MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **94** (2025) 855–862
ISSN: 0340–6253
doi: 10.46793/match.94-3.28824

Proof of a Conjecture on Sombor Index and the Least Sombor Eigenvalue of Graphs

Kinkar Chandra Das*, **Chunlei Xu**

[a] *Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea*

[b] *College of Mathematics Science, Inner Mongolia Minzu University, Tongliao 028000, P. R. China*

kinkardas2003@gmail.com, xuchunlei1981@sina.cn

(Received December 28, 2024)

Abstract

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Molecular descriptors play a significant role in quantitative studies of structure-property and structure-activity relationships. One of the popular degree-based topological indices, the Sombor index (SO), is a chemically useful descriptor. The Sombor index of a graph G is defined as

$$SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2},$$

where d_i is the degree of the vertex $v_i \in V(G)$. The Sombor matrix of G, denoted by $SM(G)$, is defined as the $n \times n$ matrix whose (i, j)-entry is $\sqrt{d_i^2 + d_j^2}$ if $v_iv_j \in E(G)$, and 0 otherwise. Let the eigenvalues of the Sombor matrix $SM(G)$ be $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. Very recently, Rabizadeh, Habibi and Gutman [**Some notes on Sombor index of graphs, MATCH Commun. Math. Comput. Chem. 93 (2025) 853–859**] proposed a conjecture about the Sombor index of graphs, stated as follows:

(a)

$$m|\sigma_n| = -m\sigma_n \geq SO(G).$$

(b) If G is connected, then the equality in (a) holds if and only if G is a complete graph. In the general case, equality holds if and only if G consists of mutually isomorphic complete graphs and some (or no) isolated vertices. In this paper, we provide a complete solution to the above conjecture.

1 Introduction

In this paper we only consider simple graphs. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. For any vertex $v_i \in V(G)$, let $N_G(v_i)$ be the set of neighbors of v_i in G. The *degree* of a vertex v_i, denoted by d_i, is the cardinality of $N_G(v_i)$. We write $v_iv_j \in E(G)$ when the vertices v_i and v_j are adjacent. Any additional notations and terminology related to graph theory used in this paper can be found in [2].

A topological descriptor is a numerical measure that captures the topology of a molecule. These descriptors are widely used to predict the physicochemical and biological properties of molecules in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [22,23]. Over time, numerous degree-based topological descriptors have been proposed and extensively studied by researchers [3,4,14,15]. Recently, a new degree-based molecular structure descriptor, known as the Sombor index, was introduced. Denoted by $SO(G)$, it is defined as [17]:

$$SO = SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}, \tag{1}$$

where d_i is the degree of vertex v_i. Fundamental mathematical properties of the Sombor index, such as lower and upper bounds, have been studied extensively (see, [1,5,6,8–11,13,14,17,24]). This index was inspired by the geometric interpretation of the degree radius of an edge v_iv_j, which represents the distance from the origin to the ordered pair (d_i, d_j).

The adjacency matrix $A(G)$ of a graph G is a $(0,1)$-square matrix of order $n \times n$, where the (i,j)-entry is 1 if $v_iv_j \in E(G)$, and 0 otherwise. The multi-set of eigenvalues of $A(G)$ is known as the spectrum of G. Since

$A(G)$ is real and symmetric, its eigenvalues are real and can be ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The mathematical properties, particularly the extremal problems and bounds, of the eigenvalues of the adjacency matrix have been studied, see [7,12,19]. The Sombor matrix of a graph G, denoted by $SM(G) = (s_{ij})_{n\times n}$, is defined as:

$$s_{ij} = \begin{cases} \sqrt{d_i^2 + d_j^2} & \text{if } v_iv_j \in E(G), \\ 0 & \text{otherwise,} \end{cases}$$

where d_i is the degree of vertex v_i. Evidently, this matrix is also real and symmetric. We denote its eigenvalues by σ_i's and order them as $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. The largest eigenvalue σ_1 of $SM(G)$ is called the "Sombor spectral radius" of G, and σ_n is the least eigenvalue of $SM(G)$. Various paper on spectral properties of Sombor matrix, like properties of Sombor eigenvalues, Sombor spectral radius and others can be found in [16, 18, 20].

The complete graphs of order n is denoted by K_n. Denote by $H_1 \cup H_2$, the **union** of two graphs $H_1 = (V_1, E_1)$ and $H_2 = (V_2, E_2)$. The union is a graph $H = (V, E)$, where $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$.

