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The Maximum Edge Eccentricity Energy of a Graph

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Abstract This paper presents a new concept in graph theory, focusing on a connected graph's edge eccentricity. We define a new matrix, the maximum edge eccentricity matrix $M_{e_e}(\Upsilon)$, which represents the maximum edge distance between all pairs of edges in the graph. This matrix is derived from the graph's structure and the eccentricity values of its edges. Our work explores the characteristics of this matrix, including the determination of specific coefficients within its characteristic polynomial, denoted as $P(\Upsilon, \nu)$. Furthermore, we introduce the concept of maximum edge eccentricity energy $M_{e_e}(\Upsilon)$ for connected graphs and provide calculations for well-known graphs. We establish upper and lower bounds for $E_{M_{e_e}}(\Upsilon)$ and prove that if the maximum edge eccentricity energy of a graph is rational, it must be an even number.

Keywords Edge distance in the graph · Edge eccentricity in the graph · Maximum edge eccentricity matrix · Maximum edge eccentricity eigenvalue · Maximum edge eccentricity energy of a graph

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1 Introduction

The spectral graph theory explores the relationship between graphs and their associated matrices. By analyzing the spectra of matrices like the adjacency

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matrix and Laplacian matrix, valuable insights into the graph's properties can be revealed. This approach borrows the concept of energy from chemistry, where it estimates the total π-electron energy in molecules. In molecular graphs, carbon atoms are vertices, and carbon-carbon bonds are edges, with hydrogen atoms omitted. The eigenvalues of these molecular graphs correspond to electron energy levels. A key focus in Hückel theory is the total π-electron energy, which is the sum of individual electron energies in a molecule.

The concept of graph energy, introduced in the 1940s [7], involves analyzing the eigenvalues of a graph's adjacency matrix. Given a simple graph G with vertices $\{v_1, v_2, \ldots, v_n\}$, the adjacency matrix $A(G)$ is an $n \times n$ matrix with entries a_{ij} indicating vertex connections. The eigenvalues of $A(G)$, denoted as $\lambda_1, \lambda_2, \ldots, \lambda_n$, are ordered non-increasingly and represent the graph's eigenvalues. The energy $E(G)$ is the sum of the absolute values of these eigenvalues [10]. Building on related work [1,14], essential definitions and notations are presented for further discussion.

Throughout this research, we will consider graphs to be simple, finite, and connected. A graph $\Upsilon = (V, E)$ is defined as a simple graph, devoid of loops, multiple edges, or directed edges. We use the standard notation $n = |V|$ and $m = |E|$ to represent the number of vertices and edges in a graph Υ, respectively. The following definitions are introduced, drawing from references [1,5]. For a given edge $e \in E$ its open neighborhood, denoted as $N(e)$, encompasses all adjacent edges, while its closed neighborhood is expressed as $N(e) = N(e) \cup \{e\}$. The degree of an edge e in Υ, denoted as $d(e)$, equals the size of its open neighborhood, $|N(e)|$. A graph Υ is classified as a k-regular graph if the degree of every vertex v in Υ is k, i.e., $d(v) = k$. The edge distance between two edges e and e' in Υ, denoted as $d(e, e')$, is the minimum number of edges connecting them. The eccentricity of an edge e in Υ, denoted as $e(e)$, is calculated as the maximum edge distance between e and any other edge e' in Υ, i.e., $e(e) = \max\{d(e, e'); e' \in E(\Upsilon)\}$. The edge radius of Υ, $r_e(\Upsilon)$, is defined as the minimum eccentricity among all edges in Υ, $r_e(\Upsilon) = \min\{e(e) : e \in E(\Upsilon)\}$, while the edge diameter, $D_e(\Upsilon)$, is the maximum eccentricity, $D_e(\Upsilon) = \max\{e(e) : e \in E(\Upsilon)\}$. Consequently, for every edge e in Υ, we have $r_e(\Upsilon) \le e(e) \le D_e(\Upsilon)$. An edge e in a connected graph Υ is considered a central edge if its eccentricity matches the edge radius, i.e., $e(e) = r_e(\Upsilon)$. Furthermore, Υ is referred to as an edge self-centered graph if the eccentricity of every edge e equals both the edge radius and edge diameter, i.e., $e(e) = r_e(\Upsilon) = D_e(\Upsilon)$.

