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Some properties of maximum deficiency energy of a graph

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Abstract

The concept of maximum deficiency matrix $M_{df}(G)$ of a simple graph G is introduced in this paper. Let $G = (V, E)$ be a simple graph of order n and let $df(v_i)$ be the deficiency of a vertex v_i, $i = 1, 2, \dots, n$, then the maximum deficiency matrix $M_{df}(G) = [f_{ij}]_{n\times n}$ is defined as:

$$f_{ij} = \begin{cases} max\{df(v_i), df(v_j)\}, & \text{if } v_iv_j \in E(G) \\ 0 \qquad\qquad\qquad\qquad\quad , & \text{otherwise.} \end{cases}$$

Further, some coefficients of the characteristic polynomial $\phi(G; \gamma)$ of the maximum deficiency matrix of G are obtained. The maximum deficiency energy $EM_{df}(G)$ of a graph G is also introduced. The bounds for $EM_{df}(G)$ are established. Moreover, maximum deficiency energy of some standard graphs is shown, and if the maximum deficiency energy of a graph is rational, then it must be an even integer.

Keywords: Deficiency, maximum deficiency matrix, maximum deficiency eigenvalues, maximum deficiency energy.

MSC 2020: 05C50.

1 Introduction

In this paper, it is assumed that all graphs are simple, finite and undirected. Let $v_1, v_2, \dots, v_n$ be vertices of graph G, then number of edges incident to vertex v is called the degree and denoted by $d(v)$. The set of vertices adjacent to v is called neighbourhood of v and denoted by $N(v)$.

Let G be a graph with maximum degree r and vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. Then deficiency is $df(v_i) = r - d(v_i)$. We define the following two measures, α_j and β_j, that will be used throughout the paper:

$\alpha_j = |\{u \in N(v_j) : df(u) < df(v_j),\ 1 \leq j \leq n\}|$

$\beta_j = |\{u_k \in N(v_j), k > j : df(u_k) = df(v_j),\ 1 \leq j \leq n\}|$.

I. Gutman [5] proposed, for the first time, that the energy of a graph G is defined as $\mathcal{E}(G) = \sum_{j=1}^{n} |\gamma_j|$, where $\gamma_1, \gamma_2, \dots, \gamma_n$ are the eigenvalues of the adjacency matrix of G. The theory of energy emerges from chemical sciences. In theoretical chemistry, the π-electron energy E in Huckel theory is the sum of the energies of all electrons in a molecule. Now-a-days the concept of graph energy is much studied in the mathematics literature ([7], [2], [11], [10], [6], [1], [9]).

Let G be a graph with vertices $v_1, v_2, \dots, v_n$ and let $d(v_i)$ be the degree of v_i, then the maximum degree matrix $M(G) = [d_{ij}]_{n \times n}$ is defined as

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

Now, the maximum degree energy of a graph G is defined as $EM(G) = \sum_{j=1}^{n} |\gamma_j|$, where $\gamma_1, \gamma_2, \dots, \gamma_n$ are the eigenvalues of the maximum degree matrix of G.

Let G be a graph with vertices $v_1, v_2, \dots, v_n$ and let $e(v_i)$ be the eccentricity of v_i, which is the maximum number of edges required to connect v_i to other vertices (or infinity in a disconnected graph), then the maximum eccentricity matrix $M_e(G) = [e_{ij}]_{n \times n}$ is defined as

$$e_{ij} = \begin{cases} max\{e(v_i), e(v_j)\}, & \text{if } v_i v_j \in E(G) \\ 0 \qquad\qquad\qquad\quad , & \text{otherwise.} \end{cases}$$

The maximum eccentricity energy of a graph G is defined as $EM_e(G) = \sum_{j=1}^{n} |\gamma_j|$, where $\gamma_1, \gamma_2, \dots, \gamma_n$ are the eigenvalues of the maximum eccentricity matrix of G.

Got motivated by the maximum degree energy [1] and maximum eccentricity energy [9], the concept of maximum deficiency energy has been introduced and studied in the following sections.

