Chapter 4

DISTANCE MATRIX OF SEMIGRAPHS AND ITS ENERGY

4.1 Introduction

Gopalapillai *et al.* [19] introduced the concept of distance matrix and energy on graphs in the year 2008, and the same will be defined as given below:

In case of connected graph G with p vertices and q edges, the distance matrix or *D*-matrix $D = [d_{ij}]$, is a square matrix of order p where, d_{ij} is the distance between the two vertices v_i and v_j.

The *D*-Matrix $D(G)$ of G is symmetric, and its eigenvalues $\mu_1, \mu_2, \mu_3, \dots \mu_p$ are all real, form *D*-spectrum of G. Then, distance energy or *D*-energy is defined as the sum of the absolute values of its *D*-eigenvalues, which is full analogy to the definition of graph energy introduced by Ivan Gutman [22] in the year 1978, for chemical graphs to approximate the total π-electron energy of a molecule.

Further, in the year 2013 M. R. Rajesh Khanna *et al.* [29] investigated minimum covering distance matrix and energy of a graph, and defined as follows:

Suppose $G(V, X)$ be a graph of order *n* and size *m*. Let *C* be a subset of the vertex set *V*, is the minimum covering set of a graph G. The minimum covering distance matrix of G is the square matrix of order n defined as $A_{MD}(G) = [d_{ij}]$,

where $d_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } v_i \in C \\ d(v_i, v_j) & \text{otherwise.} \end{cases}$

The characteristic polynomial of $A_{MD}(G)$ is denoted by $P_n(G, \lambda) = det[\lambda I - A_{MD}(G)]$. The minimum covering eigenvalues of the graph G are the eigenvalues of $A_{MD}(G)$. Since $A_{MD}(G)$ is real and symmetric, its eigenvalues are all real number and we label them in non-increasing order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. The minimum covering distance energy of G is defined as $E_{MD}(G) = \sum_{i=1}^{n} |\lambda_i|$.

E. Sampathkumar [15] in the year 1994 generalized the definition of a graph to semigraph and introduce an adjacency matrix which determines a semigraph uniquely.

In the year 2017, C. M. Deshpande, Y. S. Gaidhani and B.P. Athawale [65] defined adjacency matrix associated with a semigraph in another way as follows:

Let $G(V,X)$ be a semigraph with vertex set $V = \{v_1, v_2, \ldots, v_p\}$ and edge set $X = \{e_1, e_2, \ldots, e_q\}$. The Adjacency matrix of $G(V,X)$ is a $p \times p$ matrix $A = [a_{ij}]$ defined as follows:

1. For every edge e_i of X of cardinality, say k, let $e_i = (i_1, i_2, i_3, \ldots, i_k)$ such that $i_1, i_2, i_3, \ldots, i_k$ are distinct vertices in V, for all $i_r \in e_i$; $r = 1,2, \ldots, k$

   (a) $a_{i_1 i_r} = r - 1$ $\quad (b) a_{i_k i_r} = k - r$
2. All the remaining entries of A are zero.

On the other hand, a $p \times p$ matrix M is said to be semigraphical if there exists a semigraph G on p vertices with adjacency matrix equal to M. Again, Y. S. Gaidhani *et al.* [64] introduced energy of semigraph in the year 2019.

Thus, motivated from the above-mentioned works, our studies focus on the distance energy and minimum covering distance energy of semigraphs in this chapter.

4.2 Distance matrix and energy of semigraphs [51]

In this section we are trying to obtain the energy of distance matrix of a semigraph and some of its properties. Suppose $G(V,X)$ be a connected semigraph with vertex set $V = \{v_1, v_2, \ldots, v_p\}$ and edge set $X = \{e_1, e_2, \ldots, e_q\}$. Some definitions relating with this section are given follow:

Definition 4.2.1 Shortest path distance in semigraph

In a semigraph, shortest path distance between two vertices $d(u, v)$ is the number of edges in the shortest path between two vertices u and v. Clearly, distance between two distinct vertices on same edge is 1.

Definition 4.2.2 Distance matrix of a semigraph

If the shortest distance among all pairs of vertices in a connected semigraph $G(V, X)$ with p vertices can be arranged in a square matrix of order p. Then the matrix D obtained is a symmetric matrix known as distance matrix of a semigraph and defined as $D = [d_{ij}]_{p\times p}$

where $d_{ij}(v_i, v_j)$ = The number of edges in the shortest path from vertices v_i to v_j in G.

= 1, If vertices v_i and v_j lies in same edge.

= 0, If $v_i = v_j$.

