On Certain Upper Bounds for Energy of Graphs

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Abstract

This paper explores the energy through upper bounds for the graphs which are connected and non-singular. The bounds include maximum degree (Δ), edge cardinality, vertex cardinality, determinant of the adjacency matrix of the graph and first Zagreb index (M_1). The newly computed upper bounds show improvement in comparison with the existing classical upper bound under certain conditions.

Keywords: *Energy of graphs; connected non-singular graph; maximum degree; Zagreb index.*

1. Introduction

Let $A(G)$ denotes the adjacency matrix of a simple graph $G = (V, E)$ having n vertices and m edges i.e., $|V| = n$ and $|E| = m$. The characteristic polynomial of G is defined as $\phi(G, x) = det(xI - A(G))$ where I stands for the identity matrix. Since $A(G)$ is a real symmetric matrix, the roots of the characteristic polynomial must be real and these are called the eigenvalues of $A(G)$ represented by $\lambda_i, i = 1,2, \dots, n$ such that $\lambda_1 \geq \cdots \geq \lambda_n$. The set of eigenvalues is called the Spectrum of G. The energy of a graph G was introduced by Gutman [5] in 1978, as an approximation of the total π-electron energy within the Huckel molecular orbital model. It is defined as

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

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It was a considerably studied descriptor in chemistry but was mostly being overlooked by mathematicians until the 2000s. Early mathematical results on graph energy were reviewed by Gutman [6] and the joint appearance of this survey and the first important mathematical result (together with a conjecture) on the maximum graph energy by Koolen and Moulton [8] may have been the reason for an ever-increasing interest of mathematicians in graph energy since 2001.

Many results have been arrived at on the energy of graphs so far. Among them, McClelland's results on the energy of graphs *E(G)* via lower bound and upper bounds are remarkable. McClelland [9] in 1971 obtained the first bound (upper) for the energy of a graph in terms of *n* and *m* as

$$E(G) \leq \sqrt{2mn}$$

Later, Koolen and Moulton [8] gave an upper bound for the bipartite graph as

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}$$

Following that, Zhou [10] obtained an upper bound given by

$$E(G) \leq \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left[2m - \left(\frac{M_1}{n}\right)\right]}$$

where M_1 stands for the first Zagreb index.

This paper obtains new bounds(upper) for the energy of a connected non-singular graph through the first Zagreb index, maximum degree (Δ), edge cardinality, vertex cardinality and the determinant of the adjacency matrix.

2. Preliminaries

In this section, some basic results that are needed to determine the upper bounds for the graph energy are presented.

Definition 2.1 [1]

"A graph G is said to be *singular* if at least one of its *eigenvalues* is equal to zero. For *singular* graphs, $det\ (A) = 0$".

Definition 2.2 [1]

"A graph is *non – singular* if all its *eigenvalues* are different from zero. Then, $det\ (A) > 0$".

Definition 2.3 [1]

"The energy of a graph G, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalue of G. That is, $E(G) = \sum_{i=1}^{n} |\lambda_i|$".

Definition 2.4 [2]

The *first Zagreb index* is defined as the sum of the squares of the degrees of the vertices of a graph G. That is

$$M_1(G) = \sum_{u \in V} {d_u}^2$$

Definition 2.5 [2]

The *Second Zagreb index* is defined as the sum of the product of degrees of pair of adjacent vertices of a graph G. That is

$$M_2(G) = \sum_{uv \in E} d_u d_v$$

Lemma 2.6 [4] "Let G be a non-empty graph with maximum vertex degree, Δ. Then $\lambda_1 \geq \sqrt{\Delta}$, where the equality holds if and only if G is $\frac{n}{2}K_2$".

Lemma 2.7 [8] "The graph G has only one distinct eigenvalue if and only if G is an empty graph. It has two distinct eigenvalues μ_1 and μ_2 $(\mu_1 > \mu_2)$ with corresponding multiplicities m_1 and m_2 if and only if G is the direct sum of m_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $m_2 = m_1\mu_1$".

Lemma 2.8 [7] "Let G be a graph with m edges. Then $E(G) \geq 2\sqrt{m}$, where the equality holds if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices".

Lemma 2.9 [4] If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, then

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{i \in V} d_i^2}$$

3. Upper Bounds for Graph Energy

Two new upper bounds are obtained to calculate the graph energy. The energy computed here is through the cardinality of edges, cardinality of vertices, maximum degree (Δ), determinant of the adjacency matrix of the graph and the first Zagreb index.

Theorem 3.1 If a graph G is non-empty and non-singular having n vertices, m edges, then $E(G) \leq 2m + \sqrt{\Delta} - \Delta - log \mid det\, A \mid + log\sqrt{\Delta}$, where $det\, A (\neq 0)$ is the determinant of the adjacency matrix. Equality holds iff G is isomorphic to K_2.

