Note on Sombor index of connected graphs with given degree sequence*

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A B S T R A C T

For a simple connected graph $G = (V, E)$, let $d(u)$ be the degree of the vertex u of G. The general Sombor index of G is defined as

$$SO_\alpha(G) = \sum_{uv \in E} \left[d(u)^2 + d(v)^2\right]^\alpha$$

where $SO(G) = SO_{0.5}(G)$ is the recently invented Sombor index. In this paper, we show that in the class of connected graphs with a fixed degree sequence (for which the minimum degree being equal to one), there exists a special extremal BFS-graph with minimum general Sombor index for $0 < \alpha < 1$ (resp. maximum general Sombor index for either $\alpha > 1$ or $\alpha < 0$). Moreover, for any given tree, unicyclic, and bicyclic degree sequences with minimum degree 1, there exists a unique extremal BFS-graph with minimum general Sombor index for $0 < \alpha < 1$ and maximum general Sombor index for either $\alpha > 1$ or $\alpha < 0$.

Keywords: Sombor index; general Sombor index; degree sequence; majorization; BFS-graph

1 Introduction

Throughout this paper we consider undirected simple connected graphs. Let G be such a graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Let $d(u) = d_G(u)$ and $N(u) = N_G(u)$ denote, respectively, the degree and neighbor set of the vertex $u \in V(G)$. If $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d(v_i)$, $1 \le i \le n$, then $\pi = (d_1, d_2, \ldots, d_n)$ is said to be the

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degree sequence of G. In what follows, we always suppose that $d_1 \geq d_2 \geq \cdots \geq d_n$ and denote by $\Gamma(\pi)$ the class of connected graphs with degree sequence π. A connected graph with n vertices and $n+c-1$ edges will be referred as a c-**cyclic graph**. In particular, when $c = 0$, 1, and 2, a c-cyclic graph is also called a tree, unicyclic graph, and bicyclic graph, respectively.

Recently, Gutman proposed a geometric approach for interpreting degree-based graph invariants [9], and according to this approach, he introduced the so-called **Sombor index**, defined as,

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{(d(u)^2 + d(v)^2)}\,. \tag{1}$$

Eventually, this graph invariant attracted much attention, and in a series of researches its main mathematical properties have been determined; see, for instance [1, 4–8, 17, 18, 21] and the review [12].

One of the several modifications of the original Sombor index, Eq. (1), is the **general Sombor index** [10, 16], defined as

$$SO_\alpha = SO_\alpha(G) = \sum_{uv \in \mathbf{E}(G)} \left[d(u)^2 + d(v)^2\right]^\alpha$$

where $\alpha \neq 0$ is a real number. Evidently, $SO_{0.5}(G) = SO(G)$.

It is of evident interest to determine the elements of $\Gamma(\pi)$, extremal w.r.t. a certain graph invariant. Several such researches have been published [2, 11, 13, 14, 19]. Among these results, in many cases the extremal graphs are BFS-type (BFS = breath first search).

Definition 1. *Let G be a connected graph. We say that G is a* BFS**-graph** *if there exists a vertex ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $\mathbf{V}(G)$ satisfying:*
(i) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between v_i and v_1;
(ii) let $v \in N(u) \backslash N(w)$ and $z \in N(w) \backslash N(u)$ such that $h(v) = h(u)+1$ and $h(z) = h(w)+1$. If $u \prec w$, then $v \prec z$.

Definition 2. [14] *For a c-cyclic degree sequence $\pi = (d_1, d_2, ..., d_n)$ with $d_n = 1$ and $n \geq 3$, if G is a BFS-graph such that $\{v_1, v_2, v_3\}$ forms a triangle of G when $c \geq 1$, then G is called a* **special extremal** BFS**-graph**.

Recently, Gutman posed the problem of determining extremal graphs with minimum or maximum Sombor index among the class of connected graphs with given degree sequence (via private communication). In this paper, we settle the minimum case. Actually, we can go further by showing the following

Theorem 3. *For any given degree sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $d_n = 1$, there exists a special extremal BFS-graph with minimum $SO_\alpha(G)$ in the class of $\Gamma(\pi)$ for $0 < \alpha < 1$, and there also exists a special extremal BFS-graph with maximum $SO_\alpha(G)$ in the class of $\Gamma(\pi)$ for either $\alpha > 1$ or $\alpha < 0$.*

