

## Article

# Investigation of General Sombor Index for Optimal Values in Bicyclic Graphs, Trees, and Unicyclic Graphs Using Well-Known Transformations

Miraj Khan <sup>1,†</sup> , Muhammad Yasin Khan <sup>1,†</sup> , Gohar Ali <sup>1,\*,†</sup>  and Ioan-Lucian Popa <sup>2,3,\*,†</sup> 

<sup>1</sup> Department of Mathematics, Islamia College Peshawar, Peshawar 25120, Khyber Pakhtunkhwa, Pakistan; mirajkhan283@gmail.com (M.K.); yasin.student@icp.edu.pk (M.Y.K.)

<sup>2</sup> Department of Computing, Mathematics and Electronics, 1 Decembrie 1918 University of Alba Iulia, 510009 Alba Iulia, Romania

<sup>3</sup> Faculty of Mathematics and Computer Science, Transilvania University of Brasov, Iuliu Maniu Street 50, 500091 Brasov, Romania

\* Correspondence: gohar.ali@icp.edu.pk (G.A.); lucian.popa@uab.ro (I.-L.P.)

† These authors contributed equally to this work.

**Abstract:** The field related to indices was developed by researchers for various purposes. Optimization is one of the purposes used by researchers in different situations. In this article, a generalized Sombor index is considered. This work is related to the idea of optimization in the families of bicyclic graphs, trees, and unicyclic graphs. We investigated optimal values in the stated families by means of well-known transformations. The transformations include the following: Transformation A, Transformation B, Transformation C, and Transformation D. Transformation A and Transformation B increase the value of the generalized Sombor index, while Transformation C and Transformation D are used for minimal values.

**Keywords:** general Sombor index; transformations; optimization; bicyclic graphs; trees; unicyclic graphs



Academic Editor: Michel Planat

Received: 13 May 2025

Revised: 5 June 2025

Accepted: 10 June 2025

Published: 18 June 2025

**Citation:** Khan, M.; Khan, M.Y.; Ali, G.; Popa, I.-L. Investigation of General Sombor Index for Optimal Values in Bicyclic Graphs, Trees, and Unicyclic Graphs Using Well-Known Transformations. *Symmetry* **2025**, *17*, 968. <https://doi.org/10.3390/sym17060968>

**Copyright:** © 2025 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

## 1. Introduction

Problems related to daily life can be diagrammatically represented on paper by means of circles or dots. The relationships between these dots can be drawn using curves or lines. Mathematically, the considered structures of dots and curves have provided the concept of graphs. A graph is a mathematical structure consisting of nodes (vertices) denoted by the set  $V(G)$ . The connection between dots is called an edge, and the edge set is denoted by  $E(G)$ . In symbols, we represent a graph by  $G = (V(G), E(G))$ . Here, the order of the considered graph is the total number of vertices, and the number of edges is the size of the graph. Let  $k, l$  be two vertices of an edge  $e$ , and we denote this edge by  $kl$ . An edge joining the same vertex is called a loop. The number of incident edges to a vertex  $k$  is called its degree and is denoted by  $d(k)$ . A simple graph can be defined as a graph without loops or with multiple edges between the same pair of vertices. Two or more edges are said to be parallel if these edges are between the same pair of vertices. Furthermore, we refer to [1–3]. In this article, simple and finite graphs are considered; i.e., both  $E(G)$  and  $V(G)$  are finite.

A number in graphical terms representing the structure of a chemical is called a topological descriptor. Using the structural invariant property, a topological descriptor does not affect graph labeling. A molecular property combined with a topological descriptor is called a topological index. Furthermore, we refer to [4]. In different situations, topological indices (TIs) measure the strength of connection in chemical compounds. The Wiener index

was the first topological index to be introduced. The idea of TIs leads the researchers to theoretical chemistry. We also refer to [5]. Although TIs were used in the field of chemical graph theory, applications of TIs have also been observed in other fields. Gutman and Mohar used topological indices in networks outside of chemical structures in 1996, referring to [6]. Otte and Rousseau investigated a social network using TIs in [7]. In [8], the authors investigated indices in networks that are interconnected.

In TIs, minimization and maximization are the fields of the most interest for various researchers. The desired field of optimization is related to chemical compounds in particular. Raman and Maranas created an algorithm for optimization combined with TIs that included Randić, Wiener and Kier indices [9]. In [2], the authors found optimal graphs for a general power–sum connectivity index in different classes. In [3], the authors investigated a second form of a general power–sum connectivity index in bicyclic graphs, trees, and unicyclic graphs. In [10], an interconnectivity index was optimized by the authors for polymers. In [11], simplex algorithms were used by the authors to optimize TIs for problems in chemical graph theory. In [12], Randić and Wiener indices were optimized for a terrain problem. In [13], upper and lower bounds for forgotten TIs were investigated. The authors provided new bounds for the  $F(G)$  index. In [14], sharp optimal bounds of a symmetric VDB TI were investigated regarding  $D_n$ . In [15], lower and upper bounds for TIs in trees were investigated. In [16], the authors investigated inequalities for TIs in unicyclic graphs, and extremal unicyclic graphs were also characterized. The desired family contains the variable first Zagreb index and some others. In [17], symmetries of regular gons were considered regarding the optimal values and communication properties of dihedral groups. Topological optimization schemes for designing waveguides with symmetries in rotation and reflection were considered in [18]. Furthermore, we refer to [19–21] and the references therein.

In this work, the generalized Sombor index is considered in bicyclic graphs, trees, and unicyclic graphs. Optimal values in the families are investigated by means of well-known transformations. The generalized Sombor (GSO) index for graph  $G$  is considered as follows:

$$GSO(G) = \sum_{\varphi\delta \in E(G)} ((d_G(\varphi))^2 + (d_G(\delta))^2)^\beta, \quad \beta \text{ is real number } \geq \frac{1}{2}.$$

## 2. Transformation for Greatest Value of Generalized Sombor Index

Transformation A: Let  $\mu v \in E(G)$  with  $2 \leq d(v)$ . Let  $N(\mu) = \{v, w_1, w_2, w_3, \dots, w_t\}$ . Let  $G' = G - \{\mu w_1, \mu w_2, \mu w_3, \dots, \mu w_t\} + \{vw_1, vw_2, vw_3, \dots, vw_t\}$  and  $w_1, w_2, w_3, \dots, w_t$  be vertices of degree one, as in Figure 1.

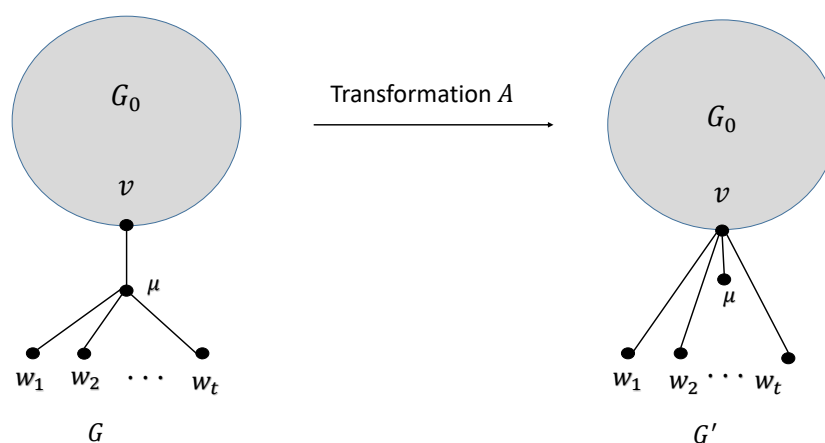


Figure 1. Graphs where Transformation A is applied on  $G$ , and  $G'$  is obtained.

**Lemma 1.** Let  $G$  be a graph, apply Transformation  $A$  on  $G$ , we obtain  $G'$  for which the following is true:

$$GSO(G') > GSO(G). \quad (1)$$

**Proof.** Using the definition of  $GSO$  for  $G'$ , we obtain

$$\begin{aligned} GSO(G') &= \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G'}(\theta))^2)^\beta + ((d_{G'}(v))^2 + (d_{G'}(\mu))^2)^\beta + ((d_{G'}(v))^2 + (d_{G'}(w_1))^2)^\beta \\ &\quad + \cdots + ((d_{G'}(v))^2 + (d_{G'}(w_t))^2)^\beta, \\ &= \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G'}(\theta))^2)^\beta + (t+1)((d_{G'}(v))^2 + 1)^\beta. \end{aligned} \quad (2)$$

Apply  $GSO$  on  $G$ , we obtain

$$\begin{aligned} GSO(G) &= \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_G(\theta))^2)^\beta + ((d_G(v))^2 + (d_G(\mu))^2)^\beta + ((d_G(\mu))^2 + (d_G(w_1))^2)^\beta \\ &\quad + ((d_G(\mu))^2 + (d_G(w_2))^2)^\beta + \cdots + ((d_G(\mu))^2 + (d_G(w_t))^2)^\beta, \\ &= \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_G(\theta))^2)^\beta + ((d_G(v))^2 + (d_G(\mu))^2)^\beta + t((d_G(\mu))^2 + 1)^\beta. \end{aligned} \quad (3)$$

We considered the difference (2)–(3), in the following

$$\begin{aligned} GSO(G') - GSO(G) &= \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G'}(\theta))^2)^\beta + (t+1)((d_{G'}(v))^2 + 1)^\beta \\ &\quad - \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_G(\theta))^2)^\beta - ((d_G(v))^2 + (d_G(\mu))^2)^\beta - t((d_G(\mu))^2 + 1)^\beta, \\ &= \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G'}(\theta))^2)^\beta + 2((d_{G'}(v))^2 + 1)^\beta + (t-1)((d_{G'}(v))^2 + 1)^\beta \\ &\quad - \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_G(\theta))^2)^\beta - ((d_G(v))^2 + (d_G(\mu))^2)^\beta - t((d_G(\mu))^2 + 1)^\beta, \\ &> 0. \end{aligned} \quad (4)$$

For positive value in Equation (4), it follows that

$$\begin{aligned} \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G'}(\theta))^2)^\beta &> \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_G(\theta))^2)^\beta, \\ (t-1)((d_{G'}(v))^2 + 1)^\beta &> t((d_G(\mu))^2 + 1)^\beta. \end{aligned} \quad (5)$$

As we have the following

$$\begin{aligned} (d_{G'}(v))^2 &> (d_G(v))^2, (d_{G'}(v))^2 > (d_G(\mu))^2, \\ \implies (d_{G'}(v))^2 + 1 &> (d_G(v))^2, (d_{G'}(v))^2 + 1 > (d_G(\mu))^2, \\ \implies 2((d_{G'}(v))^2 + 1)^\beta &> ((d_G(v))^2 + (d_G(\mu))^2)^\beta. \end{aligned} \quad (6)$$

From Equations (5) and (6), we obtain

$$GSO(G') > GSO(G).$$

□

**Remark 1.** Using Transformation A repeatedly, we transform any tree to a star and bicyclic or unicyclic graphs to bicyclic or unicyclic graphs where all the non-cyclic edges are pendent, respectively.

**Transformation B:** Consider  $\mu, v \in V(G)$ . Let adjacent leaves to  $\mu$  be  $u_\delta, u_{\delta-1}, \dots, u_2, u_1$ . Let adjacent leaves to  $v$  be  $v_t, v_{t-1}, \dots, v_2, v_1$ ,  $G'$  and  $G''$  are obtained such that  $G' = G + \{vu_1, vu_2, \dots, vu_\delta\} - \{\mu u_1, \mu u_2, \dots, \mu u_\delta\}$  and  $G'' = G - \{vv_1, vv_2, \dots, vv_t\} + \{\mu v_1, \mu v_2, \dots, \mu v_t\}$ , as shown in the Figure 2.

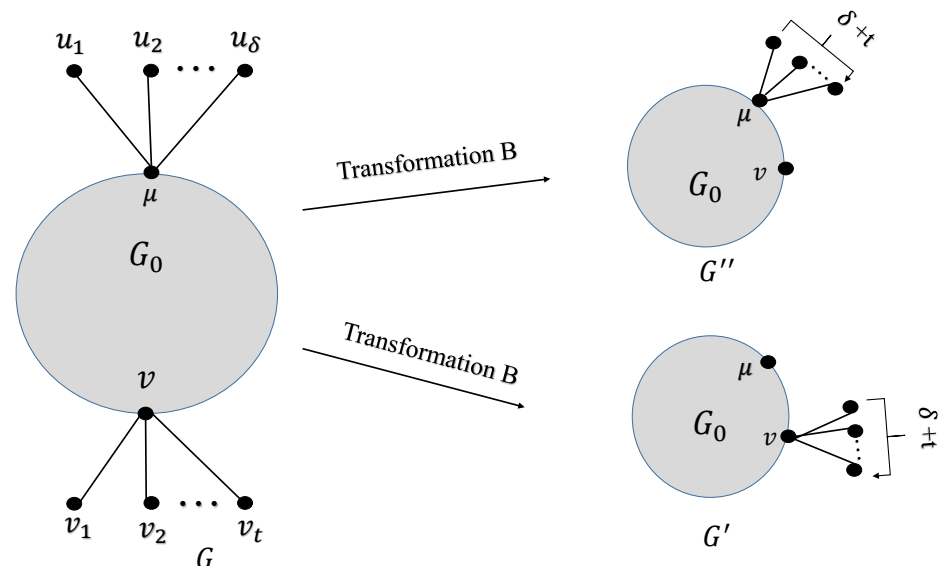


**Figure 2.** Transformation B is applied on  $G$ ,  $G'$  and  $G''$  are obtained. In  $G'$ , all the pendants are attached to  $v$ . In  $G''$ , all the pendent edges are attached to  $\mu$ .

**Lemma 2.** Consider graph  $G$ . Using Transformation B on  $G$ , we obtain  $G'$  and  $G''$ , then either  $GSO(G') > GSO(G)$  or  $GSO(G'') > GSO(G)$ .

