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ON MAXIMUM REVERSE DEGREE ENERGY OF A GRAPH AND ITS CHEMICAL APPLICABILITY

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Abstract. In this paper, we define new matrix called maximum reverse degree matrix $M_R(G)$ and reverse degree energy $EM_R(G)$ for the simple graph G and study some of their properties. The striking feature of this energy is that, they correlated with total π-electron energy of some molecules containing hetero atoms and got a good correlation with the correlation coefficient $r = 0.9536$. Further, we also find maximum reverse degree energy for standard graphs and we give upper and lower bounds for $EM_R(G)$.

1. Introduction

We consider finite undirected graph without loops and multiple edges of order n. Let $V = V(G)$ be the vertex set and $E = E(G)$ be the edge set. The adjacency matrix $A(G)$ for a simple graph G is a matrix of order n and defined as, $A(G) = (a_{ij})$ where,

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

If $|\lambda_1| \geqslant |\lambda_2| \geqslant \ldots \geqslant |\lambda_n|$ are the eigenvalues of $A(G)$. The energy of graph G was defined by Gutman [**10**] in 1978 as,

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The study of energy of a graph is found in the literature [**12, 10, 1, 11**].
Let $\Delta(G)$ denote the maximum degree among the vertices of G. The reverse vertex

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degree of a vertex v_i in G is defined as $c_{v_i} = \Delta(G) - d(v_i) + 1$, where $d(v_i)$ is degree of vertex v_i. Recently, many concept have been introduced using reverse vertex degree and found in literature see [**6, 7, 8, 4, 14, 13**]. The application of reverse vertex-degree can be found in [**5**].
In [**2**] Chandrashekar Adiga and M. Smitha have defined the following.
Let G be a simple graph with n vertices $v_1, v_2, \ldots, v_n$ and d_i be the degree of v_i for $i = 1, 2, \ldots, n$. Then maximum degree matrix $M(G) = (d_{ij})$ is defined as,

$$d_{ij} = \begin{cases} \max\{d_i, d_j\} & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

If $\mu_1, \mu_2, \ldots, \mu_n$ are eigenvalues of $M(G)$ in non-increasing order, then the maximum degree energy of a graph G is defined as $E_M(G) = \sum_{i=1}^{n} |\mu_i|$.
In this paper, we use the reverse vertex-degree concept in [**2**] and define the following definitions.
Let G be a simple graph with n vertices and size m. let c_{v_i} be the reverse vertex degree of the vertex v_i. Then maximum reverse degree matrix is defined as, $M_R(G) = (r_{ij})$ where,

$$r_{ij} = \begin{cases} \max\{c_{v_i}, c_{v_j}\} & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases} \tag{1.1}$$

Let $\phi(G; \mu)$ be the characteristic polynomial of the maximum reverse degree matrix $M_R(G)$ and it is defined as

$$\begin{aligned} \phi(G; \mu) &= det(M_R(G) - \mu I) \\ &= a_0\mu^n + a_1\mu^{n-1} + a_2\mu^{n-2} + \cdots + a_n, \end{aligned}$$

where $a_0, a_1, a_2, \ldots, a_n$ are constant coefficients and I is the identity matrix of order n. let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of $M_R(G)$ and assumed that they are in non-increasing order. The maximum reverse degree energy of a graph G is defined as

$$EM_R(G) = \sum_{i=1}^{n} |\mu_i|.$$

Since $M_R(G)$ is a real symmetric matrix with trace zero. Therefore, the sum of eigenvalues of $M_R(G)$ is also zero.

