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FIRST ECCENTRIC-DEGREE INDEX AND IT'S ENERGY FOR SOME CLASSES OF GRAPHS

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ABSTRACT. Given any simple graph G, we introduce a new distance degree based index the first eccentric-degree index $ED_1(G) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$, and compute the same for certain special class of graphs. Further, this work is extended towards defining the first eccentric-degree energy where in we investigate the bounds for any simple graph and compute the energy for complete bipartite and complete graphs.

1. Introduction

According to modern mathematics and their application the term topological indices is a widespread area of chemical graph theory. These indices play a vital role in determining the structral activity and structural property, QSAR/QSPR of the molecular structure. More specifically the topological indices are characterized into two variants namely degree base and distance based topological indices. For any molecular structure when generally converted in to a simple graph, G

Throughout this article, we consider G to be a graph of order p and size q. Here, V(G) and E(G) address the set of all vertices and edges, respectively of the graph G. we consider $u_i u_j \in E(G)$ if two vertices u_i and u_j are connected by an edge. The number of edges incident to a vertex u is the *degree* of that vertex and is denoted by d(u). The *distance* [7] between the vertices u and v, denoted by d(u,v), is the length of the shortest path joining u and v in G. The topological indices [13] are numerical graph invariants that characterizes the molecular topology of chemical compounds. It acts a crucial role in quantitative structure property relationship(QSPR) [3, 11, 9] analysis to model different properties and activities of molecules. The notion of topological indices instigated in 1947, when Harold Wiener demonstrated the widely known *Wiener index* [14] for gauging boiling point of alkanes. Subsequently, significant proportion of mathematical chemistry research was accomplished on indices based on different graph parameters

In 1972, Ivan Gutman and Nenad Trinajstic [6] have introduced the *first zagreb index* as follows.

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$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$
(1.1)

Vikas Sharma, Reena Goswami and A.K. Madan [12] have introduced a distancebased graph invariant *eccentric connectivity index* defined as,

$$\xi^c(G) = \sum_{v \in V(G)} e(v)d(v) \tag{1.2}$$

Motivated by the invariants like zagreb indicex and eccentric connectivity index, we define here *First eccentric-degree* index $ED_1(G)$ of a connected graph G as:

$$ED_1(G) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$
(1.3)

The paper is organized as follows, In section 2, the first eccentric-degree index of some graphs are computed. Section 3 concerns with the bounds on first eccentric-degree energy for connected graphs. In Section 4, we obtain first eccentric degree energy and spectra for complete bipartite graph and complete graph.

2. Computation of first eccentric-degree index of some graphs

Theorem 2.1. First eccentric-degree index of complete bipartite graph $K_{m,n}$ is

$$ED_1(K_{m,n}) = 2mn[m+n]$$

Proof. The graph $K_{m,n}$ consists of p = m + n vertices and q = mn edges, with every vertex having an eccentricity of 2. The vertex set can be split into two subsets, V_1 and V_2 , such that each edge connects a vertex u from V_1 to a vertex v from V_2 . The sizes of the sets are $|V_1| = m$ and $|V_2| = n$. Each vertex in V_1 has degree n, and each vertex in V_2 has degree m. Both sets of vertices have eccentricity 2. Therefore,

$$ED_1(K_{m,n}) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$
$$= \sum_{uv \in E(G)} [(2)(n) + (2)(m)]$$
$$= mn(2n + 2m).$$

and the expression given in Theorem 2.1 follows.

Theorem 2.2. First eccentric-degree index of complete graph K_n , is

$$ED_1(K_n) = n(n-1)^2$$

Proof. The complete graph K_n contains p = n vertices and $q = \frac{n(n-1)}{2}$ edges. Each vertex in K_n has an eccentricity of 1. The vertex set of K_n , includes vertices where each vertex u has a degree d(u) = n - 1 and an eccentricity e(u) = 1. Thus, FIRST ECCENTRIC-DEGREE INDEX AND IT'S ENERGY FOR SOME CLASSES OF GRAPHS

$$ED_1(K_n) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$

=
$$\sum_{uv \in E(G)} [(1)(n-1) + (1)(n-1)]$$

=
$$\left(\frac{n(n-1)}{2}\right) (2(n-1)).$$

and the expression given in Theorem 2.2 follows.