**Proof.** Consider  $G_0 = \{v_t, v_{t-1}, \dots, v_2, v_1, u_\delta, u_{\delta-1}, \dots, u_2, u_1\}$ . The following cases are considered for  $G$ ,  $G'$  and  $G''$ .

Let  $d_{G_0}(\mu) = \xi$  and  $d_{G_0}(v) = \varphi$ .

**Case 1.** Consider  $G$ , if  $v$  and  $\mu$  are not connected directly by an edge, then for GSO we have

$$\begin{aligned}
 GSO(G) &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((d_G(\mu))^2 + (d_{G_0}(\theta))^2)^\beta \\
 &+ \sum_{\theta \in N_{G_0}(v)} ((d_G(v))^2 + (d_{G_0}(\theta))^2)^\beta + ((d_G(\mu))^2 + 1)^\beta + ((d_G(\mu))^2 + 1)^\beta \\
 &+ \dots + ((d_G(\mu))^2 + 1)^\beta + ((d_G(v))^2 + 1)^\beta + ((d_G(v))^2 + 1)^\beta + \dots + ((d_G(v))^2 + 1)^\beta, \\
 &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
 &+ \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta + \delta((\xi + \delta)^2 + 1)^\beta + t((\varphi + t)^2 + 1)^\beta.
 \end{aligned} \tag{7}$$

Consider  $G'$ , then GSO is given by

$$\begin{aligned} GSO(G') &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} (d_{G_0}(\mu)^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad + \sum_{\theta \in N_{G_0}(v)} ((d_{G'}(v))^2 + (d_{G_0}(\theta))^2)^\beta + ((d_{G'}(v))^2 + 1)^\beta + \cdots + ((d_{G'}(v))^2 + 1)^\beta, \\ &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta. \end{aligned}$$

Taking  $G''$ , then GSO is in the following

$$\begin{aligned} GSO(G'') &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} (d_{G''}(\mu)^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad + \sum_{\theta \in N_{G_0}(v)} (d_{G_0}(v)^2 + (d_{G_0}(\theta))^2)^\beta + (d_{G''}(\mu)^2 + 1)^\beta + \cdots + (d_{G''}(\mu)^2 + 1)^\beta, \\ &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad + \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\xi + \delta + t)^2 + 1)^\beta. \end{aligned}$$

Suppose  $\Omega_1 = GSO(G') - GSO(G)$  and  $\Omega_2 = GSO(G'') - GSO(G)$ , we consider the following

$$\begin{aligned} \Omega_1 &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta \\ &\quad - \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta, \quad (8) \\ &= \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta + ((\varphi + \delta + t)^2 + \sum_{\theta \in N_{G_0}(v)} (d_{G_0}(\theta))^2)^\beta \\ &\quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\ &\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta. \end{aligned}$$

Now  $\Omega_1 > 0$ , if the following holds

$$\begin{aligned}
& \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta \\
& > [ \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad \delta((\xi + \delta)^2 + 1)^\beta + t((\varphi + t)^2 + 1)^\beta ], \\
& \Rightarrow \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta \\
& > [ \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad \delta((\xi + \delta)^2 + 1)^\beta + t((\varphi + t)^2 + 1)^\beta ].
\end{aligned} \tag{9}$$

If  $\Omega_1 > 0$  then  $\Omega_2 < 0$ , we have the following for this

$$\begin{aligned}
\Omega_2 &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\xi + \delta + t)^2 + 1)^\beta \\
& \quad - \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta \delta((\xi + \delta)^2 + 1)^\beta + t((\varphi + t)^2 + 1)^\beta, \\
& = \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta - \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta < 0.
\end{aligned} \tag{10}$$

**Case 2.** Consider graph  $G$ , if  $v$  and  $\mu$  are connected directly by an edge, then we obtain

$$\begin{aligned}
GSO(G) &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta + ((\xi + \delta)^2 + 1)^\beta + \dots + ((\xi + \delta)^2 + 1)^\beta \\
& \quad + ((\varphi + t)^2 + 1)^\beta + \dots + ((\varphi + t)^2 + 1)^\beta - ((\xi + \delta)^2 + (\varphi + t)^2)^\beta, \\
& = \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
& \quad + \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta \delta((\xi + \delta)^2 + 1)^\beta + t((\varphi + t)^2 + 1)^\beta \\
& \quad - ((\xi + \delta)^2 + (\varphi + t)^2)^\beta.
\end{aligned} \tag{11}$$

GSO for  $G'$  is given in Equation (12)

$$\begin{aligned}
GSO(G') &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta \\
&+ \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + ((\varphi + \delta + t)^2 + 1)^\beta + \dots \\
&+ ((\varphi + \delta + t)^2 + 1)^\beta - (\xi^2 + (\varphi + \delta + t)^2)^\beta, \\
&= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi)^2 + (d_{G_0}(\theta))^2)^\beta \\
&+ \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta \\
&- (\xi^2 + (\varphi + \delta + t)^2)^\beta.
\end{aligned} \tag{12}$$

GSO for  $G''$  is considered in Equation (13)

$$\begin{aligned}
GSO(G'') &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&+ \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta + ((\xi + \delta + t)^2 + 1)^\beta + \dots \\
&+ ((\delta + \xi + t)^2 + 1)^\beta - ((\xi + \delta + t)^2 + \varphi^2)^\beta, \\
&= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&+ \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\delta + \xi + t)^2 + 1)^\beta - ((\delta + \xi + t)^2 + \varphi^2)^\beta.
\end{aligned} \tag{13}$$

Let  $\Omega_1 = GSO(G') - GSO(G)$  and  $\Omega_2 = GSO(G'') - GSO(G)$ , we consider the following

$$\begin{aligned}
\Omega_1 &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi)^2 + (d_{G_0}(\theta))^2)^\beta \\
&+ \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta \\
&- (\xi^2 + (\varphi + \delta + t)^2)^\beta \\
&- \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
&- \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta \\
&+ ((\xi + \delta)^2 + (\varphi + t)^2)^\beta.
\end{aligned}$$

$$\begin{aligned}
\Omega_1 &= (\xi^2 + \sum_{\theta \in N_{G_0}(\mu)} (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta - (\xi^2 + (\varphi + \delta + t)^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta + ((\xi + \delta)^2 + (\varphi + t)^2)^\beta, \\
&= \sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta + ((\xi + \delta)^2 + (\varphi + t)^2)^\beta \\
&\quad - (\xi^2 + (\varphi + \delta + t)^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta.
\end{aligned} \tag{14}$$

If  $\Omega_1 > 0$ , then it follows that

$$\begin{aligned}
&\sum_{\theta \in N_{G_0}(\mu)} (\xi^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (\delta + t)((\varphi + \delta + t)^2 + 1)^\beta + ((\xi + \delta)^2 + (\varphi + t)^2)^\beta \\
&> -(\xi^2 + (\varphi + \delta + t)^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta. \\
\Rightarrow &\sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (\delta + t)((\varphi + \delta + t)^2 + (\delta + \xi + t)^2)^\beta + ((\delta + \xi)^2 + (\varphi + t\delta))^\beta \\
&> -(\xi^2 + (\varphi + t + \delta)^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\delta + \xi)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta.
\end{aligned} \tag{15}$$

When (15) satisfies, then we get the following

$$\begin{aligned}
\Omega_2 &= \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta + \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta + (\delta + t)((\xi + \delta + t)^2 + 1)^\beta + \dots \\
&\quad - ((\xi + \delta + t)^2 + q^2)^\beta \\
&\quad - \sum_{\theta y \in E(G - \{\mu, v\})} ((d_{G_0}(\theta))^2 + (d_{G_0}(y))^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta \\
&\quad + ((\xi + \delta)^2 + (\varphi + t)^2)^\beta.
\end{aligned}$$

$$\begin{aligned}
\Omega_2 &= \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (\delta + t)((\delta + \xi + t)^2 + 1)^\beta + ((\delta + \xi)^2 + (\varphi + t)^2)^\beta \\
&\quad - ((\xi + \delta + t)^2 + \varphi^2)^\beta - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(v)} ((\varphi + t)^2 + (d_{G_0}(\theta))^2)^\beta - \delta((\xi + \delta)^2 + 1)^\beta - t((\varphi + t)^2 + 1)^\beta. \\
\Omega_2 &< \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta + \sum_{\theta \in N_{G_0}(v)} (\varphi^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad + (t + \delta)((\delta + \xi + t)^2 + 1)^\beta + ((\delta + \xi)^2 + (\varphi + t)^2)^\beta \\
&\quad - \sum_{\theta \in N_{G_0}(\mu)} ((\xi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta - \sum_{\theta \in N_{G_0}(v)} ((\varphi + \delta + t)^2 + (d_{G_0}(\theta))^2)^\beta \\
&\quad - (\delta + t)((\varphi + \delta + t)^2 + (\xi + \delta + t)^2)^\beta - ((\xi + \delta)^2 + (\varphi + t + \delta)^2)^\beta < 0.
\end{aligned}$$

We conclude if  $\Omega_1 > 0$  then  $\Omega_2 < 0$ .

□

**Remark 2.** We transform any bicyclic graph or unicyclic graph to a bicyclic graph or unicyclic graph, respectively, in which all the vertices with degree one are connected directly to the same vertex.

### 3. GSO( $G$ ) for Greatest Values

Let  $U_n^k$  be unicyclic graph obtained from  $C_k$  in which  $n - k$  pendent edges are attached to the same vertex on  $C_k$ , then using Lemmas 1 and 2, it follows that

**Theorem 1.** Consider  $G$  be an unicyclic graph with order  $n$  and girth  $k$ , if  $G$  is not  $U_n^k$  then  $GSO(G) < GSO(\mu_n^k)$ .

Consider bicyclic graph  $G(n, n + 1)$ . Here the order is  $n$ , and the size is  $n + 1$ . The considered bicyclic graph has been investigated for the Sombor index. We consider a connected and simple graph denoted by  $\Theta(n, n + 1)$ . Furthermore, for  $G \in \Theta(n, n + 1)$ , every graph consists of cycles  $C_\xi$  and  $C_\varphi$  in  $G$ . The following cases have been observed;

- (I)  $\mathbb{A}(\xi, \varphi)$  consists of  $G \in \Theta(n, n + 1)$ , where  $C_\xi$  and  $C_\varphi$  share one vertex in common.
- (II)  $\mathbb{B}(\xi, \varphi)$  consists of  $G \in \Theta(n, n + 1)$ , where  $C_\xi$  and  $C_\varphi$  share no common vertex.
- (III)  $\mathbb{C}(\xi, \varphi, l)$  contains  $G \in \Theta(n, n + 1)$ , where the cycles  $C_\xi$  and  $C_\varphi$  are connected by a common path of length  $l$ .

In Figure 3i–iii, vertex induced subgraphs on the cycles for  $G \in \mathbb{A}(\xi, \varphi)$  (or  $\mathbb{B}(\xi, \varphi)$ ,  $\mathbb{C}(\xi, \varphi, l)$ ) are provided, respectively.

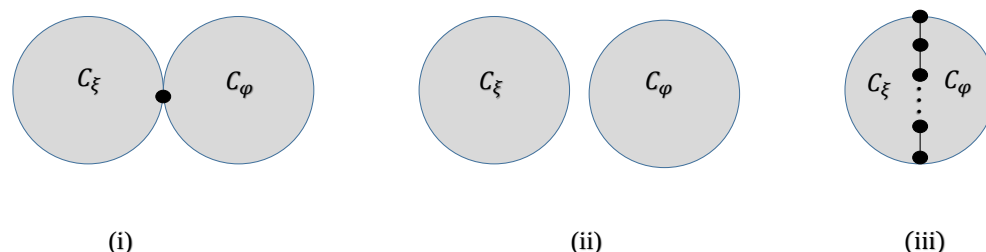


**Figure 3.** All considered bicyclic graphs. In (i), there is one common vertex between two cycles; In (ii), there is no common vertex or path; In (iii), there is a common path between two cycles.

#### 4. Greatest GSO in the Family $\mathbb{A}(\xi, \varphi)$

In this portion, we investigated GSO in  $\mathbb{A}(\xi, \varphi)$  for optimal values. Let  $S_n(\xi, \varphi)$  be from  $\mathbb{A}(\xi, \varphi)$  where  $n - \xi + 1 - \varphi$  pendent edges are attached directly to the common vertex of  $C_\xi$  and  $C_\varphi$ , for this we provide Figure 4.

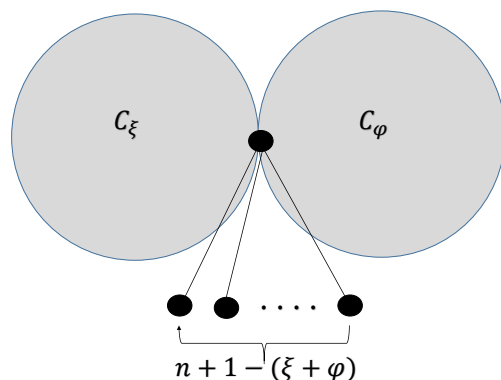


**Figure 4.** The graph  $S_n(\xi, \varphi)$ , where  $n + 1 - \xi - \varphi$  pendent edges are attached to the common vertex of the cycles.

**Theorem 2.**  $S_n(\xi, \varphi)$  is the graph with greatest GSO in  $\mathbb{A}(\xi, \varphi)$ .

**Proof.** Consider  $G$  and apply Transformation A and Transformation B. We obtain  $G'$  in which all the edges not on the cycle are connected directly to  $v$ . Using Lemmas 1 and 2, we obtain that  $GSO(G') > GSO(G)$  with equality iff, all the non-cyclic edges are connected directly to the same vertex in  $G$ . If  $G' \not\cong S_n(\xi, \varphi)$ , then  $\mu$  and  $v$  are different vertices and  $\mu$  is vertex that is common between  $C_\varphi$  and  $C_\xi$ .

