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Variations on McClelland's bound for graph energy

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Abstract

Let G be a graph of order n, size m, and spectral radius ρ. Let p and q be arbitrary real numbers such that $p \geq q > 0$. Motivated by a result from [*MATCH Commun. Math. Comput. Chem.* **84** (2020) 335–343], it is demonstrated that

$$(2m)^{\frac{p}{p+q}}\, n^{\frac{q}{p+q}} \qquad \text{and} \qquad \rho + (2m-\rho^2)^{\frac{p}{p+q}}\,(n-1)^{\frac{q}{p+q}}$$

are upper bounds on graph energy. These are shown to be closely related to the earlier known McClelland-type bounds.

Keywords: energy (of graph); spectrum (of graph); McClelland bound.

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1. Introduction

Let G be a simple graph, possessing n vertices and m edges. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of the $(0,1)$-adjacency matrix of G. Then the *energy* of G is defined as [10]

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

In this paper we are concerned with several (m,n)-type upper bounds on graph energy, that all are related to the classical McClelland bound [11]

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

In a recent article [2], the following result was communicated:

Proposition 1.1. *Let G be a graph with n vertices and m edges and suppose that all eigenvalues of G, $\lambda_1, \lambda_2, \ldots, \lambda_n$, are non-zero integers. If $\rho = \max_{1\leq i\leq n} |\lambda_i|$ and $\mu = \min_{1\leq i\leq n} |\lambda_i|$, then*

$$E(G) \leq (2m)^{\frac{\rho}{\rho+\mu}}\, n^{\frac{\mu}{\rho+\mu}}\,.$$

The aim of the present note is to show that Proposition 1.1 is a straightforward consequence of McClelland's bound (1), and also to offer an extension and generalization of this result.

For the sake of completeness, we first give a proof of (1).

Lemma 1.1. *Inequality (1) is valid for all graphs G. Equality holds if and only if $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$.*

Proof. Use the well known relation

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

and apply it to an inequality between quadratic and arithmetic means, such as

$$\left(\frac{1}{n}\sum_{i=1}^{n} |\lambda_i|\right)^2 \leq \frac{1}{n}\sum_{i=1}^{n} \lambda_i^2\,. \tag{2}$$

This implies

$$\left(\frac{E(G)}{n}\right)^2 \leq \frac{2m}{n}$$

from which (1) follows straightforwardly. □

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Recall that the condition $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$ is satisfied if G is either the empty graph, i.e., $G \cong \overline{K_n}$, $m = 0$, or G is the regular graph of degree 1, i.e., $G \cong \frac{n}{2} K_2$, provided n is even; for details see [1].

The McClelland's bound (1) is one of the most studied and most widely applied results in the theory of graph energy [10], and its chemical counterpart – the total π-electron energy [3–5].

2. Analyzing and extending Proposition 1.1

We start with an elementary result:

Lemma 2.1. *$E(G) \leq 2m$ holds for any graph G.*

Proof. Assume first that G is connected and that $n > 1$. Then the degrees of all its vertices are at least one, implying that the average vertex degree is at least one. The average vertex degree is $2m/n$. Therefore $2m \geq n$, and from inequality (1) it follows:

$$E(G) \leq \sqrt{(2m)n} \leq \sqrt{(2m)(2m)} = 2m\,.$$

confirming Lemma 2.1for connected graphs. This result holds also for $n = 1$, when $E(G) = m = 0$.

Suppose now that the graph G consists of (connected) components $G_1, G_2, \ldots, G_k$, so that G_i has m_i edges, $i = 1, 2, \ldots, k$. Then $E(G_i) \leq 2m_i$ holds for all $i = 1, 2, \ldots, k$. Recalling that the energy of a graph is equal to the sum of the energies of its components [10], we have

$$E(G) = E(G_1) + E(G_2) + \cdots + E(G_k) \leq 2m_1 + 2m_2 + \cdots + 2m_k = 2m\,,$$

confirming the validity of Lemma 2.1 also for disconnected graphs. □

Since $E(G)^2 \leq 2mn$, inequality (1) can be rewritten as

$$\frac{2m}{E(G)} \geq \frac{E(G)}{n}\,.$$

From Lemma 2.1 it follows that $2m/E(G) \geq 1$ holds for all graphs, except for the empty graph $\overline{K_n}$ (i.e., if $m = 0$).