Theorem 2.3. First eccentric-degree index of Cycle C_n , $n \ge 3$ is $ED_1(C_n) = \begin{cases} 2n^2, & \text{if } n \text{ is even} \\ 2n(n-1), & \text{if } n \text{ is odd} \end{cases}$

Proof. The cycle C_n has p = n vertices and q = n edges. In C_n , each vertex has an eccentricity of $\frac{n}{2}$ if n is even, and $\frac{n-1}{2}$ if n is odd. For any vertex $u \in V(G)$ in C_n , the degree d(u) is 2 and the eccentricity e(u) matches the aforementioned values depending on whether n is even or odd. Therefore

If n is even, then each vertex u in C_n has an eccentricity of $\frac{n}{2}$. Therefore,

$$ED_1(C_n) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$
$$= \sum_{uv \in E(G)} \left(\left(\frac{n}{2}\right)(2) + \left(\frac{n}{2}\right)(2) \right)$$
$$= n\left(\left(\frac{n}{2}\right)(2) + \left(\frac{n}{2}\right)(2) \right).$$

If n is odd, then each vertex u in C_n has an eccentricity of $\frac{n-1}{2}$. Therefore,

$$ED_1(C_n) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$

=
$$\sum_{uv \in E(G)} \left(\left(\frac{n-1}{2}\right)(2) + \left(\frac{n-1}{2}\right)(2) \right)$$

=
$$n\left(\left(\frac{n-1}{2}\right)(2) + \left(\frac{n-1}{2}\right)(2) \right).$$

d the expression given in Theorem 2.3 follows.

and

Theorem 2.4. First eccentric-degree index of a wheel W_{n+1} , $n \ge 4$, is

$$ED_1(W_{n+1}) = n(n+18)$$

Proof. The wheel graph W_{n+1} has p = n+1 vertices and q = 2n edges. We partition the edge set $E(W_{n+1})$ into two subsets E_1 and E_2 :

- E_1 contains edges where one vertex u has degree n and eccentricity 1, and the other vertex v has degree 3 and eccentricity 2. The number of such edges is $|E_1| = n$.
- E_2 contains edges where both vertices u and v have degree 3 and eccentricity 2. The number of such edges is $|E_2| = n$.

Thus,

$$ED_{1}(W_{n+1}) = \sum_{uv \in E_{1}(G)} [e(u)d(u) + e(v)d(v)] + \sum_{uv \in E_{2}(G)} [e(u)d(u) + e(v)d(v)]$$
$$= \sum_{uv \in E_{1}(G)} [(1)(n) + (2)(3)] + \sum_{uv \in E_{2}(G)} [(2)(3) + (2)(3)]$$
$$= n[(1)(n) + (2)(3)] + n[(2)(3) + (2)(3)]$$
and the summarisen in Theorem 2.4 follows

and the expression given in Theorem 2.4 follows.

Theorem 2.5. First eccentric-degree index of a Friendship graph F_n , $n \ge 2$, is

$$ED_1(F_n) = 4n(n+4)$$

Proof. The Friendship graph F_n consists of p = 2n + 1 vertices and q = 3n edges. In F_n , there is one central vertex (the coalescence vertex) with a degree of 2n, and all other vertices have a degree of 2.

The edge set $E(F_n)$ can be divided into two subsets, E_1 and E_2 , where:

- E_1 contains edges where one endpoint u has degree 2n and eccentricity 1, and the other endpoint v has degree 2 and eccentricity 2. The number of edges in E_1 is $|E_1| = 2n$.
- E_2 contains edges where both endpoints u and v have degree 2 and eccentricity 2. The number of edges in E_2 is $|E_2| = n$.

Thus,

$$\begin{split} ED_1(F_n) &= \sum_{uv \in E_1(G)} [e(u)d(u) + e(v)d(v)] + \sum_{uv \in E_2(G)} [e(u)d(u) + e(v)d(v)] \\ &= \sum_{uv \in E_1(G)} [(1)(2n) + (2)(2)] + \sum_{uv \in E_2(G)} [(2)(2) + (2)(2)] \\ &= 2n[(1)(2n) + (2)(2)] + n[(2)(2) + (2)(2)] \\ \text{and the expression given in Theorem 2.5 follows.} \end{split}$$

Theorem 2.6. First eccentric-degree index of a crown graph $H_{n,n}$, $n \ge 3$, is

$$ED_1(H_{n,n}) = 6n(n-1)^2$$

Proof. The graph $H_{n,n}$ has p = 2n vertices and q = n(n-1) edges. The vertex set of $H_{n,n}$ consists of vertices where each vertex u has a degree of d(u) = n-1 and an eccentricity of e(u) = 3.

