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A Lower (Upper) Bound for the Energy of Graphs

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ABSTRACT: Let G be a graph of order n and size m. In this paper, we determine an upper bound for the energy of non-singular graph G in terms of order n, size m, positive and negative indices of inertia of $A(G)$, and $det(A(G))$. We also obtain a lower bound for the energy of graph G, which relies on order n, size m, and maximum degree Δ. Furthermore, we identify extremal graphs that attain equality in each of these bounds.

Keywords: Adjacency matrix, graph eigenvalues, energy.

Contents

1. Introduction

All graphs considered here are finite, simple, and undirected. Let G be a graph of order n and size m. We denote its maximum degree and minimum degree by Δ and δ, respectively. The adjacency matrix of G is denoted by $A(G)$, and its i-th largest eigenvalue is denoted by $\lambda_i(G)$, or simply λ_i when the context is clear. The eigenvalues of $A(G)$ are referred as eigenvalues of graph G. A graph G is called non-singular if all its eigenvalues are non-zero. Otherwise, G is called a singular graph. The energy of a graph G, denoted by $\mathcal{E}(G)$, is the sum of absolute values of all the eigenvalues of G. Therefore, $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$. The concept of graph energy was put forward by Gutman in 1978, motivated by Hückel molecular orbital theory, which approximates the total π-electron energy of a conjugated hydrocarbon molecule using the energy of its molecular graph. An upper bound for the graph energy was first reported in [6] by McClelland in the year 1971, and it is given by $\mathcal{E}(G) \leq \sqrt{mn}$. It is interesting to note that $\mathcal{E}(G) \geq \dfrac{2m}{n} \geq 2\delta$. Initial bounds on the graph energy can be found in the book "Graph Energy" by Li, Shi and Gutman [5].

In recent years, several bounds on graph energy in terms of various graph parameters have been reported, see [1,2,3,9] for details. Motivated by the works on graph energy, we derive two bounds for the graph energy. The first is an upper bound for the energy of non-singular graph G, expressed in terms of the order n, size m, the the positive and negative indices of inertia of $A(G)$, and $det(A(G))$. The second is a lower bound that depends on the order n, size m, and maximum degree Δ. Furthermore, we identify extremal graphs that attain equality in each of these bounds. As usual, we denote the path graph, the complete graph, and the complete bipartite graph on vertices, by P_n, K_n, and $K_{p,q}$, with $p+q=n$. Further, n copies of graph G is denoted by nG.

2. Main Results

The following lemmas are crucial for proving our bounds.

Lemma 2.1 [8] *Let $(a) = (a_1, a_2, \ldots, a_n)$ and $(b) = (b_1, b_2, \ldots, b_n)$ be two set of real numbers. Then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 = \sum_{1\leq i<j\leq n} (a_i b_j - a_j b_i)^2.$$

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Lemma 2.2 [7] If $M = (m_{ij})_{n\times n}$ is a Hermitian matrix with eigenvalues $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n$, then

$$|\gamma_1 - \gamma_n| \geq 2\max_j \left(\sum_{k\neq j, k=1}^{n} |a_{jk}|^2\right)^{1/2}.$$

Lemma 2.3 [4] Let G be a connected graph of order $n \geq 2$. Then $\lambda_1 \geq \sqrt{\Delta}$, and the equality holds if and only if $G \cong K_{1,\Delta}$.

Lemma 2.4 [1] Let G be a graph of size m and $-b_1 \leq \ldots \leq -b_{n_2} \leq a_1 \leq \ldots \leq a_{n_1}$ be the eigenvalues of G, where a_1 is non-negative and b_{n_2} is positive. Then

$$\mathcal{E}(G)^2 = 4m + 4\left(\sum_{1\leq i<j\leq n_1} a_i a_j + \sum_{1\leq i<j\leq n_2} b_i b_j\right).$$

Theorem 2.1 *Let G be a non-singular graph of order n and size m. Suppose n^+ and n^- are positive and negative indices of inertia of $A(G)$, respectively. Then for $G \ncong K_n$,*

$$\mathcal{E}(G)^2 \geq 4m + 2n^2 - 4(n-\kappa)^2 - 2n + 4(\kappa - 1)\ln(|det(A(G))|).$$

where $\kappa = \min\{n^+, n^-\}$. Equality holds if and only if $G \cong P_4$, or $G \cong pK_2$, with $2p = n$ and $p \geq 2$.

