

Total Dominating Energy of Some Graphs

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Abstract : Let G be a finite, connected and not oriented graph with the vertex set $V(G)$ and edge set $E(G)$. We have estimated the total dominating energy of the complete, complete bipartite, doublestar, Barbell graph, and chemical structure of "acetaminophen". [10]

Keywords: total dominating set, total domination number, minimum total dominating matrix, minimum total dominating eigenvalues, total dominating energy of a graph.

I. INTRODUCTION

Gutman. I [5] presented the idea of "energy of the graph" during 1978. Let G be a graph with n vertices, m edges and that $A = (a_{ij})$ is the adjacency matrix of the graph. The eigen values $\lambda_1, \lambda_2, \lambda_3, \lambda_4, \dots, \lambda_{n-1}, \lambda_n$ of A , taken in descending order $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \dots \geq \lambda_{n-1} \geq \lambda_n$ are the eigenvalues of graph G . Since the adjacency matrix A of G is real and symmetric, its eigenvalues are real numbers. The "energy $E(G)$ of the graph" is the addition of the absolute values of the eigenvalues of the graph G i.e., $E(G) = \sum_{i=1}^n |\lambda_i|$. [4]

II. DEFINITIONS

2.1 Total Dominating Set : A set S of vertices on a graph $G(V, E)$ is said to be a "total dominating set" if every vertex $v \in V$ is adjoining a component of S . The "total domination number" $\gamma_t(G)$ is the smallest number of vertices detected on all the minimal total dominating set in a graph G . [9], [3]

2.2 Energy : "Energy of the graph" is the sum of the absolute values of the eigenvalues of the adjacency matrix A . It is represented by $E(G) = \sum_{i=1}^n |\lambda_i|$ where λ_i is an eigen values of A $i=1, 2, \dots, n$. [4], [6], [7]

2.3. Total Dominating Energy: Let G be a simple graph with set of vertices $V = v_1, v_2, \dots, v_n$ and the set of edges E .

Let MTDS be the minimum total dominating set of graph G . "The minimum total dominating matrix" of G is $A_{MTD}(G) = (a_{ij})$ where,

$$A_{MTD}(G) = \begin{cases} 1; & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 1; & \text{if } i = j, v_i \in MTDS \\ 0; & \text{otherwise} \end{cases}$$

The "characteristic polynomial" of $A_{MTD}(G)$ is indicated by $\text{Det}(A_{MTD}(G) - \lambda I)$. The "minimum total dominating eigenvalues" of graph G are the eigenvalues of $A_{MTD}(G)$. They are $\lambda_1, \lambda_2, \dots, \lambda_n$ in decreasing order $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. The 'total dominating energy' of G is given by $E_{TD}(G) = \sum_{i=1}^n |\lambda_i|$. [9]

Note that the trace of $(a_{ij}) = \text{Total Domination Number} = k$

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Example:

Consider a graph G with $V(G) = \{v_1, v_2, v_3, v_4, v_5, v_6\}$.

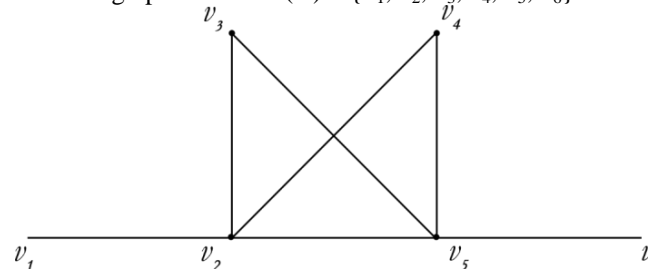


Figure (2.1)

MTDS = $\{v_2, v_5\}$

$\gamma_t(G) = 2$.

$$A_{MTD}(G) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

The characteristic equation is

$$x^6 - 2x^5 - 6x^4 + x^3 + 3x^2 = 0$$

The eigen values are $\lambda_1 = 3.5454, \lambda_2 = 0.7341, \lambda_3 = -1.5224, \lambda_4 = -0.7571, \lambda_5 = 0, \lambda_6 = 0$.

$E_{TD}(G) = 6.559$.

