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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 λ_1, λ_2, λ_3, λ_4,…..,λ_{n-1}, λ_n of A, taken in descending order $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \ldots\ldots \geq \lambda_{n-1} \geq \lambda_n$ 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∈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,……..,n. [4],[6],[7]

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

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

The "characteristic polynomial" of A_{MTD} (G) is indicated by Det (A_{MTD} (G) – λI). The "minimum total dominating eigenvalues" of graph G are the eigenvalues of $A_{MTD}(G)$. They are λ_1, λ_2,…….., λ_n in decreasing order $\lambda_1 \geq \lambda_2 \geq \ldots\ldots \lambda_n$. 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}) = 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}.

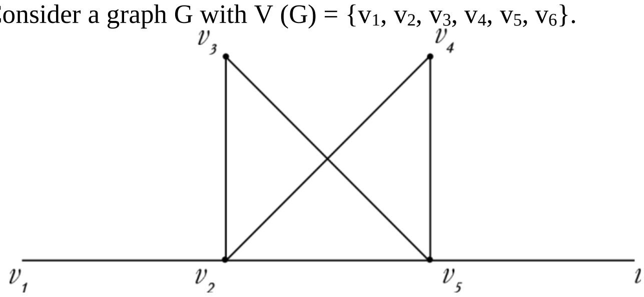

Figure (2.1)

MTDS = {v_2, v_5}

γ_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 λ_1=3.5454, λ_2 =0.7341, λ_3 = -1.5224, λ_4=-0.7571, λ_5 = 0, λ_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, ……..,x_n}. The MTDS(K_n) = {x_1, x_2} and $\gamma_t(K_n)$ = {x_1,x_2} Then,

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

The characteristic polynomial is

Det $(A_{MTD}(K_n) - \lambda I)$

$$= \begin{pmatrix} 1-\lambda & 1 & 1 & 1 & \cdots & 1 \\ 1 & 1-\lambda & 1 & 1 & \cdots & 1 \\ 1 & 1 & -\lambda & 1 & \cdots & 1 \\ 1 & 1 & 1 & -\lambda & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & \cdots & -\lambda \end{pmatrix}$$

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 $V=\{r_1, s_1, r_2, s_2, \ldots\ldots, r_n, s_n\}$. The MTDS$(K_{n,n}) = (r_1, s_1)$ and is $\gamma_t(K_{n,n}) = (r_1, s_1)$. Then

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

The characteristic polynomial is

Det $(A_{MTD}(K_{n,n}) - \lambda I) =$

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

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

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

The characteristic polynomial is

Det $(A_{MTD}(S_{r,t}) - \lambda I) =$

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

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 $V=\{w_1, w_2, w_3, w_4, \ldots\ldots, w_{2n}\}$. The MTDS$(B_{p,n})=(w_1,w_2)$ and $\gamma_t(B_{p,n}) = \{w_1, w_2\}$. Then

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

The characteristic polynomial is

Det $(A_{MTD}(B_{p,n}) - \lambda I) =$

$$\begin{pmatrix} 1-\lambda & 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -\lambda & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & -\lambda & 1 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & 1-\lambda & 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & 0 & \ldots & 1 & -\lambda & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & 0 & \ldots & 1 & 1 & -\lambda & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 1 & \cdots & -\lambda \end{pmatrix}$$

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,

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

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

Proof : B_m is a Book graph with V={m_1, m_2,………m_n}. The MTDS (B_m)= {m_1, m_2} and γ_t(B $_m$)=(m_1,m_2). Then ,

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

The Characteristic polynomial is

Det (A_{MTD}(B $_m$) – λI)=

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

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

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 γ_t= {y_1,y_2}. Then

A_{MTD}($C_8H_9NO_2$) =

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

The Characteristic polynomial is

Det (A_{MTD}($C_8H_9NO_2$) – λI) =

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

The Characteristic equation is

$\lambda^{11} - 6\lambda^{10} + 4\lambda^9 + 31\lambda^8 - 39\lambda^7 - 52\lambda^6 + 66\lambda^5 + 36\lambda^4 - 29\lambda^3 - 8\lambda^2 + 2\lambda^1 = 0$

The eigen values are

λ_1=3.0422, λ_2=2.5965, λ_3=2.0356, λ_4= 1.5127, λ_5= -1.6634, λ_6= -1.2124, λ_7= 0.7195, λ_8= -0.7800, λ_9= -0.4227,λ_{10} =0.1719, λ_{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,…..,p_n} as vertex set and q edges. MTDS={t_1,t_2,…..,t_k}. If λ_1 , λ_2 ,….., λ_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. γ_t =k. If λ_1, λ_2, …..,λ_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

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

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) [Theorem 5.1]

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

Theorem 6.2 :

If G is a graph with p vertices, q edges, (2q+k) ≥ 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

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

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

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

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

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

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 $\sqrt{\frac{2q+k}{p}} \leq \frac{2q+k}{p} \leq \lambda_1$

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

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

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

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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