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Research Paper

# Deficiency Sum Energy of Some Graph Classes

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**Abstract**

In this paper, we introduce the concept of deficiency sum matrix $S_{df}(G)$ of a simple graph $G = (V, E)$ of order $n$. The deficiency $df(v)$ of a vertex $v \in V$ is the deviation between the degree of the vertex $v$ and the maximum degree of the graph. The deficiency sum matrix $S_{df}(G)$ is a matrix of order $n$ whose $(i, j)$-th entry is $df(v_i) + df(v_j)$, if the vertices $v_i$ and $v_j$ are adjacent and 0, otherwise. In addition, we introduce deficiency sum energy $ES_{df}(G)$ of a graph $G$ and establish some bounds for $ES_{df}(G)$. Further, deficiency sum energy of some classes of graphs are obtained. Moreover, we construct an algorithm and python(3.8) code to find out spectrum and deficiency sum energy of graph $G$.



## 1 Introduction

In the study of spectral graph theory, the eigenvalues of a certain matrix corresponding to the graph can be used to obtain some useful information about the graph. In this paper, all the graphs are assumed to be simple, finite and undirected. The number of adjacent vertices on vertex $v$ is known as the degree and is denoted by $d(v)$.

Let $G$ be a graph with vertices $\{v_1, v_2, v_3, \ldots, v_n\}$ and maximum degree $r$. Then deficiency of $v_i$ would be $df(v_i) = r - d(v_i)$. For additional graph-theoretical terminologies, we refer to [1].

The concept of energy [2] was introduced almost 40 years ago as a sum of absolute eigenvalues of the adjacency matrix and has been extensively investigated, as detailed in [3–6]. Eventually, numerous other graph energies have been invented, based on the eigenvalues of matrices different from the adjacency matrix; for more details see [7–16].

Let $G = (V, E)$ be a graph with vertices $\{v_1, v_2, \ldots, v_n\}$ and let $e(v_i)$ be the eccentricity of $v_i$, which is the maximum number of edges required to connect $e(v_i)$ to other vertices(or infinity in a disconnected graph).

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One of these graph energies is the sum-eccentricity energy [17, 18], based on the eigenvalues of the sum-eccentricity matrix $S_e(G)$, whose elements are defined as:

$$s_{ij} = \begin{cases} e(v_i) + e(v_j), & \text{if } v_iv_j \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

Another recently introduced graph energy is the first Zagreb energy [12] based on the eigenvalues of the first Zagreb matrix $Z(G)$ whose elements are defined as:

$$z_{ij} = \begin{cases} d(v_i) + d(v_j), & \text{if } v_iv_j \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

Further, we have introduced maximum deficiency energy [19] based on the eigenvalues of the maximum deficiency matrix $M_{df}(G)$ whose elements are defined as:

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

We were motivated by the eccentricity sum matrix [17, 18], the first Zagreb matrix [12] and maximum deficiency energy [19]. In this paper, we have introduced deficiency sum matrix and deficiency sum energy, on the basis of this very motivation.

Let $G = (V, E)$ be a graph with vertices $\{v_1, v_2, \ldots, v_n\}$ and let deficiency of a vertex $v_i$ as $df(v_i)$. Then, the deficiency sum matrix $S_{df}(G) = [s_{ij}]_{n\times n}$ is defined as:

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

Let $\phi(G;\gamma) = det(\gamma I - S_{df}(G))$ be the characteristic polynomial of $S_{df}(G)$ and we consider $\phi(G;\gamma)$ as deficiency sum polynomial of $S_{df}(G)$(or a graph $G$) and its roots are termed as deficiency sum eigenvalues of $G$. The deficiency sum energy of a graph $G$ is defined as:

$$ES_{df}(G) = \sum_{i=1}^{n} |\gamma_i|.$$

**Remark 1**. The deficiency sum matrix $S_{df}(G)$ is a symmetric and real matrix with zero trace.

**Example 1.1.** The deficiency sum matrix of graph $G_1$(as shown in Figure 1) is

$$S_{df}(G_1) = \begin{pmatrix} 0 & 2 & 1 & 1 & 2 \\ 2 & 0 & 3 & 0 & 0 \\ 1 & 3 & 0 & 2 & 0 \\ 1 & 0 & 2 & 0 & 3 \\ 2 & 0 & 0 & 3 & 0 \end{pmatrix}.$$