In graph theory, we use the symbols K_n, C_n, S_n, P_n and $K_{m,n}$ to represent specific types of graphs: complete, cycle, star, path, and complete bipartite graphs, respectively. We refer to standard literature [3,6,11] for graph theory foundations and additional references [2,4,8,9,12,13,15,16] for supplementary concepts. Given a simple graph Υ with n vertices labeled $v_1, v_2, \ldots, v_n$, we define its maximum degree matrix $M(\Upsilon)$, where

$$d_{ij} = \begin{cases} \max\{d(v_i), d(v_j)\}, & \text{if } v_i v_j \in E(\Upsilon), \\ 0, & \text{otherwise.} \end{cases}$$

This matrix $M(\Upsilon)$ exhibits a real symmetric nature with zero traces, implying that its eigenvalues are real and sum up to zero. We extend this concept by presenting the maximum edge eccentricity matrix $M_{e_e}(\Upsilon)$ for a connected graph Υ, deriving coefficients for its characteristic polynomial $P(\Upsilon, \nu)$. Furthermore, we establish the notion of maximum eccentricity energy, denoted as $E_{M_{e_e}}(\Upsilon)$, associated with a connected graph Υ.

2 Maximum edge eccentricity energy of graph

Definition 1 For an edge e_i of Υ, the edge eccentricity is

$$e(e_i) = \max\{d(e_i, e_j); e_j \in E(\Upsilon)\},$$

that the edge distance $d(e_i, e_j)$ in a graph Υ is the minimum number of edges between e_i and e_j.

Let $\Upsilon(V, E)$ be a simple connected graph with m edge $e_1, e_2, \ldots, e_m$ and let $e(e_i)$ be the eccentricity of edge e_i, $i = 1, 2, \ldots, m$. The Maximum edge eccentricity matrix of Υ defining as,

$$M_{e_e}(\Upsilon) = \begin{pmatrix} e^*_{11} & e^*_{12} & \cdots & e^*_{1m} \\ e^*_{21} & e^*_{22} & \cdots & e^*_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ e^*_{m1} & e^*_{m2} & \cdots & e^*_{mm} \end{pmatrix},$$

where

$$e^*_{ij} = \begin{cases} \max\{e(e_i), e(e_j)\}, & \text{if } e_i, e_j \text{ are adjacent and } i \neq j, \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of the maximum edge eccentricity matrix $M_{e_e}(\Upsilon)$ is defined by $P(\Upsilon, \nu) = det(\nu I - M_{e_e}(\Upsilon))$. Where I is the identity matrix of order m. The maximum edge eccentricity eigenvalues of Υ are the eigenvalues of $M_{e_e}(\Upsilon)$. Since $M_{e_e}(\Upsilon)$ is real and symmetric with zero traces, then its eigenvalues are real numbers with sum equals to zero. We label them in non-increasing order $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_m$. The maximum edge eccentricity energy of a graph Υ is defined as

$$E_{M_{e_e}}(\Upsilon) = \sum_{i=1}^{m} |\nu_i|.$$

To clarify this concept, let's examine a specific example.

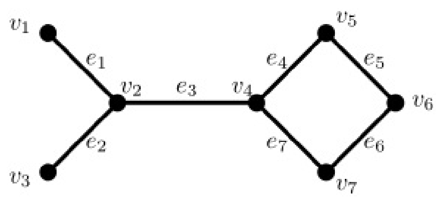

Fig. 1 graph $\varUpsilon_1$

Example 1 let $\varUpsilon_1$ be a graph in figure 1, with 7 edge $e_1, e_2, e_3, e_4, e_5, e_6$ and e_7. The edge distance matrix of $\varUpsilon_1$ is

$$M_{e_e}(\varUpsilon_1) = \begin{pmatrix} 0 & 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & 2 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 2 \\ 0 & 0 & 1 & 1 & 0 & 2 & 0 \end{pmatrix},$$