2 The maximum deficiency energy of graphs

It is assumed that $G = (V, E)$ is a simple graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, and let $df(v_i)$ be the deficiency of a vertex v_i. Then, the maximum deficiency matrix $M_{df}(G) = [f_{ij}]_{n\times n}$ is defined as:

$$f_{ij} = \begin{cases} max\{df(v_i), df(v_j)\}, & \text{if } v_iv_j \in E(G) \\ 0 \qquad\qquad\qquad\quad, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of the maximum deficiency matix $M_{df}(G)$ will be

$$\begin{aligned} \phi(G;\gamma) &= det(\gamma I - M_{df}(G)) \\ &= \gamma^n + c_1\gamma^{n-1} + c_2\gamma^{n-2} + \cdots + c_n, \end{aligned}$$

where I is the identity matrix of order n. Suppose $\gamma_1, \gamma_2, \ldots, \gamma_n$ are roots of $\phi(G;\gamma) = 0$ which have been presumed to be in non-increasing order. These roots are the eigenvalues of the given matrix $M_{df}(G)$ and termed as the maximum deficiency eigenvalues of G.

The maximum deficiency energy of a graph G is defined as

$$EM_{df}(G) = \sum_{j=1}^{n} |\gamma_j|.$$

The above formulation suggests that $M_{df}(G)$ is a real and symmetric matrix with trace zero, and its eigenvalues are real numbers with sum equal to zero.

Remark 2.1. *The adjacency energy $\mathcal{E}(G)$, maximum degree energy $EM(G)$, maximum eccentricity energy $EM_e(G)$, and maximum deficiency energy $EM_{df}(G)$ are all well-defined for unlabeled graphs.*

Theorem 2.2. *Let G be a regular graph, then maximum deficiency energy $EM_{df}(G)$ is zero.*

Proof. Let G be a r-regular graph. We know that deficiency of every vertex in regular graph is always zero. Therefore, the maximum deficiency matrix is zero matrix and each eigen value of the matrix $M_{df}(G)$ is zero. Hence, maximum deficiency energy $EM_{df}(G)$ is zero. $\square$

Example 2.3. *If G_1 is a graph in Figure 1,*

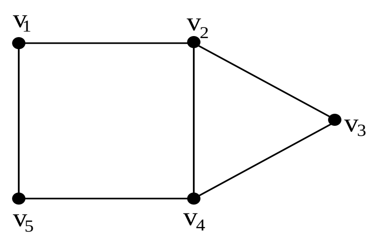

Figure 1. Graph G_1

then the maximum deficiency matrix of G_1 is

$$M_{df}(G_1) = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

The characteristic polynomial of $M_{df}(G_1)$ is

$$\phi(G_1;\gamma) = det(\gamma I - M_{df}(G_1))$$

$$= \begin{vmatrix} \gamma & -1 & 0 & 0 & -1 \\ -1 & \gamma & -1 & 0 & 0 \\ 0 & -1 & \gamma & -1 & 0 \\ 0 & 0 & -1 & \gamma & -1 \\ -1 & 0 & 0 & -1 & \gamma \end{vmatrix}$$

$$= \gamma^5 - 5\gamma^3 + 5\gamma - 2.$$

Then the maximum deficiency eigenvalues of G_1 are

$\gamma_1 = \gamma_2 = -1.618034,\ \gamma_3 = \gamma_4 = 0.618034, \gamma_5 = 2.$
Therefore,
Maximum deficiency energy $EM_{df}(G_1) = 6.472136.$
Adjacency energy $\mathcal{E}(G_1) = 6.340172.$
Maximum degree energy $EM(G_1) = 18.288101.$
Maximum eccentricity energy $EM_e(G_1) = 12.68034.$

Example 2.4. *Suppose the graph in Figure 2 is* G_2*,*

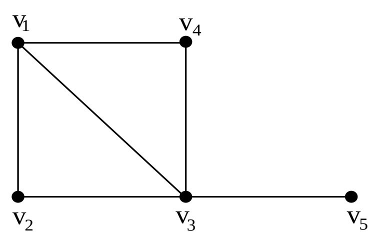

Figure 2. Graph G_2

then the maximum deficiency matrix of the graph G_2 *is*

$$M_{df}(G_2) = \begin{pmatrix} 0 & 2 & 1 & 2 & 0 \\ 2 & 0 & 2 & 0 & 0 \\ 1 & 2 & 0 & 2 & 3 \\ 2 & 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \end{pmatrix}.$$

