Research Article

Spectral Properties with the Difference between Topological Indices in Graphs

Akbar Jahanbani, Roslan Hasni, Zhibin Du, and Seyed Mahmoud Sheikholeslami

1Department of Mathematics, Azarbaijan Shahid Madani University, Tabriz, Iran
2Faculty of Ocean Engineering Technology and Informatics, University Malaysia Terengganu, 21030 UMT, Kuala Nerus, Terengganu, Malaysia
3School of Software, South China Normal University, Foshan, Guangdong 528225, China
4School of Mathematics and Statistics, Zhaoqing University, Zhaoqing, Guangdong 526061, China

Correspondence should be addressed to Roslan Hasni; hroslan@umt.edu.my

Received 29 March 2020; Accepted 19 June 2020; Published 26 July 2020

1.Introduction

Let $G$ be a graph of order $n$ with vertices labeled as $v_1, v_2, \ldots, v_n$. Let $d_i$ be the degree of the vertex $v_i$, for $i = 1, 2, \ldots, n$. The difference adjacency matrix of $G$ is the square matrix of order $n$ whose $(i, j)$ entry is equal to $(\sqrt{d_i} + d_j - 2 - 1)/\sqrt{d_i d_j}$ if the vertices $v_i$ and $v_j$ of $G$ are adjacent or $(v_i v_j \in E(G))$ and zero otherwise. Since this index is related to the degree of the vertices of the graph, our main tool will be an appropriate matrix, that is, a modification of the classical adjacency matrix involving the degrees of the vertices. In this paper, some properties of its characteristic polynomial are studied. We also investigate the difference energy of a graph. In addition, we establish some upper and lower bounds for this new energy of graph.

By equation (1), the difference between atom-bond connectivity index and Randić index (or difference index) of a graph $G$ is defined as $D(G) = \sum_{u,v \in E(G)} \frac{\sqrt{d_i} + d_j - 2 - 1}{\sqrt{d_i d_j}}$. (1)

By equation (1), the difference between atom-bond connectivity index and Randić index (or difference index) of a graph $G$ is defined as $D(G) = \frac{\sqrt{d_i} + d_j - 2 - 1}{\sqrt{d_i d_j}}$. (1)

The eigenvalues of the difference index $D(G)$ are denoted by $\vartheta_1, \vartheta_2, \ldots, \vartheta_n$ and are said to be the $D$-eigenvalues of $G$. We note that since the matrix of $D(G)$ is symmetric, its eigenvalues are real and can be ordered as $\vartheta_1 \geq \vartheta_2 \geq \cdots \geq \vartheta_n$.

Some of the most popular topological indices are given as follows: the first Zagreb index usually denoted by $M_1$ is defined as follows [3, 4]:

$$M_1(G) = \sum_{v \in V(G)} d_i^2,$$

whereas the first Zagreb index satisfies the identity...
\[ M_1(G) = \sum_{v \in V(G), v \neq v'} (d_i + d_j). \] (3)

The modified second Zagreb index \( M'_2(G) \) is equal to the sum of the reciprocals of products of degrees of pairs of adjacent vertices [5], that is,
\[ M'_2(G) = \sum_{v \in V(G), v \neq v'} \frac{1}{d_i d_j}. \] (4)

Ranjini et al. [6] redefined the Zagreb indices, i.e., the redefined first index for a graph \( G \) defined as
\[ \text{ReZG}_1(G) = \sum_{v \in V(G), v \neq v'} \frac{d_i + d_j}{d_i d_j}. \] (5)

The \( ABC \) index was defined as follows [7]:
\[ ABC(G) = \sum_{v \in V(G), v \neq v'} \frac{\sqrt{d_i + d_j} - 2}{\sqrt{d_i d_j}}. \] (6)

For the study of topological indices of graph associated with group, refer [8, 9] and the references therein.

In mathematical chemistry, observe that all these topological indices are of the form
\[ TI = TI(G) = \sum_{v \in V(G), v \neq v'} F(d_i, d_j), \] (7)
where \( F \) is a pertinently chosen function with the property \( F(x, y) = F(y, x) \). On each of such topological indices, a matrix \( TI \) can be associated, defined as
\[ (TI)_{ij} = \begin{cases} F(d_i, d_j), & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (8)

There are several degree-based topological indices introduced to test the properties of compounds and drugs, which have been widely used in chemical and pharmacy engineering. Several matrices which are related to topological indices are given as follows:

(i) First Zagreb matrix [4]:
\[ (Z^{(1)})_{ij} = \begin{cases} d_i + d_j, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (9)

(ii) Albertson matrix \( A = [a_{i,j}] \) [10]:
\[ (AL)_{ij} = a_{i,j} = \begin{cases} |d_i - d_j|, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (10)

(iii) Geometric-arithmetic matrix [11]:
\[ (GA)_{ij} = \begin{cases} \frac{2\sqrt{d_i d_j}}{d_i + d_j}, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (11)

(iv) \( ABC \) matrix [12]:
\[ (ABC)_{ij} = \begin{cases} \frac{\sqrt{d_i + d_j} - 2}{\sqrt{d_i d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (12)

(v) Sum-connectivity matrix [13]:
\[ (SCI)_{ij} = \begin{cases} \frac{1}{\sqrt{d_i + d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (13)

In this paper, we would like to introduce the matrix associated with the difference between atom-bond connectivity index and Randic index of a graph \( G \), defined as follows:

\[ (ABC - R)_{ij} = D_{ij} = d_{i,j} = \begin{cases} \frac{\sqrt{d_i + d_j} - 2 - 1}{\sqrt{d_i d_j}}, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \] (14)
We call $D$ as the difference matrix associated with the difference between atom-bond connectivity index and Randić index of graph $G$.