Let $m > 0$ and $x \geq 1$ be an arbitrary real number. Then

$$\left(\frac{2m}{E(G)}\right)^x \geq \frac{2m}{E(G)} \geq \frac{E(G)}{n}$$

i.e.,

$$(2m)^x\, n \geq E(G)^{x+1}$$

i.e.,

$$E(G) \leq (2m)^{\frac{x}{x+1}}\, n^{\frac{1}{x+1}}\,. \tag{3}$$

In a trivial manner, relation (3) holds also for the empty graph $\overline{K_n}$, since then $E(G) = m = 0$.

In order to compare the above result with Proposition 1.1, let $x = p/q$ for some $p \geq q > 0$. Then we arrive at:

Proposition 2.1. *Let G be any graph (connected or disconnected) with n vertices and $m \geq 0$ edges. No matter what the spectrum of G is, if p and q are arbitrary real numbers such that $p \geq q > 0$, then*

$$E(G) \leq (2m)^{\frac{p}{p+q}}\, n^{\frac{q}{p+q}}\,. \tag{4}$$

Conditions for equality in (4) are specified in Proposition 4.1.

Evidently, Proposition 1.1 is a special case of Proposition 2.1. In other words, in Proposition 1.1 it was not necessary to require that "all eigenvalues be non-zero integers", and the usage of the eigenvalue–based parameters ρ and μ was just one of the arbitrarily many possibilities.

3. Another McClelland–type bound for graph energy

Let, as above, $\rho = |\lambda_1| = \lambda_1 \geq 0$. Note that ρ is usually referred to as the *spectral radius* of the graph G [1].

If we apply the reasoning used in the proof of Lemma 1.1 to $\lambda_2, \ldots, \lambda_n$, then instead of inequality (2), we obtain

$$\left(\frac{1}{n-1} \sum_{i=2}^{n} |\lambda_i| \right)^2 \leq \frac{1}{n-1} \sum_{i=2}^{n} \lambda_i^2$$

which implies

$$\left(\frac{E(G) - \rho}{n-1} \right)^2 \leq \frac{2m - \rho^2}{n-1}$$

from which it directly follows

$$E(G) \leq \rho + \sqrt{(n-1)(2m - \rho^2)}\,. \tag{5}$$

Equality in (5) holds if and only if $|\lambda_2| = \cdots = |\lambda_n|$. This spectral condition is satisfied if either $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}\,K_2$ (provided n is even) or $G \cong K_t \cup \frac{n-t}{2}\,K_2$ (provided $n-t$ is even); for details see [1].

Inequality (5) is just another modification of the McClelland bound. It was used by Koolen and Moulton as the starting point for designing their famous bound [8, 9] as well as by many other authors, e.g., in [5, 7].

In full analogy to Lemma 2.1 we now have:

Lemma 3.1. *$E(G) - \rho \leq 2m - \rho^2$ holds for any graph G.*

Proof. Apply the Hong–Shu inequality [6]

$$\rho \leq \sqrt{2m - n + 1}$$

which holds for all (connected or disconnected) graphs, except for (some) graphs with isolated vertices. It can be rewritten as

$$n - 1 \leq 2m - \rho^2\,.$$

Combining this with (5), we get

$$E(G) - \rho \leq \sqrt{(n-1)(2m - \rho^2)} \leq \sqrt{(2m - \rho^2)(2m - \rho^2)} = 2m - \rho^2\,.$$

Thus, Lemma 3.1 holds provided the graph G has no isolated vertices.