Example 4.1 If $G(V, X)$ be a connected semigraph with vertex set $V = \{1,2,3,4,5,6,7,8\}$ and edge set $X = \{e_1(1,2,3), e_2(3,4), e_3(4,5,6), e_4(6,7,3), e_5(7,8)\}$. Then adjacency matrix D of the semigraph $G(V, X)$ is

$$D = \begin{bmatrix} 0 & 1 & 1 & 2 & 3 & 2 & 2 & 3 \\ 1 & 0 & 1 & 2 & 3 & 2 & 2 & 3 \\ 1 & 1 & 0 & 1 & 2 & 1 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 & 1 & 2 & 3 \\ 3 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 2 & 2 & 1 & 1 & 1 & 0 & 1 & 2 \\ 2 & 2 & 1 & 2 & 2 & 1 & 0 & 1 \\ 3 & 3 & 2 & 3 & 3 & 2 & 1 & 0 \end{bmatrix}$$

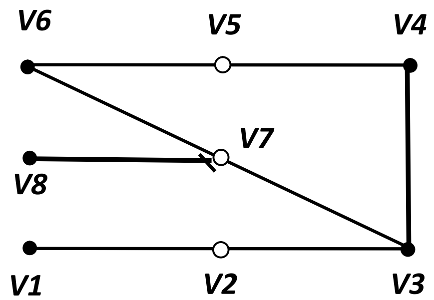

Figure 4.1

Definition 4.2.3 Eccentricity of a vertex

The maximum entry for a given row/column of the distance matrix of a semigraph is known as the eccentricity $e(v)$ of the vertex v

Definition 4.2.4 Diameter of a semigraph

The maximum eccentricity among the vertices is known as the diameter of a semigraph

Definition 4.2.5 Distance spectrum of semigraph

Distance matrix of a semigraph D is symmetric and all of its eigenvalues $\mu_1, \mu_2, \ldots \mu_p$ are real, are said to be D-eigenvalues of G and can be ordered as $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_p$ to form the distance spectrum (D-spectrum) of G.

Definition 4.2.6 Distance energy of semigraph

The distance energy of semigraph G is defined as $E_D(G) = \sum_{i=1}^{p} |\mu_i|$

Which is coincide with the definition of distance energy of a graph [19]. For a symmetric matrix, its singular values are same as their eigenvalues. Therefore, the definition of $E_D(G)$ is also put forward in full analogy to the definition of the matrix energy of semigraphs [64] denoted by $E(G)$ and is defined as the summation of the singular values of adjacency matrix of G.

4.2.1 Distance spectrum of some semigraphs and its properties:

In this section, we obtained some properties of the distance spectrum, and distance energy of semigraphs of diameter 2, and establish some theorems.

Semigraphs of diameter 2 and its distance matrix

If $G(V, X)$ be a semigraph with vertex set $V = \{v_1, v_2, .., v_p\}$ and edge set $X = \{e_1, e_2, \ldots, e_q\}$ then adjacency matrix $A = (a_{ij})$, of $G(V, X)$ is a $p \times p$ matrix whose entries are given by

a_{ij} = 1 ; if v_i, v_j are adjacent

= 0 ; otherwise.

Also, if A^c be the adjacency matrix of $\bar{G}$ (complement of *G*).

and, distance matrix $D = (d_{ij})$ of a semigraph of diameter 2 is defined as

d_{ij} = 0 ; If $v_i = v_j$.

= 1 ; If v_i, v_j are adjacent in *G*.

= 2 ; if v_i, v_j are adjacent in $\bar{G}$.

Then, the distance matrix of semigraph *G* of diameter 2 is $D = A + 2A^c$.

Example 4.2 $G(V, X)$ be a connected semigraph of diameter 2 with vertex set $V = \{1,2,3,4,5\}$ and edge set $X = \{e_1(1,2,3), e_2(3,4,5), e_3(1,5)\}$. Then adjacency matrix *D* of the semigraph $G(V, X)$ is

$$D = \begin{bmatrix} 0 & 1 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 1 & 1 \\ 2 & 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 1 & 0 \end{bmatrix}$$

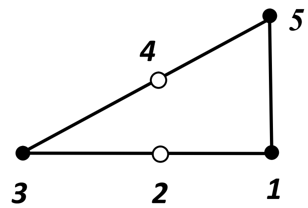

Figure 4.2

Lemma 4.1 If *G* be a semigraph of diameter 2 having order *p* and size *q*. Let $\mu_1, \mu_2, \ldots, \mu_p$ be *D*-eigenvalues of *G* then,

$$\sum_{i=1}^{p} \mu_i^2 = 2\left[2p^2 - 2p - 3\sum_{i=1}^{q} \binom{|e_i|}{2}\right]$$

Proof: In distance matrix *D* of semigraph G, there are $\left[2\sum_{i=1}^{q} \binom{|e_i|}{2}\right]$ entries equal to 1 and $\left[p(p-1) - 2\sum_{i=1}^{q} \binom{|e_i|}{2}\right]$ entries equal to 2.

