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Bounds on graph energy

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Abstract

Let G be a graph of order n and size m, and its eigenvalues λ_i , $i = 1, \ldots, n$, be labeled so that $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$. The energy $E(G)$ of G is the sum of absolute values of its eigenvalues. It was recently shown that for $t = 1$,

$$\frac{2m\,t + |\lambda_1||\lambda_n|\,n}{|\lambda_1| + |\lambda_n|}$$

is a lower bound on $E(G)$. We now establish conditions under which for $t > 1$, this expression is an upper bound on $E(G)$. We also show that for a class of r-regular graphs, $E(G) \geq 2rn/(r + 1)$, and determine the equality cases.

Keywords: graph energy; energy (of graph); spectrum (of graph); eigenvalue (of graph).

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1. Introduction

In this paper we are concerned with simple graphs, that is graphs without labeled, directed, or multiple edges, and without self loops. Let G be such a graph of order n and size m, and let the eigenvalues of its $(0, 1)$-adjacency matrix be λ_i , $i = 1, 2, \ldots, n$. These eigenvalues form the spectrum of the graph G, denoted by $Spec(G)$. In what follows, the graph eigenvalues will be labeled so that

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| \,.$$

Of the numerous known properties of graph spectrum [3], we recall that if $m \geq 1$, then $\lambda_1 > 0$, i.e., $|\lambda_1| = \lambda_1$, and that

$$\sum_{i=1}^{n} \lambda_i^2 = 2m \,. \tag{1}$$

The energy of the graph G is defined as [7]

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \,. \tag{2}$$

The theory of graph energy is nowadays well developed [7]. In particular, numerous lower and upper bounds on $E(G)$ are known; some recent publications along these lines are [1, 2, 5, 6, 8–11]. In [9], one of the present authors obtained a lower bound on E in terms of n, m, λ_1, and λ_n, namely

$$E(G) \geq \frac{2m + |\lambda_1|\,|\lambda_n|\,n}{|\lambda_1| + |\lambda_n|} \,. \tag{3}$$

Some other lower bounds of the same type were communicated in [5].

In this paper we determine conditions under which for any $t > 1$, the reverse of the inequality (3) holds, namely

$$E(G) < \frac{2m\,t + |\lambda_1|\,|\lambda_n|\,n}{|\lambda_1| + |\lambda_n|} \,. \tag{4}$$

In order to avoid trivialities, throughout this paper we assume that the graph G possesses at least one eigenvalue λ_i, such that $|\lambda_i| \neq |\lambda_1|$ and $|\lambda_i| \neq |\lambda_n|$. If so, then as shown below, the inequality (4) is strict.

We prove the following two results.

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Theorem 1.1. *Let $t > 1$ be a real number. Then the upper bound (4) holds provided*

$$|\lambda_n| \geq \left[2t - 1 - 2\sqrt{t(t-1)}\right] |\lambda_1| \,.$$

Theorem 1.2. *The upper bound (4) holds for any λ_1 and $\lambda_n \neq 0$, if*

$$t = \frac{\big(|\lambda_1| + |\lambda_n|\big)^2}{4|\lambda_1|\,|\lambda_n|} \,.$$

2. Proofs of Theorems 1.1 and 1.2

For the sake of simplicity, instead of $|\lambda_i|$ we shall write z_i. In addition, $|\lambda_n| = z_n$ and $|\lambda_1| = z_1$ will be denoted by x and y, respectively.

We start with the obvious relations

$$z_i - \frac{x}{t} \geq \frac{t-1}{t}\, x \qquad \text{and} \qquad z_i - \frac{y}{t} \geq -\frac{y}{t} \,.$$

Based on them, we may be interested when their product satisfies

$$\left(z_i - \frac{x}{t}\right)\left(z_i - \frac{y}{t}\right) \geq -\frac{t-1}{t^2}\, xy \,. \tag{5}$$

Inequality (5) can be rewritten as

$$t\, z_i^2 - (x+y) z_i + xy \geq 0 \tag{6}$$

from which, by summing over all $i = 1, 2, \ldots, n$, and by taking into account relations (1) and (2), it immediately follows

$$2m\, t - (x+y) E + xy\, n > 0 \,. \tag{7}$$

Since there exists one z_i different from x and y, the above inequality must be strict. From Equation (7) we get $E < (2m\, t + xy\, n)/(x+y)$, i.e., inequality (4).

In order that (6) be valid for all $x \leq z_i \leq y$, its opposite, namely

$$t\, z^2 - (x+y) z + xy < 0$$

must not hold for any z. This will happen if $D \leq 0$, where D is the discriminant

$$D = (x+y)^2 - 4t\, xy = x^2 - (4t-2) xy + y^2 \,. \tag{8}$$

Considering (8) as a polynomial in the variable x, $D \leq 0$ will hold if

$$x_1 \leq x \leq x_2 \,,$$

where

$$x_{1,2} = \frac{1}{2}\left(4t - 2 \pm \sqrt{(4t-2)^2 - 4}\right) y = \left(2t - 1 \pm 2\sqrt{t(t-1)}\right) y \,.$$

Thus, (4) will hold if

$$\left(2t - 1 - 2\sqrt{t(t-1)}\right) y \leq x \leq \left(2t - 1 + 2\sqrt{t(t-1)}\right) y \,.$$

Since for $t \geq 1$, $2t - 1 + 2\sqrt{t(t-1)} \geq 1$, the right–hand side requirement is satisfied in a trivial manner. What only remains is the left–hand side condition, which is just the statement of Theorem 1.1.

