On characteristic polynomial and energy of Sombor matrix

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Academic Editor: Aisha Javed
Received: 1 October 2021; Accepted: 25 October 2021; Published: 31 October 2021.

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 \( A_{SO} \) 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 \( A_{SO} \). A few results for the coefficients of the characteristic polynomial, and bounds for the energy of \( A_{SO} \) 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 \( V(G) \) and edge set \( E(G) \). 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 \( d_v \).

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

\[
TI = TI(G) = \sum_{u \leq E(G)} \varphi(d_u, d_v) \tag{1}
\]

have been considered, where \( \varphi \) 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]

\[
F(G) = \sum_{u \leq E(G)} (d_u^2 + d_v^2) = \sum_{u \in V(G)} d_u^3,
\]

the Sombor index [1]

\[
SO(G) = \sum_{u \leq E(G)} \sqrt{d_u^2 + d_v^2},
\]

and many other [16,17].
The adjacency matrix $A(G) = (a_{ij})_{n \times n}$ of the graph $G$ with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, is the symmetric matrix of order $n$, whose elements are defined as [18]:

$$
    a_{ij} = \begin{cases} 
        1 & \text{if } v_i v_j \in E(G) \\
        0 & \text{if } v_i v_j \notin E(G) \\
        0 & \text{if } i = j. 
    \end{cases} 
$$

(2)

The characteristic polynomial of $A(G)$ is $\phi(G, \lambda) = \det[\lambda I_n - A(G)]$, where $I_n$ is the unit matrix of order $n$ [18]. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $A(G)$ 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 $A_{SO}(G) = (so_{ij})_{n \times n}$ of the graph $G$ with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, is the symmetric matrix of order $n$, whose elements are

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

(3)

(2) The Sombor characteristic polynomial of the graph $G$ is $\phi_{SO}(G, \lambda) = \det[\lambda I_n - A_{SO}(G)]$. 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 $A_{SO}(G)$ form the Sombor spectrum of the graph $G$.

(4) The Sombor energy of the graph $G$ is

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

Since $A_{SO}(G)$ 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 $v_i v_j$ 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

$$
\sum_{i=1}^{n} \sigma_i = 0. 
$$
\[ \sum_{i=1}^{n} \sigma_i^2 = 2F(G), \quad (5) \]

\[ \sum_{i=1}^{n} \sigma_i^3 = 2 \sum_{\Delta} \prod_{u \in E(\Delta)} \sqrt{d_u^2 + d_v^2}, \quad (6) \]

or, equivalently,

\[ \text{so}(G, 1) = 0, \]

\[ \text{so}(G, 2) = -F(G), \]

\[ \text{so}(G, 3) = -2 \sum_{\Delta} \prod_{u \in E(\Delta)} \sqrt{d_u^2 + d_v^2}, \]

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 \( q = 1, 3, \ldots, p - 2 \),

\[ \sum_{i=1}^{n} \sigma_i^q = 0 \quad (7) \]

whereas

\[ \sum_{i=1}^{n} \sigma_i^p = 2p \sum_{C_p} \prod_{u \in E(C_p)} \sqrt{d_u^2 + d_v^2} \]

or, equivalently,

\[ \text{so}(G, p) = -2 \sum_{C_p} \prod_{u \in E(C_p)} \sqrt{d_u^2 + d_v^2}. \]

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

**Proof.** Take into account Remark 1, and use the analogous result for ordinary graphs [18]. \( \square \)

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

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

where \( M_1 = \max_{1 \leq i \leq n} a_i, M_2 = \max_{1 \leq i \leq n} b_i, m_1 = \min_{1 \leq i \leq n} a_i, \) and \( m_2 = \min_{1 \leq i \leq n} b_i \).

