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ON TOTAL ENERGY OF A GRAPH

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Abstract

The concept of total matrix and total energy of a graph G is introduced by K. Palani et al. Let $G = (V, E)$ be a (p, q) simple graph. Let $V(G) = \{v_i / i = 1, 2, \ldots, p\}$ and $E(G) = \{e_i / i = 1, 2, \ldots, q\}$. The total matrix $T = T(G)$ of G is a square matrix of order $p + q$ whose (i, j)- entry is defined as:

$$T = (t_{ij}) = \begin{cases} 1 & \text{if } v_i \text{ adjacemt to } v_j \; i \neq j \\ 1 & \text{if } e_i \text{ adjacemt to } e_j \; i \neq j \\ 1 & e_i \text{ incidentwith } v_j \\ 0 & \text{otherwise.} \end{cases}$$

The total energy of a graph is the sum of absolute value of the eigenvalues of its total matrix $T(G)$. For any (p, q) graph G, the total number of eigenvalue is $p + q$. Let $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{p+q}$ be the eigenvalues of T. Then total energy of G is $TE = \sum_{i=1}^{p+q} |\lambda_i|$. In this article we write some bounds for total energy of a graph and some theorems on total energy. Further we established the algorithms and MATLAB programs to find the total energy of (n, n)- Dragon graph, cyclic graph and $C_{n+u_1u_3}$ graph.

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I. Introduction

Throughout this article we deal with finite, simple and undirected graphs. The concept of energy of a graph was proposed by Gutman [7] in 1978 as the sum of absolute values of the eigenvalue of a graph G and is denoted by $E(G)$. The eigenvalues of the total matrix T is known as the total eigenvalues of G. In this article we write some bounds for total energy of a graph and some theorems on total energy. Further we established the algorithms and MATLAB programs to find the total energy of (n, n)- Dragon graph, cyclic graph and $C_{n+u_1u_3}$. graph.

Definition 2.1. Let $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{p+q}$ be the total eigenvalues of T. Then the spectrum of G is $Spec_T(G) = \begin{Bmatrix} \lambda_1\lambda_2\lambda_3 \ldots, \lambda_{p+q} \\ m_1m_2m_3 \ldots, m_{p+q} \end{Bmatrix}$ where m_i is the algebraic multiplicity of the total eigenvalues λ_i, for $1 \leq i \leq p+q$.

Definition 1.3 [12]**.** The cyclic graph of order n can be constructed by joining two copies of the cycle graph C_n with a common vertex.

Definition 1.4. The total graph $T(G)$ of a graph G is a graph such that (i) the vertex set of $T(G)$ corresponds to the vertices and edges of G and (ii) two vertices are adjacent in $T(G)$ if and only if their corresponding elements are either adjacent or incident in G.

Definition 1.5. Let $G = (V, E)$ be a (p, q) graph. The energy of total matrix of G is called the total energy. It is denoted as $TE(G)$. That is the total energy of $G =$ Energy of total matrix of $G = \sum_{i=1}^{p+q} | \lambda_i |$.

Theorem 1.6 [9]**.** *The entries* a_{ij} *in* A^k *represent the number of walks of length k from* v_i *to* v_j.

II. Some Results on Total Energy

Theorem 2.1. *Let G be any simple* (p, q) *graph. If* $\lambda_1, \lambda_2, \ldots, \lambda_{p+q}$ *are the total eigenvalues of the total matrix T of G then the following holds.*

(i) $\sum_{i=1}^{p+q} \lambda_i = 0$

(ii) $\sum_{i=1}^{p+q} \lambda_i^2 = 2| q' |$ *where* $q' = | E(T(G)) |$.

Proof. We know that, sum of eigenvalues of T is same as the trace of T.

i.e., $\sum_{i=1}^{p+q} \lambda_i = \sum_{i=1}^{p+q} t_{ii} = 0$ since $t_{ii} = 0 \; \forall i$.

Therefore $\sum_{i=1}^{p+q} \lambda_i = 0$.