The deficiency sum polynomial of $G_1$ is

$$\begin{aligned} \phi(G_1;\gamma) &= det(\gamma I - S_{df}(G_1)) \\ &= \begin{vmatrix} \gamma & -2 & -1 & -1 & -2 \\ -2 & \gamma & -3 & 0 & 0 \\ -1 & -3 & \gamma & -2 & 0 \\ -1 & 0 & -2 & \gamma & -3 \\ -2 & 0 & 0 & -3 & \gamma \end{vmatrix} \end{aligned}$$

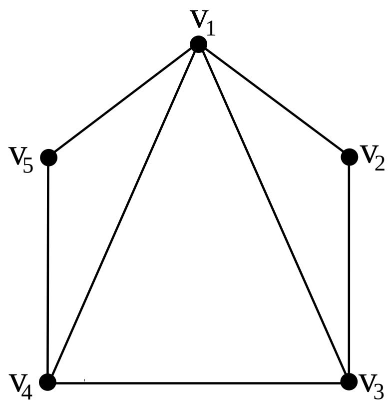


Figure 1: Graph $G_1$.

$$= \gamma^5 - 32\gamma^3 - 28\gamma^2 + 155\gamma + 72.$$

Then, the deficiency sum eigenvalues of $G_1$ are
$\gamma_1 = -4.1622777$, $\gamma_2 = -3.181567, \gamma_3 = -0.4467552, \gamma_4 = 2.1622777$ and $\gamma_5 = 5.6283239$.
Now, the deficiency sum energy of $G_1$ is

$$ES_{df}(G_1) = 15.58120315861477.$$

## 2 Properties of deficiency sum polynomial and deficiency sum eigenvalues

In this section, we obtain the exact expression of some coefficients in the deficiency sum polynomial $\phi(G;\gamma)$ of the graph $G$. In addition, some properties of the deficiency sum eigenvalues of the graph $G$ are discussed.

**Theorem 2.1.** *Let $G$ be a graph having order $n$ and let $\phi(G;\gamma) = c_0\gamma^n + c_1\gamma^{n-1} + c_2\gamma^{n-2} + \ldots + c_n$ be the deficiency sum polynomial of $G$. Then*

(i) $c_0 = 1$.

(ii) $c_1 = 0$.

(iii) $c_2 = -\sum_{i=1,i<j}^{n}(df(v_i) + df(v_j))^2, \qquad v_iv_j \in E(G)$.

*Proof.* The proof is similar to Theorem 3.1 in [18]. ■

**Theorem 2.2.** *If $G$ is assumed to be a graph having order $n$ and $\gamma_1, \gamma_2, \gamma_3, \ldots, \gamma_n$ as the deficiency sum eigenvalues of $S_{df}(G)$, then*

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

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

*Proof.* We know that

$$\sum_{i=1}^{n}\gamma_i^2 = trace(S_{df}(G))^2 = \sum_{i=1}^{n}\sum_{k=1}^{n} s_{ik}s_{ki}$$
$$= 2\sum_{i=1,i<k}^{n} s_{ik}^2 = 2\sum_{i=1,i<k}^{n}(df(v_i)+df(v_k))^2,$$

where $v_iv_k \in E(G)$. Hence by Theorem 2.1,

$$\sum_{i=1}^{n}\gamma_i^2 = -2c_2.$$

■

**Theorem 2.3.** *Let $K_{m,n}$ be a complete bipartite graph and $\gamma_1, \gamma_2, \gamma_3, \dots, \gamma_{m+n}$ are the deficiency sum eigenvalues of $K_{m,n}$. Then for $m \le n$*

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

*Proof.* Consider $K_{m,n}$ as the complete bipartite graph with vertices $\{u_1, u_2, \dots, u_m, v_1, v_2, \dots v_n\}$. Using Theorem 2.2,

$$\sum_{i=1}^{n}\gamma_i^2 = 2\sum_{i=1,i<k}^{n}(df(v_i)+df(v_k))^2, \qquad \textit{where } v_iv_k \in E(G).$$

For the graph $K_{m,n}$,

$$df(u_i) = 0,\ \forall u_i, i = 1, 2, \dots, m,$$
$$df(v_j) = n-m,\ \forall v_j, j = 1, 2, \dots, n.$$

Then, $\sum_{i=1}^{n}\gamma_i^2 = 2nm(n-m)^2$. ■

**Corollary 2.4.** *Let $K_{1,n}$ be the star graph and $\gamma_1, \gamma_2, \gamma_3, \dots, \gamma_{n+1}$ be the deficiency sum eigenvalues of the graph $K_{1,n}$. Then*

$$\sum_{i=1}^{n+1}\gamma_i^2 = 2n(n-1)^2.$$

# 3 Deficiency sum polynomial and deficiency sum energy of some special graphs

In this section, we discuss the method to obtain deficiency sum polynomial and deficiency sum energy of some special classes of graphs.