Solving $D \leq 0$ in the variable t, from (8) we obtain

$$t \geq \frac{(x+y)^2}{xy}$$

implying that inequality (4) holds for all $t \geq (x+y)^2/(xy)$. Evidently, the best choice of t is when it is as small as possible, i.e., $t = (x+y)^2/(xy)$. Theorem 1.2 follows.

3. A bound on the energy of regular graphs

In order to state the next theorem, we need some preparations.

A *matching* in G is a set of edges of G without common vertices. A *perfect matching* is a matching in which every vertex is incident to exactly one edge of the matching. The *complete graph* and the *cycle* of order n, are denoted by K_n and C_n, respectively. The *complete bipartite graph* with part sizes p and q is denoted by $K_{p,q}$. Let $r \geq 0$ be an integer and M be a perfect matching of $K_{r+1,r+1}$. By $K^{\star}_{r+1}$ we mean the r-regular graph $K_{r+1,r+1} \setminus M$. The graph $K^{\star}_{r+1}$ is called the *crown* graph of order $2r+2$. For example $K^{\star}_1 = 2K_1$, $K^{\star}_2 = 2K_2$, and $K^{\star}_3 = C_6$.

Lemma 3.1. [3] *Let H be a connected r-regular graph where $r \geq 2$. Assume that*

$$Spec(H) = \{r, \underbrace{1,\ldots,1}_{b}, \underbrace{-1,\ldots,-1}_{c}\},$$

where b and c are some non-negative integers. Then $b=0$, $c=n-1$, and $H \cong K_{r+1}$.

Lemma 3.2. [9] *Let H be a connected bipartite r-regular graph where $r \geq 2$. Assume that*

$$Spec(H) = \{r, \underbrace{1,\ldots,1}_{b}, \underbrace{-1,\ldots,-1}_{c}, -r\},$$

where b and c are some non-negative integers. Then $b=c=r$ and $H \cong K^{\star}_{r+1}$.

Lemma 3.3. *Let a and b be positive real numbers. Let α, β, x and y be non-negative real numbers such that $\beta \geq y \geq \sqrt{\frac{a}{b}} \geq x \geq \alpha$. Then*

$$\frac{a+bxy}{x+y} \geq \frac{a+b\alpha\beta}{\alpha+\beta}\,, \tag{9}$$

and the equality holds if and only if $x=\alpha=\sqrt{\frac{a}{b}}$ or $x=\beta=\sqrt{\frac{a}{b}}$ or $y=\beta=\sqrt{\frac{a}{b}}$ or $x=\alpha$ and $y=\beta$.

Proof. Let d be a positive real number and $f_d(t) = \frac{a+bdt}{d+t}$ the one-variable function on t, where $t \geq 0$. So the derivative of $f_d(t)$ with respect to t is

$$f'_d(t) = \frac{bd^2-a}{(d+t)^2}\,.$$

This shows that if $d > \sqrt{\frac{a}{b}}$, then $f_d(t)$ is strictly increasing on the interval $[0,\infty)$ and if $d < \sqrt{\frac{a}{b}}$, then $f_d(t)$ is strictly decreasing on the interval $[0,\infty)$. If $d = \sqrt{\frac{a}{b}}$, then for every $t \geq 0$, $f_d(t) = \frac{a}{d} = \sqrt{ab}$.

Since $y \leq \beta$ and $f_x(t)$ is strictly decreasing on the interval $[0,\infty)$ (if $x < \sqrt{\frac{a}{b}}$),

$$f_x(y) \geq f_x(\beta) \qquad (\text{if} \quad \beta > y \quad \text{and} \quad x \neq \sqrt{\frac{a}{b}} \quad \text{then} \quad f_x(y) > f_x(\beta))\,. \tag{10}$$

On the other hand, since $x \geq \alpha$ and $f_\beta(t)$ is strictly increasing on the interval $[0,\infty)$ (if $\beta > \sqrt{\frac{a}{b}}$),

$$f_\beta(x) \geq f_\beta(\alpha) \qquad (\text{if} \quad x > \alpha \quad \text{and} \quad \beta \neq \sqrt{\frac{a}{b}} \quad \text{then} \quad f_\beta(x) > f_\beta(\alpha))\,. \tag{11}$$

Since $f_x(\beta) = f_\beta(x)$, the Eqs. (10) and (11) show that $f_x(y) \geq f_\beta(\alpha)$. In other words, we obtain the inequality (9).