Since the sum of squares of the eigenvalues of T is the trace of $[T(G)^2]$,

$$\sum_{i=1}^{p+q} \lambda_i^2 = \sum_{i=1}^{p+q} \sum_{i=1}^{p+q} t_{ij} t_{ji}$$

$$= \sum_{i=1}^{p+q} t_{ii}^2 + \sum_{i \neq j} t_{ij} t_{ji}$$

$$= \sum_{i=1}^{p+q} t_{ii}^2 + 2 \sum_{i<j} (t_{ij})^2$$

$$= 0 + 2| E(T(G)) |$$

$\sum_{i=1}^{p+q} \lambda_i^2 = 2| q' |$ where $q' = | E(T(G)) |$.

Theorem 2.2. *Let* $G = (V, E)$ *be any simple* (p, q) *graph. If the total energy* $TE(G)$ *is a rational number then*

$$TE(G) \equiv 0 (mod\, 2).$$

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_{p+q}$ are the total eigenvalues of the total matrix T of G. Let $\lambda_1, \lambda_2, \ldots, \lambda_t$ are positive and the rest are of negative sign, then

$$\sum_{i=1}^{p+q} | \lambda_i | = (\lambda_1, \lambda_2, \ldots, \lambda_t) - (\lambda_1, \lambda_2, \ldots, \lambda_{p+q})$$

$$\sum_{i=1}^{p+q} | \lambda_i | = 2(\lambda_1, \lambda_2, \ldots, \lambda_t) - (\lambda_1, \lambda_2, \ldots, \lambda_{p+q})$$

$$\Rightarrow TE(G) = 2(\lambda_1, \lambda_2, \ldots, \lambda_t) - \sum_{i=1}^{p+q} \lambda_i$$

$$\Rightarrow TE(G) = 2(\lambda_1, \lambda_2, \ldots, \lambda_t) \text{ since } \sum_{i=1}^{p+q} \lambda_i = 0.$$

Hence $TE(G) \equiv 0 \pmod 2$.

Theorem 2.3. *Let G be a (p, q) simple graph. Let 'd' be the absolute value of determinant of the total matrix T of G, i.e., $d = | \det T(G) |$. Then $\sqrt{2q' + r(r-1)d^{(2/r)}} \leq TE(G) \leq \sqrt{2rq'}$ where $r = p + q$ and q' is the number of edges of $T(G)$.*

Proof. We know, Cauchy Schwarz inequality is

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

Put $a_i = 1$, $b_i = | \lambda_i |$ and $n = r$ then

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

$$\Rightarrow [TE(G)]^2 \leq \sum_{i=1}^{r} \lambda_i^2$$

$$= r2|E(T(G))|$$

$$= 2rq'$$

$$\Rightarrow [TE(G)] \leq \sqrt{2rq'}. \tag{1}$$

Consider $[TE(G)]^2 = (\sum_{i=1}^{r} |\lambda_i|^2)$

$$= \left(\sum_{i=1}^{r} |\lambda_i|^2\right) + \sum_{i \neq j} |\lambda_i||\lambda_j|$$

$$[TE(G)]^2 = 2q' + \sum_{i \neq j} |\lambda_i||\lambda_j| \tag{2}$$

where $2q' = (\sum_{i=1}^{r} |\lambda_i|^2)$.

We know, the geometric mean cannot exceed the arithmetic mean, we have

$$\frac{1}{r(r-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| \geq \left[\prod_{i \neq j} |\lambda_i||\lambda_j|\right]^{\frac{1}{r(r-1)}}$$

$$= \left[\prod_{i=1}^{r} |\lambda_i|^{2(r-1)}\right]^{\frac{1}{r(r-1)}}$$

$$= \left[\prod_{i=1}^{r} |\lambda_i|\right]^{\frac{2}{r}}$$

$$= \left[\prod_{i=1}^{r} \lambda_i\right]^{\frac{2}{r}}$$

$$= |\det T(G)|^{\frac{2}{r}}$$

$$= d^{\left(\frac{2}{r}\right)}$$

i.e., $\frac{1}{r(r-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| \geq d^{\left(\frac{2}{r}\right)}$

$$\Rightarrow \sum_{i \neq j} |\lambda_i||\lambda_j| \geq r(r-1)d^{\left(\frac{2}{r}\right)}. \quad (3)$$

Put (III) in (II)

$$[TE(G)]^2 \geq 2q'r(r-1)d^{\frac{2}{r}}$$

i.e.,

$$TE(G) \geq \sqrt{2q' + r(r-1)d^{2/r}} \quad (4)$$

From (I) and (IV)

$$\sqrt{2q' + r(r-1)d^{2/r}} \leq TE(G) \leq \sqrt{2rq'}.$$

Theorem 2.4. *The total spectra and total energy of the Bull graph G is* 16.81929.