This paper is organized as follows: in Section 2, we introduce some properties of characteristic polynomials of difference matrix and some properties of difference eigenvalues; in Section 3, we study the energy of graphs and introduce the difference energy; and we also obtain lower and upper bounds for this new energy.

## 2. Some Properties of Difference Matrix of Graphs

In this section, we introduce some properties of characteristic polynomials of difference matrix and some properties of difference eigenvalues of a graph $G$.

Let $G = (V, E)$ be a graph of order $n$ with $m$ edges and $D(G)$ be the adjacency difference matrix with respect to a given degree. Suppose that

$$
\mathcal{P}(G, \varrho) := \det((\varrho I - D(G))) = a_0\varrho^n + a_1\varrho^{n-1} + a_2\varrho^{n-2} + \cdots + a_n,
$$

is the characteristic polynomial of $D(G)$. Thus, in order to find nontrivial solutions to equation (15), one must demand that $D - \varrho I$ is not invertible, or equivalently,

$$
\mathcal{P}(G, \varrho) = \mathcal{P}(\varrho(G)) = \det(D(G) - \varrho I) = 0.
$$

Equation (16) is called the characteristic equation. Evaluating the determinant yields an $n$-th order polynomial in $\varrho$, called the characteristic polynomial, which we have denoted above by $\mathcal{P}(G, \varrho)$. The determinant in equation (16) can be evaluated by the usual methods. It takes the following form:

$$
\mathcal{P}(D(G) - \varrho I) = \begin{vmatrix}
d_{11} - \varrho & d_{12} & \cdots & d_{1n} \\
d_{21} & d_{22} - \varrho & \cdots & d_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
d_{n1} & d_{n2} & \cdots & d_{nn} - \varrho
\end{vmatrix}
= a_0\varrho^n + a_1\varrho^{n-1} + a_2\varrho^{n-2} + a_3\varrho^{n-3} + \cdots + a_n,
$$

where $D = [d_{ij}]$ and $d_{ij}$ are the vertices degree $v_i$ and $v_j$.

**Example 1.** The difference matrix of the graph $G_1$ in Figure 1 is

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{5}} \\
0 & 0 & \frac{2}{\sqrt{8}} & \frac{\sqrt{5} - 1}{\sqrt{12}} & \frac{\sqrt{5} - 1}{\sqrt{12}} & \frac{1}{\sqrt{20}} \\
0 & \frac{1}{\sqrt{8}} & 0 & 0 & 0 & \frac{\sqrt{5} - 1}{\sqrt{10}} \\
0 & \frac{\sqrt{5} - 1}{\sqrt{12}} & 0 & 0 & \frac{1}{3} & \frac{\sqrt{6} - 1}{\sqrt{15}} \\
0 & \frac{\sqrt{5} - 1}{\sqrt{12}} & 0 & \frac{1}{3} & \frac{\sqrt{6} - 1}{\sqrt{15}} & 0 \\
1 & \frac{\sqrt{7} - 1}{\sqrt{20}} & \frac{\sqrt{5} - 1}{\sqrt{10}} & \frac{\sqrt{6} - 1}{\sqrt{15}} & \frac{\sqrt{6} - 1}{\sqrt{15}} & -\varrho
\end{pmatrix}
$$

Figure 1: A graph $G_1$. The characteristic polynomial of the maximum degree matrix $D(G_1)$ is

$$
\mathcal{P}(D(G_1), \varrho) = \det(D(G_1) - \varrho I)
$$
and the difference eigenvalues of $G_1$ are $\varrho_1 = 1.2619117684383, \varrho_2 = 0.2094370173795, \varrho_3 = 0.088080504528, \varrho_4 = -0.3333333333333, \varrho_5 = -0.746650631759, \text{and } \varrho_6 = -0.4794453252535.$

Here, we compute some of the coefficients in equality (17).

**Lemma 1.** Let $a_0, a_1, a_2,$ and $a_3$ be the coefficients in equality (17), then

(i) $a_0 = 1,$

(ii) $a_1 = 0,$

(iii) $a_2 = -\sum_{1 \leq i < j \leq n} \left( \frac{d_i + d_j - 2 - 1}{\sqrt{d_i d_j}} \right)^2,$

(iv) $a_3 = -2P.$

**Proof**

(i) By the definition of the polynomial,

$$\mathcal{P}(\varrho) := \det(A_\varrho - \varrho I),$$

we get $a_0 = 1.$

(ii) The sum of determinants of all $1 \times 1$ principal submatrices of $D(G)$ is equal to the trace of $D$ implying that

$$a_1 = (-1)^1 \text{Tr}(D(G)) = 0.$$  \hfill (21)

