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ENERGY OF GRAPHS AND ITS NEW BOUNDS

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Abstract: In organic chemistry, finding out theoretically the total $\pi-$electron energy of conjugated carbon compound is one of the interesting concept. Later during the year 1970, I. Gutman was successful in achieving this by defining a term called energy of a graph, $\mathbb{E}(G)$ for any graph G with m edges and n vertices. It is not that easy to find energy of any general graph. This problem was solved by obtaining bounds for $\mathbb{E}(G)$. Initially bounds for energy of any graph G are obtained by using McClelland bounds. Koolen and Moulton improved the McClelland's upper bounds. In this article we established new energy bounds with the help of Holder's inequality.

Keywords and Phrases: Adjacency matrix, graph spectrum, Bounds for energy energy of graph.

2020 Mathematics Subject Classification: 05C50, 05C69.

1. Introduction

Let us consider a simple undirected graph $G = (V, E)$ having m edges and n vertices. For any vertex $v_i \epsilon V$, the degree of v_i is defined as the total number of edges that are incident to v_i and we write the degree of v_i by d_i or $d(v_i)$. When $d_i = r$, $\forall v_i$, we say that a graph G is regular graph of degree r. A graph G is said to be a bipartite graph with degree r_1 and r_2, if the vertex set can be written as, $V = U \cup V$ where $U \cap V = \phi$ and every edge of G has its vertex in U and a vertex in V. If each vertex of a bipartite graph G has same degree, then we call G a complete bipartite graph. If the graph G is bipartite and every vertex in the same partition has same degree, then we say G is semi-regular bipartite graph. A graph G is said to be a connected graph if for any two vertices u and v of the graph G has $u - v$ path. Throughout this paper we assume that the graph is connected.

It is useful to represent a graph G by means of a matrix, called Adjacency matrix. Consider a vertex set $V = \{v_1, v_2, ..., v_n\}$ the graph G, then the Adjacency matrix of G is defined by $A(G) = [a_{ij}]$, $A(G) = \begin{cases} 1 & \text{if } v_iv_j \text{ is an edge} \\ 0 & \text{otherwise} \end{cases}$

Let G be a graph with m edges and n vertices. Then energy of G is defined by $\mathbb{E}(G) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are eigenvalues of $A(G)$. The details on graph energy can be obtained from papers [6, 7, 8]. For applications on graph energy can be seen from papers [1, 2, 5].

Bounds for energy of graph in terms of m and n was initially given by McClelland [13],

$$\sqrt{2m + n(n-1)|Det(A)|^{\frac{2}{n}}} \leq \mathbb{E}(G) \leq \sqrt{2mn}. \tag{1.1}$$

Later Koolen and Moulton improvised the above upper bounds [11].

$$\mathbb{E}(G) \leq \left(\frac{2m}{n}\right) + \sqrt{(n-1)\left(2m - \left(\frac{2m}{n}\right)^2\right)} \text{ for } 2m \geq n \tag{1.2}$$

As a special case they also established an upper bound for bipartite graph in the form [12]

$$\mathbb{E}(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left(2m - 2\left(\frac{2m}{n}\right)^2\right)} \text{ for } 2m \geq n. \tag{1.3}$$

Also they arrived at the result, an upper bound for energy of a graph G in terms n vertices. $\mathbb{E}(G) \leq \frac{n}{2}(1 + \sqrt{n})$.
Improvisation of these bounds can be seen in the papers [4, 14].

Throughout this paper we use the following elementary results on eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots, \geq \lambda_n$, of adjacency matrix of a graph G.

1. $\sum_{i=1}^{n} \lambda_i = 0$ and $\sum_{i=1}^{n} \lambda_i^2 = 2m = \sum_{i=1}^{n} |\lambda_i|^2$.

Further $\prod_{i=1}^{n} \lambda_i = \mathbf{Det}(A(G))$.