Proof

For a non-singular graph G, we have $|\lambda_i| > 0$, where i is an integer. Thus, $|det\, A| = \prod_{i=1}^{n} | \lambda_i | > 0$. Consider, the function $f(x) = x^2 - x - log\, x$ where x is positive, then $f'(x) = 2x - 1 - \frac{1}{x}$. Thus, on $x \geq 1$, the function $f(x)$ increases and on $0 < x \leq 1$, the function decreases. Thus, $f(x) \geq f(1) = 0$ implies $x \leq x^2 - log\ x$, $x > 0$. The equality holds iff $x = 1$. We get the graph energy as

$$E(G) = \lambda_1 + \sum_{i=2}^{n} |\lambda_i|$$

$$\leq \lambda_1 + \sum_{i=2}^{n} (\lambda_i^2 - log|\lambda_i|)$$

$$= \lambda_1 + 2m - \lambda_1^2 - log \prod_{i=1}^{n} |\lambda_i| + log\, \lambda_1$$

$$= 2m + \lambda_1 - \lambda_1^2 - log \mid det\, A \mid + log\, \lambda_1 \quad (1)$$

We know that $\lambda_1 \geq \sqrt{\Delta}$. Since, $g(x) = 2m + x - x^2 - log \mid det\, A \mid + log\ x$ is an increasing function on $0 < x \leq 1$ and a decreasing function on $x \geq 1$, and since $x \geq \sqrt{\Delta} \geq 1$, we have

$$g(x) \leq g(\sqrt{\Delta}) = 2m + \sqrt{\Delta} - \Delta - log \mid det\, A \mid + log(\sqrt{\Delta}) .$$

Combining this with (1), the result arrives.

If G is isomorphic to K_2, then checking for equality can be done easily. Conversely, assume that equality is true. By Lemma 2.7, we observe that a graph G is non-empty and has not less than two distinct eigenvalues.

Case 1. When the absolute values of the two eigenvalues of G are the same.

We get, $\lambda_2 = -1$ and $\lambda_1 = 1$ since the absolute values of the two eigenvalues of G are the same. Thus $\lambda_1 = | \lambda_2 | = 1$. Also, $\sum_{i=2}^{n} | \lambda_i| = 0$ and since by the same Lemma $m_2 = m_1\lambda_1$, $\lambda_1 = 1$, $m_1 = m_2$. Also, we have considered the graph with two numbers of vertices has multiplicity m_1 of $\lambda_1 = 1$ be equal to $n/2 = 1$. Therefore, the graph G which is complete of order $\lambda_1 + 1 = 2$ is nothing but the direct sum of $m_1 = n/2 = 1$. Hence, the graph G is K_2.

Case 2. When the absolute values of the two eigenvalues of G are different.

We get, $\lambda_2 = -1$ and $\lambda_1 \neq 1$ since the absolute values of the two eigenvalues of G are different. Hence, $\sum_{i=2}^{n} |\lambda_i| \neq 0$, so is a contradiction.

Theorem 3.2 A graph G of order n with m edges which is not empty, connected and non-singular has its energy given by

$$E(G) \leq 2m + \sqrt{\frac{M_1}{n}} - \frac{M_1}{n} - log\,|\,det\ A\,| + log\sqrt{\frac{M_1}{n}},$$

where $det\ A(\neq 0)$ is the determinant of the adjacency matrix. Equality is true iff G is isomorphic to K_3 .

Proof:

For the non-singular graph G, we have $|\lambda_i| > 0, i = 1,2, \dots \dots, n$. Thus, $|\det A| = \prod_{i=1}^{n} |\lambda_i| > 0$. Consider the function $f(x) = x^2 - x - \log x$, $x > 0$ for which $f'(x) = 2x - 1 - \frac{1}{x}$. Thus on $x \geq 1$, the function f increases, and on $0 < x \leq 1$, the function decreases. Thus, $f(x) \geq f(1) = 0$ implying $x \leq x^2 - log\, x$ for positive x, and holds equality iff x is equal to one. We get the graph energy of G as

$$E(G) = \lambda_1 + \sum_{i=2}^{n} |\lambda_i|$$

$$\leq \lambda_1 + \sum_{i=2}^{n} (\lambda_i^2 - log|\lambda_i|)$$

$$= \lambda_1 + 2m - \lambda_1^2 - log \prod_{i=1}^{n} |\lambda_i| + \log \lambda_1$$

$$= 2m + \lambda_1 - \lambda_1^2 - log|det\ A\,| + \log\lambda_1 \qquad (2)$$

we know that $\lambda_1 \geq \sqrt{\frac{M_1}{n}}$. Since, $g(x) = 2m + x - x^2 - lo\,g|detA| + lo\,g\,x$ is an increasing function on $0 < x \leq 1$ and a decreasing function on $x \geq 1$, and since $x \geq \sqrt{\frac{M_1}{n}} \geq 1$, we have $g(x) \leq g\left(\sqrt{\frac{M_1}{n}}\right) = 2m + \sqrt{\frac{M_1}{n}} - \frac{M_1}{n} - log|det\ A\,| + log\sqrt{\frac{M_1}{n}}$.

Combining this with (2), we arrive at the result.

If G is isomorphic to K_3, then equality can be checked very easily. Conversely, if we assume that equality is true, then the non-empty graph G will have not less than two distinct eigenvalues.

Case 1. When the absolute values of the two distinct eigenvalues of G are different.