Proof: Note that the complete graph K_n $(n > 1)$ is the only non-singular graph with exactly one positive eigenvalue, and that K_2 is the only non-singular with exactly one negative eigenvalue. Therefore, $n^+, n^- \geq 2$ as $G \ncong K_n$. From Lemma 2.4,

$$\mathcal{E}(G)^2 = 4m + 4\sum_{1\leq i<j\leq n^+} \lambda_i\lambda_j + 4\sum_{n^++1\leq i<j\leq n} \lambda_i\lambda_j.$$

Since $x \geq 1 + lnx$ for all $x > 0$, with equality holding only for $x = 1$, it follows that $|\lambda_i||\lambda_j| \geq 1 + \ln(|\lambda_i|) + \ln(|\lambda_j|)$. Therefore,

$$\mathcal{E}(G)^2 \geq 4m + 4\sum_{1\leq i<j\leq n^+} [1 + \ln(\lambda_i) + \ln(\lambda_j)] + 4\sum_{n^++1\leq i<j\leq n} [1 + \ln(|\lambda_i|) + \ln(|\lambda_j|)].$$

Upon simplification, we have

$$\begin{aligned}
\mathcal{E}(G)^2 &\geq 4m + 2n^+(n^+ - 1) + 2n^-(n^- - 1) + 4(n^+ - 1)\sum_{1\leq i\leq n^+} \ln(\lambda_i) + 4(n^- - 1)\sum_{n^++1\leq i\leq n} \ln(|\lambda_i|)\\
&\geq 4m + 2n^2 - 4(n-\kappa)^2 - 2n + 4(\kappa - 1)\sum_{1\leq i\leq n} \ln(|\lambda_i|)\\
&= 4m + 2n^2 - 4(n-\kappa)^2 - 2n + 4(\kappa - 1)\ln(|det(A(G))|).
\end{aligned}$$

That is,

$$\mathcal{E}(G)^2 \geq 4m + 2n^2 - 4(n-\kappa)^2 - 2n + 4(\kappa - 1)\ln(|det(A(G))|).$$

Suppose equality holds. Then $|\lambda_i|||\lambda_j| = 1$ for all $1 \leq i < j \leq n^+$, and $|\lambda_i|||\lambda_j| = 1$ for all $n^+ + 1 \leq i < j \leq n$. Also, $n^+ = n^-$. Therefore, $\lambda_2 = \lambda_3 = \cdots = \lambda_{n^+} = \frac{1}{\lambda_1}$, and $\lambda_{n^++1} = \lambda_{n^++2} = \cdots = \lambda_{n-1} = \frac{1}{\lambda_n}$. So, $det(A(G)) = \frac{1}{\lambda_1^{n^+-2}\lambda_n^{n^--2}}$. Since G is non-singular, with $G \ncong K_n$, it follows that $n \geq 4$. If $n = 4$, then $G \cong P_4$. Otherwise, $n > 4$. Since $det(A(G))$ is a non-zero integer, we must have $-1 \leq \lambda_1\lambda_n \leq 1$. Note that, $\lambda_1 \geq 1$ for any graph G with at least one edge, and the equality holds if and only if $G \cong pK_2 \cup qK_1$. Also, $\lambda_n \leq -1$ for any graph G with at least one edge, and the equality holds if and only if each component of G is a complete graph. Thus, $-1 \leq \lambda_1\lambda_n \leq 1$ implies $\lambda_1 = |\lambda_n| = 1$, and so $G \cong pK_2$ with $2p = n$ and $p > 1$. Converse part is direct. □

The following theorem can be deduced in similar lines to Theorem 2.1 by using the fact that the eigenvalues of a bipartite graph are symmetric about the origin.

Theorem 2.2 *Let G be a non-singular bipartite graph of order n and size m. Then*

$$\mathcal{E}(G)^2 \geq 4m + n^2 - 2n + 2(n-2)\ln(|det(A(G))|).$$

Equality holds if and only if $G \cong P_4$, or $G \cong pK_2$, with $2p = n$ and $p \geq 2$.

Theorem 2.3 *Let G be a graph on n vertices. Let λ_{i+1}^* be the i-th largest number in the sequence $\left\{|\lambda_j|\right\}_{j=2}^{n-1}$. Then*

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)\left[2m - 2\Delta - \frac{1}{2}((\lambda_2^* - \lambda_{n-1}^*)^2)\right]}.$$

Equality holds if and only if $G \cong K_{1,\Delta} \cup pK_1$, with $p + \Delta + 1 = n$, or $G \cong pK_2$, with $2p = n$.

Proof: Employing Lagrange's identity (see Lemma 2.1) to the vectors $(\lambda_2^*, \lambda_3^*, \ldots, \lambda_{n-1}^*)$ and $(\underbrace{1, 1, \ldots, 1}_{n-2 \text{ times}})$, we obtain

$$\begin{aligned}
(n-2)\sum_{i=2}^{n-1} {\lambda_i^*}^2 - \left(\sum_{i=2}^{n-1} \lambda_i^*\right)^2 &= \sum_{2 \leq i < j \leq n-1} \left(\lambda_i^* - \lambda_j^*\right)^2 \\
&= \sum_{i=3}^{n-2} (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2 + (\lambda_2^* - \lambda_{n-1}^*)^2 \\
&+ \sum_{3 \leq i < j \leq n-2} \left(\lambda_i^* - \lambda_j^*\right)^2 \\
&\geq \sum_{i=3}^{n-2} (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2 + (\lambda_2^* - \lambda_{n-1}^*)^2.
\end{aligned}$$

That is,

$$(n-2)(2m - \lambda_1^2 - \lambda_n^2) - (\mathcal{E}(G) - \lambda_1 + \lambda_n)^2 \geq \sum_{i=3}^{n-2} (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*) + (\lambda_2^* - \lambda_{n-1}^*)^2. \tag{2.1}$$

