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Research

A Novel Forgotten-Sombor Energy: Bounds and Applications to Anti-Diabetes Drugs

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Abstract:
In this paper, we introduce a novel matrix naming it to be Forgotten-Sombor matrix, denoted by $\mathcal{FS}o(G)$, for a simple graph G. This matrix is defined such that for vertices v_i adjacent to v_j, the (i,j)-entry is given by $\sqrt{d_G(v_i)^4 + d_G(v_j)^4}$, where $d_G(v_i)$ represents the degree of the vertex v_i, and zero otherwise. Let $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ denote the eigenvalues of $\mathcal{FS}o(G)$, with η_1 corresponding to the spectral radius, and let the associated Forgotten-Sombor energy $E_{\mathcal{FS}o}(G)$ be defined as the sum of the absolute values of these eigenvalues. We derived new upper and lower bounds for both η_1 and $E_{\mathcal{FS}o}(G)$ in terms of the first Zagreb index $M_1(G)$. As an application, we conduct a Quantitative Structure-Property Relationship (QSPR) analysis on a dataset comprising drugs used in the treatment of Diabetese, constructing linear regression models to explore the correlation between the physicochemical properties of these drugs and their corresponding $E_{\mathcal{FS}o}(G)$ values, with results illustrated through graphical representations.

Keywords: Forgotten-Sombor matrix, spectral radius, Diabetes drugs.

2020 Mathematics Subject Classification: Primary 05C50, Secondary 05C92, 05C09.

1 Introduction

Let G be a simple graph, with vertex set $|V| = n$ and edge set $|E| = m$. The degree of a vertex $v \in V$ is the count of edges connected to v denoted by $d_G(v)$. The maximum(minimum) vertex and edge degree of a graph is denoted by $\Delta(\delta)$ and $\Delta'(\delta')$ respectively. A graph G is called s-regular if every vertex of G has degree s. In particular, the complete graph K_n is an $(n-1)$-regular graph, since each vertex is adjacent to all of the other $n-1$ vertices. For more terminologies refer the following [9].

Topological indices (TIs) are numerical descriptors derived from molecular graphs that capture chemical structural information. Degree-based topological indices are especially important in chemical graph theory and are widely used in QSPR and QSAR studies to relate molecular structure with physicochemical properties of drugs.

The first degree-based molecular descriptor, the Zagreb index, was developed by Gutman and Trinajstic [8]. It firstly emerged in the topological formula for conjugated molecules regarding their total π-electron energy. The first Zagreb index is defined as:

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$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 = \sum_{uv\in E(G)} d_G(u) + d_G(v) \tag{1}$$

The general first Zagreb index is studied in [10] and defined as

$$M_1^{(\alpha)}(G) = \sum_{v\in V(G)} d_G(v)^{(\alpha)} = \sum_{v_iv j\in E(G)} d_G(v_i)^{(\alpha-1)} + d_G(v_j)^{(\alpha-1)} \tag{2}$$

For $\alpha = 5$, we have $M_1^{(5)}(G) = \sum_{v_iv j\in E(G)} d_G(v_i)^{(4)} + d_G(v_j)^{(4)}$.

Another widely studied topological descriptor, which has attracted considerable attention in chemical graph theory, is the Sombor index [6], defined by

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}. \tag{3}$$

Inspired by the Sombor index, a new Sombor-type descriptor called the Forgotten–Sombor index was recently introduced in [12] and is defined as

$$FSO(G) = \sum_{uv\in E(G)} \sqrt{d_G(u)^4 + d_G(v)^4}. \tag{4}$$

Spectral graph theory has emerged as an active area of research in recent years, which explores the graph properties like eigenvalues and eigenvectors obtained from matrices such as the adjacency and Laplacian matrices. Among the important spectral parameters is the energy of a graph, introduced by I. Gutman in [7], which coincides with the π-electron energy of a conjugated hydrocarbon, as calculated with the Huckel molecular orbital (HMO) method.

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The adjacency matrix $A(G) = [a_{ij}]$ of order n is defined by

$$a_{ij} = \begin{cases} 1, & \text{if} v_i \text{isadjacentto} v_j, \\ 0, & \text{otherwise.} \end{cases}$$

If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $A(G)$, then the energy of the graph G, introduced by I. Gutman in [7], is given by

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

In 1994, Yang et al. [21] proposed the extended adjacency matrix $A_{ex}(G)$ for a graph G, and investigated the sum of the absolute values of its eigenvalues, which they termed the extended graph energy. Later, Ş. Burcu Bozkurt et al. [2] introduced the Randic$'$ matrix and studied the associated Randic$'$ energy, analyzing various structural properties of graphs. Zhen Lin et al. [22] explored the spectral radius, energy, and Estrada index of the Sombor matrix, while Sumedha S. Shinde et al. [18] provided bounds on the Sombor eigenvalues and energy in terms of Hyper Zagreb and Zagreb indices. Recently Sakander Hayat et al. [16] defined edge-weighted matrix of a graph and obtained bounds in terms of first reformulated Zagreb index. For more related work refer [13, 20, 19].