Consider that  $v$  is on the cycle  $C_\xi$ , we consider cases given below;

**Case 1.** Consider that  $v$  and  $\mu$  are not adjacent, the following is considered

$$\begin{aligned} GSO(S_n(\xi, \varphi)) &= ((5 - \xi - \varphi + n)^2 + 1)^\beta + ((5 - \xi - \varphi + n)^2 + 1)^\beta \\ &+ \cdots + ((5 - \xi - \varphi + n)^2 + 1)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta, \\ &= (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ (\xi - 2)8^\beta + (\varphi - 2)8^\beta. \end{aligned}$$

GSO for  $G'$ , is considered in the following

$$\begin{aligned} GSO(G') &= ((3 - \xi - \varphi + n)^2 + 1)^\beta + ((3 - \xi - \varphi + n)^2 + 1)^\beta \\ &+ \cdots + ((3 - \xi - \varphi + n)^2 + 1)^\beta + 2((3 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ (\xi - 4)(8)^\beta + (\varphi - 2)(8)^\beta + 4(20)^\beta, \\ &= (n - \xi + 1 - \varphi)((3 - \xi - \varphi + n)^2 + 1)^\beta + 2((3 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ (\xi - 4)8^\beta + (\varphi - 2)8^\beta + 4(20)^\beta. \end{aligned}$$

Consider the following difference

$$\begin{aligned}
GSO(S_n(\xi, \varphi)) - GSO(G') &= (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad + (\xi - 2)8^\beta - (n - \xi + 1 - \varphi)((3 - \xi - \varphi + n)^2 + 1)^\beta - 2((3 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad - (\xi - 4)8^\beta - 4(20)^\beta, \\
&= (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta + 2((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad + (\xi - 2)8^\beta + 2((5 - \xi - \varphi + n)^2 + 4)^\beta - (n - \xi + 1 - \varphi)((3 - \xi - \varphi + n)^2 + 1)^\beta \\
&\quad - 2((3 - \xi - \varphi + n)^2 + 4)^\beta - (\xi - 4)8^\beta - 4(20)^\beta > 0.
\end{aligned} \tag{16}$$

Here, equality holds iff  $G' \cong S_n(\xi, \varphi)$ .

**Case 2.** Consider that  $v$  and  $\mu$  are connected directly by an edge in  $G'$ . Then,

$$\begin{aligned}
GSO(G') &= ((3 - \xi - \varphi + n)^2 + 1)^\beta + ((3 - \xi - \varphi + n)^2 + 1)^\beta \\
&\quad + \dots + ((3 - \xi - \varphi + 3)^2 + 1)^\beta + ((3 - \xi - \varphi + n)^2 + (2)^2)^\beta \\
&\quad + ((n + 3 - \xi - \varphi)^2 + 4^2)^\beta + 3(4^2 + (2)^2) + (\xi - 3)((2)^2 + (2)^2)^\beta + (\varphi - 2)((2)^2 + (2)^2)^\beta, \\
&= (n - \xi + 1 - \varphi)((n + 3 - \xi - \varphi)^2 + 1)^\beta + ((n + 3 - \xi - \varphi)^2 + 4)^\beta \\
&\quad + ((n + 3 - \xi - \varphi)^2 + 16)^\beta + 3(20)^\beta + (\xi - 3)8^\beta + (\varphi - 2)8^\beta.
\end{aligned} \tag{17}$$

The following difference is considered

$$\begin{aligned}
GSO(S_n(\xi, \varphi)) - GSO(G') &= (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad + (\xi - 2)8^\beta + (\varphi - 2)8^\beta \\
&\quad - (n - \xi + 1 - \varphi)((3 - \xi - \varphi + n)^2 + 1)^\beta - ((3 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad - ((n + 3 - \xi - \varphi)^2 + 16)^\beta - 3(20)^\beta - (\xi - 3)8^\beta - (\varphi - 2)8^\beta, \\
&= (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta + ((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad + 2((5 - \xi - \varphi + n)^2 + 4)^\beta + (\xi - 2)8^\beta + ((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad - (n - \xi + 1 - \varphi)((3 - \xi - \varphi + n)^2 + 1)^\beta - ((3 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad - ((3 - \xi - \varphi + n)^2 + 16)^\beta - (\xi - 3)8^\beta - 3(20)^\beta > 0.
\end{aligned} \tag{18}$$

While equality holds iff  $G' \cong S_n(\xi, \varphi)$ .

□

For  $3 \leq \xi$  and  $3 \leq \varphi$ , applying above theorem, it follows that  $S_n(\xi, \varphi)$  is the unique graph with largest value for  $GSO$  in  $\mathbb{A}(\xi, \varphi)$ .

**Lemma 3.** (i) For  $3 < \xi$  we have  $GSO(S_n(\xi - 1, \varphi)) > GSO(S_n(\xi, \varphi))$ ; (ii) For  $3 < \varphi$ , we have  $GSO(S_n(\xi, \varphi - 1)) > GSO(S_n(\xi, \varphi))$ .

**Proof.** (i) As we have

$$\begin{aligned}
GSO(S_n(\xi, \varphi)) &= (1 - \xi - \varphi + n)((5 - \xi - \varphi + n)^2 + 1)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\
&\quad + (\xi - 2)8^\beta + (\varphi - 2)8^\beta.
\end{aligned}$$

Plug  $\xi$  by  $\xi - 1$ , it follows that

$$\begin{aligned}
GSO(S_n(\xi - 1, \varphi)) &= (2 - \xi - \varphi + n)((5 - \xi + 1 - \varphi + n)^2 + 1)^\beta \\
&\quad + 4((5 - \xi + 1 - \varphi + n)^2 + 4)^\beta + (\xi - 1 - 2)8^\beta + (\varphi - 2)8^\beta, \\
&= (2 - \xi - \varphi + n)((6 - \xi - \varphi + n)^2 + 1)^\beta \\
&\quad + 4((6 - \xi - \varphi + n)^2 + 4)^\beta + (\xi - 3)8^\beta + (\varphi - 2)8^\beta.
\end{aligned}$$

From the above calculations, the following difference is considered

$$\begin{aligned} GSO(S_n(\xi - 1, \varphi)) - GSO(S_n(\xi, \varphi)) &= (2 - \xi - \varphi + n)((6 - \xi - \varphi + n)^2 + 1)^\beta \\ &\quad + 4((6 - \xi - \varphi + n)^2 + 4)^\beta + (\xi - 3)8^\beta \\ &\quad - (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta - 4((5 - \xi - \varphi + n)^2 + 4)^\beta \\ &\quad - (\xi - 2)8^\beta > 0. \end{aligned}$$

Hence, we have  $GSO(S_n(\xi - 1, \varphi)) > GSO(S_n(\xi, \varphi))$ .

Consider (ii). We have the following:

$$\begin{aligned} GSO(S_n(\xi, \varphi - 1)) - GSO(S_n(\xi, \varphi)) &= (2 - \xi - \varphi + n)((6 - \xi - \varphi + n)^2 + 1)^\beta \\ &\quad + 4((6 - \xi - \varphi + n)^2 + 4)^\beta + (\varphi - 3)8^\beta \\ &\quad - (n - \xi + 1 - \varphi)((5 - \xi - \varphi + n)^2 + 1)^\beta - 4((5 - \xi - \varphi + n)^2 + 4)^\beta - (\varphi - 2)8^\beta > 0. \end{aligned}$$

Finally, we have  $GSO(S_n(\xi, \varphi - 1)) > GSO(S_n(\xi, \varphi))$ .  $\square$

From Theorem 2 and Lemma 3, we obtain the following:

**Theorem 3.** For every  $\xi \geq 3$  and  $\varphi \geq 3$ , the unique graph of order  $n$  with largest value of GSO is  $S_n(3, 3)$  in  $\mathbb{A}(\xi, \varphi)$ .

## 5. GSO for Greatest Values in $\mathbb{B}(\xi, \varphi)$

In the considered portion, the largest values in bicyclic graphs of GSO are considered in  $\mathbb{B}(\xi, \varphi)$ . Let  $T_n^\delta(\xi, \varphi)$  be the graph on  $n$  vertices and  $n + 1$  edges. Two cycles  $C_\xi$  and  $C_\varphi$  are connected by a path of length  $\delta$ . Here,  $n - \delta - \xi + 1 - \varphi$  pendent edges are connected directly to the common vertex of cycle  $C_\xi$  and the path. We provide Figure 5a, and  $T_n^r((\varphi, \xi))$  is given in Figure 5b.  $T_n(\xi, \varphi)$  is the graph on  $n + 1$  edges and  $n$  vertices, obtained by connecting  $C_\xi$  and  $C_\varphi$  by a path  $\mu v w$ , the remaining edges are connected directly to  $v$ ; see Figure 5c.

**Theorem 4.** Let  $G \in \mathbb{B}(\xi, \varphi)$ . Consider a common path of length  $\delta$  of  $C_\xi$  and  $C_\varphi$ , then

$$\begin{aligned} GSO(T_n^\delta(\xi, \varphi)) &\geq GSO(G) \text{ with holds iff } G \cong T_n^\delta(\xi, \varphi), \\ GSO(T_n^\delta(\varphi, \xi)) &\geq GSO(G) \text{ with equality iff } G \cong T_n^\delta(\varphi, \xi). \end{aligned} \quad (19)$$

**Proof.** Consider a path of shortest length denoted by  $P = v_1 v_2 \cdots v_\delta v_{\delta+1}$ , the considered path connects  $C_\xi$  and  $C_\varphi$  in  $G$ . Let  $v_1$  be the common vertex between  $P$  and  $C_\xi$ ,  $v_{\delta+1}$  be the common vertex of  $P$  and  $C_\varphi$ . Using Transformation A and Transformation B on  $G$  continuously, we obtain  $G'$  as provided in Figure 5. In  $G'$ , all the vertices of degree one not on the cycles are connected directly to vertex  $v$ . Applying Lemmas 1 and 2, we obtain  $GSO(G') > GSO(G)$ , with equality iff all the edges not on the cycles are pendent edges connected directly to the same vertex in  $G$ . We consider the cases given below.

**Case 1.** If  $v$  is on  $C_\xi$  with adjacent  $v$  and  $v_1$ , we provided Figure 5d. Here, the following values are considered

$$\begin{aligned} GSO(G') &= ((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + \cdots + ((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta \\ &\quad + 2((n - \delta - \xi + 3 - \varphi)^2 + 2)^\beta + (9 + d(v_2)^2)^\beta + (\xi - 4)(8)^\beta \\ &\quad + (\varphi - 2)(8)^\beta + (\delta - 2)(8)^\beta + 3(11)^\beta + 2(11)^\beta, \\ &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + 2((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\ &\quad + (9 + d(v_2)^2)^\beta + 8^\beta(\xi - 4) + 8^\beta(\varphi - 2) + 8^\beta(\delta - 2) + 5(13)^\beta. \end{aligned} \quad (20)$$

$GSO(T_n^r(\xi, \varphi))$  is given by

$$\begin{aligned} GSO(T_n^r(\xi, \varphi)) &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta \\ &+ (\delta - 2)(8)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + 3(11)^\beta, \\ &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta \\ &+ 8^\beta(\delta - 2) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta. \end{aligned} \quad (21)$$

$GSO(T_n^r(\xi, \varphi)) - GSO(G')$ , is considered in the following:

$$\begin{aligned} GSO(T_n^r(\xi, \varphi)) - GSO(G') &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta + \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta \\ &+ 8^\beta(\delta - 2) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta \\ &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - 2((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\ &- (9 + d(v_2)^2)^\beta - 8^\beta(\xi - 4) - 8^\beta(\varphi - 2) - 8^\beta(\delta - 2) - 5(13)^\beta, \\ &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta \\ &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - 2((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\ &- (9 + d(v_2)^2)^\beta + 8^\beta(\xi - 2) + 3(13)^\beta - 8^\beta(\xi - 4) - 5(13)^\beta \geq 0. \end{aligned} \quad (22)$$

Hence,  $GSO(T_n^\delta(\xi, \varphi)) - GSO(G') > 0$ , with equality iff  $G' \cong T_n^\delta(\xi, \varphi)$ , Figure 6 is provided for equality.

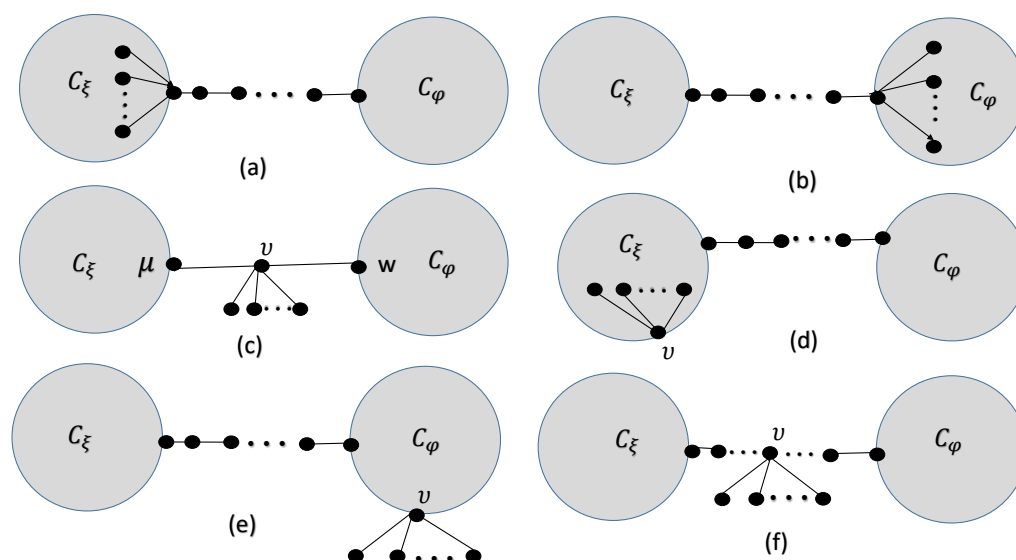


**Figure 5.** (a) The graph  $T_n^\delta(\xi, \varphi)$ , where pendent edges are attached to the common vertex between the cycle  $C_\xi$  and path; (b) The graph  $T_n^r(\varphi, \xi)$ , where the pendent edges are attached to the common vertex between the cycle  $C_\varphi$  and path; (c) The graph  $T_n(\xi, \varphi)$ , where pendent edges are attached to vertex  $v$  on the path  $\mu v w$  of length 2; (d) The graph where pendent edges are attached to  $v$  on the cycle  $C_\xi$ ; (e) The graph where pendent edges are attached to the vertex  $v$  on the cycle  $C_\varphi$ ; (f) The graph where pendent edges are attached to vertex  $v$  on the path between  $C_\xi$  and  $C_\varphi$ .