III. DEFINITIONS OF SOME GRAPHS

Definition 3.1 "Complete Graph" K_n : It is a graph in which each pair of vertices is connected by an edge. [11]

Definition 3.2 "Complete Bipartite Graph" $K_{n,n}$: It is a graph whose vertices are partitioned into two disjoint sets V_1 and V_2 such that every pair of vertices in the two sets are adjacent and no two vertices within the same set are adjacent. [11]

Definition 3.3 "Double Star Graph" $S_{r,t}$: It is obtained by joining the center of two stars $K_{1,n}$ and $K_{1,m}$ with an edge. [8]

Definition 3.4 "Barbell Graph" $B_{p,n}$: It is the graph obtained by connecting two copies of the complete graph with a cut edge. [11]

Definition 3.5 "Book Graph" B_m : It is a graph of Cartesian product of star graph and two - node path. [11]

IV. RESULTS ON TOTAL DOMINATING ENERGY OF SOME GRAPHS

Theorem 4.1 :

If $n \geq 2$ then, $E_{TD}(K_n)$ is equal to

$$|(n-3)| + \left| \frac{-(1-n) \pm \sqrt{n^2 - 2n + 9}}{2} \right|$$

Proof: K_n is the complete graph with $V = \{x_1, x_2, \dots, x_n\}$. The $MTDS(K_n) = \{x_1, x_2\}$ and $\gamma_t(K_n) = \{x_1, x_2\}$ Then,



$$A_{MTD}(K_n) = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 0 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & \dots & 0 \end{pmatrix}$$

The characteristic polynomial is

$$\text{Det}(A_{MTD}(K_n) - \lambda I) = \begin{pmatrix} 1 - \lambda & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 - \lambda & 1 & 1 & \dots & 1 \\ 1 & 1 & -\lambda & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & \dots & -\lambda \end{pmatrix}$$

The characteristic equation is

$$\lambda(\lambda + 1)^{(n-3)}(\lambda^2 - (n-1)\lambda - 2) = 0$$

The eigenvalues :

$$\lambda=0, \lambda = -1 [(n-3)\text{times}], \lambda = \frac{-(1-n) \pm \sqrt{n^2-2n+9}}{2}$$

Then,

$$E_{TD}(K_n) = |(n-3)| + \left| \frac{-(1-n) \pm \sqrt{n^2-2n+9}}{2} \right|.$$

Theorem 4.2 :

If $n \geq 2$ then, $E_{TD}(K_{n,n})$ is equal to

$$\sqrt{n^2 + 2n - 3} + (n + 1)$$

Proof: $K_{n,n}$ is the complete bipartite graph with $V = \{r_1, s_1, r_2, s_2, \dots, r_n, s_n\}$. The $MTDS(K_{n,n}) = (r_1, s_1)$ and is $\gamma_t(K_{n,n}) = (r_1, s_1)$. Then

$$A_{MTD}(K_{n,n}) = \begin{pmatrix} 1 & 0 & 0 & \dots & 1 & 1 & 1 \\ 0 & 0 & 0 & \dots & 1 & 1 & 1 \\ 0 & 0 & 0 & \dots & 1 & 1 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 0 & 0 & 0 \\ 1 & 1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 0 & 0 & 0 \end{pmatrix}$$

The characteristic polynomial is

$$\text{Det}(A_{MTD}(K_{n,n}) - \lambda I) = \begin{pmatrix} 1 - \lambda & 0 & 0 & \dots & 1 & 1 & 1 \\ 0 & -\lambda & 0 & \dots & 1 & 1 & 1 \\ 0 & 0 & -\lambda & \dots & 1 & 1 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & -\lambda & 0 & 0 \\ 1 & 1 & 1 & \dots & 0 & -\lambda & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \dots & 0 & 0 & -\lambda \end{pmatrix}$$

The characteristic equation is

$$\lambda^{2n-4} [\lambda^2 + (n-1)\lambda - (n-1)] [\lambda^2 - (n+1)\lambda + (n-1)] = 0$$

The eigenvalues are,

$$\lambda=0, \lambda = \frac{-(n-1) \pm \sqrt{n^2+2n-3}}{2}, \lambda = \frac{(n+1) \pm \sqrt{n^2-2n+5}}{2}$$

Then,

$$E_{TD}(K_{n,n}) = \sqrt{n^2 + 2n - 3} + (n+1).$$

Theorem 4.3:

If $n \geq 2$ with $r+t$ vertices then, $E_{TD}(S_{r,t})$ is equal to

$$2 \left(\sqrt{\frac{n}{2} - 1} \right) + \left| \left(1 + \sqrt{\frac{n}{2}} \right) \right| + \left| \left(1 - \sqrt{\frac{n}{2}} \right) \right|.$$

Proof: $S_{r,t}$ be the Double Star graph with

$V = \{u_1, w_1, u_2, w_2, \dots, u_n, w_n\}$. The $MTDS(S_{r,t}) = \{u_1, w_1\}$ and $\gamma_t(S_{r,t}) = \{u_1, w_1\}$. Then,

$$A_{MTD}(S_{r,t}) = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \dots & 1 & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 \end{pmatrix}$$

The characteristic polynomial is

$$\text{Det}(A_{MTD}(S_{r,t}) - \lambda I) = \begin{pmatrix} 1 - \lambda & 1 & 1 & \dots & 1 & 0 & 0 & \dots & 0 \\ 1 & -\lambda & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & -\lambda & \dots & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \dots & 1 - \lambda & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & \dots & 1 & -\lambda & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 & \dots & -\lambda \end{pmatrix}$$

The characteristic equation is

$$\lambda^{n-4} \left[\lambda^2 - \left(\frac{n}{2} - 1 \right) \right] \left[\lambda^2 - 2\lambda - \left(\frac{n}{2} - 1 \right) \right] = 0$$

The eigenvalues are

$$\lambda = 0, \lambda = \pm \sqrt{\frac{n}{2} - 1}, \lambda = 1 \pm \left(\sqrt{\frac{n}{2}} \right)$$

Then,

$$E_{TD}(S_{r,t}) = 2 \left(\sqrt{\frac{n}{2} - 1} \right) + \left| \left(1 + \sqrt{\frac{n}{2}} \right) \right| + \left| \left(1 - \sqrt{\frac{n}{2}} \right) \right|.$$

Theorem 4.4:

If $n \geq 2$ then, $E_{TD}(B_{p,n})$ is equal to

$$\frac{3n}{2} - 4 + \left| \frac{n + \sqrt{n^2 - 8n + 48}}{4} \right| + \left| \frac{n - \sqrt{n^2 - 8n + 48}}{4} \right|.$$

Proof : $B_{p,n}$ is a Barbell graph with $V = \{w_1, w_2, w_3, w_4, \dots, w_{2n}\}$. The $MTDS(B_{p,n}) = (w_1, w_2)$ and is $\gamma_t(B_{p,n}) = \{w_1, w_2\}$. Then

$$A_{MTD}(B_{p,n}) = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & 1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \dots & 1 & 1 & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & 0 & \dots & 1 & 0 & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & 0 & \dots & 1 & 1 & 0 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & 1 & 1 & 1 & \dots & 0 \end{pmatrix}$$

The characteristic polynomial is

$$\text{Det}(A_{MTD}(B_{p,n}) - \lambda I) = \begin{pmatrix} 1 - \lambda & 1 & 1 & 1 & \dots & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -\lambda & 1 & 1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & -\lambda & 1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \dots & 1 - \lambda & 1 & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & 0 & \dots & 1 & -\lambda & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & 0 & \dots & 1 & 1 & -\lambda & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & 1 & 1 & 1 & \dots & -\lambda \end{pmatrix}$$

The characteristic equation is

$$\left[\lambda - \left(\frac{n}{2} - 1 \right) \right] (\lambda + 1)^{n-3} \left[\lambda^2 - \left(\frac{n}{2} \right) \lambda + \left(\frac{n}{2} - 3 \right) \right] = 0$$

The eigenvalues are,

$$\lambda = \left(\frac{n}{2} - 1 \right), \lambda = -1 [(n-3)\text{times}], \lambda = \frac{n \pm \sqrt{n^2 - 8n + 48}}{4}$$

Then,



$$E_{TD}(B_{p,n}) = \frac{3n}{2} - 4 + \left| \frac{n + \sqrt{n^2 - 8n + 48}}{4} \right| + \left| \frac{n - \sqrt{n^2 - 8n + 48}}{4} \right|$$

Theorem 4.5:

The $E_{TD}(B_m)$ is equal to

$$(n-4) + \left| \frac{3 + \sqrt{2n-3}}{2} \right| + \left| \frac{-1 + \sqrt{2n-3}}{2} \right|$$

Proof : B_m is a Book graph with $V = \{m_1, m_2, \dots, m_n\}$. The $MTDS(B_m) = \{m_1, m_2\}$ and $\gamma_t(B_m) = (m_1, m_2)$. Then ,

$$A_{MTD}(B_m) = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 0 & \dots & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & \dots & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 & \dots & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix}$$

The Characteristic polynomial is

$$\text{Det}(A_{MTD}(B_m) - \lambda I) = \begin{vmatrix} 1-\lambda & 1 & 0 & 0 & 1 & 0 & \dots & 1 & 0 \\ 1 & 1-\lambda & 0 & 1 & 0 & 1 & \dots & 0 & 1 \\ 1 & 0 & -\lambda & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 1 & -\lambda & 1 & 1 & \dots & 0 & 0 \\ 1 & 0 & 0 & 0 & -\lambda & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & -\lambda & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \dots & -\lambda & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & \dots & 1 & -\lambda \end{vmatrix}$$

The Characteristic equation is

$$(\lambda + 1)^{\left(\frac{n}{2} - 2\right)} (\lambda - 1)^{\left(\frac{n}{2} - 2\right)} \left[\lambda^2 + \lambda - \left(\frac{n}{2} - 1\right) \right] \left[\lambda^2 + \lambda - \left(\frac{n}{2} - 3\right) \right] = 0$$

The eigenvalues are

$$\lambda = -1 \left[\left(\frac{n}{2} - 2\right) \text{ times} \right], \lambda = 1 \left[\left(\frac{n}{2} - 2\right) \text{ times} \right], \lambda = \frac{3 \pm \sqrt{2n-3}}{2}, \lambda = \frac{-1 \pm \sqrt{2n-3}}{2}$$

Then,

$$E_{TD}(B_m) = (n-4) + \left| \frac{3 + \sqrt{2n-3}}{2} \right| + \left| \frac{-1 + \sqrt{2n-3}}{2} \right|$$

Theorem 4.6:

The $E_{TD}(C_8H_9NO_2) = 14.1569$.

Proof: Consider a molecular structure of acetaminophen ($C_8H_9NO_2$) with vertices from y_1 to y_{11} .

The $MTDS = \{y_1, y_2\}$ and $\gamma_t = \{y_1, y_2\}$. Then

$$A_{MTD}(C_8H_9NO_2) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

The Characteristic polynomial is

$$\text{Det}(A_{MTD}(C_8H_9NO_2) - \lambda I) =$$

$$\begin{pmatrix} -\lambda & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1-\lambda & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & -\lambda & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1-\lambda & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1-\lambda & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1-\lambda & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1-\lambda & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1-\lambda \end{pmatrix}$$

The Characteristic equation is

$$\lambda^{11} - 6\lambda^{10} + 4\lambda^9 + 31\lambda^8 - 39\lambda^7 - 52\lambda^6 + 66\lambda^5 + 36\lambda^4 - 29\lambda^3 - 8\lambda^2 + 2\lambda = 0$$

The eigen values are

$$\lambda_1 = 3.0422, \lambda_2 = 2.5965, \lambda_3 = 2.0356, \lambda_4 = 1.5127, \lambda_5 = -1.6634, \lambda_6 = -1.2124, \lambda_7 = 0.7195, \lambda_8 = -0.7800, \lambda_9 = -0.4227, \lambda_{10} = 0.1719, \lambda_{11} = 0$$

The $E_{TD}(C_8H_9NO_2) =$

$$|3.0422| + |2.5965| + |2.0356| + |1.5127| + |-1.6634| + |-1.2124| + |0.7195| + |-0.7800| + |-0.4227| + |0.1719| + |0| = 14.1569$$

$$E_{TD}(C_8H_9NO_2) = 14.1569$$

V. PROPERTIES OF EIGENVALUES OF TOTAL DOMINATING SET

Theorem 5.1 :

We shall consider the graph with $V = \{p_1, p_2, \dots, p_n\}$ as vertex set and q edges. $MTDS = \{t_1, t_2, \dots, t_k\}$. If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigen values of $A_{MTD}(G)$ then:

- i) $\sum_{i=1}^n \lambda_i = |TD|$;
- ii) $\sum_{i=1}^n \lambda_i^2 = 2|q| + |TD|$.