Very recently, Rabizadeh, Habibi and Gutman [19] proposed a conjecture about the Sombor index of graphs, stated as follows:

Conjecture 1. [19]
(a)

$$m|\sigma_n| = -m\sigma_n \geq SO(G).$$

(b) If G is connected, then the equality in (a) holds if and only if G is a complete graph. In the general case, equality holds if and only if G consists of mutually isomorphic complete graphs and some (or no) isolated vertices.

In this paper, we provide a complete solution to the above conjecture.

2 Main Result

In this section, we confirm **Conjecture 1**. To achieve this, we first establish the following result:

Lemma 1. [21] *Let B be a $p \times p$ symmetric matrix and let B_k be its leading $k \times k$ submatrix. Then, for $i = 1, 2, \ldots, k$,*

$$\rho_{p-i+1}(B) \leq \rho_{k-i+1}(B_k) \leq \rho_{k-i+1}(B) \tag{2}$$

where $\rho_i(B)$ is the i-th greatest eigenvalue of B.

Theorem 1. *Let G be a graph of order n with m edges. Then*

$$m\,|\sigma_n(G)| = -m\,\sigma_n(G) \geq SO(G) \tag{3}$$

with equality holding if and only if $G \cong r\,K_s \cup (n - rs)\,K_1$, where $r\,(\geq 1)$ and $s\,(\geq 1)$ are positive integers.

Proof. If $m = 0$, then $G \cong n\,K_1$, $\sigma_n(G) = 0$ and $m = 0 = SO(G)$. Hence the equality holds in (3). Otherwise, $m > 0$. Let v_1 and v_2 be vertices in G such that $v_1v_2 \in E(G)$ and

$$\sqrt{d_1^2 + d_2^2} = \max_{v_k v_\ell \in E(G)} \sqrt{d_k^2 + d_\ell^2}.$$

Then we have

$$\sqrt{d_k^2 + d_\ell^2} \leq \sqrt{d_1^2 + d_2^2}$$

for any edge $v_kv_\ell \in E(G)$, that is,

$$SO(G) = \sum_{v_k v_\ell \in E(G)} \sqrt{d_k^2 + d_\ell^2} \leq m\,\sqrt{d_1^2 + d_2^2} \tag{4}$$

with equality if and only if $\sqrt{d_k^2 + d_\ell^2} = \sqrt{d_1^2 + d_2^2}$ for any edge $v_kv_\ell \in E(G)$.

Setting $p = n$, $i = 1$ and $k = 2$ in Lemma 1, we obtain

$$\sigma_n(G) = \rho_n(SM(G)) \leq \rho_2(SM_2),$$

where SM_2 is the leading 2×2 submatrix of $SM(G)$ and $\rho_2(SM_2)$ is the smallest eigenvalue of SM_2. Since $v_1v_2 \in E(G)$, the smallest eigenvalue $\rho_2(SM_2)$ satisfies

$$\begin{vmatrix} -\rho & \sqrt{d_1^2+d_2^2} \\ \sqrt{d_1^2+d_2^2} & -\rho \end{vmatrix} = 0,$$

that is,

$$\rho_2(SM_2) = -\sqrt{d_1^2+d_2^2}.$$

Thus we have

$$\sigma_n(G) \le -\sqrt{d_1^2+d_2^2} \le -\frac{SO(G)}{m},$$

$$\text{that is, } m\,|\sigma_n(G)| = -m\,\sigma_n(G) \ge SO(G). \tag{5}$$

The first part of the proof is done.

Suppose that equality holds in (3) with $m > 0$. Then all inequalities in the above argument must be equalities. In particular, from the equality in (4), we get

$$\sqrt{d_k^2+d_\ell^2} = \sqrt{d_1^2+d_2^2} \text{ for any edge } v_kv_\ell \in E(G).$$

Therefore $SM(G) = \sqrt{d_1^2+d_2^2}\,A(G)$ and hence $\sigma_n(G) = \lambda_n(G)\,\sqrt{d_1^2+d_2^2}$. From the equality in (5), we obtain

$$\sigma_n(G) = -\sqrt{d_1^2+d_2^2}.$$

From the above results, we get $\lambda_n(G) = -1$.

First we assume that G is a connected graph. If $G \cong K_n$, then $\sigma_n(G) = -(n-1)\sqrt{2}$, $SO(G) = \frac{n(n-1)^2}{\sqrt{2}}$ and hence the equality holds in (3). Otherwise, $G \ncong K_n$. Then P_3 is an induced subgraph of G. Setting $i = 1$ and $k = 3$ in Lemma 1, we obtain

$$\lambda_n(G) = \lambda_n(A(G)) \le \lambda_3(P_3) = -\sqrt{2} < -1 = \lambda_n(G),$$

a contradiction.