2. The largest eigenvalue of a connected graphs G satisfies $\lambda_1 \geq \frac{2m}{n} \geq 1$.

2. The Main Results

Lemma 2.1. *Let G represents a graph with m edges and n vertices then the adjacency matrix $A(G)$ satisfies*

$$|\mathbf{Det}(A(G))| \leq (2m)^{\frac{n}{2}}. \tag{2.1}$$

Proof. The proof easily follows with $|\mathbf{Det}(A(G))| = |\lambda_1\lambda_2 ... \lambda_n| = |\lambda_1||\lambda_2| ... |\lambda_n|$. But $|\mathbf{Det}(A(G))| \leq |\lambda_1||\lambda_1| ... |\lambda_1| = |\lambda_1|^n \leq (\sqrt{2m})^n$.
This gives $|\mathbf{Det}(A(G))| \leq (2m)^{\frac{n}{2}}$.

Lemma 2.2. *Consider a connected graph G with m edges and n vertices. The largest eigenvalue, λ_1 of G satisfies*

$$|\lambda_1| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}. \tag{2.2}$$

Proof. The relation $\lambda_1 + \lambda_2 + \cdots + \lambda_n = 0$ gives $\lambda_2 + \cdots + \lambda_n = -\lambda_1$. Since λ_1 is always positive, the sum $\lambda_2 + \cdots + \lambda_n$ should be a negative quantity.

$$\therefore \lambda_2 + \cdots + \lambda_n \leq |\lambda_2\lambda_3 \cdots \lambda_n|^{\frac{1}{n-1}}.$$

i.e.,$-\lambda_1 \leq \dfrac{|\lambda_1\lambda_2 \cdots \lambda_n|^{\frac{1}{n-1}}}{\lambda_1^{\frac{1}{n-1}}}$, which implies $-\lambda_1^{\frac{n}{n-1}} \leq |\mathbf{Det}(A(G))|^{\frac{1}{n-1}}$.
$\Rightarrow |\lambda_1|^{\frac{2n}{n-1}} \leq |\mathbf{Det}(A(G))|^{\frac{2}{n-1}}$ if $|\lambda_1| \leq 1$ and $|\lambda_1|^{\frac{2n}{n-1}} \geq |\mathbf{Det}(A(G))|^{\frac{2}{n-1}}$ if $|\lambda_1| \geq 1$.
Since G is connected $|\lambda_1| \geq 1$. Hence $|\lambda_1| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}$.

Lemma 2.3. *Let G represents a connected graph with m edges and n vertices. The largest eigenvalue, λ_1 of the graph G satisfies*

$$|\lambda_1| \geq \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{\sqrt{n}}. \tag{2.3}$$

Proof. The expressions, $\dfrac{|\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|}{n}$ and $|\lambda_1\lambda_2 \cdots \lambda_n|^{\frac{1}{n}}$ are respectively arithmetic and geometric mean of the values $|\lambda_1|, |\lambda_2|, \cdots, |\lambda_n|$.

But arithmetic mean exceeds geometric mean it follows that

$$\frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{n} \geq |\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n}}.$$

$$\frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{\sqrt{n}} \geq \frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{n} \geq |\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n}}$$

$\therefore \frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{\sqrt{n}} \geq |\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n}}$ implies $\dfrac{n|\lambda_1|}{\sqrt{n}} \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}$

$$|\lambda_1| \geq \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{\sqrt{n}}.$$

3. New Energy Bounds of a Graph

Lemma 3.1. *Let G represents a graph with m edges, n vertices and $A(G)$ be a non-singular adjacency matrix, then*

$$n|\mathbf{Det}(A(G))|^{\frac{1}{n}} \leq \mathbb{E}(G) \leq \frac{2mn}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}. \tag{3.1}$$

Proof. Making use of inequality between arithmetic and geometric mean of $|\lambda_1|, |\lambda_2|, \cdots, |\lambda_n|$ we have $\frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{n} \geq |\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n}}$.

$\Rightarrow \mathbb{E}(G) \geq n|\mathbf{Det}(A(G))|^{\frac{1}{n}}$, which is a new lower bound.

From $\frac{|\lambda_1|+|\lambda_2|+\cdots+|\lambda_n|}{n} \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}$ gives $|\lambda_1| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}$.