2. Chemical applicability of $M_R(G)$

The Huckel molecular orbital theory is mainly concentrated on conjugated, all carbon compounds. If hetero atoms are considered, then range of those compounds can be studied, by comparing energy values for hetero compounds. At the end, we need to adjust Coulomb(α) and resonance integral(β) values for hetero atoms using the relations

$$\alpha' = \alpha + h\beta \quad \text{and} \quad \beta' = k\beta$$

where h and k are correction values which are different and depending on what atom is in conjugation. So, we can take more then one value for α for a hetero atom but

depends on the number of electrons hetero atom donates to π-system [**9**]. With the help of secular matrix of the compound and taking appropriate values of α and β in that matrix, we can calculate the π-electron energy of the compound [**15, 16**]. By this idea, we calculated $EM_R(G)$ with dataset of total π-electron energy values of hetero atoms which are found in [**3**]. Further, we found that $EM_R(G)$ has good correlation hetero atoms with correlation coefficient $r = 0.9536$ and $r^2(adjusted) = 0.9091$. The Molecules containing hetero atoms with total π–electron energy and Maximum reverse degree energy are shown in the Table 1. With help of data in the Table 1, the linear regression model for the total π-electron energy (E_π) values of hetero atoms and $EM_R(G)$ is given by,

$$\pi - \text{electron energy} = 2.9429(\pm 0.64679) + 0.44735(\pm 0.02884)EM_R(G).$$

Here we found, N (The population)=26, S_e (Standard error of the estimate)=1.6341 F (F-values)=240.6119 and SF (Significance F)=5.2183×10^{14}.

3. Some results on maximum reverse degree matrix

In this section, we discuses some results related to maximum reverse degree matrix.

THEOREM 3.1. *Let G be a simple graph with n vertices and m edges. If $\mu_1, \mu_2, \mu_3, \ldots \mu_n$ are the eigenvalues of the maximum reverse degree matrix $M_R(G)$ then,*

$$(i) \quad \sum_{i=1}^{n} \mu_i = 0,$$

$$(ii) \quad \sum_{i=1}^{n} \mu_i^2 = 2\sum_{i=1}^{n} (x_i + y_i)c_{v_i}^2.$$

Where x_i= the number of vertices in the neighbourhood of v_i whose reverse vertex degree are less then c_{v_i} and y_i=the number of vertices $v_j (j > i)$ in the neighbourhood of v_i whose reverse vertex degree are equal to c_{v_i}.

PROOF. (i) Since the sum of eigenvalues of the matrix $M_R(G)$ is the trace of matrix $M_R(G)$. But from the definition, the principle diagonal elements are zero. So we have,

$$\sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n} r_{ii} = 0.$$

(ii) Similar to above, the sum of the square of the eigenvalues of matrix $M_R(G)$ is same as trace of $[M_R(G)]^2$. Therefore we have,

$$\sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} r_{ij}r_{ji} = \sum_{i=1}^{n} r_{ii}^2 + \sum_{i \neq j} r_{ij}r_{ji} = 2\sum_{i=1}^{n} (x_i + y_i)c_{v_i}^2,$$

where x_i= the number of vertices in the neighbourhood of v_i whose reverse vertex degree are less then c_{v_i}

Molecule	**Code**	E_π	$EM_R(G)$
Venyl chloride like systems	H1	2.23	5.6568
Butadiene perturbed at C2	H2	5.66	8.2421
Acrolein like systems	H3	5.76	8.2421
1,1-Dichloro-ethylene like systems	H4	6.96	10.3923
Glyoxal like and 1,2-Dichloro-ethylene like systems	H5	6.82	10.3923
Pyrrole like systems	H6	5.23	6.4721
Pyridine like systems	H7	6.69	8
Pyridazine like systems	H8	9.06	8
Pyrimidine like systems	H9	9.10	8
Pyrazine like systems	H10	9.07	8
S-Triazene like systems	H11	9.65	8
Aniline like systems	H12	8.19	18.8633
O-Phenylene-diamine like systems	H13	12.21	22.7718
m-Phenylene-diamine like systems	H14	12.22	21.6781
p-Phenylene-diamine like systems	H15	12.21	23.0880
Benzaldehyde like systems	H16	11	22.7015
Quinoline like systems	H17	14.23	26.4678
Iso-quinoline like systems	H18	14.23	26.4678
1-Naphthalein like systems	H19	16.15	28.5417
2-Naphthalein like systems	H20	16.12	29.4744
Iso-indole like systems	H21	13.46	23.5170
Indole like systems	H22	13.59	23.5170
Benzylidine–aniline-like systems	H23	20.10	37.7556
Azobenzene like systems	H24	21.02	37.7556
Acridine like systems	H25	20.56	37.3235
Phenazine like systems	H26	21.62	37.3235

