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FIRST *KCD* MATRIX AND FIRST *KCD* ENERGY OF A GRAPH

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Abstract

In this article we introduce the concept of first Karnatak College Dharwad matrix of a graph G i.e., $KCD_1(G)$ and related energy of a graph G. Further, first KCD polynomial of some graphs, bounds for the largest first KCD eigenvalue and first KCD energy of graphs is determined.

Keywords: First KCD matrix, first KCD polynomial, first KCD eigenvalues, first KCD energy.

2010 AMS classification: 05C07, 05C50.

1. Introduction

Let $G = (V, E)$ be a simple, finite and undirected graph with $|V(G)| = n$ as the vertex set and $|E(G)| = m$ as the edge set. d_i is the *degree* of vertex v_i [4]. The minimum degree and maximum degree among the vertices of G is denoted as $\delta(G)$ and $\Delta(G)$ respectively [9].

The *adjacency matrix* $A(G) = [a_{ij}]$ for a graph G [9] with n vertices is a $n \times n$ matrix defined as

$$a_{ij} = \begin{cases} 1 & if\ v_i\ is\ adjacent\ to\ v_j, \\ 0 & otherwise\,. \end{cases}$$

The *characteristic polynomial* of $A(G)$ is given as $\phi(G:\lambda) = det(\lambda I - A(G))$, where λ is a variable of degree n and I is an identity matrix. The roots of the equation $\phi(G:\lambda) = 0$ are called the *eigenvalues* of G and are denoted as $\lambda_1, \lambda_2, \ldots, \lambda_n$. The *spectrum* $Spec(G)$ of a graph G is the collection of eigenvalues of G [5]. The *energy* $E(G)$ [8] of a graph G having adjacency matrix $A(G)$ with eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The *floor function* $\lfloor x \rfloor$ [9], for a real number x is defined as the greatest integer less than or equal to x. For undefined terminologies refer [9].

The energy concept was brought forward by Gutman in 1978 [8]. Following this, mathematical literature has received numerous contributions, like maximum degree energy of a graph [1], degree sum energy [13], degree product adjacency energy [10] and others. These energies are based on vertex degree which is interesting. The vertex degree and edge degree together makes the concept more fascinating and opens new areas of research. With this motivation we introduce *first Karnatak College Dharwad matrix* $KCD_1(G)$ and *first Karnatak College Dharwad energy* $E_{KCD_1}(G)$ of a graph G.

The *first* KCD *matrix* $KCD_1(G)$ of a graph G is defined as

$$kcd_{1_{ij}} = \begin{cases} (d_i + d_j) + d_e & if\ v_i\ is\ adjacent\ to\ v_j, \\ 0 & otherwise\,. \end{cases}$$

with d_i and d_j representing degree of vertex v_i and v_j respectively, d_e is the edge degree given by $d_e = d_i + d_j - 2$. It is a square matrix of order $n \times n$.

The *first* KCD *polynomial* of a graph G is defined as

$$P_{KCD_1(G)}(\beta) = det(\beta I - KCD_1(G))$$

with β as a variable of degree n and I as an identity matrix.

$\beta_1, \beta_2, \ldots, \beta_n$ represent the *first* KCD *eigenvalues* of $KCD_1(G)$. These are arranged as $\beta_1 \geqslant \beta_2 \geqslant \ldots \geqslant \beta_n$, where β_1 is the largest and β_n is the smallest *first* KCD eigenvalue and the collection of these *first* KCD eigenvalues is the first KCD spectra of G. The sum of all absolute *first* KCD eigenvalues $\beta_1, \beta_2, \ldots, \beta_n$ is called the *first* KCD *energy* $E_{KCD_1}(G)$ of a graph G.