Hereafter, we use the symbol $p^{(q)}$ to define q copies of the real number p. In [22] the authors show that for any tree degree sequence π there exists a unique BFS-tree, here denoted by $T_M(\pi)$. The BFS-trees are also called **greedy trees** in the literature, e.g. [11, 19]. In fact, we can also construct a unique unicyclic BFS-graph $U_M(\pi)$ by the following breadth-first-search method for any unicyclic degree sequence $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$ [14]: The unique cycle of $U_M(\pi)$ is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$. Select the vertex v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices v_2, v_3, v_4, v_5,..., v_{d_1+1} as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$. Let $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$ and $N(v_3) = \{v_1, v_2, v_{d_1+d_2}, \ldots, v_{d_1+d_2+d_3-3}\}$. Then, append $d_4 - 1$ vertices to v_4 such that $N(v_4) = \{v_1, v_{d_1+d_2+d_3-2}, \ldots, v_{d_1+d_2+d_3+d_4-4}\}$, and so on. Informally, the BFS-unicyclic graph is constructed from a BFS-tree by adding an edge between v_2 and v_3. As an example, considering the unicyclic degree sequence $\pi_1 = (5, 4, 3^{(3)}, 2^{(10)}, 1^{(8)})$, $U_M(\pi_1)$ is depicted in Fig. 1.

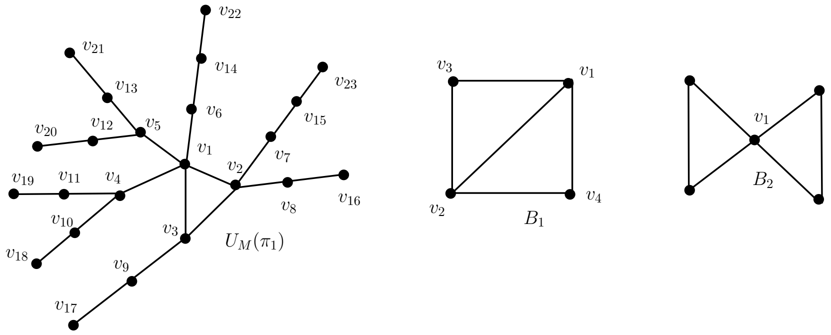

Figure 1: The graphs $U_M(\pi_1)$, B_1 and B_2.

Denote by $\mathcal{R}(G)$ the **reduced graph** obtained from G by recursively deleting pendent vertices to the resultant graph until no pendent vertices remain. If $c \geq 1$ and G is a c-cyclic graph, then $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a c-cyclic graph.

Some paths P_{l_1}, P_{l_2}, ..., P_{l_k} are said to have almost equal lengths if their lengths pairwise differ at most by 1, that is, $|l_i - l_j| \leq 1$ for $1 \leq i < j \leq k$. Let B_1 and B_2 be the two bicyclic graphs depicted in Fig. 1. If $\pi = (d_1, d_2, ..., d_n)$ is a bicyclic degree sequence with $d_n = 1$, then $\sum_{i=1}^{n} d_i = 2n + 2$, which implies that π should be one of the following two cases. When $d_n = 1$, we construct a unique bicyclic graph $B_M(\pi)$ of $\Gamma(\pi)$ as follows:

(*i*) If $d_n = 1$ and $d_1 \geq d_2 \geq 3$, then let $B_M(\pi)$ be a BFS-graph such that $\mathcal{R}(B_M(\pi)) = B_1$ and the remaining vertices appear in a BFS-ordering.

(*ii*) If $d_1 \geq 5 > d_2 = 2$ and $d_n = 1$, then let $B_M(\pi)$ be the bicyclic graph with n vertices obtained from B_2 by attaching $d_1 - 4$ paths of almost equal lengths to the v_1 of B_2 (see Fig. 1).

Definition 4. [3] *For a given degree sequence* $\pi = (d_1, d_2, \ldots, d_n)$ *with* $d_n = 1$*, we say that* G *is a* **precisely extremal graph** *of* $\Gamma(\pi)$*, if* G *has minimum* $SO_\alpha(G)$ *among all graphs of* $\Gamma(\pi)$ *for* $0 < \alpha < 1$ *and* G *has maximum* $SO_\alpha(G)$ *among all graphs of* $\Gamma(\pi)$ *for either* $\alpha > 1$ *or* $\alpha < 0$.

Theorem 5. *For any c-cyclic degree sequence* $\pi = (d_1, d_2, \ldots, d_n)$ *with* $d_n = 1$*, then*

(*i*) $T_M(\pi)$ *is a precisely extremal graph for* $c = 0$*;*

(*ii*) $U_M(\pi)$ *is a precisely extremal graph for* $c = 1$*;*

(*iii*) $B_M(\pi)$ *is a precisely extremal graph for* $c = 2$.