TABLE 1. Molecules containing hetero atoms with total π–electron energy (E_π) and maximum reverse degree energy ($EM_R(G)$).

and y_i=the number of vertices $v_j(j > i)$ in the neighbourhood of v_i whose reverse vertex degree are equal to c_{v_i}. □

REMARK 3.1. The explicit expression for the coefficient a_i of μ_{n-i}(for i=0,1,2) in characteristic polynomial of the maximum reverse degree matrix $M_R(G)$. It is also clear that $a_0 = 1$ and $a_1 = trace(M_R(G)) = 0$. Now we have,

$$\begin{aligned} a_2 &= \text{sum of determinants of all the } 2 \times 2 \text{ principal submatrices of } M_R(G) \\ &= \sum_{1 \leqslant i < j \leqslant n} \begin{vmatrix} 0 & r_{ij} \\ r_{ji} & 0 \end{vmatrix} \end{aligned}$$

But

$$\begin{vmatrix} 0 & r_{ij} \\ r_{ji} & 0 \end{vmatrix} = \begin{cases} -(max\{c_{v_i}, c_{v_j}\})^2 & , \text{ if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & , \text{ otherwise} \end{cases}$$

Thus,

$$a_2 = -\sum_{i=1}^{n} (x_i + y_j) c_{v_i}^2.$$

Note that $\sum_{i=1}^{n}(x_i + y_j)$= number of edges in graph G. Now by above theorem, we have

$$\sum_{i=1}^{n} \mu_i^2 = 2 \sum_{i=1}^{n} (x_i + y_i) c_{v_i}^2 = -2a_2.$$

4. Maximum reverse degree energy of some standard graphs

THEOREM 4.1. *For $n \geqslant 3$, the maximum reverse degree energy of the star graph S_n is*

$$EM_R(S_n) = 2\sqrt{(n-1)^3}.$$

PROOF. Consider the Star graph S_n with vertex $v_1, v_2, \ldots v_n$. Then, the maximum reverse degree matrix of the graph S_n

$$M_R(S_n) = \begin{bmatrix} 0 & n-1 & n-1 & \ldots & n-1 \\ n-1 & 0 & 0 & \ldots & 0 \\ n-1 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ n-1 & 0 & 0 & \ldots & 0 \end{bmatrix}$$

Characteristic polynomial is

$$\begin{vmatrix} -\mu & n-1 & n-1 & \dots & n-1 \\ n-1 & -\mu & 0 & \dots & 0 \\ n-1 & 0 & -\mu & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ n-1 & 0 & 0 & \dots & -\mu \end{vmatrix}$$

Characteristic equation is $(\mu)^{n-2}(\mu^2 - \sqrt{(n-1)^3}) = 0$.
The eigenvalues of maximum reverse degree matrix $M_R(G)$ of the graph are: 0 of multiplicity $n-3$ and $\pm\sqrt{(n-1)^3}$ of multiplicity one. The maximum reverse degree energy is,

$$EM_R(S_n) = |0|\,(n-2) + \left|\sqrt{(n-1)^3}\right| + \left|-\sqrt{(n-1)^3}\right| = 2\sqrt{(n-1)^3}.$$

□

THEOREM 4.2. *For $n \geqslant 3$, the maximum reverse degree energy of the Complete graph K_n is*

$$EM_R(S_n) = 2(n-1).$$

PROOF. Consider the Star graph K_n with vertex $v_1, v_2, \dots v_n$. Then, the maximum reverse degree matrix of the graph K_n

$$M_R(K_n) = \begin{bmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ 1 & 1 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 0 \end{bmatrix}$$

Characteristic polynomial is

$$\begin{vmatrix} -\mu & 1 & 1 & \dots & 1 \\ 1 & -\mu & 1 & \dots & 1 \\ 1 & 1 & -\mu & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & -\mu \end{vmatrix}$$

