REACHABILITY ENERGY AND ESTRADA INDEX

OF A CONNECTED GRAPH

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Abstract

Let $G($ T, W) be connected graph with p vertices. The reachability matrix $\mathbb{R} = (r_{ij})$ of a graph G, denoted by $\mathbb{R}(G)$ is the $p \times p$ matrix with $r_{ij} = \begin{cases} 1, & \text{if } i \leq r \text{ eachable from } t_i \\ 0, & \text{otherwise} \end{cases}$. In this paper, we introduce and obtain the reachability energy and reachability Estrada index of a graph. Also, we establish upper and lower bound for this new energy and index separately.

Keywords: Energy, Estrada Index, connected graph, spectrum of a graph.

1. INTRODUCTION

 The energy of a simple graph was introduced by Ivan Gutman in 1978[14,15]. The energy of graph is referred as the ordinary energy of graph G. The energy of a graph G, denoted by $E(G)$, is defined to be the sum of the absolute value of the eigenvalues of its adjacency matrix (i.e) $E(G)$ = $\sum_{i=1}^{p} |\lambda_i|$. There are many energies based on Distance matrix [3,13,17], Laplacian matrix [2], Harary matrix [12] etc. De la Pe na et.al., introduced the Estrada index of a graph in 2007[4]. Estrada index of the graph G is defined by $EE = EE(G) = \sum_{i=1}^{p} e^{\lambda_i}$, where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_p$ are the eigenvalues of the adjacency matrix $A(G)$ of G [5,6,7,8,9,10,11].

 Motivated by above studies, in this paper, we will introduce a new energy and index of the graph based on reachability matrix and also obtain lower and upper bounds for this new energy and new index of *.*

2. RECHABILITY ENERGY OF CONNECTED GRAPH

In this section, using reachability matrix we obtain preliminary lemmas and introduce new energy called reachability energy of graph.

Lemma 2.1:

Let G be a connected graph of order p and let $\beta_1, \beta_2, ..., \beta_p$ be its ℝ-eigenvalues. Then

$$
\sum_{i=1}^{p} \beta_i = 0 \quad \& \quad \sum_{i=1}^{p} \beta_i^2 = 2 \sum_{1 \le i < j \le p} (r_{ij})^2
$$

Proof:

We know that $\sum_{i=1}^{p} \beta_i$ is equal to the trace of a matrix and also the reachability matrix of a graph is defined as $\mathbb{R} = r_{ij} = \begin{cases} 1, & \text{if } i \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}$

Now,
$$
\sum_{i=1}^{p} \beta_i = trace \left(\mathbb{R}(G) \right) = \sum_{i=j=1}^{p} r_{ij} = 0.
$$

Moreover, for $i = 1, 2, ..., p$, the (i, i) th entry of $(\mathbb{R}(G))^2$ is equal to $\sum_{j=1}^p (r_{ij}) (r_{ji}) = \sum_{i=1}^p (r_{ij})^2$ $i=1$

$$
\sum_{i=1}^{p} {\beta_i}^2 = trace\left(\mathbb{R}(G)\right)^2 = \sum_{i=1}^{p} \sum_{j=1}^{p} (r_{ij})^2 = 2 \sum_{1 \le i < j \le p} (r_{ij})^2.
$$

Hence the result.

Lemma 2.2:

Let G be a connected graph with diameter less than or equal to 2 and let $\beta_1, \beta_2, ..., \beta_p$ be its ℝ-eigenvalues. Then

$$
\sum_{i=1}^p \beta_i^2 = p(p-1)
$$

Proof:

In the reachability matrix of the graph, there are $\frac{p(p-1)}{2}$ $\frac{y+1}{2}$ elements equal to unit for $i < j$ and $p(p-1)$ $\frac{1}{2}$ elements equal to unit for $i > j$.