**Theorem 3.1.** *Let $G$ be the regular graph. Then deficiency sum energy, $ES_{df}(G)$, of graph $G$ is zero.*

*Proof.* We know that in a regular graph deficiency of each vertex is zero. Therefore, the deficiency sum matrix is a zero matrix. Hence deficiency sum energy is always zero. ■

**Theorem 3.2.** *Let $P_n$ be a path having order $n \geq 4$. Then*

(i) the deficiency sum polynomial of $P_n$ is

$$\phi(P_n, \gamma) = \gamma^{n-4}(\gamma^2 - 1)^2,$$

(ii) the deficiency sum energy of $P_n$ is

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

*Proof.* Let $P_n$ be a path having order $n \geq 4$. Then we have

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

The deficiency sum polynomial of $P_n$ is

$$\begin{aligned} \phi(P_n; \gamma) &= det(\gamma I - S_{df}(P_n)) \\ &= \gamma^n - 2\gamma^{n-2} - \gamma^{n-4} = \gamma^{n-4}(\gamma^2 - 1)^2. \end{aligned}$$

Hence, the deficiency sum energy of $P_n$ is $ES_{df}(P_n) = 4$. ■

In the subsequent theorem $J_{m\times n}$ denotes $m \times n$ matrix with all entries 1 and $O_{n\times n}$ denotes $n \times n$ zero matrix.

**Theorem 3.3.** *Let $K_{m,n}$ be the complete bipartite graph. Then for $m < n$*

(i) the deficiency sum polynomial of $K_{m,n}$ is

$$\phi(K_{m,n}, \gamma) = \gamma^{m+n-2}(\gamma^2 - mn(n - m)^2),$$

(ii) the deficiency sum energy of $K_{m,n}$ is

$$ES_{df}(K_{m,n}) = 2(n - m)\sqrt{mn}.$$

*Proof.* Let $K_{m,n}$ be the complete bipartite graph of order $m + n$. Then, we have

$$S_{df}(K_{m,n}) = n - m \begin{pmatrix} O_{m\times m} & J_{m\times n} \\ J_{n\times m} & O_{n\times n} \end{pmatrix}_{(m+n)\times(m+n)}.$$

The deficiency sum polynomial of $K_{m,n}$ is

$$\begin{aligned} \phi(K_{m,n}; \gamma) &= det(\gamma I - S_{df}(K_{m,n})) \\ &= \gamma^{m+n} - mn(n - m)^2\gamma^{m+n-2} \\ &= \gamma^{m+n-2}(\gamma^2 - mn(n - m)^2). \end{aligned}$$

Hence, the deficiency sum energy of $K_{m,n}$ is $ES_{df}(K_{m,n}) = 2(n - m)\sqrt{mn}$.

■

**Corollary 3.4.** *Let $K_{1,n-1}$ be the star graph having order $n \geq 3$. Then*

(i) the deficiency sum polynomial of $K_{1,n-1}$ is

$$\phi(K_{1,n-1}, \gamma) = \gamma^{n-2}(\gamma^2 - (n-1)(n-2)^2),$$

(ii) the deficiency sum energy of $K_{1,n-1}$ is

$$ES_{df}(K_{1,n-1}) = 2(n-2)\sqrt{n-1}.$$

**Theorem 3.5.** *Let $B_{k,k}$ be the Bistar graph of order $2k+2$, which is obtained by joining the center vertices of two copies of $K_{1,k}$ by an edge. Then*

(i) the deficiency sum polynomial of Bistar graph $B_{k,k}$ is

$$\phi(B_{k,k}, \gamma) = \left[\gamma^{k-1}\left(\gamma^2 - k^3\right)\right]^2,$$

(ii) the deficiency sum energy of Bistar graph $B_{k,k}$ is

$$ES_{df}(B_{k,k}) = 4k\sqrt{k}.$$

*Proof.* Let $B_{k,k}$ be the Bistar graph of order $2k+2$. Then, we have

$$S_{df}(B_{k,k}) = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}_{(2k+2)\times(2k+2)},$$

where,

$$A = \begin{pmatrix} 0 & k & k & \dots & k \\ k & 0 & 0 & \dots & 0 \\ k & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}_{(k+1)\times(k+1)}.$$

The deficiency sum polynomial of $B_{k,k}$ is

$$\begin{aligned} \phi(B_{k,k};\gamma) &= det(\gamma I - S_{df}(B_{k,k})) \\ &= \left[\gamma^{k+1} - k(k)^2\gamma^{k-1}\right]^2 = \left[\gamma^{k-1}\left(\gamma^2 - k^3\right)\right]^2. \end{aligned}$$

Hence, the deficiency sum energy of $B_{k,k}$ is $ES_{df}(B_{k,k}) = 4k\sqrt{k}$.