Characteristic equation is $(\mu+1)^{n-1}(\mu^2 - (n-1)) = 0$.
The eigenvalues of maximum reverse degree matrix $M_R(G)$ of the graph are: $\mu = -1$ having the multiplicity $n-1$ and $\mu = n-1$ with multiplicity one. The maximum reverse degree energy is,

$$EM_R(K_n) = |-1|\,(n-1) + |(n-1)| = 2(n-1).$$

□

THEOREM 4.3. *For $n \geqslant 3$, the maximum reverse degree energy of the complete bipartite graph $K_{n,n}$ is*

$$EM_R(K_{n,n}) = 2n^2.$$

PROOF. Consider the complete bipartite graph $K_{n,n}$ with vertex $v_1, v_2, \ldots v_n$. Then, the maximum reverse degree matrix of the graph $K_{n,n}$

$$M_R(K_{n,n}) = \begin{bmatrix} 0 & 0 & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ 0 & 0 & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ 0 & 0 & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \ldots & 0 \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \ldots & 0 \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \ldots & 0 \end{bmatrix}_{(2n \times 2n)}$$

Characteristic polynomial is

$$\begin{vmatrix} -\mu & 0 & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ 0 & -\mu & 0 & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ 0 & 0 & -\mu & \ldots & 0 & 1 & 1 & 1 & \ldots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & -\mu & 1 & 1 & 1 & \ldots & 1 \\ 1 & 1 & 1 & \ldots & 1 & -\mu & 0 & 0 & \ldots & 0 \\ 1 & 1 & 1 & \ldots & 1 & 0 & -\mu & 0 & \ldots & 0 \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & -\mu & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \ldots & 1 & 0 & 0 & 0 & \ldots & -\mu \end{vmatrix}$$

Characteristic equation is $(\mu)^{2(n-1)}(\mu^2 - n^2) = 0$.
The eigenvalues of maximum reverse degree matrix $M_R(K_{n,n})$ of the graph are: 0 of multiplicity $2(n-1)$ and $\mu = \pm n$ of multiplicity one each. The maximum reverse degree energy is,

$$EM_R(K_{n,n}) = |0|\, 2(n-1) + |n| + |-n| = 2n.$$

□

THEOREM 4.4. *For $n \geqslant 3$, the maximum reverse degree energy of the Crown graph S_n^0 is*

$$EM_R(S_n^0) = 4(n-1).$$

PROOF. Consider the crown graph S_n^0 with vertex $v_1, v_2, \ldots v_n$. Then, the maximum reverse degree matrix of the graph S_n^0

$$M_R(S_n^0) = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 & 1 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & 1 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 1 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 & 1 & 1 & \dots & 0 \\ 0 & 1 & 1 & \dots & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 1 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix}_{(2n \times 2n)}$$

Characteristic polynomial is

$$\begin{vmatrix} -\mu & 0 & 0 & \dots & 0 & 0 & 1 & 1 & \dots & 1 \\ 0 & -\mu & 0 & \dots & 0 & 1 & 0 & 1 & \dots & 1 \\ 0 & 0 & -\mu & \dots & 0 & 1 & 1 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -\mu & 1 & 1 & 1 & \dots & 0 \\ 0 & 1 & 1 & \dots & 1 & -\mu & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 1 & 0 & -\mu & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 1 & 0 & 0 & -\mu & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & \dots & -\mu \end{vmatrix}$$

Characteristic equation is $(\mu^2 - 1)^{(n-1)}(\mu^2 - (n-1)^2) = 0$.
The eigenvalues of maximum reverse degree matrix $M_R(S_n^0)$ of the graph are: $\pm(n-1)$ of multiplicity one each and $\mu = \pm 1$ with multiplicity $(n-1)$ each. The maximum reverse degree energy is,

$$EM_R(S_n^0) = |-1|\,(n-1) + |1|\,(n-1) + |n-1| + |-(n-1)| = 4(n-1).$$

□

5. Bounds for the maximum reverse degree energy

In this section, lower and upper bounds for the maximum reverse degree energy of graphs are calculated.

