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A Short Note on Graph Energy

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Abstract

Let G be a graph with n vertices and m edges. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G. The energy of graph G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. In this note, we give improvements of two inequalities that relate to $E(G)$.

1 Introduction and preliminaries

Let G be a graph with n vertices and m edges. Denote with $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$ absolute eigenvalues of G arranged in non-increasing order, respectively. The energy of graph G is computed as [4]:

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

The energy of a given molecular graph is of interest since it can be related to the total π-electron energy of molecule represented that graph (see for example [5–7]).

The following inequalities were proved in [3] for the energy of G:

$$E(G) \geq \sqrt{2mn - \frac{n^2}{4}(|\lambda_1| - |\lambda_n|)^2} \tag{1}$$

and

$$E(G) \geq \frac{2\sqrt{2mn}\sqrt{|\lambda_1||\lambda_n|}}{|\lambda_1| + |\lambda_n|}. \tag{2}$$

In this paper we are going to prove sharper inequalities for $E(G)$ than (1) and (2).

2 Main result

Theorem 1 *Let G be a graph with n vertices and m edges. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$ be a non-increasing arrangement of eigenvalues of G. Then, the following inequality is valid*

$$E(G) \geq \sqrt{2mn - \alpha(n)(|\lambda_1| - |\lambda_n|)^2} \tag{3}$$

where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, while $[x]$ denotes integer part of a real number x.

Equality in (3) holds if and only if $G \cong \bar{K}_n$, or G or C_4.

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \ldots, n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then the following inequality is valid (see [1])

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A - a)(B - b), \tag{4}$$

where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$. Equality in (4) holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

For $a_i := |\lambda_i|$, $b_i := |\lambda_i|$, $a = b := |\lambda_n|$ and $A = B := |\lambda_1|$, $i = 1, 2, \ldots, n$, inequality (4) becomes

$$\left| n\sum_{i=1}^{n} |\lambda_i|^2 - \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \right| \leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2.$$

Since $E(G) = \sum_{i=1}^{n} |\lambda_i|$, $\sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} \lambda_i^2 = 2m$ and $E(G) \leq \sqrt{2mn}$ (see [8]), the above inequality becomes

$$2mn - E(G)^2 \leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2,$$

wherefrom the statement of Theorem 1 follows. Since equality in (4) holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$, equality in (3) holds if and only if $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$.

$\square$

Corollary 1 *Since*

$$\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right) \leq \frac{n^2}{4}$$

then according to (3) we have that

$$E(G) \geq \sqrt{2mn - \alpha(n)(|\lambda_1| - |\lambda_n|)^2} \geq \sqrt{2mn - \frac{n^2}{4}(|\lambda_1| - |\lambda_n|)^2}.$$

This means that inequality (3) is stronger of inequality (1).

Theorem 2 *Let G be a graph with n vertices and m edges. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| > 0$ be a non-increasing arrangement of eigenvalues of G. Then, the following inequality is valid*

$$E(G) \geq \frac{|\lambda_1||\lambda_n|n + 2m}{|\lambda_1| + |\lambda_n|}. \tag{5}$$

Equality in (5) holds if and only if $G \cong \bar{K}_n$.

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1, 2, \ldots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid (see [2])

$$\sum_{i=1}^{n} b_i^2 + rR \sum_{i=1}^{n} a_i^2 \leq (r + R) \sum_{i=1}^{n} a_i b_i. \tag{6}$$

Equality in (6) holds if and only if, for et least one i, $1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$.

For $b_i := |\lambda_i|$, $a_i := 1$, $r := |\lambda_n|$ and $R := |\lambda_1|$, $i = 1, 2, \ldots, n$ inequality (6) becomes

$$\sum_{i=1}^{n} |\lambda_i|^2 + |\lambda_1||\lambda_n| \sum_{i=1}^{n} 1 \leq (|\lambda_1| + |\lambda_n|) \sum_{i=1}^{n} |\lambda_i|.$$

Since $\sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} \lambda_i^2 = 2m$, $\sum_{i=1}^{n} 1 = n$ and $\sum_{i=1}^{n} |\lambda_i| = E(G)$, from the above inequality directly follows the assertion of Theorem 2, i.e. inequality (5).

If for some i holds that $ra_i = b_i = Ra_i$, then for the same i also holds $b_i = r = R$. This means that for each $j, j \neq i$ holds $|\lambda_i| \leq |\lambda_j| \leq |\lambda_i|$. Therefore equality in (6) holds if and only if $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$.

□

Corollary 2 *Using inequality between arithmetic and geometric means, according to the inequality (5) we have that*

$$E(G) \geq \frac{|\lambda_1||\lambda_n|n + 2m}{|\lambda_1| + |\lambda_n|} \geq \frac{2\sqrt{2mn}\sqrt{|\lambda_1||\lambda_i n|}}{|\lambda_1| + |\lambda_n|}.$$

This means that inequality (5) is stronger then inequality (2).

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