$\Rightarrow |\lambda_1| \sum_{i=1}^{n} |\lambda_i| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}} \sum_{i=1}^{n} |\lambda_i|$.

Since$|\lambda_i| \leq |\lambda_1|$ $\forall i$ therefore $n|\lambda_1|^2 \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}\mathbb{E}(G)$.

But $|\lambda_1|^2 \leq 2m$, hence we get $\mathbb{E}(G) \leq \dfrac{2mn}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}$, which is a new upper-bound

Thus $n|\mathbf{Det}(A(G))|^{\frac{1}{n}} \leq \mathbb{E}(G) \leq \dfrac{2mn}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}$.

With the help of Holder's inequality we can obtain new bounds for energy of graphs.

Holder's inequality. For positive real numbers $x_{ij}(i = 1, 2, ..., n$ and $j = 1, 2, 3, ..., n)$ then

$$\prod_{i=1}^{n}\Big(\sum_{j=1}^{n}x_{ij}\Big)^{\frac{1}{n}} \geq \sum_{j=1}^{n}\Big(\prod_{i=1}^{n}x_{ij}^{\frac{1}{n}}\Big)$$

Theorem 3.1. *If G represents a graph with m edges$(2m \geq n)$, n vertices and A is a adjacency non singular matrix then*

$$n^{\frac{n-1}{n}}|\mathbf{Det}(A(G))|^{\frac{1}{n}} \leq \mathbb{E}(G) < \frac{(4m)^{n^2}}{|\mathbf{Det}(A(G))|^{(n-1)}}. \tag{3.2}$$

Proof. Apply Holder's inequality using

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{|\lambda_1|} & \cdots & \frac{1}{|\lambda_1|} \\ \frac{1}{|\lambda_2|} & 1 & \cdots & \frac{1}{|\lambda_2|} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{1}{|\lambda_n|} & \frac{1}{|\lambda_n|} & \cdots & 1 \end{pmatrix}$$

and we simplify right side and left side of the inequality separately.

$$LHS=\Big(1+\frac{n-1}{|\lambda_1|}\Big)^{\frac{1}{n}}\Big(1+\frac{n-1}{|\lambda_2|}\Big)^{\frac{1}{n}}...\Big(1+\frac{n-1}{|\lambda_n|}\Big)^{\frac{1}{n}}$$
$$\leq \Big(1+\frac{n-1}{|\lambda_1|}\Big)\Big(1+\frac{n-1}{|\lambda_2|}\Big)...\Big(1+\frac{n-1}{|\lambda_n|}\Big).$$

But $2m \geq n > (n-1)$ therefore we have

$$LHS < \Big(1+\frac{2m}{|\lambda_1|}\Big)\Big(1+\frac{2m}{|\lambda_2|}\Big)...\Big(1+\frac{2m}{|\lambda_n|}\Big).$$

But $|\lambda_i| \leq \sqrt{2m} \leq 2m \Rightarrow 1 \leq \dfrac{2m}{|\lambda_i|}$ $\forall i$ so

$$LHS < \Big(\frac{2m}{|\lambda_1|}+\frac{2m}{|\lambda_1|}\Big)\Big(\frac{2m}{|\lambda_2|}+\frac{2m}{|\lambda_2|}\Big)...\Big(\frac{2m}{|\lambda_n|}+\frac{2m}{|\lambda_n|}\Big).$$
$$= \Big(\frac{4m}{|\lambda_1|}\Big)\Big(\frac{4m}{|\lambda_2|}\Big)...\Big(\frac{4m}{|\lambda_n|}\Big).$$
$$= \frac{(4m)^n}{|\lambda_1\lambda_2...\lambda_n|} = \frac{(4m)^n}{|\mathbf{Det}(A(G))|}.$$