Therefore,

$$\sum_{i=1}^{p} \mu_i^2 = \sum_{i=1}^{p} (D^2)_{ii}$$

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

As *D* is a symmetric matrix

$$\sum_{i=1}^{p} \boldsymbol{\mu_i^2} = \sum_{i=1}^{p}\sum_{j=1}^{p} \boldsymbol{d_{ij}}^2$$

$$= \left[2\sum_{i-1}^{q}\binom{|e_i|}{2}\right]1^2 + \left[p(p-1) - 2\sum_{i=1}^{q}\binom{|e_i|}{2}\right]2^2$$

$$= 2\left[2p(p-1) - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right]$$

4.2.2 Bounds for the spectral radius and distance energy:

Based on **Lemma 4.1**, and applying a technique analogous to what McClelland used for estimating graph energy [3], we arrive at the following two theorems.

Theorem 4.1 Let G be a connected semigraph of order p and degree q and of diameter 2. If $\Delta = |det\ D(G)|$ then

$$E_D \geq \sqrt{4p^2 - 4p - 6\sum_{i-1}^{q}\binom{|e_i|}{2} + p(p-1)\Delta^{2/p}}$$

With equality hold if and only if for all $1 \leq i < j \leq n$, $|\mu_i\mu_j| = c$ for some fixed real number c.

Proof: In view of the definition of *D*-energy of semigraph and using **Lemma 4.1**

$$E_D^2 = \left(\sum_{i=1}^{p}|\mu_i|\right)^2$$

$$= \sum_{i=1}^{p}\mu_i^2 + \sum_{i\neq j}|\mu_i|\,|\mu_j|$$

$$= 2\left[2p(p-1) - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right] + \sum_{i\neq j}|\mu_i\mu_j|$$

The right-hand side summation in the above expression goes over $p(p-1)$ summands. Thus, applying to it the inequality between the arithmetic and geometric means we have,

$$\frac{1}{p(p-1)}\sum_{i\neq j}|\mu_i\mu_j| \geq \left(\prod_{i\neq j}|\mu_i||\mu_j|\right)^{1/p(p-1)}$$

$$= \left(\prod_{i\neq j}|\mu_i|^{2(p-1)}\right)^{1/p(p-1)}$$

$$= \left(\prod_{i\neq j}|\mu_i|\right)^{2/p}$$

$$= \Delta^{2/p}$$

$$\sum_{i\neq j}|\mu_i|\,|\mu_j| \geq p(p-1)\Delta^{2/p}$$

Combining both the results we have,

$$E_D^2 \geq 2\left[2p(p-1) - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right] + p(p-1)\Delta^{2/p}$$

$i.e.$ $$E_D \geq \sqrt{4p^2 - 4p - 6\sum_{i-1}^{q}\binom{|e_i|}{2} + p(p-1)\Delta^{2/p}}$$

Theorem 4.2 Let G be a connected semigraph of order p and degree q and of diameter 2. Then

$$E_D \leq \sqrt{2p\left(2p^2 - 2p - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right)}$$

with equality hold if and only if for all $1 \leq i \leq n$, $|\mu_i| = c$ for some fixed real number c.

Proof: Expanding the expression given below we have,

$$\sum_{i=1}^{p}\sum_{j=1}^{p}(|\boldsymbol{\mu}_i| - |\boldsymbol{\mu}_j|)^2 = \sum_{i=1}^{p}\sum_{j=1}^{p}\left(|\mu_i|^2 + |\mu_j|^2 - 2|\mu_i||\mu_j|\right)$$

$$= p\sum_{i=1}^{p}|\mu_i|^2 + p\sum_{j=1}^{p}\left|\mu_j\right|^2 - 2\left(\sum_{i=1}^{p}|\mu_i|\right)\left(\sum_{j=1}^{p}\left|\mu_j\right|\right)$$

$$= 2\left(p\sum_{i=1}^{p}\mu_i^2 - E_D^2\right)$$

From the obvious relation

$$\sum_{i=1}^{p}\sum_{j=1}^{p}\left(|\mu_i| - \left|\mu_j\right|\right)^2 \geq 0$$

noting that equality holds if and only if all distance eigenvalues are mutually equal by absolute value.