Therefore,
$$
\sum_{i=1}^{p} \beta_i^2 = \sum_{i=1}^{p} (\mathbb{R}(G))^2 = \sum_{i=1}^{p} \sum_{j=1}^{p} (r_{ij}) (r_{ji}) = \frac{p(p-1)}{2} + \frac{p(p-1)}{2} = p(p-1).
$$

Hence the result.

Definition 2.1:

Let G be any connected graph with p vertices. The reachability matrix $\mathbb{R}(G)$ [1] of the graph G is a square matrix of order p such as reachability from t_i to t_j is '1' for $i \neq j$ and '0' for $i = j$. The Characteristic polynomial of a $\mathbb{R}(G)$ is $\phi(G,\beta) = \det(\mathbb{R}(G) - \beta I)$, where I is the idendity matrix. The roots of the equation $\phi(G, \beta) = 0$ is called the eigen values of the reachability matrix. The eigenvalues of the reachability matrix of the graph G are called as ℝ-eigenvalues of G and denoted by $\beta_1, \beta_2, ..., \beta_p$. The collection of ℝ- eigenvalues is called spectrum of a graph G[16]. The sum of the absolute values of the R-eigenvalues of G is known as reachability energy of a graph G , denoted by $\mathbb{R}E(G)$, is defined by $\mathbb{R}E(G) = \sum_{i=1}^{p} |\beta_i|$.

Theorem 2.1:

Let G be any connected graph of order p then reachability energy of the graph is $2(p-1)$.

Proof:

Consider a connected graph with p vertices. The reachability matrix $\mathbb{R}(G)$ of the graph G is a square matrix of order p such as reachability from t_i to t_j is '1' for $i \neq j$ and '0' for $i = j$. That is

$$
\mathbb{R}(G) = r_{ij} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & 1 & \cdots & 1 & 1 \\ 1 & 1 & 0 & \cdots & 1 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & 1 & \cdots & 0 & 1 \\ 1 & 1 & 1 & \cdots & 1 & 0 \end{pmatrix}
$$

Let us find the characteristic polynomial $\phi(G, \beta)$ of $\mathbb{R}(G)$ using the relation,

$$
\phi(G,\beta) = \det(\mathbb{R}(G) - \beta I), where I is the identity matrix.
$$

$$
\phi(G,\beta)=\begin{vmatrix}-\beta & 1 & 1 & \cdots & 1 & 1 \\ 1 & -\beta & 1 & \cdots & 1 & 1 \\ 1 & 1 & -\beta & \cdots & 1 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & 1 & \cdots & -\beta & 1 \\ 1 & 1 & 1 & \cdots & 1 & -\beta\end{vmatrix}=0
$$

Thus, the characteristic polynomial $\phi(G, \beta)$ of the graph G is

$$
\phi(G,\beta) = (-1)^p (\lambda - (p-1)) (\lambda + 1)^{|p-1|} \ \forall \ p \ge 2.
$$

Hence, the spectrum of $\mathbb{R}(G)$ is $\begin{pmatrix} -1 & p-1 \\ p-1 & 1 \end{pmatrix}$ $\binom{1}{1}$.

Consequently, the reachability energy $\mathbb{R}E(G)$ of the graph G can be determined as follows:

$$
\mathbb{R}E(G) = \sum_{i=1}^{p} |\beta_i|
$$

= |(-1)(p - 1)| + |(p - 1)(1)|
= 2(p - 1).

This completes the proof.

2.1. BOUNDS FOR THE REACHABILITY ENERGY

In this section, we obtain upper bound and lower bound for the reachability energy of the connected graph.

Theorem 2.1.1:

If G be a connected graph then
$$
\sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^2} \le \mathbb{R}E(G) \le \sqrt{2p \sum_{1 \le i < j \le p} (r_{ij})^2}.
$$

Proof:

By Cauchy-Schwartz inequality,

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

Consider, $a_i = 1$ and $b_i = |\beta_i|$, then

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

$$
\mathbb{R}E(G)^2 \le 2p \sum_{1 \le i < j \le p} \left(r_{ij}\right)^2
$$

$$
\mathbb{R}E(G) \le \sqrt{2p \sum_{1 \le i < j \le p} \left(r_{ij}\right)^2}.
$$

which gives the required upper bound for $\mathbb{R}E(G)$.

