Mathematics Interdisciplinary Research **4** (2019) 151 − 155

Oboudi-Type Bounds for Graph Energy

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Abstract

The graph energy is the sum of absolute values of the eigenvalues of the (0, 1)-adjacency matrix. Oboudi recently obtained lower bounds for graph energy, depending on the largest and smallest graph eigenvalue. In this paper, a few more Oboudi-type bounds are deduced.

Keywords: Spectral graph theory, spectrum (of graph), graph energy, energy (of graph), Oboudi-type bounds.

2010 Mathematics Subject Classification: 05C50.

How to cite this article
I. Gutman, Oboudi-type bounds for graph energy, *Math. Interdisc. Res.* **4** (2019) 151 − 155.

1. Introduction

Let G be a connected graph with n vertices and m edges. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of the (0, 1)-adjacency matrix of G, forming its spectrum [1, 2]. The energy of G is defined as [5]

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

Numerous upper and lower bounds for graph energy are known [5], of which we mention here only McClelland's estimate [6]

$$E(G) \leq \sqrt{2mn}\,. \tag{1}$$

Its importance lies in the fact that in the case of molecular graphs (i.e., graphs in which the vertex degrees are 4 or less), $E(G)$ can be approximated as [6]

$$E(G) \approx C\,\sqrt{2mn}, \tag{2}$$

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Academic Editor: Ottorino Ori
Received 03 November 2019, Accepted 30 November 2019
DOI: 10.22052/mir.2019.207442.1172

where C is a constant, $C \approx 0.9$. Extensive numerical testing showed that the formula (2) is the best (n,m)-type approximation for the energy of molecular graphs [3, 4].

Recently, Oboudi [7] obtained a lower bound for graph energy, whose form is similar to McClelland's upper bound (1), namely,

$$E(G) \geq \frac{2\sqrt{ab}}{a+b}\sqrt{2mn}\,. \tag{3}$$

The meaning of the parameters a and b is explained in the subsequent section.

In this paper we analyze Oboudi's results and offer a few more lower bounds for E of the same kind.

2. Oboudi's Lower Bounds for Graph Energy

Let $x_i = |\lambda_i|\,, i = 1,2,\ldots,n$, and assume that

$$x_1 \geq x_2 \geq \cdots \geq x_n\,.$$

For the sake of simplicity, we consider the case when all graph eigenvalues are non-zero, i.e., assume that $x_n > 0$.

Remark 1. If in the spectrum of the graph G there are $n_0 > 0$ zeros, i.e., if G is singular, then all formulas in this paper remain valid if n is replaced by $n - n_o$.

Denote x_1 and x_n by a and b, respectively. Thus, a is the spectral radius of the graph G, whereas b is either the smallest positive eigenvalue or the largest negative eigenvalue (with positive sign).

Evidently,

$$(x_i - a)(x_i - b) \leq 0, \qquad \text{i.e.,} \qquad x_i^2 - (a+b)x_i + ab \leq 0, \tag{4}$$

holds for all $i = 1,2,\ldots,n$, with equality for $i = 1$ and $i = n$. If $n > 2$, then there is at least one value of i for which the above inequality is strict. Summing Equation (4) over $i = 1,2,\ldots,n$, and bearing in mind that

$$\sum_{i=1}^{n} x_i = E(G) \qquad \text{and} \qquad \sum_{i=1}^{n} x_i^2 = 2m, \tag{5}$$

we arrive at

$$2m - (a+b)E(G) + ab\,n < 0,$$

from which follows Oboudi's first bound [7]:

$$E(G) > \frac{ab\,n + 2m}{a+b}\,. \tag{6}$$

Inequality (6) holds for all connected non-singular graphs with more than two vertices, and becomes equality only for $G \cong K_2$.

Using the relation $p + q \geq 2\sqrt{pq}$, from (6) we obtain Oboudi's second bound (3). Inequality (3) is also strict for all connected non-singular graphs with $n > 2$, with equality if $G \cong K_2$.

It is interesting to note that if we sum (4) over $i = 2, 3, \dots, n-1$, then

$$2m - a^2 - b^2 - (a+b)[E(G) - a - b] + ab(n-2) < 0,$$

which again leads to (6).

In the case of bipartite graphs, $x_1 = x_2 = a$ and $x_n = x_{n-1} = b$. Then, summing (4) over $i = 3, \dots, n-2$, we get

$$2m - 2a^2 - 2b^2 - (a+b)[E(G) - 2a - 2b] + ab(n-4) < 0,$$

which also results in the bound (6). In other words, Oboudi's bounds (3) and (6) cannot be strengthened for the special case of bipartite graphs.

Suppose that we know one eigenvalue of the graph G, say λ_ℓ. Let $|\lambda_\ell| = c$. Then the Oboudi's bound (6) can be improved as follows. By summing (5) over all $i = 1, 2, \dots, n$, except $i = \ell$, we obtain

$$2m - c^2 - (a+b)[E(G) - c] + ab(n-1) \leq 0,$$

which can be rewritten as

$$E(G) \geq \frac{ab\,n + 2m}{a+b} + \frac{(a-c)(c-b)}{a+b}\,.$$

The second Oboudi's bound, Equation (3), yields then

$$E(G) \geq \frac{2\sqrt{ab}}{a+b}\sqrt{2mn} + \frac{(a-c)(c-b)}{a+b}\,.$$

Evidently, if $c \neq a, b$, then $(a-c)(c-b)/(a+b) > 0$.

3. More Oboudi-Type Bounds

Instead of (4), we now consider the expression

$$(a\,x_i - b\,x_j)(a\,x_j - b\,x_i) = (a^2 + b^2)x_i\,x_j - ab(x_i^2 + x_j^2)\,. \tag{7}$$

The terms $a\,x_i - b\,x_j$ and $a\,x_j - b\,x_i$ are evidently non-negative for all $i,j = 1,2,\ldots,n$, and for some i,j are positive–valued. By summing (7) over $i,j = 1,2,\ldots,n$, and by taking into account the relations (5), we get

$$(a^2+b^2)\,E(G)^2 - ab(2mn+2mn) > 0,$$

which implies

$$E(G) > \sqrt{\frac{2ab}{a^2+b^2}}\,\sqrt{2mn}\,. \tag{8}$$

Thus, by using the expression (7), we straightforwardly arrive at a bound of McClelland-type, similar to (3). Same as in the case of (3) and (6), inequality (8) holds for all connected non-singular graphs with more than two vertices. If $G \cong K_2$, then (8) becomes equality.

It can be easily shown that Oboudi's lower bound (3) is slightly better than the new bound (8).

The main difference between Oboudi's and our approaches is seen when the summation of (7) is over $i,j = 2,3,\ldots,n-1$. This results in

$$(a^2+b^2)\,[E(G)-a-b]^2 - 2ab(n-2)(2m-a^2-b^2),$$

from which

$$E(G) > a+b+\sqrt{\frac{2ab}{a^2+b^2}}\,\sqrt{(n-2)(2m-a^2-b^2)}\,. \tag{9}$$

Analogously, in the case of bipartite graphs we obtain

$$E(G) > 2a+2b+\sqrt{\frac{2ab}{a^2+b^2}}\,\sqrt{(n-4)(2m-2a^2-2b^2)}\,. \tag{10}$$

Numerical testing shows that the bound (9) is sharper than (8), and that (10) improves (9). However, to verify the same by exact mathematical methods seems to be a tough task and remains an open problem.

Conflicts of Interest. The author declares that there are no conflicts of interest regarding the publication of this article.

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