Motivated by these developments, we introduce a novel Forgotten-Sombor matrix, denoted by $\mathcal{FSo}(G)$, which is defined as follows

$$\mathcal{FSo}(G) = \begin{cases} \sqrt{d_G(v_i)^4 + d_G(v_j)^4}, & \text{if} v_i \text{isadjacentto} v_j, \\ 0, & \text{if} i = j, \end{cases}$$

where $d_G(v_i)$ represents the degree of vertex v_i of G.

The characteristic polynomial of $\mathcal{FSo}(G)$ is given by $\psi(G,\eta) = \det(\eta I - FSo(G)) = \eta^n + r_1\eta^{n-1} + \cdots + r_n$, where I is the identity matrix of order n. Since $\mathcal{FSo}(G)$ is a real symmetric matrix, all its eigenvalues are real. Arranged in non-increasing order, the eigenvalues are $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$, with respective multiplicities $\tau_1, \tau_2, \dots, \tau_n$. Thus, the spectrum of $\mathcal{FSo}(G)$ can be represented as

$$Spectra(\mathcal{FSo}(G)) = \begin{pmatrix} \eta_1 & \eta_2 & \cdots & \eta_n \\ \tau_1 & \tau_2 & \cdots & \tau_n \end{pmatrix},$$

where η_1 is the spectral radius.

The Sombor energy associated with $\mathcal{FSo}(G)$ is defined by

$$E_{\mathcal{FSo}}(G) = \sum_{i=1}^{n} |\eta_i|.$$

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Example: Let G be a simple graph as shown in the Figure 1.

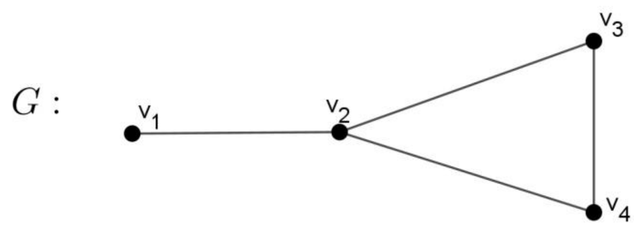

Figure 1. Simple graph G.

The degree of each vertex of G is $d_G(v_1) = 1$, $d_G(v_2) = 3$, $d_G(v_3) = 2$, $d_G(v_4) = 2$.
A new variant of Sombor matrix $\mathcal{FS}o(G)$ of G is

$$\mathcal{FS}o(G) = \begin{bmatrix} 0 & \sqrt{82} & 0 & 0 \\ \sqrt{82} & 0 & \sqrt{97} & \sqrt{97} \\ 0 & \sqrt{97} & 0 & \sqrt{32} \\ 0 & \sqrt{97} & \sqrt{32} & 0 \end{bmatrix}$$

The eigenvalues are $\eta_1 = 18.93761$, $\eta_2 = 1.64146$, $\eta_3 = -5.65685$, $\eta_4 = -14.92222$.
The Sombor energy $E_{\mathcal{FS}o}(G)$ is 41.15814.

2 Preliminaries

Lemma 2.1 *[3] (Cauchy Schwartz inequality) Let* a_i *and* b_i, $1 \le i \le s$ *be any real numbers, then*

$$(\sum_{i=1}^{s} a_i b_i)^2 \le (\sum_{i=1}^{s} a_i^2)(\sum_{i=1}^{s} b_i^2) \tag{5}$$

Lemma 2.2 *[11] Let* a_i, $1 \le i \le s$ *be any real numbers, then*

$$(\sum_{i=1}^{s} |a_i|)^2 \ge (\sum_{i=1}^{s} |a_i|^2) \tag{6}$$

Lemma 2.3 *[14] (Ozeki inequality) If* a_i *and* b_i, $(1 \le i \le s)$ *are non-negative real numbers then*

$$\sum_{i=1}^{s} a_i^2 \sum_{i=1}^{s} b_i^2 - [\sum_{i=1}^{s} a_i b_i]^2 \le \frac{n^2}{4}(N_1N_2 - n_1n_2)^2 \tag{7}$$

where $N_1 = max_{1\le i\le s}\{a_i\}$, $N_2 = max_{1\le i\le s}\{b_i\}$, $n_1 = min_{1\le i\le s}\{a_i\}$, $n_2 = min_{1\le i\le s}\{b_i\}$.

Lemma 2.4 *[15] Suppose* a_i *and* b_i, $1 \le i \le s$ *are positive real numbers, then*

$$\sum_{i=1}^{s} a_i^2 \sum_{i=1}^{s} b_i^2 \le \frac{1}{4}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)^2 (\sum_{i=1}^{s} a_i b_i)^2 \tag{8}$$

where $N_1 = max_{1\le i\le s}\{a_i\}$, $N_2 = max_{1\le i\le s}\{b_i\}$, $n_1 = min_{1\le i\le s}\{a_i\}$, $n_2 = min_{1\le i\le s}\{b_i\}$.

