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On characteristic polynomial and energy of Sombor matrix

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Abstract: Let G be a simple graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, and let d_i be the degree of the vertex v_i. The Sombor matrix of G is the square matrix $\mathbf{A}_{SO}$ of order n, whose (i, j)-element is $\sqrt{d_i^2 + d_j^2}$ if v_i and v_j are adjacent, and zero otherwise. We study the characteristic polynomial, spectrum, and energy of $\mathbf{A}_{SO}$. A few results for the coefficients of the characteristic polynomial, and bounds for the energy of $\mathbf{A}_{SO}$ are established.

Keywords: Sombor index; Sombor matrix; Energy (of Sombor matrix); Characteristic polynomial (of Sombor matrix); Degree (of vertex).

MSC: 05C07; 05C09; 05C92.

1. Introduction

The *Sombor index SO* is a recently introduced vertex-degree-based topological index [1]. It promptly attracted much attention and its mathematical properties and chemical applications became a topic of a remarkably large number of studies, e.g., [2–9]. Also promptly, the concept of Sombor index was extended to linear algebra, by defining the *Sombor matrix*, which then led to the investigation of its spectrum and various spectrum–based properties [10–14]. In particular, the *energy* of the Sombor matrix was much examined [11–14]. In the present paper we report a few additional results on this matter, with emphasis on the characteristic polynomial and energy.

In this paper, we considered simple, finite, undirected, and connected graphs. Let G be such a graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. If two vertices have a common edge then they are said to be adjacent. If the vertices u and v are adjacent, then the edge connecting them is denoted by uv. The number of edges incident to a vertex v is called the degree of that vertex v, and is denoted by d_v.

In the mathematical and chemical literature, a great number of vertex-degree-based graph invariants of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} \varphi(d_u, d_v) \tag{1}$$

have been considered, where φ is a suitably chosen function, with property $\varphi(x, y) = \varphi(y, x)$. These invariants are usually referred to as *topological indices*. Among them are the forgotten topological index [15]

$$F(G) = \sum_{uv \in \mathbf{E}(G)} \left(d_u^2 + d_v^2\right) = \sum_{u \in \mathbf{V}(G)} d_u^3,$$

the Sombor index [1]

$$SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2},$$

and many other [16,17].

The adjacency matrix $\mathbf{A}(G) = (a_{ij})_{n\times n}$ of the graph G with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$, is the symmetric matrix of order n, whose elements are defined as [18]:

$$a_{ij} = \begin{cases} 1 & \text{if } v_iv_j \in \mathbf{E}(G) \\ 0 & \text{if } v_iv_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{2}$$

The characteristic polynomial of $\mathbf{A}(G)$ is $\phi(G,\lambda) = \det\big[\lambda\, \mathbf{I}_n - \mathbf{A}(G)\big]$, where $\mathbf{I}_n$ is the unit matrix of order n [18]. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\mathbf{A}(G)$ form the spectrum of the graph G [18]. Recall that these eigenvalues coincide with the zeros of $\phi(G,\lambda)$.

The energy of the graph G is defined as [19]:

$$En(G) = \sum_{i=1}^{n} |\lambda_i|\,.$$

The theory of graph spectra, including the theory of graph energy, is nowadays a well elaborated part of discrete mathematics. In parallel with the above specified graph-spectral concepts, we now introduce their Sombor-index-related counterparts. The following definition is an application to the Sombor index of the general spectral theory of matrices associated with vertex-degree-based topological indices of the form (1) [20–22].

Definition 1. (1) The Sombor matrix $\mathbf{A}_{SO}(G) = (so_{ij})_{n\times n}$ of the graph G with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$, is the symmetric matrix of order n, whose elements are

$$so_{ij} = \begin{cases} \sqrt{d_{v_i}^2 + d_{v_j}^2} & \text{if } v_iv_j \in \mathbf{E}(G) \\ 0 & \text{if } v_iv_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{3}$$

(2) The Sombor characteristic polynomial of the graph G is $\phi_{SO}(G,\lambda) = \det\big[\lambda\, \mathbf{I}_n - \mathbf{A}_{SO}(G)\big]$. We will write it in the form

$$\phi_{SO}(G,\lambda) = \sum_{k\geq 0} so(G,k)\, \lambda^{n-k}\,.$$

(3) The eigenvalues $\sigma_1, \sigma_2, \ldots, \sigma_n$ of the Sombor matrix $\mathbf{A}_{SO}(G)$ form the Sombor spectrum of the graph G.