Let J be a matrix with all entries as 1 and I is an identity matrix, then for an r-regular graph G with n vertices $KCD_1(G) = 2(2r-1)J - 2(2r-1)I$.

$$Thus, P_{KCD_1(G)}(\beta) = (\beta - 2(2r-1)(n-1))(\beta + 2(2r-1))^{n-1}. \tag{1.1}$$

Example: Let $H = K_4$ be a complete graph. The first KCD matrix, first KCD polynomial and first KCD energy of H are as follows

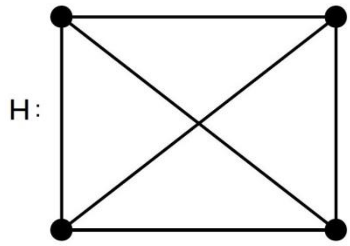

Figure 1: Complete graph

$$KCD_1(H) = \begin{pmatrix} 0 & 10 & 10 & 10 \\ 10 & 0 & 10 & 10 \\ 10 & 10 & 0 & 10 \\ 10 & 10 & 10 & 0 \end{pmatrix}$$

$$P_{KCD_1}(H) = \beta^4 - 600\beta^2 - 8000\beta - 30000$$
$$E_{KCD_1}(H) = 60.$$

2. Preliminaries

Definition 2.1 *([7]) For $n \geqslant 1$, the **ladder graph** L_n is defined as $L_n = P_2 \times P_n$, with P_n as a path graph of order n. For $n \geqslant 4$, the **wheel graph** W_n of order n is the graph $K_1 + C_{n-1}$, with K_1 as the singleton graph and C_{n-1} as the cycle graph. For $b \geqslant 3$, the **book graph** B_b is a graph defined as $B_b = K_{1,b} \times P_2$, with $K_{1,b}$ as the star graph and P_2 as the path graph. For $w \geqslant 3$, the **windmill graph** W_w^3 is the graph formed by taking 3 copies of the complete graph K_w with a vertex in common. For $f \geqslant 2$, the graph containing f copies of cycle C_3 meeting at a common vertex is the **friendship graph** F_f. For $n \geqslant 2$, the **pentagonal snake** PS_n is formed by replacing every edge of the path P_n of order n by a cycle C_5.*

Definition 2.2 *([11]) For $p \geqslant 1$, the **generalized book graph** $B_{5,p}$ is a graph having p copies of cycle C_5 with a common edge.*

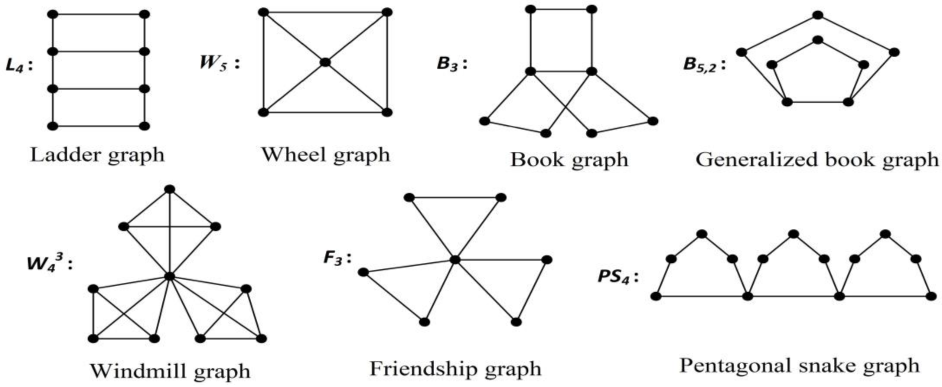

Figure 2: Examples of graphs mentioned in **Definitions 2.1** and **2.2.**

The results mentioned below are useful for computation of first KCD polynomial of some graphs, bounds for largest first KCD eigenvalue and first KCD energy of a graph.

Lemma 2.3 *([14]) If a, b, c and d are real numbers, then the determinant of the form*

$$\begin{vmatrix} (\beta + a)I_{n_1} - aJ_{n_1} & -cJ_{n_1 \times n_2} \\ -dJ_{n_2 \times n_1} & (\beta + b)I_{n_2} - bJ_{n_2} \end{vmatrix} \tag{2.1}$$

of order $n_1 + n_2$ can be expressed in the simplified form as

$$(\beta + a)^{n_1 - 1}(\beta + b)^{n_2 - 1}((\beta - (n_1 - 1)a)(\beta - (n_2 - 1)b) - n_1 n_2 cd).$$

The Cauchy-Schwarz inequality [2] says, if $(a_1, a_2, \ldots, a_n)$ and $(b_1, b_2, \ldots, b_n)$ are n real vectors, then

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leqslant \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) \tag{2.2}$$

Theorem 2.4 *([12]) Let a_i and b_i, $1 \leqslant i \leqslant n$ are nonnegative real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leqslant \frac{n^2}{4}(M_1 M_2 - m_1 m_2)^2 \qquad (2.3)$$

where $M_1 = \max_{1 \leqslant i \leqslant n}(a_i)$; $M_2 = \max_{1 \leqslant i \leqslant n}(b_i)$; $m_1 = \min_{1 \leqslant i \leqslant n}(a_i)$; $m_2 = \min_{1 \leqslant i \leqslant n}(b_i)$.