We have

$$p\sum_{i=1}^{p}\mu_i^2 - E_D^2 \geq 0$$

Using **Lemma 4.1** yields

$$E_D^2 \leq 2p\left[2p(p-1) - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right]$$

i.e. $$E_D \leq \sqrt{2p\left[2p^2 - 2p - 3\sum_{i=1}^{q}\binom{|e_i|}{2}\right]}$$

Lemma 4.2 Let the distance eigenvalues of the semigraph *G* be labeled as $\mu_1 \geq \mu_2 \geq \mu_3 \geq \ldots \geq \mu_p$. If *G* is connected of diameter 2, then

$$\mu_1 \geq \frac{2}{p}\left[p(p-1) - \sum_{i=1}^{q}\binom{|e_i|}{2}\right]$$

Proof: According to the Rayleigh-Ritz variational principle, if *I* is any *p*-dimensional row matrix, then

$$\mu_1 \geq \frac{IDI^T}{II^T}$$

Setting $I = [1,1,1,\ldots,1]$, we get

$$\boldsymbol{IDI^T} = \sum_{i=1}^{p}\sum_{j=1}^{p} d_{ij}$$

$$= \mathbf{1}\,.\left[2\sum_{i=1}^{q}\binom{|e_i|}{2}\right] + 2\,.\left[p^2 - p - 2\sum_{i=1}^{q}\binom{|e_i|}{2}\right]$$

since the distance matrix has $2\sum_{i=1}^{q}\binom{|e_i|}{2}$ elements equal to 1 and $p^2 - p - 2\sum_{i=1}^{q}\binom{|e_i|}{2}$ elements equal to 2.

In addition, $II^T = p$. Hence, we get

$$\boldsymbol{\mu_1} \geq \frac{\mathbf{2}}{\boldsymbol{p}}\left[p(p-1) - \sum_{\boldsymbol{i=1}}^{\boldsymbol{q}}\binom{|e_i|}{2}\right]$$

Using **Lemma 4.2** and following a proof technique invented by Koolen and Moulton [23] we obtain another upper bound for the distance energy of connected semigraph of diameter 2.

Theorem 4.3 Let G be a connected semigraph of order *p* and degree *q* and of diameter 2.

$$\boldsymbol{E_D} \leq \frac{\mathbf{1}}{\boldsymbol{p}}\left[\boldsymbol{2p^2 - 2p - 2\sum_{i=1}^{q}\binom{|e_i|}{2}} + \sqrt{\boldsymbol{2p^2(p-1)\left[2p(p-1) - 3\sum_{i-1}^{q}\binom{|e_i|}{2}\right] - 4(p-1)\left[p(p-1) - \sum_{i-1}^{q}\binom{|e_i|}{2}\right]^2}}\right]$$

Proof: Applying the Cauchy-Schwarz inequality to the vectors $(1,1,1,\ldots.,1)$ and $(|\mu_2|, |\mu_3|, \ldots, |\mu_p|)$ we obtained

$$\left(\sum_{i=2}^{p}|\boldsymbol{\mu}_i|\right)^2 \le (\boldsymbol{p}-\mathbf{1})\sum_{i=2}^{p}\boldsymbol{\mu}_i^2$$

from which, recalling that $\mu_1 > 0$,

$$(\boldsymbol{E_D}-\boldsymbol{\mu}_1)^2 \le (\boldsymbol{p}-\mathbf{1})\left[\sum_{i=1}^{p}\boldsymbol{\mu}_i^2-\boldsymbol{\mu}_1^2\right] = (\boldsymbol{p}-\mathbf{1})\left(\mathbf{4}\boldsymbol{p}^2-\mathbf{4}\boldsymbol{p}-\mathbf{6}\sum_{i=1}^{q}\binom{|e_i|}{2}-\boldsymbol{\mu}_1^2\right)$$

$\boldsymbol{i.e.}$

$$\boldsymbol{E_D} \le \boldsymbol{\mu}_1 + \sqrt{(\boldsymbol{p}-\mathbf{1})\left(\mathbf{4}\boldsymbol{p}^2-\mathbf{4}\boldsymbol{p}-\mathbf{6}\sum_{i=1}^{q}\binom{|e_i|}{2}-\boldsymbol{\mu}_1^2\right)} \qquad (\mathbf{4.1})$$

Consider now the function

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{x} + \sqrt{(\boldsymbol{p}-\mathbf{1})\left(\mathbf{4}\boldsymbol{p}^2-\mathbf{4}\boldsymbol{p}-\mathbf{6}\sum_{i=1}^{q}\binom{|e_i|}{2}-\boldsymbol{x}^2\right)} \qquad (\mathbf{4.2})$$

Which is monotonically decreasing in the interval (a, b) where

$$a = \frac{2}{p}\left[p(p-1)-\sum_{i=1}^{q}\binom{|e_i|}{2}\right] \quad and \quad b = \sqrt{4p^2-4p-6\sum_{i=1}^{q}\binom{|e_i|}{2}}$$

as $a \ge 1$ for $a \le x^2$. But $a \le x \le x^2$ as $x \ge 1$.