In Theorems 3 and 5, we can only confirm that there exists a (precisely) extremal BFS-graph, as the extremal graphs of $\Gamma(\pi)$ are always not uniquely. For instance, let $\pi_2 = (4, 2^{(8)}, 1^{(4)})$ and let H_1 and H_2 be the two trees as shown in Fig. 2. It is easily to see that H_1 is the unique BFS-tree of $\Gamma(\pi_2)$ and $SO_\alpha(H_1) = SO_\alpha(H_2)$ for any $\alpha \neq 0$.

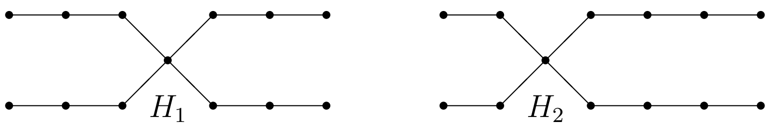

Figure 2. The trees H_1 and H_2.

The research of extremal graph in the class of connected graphs with given degree sequence has close relation with the Majorization theorem. Now, we introduce the notation of Majorization.

Definition 6. [15] *Let* $(x) = (x_1, x_2, ..., x_n)$ *and* $(y) = (y_1, y_2, ..., y_n)$ *be two different non-increasing sequences of real numbers. We write* $(x) \lhd (y)$ *if and only if* $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$*, and* $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ *for all* $j = 1, 2, ..., n$*. The ordering* $\pi \lhd \pi'$ *is said to be a* **majorization**.

Theorem 7. *Let* π *and* π' *be two c-cyclic degree sequences and let* G *and* G' *be a maximum extremal graph of* $\Gamma(\pi)$ *and* $\Gamma(\pi')$*, respectively. If* $c \in \{0, 1, 2\}$ *and* $\pi \lhd \pi'$*, then* $SO_\alpha(G) < SO_\alpha(G')$ *for* $\alpha > 1$.

2 Proof of Theorems 3 and 5

This section is dedicated to the proofs of Theorems 3 and 5. We need to introduce more notations. A symmetric bivariate function $f(x, y)$ defined on positive real numbers is called **escalating** (resp. **de-escalating**) if

$$f(x_1, x_2) + f(y_1, y_2) \geq \text{ (resp., } \leq \text{) } f(y_1, x_2) + f(x_1, y_2) \tag{2}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (2) is strict if $x_1 > y_1$ and $x_2 > y_2$.

Further, Wang [20] defined the **connectivity function** of a connected graph G associated with a symmetric bivariate function $f(x, y)$ to be

$$M_f(G) = \sum_{uv \in \mathbf{E}(G)} f(d(u), d(v)).$$

It is easily to see that $SO_\alpha(G)$ is just a special case of $M_f(G)$.

The proofs of Theorems 3 and 5 rely on the following two lemmas:

Lemma 8. [14] *For any given degree sequence* $\pi = (d_1, d_2, \ldots, d_n)$ *with* $d_n = 1$*, there exists a special extremal BFS-graph* G *such that* $M_f(G)$ *is maximized in* $\Gamma(\pi)$ *when* $f(x, y)$ *is escalating and* $M_f(G)$ *is minimized in* $\Gamma(\pi)$ *when* $f(x, y)$ *is de-escalating.*

Lemma 9. [14] *Let* $\pi = (d_1, d_2, \ldots, d_n)$ *be a given c-cyclic degree sequence with* $d_n = 1$. *In the class of* $\Gamma(\pi)$,

(i) if $c = 0$, *then* $T_M(\pi)$ *has maximum* $M_f(G)$ *when* $f(x, y)$ *is escalating, and* $T_M(\pi)$ *has minimum* $M_f(G)$ *when* $f(x, y)$ *is de-escalating;*

(ii) if $c = 1$, *then* $U_M(\pi)$ *has maximum* $M_f(G)$ *when* $f(x, y)$ *is escalating, and* $U_M(\pi)$ *has minimum* $M_f(G)$ *when* $f(x, y)$ *is de-escalating;*

(iii) if $c = 2$, *then* $B_M(\pi)$ *has maximum* $M_f(G)$ *when* $f(x, y)$ *is escalating, and* $B_M(\pi)$ *has minimum* $M_f(G)$ *when* $f(x, y)$ *is de-escalating;*

Throughout this paper, denote by $h(x, y) = \big(x^2 + y^2\big)^\alpha$, where $\min\{x, y\} > 0$. From Lemmas 8–9, to show Theorems 3 and 5, it suffices to show that the following proposition holds.