Theorem 2.5 *([3]) Let a_i and b_i, $1 \leqslant i \leqslant n$ are nonnegative real numbers, then*

$$\left|n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i\right| \leqslant \mu(n)(A-a)(B-b) \qquad (2.4)$$

where a, b, A and B are real constants, such that for each i, $1 \leqslant i \leqslant n$, $a \leqslant a_i \leqslant A$ and $b \leqslant b_i \leqslant B$. Further, $\mu(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right)$.

Theorem 2.6 *([6]) Let a_i and b_i, $1 \leqslant i \leqslant n$ are nonnegative real numbers, then*

$$\sum_{i=1}^{n} b_i^2 + c_1 c_2 \sum_{i=1}^{n} a_i^2 \leqslant (c_1 + c_2)\left(\sum_{i=1}^{n} a_i b_i\right) \qquad (2.5)$$

where c_1 and c_2 are real constants, such that for each i, $1 \leqslant i \leqslant n$ holds, $c_1 a_i \leqslant b_i \leqslant c_2 a_i$.

3. First KCD polynomial of some graphs

Theorem 3.1 *Let L_n be a ladder graph. Then*

$P_{KCD_1(L_n)}(\beta) = (\beta+6)^3(\beta+10)^{2n-5}((\beta-18)(\beta-10(2n-5)) - 256(2n-4))$.

Proof. The ladder graph L_n by definition has $2n$ vertices. Among these $2n$ vertices, 4 vertices have degree 2 and $2n-4$ vertices have degree 3.

Thus,

$$KCD_1(L_n) = \begin{bmatrix} 6(J_4 - I_4) & 8J_{4\times(2n-4)} \\ 8J_{(2n-4)\times 4} & 10(J_{2n-4} - I_{2n-4}) \end{bmatrix}$$

and

$$P_{KCD_1(L_n)}(\beta) = |\beta I - KCD_1(L_n)|$$
$$= \begin{vmatrix} (\beta+6)I_4 - 6J_4 & -8J_{4\times(2n-4)} \\ -8J_{(2n-4)\times 4} & (\beta+10)I_{2n-4} - 10J_{2n-4} \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.1 Let L_4 be a ladder graph. Then

$$P_{KCD_1(L_4)}(\beta) = (\beta+6)^3(\beta+10)^3((\beta-18)(\beta-30) - 1024).$$

Theorem 3.2 *Let W_n be a wheel graph. Then*

$$P_{KCD_1(W_n)}(\beta) = (\beta + 10)^{n-2}(\beta(\beta - 10(n-2)) - 4(n-1)(n+1)^2).$$

Proof. The wheel graph W_n by definition has n vertices. Among these n vertices, $n-1$ vertices of cycle C_{n-1} have degree 3 and a central vertex has degree $n-1$.

Thus,

$$KCD_1(W_n) = \begin{bmatrix} 10(J_{n-1} - I_{n-1}) & (2n+2)J_{(n-1)\times 1} \\ (2n+2)J_{1\times(n-1)} & J_1 - I_1 \end{bmatrix}$$

and

$$P_{KCD_1(W_n)}(\beta) = |\beta I - KCD_1(W_n)|$$

$$= \begin{vmatrix} (\beta + 10)I_{n-1} - 10J_{n-1} & -(2n+2)J_{(n-1)\times 1} \\ -(2n+2)J_{1\times(n-1)} & (\beta + 1)I_1 - J_1 \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.2 Let W_5 be a wheel graph. Then

$$P_{KCD_1(W_5)}(\beta) = (\beta + 10)^3(\beta(\beta - 30) - 576).$$

Theorem 3.3 *Let B_b be a book graph. Then*

$$P_{KCD_1(B_b)}(\beta) = (\beta + 6)^{2b-1}(\beta + 4b + 2)((\beta - 6(2b-1))(\beta - (4b+2)) - 16b(b+2)^2).$$

Proof. The book graph B_b by definition has $2b+2$ vertices. Among these $2b+2$ vertices, $2b$ vertices have degree 2 and 2 vertices have degree $b+1$.

