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Improving McClelland's Lower Bound for Energy

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Abstract

A lower bound for the energy of a graph is determined, in terms of number of vertices, edges and determinant of the adjacency matrix. It holds for nonsingular graphs, and under certain conditions improves the classical McClelland's lower bound.

1 Introduction

In this article we use the same notation as in the preceding paper [3]. In particular, by n and m we denote the numbers of vertices and edges, respectively, of the underlying graph G. The adjacency matrix of G is $\mathbf{A}$, and its eigenvalues are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. As well known,

$$\det \mathbf{A} = \prod_{i=1}^{n} \lambda_i \ .$$

A graph G is said to be singular if at least one of its eigenvalues is equal to zero. For singular graphs, evidently, $\det \mathbf{A} = 0$. A graph is nonsingular if all its eigenvalues are different from zero. Then, $|\det \mathbf{A}| > 0$.

The energy of the graph G is defined as

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

This spectrum–based graph invariant has been much studied in both chemical and mathematical literature. For details and an exhaustive list of references see the monograph [14]. What nowadays is referred to as graph energy, defined via Eq. (1), is closely related to the total π-electron energy calculated within the Hückel molecular orbital approximation; for details see in [8, 12]

Among the pioneering results of the theory of graph energy are the lower and upper bounds for E, discovered by McClelland in 1971 [15]. The famous McClelland upper bound $\sqrt{2mn}$ has been much studied in the chemical literature [4–7, 9–11, 13].

McClelland's lower bound for energy [15] depends on the parameters n, m, and $\det \mathbf{A}$, and reads:

$$E(G) \geq \sqrt{2m + n(n-1)|\det \mathbf{A}|^{2/n}} \, . \tag{2}$$

It holds for all graphs. In particular, it holds for both singular and nonsingular graphs. For bipartite graphs, it has been improved as [4]

$$E(G) \geq \sqrt{4m + n(n-2)|\det \mathbf{A}|^{2/n}} \, .$$

Caporossi et. al [1] discovered the following simple lower bound:

$$E(G) \geq 2\sqrt{m} \tag{3}$$

with equality holding if and only if G consists of a complete bipartite graph $K_{a,b}$ such that $a \cdot b = m$ and arbitrarily many isolated vertices.

In the subsequent section, we deduce a new lower bound for graph energy. It depends on the same parameters as McClelland's bound (2), namely on n, m, and $\det \mathbf{A}$. It, however, is restricted to nonsingular graphs. Under certain conditions it is better than McClelland's.

2 A lower bound on energy of nonsingular graphs

Theorem 1. *Let G be a connected nonsingular graph of order n with m edges. Then*

$$E(G) \geq \frac{2m}{n} + n - 1 + \ln|\det \mathbf{A}| - \ln \frac{2m}{n} \, . \tag{4}$$

Equality holds in (4) if and only if G is isomorphic to the complete graph K_n .

Proof. Since G is nonsingular, it is $|\lambda_i| > 0$, $i = 1, 2, \ldots, n$. Consider a function

$$f(x) = x - 1 - \ln x$$

for $x > 0$. It is elementary to prove that $f(x)$ is increasing for $x \geq 1$ and decreasing for $0 < x \leq 1$. Consequently, $f(x) \geq f(1) = 0$, implying that $x \geq 1 + \ln x$ for $x > 0$, with equality holding if and only if $x = 1$. Using the above result, we get

$$\begin{aligned} E(G) &= \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \\ &\geq \lambda_1 + n - 1 + \sum_{i=2}^{n} \ln\ |\lambda_i| \qquad (5) \\ &= \lambda_1 + n - 1 + \ln\ \prod_{i=2}^{n} |\lambda_i| \\ &= \lambda_1 + n - 1 + \ln\ |\det \mathbf{A}| - \ln\ \lambda_1 \,. \qquad (6) \end{aligned}$$

At this point, one has to recall that [2], $\lambda_1 \geq 2m/n$.

Since

$$g(x) = x + n - 1 + \ln |\det \mathbf{A}| - \ln x$$

is an increasing function on $1 \leq x \leq n$, we conclude that

$$g(x) \geq g\left(\frac{2m}{n}\right) = \frac{2m}{n} + n - 1 + \ln |\det \mathbf{A}| - \ln \frac{2m}{n}$$

for $x \geq 2m/n$. Combining the above result with (6), we arrive at (4). The first part of the proof is done.