The characteristic polynomial of $M_{df}(G_2)$ *is*

$$\phi(G_2;\gamma) = det(\gamma I - M_{df}(G_2))$$

$$= \begin{vmatrix} \gamma & -2 & -1 & -2 & 0 \\ -2 & \gamma & -2 & 0 & 0 \\ -1 & -2 & \gamma & -2 & -3 \\ -2 & 0 & -2 & \gamma & 0 \\ 0 & 0 & -3 & 0 & \gamma \end{vmatrix}$$

$$= \gamma^5 - 26\gamma^3 - 16\gamma^2 + 72\gamma.$$

Then the maximum deficiency eigenvalues of G_2 *are*
$\gamma_1 = -4.2821879,\ \gamma_2 = -2.2862586, \gamma_3 = 0, \gamma_4 = 1.4317057,$
$\gamma_5 = 5.1367409.$
Therefore,
Maximum deficiency energy $EM_{df}(G_2) = 13.1368931.$
Adjacency energy $\mathcal{E}(G_2) = 6.040894.$
Maximum degree energy $EM(G_2) = 21.92652.$
Maximum eccentricity energy $EM_e(G_2) = 12.081788.$

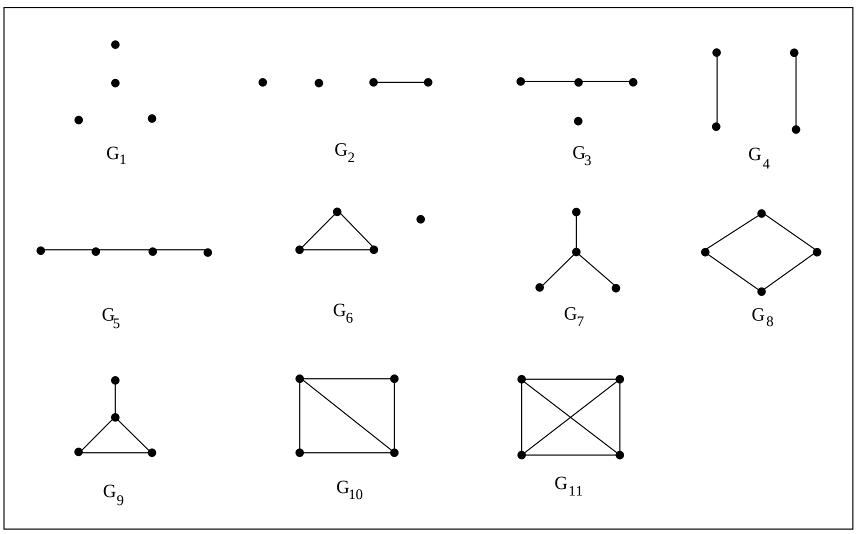

Figure 3. 11 Isomorphism classes of graphs of order 4

Table 1. Energies of isomorphism classes of graphs of order 4 as shown in Figure 3

	$\mathcal{E}(G)$	$EM(G)$	$EM_e(G)$	$EM_{df}(G)$
G_1	0	0	Not defined	0
G_2	2	2	Not defined	0
G_3	2.828427	5.656854	Not defined	2.828427
G_4	4	4	Not defined	0
G_5	4.472398	8.944796	12.649111	4
G_6	4	8	Not defined	0
G_7	3.464101	10.392303	6.928202	6.928202
G_8	4	8	8	0
G_9	4.962388	13.2915026	9.92477	6.646804
G_{10}	5.123105	15.369315	9.06226	4
G_{11}	6	18	6	0

We analyze from Table 1, in the connected graphs of order 4, the complete graph has the largest adjacency energy and the maximum degree energy, the path graph has the largest maximum eccentricity energy, while the star graph has the largest maximum deficiency energy. The maximum deficiency energy is not just complementary to maximum degree energy, since the non-regular graphs with smallest non-zero maximum deficiency energy do not always have large maximum degree energy.