Thus,

$$KCD_1(B_b) = \begin{bmatrix} 6(J_{2b} - I_{2b}) & (2b+4)J_{2b\times 2} \\ (2b+4)J_{2\times 2b} & (4b+2)(J_2 - I_2) \end{bmatrix}$$

and

$$P_{KCD_1(B_b)}(\beta) = |\beta I - KCD_1(B_b)|$$

$$= \begin{vmatrix} (\beta+6)I_{2b} - 6J_{2b} & -(2b+4)J_{2b\times 2} \\ -(2b+4)J_{2\times 2b} & (\beta+(4b+2))I_2 - (4b+2)J_2 \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.3 Let B_3 be a book graph. Then

$$P_{KCD_1(B_3)}(\beta) = (\beta+6)^5(\beta+14)((\beta-30)(\beta-14)-1200).$$

Theorem 3.4 *Let W_w^3 be a windmill graph. Then*

$$P_{KCD_1(W_w^3)}(\beta) = (\beta+4w-6)^{3w-4}(\beta(\beta-(3w-4)(4w-6)) - 12(w-1)(4w-5)^2).$$

Proof. The windmill graph W_w^3 by definition has $3w-2$ vertices. Among these $3w-2$ vertices, $3w-3$ vertices have degree $w-1$ and one vertex has degree $3(w-1)$.

Thus,

$$KCD_1(W_w^3) = \begin{bmatrix} (4w-6)(J_{3w-3} - I_{3w-3}) & (8w-10)J_{(3w-3)\times 1} \\ (8w-10)J_{1\times(3w-3)} & J_1 - I_1 \end{bmatrix}$$

and

$$P_{KCD_1(W_w^3)}(\beta) = |\beta I - KCD_1(W_w^3)|$$

$$= \begin{vmatrix} (\beta+(4w-6))I_{3w-3} - (4w-6)J_{3w-3} & -(8w-10)J_{(3w-3)\times 1} \\ -(8w-10)J_{1\times(3w-3)} & (\beta+1)I_1 - J_1 \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.4 Let W_4^3 be a windmill graph. Then

$$P_{KCD_1(W_4^3)}(\beta) = (\beta + 10)^8(\beta(\beta - 80) - 4356).$$

Theorem 3.5 *Let F_f be a friendship graph. Then*

$$P_{KCD_1(F_f)}(\beta) = (\beta + 6)^{2f-1}(\beta(\beta - 6(2f - 1)) - 8f(2f + 1)^2).$$

Proof. The friendship graph F_f by definition has $2f + 1$ vertices. Among these $2f + 1$ vertices, $2f$ vertices have degree 2 and one vertex has degree $2f$.

Thus,

$$KCD_1(F_f) = \begin{bmatrix} 6(J_{2f} - I_{2f}) & (4f + 2)J_{2f\times 1} \\ (4f + 2)J_{1\times 2f} & J_1 - I_1 \end{bmatrix}$$

and

$$P_{KCD_1(F_f)}(\beta) = |\beta I - KCD_1(F_f)|$$

$$= \begin{vmatrix} (\beta + 6)I_{2f} - 6J_{2f} & -(4f + 2)J_{2f\times 1} \\ -(4f + 2)J_{1\times 2f} & (\beta + 1)I_1 - J_1 \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.5 Let F_3 be a friendship graph. Then

$$P_{KCD_1(F_3)}(\beta) = (\beta + 6)^5(\beta(\beta - 30) - 1176).$$

Theorem 3.6 *Let PS_n be a pentagonal snake graph. Then*

$$P_{KCD_1(PS_n)}(\beta) = (\beta + 6)^{3n-2}(\beta + 14)^{n-3}((\beta - 6(3n - 2))(\beta - 14(n - 3)) - 100(3n - 1)(n - 2)).$$

Proof. The pentagonal snake PS_n by definition has $4n-3$ vertices. Among these $4n-3$ vertices, $3n-1$ vertices have degree 2 and $n-2$ vertices have degree 4.

