^\alpha d_G(v_1)^\alpha. \end{aligned} \tag{9}$$



**Figure 3.** Graph  $G$  and the resultant graph  $G_3$ .

For  $u \in V_1, v \in V_2$ ,

$$\begin{aligned} & \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_{G_3}(u)d_{G_3}(v)]^\alpha [D_{G_3}(u,v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_2}} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\ &= \sum_{v \in V_2} \{ [d_{G_3}(v_1)d_{G_3}(v)]^\alpha [D_{G_3}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \\ & \quad + \sum_{v \in V_2} \{ [d_{G_3}(v_2)d_{G_3}(v)]^\alpha [D_{G_3}(v_2, v)]^\beta - [d_G(v_2)d_G(v)]^\alpha [D_G(v_2, v)]^\beta \} \\ &= \sum_{v \in V_2} [(t + d_G(v_1))^\alpha - 2^\beta d_G(v_1)^\alpha] + \sum_{v \in V_2} [2^\beta - (t + 1)^\alpha] \\ &= \sum_{v \in V_2} [2^\beta (1 - d_G(v_1)^\alpha) + (t + d_G(v_1))^\alpha - (t + 1)^\alpha]. \end{aligned} \tag{10}$$

For  $u \in V_1, v \in V_3$ ,

$$\begin{aligned} & \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_{G_3}(u)d_{G_3}(v)]^\alpha [D_{G_3}(u,v)]^\beta - \sum_{\substack{u \in V_1 \\ v \in V_3}} [d_G(u)d_G(v)]^\alpha [D_G(u,v)]^\beta \\ &= \sum_{v \in V_2} \{ [d_{G_3}(v_1)d_{G_3}(v)]^\alpha [D_{G_3}(v_1, v)]^\beta - [d_G(v_1)d_G(v)]^\alpha [D_G(v_1, v)]^\beta \} \end{aligned}$$

$$\begin{aligned}
& + \sum_{v \in V_2} \{ [d_{G_3}(v_2)d_{G_3}(v)]^\alpha [D_{G_3}(v_2, v)]^\beta - [d_G(v_2)d_G(v)]^\alpha [D_G(v_2, v)]^\beta \} \\
& = \sum_{v \in V_2} [(t + d_G(v_1))^\alpha d_G(v)^\alpha D_G(v_1, v)^\beta - d_G(v_1)^\alpha d_G(v)^\alpha D_G(v_1, v)^\beta] \\
& \quad + \sum_{v \in V_2} [d_G(v)^\alpha (D_G(v_1, v) + 1)^\beta - (t + 1)^\alpha d_G(v)^\alpha (D_G(v_1, v) + 1)^\beta] \\
& = \sum_{v \in V_2} d_G(v)^\alpha \{ (D_G(v_1, v) + 1)^\beta [1 - (t + 1)^\alpha] \\
& \quad + D_G(v_1, v)^\beta [(t + d_G(v_1))^\alpha - d_G(v_1)^\alpha] \}. \tag{11}
\end{aligned}$$

For  $u \in V_2, v \in V_3$ ,

$$\begin{aligned}
& \sum_{\substack{u \in V_2 \\ v \in V_3}} [d_{G_3}(u)d_{G_3}(v)]^\alpha [D_{G_3}(u, v)]^\beta - \sum_{\substack{u \in V_2 \\ v \in V_3}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta \\
& = \sum_{u \in V_2, v \in V_3} d_G(v)^\alpha [(D_G(u, v) - 1)^\beta - D_G(u, v)^\beta]. \tag{12}
\end{aligned}$$

For  $\{u, v\} \subseteq V_2$  or  $\{u, v\} \subseteq V_3$ , it is obvious that

$$\sum_{\{u, v\}} [d_{G_3}(u)d_{G_3}(v)]^\alpha [D_{G_3}(u, v)]^\beta = \sum_{\{u, v\}} [d_G(u)d_G(v)]^\alpha [D_G(u, v)]^\beta,$$

since the degrees and distance between  $u$  and  $v$  are not change.

**Lemma 6.** *Let  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0. Then we have*

$$Gut_{\alpha, \beta}(G_3) < Gut_{\alpha, \beta}(G).$$

*Proof.* For  $\alpha \geq 0$ , Equation 9 is not greater than 0.

For  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$ , we have that  $2^\beta(1 - d_G(v_1)^\alpha) + (t + d_G(v_1))^\alpha - (t + 1)^\alpha \leq 0$  by Lemma 1. Thus, Equation 10 is not greater than 0. This is similar to Equation 11.

For  $\beta \geq 0$ ,  $d_G(v)^\alpha [(D_G(u, v) - 1)^\beta - D_G(u, v)^\beta] \leq 0$ . Thus, Equation 12 is not greater than 0.

Since at least one of  $\alpha$  and  $\beta$  is not 0, there exists an equation above less than 0. So,  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$ , and at least one of  $\alpha$  and  $\beta$  is not 0,

we then have  $Gut_{\alpha,\beta}(G_3) < Gut_{\alpha,\beta}(G)$ . The proof thus is complete. ■

**Lemma 7.** *Let  $\alpha \leq \beta \leq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0. Then we have*

$$Gut_{\alpha,\beta}(G_3) > Gut_{\alpha,\beta}(G).$$

The proof is similar to that of Lemma 6 and we omit it.

### 3 Extremal results for trees

Now we are ready to present and prove our main results of this paper.