3 Properties of maximum deficiency energy

In this section, the explicit expression for the coefficient c_i of γ^{n-i} $(i = 0, 1, 2, 3)$ in the characteristic polynomial $\phi(G;\gamma)$ of the maximum deficiency matrix $M_{df}(G)$ has been rendered. In addition to this, some properties of maximum deficiency eigenvalues of a graph G have been investigated.

Theorem 3.1. *If G is a simple graph of order n and $\phi(G;\gamma)$ =*

$c_0\gamma^n + c_1\gamma^{n-1} + c_2\gamma^{n-2} + \ldots + c_n$ is the characteristic polynomial of the maximum deficiency matrix of G, then,

(i) $c_0 = 1$.

(ii) $c_1 = 0$.

(iii) $c_2 = -\sum_{j=1}^{n}(\alpha_j + \beta_j)df^2(v_j)$.

(iv) $c_3 = -2\sum_{\substack{\Delta v_i v_j v_k \\ df(v_i)\leq df(v_j)\leq df(v_k)}} df^2(v_k)df(v_j)$.

Proof. The proof is similar to Theorem 2.1 in [1]. □

Remark 3.2. (a) *The sum $\sum_{j=1}^{n}(\alpha_j + \beta_j)$ represents the total number of edges in the graph G.*

(b) *The total number of terms in the sum*

$$\sum_{\substack{\Delta v_i v_j v_k \\ df(v_i)\leq df(v_j)\leq df(v_k)}} df^2(v_k)df(v_j)$$

is equal to the number of triangles in the graph G.

(c) *$c_3 = 0$ if and only if the graph is a triangle-free graph.*

(d) *$c_n = 0$ if and only if $M_{df}(G)$ is singular.*

Example 3.3. *For the graph G_1 in Figure 1, the coefficient c_2 of γ^3 in $\phi(G_1;\gamma)$ is equal to*

$$-\sum_{j=1}^{5}(\alpha_j + \beta_j)df^2(v_j)$$

$$= -[(1+1)1^2 + (0+1)0^2 + (2+0)1^2 + (0+0)0^2 + (1+0)1^2]$$

$$= -5.$$

Example 3.4. *For the graph G_2 in Figure 2, the coefficient c_2 of γ^3 in $\phi(G_2;\gamma)$ is equal to*

$$-\sum_{j=1}^{5}(\alpha_j+\beta_j)df^2(v_j)$$

$$=-[(1+0)1^2+(2+0)2^2+(0+0)0^2+(2+0)2^2+(1+0)3^2]$$

$$=-[1+8+8+9]$$

$$=-26.$$

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Theorem 3.5. *Let G be a graph of order n and $\gamma_1,\gamma_2,\gamma_3,\ldots,\gamma_n$ be the maximum deficiency eigenvalues of $M_{df}(G)$. Then*

(i) $\sum_{j=1}^{n}\gamma_j=0.$

(ii) $\sum_{j=1}^{n}\gamma_j^2=-2c_2.$

(iii) $\sum_{j=1}^{n}\gamma_j^3=-3c_3.$

Proof. The proof is based on the outcomes of Newton's identity [8] and Theorem 3.1. □

Remark 3.6. *The sum of the cubes of maximum deficiency eigenvalues is zero if and only if the graph is triangle free.*

Theorem 3.7. *If G is the complete bipartite graph $K_{m,n}$, $\gamma_1,\gamma_2,\gamma_3,\ldots,$ γ_{m+n} are its maximum deficiency eigenvalues and $m\le n$, then*

(i) $\sum_{j=1}^{m+n}\gamma_j^2=2mn(n-m)^2$

(ii) $\sum_{j=1}^{m+n}\gamma_j^3=0.$

Proof. (i) Consider $K_{m,n}$ be the complete bipartite graph with vertices $u_1,u_2,\ldots,u_m,v_1,v_2,\ldots v_n$.