(4) The Sombor energy of the graph G is

$$En_{SO}(G) = \sum_{i=1}^{n} |\sigma_i|\,. \tag{4}$$

Since $\mathbf{A}_{SO}(G)$ is a real symmetric matrix, all its eigenvalues, i.e., all roots of $\phi_{SO}(G,\lambda) = 0$, are real. Thus, they can be arranged as $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$.

Remark 1. Comparing Equations (2) and (3), we see that the Sombor matrix can be viewed as the ordinary adjacency matrix of a graph with weighted edges, such that the weight of the edge v_iv_j is $\sqrt{d_{v_i}^2 + d_{v_j}^2}$. This observation allows us to apply to the Sombor matrix and its spectrum the standard methods of graph spectral theory [18], in particular the Sachs coefficient theorem [23].

2. Preliminaries

The following elementary spectral properties of the Sombor matrix were recognized in several earlier studies [10–14].

Lemma 1. *Let G be a graph with Sombor eigenvalues $\sigma_1, \sigma_2, \ldots, \sigma_n$. Then*

$$\sum_{i=1}^{n} \sigma_i = 0,$$

$$\sum_{i=1}^{n} \sigma_i^2 = 2F(G), \tag{5}$$

$$\sum_{i=1}^{n} \sigma_i^3 = 6 \sum_{\Delta} \prod_{uv \in \mathbf{E}(\Delta)} \sqrt{d_u^2 + d_v^2}, \tag{6}$$

or, equivalently,

$$so(G,1) = 0,$$
$$so(G,2) = -F(G),$$
$$so(G,3) = -2 \sum_{\Delta} \prod_{uv \in \mathbf{E}(\Delta)} \sqrt{d_u^2 + d_v^2},$$

where $\sum_\Delta$ indicates summation over all triangles contained in the graph G.

Formula (6) can be generalized as follows:

Lemma 2. *Let p be the size of smallest odd cycle contained in the graph G, and let $\sum_{C_p}$ indicate summation over all cycles of size p contained in G. Then for $q = 1, 3, \ldots, p-2$,*

$$\sum_{i=1}^{n} \sigma_i^q = 0 \tag{7}$$

whereas

$$\sum_{i=1}^{n} \sigma_i^p = 2p \sum_{C_p} \prod_{uv \in \mathbf{E}(C_p)} \sqrt{d_u^2 + d_v^2}$$

or, equivalently,

$$so(G,p) = -2 \sum_{C_p} \prod_{uv \in \mathbf{E}(C_p)} \sqrt{d_u^2 + d_v^2}\,.$$

If G does not possess odd cycles, i.e., if G is bipartite, then relations (7) and $so(G,q) = 0$ hold for all odd values of q.

Proof. Take into account Remark 1, and use the analogous result for ordinary graphs [18]. □

Lemma 3. [24,25] *Suppose that a_i and b_i are non negative real numbers for $1 \le i \le n$. Then,*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) \le \frac{1}{4}\left(\sqrt{\frac{M_1\,M_2}{m_1\,m_2}} + \sqrt{\frac{m_1\,m_2}{M_1\,M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i\,b_i\right)^2$$

where $M_1 = \max_{1\le i\le n} a_i$, $M_2 = \max_{1\le i\le n} b_i$, $m_1 = \min_{1\le i\le n} a_i$, and $m_2 = \min_{1\le i\le n} b_i$.

Lemma 4. [24,25] *Using the same notation as in Lemma 3,*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_i\,b_i\right)^2 \le \frac{n^2}{4}\left(M_1\,M_2 - m_1\,m_2\right)^2.$$

3. New bounds for Sombor energy

Various lower and upper bounds for Sombor energy were already reported in [10–13]. In this section we establish a few more.

We first recall a result by Lin and Miao [13], that can be stated in terms of traces of the Sombor matrix. It should be compared with the below Theorem 2. The upper bound was obtained also in [12]. Note that $tr(\mathbf{A}_{SO}(G)^2) = 2F(G)$ follows from Equation (5).