Proof. Let G be the Bull graph. The total matrix of the Bull graph is

$$T_G = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of G is $x^{10} - 22x^8 - 32x^7 + 84x^6 + 18x^5 - 7x^4 - 178x^3 - 59x^2 + 30x + 12$.

And the total spectra are -0.42883, -2.27346, 2.14012, -2.13345, -1.58563, 0.96161, -1.43782, 0.46086, -0.55045, 4.84706.

Hence the total energy TE of the Bull graph is 16.81929.

Theorem 2.5. *Each entry* t_{ij} *of the total matrix* T^k *denotes the number of walks of length k from* v_i *to* v_j *in* $T(G)$, *where* $T(G)$ *is the total graph of G.*

Proof. Since the total matrix T of G is the adjacency matrix of total graph of G, the results follows from theorem 1.6.

III. Algorithms and MATLAB Programs for Total Energy of Some Graphs

3.1. Algorithm to generate the total energy of the (n, n)- Dragon graph.

Step I. Assume $G = (V, E)$ to be a (p, q) graph.

Step II. Assume that in the total matrix representation, vertices and edges appear alternatively along both rows and columns.

Step III. Let $r = p + q$.

Step IV. $t_{ii+1} = t_{u+1i} = 1 \forall 1 \leq i \leq 1$.

Step V. $t_{ii+2} = t_{i+2i} = 1 \forall \leq i \leq p - 1$ and $q + 1 \leq i \leq r - 2$.

Step VI. $t_{ip} = t_{pi} = 1$ and for $i = 1$ and 2.

Step VII. Assign $t_{1p-1} = t_{p-11} = 1$, $t_{p-1\,p+2} = t_{p+2\,p-1} = 1$, $t_{p-2\,p+1} = t_{p+1\,p-2} = 1$.

Step VIII. Assume the other entries as zero.

Step IX. Find eigenvalues of T.

Step X. Find Total Energy TE.

3.2. MATLAB program to generate the total energy of (n, n)- Dragon graph

% ‘*T*’ is the Total matrix of a graph

% ’*K*’ is the eigenvalues of the matrix

% ‘*TE*’ is the Total Energy of the graph

```
% r = p + q
% p, q refer the number of vertices and edges of (n, n)- Dragon graph.
for i = 1 : r - 1
T(i, i + 1) = 1;
T(i + 1, i) = 1;
end
for i = 1 : p - 1
T(i, i + 2) = 1;
T(i + 2, i) = 1;
end
for i = q + 1 : r - 2
T(i, i + 2) = 1;
T(i + 2, i) = 1;
end
for i = 1 : 2
T(i, p) = 1;
T(p, i) = 1;
end
T(1, p - 1) = 1;
T(p - 1, 1) = 1;
T(p - 1, p + 2) = 1;
T(p + 2, p - 1) = 1;
T(p - 2, p + 1) = 1;
T(p + 1, p - 2) = 1;
```

T

$K = eig(T);$

$TE = \text{sum}(\text{abs}(K))$

3.3. Illustration

When the above program is executed for $(5, 5)$- Dragon graph, the output will be $TE = 27.1174.$

3.4. Algorithm to generate the total energy of a cyclic graph.

Step I. Assume $G = (V, E)$ to be a (p, q) graph.

Step II. Assume that in the total matrix representation, vertices and edges appear alternatively along both rows and columns.

Step III. Let $r = p + q$.

Step IV. $t_{ii+1} = t_{i+1i} = 1 \ \forall 1 \leq i \leq r - 1$.

Step V. $t_{ii+2} = t_{i+2i} = 1 \ \forall 1 \leq i \leq p$ and $q + 1 \leq i \leq r - 2$.

Step VI. $t_{iq} = t_{qi} = 1$ for $i = 1$ and 2.

Step VII. $t_{ir} = t_{ri} = 1 \ \forall p - 1 \leq i \leq q + 1$.

Step VIII. Assign $t_{ii+3} = t_{i+3i} = 1$ for $i = p - 1$ to p.