Lemma 2.5 *[1] Suppose* a_i *and* b_i, $1 \le i \le s$ *are positive real numbers, then*

$$|s\sum_{i=1}^{s} a_i b_i - \sum_{i=1}^{s} a_i \sum_{i=1}^{s} b_i| \le \alpha(s)(A - a)(B - b) \tag{9}$$

where a, b, A and B are real constants, that for each i, $1 \le i \le s$, $a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(s) = s\lfloor\frac{s}{2}\rfloor\left(1 - \frac{1}{s}\lfloor\frac{s}{2}\rfloor\right)$.

Lemma 2.6 *[4] Let* a_i *and* b_i, $1 \le i \le s$ *are nonnegative real numbers, then*

$$\sum_{i=1}^{s} b_i^2 + tT\sum_{i=1}^{s} a_i^2 \le (t + T)(\sum_{i=1}^{s} a_i b_i) \tag{10}$$

where t and T are real constants, so that for each i, $1 \le i \le s$, holds, $ta_i \le b_i \le Ta_i$.

Lemma 2.7 *[5] Let* a_i, b_i, c_i *and* d_i *are sequences of real numbers and* p_i, q_i *are non-negative for* $i = 1,2,\ldots,s$. *Then the following inequality is valid*

$$\sum_{i=1}^{s} p_i a_i^2 \sum_{i=1}^{s} q_i b_i^2 + \sum_{i=1}^{s} p_i c_i^2 \sum_{i=1}^{s} q_i d_i^2 \geq 2 \sum_{i=1}^{s} p_i a_i c_i \sum_{i=1}^{s} q_i b_i d_i \quad (11)$$

3 Main Results

Lemma 3.1 *Consider a simple connected graph G with $d_G(v_i)$ representing the degree of the v_i vertex. Let $\mathcal{FSo}(G)$ be a new variant Sombor matrix of the graph G with eigenvalues $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ then,*

$$\sum_{i=1}^{n} \eta_i = 0$$

$$\sum_{i=1}^{n} \eta_i^2 = 2M_1^{(5)}(G)$$

Proof. Since

$$\sum_{i=1}^{n} \eta_i^2 = trace([\mathcal{FSo}(G)]^2)$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \mathcal{FSo}(G)_{ij} \mathcal{FSo}(G)_{ji}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [\mathcal{FSo}(G)_{ij}]^2$$

$$= 2 \sum_{i \neq j} \left(\sqrt{d_G(v_i)^{(4)} + d_G(v_j)^{(4)}} \right)^2$$

$$= 2 \sum_{i \neq j} \left[d_G(v_i)^{(4)} + d_G(v_j)^{(4)} \right]$$

$$= 2M_1^{(5)}(G)$$

Where

$$\sum_{i \neq j} \left[d_G(v_i)^{(4)} + d_G(v_j)^{(4)} \right] = M_1^{(5)}(G)$$

3.1 Some bounds on spectral radius (η_1) and $E_{\mathcal{FSo}(G)}$ of a new variant of Sombor matrix of a graph

Theorem 3.2 *Let G be a connected graph with n vertices and η_1 be the spectral radius (the largest eigenvalue), then*

$$\eta_1 \leq \sqrt{\frac{2(n-1)M_1^{(5)}(G)}{n}} \quad (12)$$

with equality holds if and only if G is a regular graph.

Proof: Since $\sum_{i=1}^{n} \eta_i = 0$ it can be rewritten as $\sum_{i=2}^{n} \eta_i = -\eta_1$. Further $(\sum_{i=1}^{n} (\eta_i)^2) = 2M_1^{(5)}(G)$, $(\sum_{i=2}^{n} (\eta_i)^2) = (\sum_{i=1}^{n} (\eta_i)^2 - (\eta_1)^2) = (2M_1^{(5)}(G) - (\eta_1)^2)$ and $(\sum_{i=2}^{n} 1) = (n-1)$.

Substituting $a_i = 1$ and $b_i = \eta_i$ in Lemma 2.1, we get

$$(-\eta_1)^2 \leq (n-1)(2M_1^{(5)}(G) - (\eta_1)^2)$$

$$(-\eta_1)^2 \leq 2(n-1)M_1^{(5)}(G) - (n-1)(\eta_1)^2$$

$$(-\eta_1)^2 \leq 2(n-1)M_1^{(5)}(G) - n(\eta_1)^2 + (\eta_1)^2$$

$$n(\eta_1)^2 \leq 2(n-1)M_1^{(5)}(G)$$

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$$\eta_1 \le \sqrt{\frac{2(n-1)M_1^{(5)}(G)}{n}}$$

One can verify that the equality holds if and only if G is a regular graph.