By Theorem 3.5,

$$\sum_{j=1}^{n} \gamma_j^2 = 2\sum_{j=1}^{n} (\alpha_j + \beta_j) df^2(v_j).$$

For the graph $K_{m,n}$

$$\alpha_j = 0, \forall u_j, j = 1, 2, \ldots, m,$$

$$\alpha_j = m, \forall v_j, j = 1, 2, \ldots, n,$$

$$\beta_j = 0, \forall u_j, j = 1, 2, \ldots, m,$$

$$\beta_j = 0, \forall v_j, j = 1, 2, \ldots, n,$$

$$df(u_j) = 0, \forall u_j, j = 1, 2, \ldots, m,$$

$$df(v_j) = n - m, \forall v_j, j = 1, 2, \ldots, n,$$

Then,

$$\sum_{j=1}^{m+n} \gamma_j^2 = 2mn(n-m)^2.$$

(ii) Since $K_{m,n}$ is a triangle free graph, then

$$\sum_{j=1}^{m+n} \gamma_j^3 = 0.$$

□

Theorem 3.8. *Let G be a graph of order n, in which $df(v) = df(u) = f$ and $N(v) - u = N(u) - v$. Then λ is a maximum deficiency eigenvalue of G, where*

$$\lambda = \begin{cases} -f, & \text{if } uv \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

Proof. The proof is similar to Theorem 2.5 in [1]. □

Theorem 3.9. *For a graph G, the maximum deficiency energy of G must be an even integer, if it is rational.*

Proof. We know that the characteristic polynomial of maximum deficiency matrix of a graph G is monic polynomial with integer coefficients. Therefore, roots of the characteristic polynomial are either integers or irrational numbers. Thus, the maximum deficiency energy of G is also either integer or an irrational number. Now, we know that the maximum deficiency energy of G is two times sum of positive maximum deficiency eigenvalues of G. Hence, if the maximum deficiency energy of G is rational, then it is always an even integer. □

4 The maximum deficiency energy of some classes of graphs

This section briefs about how the exact values of maximum deficiency eigenvalues and maximum deficiency energies of some well known graphs were obtained.

Theorem 4.1. *Let G be the star graph $K_{1,r-1}$ of order $r \geq 3$, then maximum deficiency eigenvalues of G are 0, $(r-2)\sqrt{(r-1)}$ and $-(r-2)\sqrt{(r-1)}$ with multiplicity $(r-2)$, 1 and 1, respectively and $EM_{df}(K_{1,r-1}) = 2(r-2)\sqrt{(r-1)}$.*

Proof. Let $K_{1,r-1}$ be the star graph with vertices $u_0, u_1, \ldots, u_{n-1}$, where u_0 is the central vertex. Then we have

$$M_{df}(K_{1,r-1}) = \begin{pmatrix} 0 & r-2 & r-2 & \dots & r-2 \\ r-2 & 0 & 0 & \dots & 0 \\ r-2 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ r-2 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

The characteristic polynomial of $M_{df}(K_{1,r-1})$ is

$$\phi(K_{1,r-1};\gamma) = \begin{vmatrix} \gamma & -(r-2) & -(r-2) & \dots & -(r-2) \\ -(r-2) & \gamma & 0 & \dots & 0 \\ -(r-2) & 0 & \gamma & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ -(r-2) & 0 & 0 & \dots & \gamma \end{vmatrix}$$

$$= \gamma^r - (r-1)(r-2)^2\gamma^{r-2}$$

$$= \gamma^{r-2}(\gamma^2 - (r-1)(r-2)^2).$$

Hence, the maximum deficiency spectrum of $K_{1,r-1}$ is

$$M_{df}SP(K_{1,r-1}) = \begin{pmatrix} (r-2)\sqrt{r-1} & 0 & -(r-2)\sqrt{r-1} \\ 1 & r-2 & 1 \end{pmatrix}.$$

Hence, the maximum deficiency energy of $K_{1,r-1}$ is

$$EM_{df}(K_{1,r-1}) = 2(r-2)\sqrt{r-1}.$$

□

Remark 4.2. *In the above theorem, for* $r = 1$ *and* $r = 2$*, the maximum deficiency eigenvalues and maximum deficiency energy is zero.*

Theorem 4.3. *Let* P_n *be the path graph of order* n*, then the maximum deficiency eigenvalues of* P_n *are* 0, 1 *and* -1 *with multiplicity* $(n-4)$, 2 *and* 2, *respectively and* $EM_{df}(P_n) = 4$.