Step IX. Assign $t_{1p} = t_{p1} = 1 t_{pr-1} = t_{r-1p} = 1$.

Step X. Assume the other entries as zero.

Step XI. Find eigenvalues of T.

Step XII. Find Total Energy TE.

3.5. MATLAB program to generate the total energy of cyclic graph.

% 'T' is the Total matrix of a graph

% 'K' is the eigenvalues of the matrix

% 'TE' is the Total Energy of the graph

```
% r = p + q
% (p, q) refers the number of vertices and edges of the cyclic graph
for i = 1 : r - 1
T(i, i + 1) = 1;
T(i + 1, i) = 1;
end
for i = 1 : p
T(i, i + 2) = 1;
T(i + 2, i) = 1;
end
for i = q + 1 : r - 2
T(i, i + 2) = 1;
T(i + 2, i) = 1;
end
for i = 1 : 2
T(i, q) = 1;
T(q, i) = 1;
end
for i = p - 1 : q + 1
T(i, r) = 1;
T(r, i) = 1;
end
for i = p - 1 : p
T(i, i + 3) = 1;
T(i + 3, i) = 1;
```

end

$T(1,\ p) = 1;$

$T(p, 1) = 1;$

$T(p,\ r-1) = 1;$

$T(r-1,\ p) = 1;$

T

$K = eig\ (T);$

$TE = \text{sum}\,(\text{abs}\,(K))$

3.6. Illustration

When the above program is executed for 4-cyclic graph, the output will be $TE = 27.7369.$

3.7. Algorithm to generate the total energy of Cycle with one chord $C_{n+u_1u_3}$.

Step I. Assume $G = (V,\ E)$ to be a $(p,\ q)$ graph.

Step II. Assume that in the total matrix representation, vertices and edges appear alternatively along both rows and columns.

Step III. Let $r = p + q$.

Step IV. $t_{ii+1} = t_{i+1i} = 1\ \forall 1 \leq i \leq r-2.$

Step V. $t_{ii+2} = t_{i+2i} = 1\ \forall 1 \leq i \leq r-3.$

Step VI. $t_{ir-1} = t_{r-1i}$ and $t_{ir} = t_{ri}$ for $i = 1$ and 2.

Step VII. $t_{ir} = t_{ri} = 1$ for $i = 4$ to 6.

Step VIII. Assign $t_{r-1r} = t_{rr-1},\ t_{15} = t_{51},\ t_{1r-2} = t_{r-21} = 1.$

Step IX. Assume the other entries as zero.

Step X. Find eigenvalues of T.

Step XI. Find Total Energy TE.

3.8. MATLAB program to generate the total energy of graph $C_{n+u_1u_3}$.

% 'T' is the Total matrix of a graph

% 'K' is the eigenvalues of the matrix

% 'TE' is the Total Energy of the graph

% $r = p + q$

% p, q refers the number of vertices and edges of $C_{n+u_1u_3}$.

for $i = 1 : r - 2$

$T(i, i+1) = 1;$

$T(i+1, i) = 1;$

end

for $i = 1 : r - 3$

$T(i, i+2) = 1;$

$T(i+2, i) = 1;$

end

for $i = 1 : r - 2$

$T(i, r-1) = 1;$

$T(r-1, i) = 1;$

$T(i, r) = 1;$

$T(r, i) = 1;$

end

for $i = 4 : 6$

$T(i, r) = 1;$

$T(r, i) = 1;$

end

$T(r-1, r) = 1;$

$T(r, r-1) = 1;$

$T(1, r-2) = 1;$

$T(r-2, 1) = 1;$

$T(1, 5) = 1;$

$T(5, 1) = 1;$

T

$K = \text{eig}(T);$

$TE = \text{sum}(\text{abs}(K))$

3.9. Illustration:

When the above program is executed for $C_{5+u_1u_3}$, the output will be $TE = 30.5445.$

Conclusion

The energy of a graph is one of the emerging concepts within graph theory. A new energy concept of total energy is discussed. We have investigated on some theorems and bounds of total energy of a graph. Furthermore we established the MATLAB programs to find the total energy of (n, n)- Dragon graph, cyclic graph and $C_{n+u_1u_3}$ graph.

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