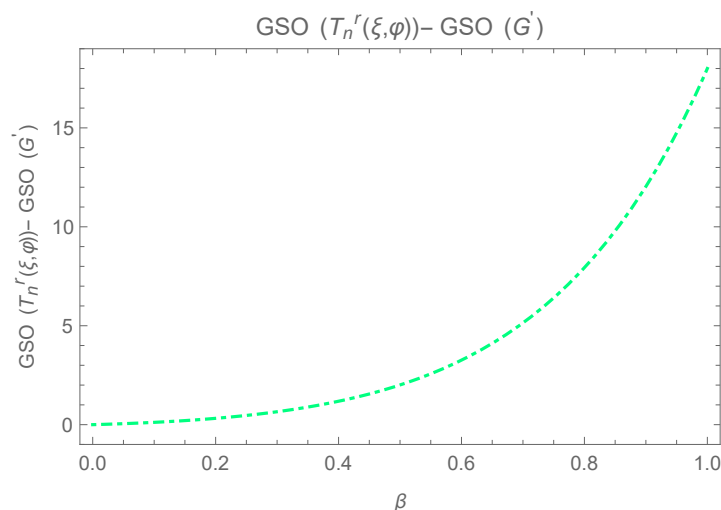


**Figure 6.** Graph for  $GSO(T_n^\delta(\xi, \varphi)) - GSO(G')$ , with adjacent  $v$  and  $v_1$ .

If the vertices  $v_1$  and  $v$  are directly connected by an edge in  $G'$ , we provide the values in the following

$$\begin{aligned}
 GSO(G') &= ((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + \dots + ((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta \\
 &+ ((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 3 - \varphi)^2 + 9)^\beta \\
 &+ (9 + d(v_2)^2)^\beta + 4(11)^\beta + (\xi - 3)(8)^\beta + (\varphi - 2)(8)^\beta + (\delta - 2)(8)^\beta, \\
 &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + ((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\
 &+ ((n - \delta - \xi + 3 - \varphi)^2 + 27)^\beta + (9 + d(v_2)^2)^\beta + 4(31)^\beta + (\xi - 3)8^\beta \\
 &+ (\varphi - 2)8^\beta + (\delta - 2)8^\beta.
 \end{aligned} \quad (23)$$

Next, we consider  $GSO(T_n^\delta(\xi, \varphi)) - GSO(G')$  in the following

$$\begin{aligned}
 GSO(T_n^r(\xi, \varphi)) - GSO(G') &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\
 &+ ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta \\
 &+ ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta + 8^\beta(\delta - 2) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta \\
 &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - ((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\
 &- ((n - \delta - \xi + 3 - \varphi)^2 + 27)^\beta - (9 + d(v_2)^2)^\beta - (\xi - 3)8^\beta - (\varphi - 2)8^\beta - (\delta - 2)8^\beta - 4(13)^\beta, \\
 &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\
 &+ ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta \\
 &+ ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta + 8^\beta(\xi - 2) + 3(13)^\beta \\
 &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - ((n - \delta - \xi + 3 - \varphi)^2 + 4)^\beta \\
 &- ((n - \delta - \xi + 3 - \varphi)^2 + 9)^\beta - (9 + d(v_2)^2)^\beta - (\xi - 3)8^\beta - 4(13)^\beta.
 \end{aligned} \quad (24)$$

Hence, we have  $GSO(T_n^\delta(\xi, \varphi)) - GSO(G') > 0$ , with equality iff  $G' \cong (T_n^\delta(\xi, \varphi))$ . Figure 7 is provided for this.

**Case 2.** Consider  $v$  on  $C_\varphi$ , this case is similar to **Case 1**. Figure 5e is provided for **Case 2**.

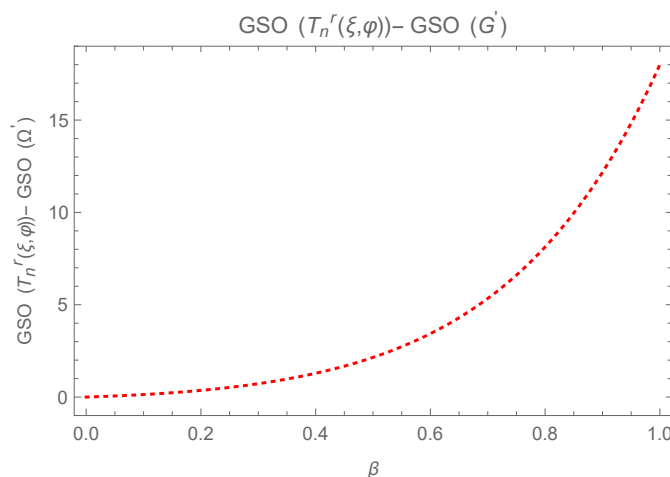


**Figure 7.** Graph for  $GSO(T_n^\delta(\xi, \varphi)) - GSO(G')$ , where  $v_1$  and  $v$  are adjacent.

**Case 3.** Consider  $v$  on  $P$  as in Figure 5f, when  $G' \not\cong T_n(\xi, \varphi)$ , then  $\delta \geq 3$ . The following is considered;

When  $\delta > t > 2$ , then  $\delta > 3$  and the following value is considered

$$\begin{aligned} GSO(T_n(\xi, \varphi)) &= ((n - \xi + 1 - \varphi)^2 + 1)^\beta + \dots + ((n - \xi + 1 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \xi + 1 - \varphi)^2 + 9)^\beta + 4(11)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta, \\ &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \xi + 1 - \varphi)^2 + 9)^\beta \\ &+ 4(13)^\beta + (\xi - 2)8^\beta + (\varphi - 2)8^\beta. \end{aligned} \quad (25)$$

$GSO$  for  $G'$  is considered in the following:

$$\begin{aligned} GSO(G') &= ((n - \delta - \xi + 1 - \varphi)^2 + 1)^\beta + \dots + ((n - \delta - \xi + 1 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 1 - \varphi)^2 + 4)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta \\ &+ (\delta - 4)(8)^\beta + 6(11), \\ &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \delta - \xi + 1 - \varphi)^2 + 4)^\beta \\ &+ (\xi - 2)8^\beta + (\varphi - 2)8^\beta + (\delta - 4)8^\beta + 6(31)^\beta. \end{aligned} \quad (26)$$

We consider the difference of  $GSO(T_n(\xi, \varphi))$  and  $GSO(G')$  in the following

$$\begin{aligned} GSO(T_n(\xi, \varphi)) - GSO(G') &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \xi + 1 - \varphi)^2 + 9)^\beta + (\xi - 2)8^\beta + (\varphi - 2)8^\beta + 4(13)^\beta \\ &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 1 - \varphi)^2 + 1)^\beta - 2((n - \delta - \xi + 1 - \varphi)^2 + 4)^\beta \\ &- (\xi - 2)8^\beta - (\varphi - 2)8^\beta - (\delta - 4)8^\beta - 6(13)^\beta, \\ &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \xi + 1 - \varphi)^2 + 9)^\beta + 4(13)^\beta \\ &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 1 - \varphi)^2 + 1)^\beta - 2((n - \delta - \xi + 1 - \varphi)^2 + 4)^\beta \\ &- (\delta - 4)8^\beta - 6(13)^\beta. \end{aligned} \quad (27)$$

Figure 8 is provided for the difference in Equation (27).

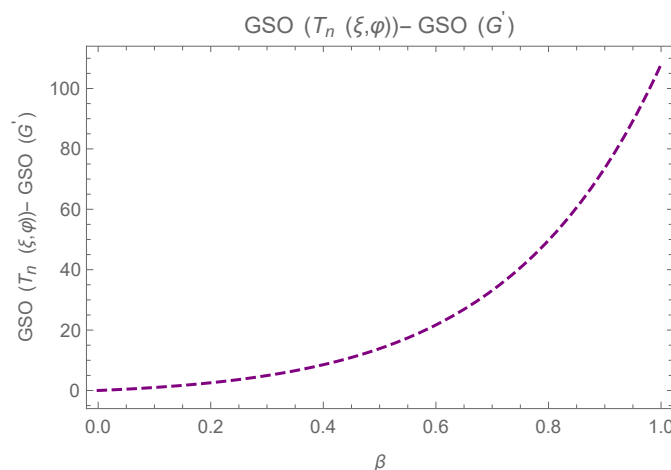


**Figure 8.** Graph for  $GSO(T_n(\xi, \varphi)) - GSO(G')$ , with  $\delta > 3$ .

If  $2 = t$  or  $t = \delta$ , then for  $G'$  the value of  $GSO$  is considered in the following

$$\begin{aligned}
 GSO(G') &= 5(11)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta \\
 &+ (9 + (n - \delta - \xi + 3 - \varphi)^2)^\beta + (4 + (n - \delta - \xi + 3 - \varphi)^2)^\beta + \\
 &((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + \dots + ((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta + (\delta - 3)(8)^\beta, \\
 &= (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + (9 + (n - \delta - \xi + 3 - \varphi)^2)^\beta + (\delta - 3)(8)^\beta \\
 &+ (4 + (n - \delta - \xi + 3 - \varphi)^2)^\beta + (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta \\
 &+ 5(13)^\beta > 0.
 \end{aligned} \tag{28}$$

The difference of  $GSO(T_n(\xi, \varphi))$  and  $GSO(G')$  is in the following

$$\begin{aligned}
 GSO(T_n(\xi, \varphi)) - GSO(G') &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta \\
 &+ 2((n - \xi + 1 - \varphi)^2 + 9)^\beta + (\xi - 2)8^\beta + (\varphi - 2)8^\beta + 4(13)^\beta \\
 &- (9 + (n - \delta - \xi + 3 - \varphi)^2)^\beta - (4 + (n - \delta - \xi + 3 - \varphi)^2)^\beta \\
 &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - (\xi - 2)8^\beta - (\varphi - 2)8^\beta \\
 &- (\delta - 3)8^\beta - 5(13)^\beta, \\
 &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \xi + 1 - \varphi)^2 + 9)^\beta \\
 &- (9 + (n - \delta - \xi + 3 - \varphi)^2)^\beta - (4 + (n - \delta - \xi + 3 - \varphi)^2)^\beta \\
 &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 3 - \varphi)^2 + 1)^\beta - (\delta - 3)8^\beta - (13)^\beta, \\
 &> 0.
 \end{aligned} \tag{29}$$

Figure 9 is provided for the difference in the Equation (29).

□

**Lemma 4.**  $GSO(T_n(3, 3)) \geq GSO(T_n(\xi, \varphi))$ , with equality iff  $\xi = 3 = \varphi$ .

**Proof.** The previous theorem provided the following value:

$$\begin{aligned}
 GSO(T_n(\xi, \varphi)) &= (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \xi + 1 - \varphi)^2 + 9)^\beta \\
 &+ 4(13)^\beta + (\xi - 2)8^\beta + (\varphi - 2)8^\beta.
 \end{aligned} \tag{30}$$

For  $GSO(T_n(3, 3))$ , the following is considered

$$\begin{aligned} GSO(T_n(3,3)) &= 4(11)^\beta + 2(8)^\beta + 2(9 + (n-5)^2)^\beta + (n-7)(1 + (n-5)^2)^\beta, \\ &= 4(13)^\beta + 2(8)^\beta + 2(1 + (n-5)^2)^\beta + (n-7)(1 + (n-5)^2)^\beta. \end{aligned} \quad (31)$$

Furthermore, we have the following difference:

$$\begin{aligned} GSO(T_n(3,3)) - GSO(T_n(\xi, \varphi)) &= 2(8)^\beta + 2(9 + (n-5)^2)^\beta + (n-7)(1 + (n-5)^2)^\beta \\ &- (n - \xi - 1 - \varphi)((n - \xi + 1 - \varphi)^2 + 1)^\beta + 2((n - \xi + 1 - \varphi)^2 + 9)^\beta \\ &+ (\xi - 2)8^\beta + (\varphi - 2)8^\beta \geq 0. \end{aligned} \quad (32)$$

Figure 10 is provided for the difference in Equation (32), with iff  $\xi = 3 = \varphi$ . For equality, Figure 11 is provided.  $\square$