Theorem 1. [13] *Denote the trace of a square matrix* $\mathbf{M}$ *by* $tr(\mathbf{M})$. *Let G be a graph on n vertices. Then*

$$\sqrt{tr(\mathbf{A}_{SO}(G)^2)} \leq En_{SO}(G) \leq \sqrt{n\, tr(\mathbf{A}_{SO}(G)^2)}$$

i.e.,

$$\sqrt{2F(G)} \leq En_{SO}(G) \leq \sqrt{2n\, F(G)}.$$

Theorem 2. *Let G be a non-trivial graph. Then*

$$En_{SO}(G) \geq \sqrt{\frac{\left[tr(\mathbf{A}_{SO}(G)^2)\right]^3}{tr(\mathbf{A}_{SO}(G)^4)}}.$$

Proof. By the Hölder inequality,

$$\sum_{i=1}^{n} a_i\, b_i \leq \left(\sum_{i=1}^{n} a_i^p\right)^{1/p} \left(\sum_{i=1}^{n} b_i^q\right)^{1/q}$$

where, $a_i, b_i \in \mathbf{R}^+$, $(i = 1, 2, 3 \ldots, n)$. Setting $a_i = |\sigma_i|^{2/3}$, $b_i = |\sigma_i|^{4/3}$, $p = 3/2$, and $q = 3$, we get

$$\sum_{i=1}^{n} |\sigma_i|^2 \leq \left(\sum_{i=1}^{n} |\sigma_i|\right)^{2/3} \left(\sum_{i=1}^{n} |\sigma_i|^4\right)^{1/3}$$

which by Equation (4), and bearing in mind that since G is not an empty graph and thus $\sum_{i=1}^{n} |\sigma_i|^4 \neq 0$, yields Theorem 2. □

Theorem 3. *If* σ_1 *is the greatest Sombor eigenvalue, then* $En_{SO}(G) \leq 2\sigma_1$. *For connected graphs, equality holds if and only if G is a complete bipartite graph.*

Proof. Bearing in mind Equation (4),

$$En_{SO}(G) = |\sigma_1| + \sum_{i=2}^{n} |\sigma_i| \geq |\sigma_1| + \left|\sum_{i=2}^{n} \sigma_i\right|.$$

On the other hand,

$$\sum_{i=1}^{n} \sigma_i = 0 \quad \Longrightarrow \quad \sigma_1 = -\sum_{i=2}^{n} \sigma_i \quad \text{and so} \quad |\sigma_1| = \left|\sum_{i=2}^{n} \sigma_i\right|.$$

Equality holds if σ_1 and σ_n are the only non-zero eigenvalues. In view of Remark 1, this happens only if G is a complete bipartite graph. □

Theorem 4. *Let G be a graph with n vertices. If no Sombor eigenvalue of G is equal to zero, then*

$$En_{SO}(G) \geq \sqrt{\frac{8n\, F(G)\, \sigma_\ell\, \sigma_s}{|\sigma_\ell| + |\sigma_s|}}$$

where, $|\sigma_\ell|$ *and* $|\sigma_s|$ *are, respectively, the largest and smallest absolute values of the eigenvalues in the Sombor spectrum of G. Of course,* $|\sigma_\ell| = \sigma_1$.

Proof. Setting in Lemma 3, $a_i = |\sigma_i|$ and $b_i = 1$ for $1 \leq i \leq n$, we get

$$\left(\sum_{i=1}^{n} |\sigma_i|^2\right)\left(\sum_{i=1}^{n} 1\right) \leq \frac{1}{4}\left(\sqrt{\frac{|\sigma_\ell|}{|\sigma_s|}} + \sqrt{\frac{|\sigma_s|}{|\sigma_\ell|}}\right)^2 \left(\sum_{i=1}^{n} |\sigma_i|\right)^2,$$

where $|\sigma_\ell| = \max_{1\le i\le n}\{|\sigma_i|\}$ and $|\sigma_s| = \min_{1\le i\le n}\{|\sigma_i|\}$. Then

$$2F(G)\,n \le \frac{1}{4}\left(\sqrt{\frac{|\sigma_\ell|}{|\sigma_s|}}+\sqrt{\frac{|\sigma_s|}{|\sigma_\ell|}}\right)^2 \left(\sum_{i=1}^{n}|\sigma_i|\right)^2$$

and thus

$$\sqrt{8n\,F(G)} \le \left(\frac{|\sigma_\ell|+|\sigma_s|}{\sqrt{\sigma_\ell\,\sigma_s}}\right) En_{SO}(G)$$

which straightforwardly leads to Theorem 4. □

Theorem 5. *Let G be a connected graph with n vertices, and σ_ℓ, σ_s same as in Theorem 4. Then*