We can easily obtain the inequality,

$$
\left(\mathbb{R}E(G)\right)^2 = \left(\sum_{i=1}^p |\beta_i|\right)^2 \ge \sum_{i=1}^p |\beta_i|^2 = 2 \sum_{1 \le i < j \le p} \left(r_{ij}\right)^2
$$
\n
$$
\mathbb{R}E(G) \ge \sqrt{2 \sum_{1 \le i < j \le p} \left(r_{ij}\right)^2}.
$$

which gives the required lower bound for $\mathbb{R}E(G)$.

Hence the result.

Example 2.1.1:

Bounds of Reachability energy from $p = 2$ to $p = 6$ is given in Table 2.1.1.

Vertices p	$(r_{ij})^2$ 2 $1 \le i < j \le p$	$\mathbb{R}E(G)$	$(r_{ij})^2$ 2p $1 \le i < j \le p$
$\overline{2}$	1.414	\overline{c}	\overline{c}
3	2.449		4.24
4	3.464	6	6.92
5	4.472	8	10
6	5.477	10	13.416

Table 2.1.1. Bounds of Reachability energy from $p = 2$ to $p = 6$.

Corollary 2.1.1: If *G* be a connected graph then $\mathbb{R}E(G) \leq p\sqrt{p-1}$.

Proof:

Since $r_{ij} = 1$ for $i \neq j$ and there are $\frac{p(p-1)}{2}$ $\frac{y-1}{2}$ pair of vertices in G. By above theorem, we have upper bound,

$$
\mathbb{R}E(G) \le \sqrt{2p \sum_{1 \le i < j \le p} (r_{ij})^2} \le \sqrt{2p \left(\frac{p(p-1)}{2}\right)} = p\sqrt{p-1}.
$$

Theorem 2.1.2:

Let G be a connected graph and let Δ be the absolute value of the determinant of the reachability matrix $\mathbb{R}(G)$ of a graph then

$$
\sqrt{2\sum_{1\leq i
$$

Proof:

By theorem 2.1.1, we have upper bound for $\mathbb{R}E(G)$.

Now, we show that the lower bound for $\mathbb{R}E(G)$ then this will finish the proof.

By definition of reachability energy,

$$
\left(\mathbb{R}E(G)\right)^{2} = \left(\sum_{i=1}^{p} |\beta_{i}| \right)^{2} = \sum_{i=1}^{p} |\beta_{i}|^{2} + 2 \sum_{1 \le i < j \le p} |\beta_{i}| |\beta_{j}|
$$

$$
= 2 \sum_{1 \le i < j \le p} (r_{ij})^{2} + \sum_{i \ne j} |\beta_{i}| |\beta_{j}|
$$

From Arithmetic – Geometric Mean inequality, we have,

$$
\frac{1}{p(p-1)}\sum_{i\neq j}|\beta_i|\,|\beta_j|\geq \left(\prod_{i\neq j}|\beta_i|\,|\beta_j|\right)^{\frac{1}{p(p-1)}}=\left(\prod_{i=1}^p|\beta_i|^{2(p-1)}\right)^{\frac{1}{p(p-1)}}=\Delta^{\frac{2}{p}}.
$$

which gives

$$
(\mathbb{R}E(G))^{2} \ge 2 \sum_{1 \le i < j \le p} (r_{ij})^{2} + p(p-1)\Delta^{\frac{2}{p}}
$$
\n
$$
\mathbb{R}E(G) \ge \sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^{2} + p(p-1)\Delta^{\frac{2}{p}}}.
$$

Hence the result.

Example 2.1.2:

Bounds of Reachability energy from $p = 2$ to $p = 6$ is given in Table 2.1.2.