Thus,

$$ED_1(H_{n,n}) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$
$$= \sum_{uv \in E(G)} [(3)(n-1) + (3)(n-1)]$$
$$= n(n-1)(6(n-1))$$

and the expression given in Theorem 2.6 follows.

Theorem 2.7. First eccentric-degree index of a cocktail party graph $CP_{n,n}$, $n \ge 2$, is

$$ED_1(CP_{n,n}) = 16n(n-1)^2$$

Proof. The graph $CP_{n,n}$ has p = 2n vertices and q = 2n(n-1) edges. For each vertex u in the vertex set V(G) of $CP_{n,n}$, the degree is d(u) = 2(n-1) and the eccentricity is e(u) = 2.

Thus,

$$ED_1(CP_{n,n}) = \sum_{uv \in E(G)} [e(u)d(u) + e(v)d(v)]$$

=
$$\sum_{uv \in E(G)} [(2)(2(n-1)) + (2)(2(n-1))]$$

=
$$2n(n-1)(8(n-1))$$

and the expression given in Theorem 2.7 follows.

3. Upper and lower bounds for first eccentric-degree energy

The spectral graph theory [2] can be viewed as a method for applying linear algebra. In particular the well-developed theory of matrices allows us to uncover many aspects of discrete mathematics and it's applications. A crucial tool in this field of research is the adjacency matrix. For a graph G, this matrix is denoted as A(G), with the (i,j)-th entry is defined as:

$$a_{ij} = \begin{cases} 1 & : if \ u_i u_j \in E(G), \\ 0 & : Otherwise. \end{cases}$$
(3.1)

The characteristic polynomial is expressed as $\Phi_A(G, \lambda) = det(\lambda I_n - A(G))$, with I_n indicating the identity matrix of dimension $n \times n$. Since A(G) is a real symmetric matrix, its eigenvalues are all real, and we can arrange them as $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$. The collection $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is referred to as the A-spectrum of G and is denoted by Sp(A(G)). If $\{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ denotes the set of distinct A-eigenvalues of G with multiplicities $\{l_1, l_2, \ldots, l_k\}$, then the spectrum of A(G) can be expressed as:

$$Sp(A(G)) = \begin{pmatrix} \lambda_1 & \lambda_2 & \dots & \lambda_k \\ l_1 & l_2 & \dots & l_k \end{pmatrix}$$

For any graph G, the graph energy is mathematically expressed as:

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \tag{3.2}$$

The comprehensive survey by Gutman and Ramane [5] delves into the intricacies of graph energy, and additional discourse on the topic can be found in references [10, 8, 1, 4].

Here, we introduce the first eccentric-degree energy of a simple graph G. as follows. The first eccentric-degree adjacency matrix of G is the $n \times n$ matrix $A_{ED_1} = (a_{ij})$ where

$$a_{ij} = \begin{cases} 0 : if \ i = j, \\ e_i d_i + e_j d_j : if \ v_i \sim v_j, \\ 0 : otherwise. \end{cases}$$
(3.3)

The eigenvalues of the graph G are the eigenvalues of A_{ED_1} . Since A_{ED_1} is real and symmetric, its eigenvalues are real numbers which are denoted by $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$, where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_n$. Then the first eccentric-degree energy of G is defined as:

$$E_{ED_1}(G) = \sum_{i=1}^{n} |\lambda_i|$$
 (3.4)

Since A_{ED_1} is a real and symmetric matrix, we have

$$\sum_{i=1}^{n} |\lambda_i| = tr(A_{ED_1}) = 0 \tag{3.5}$$

And

$$\sum_{i=1}^{n} \lambda_i^2 = tr(A_{ED_1}^2) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2 = 2 \sum_{i \sim j} (e_i d_i + e_j d_j)^2$$
(3.6)

In this section, we obtain upper and lower bounds for $E_{ED_1}(G)$.

Theorem 3.1. Let G be a simple graph of order n with no isolated vertices. Then

$$E_{ED_1}(G) \le \sqrt{2n \sum_{i \sim j} (e_i d_i + e_j d_j)^2}$$
 (3.7)

Proof. Let $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$ be the eigenvalues of A_{ED_1} . Then using Eqn, (3.6) and the Cauchy-Schwarz inequality, we have:

$$\left(\sum_{i=1}^n a_i b_i\right)^2 \le \left(\sum_{i=1}^n a_i^2\right) \cdot \left(\sum_{i=1}^n b_i^2\right),$$