**Theorem 7.** *Let  $T$  be a tree of order  $n$ . For  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0, we have*

$$\begin{aligned} (n-1)^{\alpha+1} + 2^{\beta-1}(n-1)(n-2) &= \\ Gut_{\alpha,\beta}(S_n) \leq Gut_{\alpha,\beta}(T) \leq Gut_{\alpha,\beta}(P_n) & \\ = 2^{\alpha+1} \sum_{k=1}^{n-2} k^\beta + 4^\alpha \sum_{\substack{k_1+k_2=n-2 \\ k_1, k_2 \geq 1}} k_1 k_2^\beta + (n-1)^\beta. & \end{aligned}$$

*The first equality holds if and only if  $T$  is the star  $S_n$  and the second equality holds if and only if  $T$  is the path  $P_n$ .*

*Proof.* For  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0, we can apply Operations 1 and 2 on a given tree  $T$ . By Lemma 2 and Lemma 4, we know that the general Gutman index of the resultant trees increase in each step. Finally, we obtain a path of order  $n$ .

Similarly, we can apply Operation 3 on a given tree  $T$ . By Lemma 6, the general Gutman index of the resultant trees decrease in each step, and finally we obtain a star of order  $n$ .

The calculations of the general Gutman index for a path and a star are trivial and we omit it. The proof is now complete. ■

**Theorem 8.** *Let  $T$  be a tree of order  $n$ . For  $\forall v \in V(T)$  which  $d_G(v) \geq 3$ , there are at most two vertices adjacent to  $v$  with degree greater than 1.*

Then for  $\alpha \leq 0$ ,  $\beta \leq 0$ , and at least one of  $\alpha$  and  $\beta$  is not 0, we have

$$Gut_{\alpha,\beta}(P_n) \leq Gut_{\alpha,\beta}(T).$$

The equality holds if and only if  $T$  is the path  $P_n$ .

The proof is similar for Theorem 7 and we omit it.

**Theorem 9.** Let  $T$  be a tree of order  $n$ . For  $\alpha \leq \beta \leq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0, we have

$$Gut_{\alpha,\beta}(T) \leq Gut_{\alpha,\beta}(S_n).$$

The equality holds if and only if  $T$  is the star  $S_n$ .

The proof is similar to that of Theorem 7 and we omit it.

**Corollary.** Let  $T$  be a tree of order  $n$ . For  $\forall v \in V(T)$  with  $d_G(v) \geq 3$ , there are at most two vertices adjacent to  $v$  with degree greater than 1. Then for  $\alpha \leq \beta \leq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0, we have

$$Gut_{\alpha,\beta}(P_n) \leq Gut_{\alpha,\beta}(T) \leq Gut_{\alpha,\beta}(S_n).$$

The first equality holds if and only if  $T$  is the path  $P_n$  and the second equality holds if and only if  $T$  is the star  $S_n$ .

The proof is similar to that of Theorem 7 and we omit it.

## 4 Concluding remarks

In this paper, we give three kinds of operations on trees, and discuss the changes of values of the general Gutman index under these operations. By these operations, we obtain that for  $0 \leq \alpha \leq 1$  and  $\beta \geq 0$  such that at least one of  $\alpha$  and  $\beta$  is not 0, the lower bound of the general Gutman index for trees with given order is achieved by the star and the upper bound of the general Gutman index is achieved by the path. If  $T$  is a tree such that  $\forall v \in V(T)$  with  $d_G(v) \geq 3$ , there are at most two vertices adjacent to  $v$  with degree greater than 1, then for  $\alpha \leq \beta \leq 0$  such that at least one of  $\alpha$

and  $\beta$  is not 0, the lower bound of the general Gutman index is achieved by the path and upper bound of the general Gutman index is achieved by the star.

**Acknowledgment:** The authors are very grateful to the referees for helpful comments and suggestions. This work is supported by NSFC (Grant Nos. 11871034 and 12131013).

## References

- [1] V. Andova, D. Dimitrov, J. Fink, R. Skrekovski, Bounds on Gutman index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 515–524.
- [2] S. Brezovnik, N. Tratnik, New methods for calculating the degree distance and the Gutman index, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 111–132.
- [3] K. C. Das, T. Vetrík, General Gutman index of a graph, preprint.
- [4] L. Feng, The Gutman index of unicyclic graphs, *Discr. Math. Algorithms Appl.* **4** (2012) 669–708.
- [5] M. Feng, X. Yu, J. Zhang, W. Duan, The Gutman index of the unicyclic graphs with pendent edges, *J. Phys. Conf. Ser.* **2012** (2021) #012053.
- [6] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.
- [7] I. Gutman, Gutman index – a critical personal account, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **154** (2021) 183–193.
- [8] Y. Mao, K. C. Das, Steiner Gutman index, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 779–794.
- [9] J. P. Mazorodze, S. Mukwembi, T. Vetrík, On the Gutman index and minimum degree, *Discr. Appl. Math.* **173** (2014) 77–82.
- [10] A. Sadeghieh, N. Ghanbari, S. Alikhani, Computation of Gutman index of some cactus chains, *El. J. Graph Theory Appl.* **6** (2018) 138–150.
- [11] L. Wei, H. Bian, H. Yu, X. Yang, The Gutman index and Schultz index in the random phenylene chains, *Iran. J. Math. Chem.* **12** (2021) 67–78.