Vertices p	$(r_{ij})^2 + p(p-1)\Delta^{\frac{2}{p}}$ $\overline{2}$ $1 \le i < j \le p$	$\mathbb{R}E(G)$	$(r_{ij})^2$ 2p $1 \le i < j \le p$
2	$\overline{2}$	$\overline{2}$	$\overline{2}$
3	3.9397	$\overline{4}$	4.24
4	5.726	6	6.92
$\overline{}$	7.404	8	10
6	9.0165	10	13.416

Table 2.1.2. Bounds of Reachability energy from $p = 2$ to $p = 6$.

Corollary 2.1.2: Let G be a connected graph with diameter less than or equal to 2 and let Δ be the absolute value of the determinant of its reachability matrix $\mathbb{R}(G)$ of a graph then

$$
\sqrt{p(p-1)\left(1+\Delta^{\frac{2}{p}}\right)} \leq \mathbb{R}E(G) \leq p\sqrt{p-1}.
$$

3. REACHABILITY ESTRADA INDEX OF GRAPH

In this section, we will introduce and obtain Reachability Estrada index and its bounds. Moreover, we will obtain upper bound for the reachability Estrada index involving the reachability energy of graphs.

We first recall that the Estrada index of a graph G is defined by

$$
EE(G) = \sum_{i=1}^{p} e^{\lambda_i}
$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_p$ are the eigenvalues of the adjacency matrix $A(G)$ of G [5,6,7,8,9,10,11]. Denoting by $M_k = M_k(G)$ to the k-th moment of the graph G, we get

$$
M_k(G) = \sum_{i=1}^p (\lambda_i)^k
$$

and recalling the power series expansion of e^x , we have

$$
EE = \sum_{k=0}^{\infty} \frac{M_k}{k!}
$$

It is well known that [10] $M_k(G)$ is equal to the number of closed walks of length k of the graph G. In fact Estrada index of graphs has an important role in chemistry and physics and there exists a vast literature that studies this special index. In addition to the Estrada's papers depicted above, we may also refer $[4,5]$ to the reader for detail information such as lower and upper bounds for EE in terms of the number of vertices and edges and some inequalities between EE and the energy of G .

3.1 BOUNDS FOR THE REACHABILITY ESTRADA INDEX

In this section, we will introduce and obtain the reachability Estrada index of a graph G and also its upper and lower bound.

Definition 3.1.1:

If G is a connected graph with p vertices, then the reachability Estrada index of G , denoted by \mathbb{R} *EE*(*G*), is defined by

$$
\mathbb{R}EE(G)=\sum_{i=1}^p e^{\beta_i}
$$

where $\beta_1 \geq \beta_2 \geq \beta_3 \geq \cdots \geq \beta_p$ are the R-eigenvalues of G.

Let $V_k = \sum_{i=1}^p (\beta_i)^k$. Then $\mathbb{R}EE(G) = \sum_{k=0}^{\infty} \frac{V_k}{k!}$ $k!$ $\frac{\infty}{k} = 0 \frac{v_k}{k!}$.

Reachability Estrada index can be calculated in terms of number of vertices of the connected $graph G$

$$
REE(G) = \frac{1}{e}(e^p + p - 1)
$$
 where *p* is a number of vertices of the connected graph *G*

Theorem 3.1.1:

1≤ı lt j≤p

Let G be a connected graph with diameter less than or equal to 2 then the reachability Estrada index is bounded as $\sqrt{p(3p - 2)} \leq \mathbb{R} E E(G) \leq p - 1 + e^{\sqrt{p(p-1)}}.$

Proof:

From the definition 3.1.1, $\mathbb{R} E E(G) = \sum_{i=1}^{p} e^{\beta_i}$ $i=1$

$$
\mathbb{R}EE^2(G) = \left(\sum_{i=1}^p e^{\beta_i}\right)^2 = \sum_{i=1}^p e^{2\beta_i} + 2 \sum_{1 \le i < j \le p} e^{\beta_i} e^{\beta_j}
$$