$$En_{SO}(G) \ge \sqrt{2n\,F(G) - \frac{n^2}{4}(|\sigma_\ell| - |\sigma_s|)}$$

Proof. Setting in Lemma 4, $a_i = |\sigma_i|$ and $b_i = 1$ for $1 \le i \le n$, we get

$$\left(\sum_{i=1}^{n}|\sigma_i|^2\right)\left(\sum_{i=1}^{n}1\right) - \left(\sum_{i=1}^{n}|\sigma_i|\right)^2 \le \frac{n^2}{4}\,(|\sigma_\ell| - |\sigma_s|)^2\,,$$

implying

$$2F(G)\,n - En_{SO}(G)^2 \le \frac{n^2}{4}(|\sigma_\ell| - |\sigma_s|)^2\,.$$

Theorem 5 follows. □

4. On Sombor energy of trees

In this section we focus our attention to trees. Let T be a tree on n vertices, $n \ge 2$. The main result in the spectral theory of trees is the formula [18,26,27]

$$\phi(T,\lambda) = \lambda^n + \sum_{k\ge 1}(-1)^k\, m(T,k)\,\lambda^{n-2k} \tag{8}$$

where $m(T,k)$ stands for the number of k-matchings (= selections of k mutually independent edges) in the tree T. By definition, $m(T,1) = n-1$.

As explained in Remark 1, the matrix $\mathbf{A}_{SO}(G)$ can be viewed as the adjacency matrix of a graph with weighted edges. This, of course, applies also to trees.

According to the Sachs coefficient theorem [18,23], for the Sombor characteristic polynomial of a tree T, an expression analogous to Equation (8) would hold, namely

$$\phi_{SO}(T,\lambda) = \lambda^n + \sum_{k\ge 1}(-1)^k\, m_{SO}(T,k)\,\lambda^{n-2k}\,. \tag{9}$$

The coefficient $m_{SO}(T,k)$ is equal to the sum of weights coming from all k-matchings of T. Each particular k-matching contributes to $m_{SO}(T,k)$ by the product of the squares of the terms $\sqrt{d_u^2+d_v^2}$, pertaining to the edges contained in that matching [23]. Thus, let M be a distinct k-matching of T, and let $\mathcal{M}(k)$ be the set of all such k-matchings. Then for $k \ge 1$, $\mathcal{M}(k)$ consists of $m(T,k)$ elements, i.e., $|\mathcal{M}(k)| = m(T,k)$.

The weight of a single matching M is equal to $\prod_{uv\in M}\left(d_u^2+d_v^2\right)$ and therefore

$$m_{SO}(T,k) = \sum_{M\in\mathcal{M}(k)}\ \prod_{uv\in M}\left(d_u^2+d_v^2\right) \tag{10}$$

provided $\mathcal{M}(k) \ne \varnothing$. If, on the other hand, $\mathcal{M}(k) = \varnothing$, then $m_{SO}(T,k) = 0$.

We thus see that the coefficients $m_{SO}(T,k)$ are positive if $m(T,k) > 0$ and are equal to zero if $m(T,k) = 0$. This implies:

Theorem 6. *The inertia of the Sombor matrix and of the ordinary adjacency matrix of any tree coincide.*

The energy of a tree can be computed from its matching polynomial as [28]:

$$En(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \left[1 + \sum_{k \geq 1} m(T,k)\, x^{2k} \right] dx\,. \tag{11}$$

The analogous expression for the Sombor energy is

$$En_{SO}(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \left[1 + \sum_{k \geq 1} m_{SO}(T,k)\, x^{2k} \right] dx \tag{12}$$

and can be obtained in the exactly same manner as Equation (11) [28,29].

Since, evidently, $m_{SO}(T,k) > m(T,k)$ holds whenever the tree T has at least one k-matching, by comparing Equations (11) and (12), we immediately arrive at:

Theorem 7. *For any tree T, $En_{SO}(T) > En(T)$.*

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Bibliography

[1] Gutman, I. (2021). Geometric approach to degree-based topological indices: Sombor indices. *MATCH Communications in Mathematical and in Compututer Chemistry, 86*, 11–16.

[2] Aguilar–Sánchez, R., Méndez–Bermúdez, J. A., Rodríguez, J. M., & Sigarreta, J. M. (2021). Normalized Sombor indices as complexity measures of random graphs. *Entropy, 23*(8), Article No. 976, https://doi.org/10.3390/e23080976.