The characteristic polynomial of $M_{e_e}(\varUpsilon_1)$ is

$$P(\varUpsilon_1, \nu) = det(\nu I - M_{e_e}(\varUpsilon_1)) = \nu^7 - 27\nu^5 - 18\nu^4 + 184\nu^3 + 208\nu^2 - 112\nu - 32.$$

The maximum edge eccentricity eigenvalues of $\varUpsilon_1$ are

$$\begin{array}{lll} \nu_1 = -3.5616, & \nu_2 = -2.5251, & \nu_3 = -2, \\ \nu_4 = -0.2159, & \nu_5 = 0.5616, & \nu_6 = 3.3159, \\ \nu_7 = 4.4251. & & \end{array}$$

So, the maximum edge eccentricity energy of $\varUpsilon_1$ is

$$E_{M_{e_e}}(\varUpsilon_1) = 16.6052.$$

Properties of maximum edge eccentricity energy

In this section, we obtain the values of some coefficients of the characteristic polynomial of the maximum edge eccentricity matrix and investigate some properties of maximum edge eccentricity of a graph $\varUpsilon$.

Theorem 1 *Let Υ be a graph of order m and let*

$$P(\Upsilon,\nu) = c_0\nu^m + c_1\nu^{m-1} + c_2\nu^{m-2} + \cdots + c_m,$$

be the characteristic polynomial of maximum edge eccentricity matrix of Υ. Then

(i) $c_0 = 1$,
(ii) $c_1 = 0$,
(iii) $c_2 = -\sum_{1\le i<j\le m} (e^*_{ij})^2$,
(iv) $c_3 = -2\sum_{1\le i<j<k\le m} e^*_{ij}e^*_{ik}e^*_{jk}$,
(v) $c_m = (-1)^m det(M_{e_e})$.

Proof
(i) Directly from the definition of $P(\Upsilon,\nu)$, it follows that $c_0 = 1$.
(ii) Since the trace of $M_{e_e}(\Upsilon)$ is always zero.
(iii) $(-1)^2c_2$ is equal to the sum of determinants of all the 2×2 principal submatrices of $M_{e_e}(\Upsilon)$, that is

$$\begin{aligned} c_2 = \sum_{1\le i<j\le m} \begin{vmatrix} e^*_{ii} & e^*_{ij} \\ e^*_{ji} & e^*_{jj} \end{vmatrix} &= \sum_{1\le i<j\le m} (e^*_{ii}e^*_{jj} - e^*_{ij}e^*_{ji}) \\ &= \sum_{1\le i<j\le m} e^*_{ii}e^*_{jj} - \sum_{1\le i<j\le m} (e^*_{ij})^2 \\ &= 0 - \sum_{1\le i<j\le m} (e^*_{ij})^2 \\ &= -\sum_{1\le i<j\le m} (e^*_{ij})^2. \end{aligned}$$

(iv)

$$\begin{aligned} c_3 &= (-1)^3 \sum_{1\le i<j<k\le m} \begin{vmatrix} e^*_{ii} & e^*_{ij} & e^*_{ik} \\ e^*_{ji} & e^*_{jj} & e^*_{jk} \\ e^*_{ki} & e^*_{kj} & e^*_{kk} \end{vmatrix} \\ &= -\sum_{1\le i<j<k\le m} [e^*_{ii}(e^*_{jj}e^*_{kk} - e^*_{kj}e^*_{jk}) - e^*_{ij}(e^*_{ji}e^*_{kk} - e^*_{ki}e^*_{jk}) + e^*_{ik}(e^*_{ji}e^*_{kj} - e^*_{ki}e^*_{jj})] \\ &= -\sum_{1\le i<j<k\le m} e^*_{ii}e^*_{jj}e^*_{kk} + \sum_{1\le i<j<k\le m} [e^*_{ii}(e^*_{jk})^2 + e^*_{jj}(e^*_{ik})^2 + e^*_{kk}(e^*_{ij})^2] \\ &- \sum_{1\le i<j<k\le m} e^*_{ij}e^*_{jk}e^*_{ki} - \sum_{1\le i<j<k\le m} e^*_{ik}e^*_{kj}e^*_{ji} \\ &= -0 + 0 - 2\sum_{1\le i<j<k\le m} e^*_{ij}e^*_{ik}e^*_{jk}, \end{aligned}$$

thus

$$c_3 = -2 \sum_{1 \le i < j < k \le m} e^*_{ij} e^*_{ik} e^*_{jk}.$$

(v) The proof is obvious.