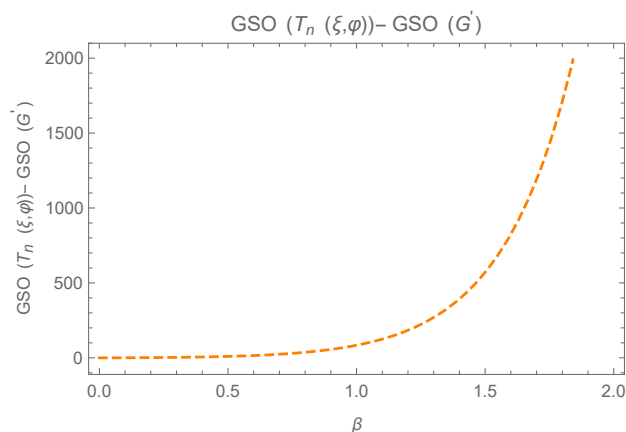


**Figure 9.** Graph representing  $GSO(T_n(\xi, \varphi)) - GSO(G')$ , where  $2 = t$  or  $\delta = t$ .

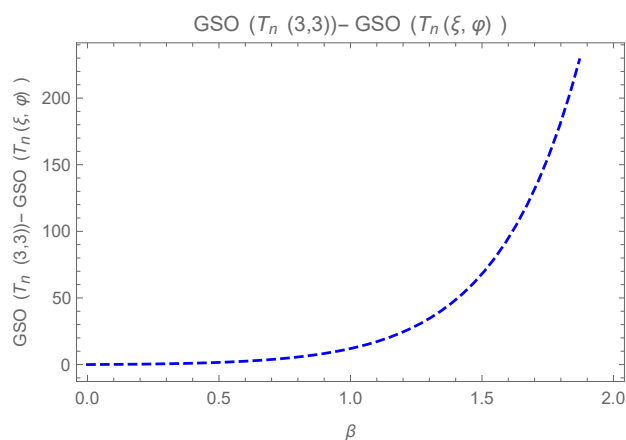


**Figure 10.** Graph for the difference  $GSO(T_n(3,3)) - GSO(T_n(\xi, \varphi))$ .

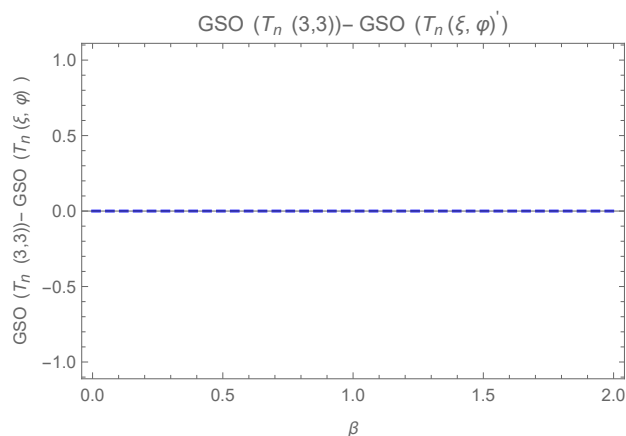


**Figure 11.** Graph for the difference  $GSO(T_n(3,3)) - GSO(T_n(\xi, \varphi))$ , where  $\xi = 3 = \varphi$ .

**Lemma 5.** For  $2 \leq \delta$ ,  $GSO(T_n^{\delta-1}(\xi, \varphi)) > GSO(T_n^\delta(\xi, \varphi))$ .

**Proof.** For the proof, we consider the following:

If  $\delta > 2$ , then  $GSO(T_n^\delta(\xi, \varphi))$ , is considered in the following

$$\begin{aligned} GSO(T_n^\delta(\xi, \varphi)) &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + d(v_2)^2)^\beta \\ &+ 8^\beta(\delta - 2) + 8^\beta(\xi - 2) + 3(13)^\beta + 8^\beta(\varphi - 2). \end{aligned}$$

Here,  $d(v_2) = 2$ , it follows that

$$\begin{aligned} GSO(T_n^\delta(\xi, \varphi)) &= (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &+ 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta + ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta \\ &+ 8^\beta(\delta - 2) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta. \end{aligned} \quad (33)$$

Replacing  $\delta$  by  $\delta - 1$  in (33), it follows that

$$\begin{aligned} GSO(T_n^{\delta-1}(\xi, \varphi)) &= (2 - \xi - \varphi - \delta + n)((5 - \xi - \varphi + n - \delta)^2 + 1)^\beta \\ &+ 2((5 - \xi - \varphi + n - \delta)^2 + 4)^\beta + ((5 - \xi - \varphi + n - \delta)^2 + 4)^\beta \\ &+ 8^\beta(\delta - 3) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta. \end{aligned}$$

The difference of  $GSO(T_n^\delta(\xi, \varphi))$  and  $GSO(T_n^{\delta-1}(\xi, \varphi))$  is considered in the following

$$\begin{aligned} GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi)) &= (n + 2 - \xi - \varphi - \delta)((5 - \xi - \varphi + n - \delta)^2 + 1)^\beta \\ &+ 2((5 - \xi - \varphi + n - \delta)^2 + 4)^\beta + ((5 - \xi - \varphi + n - \delta)^2 + 4)^\beta \\ &+ 8^\beta(\delta - 3) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta \\ &- (n - \delta - \xi + 1 - \varphi)((n - \delta - \xi + 4 - \varphi)^2 + 1)^\beta \\ &- 2((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta - ((n - \delta - \xi + 4 - \varphi)^2 + 4)^\beta \\ &- 8^\beta(\delta - 2) - 8^\beta(\xi - 2) - 8^\beta(\varphi - 2) - 3(13)^\beta. \end{aligned}$$

The difference  $GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi)) > 0$  is observed in Figure 12.

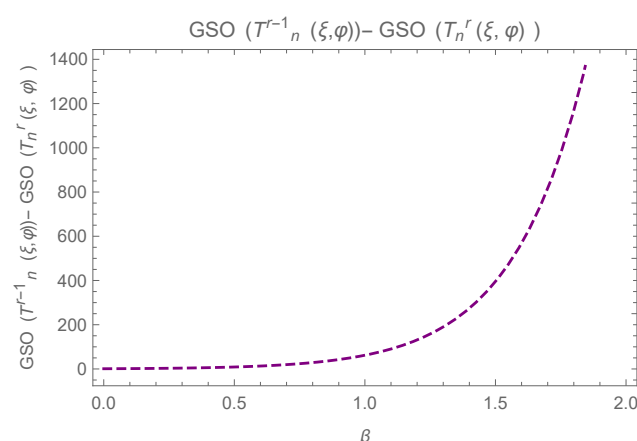


**Figure 12.** Graph for the difference  $GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi))$ , where  $\delta > 2$ .

If  $\delta = 2$ , then the following is considered

$$\begin{aligned} GSO(T_n^\delta(\xi, \varphi)) &= (n - \xi - 1 - \varphi)((2 - \xi - \varphi + n)^2 + 1)^\beta \\ &+ 2((2 - \xi - \varphi + n)^2 + 4)^\beta + ((2 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ 8^\beta(2 - 2) + 8^\beta(\xi - 2) + 8^\beta(\varphi - 2) + 3(13)^\beta. \end{aligned}$$

For  $GSO(T_n^{\delta-1}(\xi, \varphi))$ , it follows that

$$\begin{aligned} GSO(T_n^{\delta-1}(\xi, \varphi)) &= (n - \xi - \varphi)(1 + (3 - \xi - \varphi + n)^2)^\beta + 2(4 + (3 - \xi - \varphi + n)^2)^\beta \\ &+ (9 + (3 - \xi - \varphi + n)^2)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + 2(11)^\beta, \\ &= (n - \xi - \varphi)((n - \xi - \varphi + 3)^2 + 1)^\beta + 2((3 - \xi - \varphi + n)^2 + 4)^\beta \\ &+ ((3 - \xi - \varphi + n)^2 + 9)^\beta + (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + 2(13)^\beta. \end{aligned}$$

Consider  $GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi))$  in the following

$$\begin{aligned} GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi)) &= (n - \xi - \varphi)(1 + (3 - \xi - \varphi + n)^2)^\beta \\ &+ 2(4 + (3 - \xi - \varphi + n)^2)^\beta + (9 + (3 - \xi - \varphi + n)^2)^\beta \\ &+ (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + 2(13)^\beta - (n - \xi - 1 - \varphi)((2 - \xi - \varphi + n)^2 + 1)^\beta \\ &- 2((2 - \xi - \varphi + n)^2 + 4)^\beta - ((n + 2 - \xi - \varphi)^2 + 4)^\beta \\ &- 8^\beta(2 - 2) - 8^\beta(\xi - 2) - 8^\beta(\varphi - 2) - 3(13)^\beta \\ &> 0. \end{aligned} \quad (34)$$

Figure 13 is provided for the difference in Equation (34).  $\square$

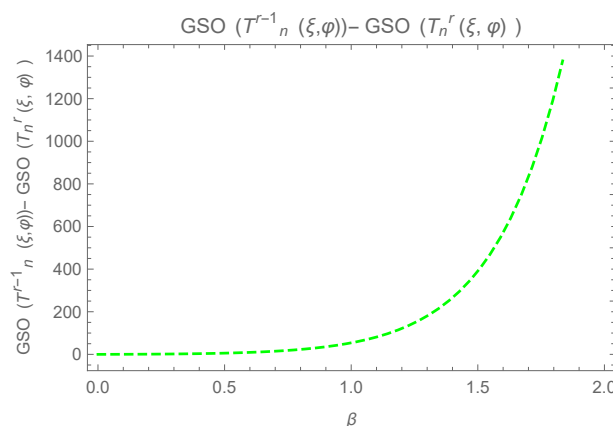


Figure 13. Graph for the difference  $GSO(T_n^{\delta-1}(\xi, \varphi)) - GSO(T_n^\delta(\xi, \varphi))$ , where  $\delta = 2$ .

**Lemma 6.**  $GSO(T_n^1(3, 3)) \geq GSO(T_n^1(\xi, \varphi))$ , with equality iff  $\xi = \varphi = 3$ .

**Proof.** We know that

$$\begin{aligned} GSO(T_n^1(\xi, \varphi)) &= (n - \xi - \varphi)(1 + (3 - \xi - \varphi + n)^2)^\beta + 2(4 + (3 - \xi - \varphi + n)^2)^\beta \\ &+ (9 + (3 - \xi - \varphi + n)^2)^\beta + (\xi - 2)(8)^\beta + 2(13)^\beta + (\varphi - 2)(8)^\beta. \end{aligned} \quad (35)$$

Put  $\xi = 3 = \varphi$  in (35), we obtain

$$\begin{aligned} GSO(T_n^1(3, 3)) &= (n - 6)(1 + (n - 3)^2)^\beta + 2(4 + (n - 3)^2)^\beta + (9 + (n - 3)^2)^\beta \\ &+ (\xi - 2)(8)^\beta + (\varphi - 2)(8)^\beta + 2(13)^\beta. \end{aligned}$$

The following difference is considered:

$$GSO(T_n^1(3,3)) - GSO(T_n^1(\xi, \varphi)) = (n-6)(1+(n-3)^2)^\beta + 2(4+(n-3)^2)^\beta + (9+(n-3)^2)^\beta - (n-\xi-\varphi)(1+(n-\xi-\varphi+3)^2)^\beta - 2(4+(3-\xi-\varphi+n)^2)^\beta - (9+(3-\xi-\varphi+n)^2)^\beta \geq 0. \quad (36)$$

Figures 14 and 15 are provided for the difference in Equation (36), with equality iff  $\xi = 3 = \varphi$ .  $\square$

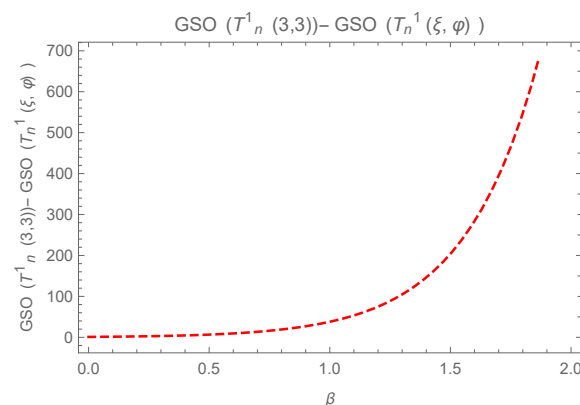


Figure 14. Graph for the difference  $GSO(T_n^1(3,3)) - GSO(T_n^1(\xi, \varphi))$ , where  $\xi$  and  $\delta$  are not both 3.

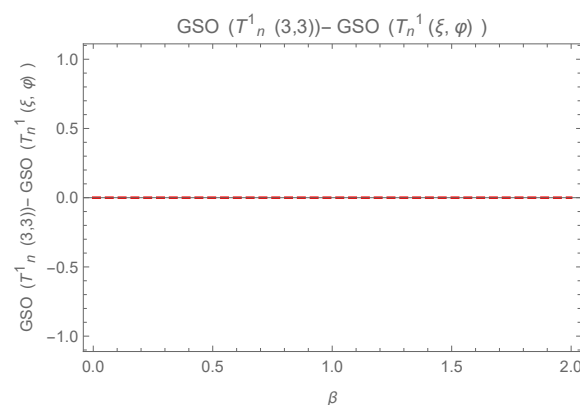


Figure 15. Graph for the difference  $GSO(T_n^1(3,3)) - GSO(T_n^1(\xi, \varphi))$ , where  $\xi = 3 = \delta$ .

The value of  $GSO$  for  $T_n^1(3,3)$  and  $T_n(3,3)$  are easy to find, and we have  $GSO(T_n^1(3,3)) > GSO(T_n(3,3))$ .

**Theorem 5.** In  $\mathbb{B}(\xi, \varphi)$ ,  $T_n^1(3,3)$  is the unique tree with greatest  $GSO$  for all  $\varphi \geq 3$  and  $\xi \geq 3$ .

## 6. Greatest $GSO$ in $\mathbb{C}(\xi, \varphi, l)$

Bicyclic graph on cycles  $C_\xi$  and  $C_\varphi$  is denoted by  $\mathbb{C}(\xi, \varphi, l)$ , where  $l$  is the length of the common path between  $C_\xi$  and  $C_\varphi$ . Let  $L_n^l(\xi, \varphi)$  be the resultant of the Figure 3iii, obtained by connecting  $1 + l - \xi - \varphi + n$  vertices to the vertex of degree 3, as given in Figure 16i.

**Theorem 6.** Consider a graph  $G \in \mathbb{C}(\xi, \varphi, l)$ , then  $GSO(G) \leq GSO(G_0)$ , with equality iff  $G \cong G_0$ .