Theorem 3.3 *Let G be a connected graph with n vertices then*

$$\sqrt{2M_1^{(5)}(G)} \le E_{\mathcal{FSo}(G)} \le \sqrt{2nM_1^{(5)}(G)} (13)$$

Proof: Since $E_{\mathcal{FSo}(G)} = \sum_{i=1}^{n} |\eta_i|$, $\sum_{i=1}^{n} 1 = n$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2M_1^{(5)}(G)$
Substituting $a_i = |\eta_i|$ and $b_i = 1$ in Lemma 2.1, we get

$$E_{\mathcal{FSo}(G)}^2 \le 2nM_1^{(5)}(G)$$

$$E_{\mathcal{FSo}(G)} \le \sqrt{2nM_1^{(5)}(G)}$$

Also, substituting $a_i = |\eta_i|$ in Lemma 2.2, we get

$$E_{\mathcal{FSo}(G)}^2 \ge 2M_1^{(5)}(G)$$

$$E_{\mathcal{FSo}(G)} \ge \sqrt{2M_1^{(5)}(G)}$$

This gives us both the upper and lower bound.

Theorem 3.4 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{FSo}(G)} \ge \frac{2\sqrt{2M_1^{(5)}(G)|\eta_1||\eta_n|}}{|\eta_1|+|\eta_n|} \quad (14)$$

Proof: Let $|\eta_1|$ and $|\eta_n|$ be the largest and the smallest eigenvalues. Since $E_{\mathcal{FSo}(G)} = \sum_{i=1}^{n} |\eta_i|$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2M_1^{(5)}(G)$
Substituting $a_i = |\eta_i|$, $b_i = 1$, $M_1 = |\eta_1|$, $m_1 = |\eta_n|$, $M_2 = 1$ and $m_2 = 1$ in Lemma 2.4, we get

$$\sum_{i=1}^{n} |\eta_i|^2 \sum_{i=1}^{n} 1 \le \frac{1}{4}\left(\sqrt{\frac{|\eta_1|}{|\eta_n|}} + \sqrt{\frac{|\eta_n|}{|\eta_1|}}\right)^2 \left(\sum_{i=1}^{n} |\eta_i|\right)^2$$

$$2M_1^{(5)}(G)n \le \frac{1}{4}\left(\frac{(|\eta_1| + |\eta_n|)}{\sqrt{|\eta_n||\eta_1|}}\right)^2 E_{\mathcal{FSo}(G)}^2$$

$$2nM_1^{(5)}(G) \le \frac{1}{4}\left(\frac{(|\eta_1| + |\eta_n|)^2}{|\eta_n||\eta_1|}\right) E_{\mathcal{FSo}(G)}^2$$

$$\frac{8nM_1^{(5)}(G)|\eta_n||\eta_1|}{(|\eta_1| + |\eta_n|)^2} \le E_{\mathcal{FSo}(G)}^2$$

$$E_{\mathcal{FSo}(G)} \ge \sqrt{\frac{8nM_1^{(5)}(G)|\eta_1||\eta_n|}{(|\eta_1| + |\eta_n|)^2}}$$

$$E_{\mathcal{FSo}(G)} \ge \frac{2\sqrt{2nM_1^{(5)}(G)|\eta_1||\eta_n|}}{|\eta_1| + |\eta_n|}$$

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Theorem 3.5 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{FSo}(G)} \geq \frac{\sqrt{8nM_1^{(5)}(G)-n^2(|\eta_1|-|\eta_n|)^2}}{2} \qquad (15)$$

Proof: Let $|\eta_1|$ and $|\eta_n|$ be the largest and the smallest eigenvalues. Since $E_{\mathcal{FSo}(G)} = \sum_{i=1}^{n} |\eta_i|$ and $\sum_{i=1}^{n} |\eta_i|^2 = 2M_1^{(5)}(G)$

Substituting $a_i = |\eta_i|$, $b_i = 1$, $M_1 = |\eta_1|$, $m_1 = |\eta_n|$, $M_2 = 1$ and $m_2 = 1$ in Lemma 2.3, we get

$$\sum_{i=1}^{n} |\eta_i|^2 \sum_{i=1}^{n} 1 - \left(\sum_{i=1}^{n} |\eta_i|\right)^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$2M_1^{(5)}(G)n - E_{\mathcal{FSo}(G)}^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$2nM_1^{(5)}(G) - \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2 \leq E_{\mathcal{FSo}(G)}^2$$

$$\frac{8nM_1^{(5)}(G)-n^2(|\eta_1|-|\eta_n|)^2}{4} \leq E_{\mathcal{FSo}(G)}^2$$

$$E_{\mathcal{FSo}(G)} \geq \frac{\sqrt{8nM_1^{(5)}(G)-n^2(|\eta_1|-|\eta_n|)^2}}{2}$$

Theorem 3.6 *Let G be a connected graph with n vertices then*

$$E_{\mathcal{FSo}(G)} \leq |\eta_1| + \sqrt{(2M_1^{(5)}(G) - |\eta_1|^2)(n-1)} \qquad (16)$$