■

If $\vartheta$ is considered a positive integer, then the friendship graph $F_\vartheta$ will be a collection of $\vartheta$ - cycles with a common vertex and the length of each cycle being 3. Now, we compute the deficiency sum polynomial and the deficiency sum energy of friendship graphs.

**Theorem 3.6.** *For $\vartheta \geq 2$,*

(i) the deficiency sum polynomial of friendship graph $F_\vartheta$ is

$$\begin{aligned} \phi(F_\vartheta, \gamma) = \left[\gamma^2 - 4(2\vartheta-2)^2\right]^{\vartheta-1} &\left(\gamma - \left[(2\vartheta-2) + (2\vartheta-2)\sqrt{1+2\vartheta}\right]\right) \\ \left(\gamma - \left[(2\vartheta-2) - (2\vartheta-2)\sqrt{1+2\vartheta}\right]\right) &\left(\gamma + 2(2\vartheta-2)\right), \end{aligned}$$

(ii) the deficincy sum energy of friendship graph $F_\vartheta$ is

$$ES_{df}(F_\vartheta) = 2(2\vartheta - 2)[2\vartheta - 1 + \sqrt{1 + 2\vartheta}].$$

*Proof.* Let $F_\vartheta$ be the friendship graph of order $2\vartheta + 1$. Then the deficiency sum polynomial of $F_\vartheta$ is

$$\phi(F_\vartheta; \gamma) = det(\gamma I - S_{df}(F_\vartheta))$$

$$= \begin{vmatrix} \gamma & -(2\vartheta-2) & -(2\vartheta-2) & \dots & -(2\vartheta-2) & -(2\vartheta-2) \\ -(2\vartheta-2) & \gamma & -2(2\vartheta-2) & \dots & 0 & 0 \\ -(2\vartheta-2) & -2(2\vartheta-2) & \gamma & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -(2\vartheta-2) & 0 & 0 & \dots & \gamma & -2(2\vartheta-2) \\ -(2\vartheta-2) & 0 & 0 & \dots & -2(2\vartheta-2) & \gamma \end{vmatrix}_{(2\vartheta+1)\times(2\vartheta+1)}.$$

Now, the first array cofactor in the first row is

$$\begin{vmatrix} \gamma & -2(2\vartheta-2) & 0 & 0 & \dots & 0 & 0 \\ -2(2\vartheta-2) & \gamma & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \gamma & -2(2\vartheta-2) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \gamma & -2(2\vartheta-2) \\ 0 & 0 & 0 & 0 & \dots & -2(2\vartheta-2) & \gamma \end{vmatrix}_{(2\vartheta)\times(2\vartheta)},$$

and the another arrays cofactor in the first row are indistinguishable from

$$\begin{vmatrix} -(2\vartheta-2) & -2(2\vartheta-2) & \dots & 0 & 0 \\ -(2\vartheta-2) & \gamma & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ -(2\vartheta-2) & 0 & \dots & \gamma & -2(2\vartheta-2) \\ -(2\vartheta-2) & 0 & \dots & -2(2\vartheta-2) & \gamma \end{vmatrix}_{(2\vartheta)\times(2\vartheta)}.$$

Now, solving determinants, we get

$$\begin{aligned} \phi(F_\vartheta; \gamma) &= \gamma\big[\gamma^2 - 4(2\vartheta-2)^2\big]^{\vartheta} + 2\vartheta(2\vartheta-2)\big[\gamma^2 - 4(2\vartheta-2)^2\big]^{\vartheta-1} \\ &\quad [-\gamma(2\vartheta-2) - 2(2\vartheta-2)^2] \\ &= \big[\gamma^2 - 4(2\vartheta-2)^2\big]^{\vartheta-1}[\gamma + 2(2\vartheta-2)][\gamma(\gamma - 2(2\vartheta-2)) - 2\vartheta(2\vartheta-2)^2] \\ &= \big[\gamma^2 - 4(2\vartheta-2)^2\big]^{\vartheta-1}\Big[\gamma - \big[(2\vartheta-2) + (2\vartheta-2)\sqrt{1+2\vartheta}\big]\Big] \\ &\quad \big(\gamma + 2(2\vartheta-2)\big)\Big[\gamma - \big[(2\vartheta-2) - (2\vartheta-2)\sqrt{1+2\vartheta}\big]\Big]. \end{aligned}$$