(iii) $(-1)^2 a_2 =$ sum of determinants of all the $2 \times 2$ principal submatrices of $D(G):$

\[
(-1)^2 a_3 = \sum_{1 \leq i < j < k \leq n} \left| \begin{array}{ccc}
    d_{ii} & d_{ij} & d_{ik} \\
    d_{ji} & d_{jj} & d_{jk} \\
    d_{ki} & d_{kj} & d_{kk}
  \end{array} \right| 
- \sum_{1 \leq i \leq k < j \leq n} d_{ii} d_{jj} \sum_{1 \leq k < j \leq n} \left( \frac{d_i + d_j - 2 - 1}{\sqrt{d_i d_j}} \right)^2,
\]

\[
= \sum_{1 \leq i \leq k \leq n} \left( d_{ii} [d_{jj}d_{kk} - d_{kk}a_{kj}] - d_{ij} [d_{jj}d_{kk} - d_{kk}a_{jk}] + d_{ik} [d_{jj}d_{kk} - d_{kk}d_{jj}] \right),
\]

\[
= - \sum_{1 \leq i \leq k < j \leq n} \left( d_{ii} d_{ij} d_{kk} + \sum_{1 \leq k < j \leq n} \left[ d_{ii} d_{kk}^2 + d_{ij} d_{kk}^2 + d_{kk} d_{ij}^2 \right] + 2 \sum_{1 \leq k < j \leq n} d_{kk} d_{ij} d_{jk} \right),
\]

\[
= -2 \sum_{1 \leq i \leq k < j \leq n} \left( \frac{d_i + d_j - 2 - 1}{\sqrt{d_i d_j}} \right)^2 \left( \frac{d_k + d_j - 2 - 1}{\sqrt{d_k d_j}} \right) = -2P,
\]

where $P = \sum_{1 \leq i < j \leq n} \left( \frac{\sqrt{d_i + d_j - 2 - 1}}{\sqrt{d_i d_j}} \right)^2 \left( \frac{\sqrt{d_i + d_j - 2 - 1}}{\sqrt{d_i d_j}} \right) \left( \frac{\sqrt{d_i + d_j - 2 - 1}}{\sqrt{d_i d_j}} \right).$

We are dealing this part with some results related to the traces of powers of $D.$ Recall that we denote $N_k = \text{Tr}(D^k).$
Now, we prove the following lemma that will need to obtain the main results.

\begin{equation}
(1) \ N_0 = \sum_{i=1}^{n} \theta_i = n,
\end{equation}

\begin{equation}
(2) \ N_1 = \sum_{i=1}^{n} \theta_i^2 = 0,
\end{equation}

\begin{equation}
(3) \ N_2 = \sum_{i=1}^{n} \theta_i^2 = 2 \sum_{i \neq j} \left( \frac{d_i + d_j - 2}{\sqrt{d_i d_j}} \right)^2 ,
\end{equation}

\begin{equation}
(4) \ N_3 = \sum_{i=1}^{n} \theta_i^3 = 2 \sum_{i \neq j} \left( \frac{d_i + d_j - 2}{\sqrt{d_i d_j}} \right)^2 \sum_{k \in V(G)} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \frac{\sqrt{d_j + d_k - 2} - 1}{\sqrt{d_j d_k}} ,
\end{equation}

\begin{equation}
(5) \ N_4 = \sum_{i=1}^{n} \theta_i^4 = \sum_{i \neq j} \sum_{k \in V(G)} \left( \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 \sum_{k \in V(G)} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \frac{\sqrt{d_j + d_k - 2} - 1}{\sqrt{d_j d_k}} ,
\end{equation}

where $\sum_{i \neq j}$ indicates summation over all pairs of adjacent vertices $v_i$ and $v_j$.

**Proof.** By definition, the diagonal elements of $D$ are equal to zero. Therefore, the trace of $D$ is zero.

Next, we calculate the matrix $D^2$. For $i = j$,

\begin{equation}
(D^2)_{ii} = \sum_{j=1}^{n} D_{ij} D_{ji} = \sum_{j=1}^{n} (D_{ij})^2 = \sum_{i=1}^{n} (D_{ij})^2 = \sum_{i \neq j} \left( \frac{d_i + d_j - 2}{\sqrt{d_i d_j}} \right)^2 ,
\end{equation}

whereas for $i \neq j$,

\begin{equation}
(D^2)_{ij} = \sum_{j=1}^{n} D_{ij} D_{ji} = D_{ii} D_{jj} + \sum_{k \in V(G)} D_{ik} D_{kj} = \sum_{k \in V(G)} D_{ik} D_{kj} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \frac{\sqrt{d_j + d_k - 2} - 1}{\sqrt{d_j d_k}} ,
\end{equation}

\begin{equation}
= \sum_{k \in V(G)} D_{ik} D_{kj} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \frac{\sqrt{d_j + d_k - 2} - 1}{\sqrt{d_j d_k}} ,
\end{equation}

Therefore,

\begin{equation}
\text{tr}(D^2) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 = 2 \sum_{i \neq j} \left( \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 .
\end{equation}

We next calculate $N_4$. The diagonal elements of $D^4$ are
tr(D^4) = \left( \sum_{i \neq j} \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 \\
+ \sum_{i \in V(G)} \left( \sum_{k \neq i, k \neq j} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \right)^2.

Then, we obtain
\[ N_4 = \sum_{i \in V(G)} \left( \sum_{j \neq i} \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 \\
+ \sum_{i \in V(G)} \sum_{j \neq i} \left( \sum_{k \neq i, k \neq j} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \right)^2 \]
\[ = \sum_{i \in V(G)} \left( \sum_{j \neq i} \frac{\sqrt{d_i + d_j - 2} - 1}{\sqrt{d_i d_j}} \right)^2 \\
+ \sum_{i,j \in V(G)} \left( \sum_{k \neq i, k \neq j} \frac{\sqrt{d_i + d_k - 2} - 1}{\sqrt{d_i d_k}} \right)^2. \]

Equality holds if and only if X is an eigenvector of B, corresponding to the largest eigenvalue \( \lambda_1(B) \).