Proof. Let P_n be the path graph with vertices $v_1, v_2, \ldots, v_n$, then we have

$$M_{df}(P_n) = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 & 0 \\ 1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & 0 & \ldots & 1 & 0 \end{pmatrix}.$$

The characteristic polynomial of $M_{df}(P_n)$ is

$$\phi(P_n;\gamma) = \begin{vmatrix} \gamma & -1 & 0 & \ldots & 0 & 0 \\ 1 & \gamma & 0 & \ldots & 0 & 0 \\ 0 & 0 & \gamma & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \gamma & -1 \\ 0 & 0 & 0 & \ldots & -1 & \gamma \end{vmatrix}$$

$$= \gamma^n - 2\gamma^{n-2} - \gamma^{n-4}$$

$$= \gamma^{n-4}(\gamma^2 - 1)^2.$$

Hence, the maximum deficiency spectrum of P_n is

$$M_{df}SP(P_n) = \begin{pmatrix} 0 & 1 & -1 \\ n-4 & 2 & 2 \end{pmatrix}.$$

Hence, the maximum deficiency energy of P_n is

$$EM_{df}(P_n) = 4.$$

□

5 Bounds for maximum deficiency energy

The formulation of the lower bound and upper bound for the maximum deficiency energy of a graph has been detailed in this section.

Theorem 5.1. *Let G be a simple graph of order $n \geq 2$. Then*

$$\sqrt{-2c_2 + n(n-1)|det(M_{df}(G))|^{\frac{2}{n}}} \leq EM_{df}(G) \leq \sqrt{-2nc_2}.$$

Proof. The similar theorem is proved in [1] for maximum degree energy. We know that

$$(EM_{df}(G))^2 = \left(\sum_{j=1}^{n}|\gamma_j|\right)^2$$

$$= \left(\sum_{j=1}^{n}|\gamma_j|^2\right) + \left(\sum_{i\neq j}|\gamma_i||\gamma_j|\right).$$

From the arithemetic and geometric mean inequality, we get

$$\frac{1}{n(n-1)}\sum_{i\neq j}|\gamma_i||\gamma_j| \geq \left(\prod_{i\neq j}|\gamma_i||\gamma_j|\right)^{1/n(n-1)}.$$

By Theorem 3.5 and this inequality, we get

$$(EM_{df}(G))^2 \geq \left(\sum_{j=1}^{n}|\gamma_j|^2\right) + n(n-1)\left(\prod_{i\neq j}|\gamma_i||\gamma_j|\right)^{1/n(n-1)}$$

$$\geq \left(\sum_{j=1}^{n}|\gamma_j|^2\right) + n(n-1)|\prod_{j=1}\gamma_j|^{2/n}$$

$$\geq -2c_2 + n(n-1)|det(M_{df}(G))|^{\frac{2}{n}}.$$

For the upper bound, consider the cauchy-schwartz inequality

$$\left(\sum_{j=1}^{n}|x_j y_j|\right)^2 \leq \left(\sum_{j=1}^{n}|x_j|^2\right)\left(\sum_{j=1}^{n}|y_j|^2\right).$$

By choosing $x_j = 1$ and $y_j = |\gamma_j|$, we get

$$\begin{aligned} EM_{df}(G) &\leq \sqrt{n\sum_{j=1}^{n}|\gamma_j|^2} \\ &= \sqrt{-2nc_2}. \end{aligned}$$

Hence,

$$\sqrt{-2c_2 + n(n-1)|det(M_{df}(G))|^{\frac{2}{n}}} \leq EM_{df}(G) \leq \sqrt{-2nc_2}.$$

□

Remark 5.2. *For the graph shown in Figure* 2*,* $c_2 = -26$*. Thus, from Theorem 5.1,*

$$\begin{aligned} \sqrt{52} \leq EM_{df}(G_2) \leq \sqrt{260} \\ 7.211 \leq 13.136 \leq 16.1245. \end{aligned}$$

Lemma 5.3. [3].