Now we consider the equality. Assume that $\frac{a+bxy}{x+y} = \frac{a+b\alpha\beta}{\alpha+\beta}$. So $f_x(y) = f_\beta(\alpha)$. Hence by (10) and (11) we find that $f_x(y) = f_x(\beta)$ and $f_\beta(x) = f_\beta(\alpha)$. Using (10) and (11) one can easily obtain the result. □

Theorem 3.1. *Let G be an r-regular graph of order n where $r > 0$. Suppose that G has no eigenvalue in the interval $(-1,1)$. Then*

$$E(G) \geq \frac{2rn}{r+1}\,. \tag{12}$$

Equality holds if and only if every connected component of G is the complete graph K_{r+1} or the crown graph $K^{\star}_{r+1}$.

Proof. For an r-regular graph, $\lambda_1 = r$ [3]. Since G has no eigenvalue in the interval $(-1,1)$, $|\lambda_n| \geq 1$. As well known [3], for any (n,m)-graph,

$$|\lambda_n| \leq \sqrt{\frac{2m}{n}} \leq |\lambda_1|\,. \tag{13}$$

Let $\alpha = 1$, $\beta = r$, $a = 2m = nr$, $b = n$, $x = |\lambda_n|$ and $y = |\lambda_1|$. By (13) we get

$$\beta \geq y \geq \sqrt{\frac{a}{b}} \geq x \geq \alpha\,.$$

By applying Lemma 3.3 and bearing in mind Equation (3), we find that

$$E(G) \geq \frac{a+bxy}{x+y} \geq \frac{a+b\alpha\beta}{\alpha+\beta}\,, \tag{14}$$

which bearing in mind the definitions of α, β, a, b, implies the bound (12).

Now we investigate the equality of Equation (12). We note that for every disjoint graphs G_1 and G_2, $E(G_1 \cup G_2) = E(G_1) + E(G_2)$. Since $E(K_{r+1}) = 2r$ and $E(K^{\star}_{r+1}) = 4r$, it is easy to check that if $G = p\,K_{r+1} \cup q\,K^{\star}_{r+1}$, where p and q are non-negative integers, then the equality holds. Hence it remains to consider the converse. Thus assume that G is an r-regular graph of order n such that G has no eigenvalue in the interval $(-1, 1)$, and $E(G) = 2rn/(r+1)$. Using Equation (14) we obtain

$$E(G) = \frac{a+bxy}{x+y} \qquad \text{and} \qquad \frac{a+bxy}{x+y} = \frac{a+b\alpha\beta}{\alpha+\beta}\,. \tag{15}$$

In [9] it was shown that if (3) is equality, then there exists $s \in \{1, \ldots, n\}$ such that $|\lambda_1| = \cdots = |\lambda_s|$ and $|\lambda_{s+1}| = \cdots = |\lambda_n|$ (we note that $|\lambda_1| = r$). On the other hand, by Lemma 3.3, $|\lambda_1| = \sqrt{\frac{a}{b}}$ or $|\lambda_n| = \sqrt{\frac{a}{b}}$ or $|\lambda_n| = 1$. If $|\lambda_1| = \sqrt{\frac{a}{b}}$ or $|\lambda_n| = \sqrt{\frac{a}{b}}$, then we obtain that $|\lambda_1| = \cdots = |\lambda_n|$. By combining these conditions, we find that there are two possible cases:

(I) $|\lambda_1| = \cdots = |\lambda_n| = r$. Hence every eigenvalue of G is r or $-r$. By Equation (1), we conclude that $nr^2 = nr$. Thus $r = 1$, i.e., every connected component of G is K_2.

(II) $|\lambda_1| = \cdots = |\lambda_s| = r$ and $|\lambda_{s+1}| = \cdots = |\lambda_n| = 1$. Then every eigenvalue of G is either r or $-r$ or 1 or -1. If $r = 1$, then every connected component of G is K_2. Therefore, assume that $r \geq 2$. Let H be a connected component of G. Since H is r-regular, r is the largest eigenvalue of H and its multiplicity is one. Suppose first that H is bipartite. Then $-r$ is also one of the eigenvalues of H with multiplicity one. Then the spectrum of H consists of one r, one $-r$ and the other elements are 1 and -1. By Lemma 3.2, $H \cong K^{\star}_{r+1}$. Assume now that H is not bipartite. Then $-r$ is not an eigenvalue of H [3]. Therefore the spectrum of H consist of one r and the other elements are 1 or -1. By Lemma 3.1, $H \cong K_{r+1}$.

The proof of Theorem 3.1 is complete. □

Remark 3.1. *In [4] it was shown that for all r-regular graphs, $r > 0$, $E(G) \geq n$. If $r \geq 3$, then $\frac{2r}{r+1} \geq 1.5$. Thus, by Theorem 3.1 we improve this result for a certain family of r-regular graphs.*

We conclude this paper by two examples. The cycle C_6 is the crown graph $K^{\star}_3$ and $Spec(C_6) = \{2, 1, 1, -1, -1, -2\}$. Thus $E(C_6) = 8$ which is an equality case in Theorem 3.1. For the Petersen graph P, $Spec(P) = \{3, 1, 1, 1, 1, 1, -2, -2, -2, -2\}$. Thus $E(P) = 16$ whereas the lower bound of Theorem 3.1 is 15.

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