[3] Cruz, R., Rada, J., & Sigarreta, J. M. (2021). Sombor index of trees with at most three branch vertices. *Applied Mathematics and Computation, 409*, Article No. 126414, https://doi.org/10.1016/j.amc.2021.126414.

[4] Das, K. C., & Gutman, I. (2022). On Sombor index of trees. *Applied Mathematics and Computation*, *412*, Article No. 126525, https://doi.org/10.1016/j.amc.2021.126575.

[5] Das, K. C., & Shang, Y. (2021). Some extremal graphs with respect to Sombor index. *Mathematics*, *9*(11), Article No. 1202, https://doi.org/10.3390/math9111202.

[6] Gutman, I. (2021). Some basic properties of Sombor indices. *Open Journal of Discrete Applied Mathematics*, *4(1)*, 1–3.

[7] Rada, J., Rodríguez, J. M., & Sigarreta, J. M. (2021). General properties on Sombor indices. *Discrete Applied Mathematics*, *299*, 87–97.

[8] Redžepović, I. (2021). Chemical applicability of Sombor indices. *Journal of the Serbian Chemical Society*, *86*, 445–457.

[9] Réti, T., Došlić, T., & Ali, A. (2021). On the Sombor index of graphs. *Contributions to Mathematics*, *3*, 11–18.

[10] Ghanbari, B. (2021). On the Sombor characteristic polynomial and Sombor energy of a graph. *arXiv*, arXiv:2108.08552.

[11] Gowtham, K. J., & Swamy, N. N. (2021). On Sombor energy of graphs. *Nanosystems: Physics, Chemistry, Mathematics*, *12*, 411–417.

[12] Gutman, I. (2021). Spectrum and energy of the Sombor matrix. *Milirary Technical Courier, 69*, 551–561.

[13] Lin, Z., & Miao, L. (2021). On the spectral radius, energy and Estrada index of the Sombor matrix of graphs. *arXiv*, arXiv: 2102.03960.

[14] Wang, Z., Mao, Y., Gutman, I., Wu, J., & Ma, Q. (2022). Spectral radius and energy of Sombor matrix of graphs. *Filomat*, In Press.

[15] Furtula, B., & Gutman, I. (2015). A forgotten topological index. *Journal of Mathematical Chemistry*, *53*, 1184–1190.

[16] Kulli, V. R. (2020). Graph indices, in: Pal, M., Samanta, S., & Pal A. (Eds.). *Handbook of Research of Advanced Applications of Graph Theory in Modern Society*. Hershey: Global, pp. 66–91.

[17] Vukičević, D., & Gašperov, M. (2010). Bond additive modeling 1. Adriatic indices. *Croatica Chemica Acta*, *83*, 243–260.

[18] Cvetković, D., Rowlinson, P., Simić, S. K. (2010). *An Introduction to the Theory of Graph Spectra*. Cambridge: Cambridge University Press.

[19] Li, X., Shi, Y., & Gutman, I. (2012). *Graph Energy*. New York: Springer.

[20] Li, X., & Wang, Z. (2021). Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree-based indices. *Linear Algebra and Its Applications, 620*, 61–75.

[21] Das, K. C., Gutman, I., Milovanović, I., Milovanović, E., & Furtula, B. (2018). Degree-based energies of graphs. *Linear Algebra and Its Applications, 554*, 185–204.

[22] Shao, Y., Gao, Y., Gao, W., & Zhao, X. (2021). Degree-based energies of trees. *Linear Algebra and Its Applications, 621*, (2021) 18–28.

[23] Sachs, H. (1964). Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem charakteristischen Polynom. *Publicationes Mathematica (Debrecen), 11*, 119–134.

[24] Mitrinović, D. S., & Vasić, P. M. (1970). *Analytic Inequalities*. Berlin: Springer.

[25] Ozeki, N. (1968). On the estimation of inequalities by maximum and minimum values. *Journal of the College of Arts and Science Chiba University, 5*, 199–203.

[26] Godsil, C. D., & Gutman, I. (1981). On the theory of the matching polynomial. *Journal of Graph Theory, 5*, 137–144.

[27] Godsil, C. D., & Royle, G. (2001). *Algebraic Graph Theory*. New York: Springer.

[28] Gutman, I. (1977). Acyclic systems with extremal Hückel π-electron energy. *Theoretica Chimica Acta, 45*, 79–87.

[29] Mateljević, M., Božin, V., & Gutman, I. (2010). Energy of a polynomial and the Coulson integral formula. *Journal of Mathematical Chemistry, 48*, 1062–1068.