Thus,

$$KCD_1(PS_n) = \begin{bmatrix} 6(J_{3n-1} - I_{3n-1}) & 10J_{(3n-1)\times(n-2)} \\ 10J_{(n-2)\times(3n-1)} & 14(J_{n-2} - I_{n-2}) \end{bmatrix}$$

and

$$P_{KCD_1(PS_n)}(\beta) = |\beta I - KCD_1(PS_n)|$$

$$= \begin{vmatrix} (\beta+6)I_{3n-1} - 6J_{3n-1} & -10J_{(3n-1)\times(n-2)} \\ -10J_{(n-2)\times(3n-1)} & (\beta+14)I_{n-2} - 14J_{n-2} \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.6 Let PS_4 be a pentagonal snake graph. Then

$$P_{KCD_1(PS_4)}(\beta) = (\beta+6)^{10}(\beta+14)((\beta-60)(\beta-14)-2200).$$

Theorem 3.7 *Let $B_{5,p}$ be a generalized book graph. Then*

$$P_{KCD_1(B_{5,p})}(\beta) = (\beta+6)^{3p-1}(\beta+4p+2)((\beta-6(3p-1))(\beta-(4p+2)) - 24p(p+2)^2).$$

Proof. The generalized book graph $B_{5,p}$ by definition has $3p+2$ vertices. Among these $3p+2$ vertices, $3p$ vertices have degree 2 and 2 vertices have degree $p+1$.

Thus,

$$KCD_1(B_{5,p}) = \begin{bmatrix} 6(J_{3p} - I_{3p}) & (2p+4)J_{3p\times 2} \\ (2p+4)J_{2\times 3p} & (4p+2)(J_2 - I_2) \end{bmatrix}$$

and

$$P_{KCD_1(B_{5,p})}(\beta) = |\beta I - KCD_1(B_{5,p})|$$

$$= \begin{vmatrix} (\beta+6)I_{3p} - 6J_{3p} & -(2p+4)J_{3p\times 2} \\ -(2p+4)J_{2\times 3p} & (\beta+(4p+2))I_2 - (4p+2)J_2 \end{vmatrix}.$$

Using Lemma (2.3), the desired result is obtained.

□

Illustration 3.7 Let $B_{5,2}$ be a generalized book graph. Then

$P_{KCD_1(B_{5,2})}(\beta) = (\beta+6)^5(\beta+10)((\beta-30)(\beta-10)-768)$.

4. Bounds for the largest first KCD eigenvalue and first KCD energy

Theorem 4.1 *The eigenvalues of* $KCD_1(G)$ *satifies the relations*

1. $\sum_{i=1}^{n} \beta_i = 0$

2. $\sum_{i=1}^{n} \beta_i^2 = 2Q, \quad where \quad Q = \sum_{i<j} 4(d_i + d_j - 1)^2.$

Proof. By the definition of $KCD_1(G)$,

$$\sum_{i=1}^{n} \beta_i = 0. \tag{4.1}$$

Further,

$$\sum_{i=1}^{n} \beta_i^2 = trace((KCD_1(G))^2)$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} d_{ji}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}^2$$

$$= 2\sum_{i<j} ((d_i + d_j) + d_e)^2, \; where \quad d_e = d_i + d_j - 2$$

$$= 2\sum_{i<j} 4(d_i + d_j - 1)^2$$

$$= 2Q, \; where \quad Q = \sum_{i<j} 4(d_i + d_j - 1)^2. \tag{4.2}$$

□

Illustration 4.1 For the graph H in the Figure 1, $\sum_{i=1}^{4} \beta_i = 0$ and $\sum_{i=1}^{4} \beta_i^2 = 2Q = 1200$.