LEMMA 5.1. *Suppose a_i and b_i are non negative real numbers for $1 \leqslant i \leqslant n$ then,*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) \leqslant \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} a_ib_i\right)^2,$$

where $M_1 = \max_{1\leqslant i\leqslant n} a_i,\ M_2 = \max_{1\leqslant i\leqslant n} b_i,\ m_1 = \min_{1\leqslant i\leqslant n} a_i$ *and* $m_2 = \min_{1\leqslant i\leqslant n} b_i$

LEMMA 5.2. *If a_i and b_i are non negative real numbers for $1 \leqslant i \leqslant n$ then,*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_ib_i\right)^2 \leqslant \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2,$$

where $M_1 = \max_{1\leqslant i\leqslant n} a_i,\ M_2 = \max_{1\leqslant i\leqslant n} b_i,\ m_1 = \min_{1\leqslant i\leqslant n} a_i$ *and* $m_2 = \min_{1\leqslant i\leqslant n} b_i.$

LEMMA 5.3. *If a_i and b_i are any sequences of real and complex numbers for $1 \leqslant i \leqslant n$ then,*

$$\left(\sum_{i=1}^{n} a_ib_i\right)^2 = \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \sum_{1\leqslant i\leqslant j\leqslant n} (a_ib_j - a_jb_i)^2.$$

THEOREM 5.1. *Let G be a simple graph with n vertices, m size. Let $\mu_1, \mu_2, \mu_3, \ldots \mu_n$ be the eigenvalues of the maximum reverse degree matrix, $M_R(G)$ then,*

$$\sqrt{2\sum_{i=1}^{n}(x_i + y_i)c_{v_i}^2 + n(n-1)P^{\frac{2}{n}}} \leqslant EM_R(G) \leqslant \sqrt{2n\left(\sum_{i=1}^{n}(x_i + y_i)c_{v_i}^2\right)}$$

where $P = det(M_R(G))$.

PROOF. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of the Laplacian edge dominating matrix $M_R(G)$. In Cauchy-Schwarz inequality, put $a_i = 1$ and $b_i = |\mu_i|$ we get,

$$\left(\sum_{i=1}^{n} |\mu_i|\right)^2 \leqslant \left(\sum_{i=1}^{n} 1\right)\left(\sum_{i=1}^{n} |\mu_i|^2\right),$$

From Theorem 3.1, we have

$$(EM_R(G)) \leqslant \sqrt{\left(2n\sum_{i=1}^{n}(x_i + y_i)c_{v_i}^2\right)} \tag{5.1}$$

For lower bound consider,

$$(EM_R(G))^2 = \left(\sum_{i=1}^{n} |\mu_i|^2\right) = \sum_{i=1}^{n} \mu_i^2 + \sum_{i\neq j} |\mu_i||\mu_j| \tag{5.2}$$

Since the geometric means of positive number is not greater then arithmetic mean so we get,

$$\frac{1}{n(n-1)}\sum_{i\neq j}|\mu_i||\mu_j| \geqslant \prod_{i\neq j}(|\mu_i||\mu_j|)^{\frac{1}{n(n-1)}} = \left(\prod_{i=1}^{n}|\mu_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}$$
$$= P^{\frac{2}{n}}.$$

Where $P = det(M_R(G))$ and now, using above equation in (5.2) we get,

$$(EM_R(G)) \geqslant \sqrt{2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2 + n(n-1)P^{\frac{2}{n}}} \tag{5.3}$$

Rearranging equation (5.1) and (5.3) the result follows. □

THEOREM 5.2. *If the maximum reverse degree energy $EM_R(G)$ is a rational number then $EM_R(G)$ it must be an even integer.*