We get, $\lambda_2 = -1$ and $\lambda_1 \neq 1$ since the absolute values of the two distinct eigenvalues of G are not the same by Lemma 2.7. Thus $\lambda_2 = \lambda_3 = -1$. Also, since $\sum_{i=1}^{3} \lambda_i = 0$ and since by the same Lemma, 2 is the multiplicity of -1, $n - 1 = \lambda_1 = 2$; λ_1 has the multiplicity $m_1 = 1$. Therefore, the graph G which is complete of order $\lambda_1 + 1 = 2$ is nothing but the direct sum of $m_1 = 1$. Hence, the graph G is K_3 or C_3.

Case 2. When the absolute values of the two distinct eigenvalues of G are the same.

We get, $\lambda_2 = -1$ and $\lambda_1 = 1$ since the absolute values of the two distinct eigenvalues of G are the same and can be concluded from Lemma 2.7. Thus, $m_2 = m_1\lambda_1, \lambda_1 = 1$ i.e., $(m_2 = m_1)$. Also, for the integers *m, n* the graph we have considered is with three number of vertices having $n = 2m$, this contradicts the assumption.

Case 3. When there are three different eigenvalues exist for graph G.

For the bipartite graph G, we get $\lambda_1 = -\lambda_n \neq 0$ since there are three distinct eigenvalues, so $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = 0$. Hence $E(G) = 2\lambda_1$. Also, it is understood by Lemma 2.8 that $2\lambda_1 \geq 2\sqrt{m}$. Thus, $2\lambda_1^2 \geq 2m$. Notice that $2m = \sum_{i=1}^{n} \lambda_i^2 = 2\lambda_1^2$. Therefore $\lambda_1 = \sqrt{m}$ and $2\sqrt{m} = E(G)$. Therefore, Lemma 2.8 says that graph G is a complete bipartite having many arbitrary isolated vertices. When there exists integers $r_1 \geq 1$ and $r_2 \geq 1$, then G is $K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1 r_2 = m$, here $r_1 = 1$ and $n - 1 = r_2$. This gives a contradiction with equality.

4. Conclusion

Many researchers are trying to improve the bounds for various graph energies. In this work, two new upper bounds are obtained for the energy of a graph. The newly obtained upper bounds of graphs are compared with classical upper bound as given below.

Illustration

Consider a graph *G*:

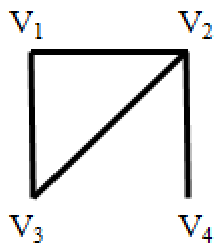

Fig 3.1 Graph *G*

	v_1	v_2	v_3	v_4
v_1	0	1	1	0
v_2	1	0	1	1
v_3	1	1	0	0
v_4	0	1	0	0

Table 3.1 Adjacency matrix

Here $n = 4$, $m = 4$

The energy of *G*:

$$E(G) = \sum_{i=1}^{n} |\lambda i| = 4.9624$$

Ivan Gutman and K.C. Das bound [3]

$$E(G) \leq 2m - \frac{2m}{n}\left(\frac{2m}{n} - 1\right) - ln\left(\frac{n\,|\,det\,A\,|}{2m}\right) = 6.6931$$

New upper bound:

$$E(G) \leq 2m + \sqrt{\Delta} - \Delta - log\,|\,det\,A\,| + log\sqrt{\Delta} = 6.903$$

$$E(G) \leq 2m + \sqrt{\frac{M_1}{n}} - \frac{M_1}{n} - log\,|\,det\,A\,| + log\sqrt{\frac{M_1}{n}} = 5.94$$

Thus, the obtained new upper bounds improve the existing classical upper bound under certain conditions.

References

[1] Balakrishnan R., “The energy of a graph”, Linear algebra Appl. 387 (2004) 287-295.

[2] Das K. C., Mojallal S.A., Gutman I., “Improving McClellands lower bound for energy”, MATCH Commun. Math. Comput. Chem. 70 (2013) 663–668.

[3] Das K. C. and Gutman. I., “Bounds for the energy of graphs”, Hacettepe Journal of Mathematics and Statistics, 45(3) (2016) 695-703.

[4] Favaron O., Mahéo M., Saclé J.F., “Some eigenvalue properties in graphs”, Discrete Math. 111 (1993) 197–220.

[5] Gutman I., “The energy of a graph”, Ber. Math.-Statist. Sekt. Forschungsz Graz. 103 (1978) 1–22.

[6] Gutman I, et al., “The energy of a graph: Old and new results”, Algebraic Combinatorics and Applications, Springer–Verlag Berlin; (2001) 196–211.

[7] Hong Y., “On the spectra of unicyclic graphs”, J. East China Norm. Univ. Nat. Sci. Ed. 1 (1986) 31–34.

[8] Koolen J. H. and Moulton V., “Maximal Energy Graphs”, Adv. Appl. Math. 26 (2001) 47–52.

[9] Mc Clelland B.J., “Properties of the latent roots of a matrix: the estimation of π-electron energies”, J. Chem. Phys. 54 (1971) 640–643.

[10] Zhou B., “Energy of graphs”, MATCH Commun. Math. Comput. Chem. 51 (2004) 111–118.