Proof: Let $|\eta_1|$ be the largest eigenvalue. Since $E_{\mathcal{FSo}(G)} = \sum_{i=1}^{n} |\eta_i|$,

$$E_{\mathcal{FSo}(G)} - |\eta_1| = \sum_{i=2}^{n} |\eta_i|$$

Squaring both sides and applying Lemma 2.1, we get

$$(E_{\mathcal{FSo}(G)} - |\eta_1|)^2 = \left(\sum_{i=2}^{n} |\eta_i|\right)^2$$

$$(E_{\mathcal{FSo}(G)} - |\eta_1|)^2 = \left(\sum_{i=2}^{n} |\eta_i| \cdot 1\right)^2 \leq \left(\sum_{i=2}^{n} |\eta_i|^2\right)\left(\sum_{i=2}^{n} 1^2\right)$$

$$(E_{\mathcal{FSo}(G)} - |\eta_1|)^2 \leq \left(2M_1^{(5)}(G) - |\eta_1|^2\right)(n-1)$$

$$(E_{\mathcal{FSo}(G)} - |\eta_1|) \leq \sqrt{\left(2M_1^{(5)}(G) - |\eta_1|^2\right)(n-1)}$$

$$E_{\mathcal{FSo}(G)} \leq |\eta_1| + \sqrt{\left(2M_1^{(5)}(G) - |\eta_1|^2\right)(n-1)}$$

Theorem 3.7 *Let G be a graph of order n and size m. Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the eigenvalues of $\mathcal{FSo}(G)$. Then*

$$E_{\mathcal{FSo}}(G) \geq \sqrt{2nM_1^{(5)}(G) - \alpha(n)(|\eta_1| - |\eta_n|)^2} \qquad (17)$$

where $\alpha(n) = n\lfloor\frac{n}{2}\rfloor\left(1 - \frac{1}{n}\lfloor\frac{n}{2}\rfloor\right)$.

Proof: Let $|\eta_1| \geq |\eta_2| \geq \ldots \geq |\eta_n|$ be the eigenvalues of $\mathcal{FSo}(G)$. By putting $a_i = |\eta_i| = b_i$, $A = |\eta_1| = B$ and $a = |\eta_n| = b$ in Lemma 2.5, we get

$$\left|n\sum_{i=1}^{n} |\eta_i|^2 - \left(\sum_{i=1}^{n} |\eta_i|\right)^2\right| \leq \alpha(n)(|\eta_1| - |\eta_n|)^2$$

$$\left|2nM_1^{(5)}(G) - (E_{\mathcal{FSo}}(G))^2\right| \leq \alpha(n)(|\eta_1| - |\eta_n|)^2$$

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$$2nM_1^{(5)}(G)-\alpha(n)(|\eta_1|-|\eta_n|)^2\le(E_{\mathcal{FS}o}(G))^2$$

$$E_{\mathcal{FS}o}(G)\ge\sqrt{2nM_1^{(5)}(G)-\alpha(n)(|\eta_1|-|\eta_n|)^2}$$

Theorem 3.8 *Let G be a graph of order n and size m. Let $\eta_1\ge\eta_2\ge\ldots\ge\eta_n$ be the eigenvalues of $\mathcal{FS}o(G)$. Then*

$$E_{\mathcal{FS}o}(G)\ge\frac{2M_1^{(5)}(G)+n(\eta_1\eta_n)}{\eta_1+\eta_n}\tag{18}$$

Proof: Let $\eta_1\ge\eta_2\ge\ldots\ge\eta_n$ be the eigenvalues of $\mathcal{FS}o(G)$. By putting $a_i=1,\ b_i=|\eta_i|,\ r=\eta_n$ and $R=\eta_1$, in Lemma 2.6, we get

$$\sum_{i=1}^{n}|\eta_i|^2+\eta_n\eta_1\sum_{i=1}^{n}1^2\le(\eta_n+\eta_1)\left(\sum_{i=1}^{n}|\eta_i|\right)$$

$$2M_1^{(5)}(G)+n(\eta_n\eta_1)\le(\eta_n+\eta_1)E_{\mathcal{FS}o}(G)$$

$$E_{\mathcal{FS}o}(G)\ge\frac{2M_1^{(5)}(G)+n(\eta_1\eta_n)}{\eta_1+\eta_n}$$

Hence the proof.

Theorem 3.9 *Let G be a non-empty graph with n vertices. Then*

$$E_{\mathcal{FS}o}(G)\le\sqrt{2(M_1^{(5)}(G))^2+\frac{n^2}{2}}\tag{19}$$

Proof: Let $\eta_1\ge\eta_2\ge\ldots\ge\eta_n$ be the eigenvalues of $\mathcal{FS}o(G)$. Substituting $a_i=|\eta_i|=b_i$ and $c_i=d_i=p_i=q_i=1$ in Lemma 2.7, we get

$$\sum_{i=1}^{n}1\cdot|\eta_i|^2\sum_{i=1}^{n}1\cdot|\eta_i|^2+\sum_{i=1}^{n}1\cdot1^2\sum_{i=1}^{n}1\cdot1^2\ge2\sum_{i=1}^{n}1\cdot|\eta_i|\cdot1\sum_{i=1}^{n}1\cdot|\eta_i|\cdot1$$