Proposition 10. $SO_\alpha(G)$ *is escalating for* $\alpha > 1$ *or* $\alpha < 0$, *and* $SO_\alpha(G)$ *is de-escalating for* $0 < \alpha < 1$.

Proof. In what follows, we suppose that $x_1 \geq y_1 \geq 1$ and $x_2 \geq y_2 \geq 0$. It suffices to show that $h(x, y)$ satisfies (2). Since the equality holds in (2) for either $x_1 = y_1$ or $x_2 = y_2$, we may suppose that $x_1 > y_1$ and $x_2 > y_2$.

One can easily check that

$$\begin{aligned} & h(x_1, x_2) + h(y_1, y_2) - h(y_1, x_2) - h(x_1, y_2) \\ = & \int_{y_1}^{x_1} 2t\alpha(t^2 + x_2^2)^{\alpha-1} dt - \int_{y_1}^{x_1} 2t\alpha(t^2 + y_2^2)^{\alpha-1} dt. \end{aligned} \tag{3}$$

Case 1. $0 < \alpha < 1$. Since $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 0$ and $2t\alpha(t^2 + y_2^2)^{\alpha-1} > 0$ for $t \geq y_1 > 0$, we have

$$2t\alpha(t^2 + x_2^2)^{\alpha-1} < 2t\alpha(t^2 + y_2^2)^{\alpha-1}, \tag{4}$$

as $x_2 > y_2 > 0$ and $0 < \alpha < 1$. Combining (4) with $x_1 > y_1 > 0$, we can conclude that $h(x_1, x_2) + h(y_1, y_2) < h(y_1, x_2) + h(x_1, y_2)$ by (3). Thus, $SO_\alpha(G)$ is de-escalating for $0 < \alpha < 1$.

Case 2. $\alpha < 0$ **or** $\alpha > 1$. If $\alpha > 1$, then $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 2t\alpha(t^2 + y_2^2)^{\alpha-1}$ for $t \geq y_1 > 0$ and $x_2 > y_2$. Combining this with $x_1 > y_1 > 0$, we can conclude that $h(x_1, x_2) + h(y_1, y_2) > h(y_1, x_2) + h(x_1, y_2)$ by (3), which implies that $SO_\alpha(G)$ is escalating for $\alpha > 1$.

Otherwise, $\alpha < 0$. Since $2t\alpha(t^2 + x_2^2)^{\alpha-1} < 0$ and $2t\alpha(t^2 + y_2^2)^{\alpha-1} < 0$, we have $2t\alpha(t^2 + x_2^2)^{\alpha-1} > 2t\alpha(t^2 + y_2^2)^{\alpha-1}$ for $t \geq y_1 > 0$ and $x_2 > y_2 > 0$. Taking this with $x_1 > y_1 > 0$ into consideration, we also deduce that $SO_\alpha(G)$ is escalating for $\alpha < 0$. □

3 Proof of Theorem 7

The following definition will play a crucial role in the proof of Theorem 7.

Definition 11. [14] *A non-negative escalating function $f(x, y)$ is called a* **good escalating** *function, if $f(x, y)$ satisfies $\frac{\partial f(x,y)}{\partial x} > 0$, $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$, and*

$$f(x_1 + 1, x_2) + f(x_1 + 1, y_2) + f(x_1 + 1, y_1 - 1) > f(x_1, x_2) + f(y_1, y_2) + f(x_1, y_1)$$

holds for any $x_1 \geq y_1 \geq 2$ and $x_2 \geq y_2 \geq 1$.

Lemma 12. [13] *Let π and π' be two c-cyclic degree sequences with $\pi \lhd \pi'$ and $c \in \{0, 1, 2\}$. Let G and G' have maximum $M_f(G)$ and $M_f(G')$ in the class of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is good escalating, then $M_f(G) < M_f(G')$.*

Proof of Theorem 7: By Lemma 12, to complete the proof of Theorem 7, it suffices to show that $h(x, y)$ is a good escalating function for $\alpha > 1$. We already know that $h(x, y)$ is a non-negative escalating function for $\alpha > 1$ by Proposition 10.