From definition of deficiency sum energy $ES_{df}(G)$, we get

$$ES_{df}(F_\vartheta) = 2(2\vartheta - 2)[2\vartheta - 1 + \sqrt{1 + 2\vartheta}].$$

■

Let $\vartheta$ be a positive integer, then the Dutch Windmill graph $D_4^\vartheta$ is a collection of $\vartheta$-cycles with a common vertex and the length of each cycle being 4. Now, we compute the deficiency sum polynomial and the deficiency sum energy of Dutch Windmill graph $D_4^\vartheta$.

**Theorem 3.7.** *For $\vartheta \geq 2$,*

(i) the deficiency sum polynomial of Dutch Windmill graph $D_4^\vartheta$ is
$\phi(D_4^\vartheta, \gamma) = \gamma^{\vartheta+1}\big(\gamma^2 - 8(2\vartheta-2)^2\big)^{\vartheta-1}\big[\gamma^2 - 8(2\vartheta-2)^2 - 2\vartheta(2\vartheta-2)^2\big]$,

(ii) the deficiency sum energy of Dutch Windmill graph $D_4^\vartheta$ is

$$ES_{df}(D_4^\vartheta) = 2\sqrt{2}(2\vartheta-2)[2(\vartheta-1) + \sqrt{\vartheta+4}].$$

*Proof.* Let $D_4^\vartheta$ be the Dutch Windmill graph of order $3\vartheta+1$. Then the deficiency sum polynomial of $D_4^\vartheta$ is

$$\phi(D_4^\vartheta;\gamma) = det(\gamma I - S_{df}(D_4^\vartheta))$$

$$= \begin{vmatrix} \gamma & -(2\vartheta-2) & -(2\vartheta-2) & 0 & \dots & -(2\vartheta-2) & -(2\vartheta-2) & 0 \\ -(2\vartheta-2) & \gamma & 0 & -2(2\vartheta-2) & \dots & 0 & 0 & 0 \\ -(2\vartheta-2) & 0 & \gamma & -2(2\vartheta-2) & \dots & 0 & 0 & 0 \\ 0 & -2(2\vartheta-2) & -2(2\vartheta-2) & \gamma & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -(2\vartheta-2) & 0 & 0 & 0 & \dots & \gamma & 0 & -2(2\vartheta-2) \\ -(2\vartheta-2) & 0 & 0 & 0 & \dots & 0 & \gamma & -2(2\vartheta-2) \\ 0 & 0 & 0 & 0 & \dots & -2(2\vartheta-2) & -2(2\vartheta-2) & \gamma \end{vmatrix}_{(3\vartheta+1)\times(3\vartheta+1)}.$$

In order to solve the determinant, we consider its first row.
Let

$$M = \begin{pmatrix} \gamma & 0 & -2(2\vartheta-2) \\ 0 & \gamma & -2(2\vartheta-2) \\ -2(2\vartheta-2) & -2(2\vartheta-2) & \gamma \end{pmatrix},$$

$$N = \begin{pmatrix} -(2\vartheta-2) & 0 & 0 \\ -(2\vartheta-2) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad P = \begin{pmatrix} -(2\vartheta-2) & 0 & -2(2\vartheta-2) \\ -(2\vartheta-2) & \gamma & -2(2\vartheta-2) \\ 0 & -2(2\vartheta-2) & \gamma \end{pmatrix}.$$

Then

$$\phi(D_4^\vartheta, \gamma) = \gamma(det(M))^\vartheta + 2\vartheta(2\vartheta-2)det\begin{pmatrix} P & 0 & 0 & \dots & 0 \\ N & M & 0 & \dots & 0 \\ N & 0 & M & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ N & 0 & 0 & \dots & M \end{pmatrix}.$$

By computing, we get

$$\phi(D_4^\vartheta, \gamma) = \gamma^{\vartheta+1}\big(\gamma^2 - 8(2\vartheta-2)^2\big)^{\vartheta-1}\big[\gamma^2 - 8(2\vartheta-2)^2 - 2\vartheta(2\vartheta-2)^2\big].$$

From definition of deficiency sum energy $ES_{df}(G)$, we get

$$ES_{df}(D_4^\vartheta) = 2\sqrt{2}(2\vartheta-2)[2(\vartheta-1) + \sqrt{\vartheta+4}].$$

■

Let $\vartheta$ be a positive integer, then the $k_4$-Windmill graph $K_4^\vartheta$ is a collection of $\vartheta$ complete graphs with a common vertex and the length of each complete graph being 4. Now, we compute the deficiency sum polynomial and the deficiency sum energy of $K_4$-Windmill graph $K_4^\vartheta$.