The following result is related with the large eigenvalue \( \lambda_1(B) \).

**Lemma 3** (Rayleigh–Ritz [14]). If B is a real symmetric \( n \times n \) matrix with eigenvalues \( \lambda_1(B) \leq \lambda_2(B) \leq \cdots \leq \lambda_n(B) \), then for any \( X \in \mathbb{R}^n \) (\( X \neq 0 \)), \n\[ X'BX \leq \lambda_1(B)X'X. \]

This completes the proof.

Here, we recall the following lemma that we need to prove the next lemma.

**Lemma 4.** Let G be a connected graph with \( n \geq 2 \) vertices. Then, the spectral radius of the difference matrix is bounded from below as
\[ \theta_1 \geq \frac{2D(G)}{n}. \]

**Proof.** Let \( D = [d_{ij}] \) be the difference matrix corresponding to D. By Lemma 3, for any vector \( X = (x_1, x_2, \ldots, x_n)' \),
\[ X'DX = \left( \sum_{j=1}^{n} x_j d_{j1}, \sum_{j=2}^{n} x_j d_{j2}, \ldots, \sum_{j=n}^{n} x_j d_{jn} \right)'X \]
\[ = 2 \sum_{j=1}^{n} d_{jj} x_j^2, \]
because \( d_{ij} = d_{ji} \). Also,
\[ X'X = \sum_{i=1}^{n} x_i^2. \]

Using equations (34) and (35), by Lemma 3, we obtain
\[ \theta_1 \geq \frac{2\sum_{j=1}^{n} x_j^2}{n} \]
\[ = \frac{2\sum_{j=1}^{n} x_j^2}{n}. \]

Since (36) is true for any vector X, by putting \( X = (1, 1, \ldots, 1)' \), we have
\[ \theta_1 \geq \frac{2D(G)}{n}. \]

This completes the proof.

Now, we obtain a lower bound for the maximum eigenvalue.

**Lemma 5.** Let G be a graph with \( n \) vertex and \( m \) edges:
\[ \theta_1 \geq \frac{ABC(G)}{n} - \frac{2m}{n^6}. \]

**Proof.** Let \( x \in \mathbb{R}^n \) be a unit vector, then
\[ x'THx = \sum_{u,v \in E(G)} \left( \frac{\sqrt{d_u + d_v - 2} - 1}{\sqrt{d_u d_v}} \right) x_u x_v \]
\[ = \sum_{u,v \in E(G)} \left( \frac{\sqrt{d_u + d_v - 2} - 1}{\sqrt{d_u d_v}} \right) x_u x_v \]
\[ \geq \sum_{u,v \in E(G)} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u d_v}} x_u x_v - \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u d_v}} x_u x_v \]
\[ \geq \sum_{u,v \in E(G)} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u d_v}} x_u x_v - \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u d_v}} x_u x_v. \]

If we put \( x^T = (1/\sqrt{n}, 1/\sqrt{n}, \ldots, 1/\sqrt{n}) \), we get
\[ x'THx \geq \sum_{u,v \in E(G)} \frac{\sqrt{d_u + d_v - 2}}{n^{d_u d_v}} - \frac{2m}{n^6}. \]

Therefore, by Lemma 3, the proof is now complete.

Here, we obtain an upper bound for \( N_4 \) that will need to obtain upper and lower bounds for new energy.

**Lemma 6.** Let G be a simple graph with \( m \) edges and the redefined first \( \text{Re}Z(G) \) index. Then,
\[ N_4 \leq 2 \left( \text{Re}Z_1(G) - \frac{2\sqrt{2} - 2}{\Delta^2} - \mathcal{M}_4(G) \right). \]

**Proof.** By Lemma 2, we know that
\[ \text{tr}(D^2) = 2 \sum_{u,v \in E(G)} \left( \frac{\sqrt{d_i + d_j - 2}}{\sqrt{d_id_j}} \right)^2 \]

\[ = 2 \sum_{u,v \in E(G)} \left( \frac{d_i + d_j}{d_id_j} - \frac{2\sqrt{d_i + d_j - 2}}{d_id_j} - \frac{1}{d_id_j} \right) \]

\[ = 2 \left( \text{Re}Z_1(G) - \sum_{u,v \in E(G)} \frac{2\sqrt{d_i + d_j - 2}}{d_id_j} - \mathcal{M}_2^*(G) \right). \]

Now, since \( 2\delta \leq d_i + d_j \leq 2\Delta \) for all edges \( v_iv_j \in E(G) \), \( \delta \leq d_i \leq \Delta \) for all vertices \( v_i \in V(G) \),

\[ 2 \left( \text{Re}Z_1(G) - \sum_{u,v \in E(G)} \frac{2\sqrt{d_i + d_j - 2}}{d_id_j} - \mathcal{M}_2^*(G) \right) \leq 2 \left( \text{Re}Z_1(G) - \frac{2\sqrt{2\delta - 2}}{\Delta^2} - \mathcal{M}_2^*(G) \right) \]

This completes the proof. \( \square \)

### 3. Bounds for the Difference Energy of Graphs

In this section, we study the energy of graphs and introduce the difference energy. We also obtain lower and upper bounds for the new energy.