Theorem 4.2 *If G is a graph with n vertices, then*

$$\beta_1 \leqslant \sqrt{\frac{2Q(n-1)}{n}}. \tag{4.3}$$

Proof. Let $a_i = 1$ and $b_i = \beta_i$ for $i = 1,2,\ldots,n$ in inequality (2.2)

then,

$$\left(\sum_{i=1}^{n} \beta_i\right)^2 \leqslant (n-1)\left(\sum_{i=1}^{n} \beta_i^2\right) \tag{4.4}$$

From Eqs. (4.1) and (4.2), we get

$$\sum_{i=2}^{n} \beta_i = -\beta_1 \quad and \quad \sum_{i=2}^{n} \beta_i^2 = 2Q - \beta_1^2.$$

Thus inequality (4.4) implies,

$$(-\beta_1^2) \leqslant (n-1)(2Q - \beta_1^2).$$

Hence,

$$\beta_1 \leqslant \sqrt{\frac{2Q(n-1)}{n}}.$$

Equality for β_1 holds if graph G is regular.

□

Illustration 4.2 Consider the graph W_5 in the Figure 2. It has $\beta_1 = 36$ and $2Q = 1952$, therefore satisfies inequality in Theorem 4.2. Further, for the regular graph H in the Figure 1, $\beta_1 = 30$ and $2Q = 1200$, thus satisfying the equality in the Theorem 4.2.

Theorem 4.3 *If G is a graph with n vertices, then*

$$\sqrt{2Q} \leqslant E_{KCD_1}(G) \leqslant \sqrt{2nQ}.$$

Proof. For $a_i = 1$ and $b_i = \beta_i$ in inequality (2.2)

we obtain,

$$\left(\sum_{i=1}^{n} |\beta_i|\right)^2 \leqslant n\left(\sum_{i=1}^{n} |\beta_i|^2\right)$$

Using definition of first KCD energy of a graph G and Eq. (4.2), we get

$$(E_{KCD_1}(G))^2 \leqslant 2nQ.$$

Thus,

$$E_{KCD_1}(G) \leqslant \sqrt{2nQ}. \tag{4.5}$$

Since,

$$(E_{KCD_1}(G))^2 = \left(\sum_{i=1}^{n} |\beta_i|\right)^2 \geqslant \sum_{i=1}^{n} |\beta_i|^2 = 2Q.$$

Thus,

$$E_{KCD_1}(G) \geqslant \sqrt{2Q}. \tag{4.6}$$

From Eqs. (4.5) and (4.6), required result is generated.

□

Illustration 4.3 Consider the graph W_5 in the Figure 2. It has $E_{KCD_1}(W_5) = 72$. Further, $2Q = 1952$ and $2nQ = 9760$, therefore satisfying the Theorem 4.3.

Theorem 4.4 *If G is a graph with n vertices, then*

$$E_{KCD_1}(G) \geqslant \sqrt{2nQ - \frac{n^2}{4}(|\beta_1| - |\beta_n|)^2}.$$

where $|\beta_1|$ is maximum and $|\beta_n|$ is minimum of the absolute value of $\beta_i's$.

Proof. For $a_i = 1$ and $b_i = \beta_i$ in inequality (2.3)

we obtain,

$$\sum_{i=1}^{n} 1^2 \sum_{i=1}^{n} |\beta_i|^2 - \left(\sum_{i=1}^{n} |\beta_i|\right)^2 \leqslant \frac{n^2}{4}(|\beta_1| - |\beta_n|)^2$$

$$2nQ - (E_{KCD_1}(G))^2 \leqslant \frac{n^2}{4}(|\beta_1| - |\beta_n|)^2$$

$$E_{KCD_1}(G) \geqslant \sqrt{2nQ - \frac{n^2}{4}(|\beta_1| - |\beta_n|)^2}.$$

□

Illustration 4.4 Consider the graph H in the Figure 1. It has $|\beta_1| = 30$, $|\beta_4| = 10$, $2nQ = 4800$, $n = 4$. Further $E_{KCD_1}(H) = 60$. Therefore it satisfies the Theorem 4.4.

Theorem 4.5 *If G is a (n, m) graph, then*

$$E_{KCD_1}(G) \geqslant \sqrt{2nQ - \mu(n)(|\beta_1| - |\beta_n|)^2}$$

where $\mu(n) = n\left\lfloor\frac{n}{2}\right\rfloor\left(1 - \frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\right)$.