Theorem 2 *Let $\nu_1, \nu_2, \ldots, \nu_m$ be eigenvalues of the maximum edge eccentricity of $M_{e_e}(\Upsilon)$, then*

(i) $\sum\limits_{i=1}^{m} \nu_i = 0.$

(ii) $\sum\limits_{i=1}^{m} \nu_i^2 = 2 \sum\limits_{1 \le i < j < k \le m} (e^*_{ij})^2.$

(iii) $\sum\limits_{i=1}^{m} \nu_i^3 = 6 \sum\limits_{1 \le i < j < k \le m} e^*_{ij} e^*_{ik} e^*_{jk}.$

Proof The proof is the consequences of binomial expansions and Theorem 1.

Corollary 1 *let $\nu_1, \nu_2, \ldots, \nu_m$ be the eigenvalues of maximum edge eccentricity of a graph Υ, then*

(i) If $\Upsilon = K_n$, then $\sum\limits_{i=1}^{m} \nu_i^2 = n(n-1)(n-2),$

(ii) If $\Upsilon = C_n$, then $\sum\limits_{i=1}^{m} \nu_i^2 = 2mD_e^2(\Upsilon),$

(iii) If $\Upsilon = K_{m,n}$, then $\sum\limits_{i=1}^{m} \nu_i^2 = \sum\limits_{i=1}^{m} deg(e_i) = m \cdot deg(e),$

(iv) If $\Upsilon = S_n$, then $\sum\limits_{i=1}^{m} \nu_i^2 = 0,$ *and* $\sum\limits_{i=1}^{m} \nu_i^3 = \sum\limits_{i=1}^{m} \nu_i^4 = \cdots = \sum\limits_{i=1}^{m} \nu_i^j = 0,$ $j = 1, \ldots, m.$

Theorem 3 *Let Υ be an edge eccentricity set of a graph. Then*

$$E_{M_{e_e}}(\Upsilon) = 2 \sum \nu_r.$$

Proof Let $\nu_1, \nu_2, \ldots, \nu_r$ be positive eigenvalues, and the rest of the eigenvalues non-positive, so

$$E_{M_{e_e}}(\Upsilon) = \sum_{i=1}^{m} |\nu_i| = (\nu_1 + \nu_2 + \cdots + \nu_r) - (\nu_{r+1} + \nu_{r+2} + \cdots + \nu_m),$$

implying

$$E_{M_{e_e}}(\Upsilon) = 2(\nu_1 + \nu_2 + \cdots + \nu_r).$$

Since, $\nu_1, \nu_2, \cdots, \nu_r$ are algebraic integers, so is their sum. Hence,

$$E_{M_{e_e}}(\Upsilon) = 2 \sum \nu_r.$$

Theorem 4 *Let Υ be an edge eccentricity set of a complete graph. Then*

$$E_{M_{e_e}}(\Upsilon) = 2\sum \nu_r = 4(m-n).$$

Proof Let $\nu_1, \nu_2, \ldots, \nu_r$ be positive eigenvalues, and the rest of the eigenvalues non-positive, so

$$E_{M_{e_e}}(\Upsilon) = \sum_{i=1}^{m} |\nu_i| = (\nu_1 + \nu_2 + \cdots + \nu_r) - (\nu_{r+1} + \nu_{r+2} + \cdots + \nu_m),$$

implying

$$E_{M_{e_e}}(\Upsilon) = 2(\nu_1 + \nu_2 + \cdots + \nu_r),$$

Since, $\nu_1, \nu_2, \ldots, \nu_r$ are algebraic integers, so is their sum. Thus

$$E_{M_{e_e}}(\Upsilon) = 2\sum \nu_r = 2(2(m-n)) = 4(m-n).$$

Proposition 1 *If $\Upsilon = S_n$, then $E_{M_{e_e}}(\Upsilon) = \sum\limits_{i=1}^{m} |\nu_i| = 0$.*

Proof The proof is obvious.