PROOF. Let $\mu_1, \mu_2, \ldots \mu_n$ be the eigenvalues of the maximum reverse degree matrix $M_R(G)$ such that, $\mu_1, \mu_2, \ldots, \mu_t$ are positive and rest are non-positive. By the definition we have,

$$\begin{aligned} EM_R(G) &= \sum_{i=1}^{n}|\mu_i| \\ &= (\mu_1+\mu_2+\cdots+\mu_t) - (\mu_{(t+1)}+\mu_{(t+2)}+\cdots+\mu_n) \\ &= 2(\mu_1+\mu_2+\cdots+\mu_t) - (\mu_1+\mu_2+\cdots+\mu_n) \\ &= 2(\mu_1+\mu_2+\cdots+\mu_t) - \sum_{i=1}^{n}\mu_i \end{aligned}$$

This follows the required result. □

THEOREM 5.3. *Let G be a graph with n vertices and m edges, then*

$$EM_R(G) \leqslant |\mu_1| + \sqrt{(n-1)(\beta - |\mu_1|^2)) \quad where \quad \beta = 2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2}$$

and with property $\mu \geqslant m$.

PROOF. Let $\mu_1 \geqslant \mu_2 \geqslant \ldots \mu_n$ be the non increasing order of eigenvalues of the maximum reverse degree matrix $M_R(G)$. With considering $a_i = 1$ and $b_i = |\mu_i|$ in Cauchy-Schwarz inequalityand we get,

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

We get,

$$(EM_R(G) - |\mu_1|)^2 \leqslant (n-1)\left(2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2 - |\mu_1|^2\right). \tag{5.4}$$

Take $2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2 = \beta$.

Now using above in equation (5.4) and simplifying we get the required result. □

We obtain the results for bounds of $EM_R(G)$ in terms of the largest and smallest absolute eigenvalues of the the maximum reverse degree matrix $M_R(G)$. We use some previously known inequalities that will be needed in the proof of the next results.

THEOREM 5.4. *Let G be a graph with n vertices and m edges, then*

$$EM_R(G) \geqslant \frac{2\sqrt{n\beta}\sqrt{|\mu_l^*||\mu_s^*|}}{|\mu_l^*| + |\mu_s^*|}$$

where $\beta = 2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2$,$|\mu_l^*|$ and $|\mu_s^*|$ are the largest and smallest absolute eigenvalues of the matrix $M_R(G)$ respectively.

PROOF. Let $\mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_n$ be the eigenvalues of the the maximum reverse degree matrix $M_R(G)$.
Putting $a_i = |\mu_i|$ and $b_i = 1$ for $1 \leqslant i \leqslant n$, in Cauchy-Schwarz inequality, we get

$$\left(\sum_{i=1}^{n}|\mu_i|^2\right)\left(\sum_{i=1}^{n}1\right) \leqslant \frac{1}{4}\left(\sqrt{\frac{|\mu_1^*|}{|\mu_s^*|}} + \sqrt{\frac{|\mu_s^*|}{|\mu_1^*|}}\right)^2\left(\sum_{i=1}^{n}\mu_i\right)^2,$$

$$\text{where } |\mu_l^*| = \max_{1\leqslant i\leqslant n}\{|\mu_i|\} \text{ and } |\mu_s^*| = \min_{1\leqslant i\leqslant n}\{|\mu_i|\}$$

$$\therefore \quad n\beta \leqslant \frac{1}{4}\left(\sqrt{\frac{|\mu_l^*|}{|\mu_s^*|}} + \sqrt{\frac{|\mu_s^*|}{|\mu_l^*|}}\right)^2 (EM_R(G))^2$$

$$\implies \quad 2\sqrt{n\beta} \leqslant \frac{(|\mu_l^*| + |\mu_s^*|)}{\sqrt{|\mu_s^*||\mu_l^*|}}\,(EM_R(G))$$

With rearranging , the result holds. □

THEOREM 5.5. *Let G be a connected graph, then*

$$EM_R(G) \geqslant \sqrt{n\beta - \frac{n^2}{4}\,(|\mu_l^*| + |\mu_s^*|)^2},$$

where $\beta = 2\sum_{i=1}^{n}(x_i+y_i)c_{v_i}^2$,$|\mu_1^*|$ and $|\mu_s^*|$ are the largest and smallest absolute eigenvalues of the matrix $M_R(G)$ respectively.