The energy \( E = E(G) \) of a graph \( G \) is the sum of the absolute values of the eigenvalues of \( G \). The motivation for the introduction of this invariant comes from chemistry, where results on \( E \) were obtained already in the 1940s. The graph energy is a graph-spectrum-based quantity, introduced in the 1970s. After a latent period of 20–30 years, it became a popular topic of research both in mathematical chemistry and in “pure” spectral graph theory. In 1978, Gutman defined energy mathematically for all graphs [15]. The energy of different graphs including regular, nonregular, circulant, and random graphs is also under study. The energy of the graph \( G \) is defined as

\[ E = E(G) = \sum_{i=1}^{n} |\lambda_i|, \]

where \( \lambda_i, i = 1, 2, \ldots, n \), are the eigenvalues of graph \( G \).

The difference energy \( (E_D) \) of graph \( G \) is defined in an analogue way as

\[ E_D(G) = \sum_{i=1}^{n} |\lambda_i - \lambda_i'|. \]

It is usual and useful to define some modified energies such as Zagreb energy, harmonic energy, Albertson energy, matching energy, Laplacian energy, and geometric-arithmetic energy (refer [16–18] and [10, 19–26]). These modified energies have applications in theoretical organic chemistry [27], image processing [28], and information theory [29].

**Example 2.** The difference energy of the graph \( G_1 \) in Figure 1 is

\[ E_D(G_1) = 3.1188585806916. \] (46)

We start with upper bound for difference energy.

**Theorem 1.** Let \( G \) be a graph with \( n \) vertices. Then,

\[ E_D(G) \leq \frac{2n}{\Delta^2} \left( \text{REZ}_1(G) - \frac{2\sqrt{\Delta - 2}}{\Delta^2} - \mathcal{M}_2^*(G) \right). \] (47)

**Proof.** By Cauchy Schwarz inequality and Lemma 6, we have

\[ \sum_{i=1}^{n} |\lambda_i - \lambda_i'| \leq \sqrt{n \sum_{i=1}^{n} \lambda_i^2} \]

\[ \leq \sqrt{2n \left( \text{REZ}_1(G) - \frac{2\sqrt{\Delta - 2}}{\Delta^2} - \mathcal{M}_2^*(G) \right)}. \] (48)

Hence,

\[ E_D(G) \leq \frac{2n}{\Delta^2} \left( \text{REZ}_1(G) - \frac{2\sqrt{\Delta - 2}}{\Delta^2} - \mathcal{M}_2^*(G) \right). \] (49)

This completes the proof.

We need the following lemma to obtain lower and upper bounds of the difference energy involving \( N_2 \).

**Lemma 7 (see [30]).** Let \( a_1, \ldots, a_n \) and \( b_1, \ldots, b_n \) be real numbers such that \( a \leq a_i \leq A \) and \( b \leq b_i \leq B \), \( i = 1, \ldots, n \). Then,

\[ - (A + a)(B - b)n^2 \alpha(\lambda) \leq \sum_{i=1}^{n} a_i b_i - \frac{1}{n} \sum_{i=1}^{n} a_i \sum_{j=1}^{n} b_j \leq (A + a)(B - b)n^2 \alpha(\lambda), \]

where \( \alpha(\lambda) = (1/4)(1 - ((-1)^{n+1} + 1/2n^2)). \) (50)

Here, we obtain lower and upper bounds for new energy.

**Theorem 2.** Let \( G \) be a graph with \( n \) vertices. Then,

\[ \sqrt{nN_2 - n^2 \alpha(\lambda)} \leq E_D(G) \leq \sqrt{nN_2 + n^2 \alpha(\lambda)} \]

\[ \leq \sqrt{nN_2 + n^2 \alpha(\lambda)} \] (51)

Equality holds if and only if \( G = \mathcal{G}. \)

**Proof.** For \( a_i = b_i = |\lambda_i| \), \( A = B = |\lambda_1| \), \( a = b = |\lambda_n| \), and \( \mathcal{M}_2 = m_2 = 1 \), inequality (50) becomes

\[ \leq - \left( |\lambda_1| - |\lambda_n| \right) n \alpha(\lambda) \leq \sum_{i=1}^{n} \lambda_i^2 - \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j \]

\[ \leq (|\lambda_1| - |\lambda_n|) \left( |\lambda_1| - |\lambda_n| \right) n \alpha(\lambda). \] (52)

Therefore, by Lemma 2 and definition of difference energy, inequality (52) becomes
\[-na(n)(\lvert e_1 \rvert - \lvert e_n \rvert)^2 - N_2 \leq - \frac{1}{n} E_D(G) \leq na(n)(\lvert e_1 \rvert - \lvert e_n \rvert)^2 - N_2. \]

(53)

Clearly, if \( G \cong \overline{G} \), then \( e_1 = e_2 = \cdots = e_n = 0 \); hence, \( E_D(G) = 0 \), and also, \( nN_2 = 0 \); therefore by (51), we have \( 0 = E_D(G) = 0 \). Conversely, if \( e \) is held on both sides of (51), then equality holds in (52) and (53); therefore, we have

\[-na(n)(\lvert e_1 \rvert - \lvert e_n \rvert)^2 - N_2 = \frac{1}{n} E_D(G) = na(n)(\lvert e_1 \rvert - \lvert e_n \rvert)^2 - N_2. \]

(54)

So by equality on both sides of (54), we get

\( na(n)(\lvert e_1 \rvert - \lvert e_n \rvert)^2 = 0 \); since \( n, n \neq 0 \), therefore, \( (\lvert e_1 \rvert - \lvert e_n \rvert)^2 = (\lvert e_1 \rvert - \lvert e_n \rvert)^2 = 0 \); in other words, \( e_1 = e_n \), or \( e_n = \pm e_1 \); hence, \( e_1 = e_n = 0 \), then \( G \cong \overline{G} \).