**Theorem 3.8.** *For $\vartheta \geq 2$,*

(i) the deficiency sum polynomial of $K_4$-Windmill graph $K_4^{\vartheta}$ is

$$\phi(K_4^{\vartheta}, \gamma) = \big(\gamma + 2(3\vartheta - 3)\big)^{\vartheta}\big(\gamma^2 - 2\gamma(3\vartheta - 3) - 8(3\vartheta - 3)\big)^{\vartheta-1} \gamma\big[\gamma^2 - 2\gamma(3\vartheta - 3) - 8(3\vartheta - 3) - 3\vartheta(3\vartheta - 3)^2\big],$$

(ii) the deficiency sum energy of Dutch Windmill graph $K_4^{\vartheta}$ is

$$ES_{df}(K_4^{\vartheta}) = 2\vartheta(3\vartheta - 3) + 2(\vartheta - 1)\sqrt{(3\vartheta - 3)^2 + 8(3\vartheta - 3)} + 2\sqrt{(3\vartheta - 3)^2 + 8(3\vartheta - 3) + 3\vartheta(3\vartheta - 3)^2}.$$

*Proof.* Let $K_4^{\vartheta}$ be the $K_4$-Windmill graph of order $4\vartheta + 1$. Then the deficiency sum polynomial of $K_4^{\vartheta}$ is

$$\phi(K_4^{\vartheta}; \gamma) = det(\gamma I - S_{df}(K_4^{\vartheta}))$$

$$= \begin{vmatrix} \gamma & -(3\vartheta-3) & -(3\vartheta-3) & -(3\vartheta-3) & \dots & -(3\vartheta-3) & -(3\vartheta-3) & (3\vartheta-3) \\ -(3\vartheta-3) & \gamma & -2(3\vartheta-3) & -2(3\vartheta-3) & \dots & 0 & 0 & 0 \\ -(3\vartheta-3) & -2(3\vartheta-3) & \gamma & -2(3\vartheta-3) & \dots & 0 & 0 & 0 \\ -(3\vartheta-3) & -2(3\vartheta-3) & -2(3\vartheta-3) & \gamma & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -(3\vartheta-3) & 0 & 0 & 0 & \dots & \gamma & -2(3\vartheta-3) & -2(3\vartheta-3) \\ -2(3\vartheta-3) & 0 & 0 & 0 & \dots & -2(3\vartheta-3) & \gamma & -2(3\vartheta-3) \\ 0 & 0 & 0 & 0 & \dots & -2(3\vartheta-3) & -2(3\vartheta-3) & \gamma \end{vmatrix}_{(3\vartheta+1)\times(3\vartheta+1)}.$$

In order to solve the determinant, we consider its first row.
Let

$$M = \begin{pmatrix} \gamma & -2(3\vartheta-3) & -2(3\vartheta-3) \\ -2(3\vartheta-3) & \gamma & -2(3\vartheta-3) \\ -2(3\vartheta-3) & -2(3\vartheta-3) & \gamma \end{pmatrix},$$

$$N = \begin{pmatrix} -(3\vartheta-3) & 0 & 0 \\ -(3\vartheta-3) & 0 & 0 \\ -(3\vartheta-3) & 0 & 0 \end{pmatrix} \text{ and } P = \begin{pmatrix} -(3\vartheta-3) & -2(3\vartheta-3) & -2(3\vartheta-3) \\ -(3\vartheta-3) & \gamma & -2(3\vartheta-3) \\ -(3\vartheta-3) & -2(3\vartheta-3) & \gamma \end{pmatrix}.$$

Then

$$\phi(K_4^{\vartheta}, \gamma) = \gamma(det(M))^{\vartheta} + 3\vartheta(3\vartheta - 3)det \begin{pmatrix} P & 0 & 0 & \dots & 0 \\ N & M & 0 & \dots & 0 \\ N & 0 & M & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ N & 0 & 0 & \dots & M \end{pmatrix}.$$

By computing, we get

$$\phi(K_4^{\vartheta}, \gamma) = \big(\gamma + 2(3\vartheta - 3)\big)^{\vartheta}\big(\gamma^2 - 2\gamma(3\vartheta - 3) - 8(3\vartheta - 3)\big)^{\vartheta-1} \gamma\big[\gamma^2 - 2\gamma(3\vartheta - 3) - 8(3\vartheta - 3) - 3\vartheta(3\vartheta - 3)^2\big].$$