$$RHS=\frac{1}{|\lambda_2|^{\frac{1}{n}}|\lambda_3|^{\frac{1}{n}}...|\lambda_n|^{\frac{1}{n}}}+\frac{1}{|\lambda_1|^{\frac{1}{n}}|\lambda_3|^{\frac{1}{n}}...|\lambda_n|^{\frac{1}{n}}}+...+\frac{1}{|\lambda_1|^{\frac{1}{n}}|\lambda_2|^{\frac{1}{n}}...|\lambda_{n-1}|^{\frac{1}{n}}}.$$
$$= \frac{|\lambda_1|^{\frac{1}{n}}}{|\lambda_1\lambda_2...\lambda_n|^{\frac{1}{n}}}+\frac{|\lambda_2|^{\frac{1}{n}}}{|\lambda_1\lambda_2...\lambda_n|^{\frac{1}{n}}}+...+\frac{|\lambda_n|^{\frac{1}{n}}}{|\lambda_1\lambda_2...\lambda_n|^{\frac{1}{n}}}.$$
$$= \frac{1}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}\sum_{i=1}^{n}|\lambda_i|^{\frac{1}{n}}.$$

$$\therefore \frac{1}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}} \sum_{i=1}^{n} |\lambda_i|^{\frac{1}{n}} < \frac{(4m)^n}{|\mathbf{Det}(A(G))|}.$$

$$\sum_{i=1}^{n} |\lambda_i|^{\frac{1}{n}} < \frac{(4m)^n}{|\mathbf{Det}(A(G))|^{(1-\frac{1}{n})}}.$$

But $\left(\sum_{i=1}^{n} |\lambda_i|\right)^{\frac{1}{n}} \leq \sum_{i=1}^{n} |\lambda_i|^{\frac{1}{n}}$. Hence $\left(\sum_{i=1}^{n} |\lambda_i|\right)^{\frac{1}{n}} < \frac{(4m)^n}{|\mathbf{Det}(A(G))|^{(\frac{n-1}{n})}}$.

$$\mathbb{E}(G) < \frac{(4m)^{n^2}}{|\mathbf{Det}(A(G))|^{(n-1)}}.$$

For lower bound we use the following substitution in Holder's inequality

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{pmatrix} = \begin{pmatrix} |\lambda_1| & |\lambda_1| & \cdots & |\lambda_1| \\ |\lambda_2| & |\lambda_2| & \cdots & |\lambda_2| \\ \vdots & \vdots & \cdots & \vdots \\ |\lambda_n| & |\lambda_n| & \cdots & |\lambda_n| \end{pmatrix}$$

$$(n|\lambda_1|)^{\frac{1}{n}} + (n|\lambda_2|)^{\frac{1}{n}} + \cdots + (n|\lambda_n|)^{\frac{1}{n}} \geq n(|\lambda_1||\lambda_2|\cdots|\lambda_n|)^{\frac{1}{n}}.$$

$$|\lambda_1|^{\frac{1}{n}} + |\lambda_2|^{\frac{1}{n}} + \cdots + |\lambda_n|^{\frac{1}{n}} \geq n^{\frac{n-1}{n}}(|\mathbf{Det}(A(G))|)^{\frac{1}{n}}.$$

But $(|\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|) \geq |\lambda_1|^{\frac{1}{n}} + |\lambda_2|^{\frac{1}{n}} + \cdots + |\lambda_n|^{\frac{1}{n}}$.

$$\therefore \mathbb{E}(G) \geq n^{\frac{n-1}{n}}|\mathbf{Det}(A(G))|^{\frac{1}{n}}.$$

Thus the bounds for $\mathbb{E}(G)$ is, $n^{\frac{n-1}{n}}|\mathbf{Det}(A(G))|^{\frac{1}{n}} \leq \mathbb{E}(G) < \frac{(4m)^{n^2}}{|\mathbf{Det}(A(G))|^{(n-1)}}$.

4. New Energy Lower Bounds and new Energy Upper Bounds

Theorem 4.1. *The energy of a graph G has a lower bound*

$$\mathbb{E}(G) \geq \frac{2m}{n} + \Big(\frac{|\boldsymbol{Det}(A(G))|}{\frac{2m}{n}}\Big)^{\frac{1}{n-1}}. \tag{4.1}$$

where G is graph with m edges and n vertices with $2m \geq n$.