Now, we obtain lower bound for new energy involving \( N_2 \) and \( N_3 \).

**Theorem 3.** Let \( G \) be a graph with \( n \) vertices and at least one edge. Then,

\[ E_D(G) > \sqrt{\frac{N_3}{N_4}}. \]

(55)

**Proof.** Using Hölder inequality, we have

\[
\sum_{i=1}^{n} a_i^{\nu} \leq \left( \sum_{i=1}^{n} a_i^{p} \right)^{\frac{1}{p}} \left( \sum_{i=1}^{n} a_i^{q} \right)^{\frac{1}{q}},
\]

(56)

which holds for any nonnegative real numbers \( a_1, a_2, \ldots, a_n \). Setting \( a_i = |e_1|^{2/3}, b_i = |e_i|^{0/3}, p = (3/2), \) and \( q = 3 \), we obtain

\[
\sum_{i=1}^{n} |e_i|^2 = \sum_{i=1}^{n} |e_i|^{2/3} \sum_{i=1}^{n} |e_i|^{4/3} \leq \left( \sum_{i=1}^{n} |e_i|^{2/3} \right)^{2/3} \left( \sum_{i=1}^{n} |e_i|^{4/3} \right)^{4/3},
\]

(57)

since \( G \) is nonempty graph; hence, we have

\[
\sum_{i=1}^{n} |e_i|^2 = \frac{\left( \sum_{i=1}^{n} |e_i|^{2/3} \right)^{2} \left( \sum_{i=1}^{n} |e_i|^{4/3} \right)^{4/3}}{\sum_{i=1}^{n} |e_i|^{4/3}} \leq \sqrt{\frac{N_3}{N_4}}.
\]

(58)

Hence, we get the result.

Now, we obtain an upper bound for new energy involving vertices, edges, minimum degree, and \( ABC \) index.

**Theorem 4.** Let \( G \) be a nonempty graph with \( n \) vertices. Then,

\[ E_D(G) < \frac{ABC(G)}{n} - \frac{2m}{n^\delta} + \sqrt{(n-1) \left( \frac{ABC(G)}{n} - \frac{2m}{n^\delta} \right)^2}. \]

(59)

**Proof.** Let \( \varphi_1, \varphi_2, \ldots, \varphi_{n-1}, \varphi_n \) be the eigenvalues of \( G \). By the Cauchy–Schwartz inequality,

\[ \sum_{i=1}^{n} |e_i|^2 \leq \sqrt{(n-1) \sum_{i=2}^{n} \varphi_i^2} = \sqrt{(n-1)(N_2 - \varphi_n^2)}. \]

(60)

Hence,

\[ E_D(G) \leq \varphi_1 + \sqrt{(n-1)(N_2 - \varphi_1^2)}. \]

(61)

Note that the function \( f(x) = x + \sqrt{(n-1)(N_2 - x^2)} \) decreases for \( (ABC(G)/n) - (2m/n^\delta) \leq x \leq (ABC(G)/n^2) - (2m/n^\delta) \). By Lemma 5, we have \( \varphi_1 \geq (ABC(G)/n) - (2m/n^\delta) \); therefore,

\[ \varphi_1 \geq \frac{ABC(G)}{n} - \frac{2m}{n^\delta} \geq ABC(G) n^2 - \frac{2m}{n^\delta} \]

(62)

So \( f(\varphi_1) \leq f((ABC(G)/n) - (2m/n^\delta)) \), since \( G \) is nonempty graph which implies that

\[ E_D(G) < \frac{ABC(G)}{n} - \frac{2m}{n^\delta} + \sqrt{(n-1) \left( \frac{ABC(G)}{n} - \frac{2m}{n^\delta} \right)^2}. \]

(63)

This completes the proof.

Similarly, by Lemma 4, we have the following lemma.

**Lemma 8.** Let \( G \) be a nonempty graph with \( n \) vertices:

\[ E_D(G) \leq \frac{2D(G)}{n} + \sqrt{(n-1) \left( \frac{2D(G)}{n} \right)^2}. \]

(64)

Here, we obtain an upper bound for new energy involving vertices and \( N_2 \).

**Theorem 5.** Let \( G \) be a graph with \( n \) vertices. Then,

\[ E_D(G) \leq \frac{N_2 + n}{2}. \]

(65)

Equality holds if and only if \( G \cong (n/2)K_2, (n = 2m) \).