$$2M_1^{(5)}(G)\cdot2M_1^{(5)}(G)+n\cdot n\ge2(E_{\mathcal{FS}o}(G))^2$$

$$4(M_1^{(5)}(G))^2+n^2\ge2(E_{\mathcal{FS}o}(G))^2$$

$$\sqrt{\frac{4(M_1^{(5)}(G))^2+n^2}{2}}\ge E_{\mathcal{FS}o}(G)$$

$$E_{\mathcal{FS}o}(G)\le\sqrt{2(M_1^{(5)}(G))^2+\frac{n^2}{2}}$$

4 Applications on energy of a novel Forgotten-Sombor matrix

Diabetes is a chronic metabolic disorder arising from inadequate insulin secretion or ineffective insulin action, leading to elevated blood glucose levels. Glucose, obtained from food, functions as a key energy source, and its uptake into cells is mediated by insulin produced by the pancreas. Glucagon complements insulin in regulating glucose levels. In certain cases, immune dysfunction destroys insulin-producing cells, resulting in impaired glucose utilization and its accumulation in the bloodstream. Prolonged hyperglycemia causes damage to nerves and blood vessels and contributes to various complications. Although no definitive cure exists, proper management can control the disease. Several antidiabetic drugs, including Acarbose, Tolazamide, Miglitol, Repaglinide, Metformin, Glimepiride, Linagliptin, Pioglitazone, Bromocriptine and Alogliptin and its molecular structures are considered for our study from [17].

Chemical structures of drugs possess inherent properties that can be analyzed via their corresponding molecular graphs. Topological indices

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derived from these graphs are widely used in QSPR/QSAR models to estimate physicochemical properties. Graph energy is another significant parameter employed in such analyses. The physicochemical properties [17], namely refractive index (RI), flash point (FP), molar volume (MV), polarity (P), boiling point (BP), and complexity (C), along with the computed $E_{\mathcal{FS}o}(G)$, are presented in Table 1. Linear regression analysis was performed to examine the relationship between these physicochemical properties and $E_{\mathcal{FS}o(G)}$. In the regression models, n', F, SE, and Sig, denote the sample size, F-statistic, standard error of estimate, and statistical significance, respectively.

Drugs	RI	FP	MV	P	BP	C	$E_{\mathcal{FS}o}(G)$
Acarbose	139.02	541.4	369.8	60.87	675.05	962	650.24782
Tolazamide	81.34	246.8	237.9	32.82	300	431	238.70578
Miglitol	48.16	284.3	142.1	20.81	453.7	179	140.67092
Prandin/ Repaglinide	131.83	360.8	397.9	51.49	672.9	619	358.50017
Metformin	56.64	58.1	100.8	13.43	224	132	89.13415
Glimepiride	129.8	363.2	378.8	53.49	–	895	383.62647
Linagliptin	133.43	353.7	338	51.24	661.2	885	390.52862
Pioglitazone	97.39	301.8	282.8	37.91	–	466	274.42235
Bromocriptine	165.51	492.8	429.4	66.44	891.3	1230	604.53332
Alogliptin	104.26	267.8	252.9	35.44	519.2	622	284.48388

Table 1: Physicochemical Properties and calculated Forgotten-Sombor energy of Selected Drugs.

4.1 Linear Regression Model

	RI	FP	MV	P	BP	C
$E_{\mathcal{FS}o}(G)$	0.898	0.932	0.852	0.938	0.844	0.926

Table 2: Correlation coefficient r between physicochemical properties and $E_{\mathcal{FS}o}(G)$ for antidiabetic drugs.