**Proof.** Apply Transformation A and Transformation B continuously and repeatedly on  $G$ .  $G'$  is obtained where vertices not on the cycles with degree one are directly connected to vertex  $v_0$ , that is  $G'$  in Figure 16. Apply Lemmas 1 and 2,  $GSO(G') \geq GSO(G)$  with equality iff all the vertices not on the cycles with degree one are connected directly to the same vertex in  $G$ .

Let  $R_1 = vx_{t-1}x_{t-2} \cdots x_2x_1\mu$  be the path common between  $C_\xi$  and  $C_\varphi$  in  $G'$ ; Figure 16 is provided for this. Let  $Q_2 = vy_\delta y_{\delta-1} \cdots y_2y_1\mu$  and  $Q_3 = vz_tz_{t-1} \cdots z_2z_1\mu$  be other paths joining  $\mu$  and  $v$  on the cycles  $C_\xi$  and  $C_\varphi$ , respectively;  $\delta = \xi - 1 - l$ ,  $t = \varphi - 1 - l$ ,  $r \geq 0$ ,  $t \geq 0$ ,  $l \geq 1$  and  $l + \delta + t \geq 3$ .

Let  $gh$  is in  $G_1$  where  $d(g) = d(h) = 2$ ,  $G'_1$  is obtain where the edge  $gh$  is contracted and attach a pendent edge  $\mu u' = e'$  to  $\mu$ . Then, we find that  $GSO(G'_1) > GSO(G_1)$ , since  $(d_{G_1}(g)^2 + d_{G_1}(h)^2)^\beta = (8)^\beta$  and  $(d_{G_1}(\mu)^2 + d_{G_1}(\mu')^2)^\beta > 8^\beta$ . Hence,  $GSO(G_0) \geq GSO(G_1)$  with equality iff  $G_1 \cong G_0$ .

Similarly, if two edges are in graph  $G_2$  have end vertices of degree 2, then  $G'_2$  is obtained by deleting such edges and attaching two pendent edges to  $x_i$ . Then,  $GSO(G'_2) \geq GSO(G_2)$ , therefore  $GSO(G_1) \leq GSO(G_1)$  and  $GSO(G_2) \leq GSO(G_4)$ . One can easily obtain that  $GSO(G_0) > GSO(G_3)$  and  $GSO(G_0) > GSO(G_4)$ .  $\square$

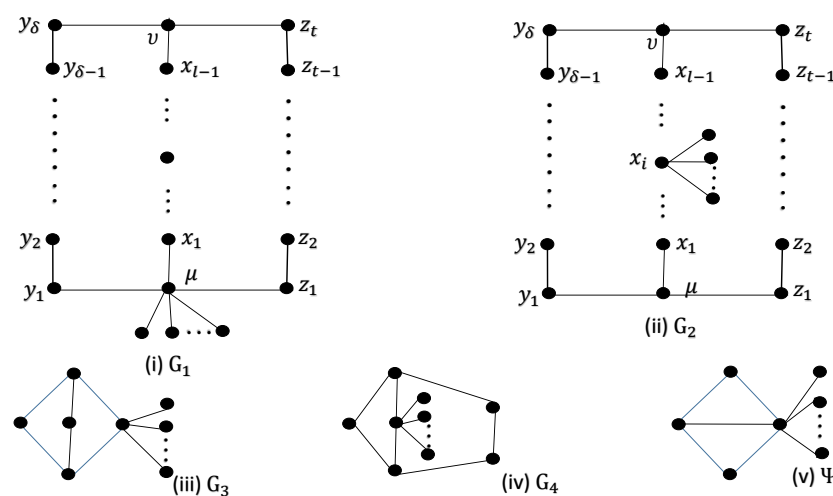


**Figure 16.** (i) The graph  $G_1$ , where all the pendent edges are attached to the vertex  $\mu$  of degree three; (ii) The graph  $G_2$ , where all the pendent edges are attached to the vertex  $x_i$  of degree two; (iii) The graph  $G_3$ , where all the pendent edges are attached to the vertex of degree two and there is a common path of length two between the cycles; (iv) The graph  $G_4$ , where all the pendent edges are attached to the vertex of degree two on the common path of length two; (v) The graph  $\Psi$ , where all the pendent edges are attached to the vertex of degree two and there is a common path of length one between the cycles.

From the above discussion, we have

**Theorem 7.** In bicyclic graphs,  $G_0$  is unique and has the largest GSO.

**Proof.** From Theorems 3, 5 and 6, in the following we compare general Sombor index of  $S_n(3, 3)$ ,  $T_n^1(3, 3)$  and  $G_0$ .

$$GSO(T_n^1(3, 3)) < GSO(S_n(3, 3)) < GSO(G_0).$$

The inequality is given in Figures 17 and 18, where

$$GSO(T_n^1(3, 3)) = (n-6)(1 + (n-3)^2)^\beta + 2(4 + (n-3)^2)^\beta + (9 + (n-3)^2)^\beta + (\xi-2)(8)^\beta + (\varphi-2)(8)^\beta + 2(13)^\beta.$$

For  $GSO(S_n(3, 3))$ , it follows that

$$GSO(S_n(3, 3)) = 2(8)^\beta + 4((5 - \xi - \varphi + n)^2 + 4)^\beta + (1 - \xi - \varphi + n)(1 + (5 - \xi - \varphi + n)^2)^\beta.$$

For  $GSO(G_0)$ , it follows that

$$GSO(G_0) = 2(13)^\beta + 2(4 + (2 + 3 - \xi - \varphi + n)^2)^\beta + (9 + (n - \xi - \varphi + 2 + 3)^2)^\beta + (n - \xi - \varphi + 2)(1 + (2 + 3 + n - \xi - \varphi)^2)^\beta.$$

□

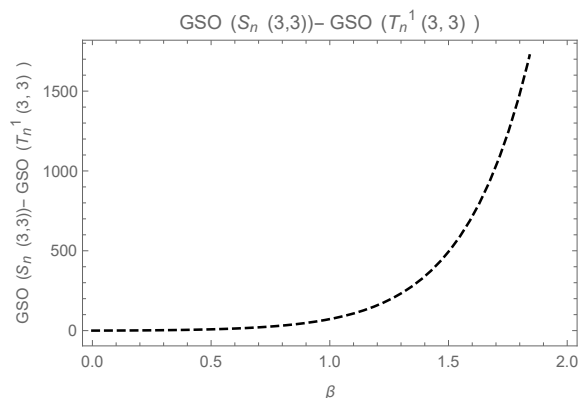


Figure 17. Graph for the difference  $GSO(S_n(3,3)) - GSO(T_n^1(3,3))$ .

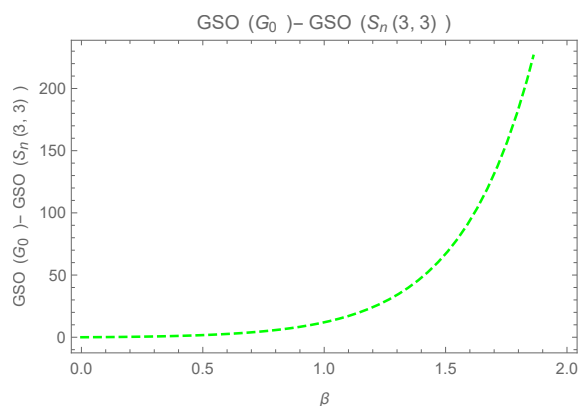


Figure 18. Graph for the difference  $GSO(G_0) - GSO(S_n(3,3))$ .

## 7. Transformation for Decreasing GSO

In this section, we investigated the transformation used for decreasing GSO.

Transformation C: Consider a simple connected graph  $G$  not  $P_1$ , choose  $\mu$  form  $V(G)$ . Let  $G_1$  is obtained from  $G$  by labeling  $\mu$  with  $v_k$  of the path  $v_1v_2v_3 \cdots v_n$ , here  $1 < k < n$ . Consider  $G_1$ , we obtain  $G_2$  by deleting  $v_{k-1}v_k$  and adding  $v_nv_{k-1}$ , we provide Figure 19.

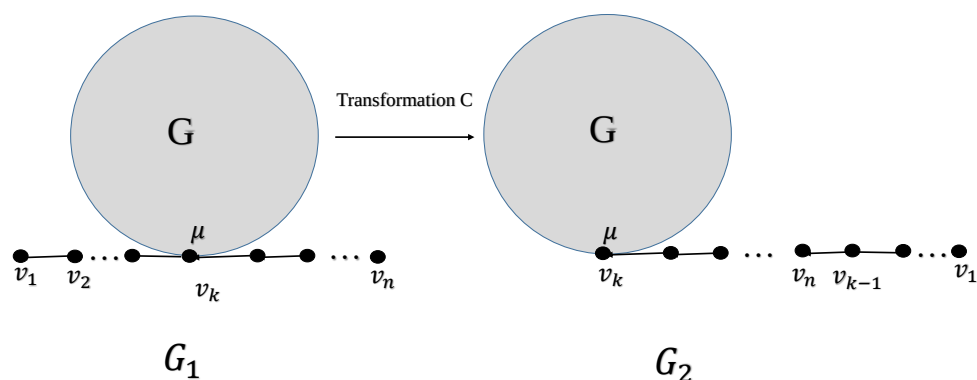


Figure 19. Graph provided for Transformation C.

**Lemma 7.** Consider Figure 19, then  $GSO(G_1) > GSO(G_2)$ .

**Proof.** Applying GSO, it follows that

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 2)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 2)^2 + (d_{G_1}(v_{k-1}))^2)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + (d_{G_1}(v_{k+1}))^2)^\beta + ((d_{G_1}(v_{n-1}))^2 + (d_{G_1}(v_n))^2)^\beta. \end{aligned}$$

$G_2$  follows that

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + (d_{G_2}(v_{k+1}))^2)^\beta \\ &\quad + ((d_{G_2}(v_{n-1}))^2 + (d_{G_2}(v_n))^2)^\beta + ((d_{G_2}(v_n))^2 + (d_{G_2}(v_{k-1}))^2)^\beta. \end{aligned}$$

Here we considered the following:

**Case 1:** If  $k = 2$  and  $n = 3$ .

In the considered case, the following value is considered:

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + d_{G_1}(v_1)^2)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + d_{G_1}(v_3)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 1)^\beta + ((2 + d_G(\mu))^2 + 1)^\beta. \end{aligned}$$

GSO for  $G_2$  is given by

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + d_{G_2}(v_3)^2)^\beta \\ &\quad + ((d_{G_2}(v_3))^2 + d_{G_2}(v_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + 4)^\beta + (5)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 1)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + 1)^\beta - \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta \\ &\quad - ((1 + d_G(\mu))^2 + 4)^\beta - (5)^\beta > 0. \end{aligned}$$

Comparing terms of the above last inequality, we obtain  $GSO(G_1) > GSO(G_2)$ .

**Case 2:** If  $k = 2$  and  $3 < n$ .

The following value is considered:

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + d_{G_1}(v_1)^2)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + d_{G_1}(v_3)^2)^\beta + ((d_{G_1}(v_{n-1}))^2 + (d_{G_1}(v_n))^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + 1)^\beta + (5)^\beta. \end{aligned}$$

GSO for  $(G_2)$  is given by

$$\begin{aligned} \text{GSO}(G_1) &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + d_{G_1}(v_3)^2)^\beta \\ &\quad + ((d_{G_2}(\mu_{n-1}))^2 + d_{G_2}(v_n)^2)^\beta + ((d_{G_2}(v_n))^2 + (d_{G_2}(v_1))^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + 4)^\beta + (8)^\beta + (5)^\beta. \end{aligned}$$

The difference of  $\text{GSO}(G_1)$  and  $\text{GSO}(G_2)$  is given in the following

$$\begin{aligned} \text{GSO}(G_1) - \text{GSO}(G_2) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + 1)^\beta + (5)^\beta - \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta ((1 + d_G(\mu))^2 + 4)^\beta \\ &\quad - (8)^\beta - (5)^\beta > 0. \end{aligned}$$

Comparing terms of the above last inequality we obtain that  $\text{GSO}(G_1) > \text{GSO}(G_2)$ .

**Case 3:** Consider  $2 < k$  and  $n = k + 1$ .

The following value is considered:

$$\begin{aligned} \text{GSO}(G_1) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + d_{G_1}(v_{k+1})^2)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + d_{G_1}(v_{k-1})^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta \end{aligned}$$

GSO for  $G_2$  is given in the following:

$$\begin{aligned} \text{GSO}(G_2) &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + d_{G_2}(v_{k+1})^2)^\beta \\ &\quad + ((d_{G_2}(v_{k+1}))^2 + d_{G_2}(v_{k-1})^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + 4)^\beta + (8)^\beta. \end{aligned}$$

The difference of  $\text{GSO}(G_1)$  and  $\text{GSO}(G_2)$  is considered in the following:

$$\begin{aligned} \text{GSO}(G_1) - \text{GSO}(G_2) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta \\ &\quad + ((2 + d_G(\mu))^2 + 4)^\beta - \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta - ((1 + d_G(\mu))^2 + 4)^\beta - (8)^\beta, \\ &> 0. \end{aligned}$$

Term by term comparison provided that  $\text{GSO}(G_1) - \text{GSO}(G_2) > 0$ , hence  $\text{GSO}(G_1) > \text{GSO}(G_2)$ .