Definition 2 A graph Υ is called an edge self-centered graph if

$$e(e) = r_e(\Upsilon) = D_e(\Upsilon),$$

for every edge $e \in E(\Upsilon)$.

Theorem 5 *If Υ is an edge self-centered k-regular graph with diameter D_e, then kD_e is a maximum edge eccentricity eigenvalue of Υ and*

$$E_{M_{e_e}}(\Upsilon) = D_e E(\Upsilon).$$

Proof Consider a graph Υ, which is edge self-centered and k-regular, with a diameter denoted as D_e. For any edge e in Υ, we have $e(e) = D_e$. From the definition of the edge eccentricity matrix $M_{e_e}(\Upsilon)$, we observe that each row contains K entries equal to D_e. By replacing the first raw of $det(\nu I - M_{e_e}(\Upsilon))$ by the sum of all raw, we find that $(\nu - kD_e)$ is a factor of this determinant. Consequently, kD_e is established as a maximum edge eccentricity eigenvalue of Υ. Given that Υ is an edge self-centered k-regular graph, we can deduce from the definitions of edge adjacency and maximum edge eccentricity matrices that $M_{e_e}(\Upsilon) = D_e A_e(\Upsilon)$. This leads to the conclusion that if ν_i is an eigenvalue of Υ, then $D_e \nu_i$ is a maximum edge eccentricity eigenvalue for all $1 \leq i \leq m$. As a result, $E_{M_{e_e}}(\Upsilon) = D_e E(\Upsilon)$.

Corollary 2 *If Υ is an edge self-centered k-regular graph with n vertices and diameter D_e, then $E_{M_{e_e}}(\Upsilon) = E(\Upsilon)$ for $n > 3$.*

Theorem 6 *If the maximum edge eccentricity energy of a graph Υ is rational, then it must be an even integer.*

Proof *Let Υ be a graph of order m and $\nu_1, \nu_2, \ldots, \nu_m$ be the maximum edge eccentricity eigenvalues of Υ. Since, $\sum_{i=1}^{m} \nu_i = 0$, then $\nu_1, \nu_2, \ldots, \nu_r$ be the positive eigenvalues of Υ and the remaining are non-positive. Then*

$$\begin{aligned} E_{M_{ee}}(\Upsilon) &= \nu_1 + \nu_2 + \cdots + \nu_r - (\nu_{r+1} + \nu_{r+2} + \cdots + \nu_m) \\ &= 2(\nu_1 + \nu_2 + \cdots + \nu_r). \end{aligned}$$

Since, $\nu_1, \nu_2, \ldots, \nu_r$ are algebraic numbers, so is their sum and so must be an integer if $E_{M_{ee}}$, is rational.

3 Bounds for maximum edge eccentricity energy

In this section, we established upper and lower bounds for the maximum edge eccentricity energy of a graph.

Theorem 7 *Let Υ be a connected graph of order $n \geq 2$ and size m and let $r_e(\Upsilon)$ and $D_e(\Upsilon)$ be the radius and the diameter of Υ respectively. Then*

$$r_e(\Upsilon)\sqrt{\sum_{i=1}^{m} dege_i} \leq E_{M_{ee}}(\Upsilon) \leq D_e(\Upsilon)\sqrt{m\sum_{i=1}^{m} dege_i}.$$

Proof *Consider the Cauchy-Schwarz inequality and Theorem 2, we get*

$$\begin{aligned} (E_{M_{ee}}(\Upsilon))^2 = \Big(\sum_{i=1}^{m} |\nu_i|\Big)^2 &\leq \Big(\sum_{i=1}^{m} 1\Big)\Big(\sum_{i=1}^{m} \nu_i\Big)^2 \\ &\leq m\Big(\ 2\sum_{1\leq i<j<k\leq m} (e^*_{ij})^2\Big) \\ &\leq m\Big(\ 2\sum_{i=1}^{m}(x_i + y_i)e^2(e_i)\Big). \end{aligned}$$