The linear regression model is given by

$$PP = a(E_{\mathcal{FS}o}(G)) + b$$

$$RI = 0.204(E_{\mathcal{FS}o}(G)) + 46.529$$

$$n' = 10 \quad F = 33.173 \quad SE = 17.7759 \quad Sig = 0.000$$

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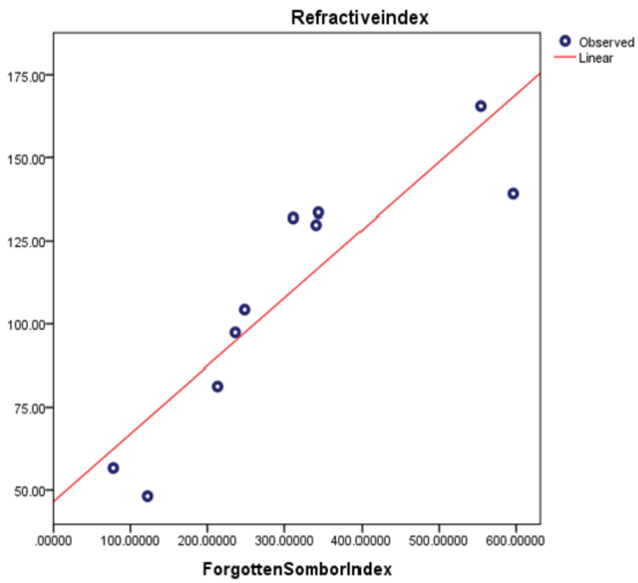
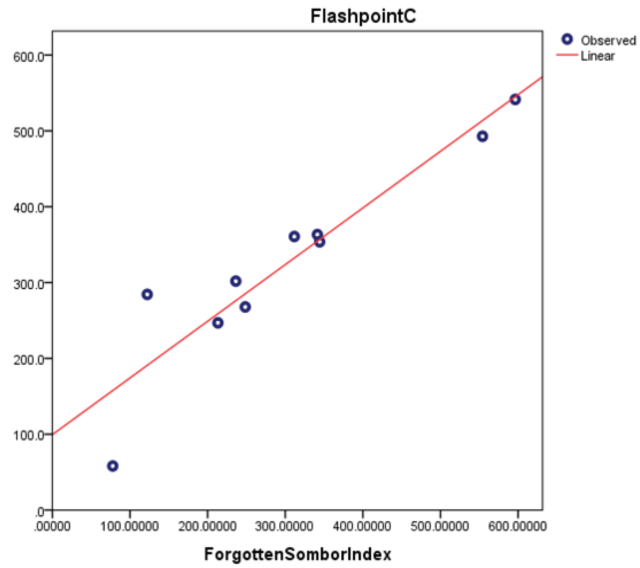
$$FP = 0.747(E_{\mathcal{FS}o}(G)) + 99.519$$





$$n' = 10 \quad F = 53.238 \quad SE = 51.326 \quad Sig = 0.000$$

$$MV = 0.562(E_{\mathcal{FS}o}(G)) + 121.830$$

$$n' = 10 \quad F = 21.203 \quad SE = 61.193 \quad Sig = 0.002$$

$$P = 0.097(E_{\mathcal{FS}o}(G)) + 12.945$$

$$n' = 10 \quad F = 58.798 \quad SE = 6.321 \quad Sig = 0.000$$

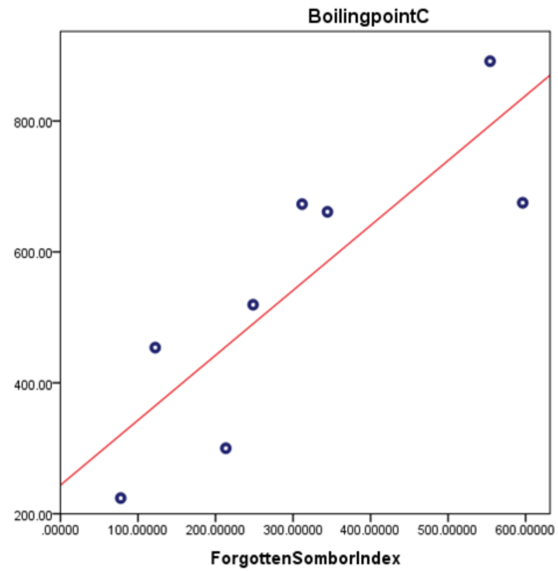
$$BP = 0.992(E_{\mathcal{FS}o}(G)) + 243.752$$

$$n' = 10 \quad F = 14.822 \quad SE = 127.520 \quad Sig = 0.008$$

$$C = 1.956(E_{\mathcal{FS}o}(G)) + 46.356$$

$$n' = 10 \quad F = 47.830 \quad SE = 141.768 \quad Sig = 0.008$$

The linear regression models are depicted in the following figures.



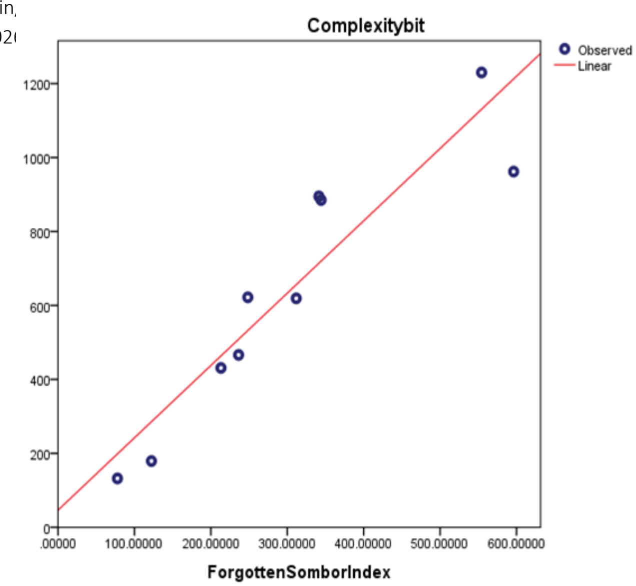
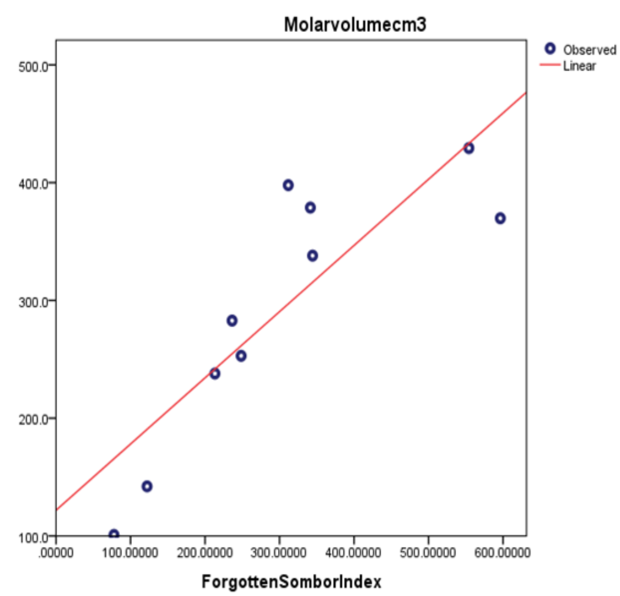