If G has $\ell > 0$ isolated vertices, then $G \cong G^* \cup \overline{K_\ell}$. The graph G^* has no isolated vertices and therefore

$$E(G^*) - \rho(G^*) \leq 2m(G^*) - \rho(G^*)^2\,.$$

Since $E(G) = E(G^*)$, $\rho(G) = \rho(G^*)$, $m(G) = m(G^*)$, Lemma 3.1 holds also for graphs with isolated vertices.

Finally, it remains to verify that Lemma 3.1 holds also for $G \cong \overline{K_n}$. This is evident, since for the empty graph, $E(\overline{K_n}) = \rho = m = 0$. □

Assuming that $m > 0$, from Lemma 3.1 it follows that

$$\frac{2m - \rho^2}{E(G) - \rho} \geq 1\,. \tag{6}$$

On the other hand, inequality (5) can be written in the form

$$\frac{2m - \rho^2}{E(G) - \rho} \geq \frac{E(G) - \rho}{n-1}\,. \tag{7}$$

Let $x \geq 1$ be an arbitrary real number. Then, combining (6) and (7) we get

$$\left(\frac{2m - \rho^2}{E(G) - \rho} \right)^x \geq \frac{E(G) - \rho}{n-1}$$

i.e.,

$$(2m - \rho^2)^x\,(n-1) \geq \big(E(G) - \rho\big)^{x+1}$$

i.e.,

$$E(G) \leq \rho + (2m - \rho^2)^{\frac{x}{x+1}}\,(n-1)^{\frac{1}{x+1}}\,. \tag{8}$$

Again, in an obvious manner, inequality (8) holds also for $m = 0$.

Let, as before, $x = p/q$ for some $p \geq q > 0$. Then from (8) we obtain:

Proposition 3.1. *Let G be any graph (connected or disconnected) with n vertices, $m \geq 0$ edges, and spectral radius ρ. No matter what the spectrum of G is, if p and q are arbitrary real numbers such that $p \geq q > 0$, then*

$$E(G) \leq \rho + (2m - \rho^2)^{\frac{p}{p+q}} (n-1)^{\frac{q}{p+q}} . \tag{9}$$

Conditions for equality in (9) are specified in Proposition 4.1.

Note that in Proposition 3.1, ρ may stand for any $|\lambda_i|$, $i = 1, 2, \ldots, n$. However, if $\rho = |\lambda_i|$ for some $i \neq 1$, then the corresponding bound would be weaker than the bound for $\rho = |\lambda_1| = \lambda_1$.

4. Final comments

There is a concealed problem with Propositions 2.1 and 3.1. The right–hand sides of (3) and (8) can be rewritten as

$$n \left(\frac{2m}{n}\right)^{\frac{x}{x+1}} \qquad \text{and} \qquad \rho + (n-1)\left(\frac{2m-\rho^2}{n-1}\right)^{\frac{x}{x+1}} .$$

Because for $x \geq 1$, the function $x/(x+1)$ monotonically increases, the best upper bounds for graph energy of the form (3) and (8) are for $x = 1$, which reduce (3) and (8) to the McClelland's bounds (1) and (5), respectively. In other words, both Propositions 2.1 and 3.1 provide upper bounds for graph energy not better than the original results of McClelland, formula (1) from year 1971 [11], and its variant, formula (5) from year 2000 [8, 9]. Based on these observations, we get:

Proposition 4.1. *(a) Equality in (4) holds if and only if $p = q$ and either $G \cong \overline{K_n}$ or $G \cong \frac{n}{2} K_2$ (provided n is even). If $p > q$, then the inequality in (4) is strict for all graphs.*
(b) Equality in (9) holds if and only if $p = q$ and either $G \cong \overline{K_n}$ or $G \cong \frac{n}{2} K_2$ (provided n is even), or $G \cong K_t \cup \frac{n-t}{2} K_2$ (provided $n - t$ is even). If $p > q$, then the inequality in (9) is strict for all graphs.

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