PROOF. Let $\mu_1 \geqslant \mu_2 \geqslant \ldots \mu_n$ be the eigenvalues of maximum reverse degree matrix $M_R(G)$.
Putting $a_i = |\mu_i|$ and $b_i = 1$ for $1 \leqslant i \leqslant n$, in lemma 5.2, we get

$$\left(\sum_{i=1}^{n} |\mu_i|^2\right)\left(\sum_{i=1}^{n} 1\right) - \left(\sum_{i=1}^{n} |\mu_i|\right)^2 \leqslant \frac{n^2}{4}\left(|\mu_1^*| - |\mu_s^*|\right)^2, \tag{5.5}$$

where $|\mu_l^*| = \max_{1\leqslant i\leqslant n}\{|\mu_i|\}$, $|\mu_s^*| = \min_{1\leqslant i\leqslant n}\{|\mu_i|\}$ and $\beta = 2\sum_{i=1}^{n}(x_i + y_i)c_{v_i}^2$
Using those in equation (5.5) we get,

$$(n\beta) - \left(EM_R(G)\right)^2 \leqslant \frac{n^2}{4}\left(|\mu_l^*| - |\mu_s^*|\right)^2 \tag{5.6}$$

By rearranging we get the result. □

References

1. R. Balakrishnan, *The energy of a graph*, Linear Algebra Appl., **387**(2004), 287–295.
2. A. Chandrashekar and M. Smitha, *On maximum degree energy of a graph*, Int. J. Contemp. Math. Sciences, **4**(8)(2009), 385–396.
3. C. A. Coulson and J. Streitwieser, *Dictionary of π-Electron Calculations* Freeman, San Francisco, 1965.
4. S. Ediz and Murat Cancan, *Reverse Zagreb indices of cartesian product of graphs*, International Journal of Mathematics and Computer Science, **11(1)**(2016), 51–58.
5. K. J. Gowtham, *A study of reverse topological indices and their importance in chemical sciences*, Applied Mathematics E-Notes, In press.
6. K. J. Gowtham and N. N. Swamy, *Multiplicative reverse Geometric-Arithmetic indices and Arithmetic-Geometric of silicate network*, Biointerface applied rescarch in chemistry, **12**(3)(2022), 4192–4199.
7. K. J. Gowtham, *On reverse laplacian energy of a graph*, Letters in Applied NanoBioScience **12**(1)(2022), DOI: 10.33263/lianbs121.019.
8. K. J. Gowtham, *Reverse Hyper-Zagreb indices of the Cartesian product of graphs*, International Journal of Mathematical Combinatorics, **4**(2021), 49–56.
9. K. J. Gowtham and N. N. Swamy, *On Sombor energy of graphs*, Nanosystems: Physics, Chemistry, Mathematics, **12:4** (2021), 411–417.
10. I. Gutman, *The energy of a graph*, Ber. Math. Stat. Sekt.Forschungszent Graz, **103**(1978), 1–22.
11. I. Gutman, *Topology and stability of conjugated hydrocarbons. The dependence of total pi-electron energy on molecular topology*, J. Serb. Chem. Soc. **70**(2005), 441–456.
12. I. Gutman, *The Energy of a Graph: Old and new results*, Algebraic combinatorics and applications, Springer, Berlin, 196–211 (2001).
13. V. R. Kulli, *Reverse Zagreb and Reverse Hyper-Zagreb Indices and their Polynomials of Rhombus Silicate Networks*, Annals of Pure and Applied Mathematics, Vol. **16**(1)(2018), 47–51.
14. V. R. Kulli, *Computing F-reverse index and F-reverse polynomial of certain networks*,International Journal of Mathematical Archive, **9**(8)(2018), 27–33.
15. K. I. Ramachandran, G. Deepa, K. Namboori *Computational Chemistry and Molecular Modelling:Principles and Applications*. Springer, Berlin, 2008.
16. K. Yates, *Huckel Molecular Orbital Theory* Academic Press, New York (1978).

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