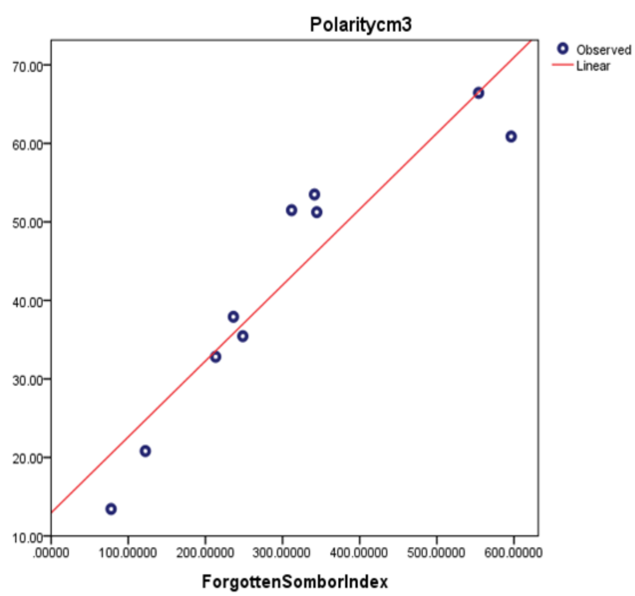
Figure 2: Linear regression model of RI and FP with $E_{\mathcal{FS}o}(G)$

Figure 3: Linear regression model of MV and P with $E_{\mathcal{FS}o}(G)$

Figure 4: Linear regression model of BP and C with $E_{\mathcal{FS}o}(G)$

4.2 Analysis





- The present study examines the relationship between the topological descriptor $E_{\mathcal{FS}o}(G)$ and various physicochemical properties using correlation and linear regression analysis.

- The obtained correlation coefficients indicate a strong positive relationship between $E_{\mathcal{FS}o}(G)$ and all the considered physicochemical parameters.
- Polarity (P) exhibits the highest correlation with $E_{\mathcal{FS}o}(G)$ with $r = 0.938$, indicating a very strong linear association.
- Flash point (FP) and molecular complexity (C) also show strong correlations with $r = 0.932$ and $r = 0.926$, respectively.
- The refractive index (RI) demonstrates a strong correlation with $r = 0.898$, while molar volume (MV) and boiling point (BP) show moderate but significant correlations with $r = 0.852$ and $r = 0.844$, respectively.
- The linear regression models confirm that each physicochemical property can be represented as a linear function of $E_{\mathcal{FS}o}(G)$.
- The regression models for refractive index, flash point, and complexity are highly significant, with $F = 33.173$, $F = 53.238$, and $F = 47.830$, respectively.
- The polarity model provides the best predictive performance, with the highest F-value ($F = 58.798$) and the lowest standard error ($SE = 6.321$).
- The molar volume and boiling point models also remain statistically significant, with $F = 21.203$ and $F = 14.822$, respectively.
- The consistently low p-values across all models and the sample size $n' = 10$ support the statistical validity of the obtained results.

5 Conclusion

In this paper, we introduce a novel matrix naming it to be Forgotten-Sombor matrix, denoted by $\mathcal{FS}o(G)$, for a simple graph G. This matrix is defined such that for vertices v_i adjacent to v_j, the (i,j)-entry is given by $\sqrt{d_G(v_i)^4 + d_G(v_j)^4}$, where $d_G(v_i)$ represents the degree of the vertex v_i, and zero otherwise. The Sombor energy $E_{\mathcal{FS}}o(G)$ is defined as the sum of the absolute values of its eigenvalues. Upper and lower bounds for both the spectral radius η_1 and $E_{\mathcal{FS}O}(G)$ are established in terms of the first Zagreb index $M_1(G)$ .As an application, a Quantitative Structure-Property Relationship (QSPR) analysis is conducted using a dataset of drugs employed in diabetes treatment. Linear regression models are developed to investigate the relationship between the physicochemical properties of these compounds and their corresponding $E_{\mathcal{FS}o}(G)$ values, with the results illustrated through graphical representations.

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