From definition of deficiency sum energy $ES_{df}(G)$, we get

$$ES_{df}(K_4^{\vartheta}) = 2\vartheta(3\vartheta - 3) + 2(\vartheta - 1)\sqrt{(3\vartheta - 3)^2 + 8(3\vartheta - 3)} + 2\sqrt{(3\vartheta - 3)^2 + 8(3\vartheta - 3) + \upsilon(3\vartheta - 3)^2}.$$

■

# 4 Bounds for deficiency sum energy

In this section, the formulation of the lower and upper bound for the deficiency sum energy of a graph $G$ has been detailed.

**Lemma 4.1.** ([16]). Let $\xi_1, \xi_2, \xi_3, \ldots, \xi_m$ be non-negetive numbers. Then

$$n\left[\frac{1}{n}\sum_{k=1}^{n}\xi_k - \left(\prod_{k=1}^{n}\xi_k\right)^{\frac{1}{n}}\right] \leq n\sum_{k=1}^{n}\xi_k - \left(\sum_{k=1}^{n}\sqrt{\xi_k}\right)^2 \leq n(n-1)\left[\frac{1}{n}\sum_{k=1}^{n}\xi_k - \left(\prod_{k=1}^{n}\xi_k\right)^{\frac{1}{n}}\right].$$

**Theorem 4.2.** *If $G$ is considered to be a graph having order $n \geq 2$, then*

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

*Proof.* Lower bound:

For $k = 1, \ldots, n$ let $\xi_k = \gamma_k^2$ in Lemma 4.1, we get

$$n\sum_{k=1}^{n}\gamma_k^2 - \left(\sum_{k=1}^{n}|\gamma_k|\right)^2 \leq n(n-1)\left[\frac{1}{n}\sum_{k=1}^{n}\gamma_k^2 - \left(\prod_{k=1}^{n}\gamma_k^2\right)^{\frac{1}{n}}\right].$$

Using Theorem 2.2, we have

$$\sum_{k=1}^{n}\gamma_k^2 = -2c_2.$$

Therefore

$$-2nc_2 - ES_{df}^2(G) \leq -2(n-1)c_2 - n(n-1)\left(\prod_{k=1}^{n}|\gamma_j|\right)^{\frac{2}{n}}.$$

Hence

$$ES_{df}(G) \geq \sqrt{-2c_2 + n(n-1)det(S_{df}(G))^{\frac{2}{n}}}.$$

Upper bound :

By using Cauchy-Schwartz inequality, we have

$$\left(\sum_{k=1}^{n}|\gamma_k|\right)^2 \leq n\sum_{k=1}^{n}|\gamma_k|^2,$$

$$ES_{df}(G) \leq \sqrt{n\sum_{k=1}^{n}|\gamma_k|^2}.$$

By Theorem 2.2, we have $ES_{df}(G) \leq \sqrt{-2nc_2}$. ∎

**Lemma 4.3.** ([20]). *Suppose that $x_j$ and $y_j$, $1 \leq j \leq n$, are non-negative real numbers. Then*

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

*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 4.4.** ([21]). *Suppose that $x_j$ and $y_j$, $1 \leq j \leq n$, are non-negative real numbers. Then*

$$\sum_{j=1}^{n} x_j^2 \sum_{j=1}^{n} y_j^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{j=1}^{n} x_jy_j\right)^2,$$

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

**Lemma 4.5.** ([22]). *Suppose that $x_j$ and $y_j$, $1 \leq j \leq n$, are non-negetive real numbers. Then*

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

*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 4.6.** *Suppose $G$ is a graph with $n$ vertices. Let $\gamma_j$, $j = 1, 2, \ldots, n$ are the deficiency sum eigenvalues of $G$. Let* $\gamma_{min} = \min_{1\leq j\leq n}(|\gamma_j|)$, $\gamma_{max} = \max_{1\leq j\leq n}(|\gamma_j|)$ *and* $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, *Then*

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

*Proof.* Applying Lemma 4.3 and put $x_j = |\gamma_j| = y_j$, $x = \gamma_{min} = y$ and $X = \gamma_{max} = Y$ implies 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 2.2, we get