Since, $e(e) \leq D_e(\Upsilon)$, for every $e \in E(\Upsilon)$ and by $\sum_{i=1}^{m}(x_i + y_i) = \frac{1}{2}\sum_{i=1}^{m} deg(e_i)$ it follows that

$$E_{M_{ee}}(\Upsilon) \leq D_e(\Upsilon)\sqrt{m\sum_{i=1}^{m} dege_i}.$$

Now, since $(\sum_{i=1}^{m} |\nu_i|)^2 \geq \sum_{i=1}^{m} \nu_i^2$, it follows that

$$(E_{M_{ee}}(\Upsilon))^2 \geq 2\sum_{i=1}^{m}(x_i + y_i)e^2(e_i).$$

Since, $e(e) \geq r_e(\Upsilon)$ for every $e \in E(\Upsilon)$, then

$$E_{M_{e_e}}(\Upsilon) \geq r_e(\Upsilon)\sqrt{\sum_{i=1}^{m} dege_i}.$$

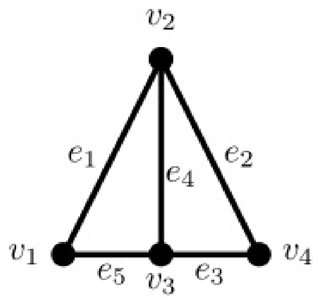

Fig. 2 graph Υ_2

Example 2 Let Υ_2 be the graph in figure 2, with 5 edge e_1, e_2, e_3, e_4 and e_5. The maximum edge eccentricity matrix of Υ_2 is

$$M_{e_e}(\Upsilon_2) = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$

The characteristic polynomial of $M_{e_e}(\Upsilon_2)$ is

$$P(\Upsilon_2, \nu) = det(\nu I - M_{e_e}(v_2)) = \begin{vmatrix} \nu & -1 & 0 & -1 & -1 \\ -1 & \nu & -1 & -1 & 0 \\ 0 & -1 & \nu & -1 & -1 \\ -1 & -1 & -1 & \nu & -1 \\ -1 & 0 & -1 & -1 & \nu \end{vmatrix} = \nu^5 - 8\nu^3 - 8\nu^2.$$

The maximum edge eccentricity eigenvalues of Υ_2 are

$\nu_1 = -2,$ $\nu_2 = -1.2361,$ $\nu_3 = 0,$
$\nu_4 = 0,$ $\nu_5 = 3.2361.$

The maximum edge eccentricity energy of (Υ_2) is $E_{M_{e_e}}(\Upsilon_2) = 6.4722$. In this graph $r_e(\Upsilon) = 0$, $D_e(\Upsilon) = 1$ and $\sum_{i=1}^{5} dege_i = 16$. So,

$$0 \leq EM_{e_e}(\Upsilon) \leq \sqrt{5 \times 16} \quad \Rightarrow 0 \leq 6.4722 \leq 8.9443.$$

4 Conclusion

This research presents a new concept, the maximum edge eccentricity matrix $M_{e_e}(\Upsilon)$, for connected graphs. $M_{e_e}(\Upsilon)$ is derived from the graph's structure and edge eccentricities. We have calculated specific coefficients of the characteristic polynomial of $M_{e_e}(\Upsilon)$. For a connected edge self-centered k-regular graph with diameter D_e, M_{e_e} is equivalent to D_e times the edge adjacency matrix $A_e(\Upsilon)$. Our focus extends to exploring the mathematical properties of the maximum edge eccentricity energy $E_{M_{e_e}}(\Upsilon)$ of graphs. We prove that in an edge self-centered k-regular graph with diameter D_e, kD_e is a maximum edge eccentricity eigenvalue. Additionally, we establish upper and lower limits for $E_{M_{e_e}}$. Interestingly, we demonstrate that if $E_{M_{e_e}}$ is rational, it must be an even integer. The characteristic polynomial of the maximum edge matrix, as discussed in this paper, offers a valuable tool for investigating Laplacian and signless Laplacian variations of the issue. This concept is further explored in the literature, specifically in the study of digraph characteristic polynomials. Moreover, the maximum edge energy concept presented here could find practical use in chemistry and other fields.

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