Therefore, inequality (4.1) remains valid if on the right-hand side of (4.2) the variable *x* is replaced by the lower bound for μ_1 from **Lemma 2**.

Hence, we have

$\boldsymbol{E_D} \le$

$\frac{\mathbf{1}}{\boldsymbol{p}}\Bigg[\mathbf{2}\boldsymbol{p}^2-\mathbf{2}\boldsymbol{p}-$

$$2\sum_{i=1}^{q}\binom{|e_i|}{2}+$$

$$\sqrt{2p^2(p-1)\left[2p(p-1)-3\sum_{i-1}^{q}\binom{|e_i|}{2}\right]-4(p-1)\left[p(p-1)-\sum_{i-1}^{q}\binom{|e_i|}{2}\right]^2}\Bigg]$$

4.3 On minimum covering distance matrix and energy of semigraphs:

Definition 4.3.1 Suppose $G(V,X)$ be a connected semigraph of order n and size m with vertex set $V=\{v_1,v_2,\dots\dots,v_n\}$ and edge set $X=\{e_1,e_2,\dots\dots,e_m\}$. Let $C\subseteq V$ be the minimum covering set. The minimum covering distance matrix of G is the square matrix $D_{mc}(G)=[d_{ij}]$ of order n, whose (i,j)-element,

$$d_{ij}=\begin{cases}1 & if\ i=j\ and\ v_i\in C\\ d(v_i\,,v_j) & otherwise\end{cases}$$

where $d(v_i,v_j)$ is the distance between two vertices v_i and v_j in G.

Example 4.3 $G(V,X)$ be a connected semigraph as shown in **Figure 4.1** with vertex set $V=\{1,2,3,4,5,6,7,8\}$ and edge set

$X=\{e_1(1,2,3),e_2(3,4),e_3(4,5,6),e_4(6,7,3),e_5(7,8)\}$.

Let $C=\{3,4,7\}$ be the minimum covering set. Then,

Minimum covering distance matrix $D_{mc}(G)$ of the semigraph $G(V,X)$ is

$$D_{mc}(G)=\begin{bmatrix}0&1&1&2&3&2&2&3\\1&0&1&2&3&2&2&3\\1&1&1&1&2&1&1&2\\2&2&1&1&1&1&2&3\\3&3&2&1&0&1&2&3\\2&2&1&1&1&0&1&2\\2&2&1&2&2&1&1&1\\3&3&2&3&3&2&1&0\end{bmatrix}$$

Definition 4.3.2 The minimum covering distance matrix $D_{mc}(G)$ of a semigraph G is symmetric and hence its eigenvalues $\xi_1,\xi_2,\xi_3,\dots\dots,\xi_n$ are all real, called minimum covering distance eigenvalues of G. The minimum covering distance energy of a semigraph G is denoted by $E_{mc}^{D}(G)$ and defined as $E_{mc}^{D}(G) = \sum_{i=1}^{n}|\xi_i|$.

In this section, we are interested in realizing the mathematical aspects of the minimum covering distance energy of semigraphs. Some properties and bounds for minimum covering distance matrix and energy for a semigraph of diameter 2 are investigated as follows:

4.3.1 Properties of minimum covering distance energy of semigraphs:

Suppose $G(V,X)$ be a semigraph of diameter 2 having order n and size m, and let $C \subseteq V$ be the minimum covering set. Suppose $D_{mc}(G) = (d_{ij})_{n\times n}$ be the minimum covering distance matrix of G. Suppose characteristic polynomial of $D_{mc}(G)$ be

$$P_{mc}^{D}(G,\xi) = det(\xi I - D_{mc}(G)) = a_0\xi^n + a_1\xi^{n-1} + a_2\xi^{n-2} + a_3\xi^{n-3} + \ldots + a_n$$

Lemma 4.3. **[45]** If A is a real or complex square matrix of order n with eigenvalues $\xi_1, \xi_2, \xi_3, \ldots, \xi_n$, then for each $k \in \{1,2,3\ldots, n\}$, the number $S_k = (-1)^k a_k =$ the sum of the $k \times k$ principal minors of A, where a_k's are the coefficients of the characteristic polynomial of A, and S_k the k^{th} symmetric function of $\xi_1, \xi_2, \xi_3, \ldots, \xi_n$, is the sum of the products of the eigenvalues taken k at a time.