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

Hence,

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

■

**Corollary 4.7.** *Since $\alpha(n) \leq \frac{n^2}{4}$, then by Theorem 4.6, we get*

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

**Remark 2.**

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

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

**Theorem 4.8.** *Suppose $G$ is a graph with $n$ vertices. Let $\gamma_j$, $j = 1, 2, \ldots, n$ are the deficiency sum eigenvalues of $G$. If zero is not an eigenvalue of $S_{df}(G)$. Then*

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

*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 4.4 for $x_i = |\gamma_j|$ and $y_j = 1$ we get

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

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

Hence

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

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 4.9.** *If $G$ is a graph of order $n$. Let $\gamma_j, i = 1, 2, \ldots, n$ are the deficiency sum eigenvalues of $G$. Then*

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

*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 4.5 and setting $x_j = 1, y_j = |\gamma_j|, r = \gamma_{min}$ and $R = \gamma_{max}$, we get

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

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

Hence

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

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 3**. Using inequality between arithmetic and geometric means,

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

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

# 5 Algorithm to find spectrum and deficiency sum energy

In this section, we present an algorithm that helps in finding the spectrum and deficiency sum energy of a graph $G$. This algorithm consists of several functions and sub-algorithms. It takes $n$(order), $m$(size) and edge list of graph as inputs to give the exact value of spectrum and deficiency sum energy of $G$.

(i) Take $n$(order), $m$(size) and edge list of graph G as inputs.

(ii) Make adjacency matrix as adj.

(iii) Find the degree of each vertex and the maximum degree among these vertices.

```
deg = [ ]
for i = 0 to n − 1 :
        deg.append(sum(adj[i]))
maximum_degree = max(deg)
```

(iv) Find deficiency of each vertex.

```
def=[ ]
for i = 0 to n − 1 :
        def.append(maximum_degree-deg[i])
```

(v) Find deficiency sum matrix.

```
def_sum = [ ]
for i = 0 to n − 1 :
        for j = 0 to n − 1 :
                if adj[i][j] == 0 :
                    def_sum[i][j] = 0
                else:
                    def_sum[i][j]=def[i] + def[j]
```

(vi) Find eigenvalues of deficiency sum matrix.

(vii) Find deficiency sum energy by using absolute sum of eigenvalues.

A Python(3.8) code to find spectrum and deficiency sum energy of a graph $G$ is added as Appendix I

# 6 Conclusion

In this paper, we investigated the newly developed deficiency sum matrix $S_{df}(G)$ of a graph $G$. The deficiency sum polynomial of the graph $G$ has been solved for some of its coefficients. The deficiency sum energy $ES_{df}(G)$ has also been formulated for graph G. The influencing factors of deficiency sum energy $ES_{df}(G)$ are the underlying graph along with the deficiency on its vertices. Further, we have developed an algorithm and a python(3.8) code to find out spectrum and deficiency sum energy of $G$. The deficiency sum energy that is considered in this study may possibly have few applications in the field of chemistry along with some other study areas.

**Authors' contributions**: Omendra Singh wrote the main manuscript text, Pravin Garg wrote the algorithm to find spectrum and deficiency sum energy and Neha Kansal prepared Python 3.8 coding to find spectrum and deficiency sum energy. All authors reviewed the manuscript.
**Conflicts of Interest.** The authors declare that they have no conflicts of interest regarding the publication of this article.

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# Appendix I Coding (Python 3.8) to find spectrum and deficiency sum energy

```
from numpy.linalg import eig
import numpy as np
n = int(input())
m = int(input())
adj = []
for i in range(n):
    temp = []
    for j in range(n):
        temp.append(0)
    adj.append(temp)
for i in range(m):
    a,b = map(int,input().split())
    adj[a][b] = 1
    adj[b][a] = 1
deg = []
for i in range(n):
    deg.append(sum(adj[i]))
maximum_degree = max(deg)
defi = []
for i in range(n):
    defi.append(maximum_degree-deg[i])
def_sum = []
for i in range(n):
    def_sum.append([])
    for j in range(n):
        def_sum[i].append(0)
        if adj[i][j]==0:
```

```
            def_sum[i][j]=0
        else:
            def_sum[i][j] = defi[i]+defi[j]
print()
print("deficiency matrix of this graph is as following:")
for i in range(len(def_sum)):
    for j in range(len(def_sum[0])):
        print(def_sum[i][j],end=" ")
    print()
print()
m = np.array(def_sum)
w,v = eig(m)
print("Eigen values of this graph is = (",end="")
for i in range(len(w)):
    if i!=0:
        print("",end=",")
        print("",end="")
    print(w[i],end="")
print(")")
print()
ans = 0
for i in w:
    ans+=abs(i)
print("Energy of this graph is = ",end="")
print(ans)
```