Consider the 2nd term of the above equation, by using Arithmetic-Geometric Mean Inequality, we have

$$
2\sum_{1 \le i < j \le p} e^{\beta_i} e^{\beta_j} \ge p(p-1) \left(\prod_{1 \le i < j \le p} e^{\beta_i} e^{\beta_j} \right)^{\frac{2}{p(p-1)}}
$$
\n
$$
= p(p-1) \left(\left(\prod_{i=1}^p e^{\beta_i} \right)^{p-1} \right)^{\frac{2}{p(p-1)}}
$$
\n
$$
= p(p-1)(e^{\gamma_1})^{\frac{2}{p}} = p(p-1).
$$

By means of power series expansion and we have three moments as $V_0 = p, V_1 = 0$ & $V_2 =$ $2\sum_{1\leq i < j \leq p} (r_{ij})^2$

$$
\sum_{i=1}^{p} e^{2\beta_i} = \sum_{i=1}^{p} \sum_{k \ge 0} \frac{(2\beta_i)^k}{k!} = p + 4 \sum_{1 \le i < j \le p} (r_{ij})^2 + \sum_{i=1}^{p} \sum_{k \ge 3} \frac{(2\beta_i)^k}{k!}
$$

Since we require lower bound as good as possible, it holds reasonable to replace $\sum_{k\geq 3} \frac{(2\beta_i)^k}{k!}$ by $4 \frac{(\beta_i)^k}{k!}$ $\frac{\partial v}{\partial k!}$. Further, we use a multiplier $t \in [0,4]$ instead of 4. We get,

$$
\sum_{i=1}^{p} e^{2\beta_i} \ge p + 4 \sum_{1 \le i < j \le p} (r_{ij})^2 + t \sum_{i=1}^{p} \sum_{k \ge 3} \frac{(\beta_i)^k}{k!}
$$
\n
$$
\sum_{i=1}^{p} e^{2\beta_i} \ge p + 4 \sum_{1 \le i < j \le p} (r_{ij})^2 - tp - t \sum_{1 \le i < j \le p} (r_{ij})^2 + t \sum_{i=1}^{p} \sum_{k \ge 0} \frac{(\beta_i)^k}{k!}
$$
\n
$$
\sum_{i=1}^{p} e^{2\beta_i} \ge p(1-t) + (4-t) \sum_{1 \le i < j \le p} (r_{ij})^2 + t \cdot \mathbb{R}EE(G)
$$

By Lemma 2.1 & 2.2, we get,

$$
\sum_{i=1}^{p} e^{2\beta_i} \ge p(1-t) + (4-t) \left(\frac{p(p-1)}{2} \right) + t. \mathbb{R} E E(G)
$$

Then solving for $\mathbb{R}EE(G)$,

$$
\mathbb{R}EE^{2}(G) \ge p(1-t) + (4-t)\left(\frac{p(p-1)}{2}\right) + t \cdot \mathbb{R}EE(G) + p(p-1)
$$

$$
\mathbb{R}EE^{2}(G) \ge p + 3(p^{2} - p) + t\left[\mathbb{R}EE(G) - \frac{1}{2}(p^{2} - p) - p\right]
$$

For $p \ge 2$, the best lower bound for $\mathbb{R} E E(G)$ is attained when $t = 0$.

$$
\mathbb{R}EE^2(G) \ge p + 3(p^2 - p)
$$

$$
\mathbb{R}EE(G) \ge \sqrt{p(3p - 2)}.
$$

which gives the required lower bound for $\mathbb{R}EE(G)$.