**Case 4:** Consider  $2 < K$  and  $n > k + 1$ .

In the desired case, the following value is considered

$$\begin{aligned} \text{GSO}(G_1) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + d_{G_1}(v_{k-1})^2)^\beta \\ &\quad + ((d_G(\mu) + 2)^2 + d_{G_1}(v_{k+1})^2)^\beta + ((d_{G_1}(v_{n-1}))^2 + d_{G_1}(v_n)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta + (5)^\beta. \end{aligned}$$

$GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + d_{G_2}(v_{k+1})^2)^\beta \\ &\quad + ((d_{G_2}(v_{n-1}))^2 + d_{G_2}(v_n)^2)^\beta + ((d_{G_2}(v_n))^2 + d_{G_2}(v_{k-1})^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((1 + d_G(\mu))^2 + 4)^\beta + (8)^\beta + (8)^\beta. \end{aligned}$$

The difference of  $GSO(G_1)$  and  $GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((2 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta + ((2 + d_G(\mu))^2 + 4)^\beta + (5)^\beta \\ &\quad - \sum_{\theta \in N_G(\mu)} ((1 + d_G(\mu))^2 + (d_G(\theta))^2)^\beta - ((1 + d_G(\mu))^2 + 4)^\beta - (8)^\beta - (8)^\beta, \\ &> 0. \end{aligned}$$

Term by term comparison provided that  $((2 + d_G(\mu))^2 + 4)^\beta + (5)^\beta - (8)^\beta - (8)^\beta > 0$ . Hence it follows that  $GSO(G_1) - GSO(G_2) > 0$ .

□

**Remark 3.** Using Transformation C repeatedly, we transform any tree to a path and GSO decreases, Figure 20 is given for this.

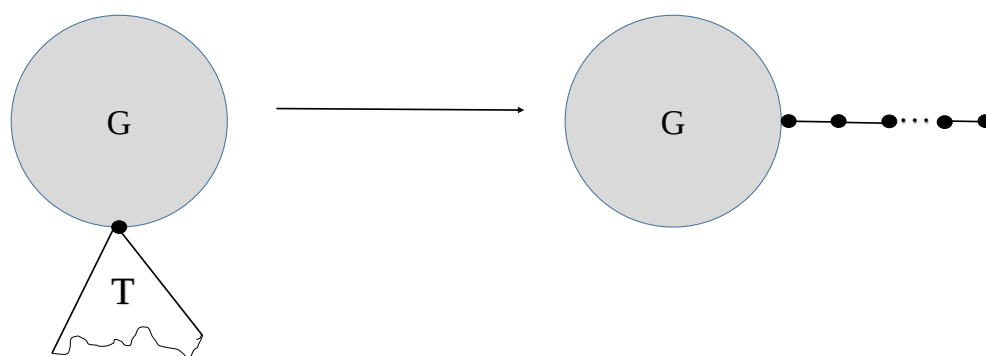


Figure 20. Remark of Transformation C.

Transformation D: Consider a graph  $G$ , let  $\mu$  and  $v$  are in  $G$ . We obtain  $G_1$  by marking  $\mu$  with  $u_0$  and  $v$  with  $v_0$  of the considered paths  $u_0u_1 \cdots u_{\delta-1}u_\delta$  and  $v_0v_1 \cdots v_{t-1}v_t$ , respectively. Let  $G_2$  be the graph which is obtained from  $G_1$  by removing  $u_0u_1$  and add  $v_tu_1$  as in Figure 21.

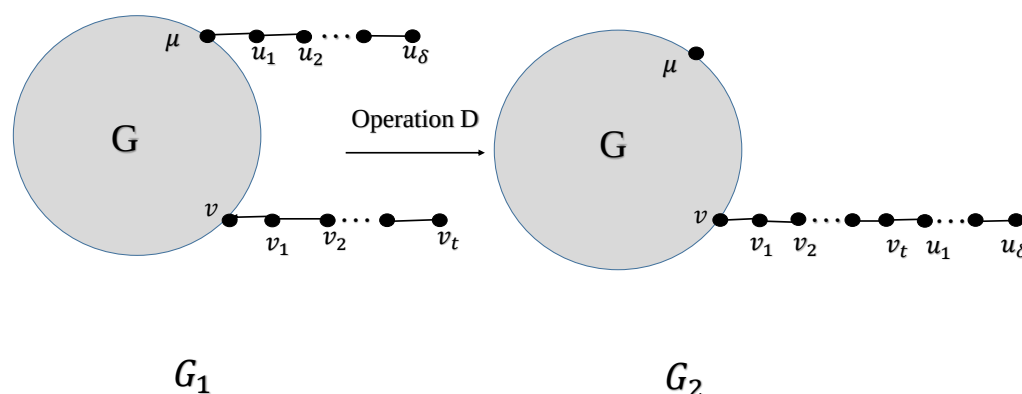


Figure 21. Graphical representation of Transformation D.

**Lemma 8.** Consider  $G_1$  and  $G_2$  as in Figure 21, with  $1 < d_G(v) \leq d_G(\mu)$ ,  $1 \leq \delta$  and  $0 \leq t$ , then

- (i) For  $0 < t$ , we have  $GSO(G_2) < GSO(G_1)$ ;
- (ii) For  $t = 0$  and  $\sum_{y \in \{N_G(v) - \{\mu\}\}} d_G(y) < \sum_{\theta \in \{N_G(\mu) - \{v\}\}} d_G(\theta)$ , we have  $GSO(G_2) < GSO(G_1)$ .

**Proof.** (i) As  $1 < d_G(\mu)$  and  $0 < t$ , then we consider the following cases;

**Case 1.** For  $t = 1$  and  $\delta = 1$ .

In the considered case, for  $GSO(G_1)$  we have the following:

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + ((d_G(v) + 1)^2 + d_{G_1}(v_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 1)^\beta + ((d_G(v) + 1)^2 + 1)^\beta. \end{aligned}$$

$GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + d_{G_2}(v_1)^2)^\beta \\ &\quad + ((d_{G_2}(v_1))^2 + d_{G_2}(\mu_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + 4)^\beta + (5)^\beta. \end{aligned}$$

The difference of  $GSO(G_1)$  and  $GSO(G_2)$  is considered in the following

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 1)^\beta \\ &\quad + ((d_G(v) + 1)^2 + 1)^\beta - \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta - ((d_G(v) + 1)^2 + 4)^\beta - (5)^\beta, \\ &> 0, \quad \because d_G(\mu) \geq d_G(v). \end{aligned}$$

Hence  $GSO(G_1) > GSO(G_2)$ .

**Case 2.** If  $t > 1$  and  $\delta = 1$ .

In the considered case, we have  $GSO(G_1)$  in the following

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + ((d_{G_1}(v_{t-1}))^2 + d_{G_1}(v_t)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 1)^\beta + (5)^\beta \end{aligned}$$

$GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_{G_2}(v_{t-1}))^2 + d_{G_2}(v_t)^2)^\beta \\ &\quad + ((d_{G_2}(v_t))^2 + d_{G_2}(\mu_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + (8)^\beta + (5)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 1)^\beta + (5)^\beta \\ &\quad - \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta - (8)^\beta - (5)^\beta > 0. \end{aligned}$$

Hence  $GSO(G_1) > GSO(G_2)$ .

**Case 3.** If  $1 < \delta$  and  $t = 1$ .

In the considered case,  $GSO(G_1)$  is given by

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + ((d_G(v) + 1)^2 + d_{G_1}(v_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 4)^\beta + ((d_G(v) + 1)^2 + 1)^\beta. \end{aligned}$$

The value of  $GSO(G_2)$  is considered below

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + d_{G_2}(v_1)^2)^\beta \\ &\quad + ((d_{G_2}(v_1))^2 + d_{G_2}(\mu_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + 4)^\beta + (8)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 4)^\beta \\ &\quad + ((d_G(v) + 1)^2 + 1)^\beta - \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta \\ &\quad - ((d_G(v) + 1)^2 + 4)^\beta - (8)^\beta > 0. \end{aligned}$$

Here we have  $GSO(G_1) > GSO(G_2)$ .

**Case 4.** If  $1 < \delta$  and  $t > 1$ .

In the considered case,  $GSO(G_1)$  is given by

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + ((d_{G_1}(v_{t-1}))^2 + d_{G_1}(v_t)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 4)^\beta + (5)^\beta. \end{aligned}$$

$GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_{G_2}(v_{t-1}))^2 + d_{G_2}(v_t)^2)^\beta \\ &\quad + ((d_{G_2}(v_t))^2 + d_{G_2}(\mu_1)^2)^\beta, \\ &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + (8)^\beta + (5)^\beta. \end{aligned}$$

The following difference is considered

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + 4)^\beta + (5)^\beta \\ &\quad - \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + (8)^\beta + (5)^\beta > 0. \end{aligned}$$

Hence  $GSO(G_1) - GSO(G_2)$  and  $GSO(G_1) > GSO(G_2)$ .

(ii). For  $t = 0$  and  $\sum_{y \in N_G(v) - \{\mu\}} d_G(y) < \sum_{\theta \in N_G(\mu) - \{v\}} d_G(\theta)$ , if  $v$  and  $\mu$  are adjacent then the following is considered:

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + \sum_{y \in N_G(v)} ((d_G(v))^2 + d_G(y)^2)^\beta. \end{aligned}$$

$GSO(G_2)$  is considered below.

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + d_{G_2}(\mu_1)^2)^\beta \\ &\quad + \sum_{y \in N_G(v)} ((d_G(v) + 1)^2 + d_G(y)^2)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is considered in the following:

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= \sum_{\theta \in N_G(\mu)} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + \sum_{y \in N_G(v)} ((d_G(v))^2 + d_G(y)^2)^\beta - \sum_{\theta \in N_G(\mu)} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta \\ &\quad - ((d_G(v) + 1)^2 + d_{G_2}(\mu_1)^2)^\beta - \sum_{y \in N_G(v)} ((d_G(v) + 1)^2 + d_G(y)^2)^\beta, \\ &> 0. \quad \because d_{G_1}(\mu_1) = d_{G_2}(\mu_1) \end{aligned}$$

The above inequality provided that  $GSO(G_1) > GSO(G_2)$ .

If  $v$  and  $\mu$  are adjacent, then

$$\begin{aligned} GSO(G_1) &= \sum_{\theta \in N_G(\mu) - \{v\}} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\ &\quad + \sum_{y \in N_G(v) - \{\mu\}} ((d_G(v))^2 + d_G(y)^2)^\beta + ((d_G(\mu) + 1)^2 + (d_G(v))^2)^\beta. \end{aligned}$$

For  $GSO(G_2)$ , it follows that

$$\begin{aligned} GSO(G_2) &= \sum_{\theta \in N_G(\mu) - \{v\}} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta + ((d_G(v) + 1)^2 + d_{G_2}(\mu_1)^2)^\beta \\ &\quad + \sum_{y \in N_G(v) - \{\mu\}} ((d_G(v) + 1)^2 + d_G(y)^2)^\beta + ((d_G(\mu))^2 + (d_G(v) + 1)^2)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is considered in the following:

$$\begin{aligned}
 GSO(G_1) - GSO(G_2) = & \sum_{\theta \in N_G(\mu) - \{v\}} ((d_G(\mu) + 1)^2 + (d_G(\theta))^2)^\beta + ((d_G(\mu) + 1)^2 + d_{G_1}(\mu_1)^2)^\beta \\
 & + \sum_{y \in N_G(v) - \{\mu\}} ((d_G(v))^2 + d_G(y)^2)^\beta + ((d_G(\mu) + 1)^2 + (d_G(v))^2)^\beta \\
 & - \sum_{\theta \in N_G(\mu) - \{v\}} ((d_G(\mu))^2 + (d_G(\theta))^2)^\beta - ((d_G(v) + 1)^2 + d_{G_2}(\mu_1)^2)^\beta \\
 & - \sum_{y \in N_G(v) - \{\mu\}} ((d_G(v) + 1)^2 + d_G(y)^2)^\beta - ((d_G(\mu))^2 + (d_G(v) + 1)^2)^\beta, \\
 & > 0. \qquad \qquad \qquad \because d_{G_1}(\mu_1) = d_{G_2}(\mu_1)
 \end{aligned}$$

Hence  $GSO(G_1) - GSO(G_2)$  and  $GSO(G_1) > GSO(G_2)$ .

□

**Remark 4.** Apply Transformation C and Transformation D repeatedly. We change every tree to a path and every unicyclic graph to a unicyclic graph in which the path is attached to the cycle. Any bicyclic graph can be transformed to a bicyclic graph where the path is attached to the graph in Figure 22 (Lemma 8(i)). We transform any bicyclic graph to a new bicyclic graph where the path is attached to the vertex of degree 2 (Lemma 8(ii)), general Sombor index minimizes.

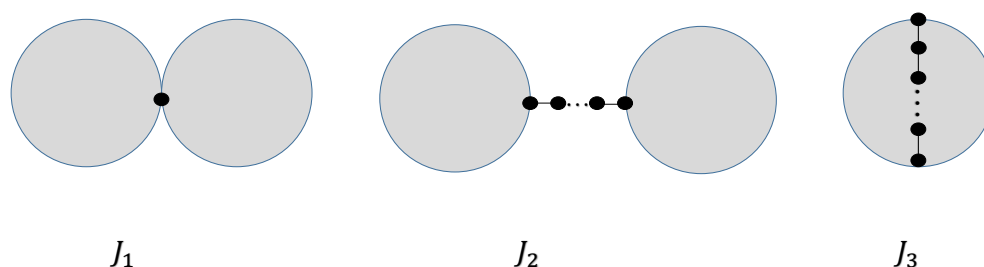


Figure 22. The considered bicyclic graphs  $J_1$ ,  $J_2$  and  $J_3$ .

**Lemma 9.** Consider a graph  $G_1$  given in the Figure 23, let us consider a path  $x_k, x_{k-1}, x_{k-2}, \dots, x_3, x_2, x_1$ , where  $1 < k$  attached to vertex  $x_1$ . We obtain  $G_2$  from  $G_1$  by removing  $vx_1$  and attach  $vx_k$ , then  $GSO(G_1) > GSO(G_2)$ .