Suppose now that the equality holds in (4). Then all the inequalities in the above considerations must be equalities. From the equality (5), we get

$$|\lambda_2| = |\lambda_3| = \cdots = |\lambda_n| = 1 \,. \qquad (7)$$

Since G is assumed to be connected, condition (7) is obeyed if and only if $G \cong K_n$ [2]. $\square$

In the general case, the lower bound (4) is not better than McClelland's (2). In Fig. 1 is depicted a class of graphs for which by numerical checking we established that (4) is superior to (2). The graph in Fig. 1 has n vertices and $4n-2$ edges, where

n is even but not a multiple of 6. (If n is multiple of 6, then $\det \mathbf{A} = 0$ and inequality (4) is not applicable.) The maximal vertex degree is 4 and thus, formally speaking, the graphs depicted in Fig. 1 belongs to the class of molecular graphs.

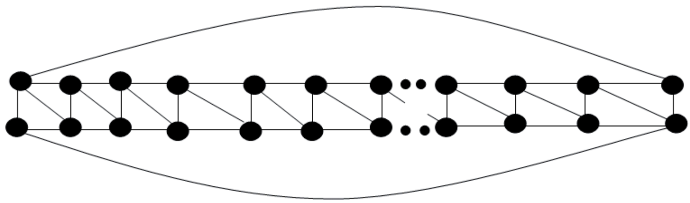

Fig. 1. A class of chemical graph for which the lower bound (4) is better than McClelland's lower bound (2).

Let Γ_1 be the class of connected graphs of order n, for which the following conditions are satisfied:

$$16 \leq \frac{n}{2} \leq \frac{2m}{n} \leq |\det \mathbf{A}| \leq n-1 \ . \tag{8}$$

For instance, K_n, $K_{n,n-1} \in \Gamma_1$.

Theorem 2. *Inequality (4) is better than (2) for any graph in* Γ_1*.*

Proof. From (8) it follows

$$\ln|\det \mathbf{A}| - \ln\frac{2m}{n} = \ln\left(\frac{|\det \mathbf{A}|}{\frac{2m}{n}}\right) \geq 0 \ .$$

Moreover, for $n \geq 32$,

$$(n-1)^{2/n} \leq \frac{5}{4} \ .$$

From (4) we now get

$$\frac{2m}{n} + n - 1 + \ln|\det \mathbf{A}| - \ln\frac{2m}{n} \geq \frac{2m}{n} + n - 1 \, .$$

In order to show that under the conditions (8), (4) is better than (2), we need to demonstrate that

$$2m+n(n-1)|\det \mathbf{A}|^{2/n} \leq 2m+n(n-1)\,(n-1)^{2/n} \leq 2m+n(n-1)\,\frac{5}{4} \leq \left(\frac{2m}{n} + n - 1\right)^2$$

that is,

$$2m + n(n-1)\,\frac{5}{4} \leq \left(\frac{2m}{n} - 1\right)^2 + n^2 + 4m - 2n$$

that is,

$$\left(\frac{2m}{n} - 1\right)^2 + 2m \geq \frac{n^2 + 3n}{4}$$

that is,

$$\left(\frac{2m}{n} - 1\right)^2 + 2m \geq \frac{3n^2 - 4n + 4}{4} \geq \frac{n^2 + 3n}{4}$$

which, because of $2m/n \geq n/2$ is always obeyed. $\square$

Let Γ_2 be the class of connected graphs of order n for which the following condition is satisfied:

$$|\det \mathbf{A}| \geq \frac{2m}{n}\ . \tag{9}$$

For instance, $K_n,\ K_{n,n-1} \in \Gamma_2$.

Theorem 3. *Inequality (4) is better than (3) for any graph in Γ_2.*

Proof. From (9) it follows

$$\frac{2m}{n} + n - 1 + \ln|\det \mathbf{A}| - \ln\frac{2m}{n} \ \geq\ \frac{2m}{n} + n - 1$$

$$\geq \sqrt{\left(\frac{2m}{n} - 1\right)^2 + n^2 + 4m - 2n} \ \geq\ 2\sqrt{m}\ .$$

$\square$

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