Next we assume that G is disconnected. Let $H_i\,(1 \le i \le r)$ be the i-th connected component in G with n_i vertices and $m_i\,(> 0)$ edges such that $m_1 \ge m_2 \ge \cdots \ge m_r > 0$. Thus we have

$$G \cong H_1 \cup H_2 \cup \cdots \cup H_r \cup (n - n_1 - n_2 - \cdots - n_r)\, K_1.$$

Since $m_i > 0\,(1 \le i \le r)$, by Lemma 1, one can easily see that $\lambda_n(H_i) \le -1$. Thus we have

$$-1 = \lambda_n(G) = \min_{1\le i\le r} \lambda_{n_i}(H_i) \le -1.$$

Hence $\lambda_{n_i}(H_i) = -1$ for $1 \le i \le r$. Since $H_i\,(1 \le i \le r)$ is connected, from the above, we have $H_i \cong K_{n_i}$. For $1 \le i \le r$, we have

$$(n_i - 1)\,\sqrt{2} = \sqrt{d_1^2 + d_2^2} \;\text{ for any edge } v_k v_\ell \in E(H_i),$$

that is, $n_1 = n_2 = \cdots = n_r = s$, (say). Hence $G \cong r\,K_s \cup (n - rs)\,K_1$, where $r\,(\ge 1)$ and $s\,(\ge 2)$ are positive integers.

Conversely, let $G \cong r\,K_s \cup (n - rs)\,K_1$, where $r\,(\ge 1)$ and $s\,(\ge 2)$ are positive integers. Then $\sigma_n(G) = -\sqrt{2}\,(s-1)$, $m = \frac{rs(s-1)}{2}$ and $SO(G) = \frac{rs(s-1)^2}{\sqrt{2}}$. Then $m\,|\sigma_n(G)| = -m\,\sigma_n(G) = SO(G)$. This completes the proof of the theorem. ■

***Acknowledgment*:** C. Xu is supported by the Doctoral Scientific Research Funds of Inner Mongolia Minzu University (BSZ013, BSZ014, BS643) and the Natural Science Foundation of Inner Mongolia Autonomous Regions (2022LHMS01006).

References

[1] S. Ahmad, R. Farooq, K. C. Das, The general Sombor index of extremal trees with a given maximum degree, *MATCH Commun. Math. Comput. Chem.*, in press.

[2] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, MacMillan, London, 1976.

[3] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Zagreb indices: Bounds and extremal graphs, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.

[4] L. Buyantogtokh, B. Horoldagva, K. C. Das, On reduced second Zagreb index, *J. Comb. Opt.* **39** (2020) 776–791.

[5] R. Cruz, I. Gutman, J. Rada, Sombor index of chemical graphs, *Appl. Math. Comput.* **339** (2021) #126018.

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

[7] D. M. Cvetković, P. Rowlison, S. Simić, *An Introduction to Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.

[8] K. C. Das, Open problems on Sombor index of unicyclic and bicyclic graphs, *Appl. Math. Comput.* **473** (2024) #128647.

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

[10] K. C. Das, A. Ghalavand, A. R. Ashrafi, On a conjecture about the Sombor index of graphs, *Symmetry* **13** (2021) #1830.

[11] K. C. Das, I. Gutman, On Sombor index of trees, *Appl. Math. Comput.* **412** (2022) #126575.

[12] K. C. Das, P. Kumar, Some new bounds on the spectral radius of graphs, *Discr. Math.* **281** (2004) 149–161.

[13] K. C. Das, M. Imran, T. Vetrík, General Sombor index of graphs and trees, *J. Discr. Math. Sci. Crypt.*, in press.

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

[15] H. Deng, Z. Tang, R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum Chem.* **11** (2021) #e26622.

[16] N. Ghanbari, On the Sombor characteristic polynomial and Sombor energy of a graph, *Comput. Appl. Math.* **41** (2022) #242.

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

[18] S. Pirzada, B. A. Rather, K. C. Das, Y. Shang, On spectrum of Sombor matrix and Sombor energy of graphs, *Georgian Math. J.*, in press.

[19] S. Rabizadeh, M. Habibi, I. Gutman, Some notes on Sombor index of graphs, *MATCH Commun. Math. Comput. Chem.* **93** (2025) 853–859.

[20] B. A. Rather, M. Imran, Sharp bounds on the Sombor energy of graphs, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 605–624.

[21] J. R. Schott, *Matrix Analysis for Statistics*, Wiley, New York, 1997.

[22] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[23] N. Trinajsti c, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983.

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