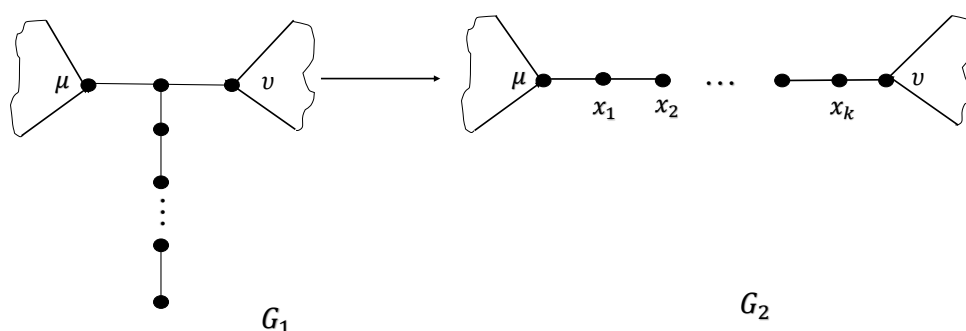


Figure 23. Graph provided for Lemma 9.

**Proof.** Here,  $d(x_k)$  and  $d(x_1)$  are not same. If  $k = 2$ , then the following is considered

$$\begin{aligned}
 GSO(G_1) &= (d(\mu)^2 + d_{G_1}(x_1)^2)^\beta + (d_{G_1}(x_1)^2 + d_{G_1}(x_2)^2)^\beta + (d_{G_1}(x_1)^2 + d(v)^2)^\beta, \\
 &= (d(\mu)^2 + 9)^\beta + (10)^\beta + (9 + d(v)^2)^\beta.
 \end{aligned}$$

$GSO(G_2)$  is considered below.

$$\begin{aligned} GSO(G_2) &= (d(\mu)^2 + d_{G_2}(x_1)^2)^\beta + (d_{G_2}(x_1)^2 + d_{G_2}(x_2)^2)^\beta + (d_{G_2}(x_2)^2 + d(v)^2)^\beta, \\ &= (d(\mu)^2 + 4)^\beta + (8)^\beta + (4 + d(v)^2)^\beta. \end{aligned}$$

Considering  $GSO(G_1) - GSO(G_2)$  below

$$\begin{aligned} GSO(G_1) - GSO(G_2) &= (d(\mu)^2 + 27)^\beta + (28)^\beta + (27 + d(v)^2)^\beta \\ &\quad - (d(\mu)^2 + 4)^\beta - (8)^\beta - (4 + d(v)^2)^\beta, \\ &> 0. \end{aligned}$$

Let  $2 < k$ , then for  $GSO(G_1)$  the following is considered

$$\begin{aligned} GSO(G_1) &= (d(\mu)^2 + d_{G_1}(x_1)^2)^\beta + (d_{G_1}(x_1)^2 + d_{G_1}(x_2)^2)^\beta \\ &\quad + (d_{G_1}(x_1)^2 + d(v)^2)^\beta + (d_{G_1}(x_{k-1})^2 + d_{G_1}(x_k)^2)^\beta, \\ &= (d(\mu)^2 + 9)^\beta + (13)^\beta + (9 + d(v)^2)^\beta + (5)^\beta. \end{aligned}$$

$GSO(G_1)$  is considered in the following:

$$\begin{aligned} GSO(G_2) &= (d(\mu)^2 + d_{G_2}(x_1)^2)^\beta + (d_{G_2}(x_1)^2 + d_{G_2}(x_2)^2)^\beta \\ &\quad + (d_{G_2}(x_k)^2 + d(v)^2)^\beta + (d_{G_2}(x_{k-1})^2 + d_{G_2}(x_k)^2)^\beta, \\ &= (d(\mu)^2 + 4)^\beta + (8)^\beta + (4 + d(v)^2)^\beta + (8)^\beta. \end{aligned}$$

$GSO(G_1) - GSO(G_2)$  is in the following:

$$\begin{aligned} GSO(G_1) - GSO(G_{12}) &= (d(\mu)^2 + 9)^\beta + (9 + d(v)^2)^\beta - (d(\mu)^2 + 4)^\beta - (4 + d(v)^2)^\beta \\ &\quad + (13)^\beta + (5)^\beta - 2(8)^\beta > 0. \end{aligned}$$

We obtain that  $GSO(G_1) - GSO(G_2) > 0$  and  $GSO(G_1) > GSO(G_2)$ .  $\square$

## 8. The Smallest $GSO$ in Trees, Unicyclic, and Bicyclic Graphs

In this section, the general Sombor index is investigated in trees, unicyclic, and bicyclic graphs for minimum values. From Lemma 7, it follows that

**Theorem 8.** Consider a tree  $T$  of order  $n$ , if  $T \neq P_n$  then  $GSO(T_n) > GSO(P_n)$ .

Consider  $U_n^k$  be a unicyclic graph obtained by attaching a path of length  $n - k$  to  $C_k$ . Using Lemmas 7 and 8, it follows that

**Theorem 9.** Consider a unicyclic graph  $G$  with order  $n$  and girth  $k$ . If  $G \neq U_n^k$ , then  $GSO(U_n^k) < GSO(G)$ .

By means of Lemma 9, the following is obtained:

**Theorem 10.**  $C_n$  is the unique graph with smallest  $GSO$ .

Let  $J_1$ ,  $J_2$ , and  $J_3$  be as shown in Figure 22. From Lemmas 7 and 9, the bicyclic graph with the smallest general Sombor index is given by

$$GSO(J_1) = (n - 3)8^\beta + 4(20)^\beta.$$

$$GSO(J_2) = GSO(J_3) = (n - 4)8^\beta + 4(13)^\beta + (18)^\beta,$$

if  $v$  and  $\mu$  are directly connected by an edge

$$GSO(J_2) = GSO(J_3) = (n - 5)8^\beta + 6(13)^\beta,$$

if  $v$  and  $\mu$  are not connected directly by an edge. We have the following differences:

$$GSO(J_1) - GSO(J_2) = 8^\beta + 4(20)^\beta - 4(13)^\beta - (18)^\beta > 0.$$

Figure 24 is provided for the difference.

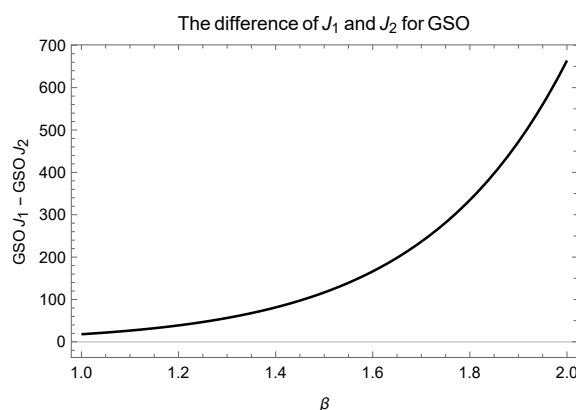


**Figure 24.** Graph for the difference  $GSO(J_1) - GSO(J_2)$ .

$$GSO(J_1) - GSO(J_3) = 2(8^\beta) + 4(20)^\beta - 6(13)^\beta > 0.$$

$$GSO(J_2) - GSO(J_3) = 8^\beta + 4(13)^\beta + (18)^\beta - 6(13)^\beta > 0.$$

For the last inequality, we provide Figure 25.

Hence, it follows that

**Theorem 11.** Let  $G$  be the family of bicyclic graphs of order  $n$ , then the largest GSO is for the graph  $J_1$ .

**Theorem 12.** Let  $G$  be the family of bicyclic graphs of order  $n$ , then the smallest GSO is for  $J_3$  where the vertices of degree 3 are not adjacent, that is  $GSO(J_1) > GSO(J_2) > GSO(J_3)$ .

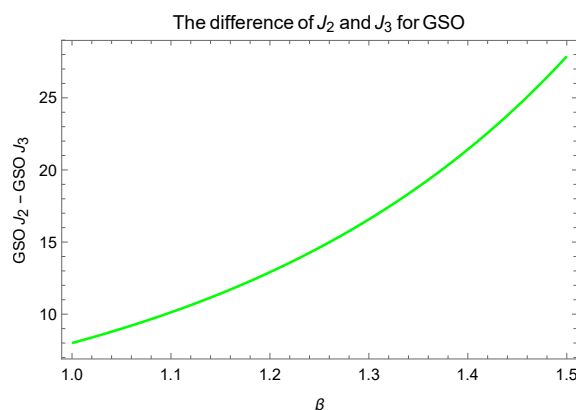


**Figure 25.** Graph for the difference  $GSO(J_2) - GSO(J_3)$ .

## 9. Conclusions

In this work, the generalized Sombor index is investigated for optimal values in graphs. Various transformations are used for obtaining graphs with optimal values in the family of bicyclic graphs, trees, and unicyclic graphs. The considered transformations are simple and

very easy to understand. The effectiveness of these transformations has been demonstrated through rigorous theorems and visualized using comparative plots. Our results contribute to the deeper understanding of the behavior of the generalized Sombor index and offer useful tools for future studies in topological indices.

**Author Contributions:** Conceptualization, G.A. and I.-L.P.; Methodology, M.K., M.Y.K. and I.-L.P.; Software, M.K. and M.Y.K.; Formal analysis, G.A.; Resources, I.-L.P.; Writing—original draft, M.K. and M.Y.K.; Writing—review & editing, G.A.; Funding acquisition, I.-L.P. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research received no external funding.

**Data Availability Statement:** Data are contained within the article.

**Conflicts of Interest:** The authors declare no conflicts of interest.

## References

- Balakrishnan, V.K. *Schaum's Outline of Theory and Problems of Graph Theory*; McGraw-Hill: New York, NY, USA, 1997.
- Khan, M.Y.; Ali, G.; Popa, I.L. Optimization of General Power-Sum Connectivity Index in Uni-Cyclic Graphs, Bi-Cyclic Graphs and Trees by Means of Operations. *Axioms* **2024**, *13*, 840. [[CrossRef](#)]
- Khan, M.Y.; Ali, G.; Popa, I.L. Optimization in Symmetric Trees, Unicyclic Graphs, and Bicyclic Graphs with Help of Mappings Using Second Form of Generalized Power-Sum Connectivity Index. *Symmetry* **2025**, *17*, 122. [[CrossRef](#)]
- Diudea, M.V.; Gutman, I.; Jantschi, L. *Molecular Topology*; Nova Science Publishers: Huntington, NY, USA, 2001.
- Mahasinghe, A.C.; Erandi, K.K.W.H.; Perera, S.S.N. Optimizing Wiener and Randić Indices of Graphs. *Adv. Oper. Res.* **2020**, *2020*, 3139867. [[CrossRef](#)]
- Gutman, I.; Mohar, B. The quasi-Wiener and the Kirchhoff indices coincide. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 982–985. [[CrossRef](#)]
- Otte, E.; Rousseau, R. Social network analysis: A powerful strategy, also for the information sciences. *J. Inf. Sci.* **2002**, *28*, 441–453. [[CrossRef](#)]
- Imran, M.; Hayat, S.; Mailk, M.Y.H. On topological indices of certain interconnection networks. *Appl. Math. Comput.* **2014**, *244*, 936–951. [[CrossRef](#)]
- Kier, L.B. Indexes of molecular shape from chemical graphs. *Med. Res. Rev.* **1987**, *7*, 417–440. [[CrossRef](#)] [[PubMed](#)]
- Camarda, K.V.; Maranas, C.D. Optimization in polymer design using connectivity indices. *Ind. Eng. Chem. Res.* **1999**, *38*, 1884–1892. [[CrossRef](#)]
- Matamala, A.R.; Estrada, E. Generalised topological indices: Optimisation methodology and physico-chemical interpretation. *Chem. Phys. Lett.* **2005**, *410*, 343–347. [[CrossRef](#)]
- Preuß, M.; Dehmer, M.; Pickl, S.; Holzinger, A. On terrain coverage optimization by using a network approach for universal graph-based data mining and knowledge discovery. In *Brain Informatics and Health, Proceedings of the International Conference, BIH 2014, Warsaw, Poland, 11–14 August 2014*; Proceedings; Springer International Publishing: Berlin/Heidelberg, Germany, 2014; pp. 564–573.
- Che, Z.; Chen, Z. Lower and upper bounds of the forgotten topological index. *MATCH Commun. Math. Comput. Chem.* **2016**, *76*, 635–648.
- Monsalve, J.; Rada, J. Sharp upper and lower bounds of VDB topological indices of digraphs. *Symmetry* **2021**, *13*, 1903. [[CrossRef](#)]
- Martínez-Pérez, Á.; Rodríguez, J.M. New bounds for topological indices on trees through generalized methods. *Symmetry* **2020**, *12*, 1097. [[CrossRef](#)]
- Martínez-Pérez, Á.; Rodríguez, J.M. Upper and lower bounds for topological indices on unicyclic graphs. *Topol. Its Appl.* **2023**, *339*, 108591. [[CrossRef](#)]
- Wei, C.C.; Salman, M.; Ali, U.; Rehman, M.U.; Khan, M.A.A.; Chaudary, M.H.; Ahmad, F. Some topological invariants of graphs associated with the group of symmetries. *J. Chem.* **2020**, *2020*, 6289518. [[CrossRef](#)]
- Chu, P.; Li, Y.; He, Z.; Li, E.; Ozgun, O.; Venbosch, G.A.; Zheng, X. A group theory based topology optimization scheme for the design of inhomogeneous waveguides with dihedral group symmetries. *Eng. Anal. Bound. Elem.* **2024**, *166*, 105845. [[CrossRef](#)]
- Öztürk Sözen, E.; Alsuraiheed, T.; Abdioglu, C.; Ali, S. Computing topological descriptors of prime ideal sum graphs of commutative rings. *Symmetry* **2023**, *15*, 2133. [[CrossRef](#)]

20. Balasubramanian, K. Topological indices, graph spectra, entropies, Laplacians, and matching polynomials of n-dimensional hypercubes. *Symmetry* **2023**, *15*, 557. [\[CrossRef\]](#)
21. Kosaka, I.; Swan, C.C. A symmetry reduction method for continuum structural topology optimization. *Comput. Struct.* **1999**, *70*, 47–61. [\[CrossRef\]](#)

**Disclaimer/Publisher’s Note:** The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.