Proof: (i) since “trace of $A_{MTD}(G) = \sum_{i=1}^n \lambda_i$ ” [1]

$$\sum_{i=1}^n \lambda_i = \sum_{i=1}^n a_{ii} = |TD| = k$$

(ii) Since “trace of $[A_{MTD}(G)]^2 = \sum_{i=1}^n \lambda_i^2$ ” [1]

$$\begin{aligned} \sum_{i=1}^n \lambda_i^2 &= \sum_{i=1}^n \sum_{j=1}^n a_{ij} a_{ji} \\ &= \sum_{i=1}^n (a_{ii})^2 + \sum_{i \neq j} a_{ij} a_{ji} \\ &= \sum_{i=1}^n (a_{ii})^2 + 2 \sum_{i < j} (a_{ij})^2 \\ &= |TD| + 2|q| \end{aligned}$$

VI. BOUNDS FOR TOTAL DOMINATING ENERGY

Theorem 6.1:

Let us take the graph with p vertices , and q edges. $\gamma_t = k$. If $\lambda_1, \lambda_2, \dots, \lambda_p$ are the eigen values of minimum total dominating matrix $A_{TD}(G)$ then $E_{TD}(G) \leq \sqrt{p(2q+k)}$.

Proof : Cauchy Schwarz inequality is

$$\left(\sum_{i=1}^p a_i b_i \right)^2 \leq \left(\sum_{i=1}^p a_i^2 \right) \left(\sum_{i=1}^p b_i^2 \right)$$

If $a_i = 1, b_i = |\lambda_i|$ then,

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

$$[E_{TD}(G)]^2 \leq p(2q+k) \quad [\text{Theorem 5.1}]$$

$$\Rightarrow E_{TD}(G) \leq \sqrt{p(2q+k)}$$

Theorem 6.2 :

If G is a graph with p vertices, q edges, $(2q+k) \geq p$, and $\lambda_1(G) \geq \frac{2q+k}{p}$ then

$$E_{TD}(G) \leq \frac{(2q+k)}{p} + \sqrt{(p-1)\left[(2q+k) - \left(\frac{2q+k}{p}\right)^2\right]}$$

Where k = total domination number.

Proof : Cauchy Schwarz inequality is

$$\left(\sum_{i=1}^p a_i b_i\right)^2 \leq \left(\sum_{i=1}^p a_i^2\right) \left(\sum_{i=1}^p b_i^2\right)$$

Put $a_i = 1, b_i = |\lambda_i|$ then

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

$$\Rightarrow [E_{TD}(G) - \lambda_1]^2 \leq (p-1)(2q+k - \lambda_1^2)$$

$$\Rightarrow E_{TD}(G) \leq \lambda_1 + \sqrt{(p-1)(2q+k - \lambda_1^2)}$$

Let $f(x) = x + \sqrt{(p-1)(2q+k - x^2)}$

For decreasing function,

$$f'(x) \leq 0 \Rightarrow 1 - \frac{x(p-1)}{\sqrt{(p-1)(2q+k-x^2)}} \leq 0$$

$$\Rightarrow x \geq \sqrt{\frac{2q+k}{p}}$$

Since $(2q+k) \geq p$, we have $\sqrt{\frac{2q+k}{p}} \leq \frac{2q+k}{p} \leq \lambda_1$

$$f(\lambda_1) \leq f\left(\frac{2q+k}{p}\right)$$

$$\text{i.e., } E_{TD} \leq f(\lambda_1) \leq \left(\frac{2q+k}{p}\right)$$

$$\text{i.e., } E_{TD} \leq f\left(\frac{2q+k}{p}\right)$$

$$\text{i.e., } E_{TD} \leq \frac{(2q+k)}{p} + \sqrt{(p-1)\left[(2q+k) - \left(\frac{2q+k}{p}\right)^2\right]}$$

VII. CONCLUSION

We evaluated E_{TD} of complete, complete bipartite, double star, Barbell, Book graph and chemical structure of acetaminophen. In future, we will work on double domination.

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