Proof. We make use of inequality between arithmetic mean and geometric mean for $(n-1)$ real numbers $|\lambda_2|, |\lambda_3|, \cdots, |\lambda_n|$, $\frac{|\lambda_2| + |\lambda_3| + \cdots + |\lambda_n|}{n-1} \geq |\lambda_2\lambda_3\cdots\lambda_n|^{\frac{1}{n-1}}$.

$$\Big(|\lambda_2| + |\lambda_3| + \cdots + |\lambda_n|\Big) \geq \frac{|\lambda_2| + |\lambda_3| + \cdots + |\lambda_n|}{n-1} \geq |\lambda_2\lambda_3\cdots\lambda_n|^{\frac{1}{n-1}}.$$

$$\Rightarrow \mathbb{E}(G) - |\lambda_1| \geq \frac{|\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n-1}}}{|\lambda_1|_{\frac{1}{n-1}}}.$$

$$\Rightarrow \ \mathbb{E}(G) \geq |\lambda_1| + \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n-1}}}{|\lambda_1|^{\frac{1}{n-1}}}.$$

Put $f(x) = x + \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n-1}}}{x^{\frac{1}{n-1}}}$ with $|\lambda_1| = x$. In order to minimize the function we find $f'(x)$ and $f''(x)$. But at minima or maxima point $f'(x) = 0$. Thus the function $f(x)$ has minima or maxima at $x = \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-1)^{\frac{n-1}{n}}}$.
At this point the value of $f''(x)$ is given by,
$f''(x) = \dfrac{n}{(n-1)^2}|\mathbf{Det}(A(G))|^{\frac{1}{n-1}} x^{\frac{1-2n}{n-1}} \geq 0.$

This implies at this particular point the function has the minimum value. Its value is given by $f\Big(\dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-1)^{\frac{n-1}{n}}}\Big) = \frac{n|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-1)^{\frac{(n-1)}{n}}}$.

Since the function becomes an increasing function in
$\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-1)^{\frac{n-1}{n}}} \leq |detA|^{\frac{1}{n}} \leq \frac{2m}{n} \leq |\lambda_1| \leq \sqrt{2m}.$

$$\mathbb{E}(G) \geq f\Big(\frac{2m}{n}\Big).$$
$$\mathbb{E}(G) \geq \frac{2m}{n} + \Big(\frac{|\mathbf{Det}(A(G))|}{\frac{2m}{n}}\Big)^{\frac{1}{n-1}}.$$

Theorem 4.2. *Consider a graph G having m edges and $n(\geq 3)$ vertices with $2m \geq n$. Then*

$$\mathbb{E}(G) \geq \frac{2m}{n} + \frac{(n-2)^{\frac{1}{n}}|\mathbf{Det}(A(G))|^{\frac{n-1}{n(n-2)}}}{(\frac{2m}{n})^{\frac{1}{n-2}}}. \tag{4.2}$$

Proof. We make use of inequality between arithmetic mean and geometric mean for $(n-2)$ real numbers
$|\lambda_2|, |\lambda_3|, \cdots, |\lambda_{n-1})|,\ \dfrac{|\lambda_2| + |\lambda_3| + \cdots + |\lambda_{n-1}|}{n-2} \geq |\lambda_2\lambda_3\cdots\lambda_{n-1}|^{\frac{1}{n-2}}$

$$\Big(|\lambda_2| + |\lambda_3| + \cdots + |\lambda_{n-1}|\Big) \geq \frac{|\lambda_2| + |\lambda_3| + \cdots + |\lambda_{n-1}|}{n-2} \geq |\lambda_2\lambda_3\cdots\lambda_{n-1}|^{\frac{1}{n-2}}.$$

$$\Rightarrow \ \mathbb{E}(G) - |\lambda_1| - |\lambda_n| \geq \frac{|\lambda_1\lambda_2\cdots\lambda_n|^{\frac{1}{n-2}}}{|\lambda_1\lambda_n|^{\frac{1}{n-2}}}.$$
$$\Rightarrow \ \mathbb{E}(G) \geq |\lambda_1| + |\lambda_n| + \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{|\lambda_1\lambda_n|^{\frac{1}{n-2}}}.$$

Let $|\lambda_1| = x$, $|\lambda_n| = y$ with $g(x, y) = x + y + \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{(xy)^{\frac{1}{n-2}}}$.