From the definition 3.1.1,

$$
\mathbb{R}EE(G) = \sum_{k=0}^{\infty} \frac{V_k}{k!} = p + \sum_{k=1}^{\infty} \frac{V_k}{k!}
$$

\n
$$
\mathbb{R}EE(G) \le p + \sum_{i=1}^{p} \sum_{k\ge 1} \frac{(\beta_i)^k}{k!}
$$

\n
$$
\mathbb{R}EE(G) \le p + \sum_{i=1}^{p} \sum_{k\ge 1} \frac{|\beta_i|^k}{k!}
$$

\n
$$
\le p + \sum_{k\ge 1} \frac{1}{k!} \sum_{i=1}^{p} ((\beta_i)^2)^{\frac{k}{2}} = p + \sum_{k\ge 1} \frac{1}{k!} \left(2 \sum_{1 \le i < j \le p} (r_{ij})^2 \right)^{\frac{k}{2}}
$$

\n
$$
= p - 1 + \sum_{k\ge 0} \frac{\left(\sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^2} \right)^k}{k!} = p - 1 + e^{\sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^2}}
$$

By Lemma 2.1 & 2.2, we get, $\mathbb{R} E E(G) \le p - 1 + e^{\sqrt{p(p-1)}}$.

which gives required upper bound for $\mathbb{R} \mathbb{E} \mathbb{E} \left(G \right)$.

Example 3.1.1:

Bounds of Reachability Estrada index from $p = 2$ to $p = 6$ is given in Table 3.1.1.

Table 3.1.1. Bounds for Reachability Estrada index from $p = 2$ to $p = 6$.

3.2 AN UPPER BOUND FOR THE REACHABILITY ESTRADA INDEX INVOLVING THE REACHABILITY ENERGY

In this section, using reachability energy we will show that there exist two upper bounds for the reachability Estrada index $\mathbb{R}E E(G)$ where G is a connected graph of diameter not greater than 2.

Theorem 3.2.1:

Let G be a connected graph of diameter not greater than 2 then

$$
REE(G) - RE(G) \le p - 1 - \sqrt{p(p-1)} + e^{\sqrt{p(p-1)}} \text{ and } REE(G) \le p - 1 + e^{RE(G)}.
$$

Proof:

From the proof of theorem 3.1.1, we have,

$$
\mathbb{R}EE(G) = p + \sum_{i=1}^{p} \sum_{k\geq 1} \frac{(\beta_i)^k}{k!}
$$

$$
\leq p + \sum_{i=1}^{p} \sum_{k\geq 1} \frac{|\beta_i|^k}{k!}
$$

By definition of reachability energy,

$$
\mathbb{R}EE(G) \le p + \mathbb{R}E(G) + \sum_{i=1}^{p} \sum_{k \ge 2} \frac{|\beta_i|^k}{k!}
$$

$$
\mathbb{R}EE(G) - \mathbb{R}E(G) \le p - 1 - \sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^2} + e^{\sqrt{2 \sum_{1 \le i < j \le p} (r_{ij})^2}}
$$

$$
\mathbb{R}EE(G) - \mathbb{R}E(G) \le p - 1 - \sqrt{p(p - 1)} + e^{\sqrt{p(p - 1)}}
$$

Another approximation to connect $\mathbb{R}E E(G)$ and $\mathbb{R}E(G)$ can be seen as follows:

$$
\begin{aligned} \mathbb{R}EE(G) &\le p + \sum_{i=1}^{p} \sum_{k\ge 1} \frac{|\beta_i|^k}{k!} \le p + \sum_{k\ge 1} \frac{1}{k!} \left(\sum_{i=1}^{p} |\beta_i|^k \right) \\ &\le p - 1 + \sum_{k\ge 0} \frac{\left(\mathbb{R}E(G) \right)^k}{k!} \\ \mathbb{R}EE(G) &\le p - 1 + e^{\mathbb{R}E(G)}. \end{aligned}
$$

Hence the result.

Example 3.2.1:

Upper Bounds of Reachability Estrada index involving reachability energy from

 $p = 2$ to $p = 6$ is given in Table 3.2.1.

Table 3.2.1. Upper bounds for the reachability Estrada index involving reachability energy from $p = 2$ to $p = 6$.

Conclusion:

 In this paper, we have introduced and obtained the reachability energy and reachability Estrada index of the connected graph of order p . Also, we have found its bounds of this energy and index of the connected graph of order p .

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