Suppose that x_j *and* y_j*,* $1 \leq j \leq n$*, are non-negative real numbers. Then*

$$\left| n\sum_{j=1}^{n} x_j y_j - \sum_{j=1}^{n} x_j \sum_{j=1}^{n} y_j \right| \leq \alpha(n)(X-x)(Y-y),$$

where x*,* y*,* X *and* Y *are real constants, such that for each* j*,* $1 \leq j \leq n$*, the conditions* $x \leq x_j \leq X$ *and* $y \leq y_j \leq Y$ *are satisfied. Further,* $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$*, while* $[x]$ *denotes integer part of a real number* x*.*

Lemma 5.4. [12]. *Suppose that* x_j *and* y_j*,* $1 \leq j \leq n$*, are non-negative real numbers. Then*

$$\sum_{j=1}^{n} x_j^2 \sum_{j=1}^{n} y_j^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{j=1}^{n} x_j y_j\right)^2,$$

where $M_1 = \max\limits_{1\leq j\leq n}(x_j), M_2 = \max\limits_{1\leq j\leq n}(y_j), m_1 = \min\limits_{1\leq j\leq n}(x_j)$ *and* $m_2 = \min\limits_{1\leq j\leq n}(y_j)$*.*

Lemma 5.5. [4].

Suppose that x_j and y_j, $1 \leq j \leq n$, are non-negative real numbers. Then

$$\sum_{j=1}^{n} y_j^2 + rR\sum_{j=1}^{n} x_j^2 \leq (r+R)\left(\sum_{j=1}^{n} x_j y_j\right),$$

where r, R are real constants, such that for each j, $1 \leq j \leq n$, the conditions $rx_j \leq y_j \leq Rx_j$ are satisfied.

Theorem 5.6. *Suppose G is a graph with n vertices. Let γ_j, $j = 1, 2, \ldots, n$ be the maximum deficiency eigenvalues of G. Let $\gamma_{min} = \min_{1\leq j\leq n}(|\gamma_j|)$ and $\gamma_{max} = \max_{1\leq j\leq n}(|\gamma_j|)$ and $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, while [x] denotes integer part of a real number x.*

Then

$$EM_{df}(G) \geq \sqrt{-2nc_2 - \alpha(n)(\gamma_{max} - \gamma_{min})^2}. \tag{1}$$

Proof. Applying Lemma 5.3 and putting $x_j = |\gamma_j| = y_j$, $x = \gamma_{min} = y$ and $X = \gamma_{max} = Y$ imply that

$$\left| n\sum_{j=1}^{n} |\gamma_j|^2 - \left(\sum_{j=1}^{n} |\gamma_j\right)^2 \right| \leq \alpha(n)(\gamma_{max} - \gamma_{min})^2.$$

By Theorem 3.5, we get

$$-2nc_2 - EM_{df}(G)^2 \leq \alpha(n)(\gamma_{max} - \gamma_{min})^2.$$

Hence

$$EM_{df}(G) \geq \sqrt{-2nc_2 - \alpha(n)(\gamma_{max} - \gamma_{min})^2}.$$

□

Corollary 5.7. *Since $\alpha(n) \leq \frac{n^2}{4}$, then by Theorem 5.6, we get*

$$EM_{df}(G) \geq \sqrt{-2nc_2 - \frac{n^2}{4}(\gamma_{max} - \gamma_{min})^2}. \tag{2}$$

Remark 5.8.

$$EM_{df}(G) \geq \sqrt{-2nc_2 - \alpha(n)(\gamma_{max} - \gamma_{min})^2} \geq$$
$$\geq \sqrt{-2nc_2 - \frac{n^2}{4}(\gamma_{max} - \gamma_{min})^2}.$$

Thus, inequality (1) is stronger than inequality (2).

Theorem 5.9. *Suppose G is a graph with n vertices. Let γ_j, $j = 1, 2, \ldots, n$ be the maximum deficiency eigenvalues of G. If zero is not an eigenvalue of $M_{df}(G)$, then*

$$EM_{df}(G) \geq \frac{2\sqrt{-2nc_2\gamma_{max}\gamma_{min}}}{\gamma_{max} + \gamma_{min}}, \tag{3}$$

where $\gamma_{min} = \min\limits_{1\leq j\leq n}(|\gamma_j|)$ and $\gamma_{max} = \max\limits_{1\leq j\leq n}(|\gamma_j|)$.