Theorem 4.4 Using the notations given above, we have

(a) $a_0 = 1$

(b) $a_1 = -|C|$

(c) $a_2 = \binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}$

where $|e_i|$ is the number of vertices in the edge $e_i \in X$.

Proof: (a) From the definition of the characteristic polynomial $P_{mc}^{D}(G,\xi) = det(\xi I - D_{mc}(G))$ of $D_{mc}(G)$, it is clear that $a_0 = 1$.

(b) $(-1)^1 a_1$ = Sum of all first order principal minors of $D_{mc}(G)$

= Trace of $D_{mc}(G) = |C|$

Thus $a_1 = -|C|$

(c) $(-1)^2 a_2$ = Sum of all the 2×2 principal minors of $D_{mc}(G)$

$$= \sum_{1 \le i < j \le n} \begin{vmatrix} d_{ii} & d_{ij} \\ d_{ji} & d_{jj} \end{vmatrix} = \sum_{1 \le i < j \le n} (d_{ii}d_{jj} - d_{ij}d_{ji}) = \binom{|C|}{2} - \sum_{i<j} d^2{}_{ij}$$

Since, G is a semigraph of diameter 2, then in its minimum covering distance matrix $D_{mc}(G)$, there are $|C|$ diagonal elements equal to 1 and other diagonal elements are 0.

Also, in $D_{mc}(G)$ there are $2\sum_{i=1}^{m}\binom{|e_i|}{2}$ non-diagonal entries are equal to 1 and other $n^2 - n - 2\sum_{i=1}^{m}\binom{|e_i|}{2}$ non-diagonal elements are equal to 2.

Thus, we have

$$2\sum_{i<j} d^2{}_{ij} = 1^2\left[2\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + 2^2\left[n(n-1) - 2\sum_{i=1}^{m}\binom{|e_i|}{2}\right]$$

$$\Rightarrow \sum_{i<j} d^2{}_{ij} = n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}$$

Hence, $$a_2 = \binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}$$

Theorem 4.5 If $\xi_1, \xi_2, \xi_3, \ldots, \xi_n$ are the eigenvalues of the minimum covering distance matrix $D_{mc}(G)$ of a semigraph $G(V, X)$ of order n, having m edges of diameter 2, and if C be the minimum covering set of G, then

$i.$ $$\sum_{i=1}^{n} \xi_i = |C|$$

$ii.$ $$\sum_{i=1}^{n} \xi_i^2 = 2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

where $|e_i|$ is the number of vertices in the edge $e_i \in X$.

Proof: i. Since, the sum of the eigenvalues of $D_{mc}(G)$ = The trace of $D_{mc}(G)$

Hence,

$$\sum_{i=1}^{n} \xi_i = \sum_{i=1}^{n} d_{ii} = |C|$$

ii. Consider

$$\sum_{i=1}^{n} \xi_i^2 = \sum_{i=1}^{n} \left((D_{mc})^2\right)_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}\, d_{ji}$$

As $D_{mc}(G)$ is a symmetric matrix

$$\sum_{i=1}^{n} \xi_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} {d_{ij}}^2 = 2\sum_{i<j}\left(d_{ij}\right)^2 + \sum_{i=1}^{n}(d_{ii})^2$$

$$= 2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

4.3.2 Bounds for minimum covering distance energy of semigraphs:

Using **Theorem 4.5**, and applying technique adopted by McClelland used for estimating graph energy [3], we obtain the following two theorems.

Theorem 4.6 If $G(V,X)$ be a semigraph having *n* vertices and *m* edges of diameter 2. Let C be the minimum covering set G, then

$$E_{mc}^{D}(G) \le \sqrt{2n\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + n|C|}$$

Proof: The minimum covering distance matrix $D_{mc}(G)$ of a semigraph G is symmetric and hence its eigenvalues are real and can be ordered as $\xi_1 \ge \xi_2 \ge \xi_3 \ge \ldots \ge \xi_n$.

Appling the Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^{n} u_i v_i\right)^2 \le \left(\sum_{i=1}^{n} u_i^2\right)\left(\sum_{i=1}^{n} v_i^2\right)$$

Substituting $u_i = 1$, $v_i = |\xi_i|$ in the above inequality and by **Theorem 4.5** we have

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

$$i.e. \qquad [E_{mc}^D(G)]^2 = n\left[2\left\{2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right\} + |C|\right]$$

$$Hence, \qquad E_{mc}^D(G) \leq \sqrt{2n\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + n|C|}$$

Theorem 4.7 Let $G(V,X)$ be a semigraph having *n* vertices and *m* edges of diameter 2, with the minimum covering set *C*. If $\Delta = |det\, D_{mc}(G)|$ then

$$E_{mc}^D(G) \geq \sqrt{2\left(2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right) + |C| + n(n-1)\Delta^{2/n}}$$