To minimize the above function of two variables, we make use of partial differentiation method by finding $g_x(x,y)$, $g_y(x,y)$, $g_{xx}(x,y)$, $g_{yy}(x,y)$, $g_{xy}(x,y)$ and $\Delta = g_{xx}g_{yy} - g_{xy}^2$.

$$g_x = 1 - \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{n-2}(xy)^{\frac{1-n}{n-2}}y, \quad g_y = 1 - \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{n-2}(xy)^{\frac{1-n}{n-2}}x$$

$$g_{xx} = -\frac{y^2(1-n)|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{(n-2)^2}(xy)^{\frac{3-2n}{n-2}}, g_{yy} = -\frac{x^2(1-n)|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{(n-2)^2}(xy)^{\frac{3-2n}{n-2}}$$

$$g_{xy} = -\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}{n-2}\Big((xy)^{\frac{1-n}{n-2}} + y\frac{n-1}{n-2}(xy)^{\frac{3-2n}{n-2}}\Big),$$

$$\Delta = \tfrac{(xy)^2(1-n)^2|\mathbf{Det}(A(G))|^{\frac{2}{n-2}}}{(n-2)^4}(xy)^{\frac{6-4n}{n-2}} - \tfrac{|\mathbf{Det}(A(G))|^{\frac{2}{n-2}}}{(n-2)^2}\Big((xy)^{\frac{1-n}{n-2}} + y\tfrac{n-1}{n-2}(xy)^{\frac{3-2n}{n-2}}\Big)^2.$$

At minima or maxima $g_x = 0$, $g_y = 0$. This gives us two equations $(xy)^{\frac{1-n}{n-2}}y = \dfrac{n-2}{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}$ and $(xy)^{\frac{1-n}{n-2}}x = \dfrac{n-2}{|\mathbf{Det}(A(G))|^{\frac{1}{n-2}}}$. On solving, we have $x = y = \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}$.

This implies the function $g(x,y)$ has minima or maxima for $x = y = \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}$.

For this point, $g_{xx} \geq 0$, $g_{yy} \geq 0$ and $\Delta \leq 0$. Hence the function has the minimum value at this point, which is given by, $g\Big(\dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}, \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}\Big)$.

Since $2m \geq n$, so $g(x,y)$ is an increasing function in

$|\det(A(G))|^{\frac{1}{n}} \leq \frac{2m}{n} \leq x \leq \sqrt{2m}$ and $0 \leq y \leq |\det(A(G))|^{\frac{1}{n}} \leq \frac{2m}{n} \leq \sqrt{2m}$.

At $y = \dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}$, $g(x,y) = x + \dfrac{(n-2)^{\frac{1}{n}}|\mathbf{Det}(A(G))|^{\frac{n-1}{n(n-2)}}}{x^{\frac{1}{n-2}}}$.

$$\therefore \mathbb{E}(G) \geq g\Big(x, \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}\Big) \geq g\Big(\frac{2m}{n}, \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{(n-2)^{\frac{n-2}{n}}}\Big).$$

Hence, $\mathbb{E}(G) \geq \dfrac{2m}{n} + \dfrac{(n-2)^{\frac{1}{n}}|\mathbf{Det}(A(G))|^{\frac{n-1}{n(n-2)}}}{(\frac{2m}{n})^{\frac{1}{n-2}}}$.

Theorem 4.3. *If G represents a graph with m edges, $n \geq 2$ vertices and $A(G)$ is the adjacency non-singular matrix then*

$$\mathbb{E}(G) \leq \sqrt{2m} + \frac{(n-1)(2m)}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}. \tag{4.3}$$

Proof. We know that $|\lambda_1| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}$, which implies

$$|\lambda_1|\sum_{i=2}^{n}|\lambda_i| \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}\sum_{i=2}^{n}|\lambda_i|.$$

Since$|\lambda_i| \leq |\lambda_1|\ \forall i$, therefore $(n-1)|\lambda_1|^2 \geq |\mathbf{Det}(A(G))|^{\frac{1}{n}}\Big(\mathbb{E}(G) - |\lambda_1|\Big)$.