Let $a_i = 1$ and $b_i = |\lambda_i|$. Applying this inequality, we obtain:

$$E_{ED_1}(G) = \sum_{i=1}^n |\lambda_i| \le \sqrt{\left(\sum_{i=1}^n |\lambda_i|^2\right)}.$$

Using the fact that the sum of squares of the eigenvalues is related to the trace of the matrix, we get:

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$$E_{ED_1}(G) \le \sqrt{n \sum_{i=1}^n \lambda_i^2} = \sqrt{2n \sum_{i \sim j} (e_i d_i + e_j d_j)^2}.$$

Theorem 3.2. Let G be a simple graph of order n with no isolated vertices. Then

$$E_{ED_1}(G) \ge 2\sqrt{\sum_{i \sim j} (e_i d_i + e_j d_j)^2}$$
 (3.8)

Proof. From Eqn. (3.5), we have

$$\sum_{i=1}^{n} \lambda_i^2 + 2 \sum_{1 \le i \le j \le n} \lambda_i \lambda_j = 0.$$

Therefore,

$$-\sum_{i=1}^{n} \lambda_i^2 = 2 \sum_{1 \le i \le j \le n} \lambda_i \lambda_j.$$
(3.9)

Thus,

$$(E_{ED_1}(G))^2 = \left(\sum_{i=1}^n |\lambda_i|\right)^2 = \sum_{i=1}^n \lambda_i^2 + 2 \sum_{1 \le i \le j \le n} |\lambda_i \lambda_j|.$$

$$\geq \sum_{i=1}^n \lambda_i^2 + 2 \left|\sum_{1 \le i \le j \le n} \lambda_i \lambda_j\right|.$$

$$= 2 \sum_{i=1}^n \lambda_i^2, \text{ on using (3.9).}$$
(3.10)

Using Eqn. (3.10) together with Eqn. (3.6), we obtain

$$(E_{ED_1}(G))^2 \ge 4 \sum_{i \sim j} (e_i d_i + e_j d_j)^2.$$

Thus,

$$E_{ED_1}(G) \ge 2\sqrt{\sum_{i \sim j} (e_i d_i + e_j d_j)^2}.$$

4. First eccentric-degree energy of some graphs

Theorem 4.1. The First eccentric-degree energy of the complete bipartite graph $K_{m,n}$ is $4(m+n)\sqrt{mn}$.

Proof. Let the vertex set of the complete bipartite graph $K_{m,n}$ be $V(K_{m,n}) = \{u_1, u_2, \ldots, u_m, v_1, v_2, \ldots, v_n\}$. Then the first eccentric-degree matrix of the complete bipartite graph is given by:

Its characteristic polynomial is

$$|\lambda I - A_{ED_1}| = \begin{vmatrix} \lambda & 0 & \cdots & 0 & -2(m+n) & -2(m+n) & \cdots & -2(m+n) \\ 0 & \lambda & \cdots & 0 & -2(m+n) & -2(m+n) & \cdots & -2(m+n) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda & -2(m+n) & -2(m+n) & \cdots & -2(m+n) \\ -2(m+n) & -2(m+n) & \cdots & -2(m+n) & \lambda & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -2(m+n) & -2(m+n) & \cdots & -2(m+n) & 0 & 0 & \cdots & \lambda \end{vmatrix}$$

This can be written as:

$$|\lambda I - A_{ED_1}| = \begin{vmatrix} \lambda I_m & -2(m+n)J \\ -2(m+n)J^T & \lambda I_n \end{vmatrix}$$

where J is an $n \times m$ matrix with all entries equal to 1. Hence the characteristic equation is:

$$\begin{vmatrix} \lambda I_m & -2(m+n)J \\ -2(m+n)J^T & \lambda I_n \end{vmatrix} = 0$$

which can be written as:

$$\left|\lambda I_m\right| \left|\lambda I_n - \left(-2(m+n)J\right)\frac{I_m}{\lambda}\left(-2(m+n)J^T\right)\right| = 0$$

$$\left|\lambda I_{m}\right|\left|\lambda I_{n}-\left(-aJ\right)\frac{I_{m}}{\lambda}\left(-aJ^{T}\right)\right|=0$$

On simplification, we obtain:

$$\lambda^{m+n-2} \cdot a^2 \left(\frac{\lambda^2}{a^2} - mn\right) = 0$$
$$\lambda^{m+n-2} \left(\lambda^2 - a^2 mn\right) = 0$$

where a = 2(m+n).