Proof: We have,

$$[E_{mc}^D(G)]^2 = \left(\sum_{i=1}^{n}|\xi_i|\right)^2 = \sum_{i=1}^{n}\xi_i^2 + \sum_{i\neq j}|\xi_i|\,|\xi_j|$$

By applying $AM \geq GM$, we have

$$\frac{1}{n(n-1)}\sum_{i\neq j}|\xi_i|\,|\xi_j| \geq \left(\prod_{i\neq j}|\xi_i||\xi_j|\right)^{1/n(n-1)}$$

$$= \left(\prod_{i\neq j}|\xi_i|^{2(n-1)}\right)^{1/n(n-1)}$$

$$= \left|\prod_{i\neq j}\xi_i\right|^{2/n}$$

$$= \Delta^{2/n}$$

$$i.e. \quad \sum_{i\neq j}|\xi_i|\,|\xi_j| \geq n(n-1)\Delta^{2/n}$$

$$Thus, \qquad [E^D_{mc}(G)]^2 \geq \sum_{i=1}^{n} \xi_i^2 + n(n-1)\Delta^{2/n}$$

Now using **Theorem 4.5**

$$[E^D_{mc}(G)]^2 \geq 2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C| + n(n-1)\Delta^{2/n}$$

Hence the result.

4.3.3 Some other bounds for minimum covering distance energy of semigraphs:

Theorem 4.8 Let $G(V,X)$ be semigraph of diameter 2 having order *n*, size *m* and if *C* be the minimum covering set. Then

$$E^D_{mc}(G) \geq \sqrt{2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2} + \left|\binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right|\right] + |C|}$$

Proof: Consider

$$[E^D_{mc}(G)]^2 = \left(\sum_{i=1}^{n}|\xi_i|\right)^2$$

$$= \sum_{i=1}^{n}|\xi_i|^2 + \sum_{i\neq j}|\xi_i|\,|\xi_j|$$

$$= \textstyle\sum_{i=1}^{n} {\xi_i}^2 + 2\sum_{i<j}|\xi_i|\,|\xi_j| \qquad (4.3)$$

$$We\ have, \qquad \sum_{1\leq i<j\leq n} \xi_i\xi_j = \sum_{1\leq i<j\leq n}\begin{vmatrix} d_{ii} & d_{ij} \\ d_{ji} & d_{jj}\end{vmatrix}$$

$$= \sum_{1\leq i<j\leq n}\left(d_{ii}d_{jj} - d_{ij}d_{ji}\right)$$

The minimum covering distance matrix $D_{mc}(G)$ is symmetric, thus $d_{ij} = d_{ji}$,

Therefore we have,

$$\sum_{1\leq i<j\leq n} \xi_i\xi_j = \sum_{1\leq i<j\leq n} d_{ii}d_{jj} - \sum_{1\leq i<j\leq n} d_{ij}d_{ji}$$

$$= \sum_{1\leq i<j\leq n} d_{ii}d_{jj} - \sum_{1\leq i<j\leq n} \left(d_{ij}\right)^2$$

$$= \binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}$$

$We\ know\ that,$ $$\sum_{i<j} |\xi_i|\,|\xi_j| \geq |\sum_{i<j} \xi_i\xi_j\,|$$

Thus $$\sum_{i<j} |\boldsymbol{\xi_i}|\,|\boldsymbol{\xi_j}| \geq \left|\binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right| \qquad (4.4)$$

Using inequation (4.3) and (4.4) and **Theorem 4.5**, we obtain

$$[\boldsymbol{E^D_{mc}(G)}]^2 \geq 2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2} + \left|\binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right|\right] + |C|$$

Taking positive square-root, we get

$$\boldsymbol{E^D_{mc}(G)} \geq \sqrt{2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2} + \left|\binom{|C|}{2} - 2n(n-1) + 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right|\right] + |C|}$$

Hence the result.