Now, for $\lambda_i \neq \lambda_2^*, \lambda_{n-1}^*$,

$$\begin{aligned}
(\lambda_2^* - \lambda_{n-1}^*)^2 &= ((\lambda_2^* - \lambda_i^*) + (\lambda_i^* - \lambda_{n-1}^*))^2 \\
&= (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2 + 2(\lambda_2^* - \lambda_i^*)(\lambda_i^* - \lambda_{n-1}^*) \\
&\leq (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2 + \left(\frac{\lambda_2^* - \lambda_i^*}{\lambda_i^* - \lambda_{n-1}^*} + \frac{\lambda_i^* - \lambda_{n-1}^*}{\lambda_2^* - \lambda_i^*}\right)(\lambda_2^* - \lambda_i^*)(\lambda_i^* - \lambda_{n-1}^*) \\
&= 2\left((\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2\right).
\end{aligned}$$

Thus, for $3 \leq i \leq n-1$,

$$\frac{1}{2}(\lambda_2^* - \lambda_{n-1}^*)^2 \leq (\lambda_2^* - \lambda_i^*)^2 + (\lambda_i^* - \lambda_{n-1}^*)^2 \tag{2.2}$$

Employing equation (2.2) in (2.1), and upon simplification, we get

$$\mathcal{E}(G) \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\left[2m - \lambda_1^2 - \lambda_n^2 - \frac{1}{2}((\lambda_2^* - \lambda_{n-1}^*)^2)\right]}.$$

From Cauchy's-Schwarz inequality, $(\lambda_1-\lambda_n)^2 \leq 2(\lambda_1^2+\lambda_n^2)$ with equality holding if and only if $\lambda_1 = -\lambda_n$. Therefore,

$$\mathcal{E}(G) \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\left[2m - \frac{1}{2}(\lambda_1-\lambda_n)^2 - \frac{1}{2}((\lambda_2^* - \lambda_{n-1}^*)^2)\right]}. \tag{2.3}$$

Let $f(x) = 2x + \sqrt{(n-2)\left[2m - 2x^2 - \frac{1}{2}((\lambda_2^* - \lambda_{n-1}^*)^2)\right]}$. Then

$f'(x) = 2\left(1 - \frac{(n-2)x}{\sqrt{(n-2)(2m-2x^2-\frac{1}{2}((\lambda_2^*-\lambda_{n-1}^*)^2))}}\right)$. By first derivative test, $f(x)$ is strictly decreasing for $\sqrt{\frac{2m-\frac{1}{2}((\lambda_2^*-\lambda_{n-1}^*)^2)}{n}} < x < \sqrt{m - \frac{1}{4}(\lambda_2^*-\lambda_{n-1}^*)^2}$. By Lemma 2.2, $\frac{\lambda_1-\lambda_n}{2} \geq \sqrt{\Delta} \geq \sqrt{\frac{2m-\frac{1}{2}((\lambda_2^*-\lambda_{n-1}^*)^2}{n}}$.

Therefore, $f\left(\frac{\lambda_1-\lambda_n}{2}\right) \leq f(\sqrt{\Delta})$, and so by equation (2.3), we have

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)\left[2m - 2\Delta - \frac{1}{2}((\lambda_2^*-\lambda_{n-1}^*)^2)\right]}.$$

Suppose the equality holds. Then all the inequalities mentioned previously must actually be equalities. Therefore, we must have $\lambda_1 = -\lambda_n$, $\lambda_1 - \lambda_n = 2\sqrt{\Delta}$, and $\lambda_3^* = \cdots = \lambda_{n-2}^* = \frac{\lambda_2^*+\lambda_{n-1}^*}{2}$. From $\lambda_1 = -\lambda_n$, $\lambda_1-\lambda_n = 2\sqrt{\Delta}$, it follows that $\lambda_1 = \sqrt{\Delta} = -\lambda_n$. Hence, by Lemma 2.3, one of the connected components of G, say G_1, must be isomorphic to the star graph $K_{1,\Delta}$. Observe that, if 0 is an eigenvalue of G with multiplicity at least 2, then, $\lambda_2^* = \lambda_3^* = \cdots = \lambda_{n-2}^* = \lambda_{n-1}^* = 0$, and so $G \cong K_{1,\Delta} \cup pK_1$, where $1+\Delta+p = n$.

Case 1: $\Delta \geq 3$. Then 0 is an eigenvalue of G_1 with multiplicity at least 2. So, $G \cong K_{1,\Delta} \cup pK_1$.

Case 2: $\Delta = 2$. By Lemma 2.3, any component of G, other than G_1 is isomorphic to $K_{1,2}$, K_2, or K_1. To satisfy the condition $\lambda_3^* = \cdots = \lambda_{n-2}^* = \frac{\lambda_2^*+\lambda_{n-1}^*}{2}$, the graph must be $K_{1,2} \cup pK_1$, with $p+3 = n$.

Case 3: $\Delta = 1$. Again, by Lemma 2.3, the graph must be either $K_2 \cup pK_1$, with $p+2 = n$, or pK_2, with $2p = n$. Converse part is direct. □

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