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

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

### 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 \( \text{tr}(A_{SO}(G)) = 2F(G) \) follows from Equation (5).
Theorem 1. [13] Denote the trace of a square matrix $M$ by $tr(M)$. Let $G$ be a graph on $n$ vertices. Then

$$\sqrt{tr(A_{SO}(G)^2)} \leq En_{SO}(G) \leq \sqrt{n tr(A_{SO}(G)^2)}$$

i.e.,

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

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

$$En_{SO}(G) \geq \sqrt{\frac{[tr(A_{SO}(G)^2)]^3}{tr(A_{SO}(G)^4)}} .$$

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

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

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 $\sigma_1$ 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),

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

On the other hand,

$$\sum_{i=1}^{n} \sigma_i = 0 \implies \sigma_1 = -\sum_{i=2}^{n} \sigma_i$$

and so $|\sigma_1| = \left| \sum_{i=2}^{n} \sigma_i \right| .$

Equality holds if $\sigma_1$ and $\sigma_n$ 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

$$En_{SO}(G) \geq \sqrt{\frac{8n F(G) \sigma_1 \sigma_3}{|\sigma_1| + |\sigma_3|}}$$

where, $|\sigma_1|$ and $|\sigma_3|$ are, respectively, the largest and smallest absolute values of the eigenvalues in the Sombor spectrum of $G$. Of course, $|\sigma_1| = \sigma_1$.

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

$$\left( \sum_{i=1}^{n} |\sigma_i|^2 \right) \left( \sum_{i=1}^{n} 1 \right) \leq \frac{1}{4} \left( \sqrt{\frac{|\sigma_1|}{|\sigma_3|}} + \sqrt{\frac{|\sigma_3|}{|\sigma_1|}} \right)^2 \left( \sum_{i=1}^{n} |\sigma_i| \right)^2 .$$
where \( |\sigma_t| = \max_{1 \leq i \leq n} |\sigma_i| \) and \( |\sigma_s| = \min_{1 \leq i \leq n} |\sigma_i| \). Then

\[
2F(G) n \leq \frac{1}{4} \left( \sqrt{\frac{|\sigma_t|}{|\sigma_s|}} + \sqrt{\frac{|\sigma_s|}{|\sigma_t|}} \right)^2 \left( \sum_{i=1}^{n} |\sigma_i| \right)^2
\]

and thus

\[
\sqrt{8n F(G)} \leq \left( \frac{|\sigma_t| + |\sigma_s|}{\sqrt{|\sigma_t| |\sigma_s|}} \right) \text{En}_{SO}(G)
\]

which straightforwardly leads to Theorem 4.

Theorem 5. Let \( G \) be a connected graph with \( n \) vertices, and \( \sigma_t, \sigma_s \) same as in Theorem 4. Then

\[
\text{En}_{SO}(G) \geq \sqrt{2n F(G) - \frac{n^2}{4} (|\sigma_t| - |\sigma_s|)}
\]

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

\[
\left( \sum_{i=1}^{n} |\sigma_i|^2 \right) \left( \sum_{i=1}^{n} 1 \right) - \left( \sum_{i=1}^{n} |\sigma_i| \right)^2 \leq \frac{n^2}{4} (|\sigma_t| - |\sigma_s|)^2,
\]

implying

\[
2F(G) n - \text{En}_{SO}(G)^2 \leq \frac{n^2}{4} (|\sigma_t| - |\sigma_s|)^2.
\]

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, \( n \geq 2 \). The main result in the spectral theory of trees is the formula \[18,26,27]\]

\[
\phi(T, \lambda) = \lambda^n + \sum_{k \geq 1} (-1)^k m(T, k) \lambda^{n-2k}
\]

(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 \( A_{SO}(G) \) 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

\[
\phi_{SO}(T, \lambda) = \lambda^n + \sum_{k \geq 1} (-1)^k m_{SO}(T, k) \lambda^{n-2k}.
\]

(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 \( k \geq 1 \), \( \mathcal{M}(k) \) consists of \( m(T, k) \) elements, i.e., \( |\mathcal{M}(k)| = m(T, k) \).

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

\[
m_{SO}(T, k) = \sum_{M \in \mathcal{M}(k)} \prod_{u \in M} (d_u^2 + d_v^2)
\]

(10)

provided \( \mathcal{M}(k) \neq \emptyset \). If, on the other hand, \( \mathcal{M}(k) = \emptyset \), 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 \(T\), \(En_{SO}(T) > En(T)\).

Author Contributions: All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

Conflicts of Interest: “The authors declare no conflict of interest.”

Bibliography


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