Theorem 4.9 Let $G(V,X)$ be a semigraph of order *n*, size *m* and having *C* be the minimum covering set, of diameter 2. Then

$$E^D_{mc}(G) \leq \mathbf{2}\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

Proof: Clearly,

$$n \leq 2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

Thus,

$$\boldsymbol{n}\left[2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|\right] \leq \left[\mathbf{2}\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|\right]^{\mathbf{2}}$$

Taking positive square-root, we get

$$\sqrt{2n\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + n|C|} \leq \mathbf{2}\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

Thus, by using **Theorem 4.6**

$$E_{mc}^{D}(G) \le \mathbf{2}\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C|$$

Theorem 4.10 Let $G(V, X)$ be a semigraph having order *n* and size *m* of diameter *2*, with the minimum covering set *C*. Let minimum covering distance eigenvalues of the matrix $D_{mc}(G)$ be $\xi_1 \ge \xi_2 \ge \xi_3 \ge \ldots \ge \xi_n$. Then

$$E_{mc}^{D}(G) \le |\xi_1| + \sqrt{(n-1)\left[2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C| - \xi_1^2\right]}$$

Proof: Let $\xi_1 \ge \xi_2 \ge \xi_3 \ge \ldots\ldots\ldots \ge \xi_n$ be the minimum covering distance eigenvalues of $D_{mc}(G)$. Appling the Cauchy-Schwarz inequality on to vectors $(|\xi_2|, |\xi_3|, \ldots, |\xi_n|)$ and $(1,1,\ldots,1)$ with $n-1$ entries,

$$\left(\sum_{i=2}^{n}|\xi_i|\right)^2 \le (n-1)\left(\sum_{i=2}^{n}|\xi_i|^2\right)$$

$i.e.$
$$\sum_{i=2}^{n}|\xi_i| \le \sqrt{(n-1)\left(\sum_{i=2}^{n}|\xi_i|^2\right)}$$

$i.e.$
$$\sum_{i=1}^{n}|\xi_i| - |\xi_1| \le \sqrt{(n-1)\left(\sum_{i=1}^{n}{\xi_i}^2 - \xi_1^2\right)}$$

By using **Theorem 4.5,** we have

$$E_{mc}^{D}(G) \le |\xi_1| + \sqrt{(n-1)\left[2\left[2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + |C| - \xi_1^2\right]}$$

Theorem 4.11 Let $G(V, X)$ be a semigraph having order *n* and size *m* of diameter *2* with the minimum covering set *C*. Let ξ_{max} be the largest absolute value of minimum covering distance eigenvalue. Then

$$E_{mc}^{D}(G) \ge \frac{1}{\xi_{max}}\left[2\left\{2n(n-1) - 3\sum_{i=1}^{m}\binom{|e_i|}{2}\right\} + |C|\right]$$

Proof: Let ξ_{max} be the largest absolute value of the minimum covering distance eigenvalue of $D_{mc}(G)$. Then

$$\xi_{max}|\xi_i| \geq \xi_i^2$$

Thus, $$\sum_{i=1}^{n} \xi_{max} |\xi_i| \geq \sum_{i=1}^{n} \xi_i^2$$

By **Theorem 4.5,** we have

$$\xi_{max} \sum_{i=1}^{n} |\xi_i| \geq \mathbf{2} \left[2n(n-1) - 3 \sum_{i=1}^{m} \binom{|e_i|}{2} \right] + |\boldsymbol{C}|$$

Hence, $$E_{mc}^{D}(G) \geq \frac{1}{\xi_{max}} \left[2 \left\{ 2n(n-1) - 3 \sum_{i=1}^{m} \binom{|e_i|}{2} \right\} + |C| \right]$$

Theorem 4.12 If $G(V, X)$ is a semigraph having order *n* and size *m* of diameter 2, and *C* be the minimum covering set of *G*. Let ξ_1 be the greatest minimum covering distance eigenvalue of $D_{mc}(G)$, then

$$\xi_1 \geq \frac{\mathbf{1}}{\boldsymbol{n}} \left[2n^2 - 2n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2} + |C| \right]$$

Proof: According to the Rayleigh-Ritz variational principle, if $I = [1, 1, \ldots, 1]^T$ is a n-dimensional column vector. Then $\xi_1 \geq \frac{I^T D_{mc}(G) I}{I^T I}$

Since in the minimum covering distance matrix $D_{mc}(G)$, there are $|C|$ diagonal elements equal to 1 and other diagonal elements are 0. Also, there are $2 \sum_{i=1}^{m} \binom{|e_i|}{2}$ non-diagonal entries are equal to 1 and other $n^2 - n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2}$ non-diagonal elements are equal to 2. In addition, $I^T I = n$ we have

$$\frac{1}{I^T I} [I^T D_{mc}(G) I] = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}$$

i.e. $$\frac{1}{I^T I} [I^T D_{mc}(G) I] = \frac{1}{n} \left[1 \left\{ 2 \sum_{i=1}^{m} \binom{|e_i|}{2} + |C| \right\} + 2 \left\{ n^2 - n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2} \right\} \right]$$

Thus, $$\xi_1 \geq \frac{\mathbf{1}}{\boldsymbol{n}} \left[|C| + 2n^2 - 2n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2} \right]$$

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