Therefore, the spectrum of $K_{m,n}$ is:

Spec
$$(K_{m,n}) = \begin{pmatrix} 0 & -2(m+n)\sqrt{mn} & 2(m+n)\sqrt{mn} \\ m+n-2 & 1 & 1 \end{pmatrix}$$

Hence, the first eccentric-degree energy of the complete bipartite graph is:

$$E_{ED_1}(K_{m,n}) = 4(m+n)\sqrt{mn}$$

Theorem 4.2. The First eccentric-degree energy of complete graph K_n is $4(n-1)^2$. *Proof.* Let the vertex set of complete graph be $V(K_n) = \{v_1, v_2, ..., v_n\}$. Then the first eccentric-degree energy of the complete graph K_n is given by

$$A_{ED_1} = \begin{pmatrix} 0 & 2(n-1) & 2(n-1) & \cdots & 2(n-1) \\ 2(n-1) & 0 & 2(n-1) & \cdots & 2(n-1) \\ 2(n-1) & 2(n-1) & 0 & \cdots & 2(n-1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(n-1) & 2(n-1) & 2(n-1) & \cdots & 0 \end{pmatrix}$$

Hence the characteristic polynomial is given by

$$|\lambda I - A_{ED_1}| = = \begin{vmatrix} \lambda & -2(n-1) & -2(n-1) & \cdots & -2(n-1) \\ -2(n-1) & \lambda & -2(n-1) & \cdots & -2(n-1) \\ -2(n-1) & -2(n-1) & \lambda & \cdots & -2(n-1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -2(n-1) & -2(n-1) & -2(n-1) & \cdots & \lambda \end{vmatrix}$$

$$= (2(n-1))^{n} \begin{vmatrix} \mu & -1 & -1 & \cdots & -1 \\ -1 & \mu & -1 & \cdots & -1 \\ -1 & -1 & \mu & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & \mu \end{vmatrix} \qquad \left(where \ \mu = \frac{\lambda}{2(n-1)} \right)^{n}$$
$$|\lambda I - A_{ED_{1}}| = \phi_{n}(\mu) \ (2(n-1))^{n} \qquad (4.1)$$

Then

where

$$\phi_n(\mu) = \begin{vmatrix} \mu & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & \mu & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & \cdots & \mu & -1 \\ -1 & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & \mu & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & \cdots & \mu & -1 \\ 0 & 0 & 0 & 0 & \cdots & -1 - \mu & \mu + 1 \end{vmatrix}$$

$$= (\mu + 1) \begin{vmatrix} \mu & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & \mu & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & \cdots & \mu & -1 \\ -1 & -1 & -1 & -1 & \cdots & -1 & -1 \end{vmatrix}$$
$$+ (\mu + 1) \begin{vmatrix} \mu & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & \mu & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & \cdots & \mu & -1 \\ -1 & -1 & -1 & -1 & \cdots & -1 & \mu \end{vmatrix}$$

$$= (\mu+1) \begin{vmatrix} \mu & -1 & -1 & -1 & \cdots & -1 & -1 \\ -1 & \mu & -1 & -1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & \cdots & \mu & -1 \\ -1 & -1 & -1 & -1 & \cdots & -1 & -1 \end{vmatrix} + (\mu+1) \phi_{n-1}(\mu)$$

Iterating this, we obtain

$$\phi_n(\mu) = (\mu + 1)^{n-1} (\mu - (n-1)) \tag{4.2}$$

substitute (4.2) in (4.1) we get,

$$|\lambda I - A_{ED_1}| = (\mu + 1)^{n-1} (\mu - (n-1))(2(n-1))^n$$

Characteristic equation is given by

$$(\mu+1)^{n-1}(\mu-(n-1))(2(n-1))^n = 0$$

Hence

$$Spec(K_n) = \begin{pmatrix} -2(n-1) & 2(n-1)^2 \\ n-1 & 1 \end{pmatrix}$$

Hence the first eccentric-degree energy of K_n is

$$E_{ED_1}(K_n) = 4(n-1)^2$$

Conclusion

In this work, we present a new topological indexcalled the first eccentric degree index, which expands on the traditional definition of eccentricity to describe graph structural characteristics in terms of vertex degrees. We meticulously determined the this indexfor several graph families, such as the friendship, crown, wheel, complete graph, and complete bipartite graph. Simultaneously, we determined the first eccentric degree energy that corresponds to the aforementioned index and set potential bounds for this energy across different graph classes. We demonstrated its usefulness in quantifying graph energy in relation to the first eccentric degree index by computing the first eccentric degree energy for both the completegraph and the complete bipartite graph.

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