Proof. Let $a_i = |\beta_i| = b_i$, $A = |\beta_1| = B$ and $a = |\beta_n| = b$ in inequality (2.4) then,

$$\left|n\sum_{i=1}^{n}|\beta_i|^2 - \left(\sum_{i=1}^{n}|\beta_i|\right)^2\right| \leqslant \mu(n)(|\beta_1| - |\beta_n|)^2 \tag{4.7}$$

Since,

$$E_{KCD_1(G)} = \sum_{i=1}^{n}|\beta_i| \quad and \quad \sum_{i=1}^{n}|\beta_i|^2 = 2Q.$$

Inequality (4.7) gives

$$2nQ - (E_{KCD_1}(G))^2 \leqslant \mu(n)(|\beta_1| - |\beta_n|)^2. \tag{4.8}$$

Simplification of inequality (4.8) generates desired result.

□

Illustration 4.5 For the graph H in the Figure 1, $|\beta_1| = 30$, $|\beta_4| = 10$, $2nQ = 4800$, $n = 4$, $\mu(n) = 4$. Further $E_{KCD_1}(H) = 60$. Thus it satisfies the Theorem 4.5.

Theorem 4.6 *If G is a (n, m) graph , then*

$$E_{KCD_1}(G) \geqslant \frac{2Q + n|\beta_1||\beta_n|}{|\beta_1| + |\beta_n|}$$

where $|\beta_1|$ is maximum and $|\beta_n|$ is minimum of the absolute value of $\beta_i's$.

Proof. Let $a_i = 1$, $b_i = |\beta_i|$, $c_1 = |\beta_n|$ and $c_2 = |\beta_1|$ in inequality (2.5) then,

$$\sum_{i=1}^{n} |\beta_i|^2 + |\beta_1||\beta_n| \sum_{i=1}^{n} 1^2 \leqslant (|\beta_1| + |\beta_n|)(\sum_{i=1}^{n} |\beta_i|) \tag{4.9}$$

Since,

$$E_{KCD_1(G)} = \sum_{i=1}^{n} |\beta_i| \quad and \quad \sum_{i=1}^{n} |\beta_i|^2 = 2Q.$$

Simplification of inequality (4.9) is

$$2Q + n|\beta_1||\beta_n| \leqslant (|\beta_1| + |\beta_n|)E_{KCD_1(G)}. \tag{4.10}$$

Simple calculation of inequality (4.10) yields the required result.

□

Illustration 4.6 Consider the graph H in the Figure 1, it has $|\beta_1| = 30$, $|\beta_4| = 10$, $2Q = 1200$, $n = 4$. Further $E_{KCD_1}(H) = 60$. Hence it satisfies the Theorem 4.6.

Theorem 4.7 *If G is a r-regular graph, then the first KCD eigenvalues of G are $-2(2r-1)$ and $2(n-1)(2r-1)$ with multiplicities (n-1) and 1 respectively and $E_{KCD_1}(G) = 4(n-1)(2r-1)$.*

Proof.

$$|\beta I - KCD_1(G)| = \begin{vmatrix} \beta & -2(2r-1) & -2(2r-1) & \cdots & -2(2r-1) \\ -2(2r-1) & \beta & -2(2r-1) & \cdots & -2(2r-1) \\ -2(2r-1) & -2(2r-1) & \beta & \cdots & -2(2r-1) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -2(2r-1) & -2(2r-1) & -2(2r-1) & \cdots & \beta \end{vmatrix}$$

$$= (\beta + 2(2r-1))^{n-1} \begin{vmatrix} \beta & -2(2r-1) & -2(2r-1) & \cdots & -2(2r-1) \\ -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & \cdots & 1 \end{vmatrix}$$

$$= (\beta - (n-1)2(2r-1))(\beta + 2(2r-1))^{n-1}.$$

Hence,

$$E_{KCD_1}(G) = 4(n-1)(2r-1).$$

□

Illustration 4.7 For the regular graph H in the Figure 1, the first KCD eigenvalues of H are -10 (3 times) and 30 (1 time). Thus $E_{KCD_1}(H) = 60$.

5. Conclusion

In this article, we have introduced a new graph matrix called first KCD matrix and its related energy. Further, the computation of first KCD polynomials of some graphs has added a depth to this concept. The work is extended with the calculation of bounds for the largest first KCD eigenvalue and first KCD energy of a graph.

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