Proof. Using Lemma 5.4 for $x_i = |\gamma_j|$ and $y_j = 1$, we get

$$\sum_{j=1}^{n}|\gamma_j|^2 \sum_{j=1}^{n} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{\gamma_{max}}{\gamma_{min}}} + \sqrt{\frac{\gamma_{min}}{\gamma_{max}}}\right)^2 \left(\sum_{j=1}^{n}|\gamma_j|\right)^2$$

$$\Rightarrow -2nc_2 \leq \frac{1}{4}\left(\sqrt{\frac{\gamma_{max}}{\gamma_{min}}} + \sqrt{\frac{\gamma_{min}}{\gamma_{max}}}\right)^2 EM_{df}(G)^2.$$

Hence

$$EM_{df}(G) \geq \frac{2\sqrt{-2nc_2\gamma_{max}\gamma_{min}}}{\gamma_{max} + \gamma_{min}},$$

where $\gamma_{min} = \min\limits_{1\leq j\leq n}(|\gamma_j|)$ and $\gamma_{max} = \max\limits_{1\leq j\leq n}(|\gamma_j|)$.

□

Theorem 5.10. *Suppose G is a graph of order n. Let $\gamma_j, i = 1, 2, \ldots, n$ be the maximum deficiency eigenvalues of G. Then*

$$EM_{df}(G) \geq \frac{-2c_2 + n\gamma_{max}\gamma_{min}}{\gamma_{max} + \gamma_{min}}, \tag{4}$$

where $\gamma_{min} = \min\limits_{1\leq j\leq n}(|\gamma_j|)$ and $\gamma_{max} = \max\limits_{1\leq j\leq n}(|\gamma_j|)$.

Proof. Using Lemma 5.5 and setting $x_j = 1, y_j = |\gamma_j|, r = \gamma_{min}$ and $R = \gamma_{max}$, we get

$$\sum_{j=1}^{n} |\gamma_j|^2 + \gamma_{min}\gamma_{max} \sum_{j=1}^{n} 1 \leq (\gamma_{min} + \gamma_{max}) \sum_{j=1}^{n} |\gamma_j|$$

$$\Rightarrow -2c_2 + n\gamma_{min}\gamma_{max} \leq (\gamma_{min} + \gamma_{max}) EM_{df}(G).$$

Hence

$$EM_{df}(G) \geq \frac{-2c_2 + n\gamma_{max}\gamma_{min}}{\gamma_{max} + \gamma_{min}},$$

where $\gamma_{min} = \min\limits_{1 \leq j \leq n} (|\gamma_j|)$ and $\gamma_{max} = \max\limits_{1 \leq j \leq n} (|\gamma_j|)$. □

Remark 5.11. Using inequality between arithmetic and geometric means,

$$EM_{df}(G) \geq \frac{-2c_2 + n\gamma_{max}\gamma_{min}}{\gamma_{max} + \gamma_{min}} \geq \frac{2\sqrt{-2nc_2\gamma_{max}\gamma_{min}}}{\gamma_{max} + \gamma_{min}}.$$

Thus, inequality (4) is stronger than inequality (3).

Remark 5.12. *There are analogous bounds for the adjacency energy $\mathcal{E}(G)$, the maximum degree energy $EM(G)$ and the maximum eccentricity energy $EM_e(G)$*

6 Conclusion

A newly developed matrix of a graph G called maximum deficiency matrix $M_{df}(G)$ has been introduced in this paper. The underlying graph along with the deficiency on its vertices are found to be the influencing factors of it. Some coefficients of the characteristic polynomial of the maximum deficiency matrix are found. For a graph, the maximum deficiency energy $EM_{df}(G)$ has been formulated and the upper and lower bounds have been obtained. It is possible that the maximum deficiency energy that we are considering in this paper may have some applications in chemistry as well as in other areas.

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