Since $\alpha > 1$, we have

$$\frac{\partial h(x,y)}{\partial x} = 2x\alpha(x^2 + y^2)^{\alpha-1} > 0 \text{ and } \frac{\partial^2 h(x,y)}{\partial x^2} = 2\alpha(x^2 + y^2)^{\alpha-2}\big[(x^2 + y^2) + 2x^2(\alpha - 1)\big] > 0.$$

Since $h(x, y)$ is a strictly increasing function on x, we have $h(x_1 + 1, x_2) > h(x_1, x_2)$ and $h(x_1 + 1, y_2) > h(y_1, y_2)$, as $x_1 \geq y_1$.

Since $\big[(x_1 + 1)^2 + (y_1 - 1)^2\big] - \big[x_1^2 + y_1^2\big] = 2(x_1 - y_1 + 1) > 0$ for $x_1 \geq y_1$, we have

$$h(x_1 + 1, y_1 - 1) - h(x_1, y_1) = \big[(x_1 + 1)^2 + (y_1 - 1)^2\big]^\alpha - \big(x_1^2 + y_1^2\big)^\alpha > 0$$

for $\alpha > 1$. Now, we can see that $h(x, y)$ is a good escalating function for $\alpha > 1$. □

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References

[1] A. Aashtab, S. Akbari, S. Madadinia, M. Noei, F. Salehi, On the graphs with minimum Sombor index, MATCH Commun. Math. Comput. Chem. 88 (2022) 553–559.

[2] E. O. D. Andriantiana, V. R. Misanantenaina, S. Wagner, Extremal trees with fixed degree sequence, Electron. J. Combin. 28 (2021) #P1.1.

[3] C. Chen, M. Liu, X. Chen, W. Lin, On general ABC-type index of connected graphs, Discrete Appl. Math. 315 (2022) 27–35.

[4] H. Chen, W. Li, J. Wang, Extremal values on the Sombor index of trees, MATCH Commun. Math. Comput. Chem. 87 (2022) 23–49.

[5] R. Cruz, J. Rada, Extremal values of the Sombor index in unicyclic and bicyclic graphs, J. Math. Chem. 59 (2021) 1098–1116.

[6] K. C. Das, A. S. Çevik, I. N. Cangul, Y. Shang, On Sombor index, Symmetry 13 (2021) #140.

[7] K. C. Das, Y. Shang, Some extremal graphs with respect to Sombor index, Mathematics 9 (2021) #1202.

[8] I. Gutman, Some basic properties of Sombor indices, Open J. Discret. Appl. Math. 4 (2021) 1–3.

[9] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, MATCH Commun. Math. Comput. Chem. 86 (2021) 11–16.

[10] J. C. Hernández, J. M. Rodríguez, O. Rosario, J. M. Sigarreta, Extremal problems on the general Sombor index of a graph, AIMS Math. 7 (2022) 8330–8343.

[11] W. Lin, T. Gao, Q. Chen, X. Lin, On the minimal ABC index of connected graphs with given degree sequence, MATCH Commun. Math. Comput. Chem. 69 (2013) 571–578.

[12] H. Liu, I. Gutman, L. You, Y. Huang, Sombor index: Review of extremal results and bounds, J. Math. Chem. 66 (2022) 771–798.

[13] M. Liu, I. Tomescu, J. Liu, Unified extremal results for k-apex unicyclic graphs (trees), Discrete Appl. Math. 288 (2021) 35–49.

[14] M. Liu, K. Xu, X.-D. Zhang, Extremal graphs for vertex-degree-based invariants with given degree sequences, Discrete Appl. Math. 255 (2019), 267–277.

[15] A. W. Marshall, I. Olkin, Inequalities: Theory of Majorization and its Applications, Academic Press, New York, 1979.

[16] C. Phanjoubam, S. M. Mawiong, A. M. Buhphang, On general Sombor index of graphs, Asian-European J. Math., DOI 10.1142/S1793557123500523.

[17] J. Rada, J. M. Rodríguez, J. M. Sigarreta, General properties on Sombor indices, Discrete Appl. Math. 299 (2021) 87–97.

[18] T. Réti, T. Došlić, A. Ali, On the Sombor index of graphs, Contrib. Math. 3 (2021) 11–18.

[19] H. Wang, Extremal trees with given degree sequence for the Randić index, Discrete Math. 308 (2008) 3407–3411.

[20] H. Wang, Functions on adjacent vertex degrees of trees with given degree sequence, Central Eur. J. Math. 12 (2014) 1656–1663.

[21] C. Yang, M. Ji, K. C. Das, Y. Mao, Extreme graphs on the Sombor indices, AIMS Math. 7 (2022) 19126–19146.

[22] X. -D. Zhang, The Laplacian spectral radii of trees with degree sequences, Discrete Math. 308 (2008) 3143–3150.