Thus $\quad \mathbb{E}(G) \leq |\lambda_1| + \dfrac{(n-1)|\lambda_1|^2}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}$.

Let $|\lambda_1| = x$ and $h(x) = x + \dfrac{(n-1)x^2}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}$. The condition for minima or maxima is $h'(x) = 0$ which implies $1 + \dfrac{(n-1)2x}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}} = 0$. So the function has minimum or maximum value at $x = -\dfrac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{2(n-1)}$.

But $h''(x) = \dfrac{2(n-1)}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}} > 0$, so at this point the given function has minimum value.

The minimum value is

$$h\Big(-\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{2(n-1)}\Big) = -\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{2(n-1)} + \frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{4(n-1)} = -\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{4(n-1)}.$$

But $h(x)$ becomes an increasing function in the interval $-\frac{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}{2(n-1)} \leq x \leq \sqrt{2m}$.

Hence $h(x) \leq f(\sqrt{2m})$.

This gives us a new upper bound $\mathbb{E}(G) \leq \sqrt{2m} + \dfrac{(n-1)(2m)}{|\mathbf{Det}(A(G))|^{\frac{1}{n}}}$.

5. Brief Summary and Conclusion

Energy of graph is an interesting subject in mathematical chemistry. In this paper we obtain new bounds for energy of graph using Holder's inequality. Are these lower and upper bounds superior to McClelland and Koolen-Moulton bound? It is yet to be investigated and is an area of further research.

References

[1] Cvetković D. and Gutman I., Applications of Graph Spectra, Mathematical Institution, Belgrade, 2009.

[2] Cvetković D. and Gutman I., Selected Topics on Applications of Graph Spectra, Mathematical Institute Belgrade, 2011.

[3] Das K. C., Mojallal S. A. and Gutman I., Improving the McCelland inequality for energy, MATCH Commun. Math. Comput. Chem., Vol. 70 (2013), 663-668.

[4] Das K. C., Gutman I., Bounds for energy of graphs, Hacettepe Journal of Mathematics and Statistics, Vol. 45 (2016), 695-703.

[5] Graovac A., Gutman I. and Trinajstić N., Topological Approach to the Chemistry of Conjugated Molecules, Springer, Berlin, Vol. 4, 1977.

[6] Gutman I., The energy of a graph, Ber. Ber. Math-Statist. Sekt. Forschungszentrum Graz, 103 (1978), 1-22.

[7] Gutman I., The energy of a graph: Old and New Results, ed. by A. Betten, A. Kohnert, R. Laue, A. Wassermann, Algebraic Combinatorics and Applications, Springer, Berlin, (2001), 196-211.

[8] Gutman I. and Polansky O. E., Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[9] Huiqing L., Mei L. and Feng T., Some upper bounds for the energy of graphs, Journal of Mathematical Chemistry, Vol. 41, No. 1 (2007), 45-57.

[10] Koolen J. H., Moulton V. and Gutman I., Improving the McCelland inequality for π-electron energy, Chem. Phys. Lett., Vol. 320 (2000), 213-216.

[11] Koolen J. H. and Moulton V., Maximal energy of graphs, Adv. Appl. Math, Vol. 26 (2001), 47-52.

[12] Koolen J. H. and Moulton V., Maximal energy of bipartite graphs, Graphs and Combinatorics, Vol. 19 (2003), 131-135.

[13] McClelland B. J., Properties of the latent root of a matrix: The estimation of π-electron energies, J. Chem. Phys., Vol. 54 (1971), 640-643.

[14] Sridhara G., Rajesh Kanna M. R., Jagadeesh R. and Cangul I. N., Improved McClelland and Koolen-Moulton bounds for the energy of graphs, Scientia Magna, Vol. 13, No. 1 (2018), 48-62.