**Proof.** Let \( a_1, a_2, \ldots, a_n \) and \( b_1, b_2, \ldots, b_n \) be sequences of real numbers and \( c_1, c_2, \ldots, c_n \) and \( d_1, d_2, \ldots, d_n \) are nonnegative. Then, the following inequality is valid (see [31]):

\[ \sum_{i=1}^{n} d_i \sum_{i=1}^{n} c_i a_i^2 + \sum_{i=1}^{n} c_i d_i b_i^2 \geq \sum_{i=1}^{n} a_i c_i \sum_{i=1}^{n} b_i d_i. \]

(66)

For \( a_i = |e_i|, b_i = c_i = d_i = 1, i = 1, 2, \ldots, n \), inequality (66) becomes

\[ \sum_{i=1}^{n} \sum_{i=1}^{n} |e_i|^2 + \sum_{i=1}^{n} \sum_{i=1}^{n} |e_i|^2 \geq \sum_{i=1}^{n} |e_i|^2 \sum_{i=1}^{n} 1. \]

(67)

Therefore, by Lemma 2, we have

\[ E_D(G) \leq \frac{N_2 + n}{2}. \]

(68)
Let $G$ be a nonempty graph with $n \geq 2$ vertices. Then,
$$E_D(G) \geq \frac{N_2}{\ell_1}. \quad (73)$$

Equality holds if and only if $G \equiv (n/2)K_2$, $(n = 2m)$.

Proof. Let $a_i$ and $b_i$ be decreasing nonnegative sequences with $a_i, b_i \neq 0$ and $w_i$ a nonnegative sequence, for $i = 1, 2, \ldots, n$. Then, the following inequality is valid (see [32], p. 85):
$$\sum_{i=1}^{n} w_i a_i^2 \sum_{i=1}^{n} w_i b_i^2 \leq \max \left\{ b_1 \sum_{i=1}^{n} w_i a_i, a_1 \sum_{i=1}^{n} w_i b_i \right\} \sum_{i=1}^{n} w_i a_i b_i. \quad (74)$$

For $a_i = b_i = |e_i|$ and $w_i = 1$, $i = 1, 2, \ldots, n$, inequality (74) becomes
$$\sum_{i=1}^{n} e_i^2 = \max \left\{ e_1 \sum_{i=1}^{n} |e_i|, e_1 \sum_{i=1}^{n} |e_i| \right\} \sum_{i=1}^{n} e_i^2. \quad (75)$$

Since
$$\sum_{i=1}^{n} |e_i|^2 = \sum_{i=1}^{n} e_i^2 = N_2, \quad (76)$$
$$\sum_{i=1}^{n} |e_i| = E_D(G),$$
then the above inequality follows directly from the assertion of Theorem 6, i.e., inequality (73).

If $G \equiv (n/2)K_2$, then it is easy to check that the equality in (73) holds. Conversely, if the equality in (73) hold, then equality also holds in (74) and (75); therefore, we have
$$\sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} e_i^2 = \max \left\{ e_1 \sum_{i=1}^{n} |e_i|, e_1 \sum_{i=1}^{n} |e_i| \right\} \sum_{i=1}^{n} e_i^2. \quad (77)$$

From equality (77), we get
$$\sum_{i=1}^{n} e_i^2 = \sigma_1 \sum_{i=1}^{n} |e_i|. \quad (78)$$

By equality (78), we have
$$\left( |e_1|^2 + |e_2|^2 + \cdots + |e_n|^2 \right) - e_1 \left( |e_1|^2 + |e_2|^2 + \cdots + |e_n|^2 \right) = 0. \quad (79)$$

Equality (79) implies that
$$\left( |e_1|^2 + |e_2|^2 + \cdots + |e_n|^2 \right) - e_1 \left( 1 + 1 + \cdots + 1 \right) = 0. \quad (80)$$

Since $G$ is a nonempty graph, then $(|e_1|^2 + |e_2|^2 + \cdots + |e_n|^2) = E_D(G) \neq 0$; therefore, by equality (80), we have
$$\left( |e_1|^2 + |e_2|^2 + \cdots + |e_n|^2 \right) = e_1 \left( 1 + 1 + \cdots + 1 \right). \quad (81)$$

Hence, we have $|e_1| = |e_2| = \cdots = |e_n| = 1$. Therefore, $G \equiv (n/2)K_2$, $(n = 2m)$.

Analogy with the paper [24], we obtain the following theorems.

Theorem 7. Let $G$ be a graph with $n$ vertices. Then,
$$\sqrt{N_2} \leq E_D(G) \leq \sqrt{nN_2}. \quad (82)$$

Theorem 8. Let $G$ be a connected graph with $n$ vertices. Then,
$$E_D(G) \geq \sqrt{N_2 + n(n-1)|\det D|^{2/n}}. \quad (83)$$

4. Conclusion

In this paper, the spectral properties of the difference between the atom-bond connectivity index and Randić index were studied. Our main tool was the modification of the classical adjacency matrix involving the degree of the vertices in graph $G$. Some properties of its characteristic polynomial were established. In addition, bounds for the difference energy were obtained, as well as the relations between them.

Data Availability

No data were used in this research.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.
Authors’ Contributions

All authors contributed equally to this work.

Acknowledgments

The research of the second author was supported by the Research Intensified Grant Scheme (RIGS), Phase 1/2019, Universiti Malaysia Terengganu, Malaysia, with Grant Vot. 55192/6.

References

[1] H. Wiener, “Structural determination of paraffin boiling points,” Journal of the American Chemical Society, vol. 69, no. 1, pp. 17–20, 1947.
[2] A. Ali and Z. Du, “On the difference between atom-bond connectivity index and randic index of binary and chemical trees,” International Journal of Quantum Chemistry, vol. 117, no. 23, Article ID e25446, 2017.
[3] I. Gutman and N. Trinajstić, “Graph theory and molecular orbitals. Total ϕ-electron energy of alternant hydrocarbons,” Chemical Physics Letters, vol. 17, no. 4, pp. 535–538, 1972.
[4] N. J. Rad, A. Jahanbani, and I. Gutman, “Zagreb energy and Zagreb estrada index of graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 79, pp. 371–386, 2018.
[5] A. Milčević, S. Nikolić, and N. Trinajstić, “On reformulated Zagreb indices,” Molecular Diversity, vol. 8, no. 4, pp. 393–399, 2004.
[6] P. S. Ranjini, V. Lokesha, and A. Usha, “Relation between phenylene and hexagonal squeeze using harmonic index,” International Journal of Graph Theory, vol. 1, pp. 116–121, 2013.
[7] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, “An atom-bond connectivity index: modelling the enthalphy of formation of alkanes,” Indian Journal of Chemistry -Section A, vol. 37, pp. 849–855, 1998.
[8] Z. Du, A. Jahanbani, and S. M. Sheikholeslami, “Relationships between Randić index and other topological indices,” Communications in Combinatorics and Optimization (To Appear), 2020.
[9] N. H. Sarmin, N. I. Alimon, and A. Erfanian, “Topological indices of the non-commuting graph for generalised quaternion group,” Bulletin of the Malaysian Mathematical Sciences Society, 2019.
[10] A. Jahanbani, “Albertson energy and Albertson-Estrada index of graphs,” Journal of Linear and Topological Algebra, vol. 8, pp. 11–24, 2019.
[11] J. M. Rodriguez and J. M. Siganreta, “Spectral properties of geometric-arithmetic index,” Applied Mathematics and Computation, vol. 277, pp. 142–153, 2016.
[12] E. Estrada, “The ABC matrix,” Journal of Mathematical Chemistry, vol. 55, no. 4, pp. 1021–1033, 2017.
[13] B. Zhou and N. Trinajstić, “On sum-connectivity matrix and sum-connectivity energy of (molecular) graphs,” Acta Chimica Slovenica, vol. 57, no. 3, pp. 518–523, 2010.
[14] R. A. Horn and C. R. Johnson, Matrix Analysis, Cambridge University Press, New York, NY, USA, 1985.
[15] I. Gutman, “The energy of a graph,” Ber. Math Statist. Sekt. Forschungsz. Graz vol. 103, pp. 1–22, 1978.
[16] L. Chen and Y. Shi, “Maximal matching energy of tricyclic graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 73, pp. 105–119, 2015.
[17] K. C. Das and I. Gutman, “On incidence energy of graphs,” Linear Algebra and Its Applications, vol. 446, pp. 329–344, 2014.
[18] K. C. Das, S. A. Mojallal, and I. Gutman, “On energy and Laplacian energy of bipartite graphs,” Applied Mathematics and Computation, vol. 273, pp. 759–766, 2016.
[19] A. Jahanbani and J. R. Zambrano, “Koolen-moultton-type upper bounds on the energy of a graph,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 83, pp. 497–518, 2020.
[20] A. Jahanbani, “Upper bounds for the energy of graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 79, pp. 275–286, 2018.
[21] A. Jahanbani, “Some new lower bounds for energy of graphs,” Applied Mathematics and Computation, vol. 296, pp. 233–238, 2017.
[22] A. Jahanbani, “Lower bounds for the energy of graphs,” AKCE International Journal of Graphs and Combinatorics, vol. 15, no. 1, pp. 88–96, 2018.
[23] A. Jahanbani, “New bounds for the harmonic energy and harmonic estrada index of graphs,” Computer Science Journal of Moldova, vol. 26, pp. 270–300, 2018.
[24] A. Jahanbani and H. H. Raz, “On the harmonic energy and estrada index of graphs,” Mathematical Aspects of Topological Indices, vol. 1, pp. 1–20, 2019.
[25] A. Jahanbani, “Hermitian energy and hermitian estrada index of digraphs,” Asian-European Journal of Mathematics, 2019.
[26] A. Jahanbani, “New bounds for the Harary energy and Harary Estrada index of graphs,” Mathematical Aspects of Topological Indices, vol. 1, pp. 40–51, 2019.
[27] S. Renqian, Y. Ge, B. Huo, S. Ji, and Q. Diao, “On the tree with diameter 4 and maximal energy,” Applied Mathematics and Computation, vol. 268, pp. 364–374, 2015.
[28] Y. Z. Song, P. Arbelaez, P. Hall, C. Li, and A. Balikai, “Finding semantic structures in image hierarchies using Laplacian graph energy,” in Proceedings of the Eleventh European Conference on Computer Vision(ECCV), Part IV, Springer-Verlag, Heraklion, Greece, pp. 694–707, September 2010.
[29] X. Li, Z. Qin, M. Wei, I. Gutman, and M. Dehmer, “Novel inequalities for generalized graph entropies—graph energies and topological indices,” Applied Mathematics and Computation, vol. 259, pp. 470–479, 2015.
[30] D. S. Mitroinić and P. Vasić, Analytic Inequalities, Springer, Berlin, Germany, 1970.
[31] S. S. Dragomir, On Some Inequalities (Romanian), Mathematica, No. 13, University of Timișoara, Timișoara, Romania, 1984.
[32] S. S. Dragomir, “A survey on Cauchy-Bunyakovsky-Schwarz type discrete inequalities,” Journal of Inequalities in Pure and Applied Mathematics, vol. 4, pp. 1–142, 2003.