

Bounds for the energy of graphs

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Abstract

The energy of a graph G , denoted by $E(G)$, is the sum of the absolute values of all eigenvalues of G . In this paper we present some lower and upper bounds for $E(G)$ in terms of number of vertices, number of edges, and determinant of the adjacency matrix. Our lower bound is better than the classical McClelland's lower bound. In addition, Nordhaus–Gaddum type results for $E(G)$ are established.

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1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \dots, n$. The maximum and minimum vertex degrees are denoted by Δ and δ , respectively. If the vertices v_i and v_j are adjacent, we denote that by $v_i v_j \in E(G)$. The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of G is defined by its entries as $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ denote the eigenvalues of $\mathbf{A}(G)$. λ_1 is called the spectral radius of the graph G . Some well known properties of graph eigenvalues are:

$$\sum_{i=1}^n \lambda_i = 0, \quad \sum_{i=1}^n \lambda_i^2 = 2m \quad \text{and} \quad \det \mathbf{A} = \prod_{i=1}^n \lambda_i.$$

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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, $\det \mathbf{A} \neq 0$.

The energy of the graph G is defined as

$$(1.1) \quad E(G) = \sum_{i=1}^n |\lambda_i|$$

where λ_i , $i = 1, 2, \dots, n$, are the eigenvalues of graph G .

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. (1.1), is closely related to the total π -electron energy calculated within the Hückel molecular orbital approximation; for details see in [8, 11, 18].

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present a lower bound on the energy $E(G)$. In Section 4, we obtain an upper bound on $E(G)$. In Section 5, Nordhaus–Gaddum type results for $E(G)$ are established.

2. Preliminaries

In this section, we shall list some previously known results that will be needed in the next two sections.

2.1. Lemma. (*Cauchy interlace theorem*) [3, 17] *Let B be a $p \times p$ symmetric matrix and let B_k be its leading $k \times k$ submatrix; that is, B_k is a matrix obtained from B by deleting its last $p - k$ rows and columns. Then for $i = 1, 2, \dots, k$,*

$$(2.1) \quad \rho_{p-i+1}(B) \leq \rho_{k-i+1}(B_k) \leq \rho_{k-i+1}(B)$$

where $\rho_i(B)$ is the i -th largest eigenvalue of B .

2.2. Lemma. [13] *Let x_1, x_2, \dots, x_N be non-negative numbers, and let*

$$\alpha = \frac{1}{N} \sum_{i=1}^N x_i \quad \text{and} \quad \gamma = \left(\prod_{i=1}^N x_i \right)^{1/N}$$

be their arithmetic and geometric means. Then

$$\frac{1}{N(N-1)} \sum_{i < j} (\sqrt{x_i} - \sqrt{x_j})^2 \leq \alpha - \gamma \leq \frac{1}{N} \sum_{i < j} (\sqrt{x_i} - \sqrt{x_j})^2.$$

Moreover, equality holds if and only if $x_1 = x_2 = \dots = x_N$.

2.3. Lemma. [6] *Let a_1, a_2, \dots, a_n and b_1, b_2, \dots, b_n be non-negative real numbers. If $p > 1$, then*

$$\left(\sum_{i=1}^n (a_i + b_i)^p \right)^{1/p} \leq \left(\sum_{i=1}^n a_i^p \right)^{1/p} + \left(\sum_{i=1}^n b_i^p \right)^{1/p}.$$

Moreover, the above equality holds if and only if the rows $\{a_i\}$ and $\{b_i\}$ are proportional.

2.4. Lemma. [1] For a graph G ,

$$-\sqrt{\frac{2m(r-1)}{n(n-r+1)}} \leq \lambda_r \leq \sqrt{\frac{2m(n-r)}{nr}}, \quad 1 \leq r \leq n$$

2.5. Lemma. [2, 3] Let G be a connected graph of order n . Then

$$\lambda_1 \geq \frac{2m}{n}$$

with equality if and only if G is a regular graph.

3. Lower bound on graph energy

In this section we give a lower bound on energy $E(G)$ in terms of n , m and the determinant of the adjacency matrix.

First we mention some popular lower bounds on graph energy.

In the monograph [14] the following simple lower bound in terms of m is mentioned:

$$(3.1) \quad E(G) \geq 2\sqrt{m}$$

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.

McClelland [18] obtained the following lower bound in terms of n , m and the determinant of the adjacency matrix:

$$(3.2) \quad E(G) \geq \sqrt{2m + n(n-1)|\det \mathbf{A}|^{2/n}}.$$

Recently, Das et al. [5] have given the following lower bound, valid for non-singular graphs:

$$(3.3) \quad E(G) \geq \frac{2m}{n} + n - 1 + \ln \left(\frac{n|\det \mathbf{A}|}{2m} \right).$$

We now give an additional such lower bound, applicable for any graphs:

3.1. Theorem. Let G be a simple graph of order $n > 2$ with m edges. Then

$$(3.4) \quad E(G) \geq \sqrt{2m + n(n-1)|\det \mathbf{A}|^{2/n} + \frac{4}{(n+1)(n-2)} \left[\sqrt{\frac{2m}{n}} - \left(\frac{2m}{n} \right)^{1/4} \right]^2}$$

where equality holds if and only if $G \cong \frac{n}{2} K_2$ (n is even) or $G \cong \overline{K_n}$.

Proof. When $G \cong \overline{K_n}$, we have $m = 0$, $\det \mathbf{A} = 0$ and $E(G) = 0$. Hence the equality holds in (3.4). When $G \cong \frac{n}{2} K_2$ (n is even), we have $2m = n$, $\det \mathbf{A} = (-1)^{n/2}$ and $E(G) = n$. Hence the equality holds in (3.4). When $G \cong p K_2 \cup (n-2p) K_1$ ($\lceil \frac{n}{2} \rceil > p \geq 1$), we have $2m = 2p < n$, $\det \mathbf{A} = 0$ and $E(G) = 2p$. Hence the inequality in (3.4) is strict. Otherwise, G has at least one connected component with $m_1 \geq 2$ (m_1 is the number of edges in the connected component).

From Lemma 2.2, we get

$$(3.5) \quad \sum_{i=1}^N x_i \geq N \left(\prod_{i=1}^N x_i \right)^{1/N} + \frac{1}{(N-1)} \sum_{i < j} (\sqrt{x_i} - \sqrt{x_j})^2.$$

Putting $N = \frac{n(n-1)}{2}$ and

$$(x_1, x_2, \dots, x_N) = \left(|\lambda_1||\lambda_2|, |\lambda_1||\lambda_3|, \dots, |\lambda_1||\lambda_n|, |\lambda_2||\lambda_3|, \dots, |\lambda_2||\lambda_n|, \dots, |\lambda_{n-1}||\lambda_n| \right)$$

in (3.5), we get

$$\begin{aligned} \sum_{1 \leq i < j \leq n} |\lambda_i||\lambda_j| &\geq \frac{n(n-1)}{2} \left(\prod_{i=1}^n |\lambda_i| \right)^{2/n} \\ &+ \frac{2}{(n^2 - n - 2)} \sum_{i < j \leq k < \ell} \left(\sqrt{|\lambda_i||\lambda_j|} - \sqrt{|\lambda_k||\lambda_\ell|} \right)^2 \end{aligned}$$

that is,

$$(3.6) \quad \begin{aligned} 2 \sum_{1 \leq i < j \leq n} |\lambda_i||\lambda_j| &\geq n(n-1) |\det \mathbf{A}|^{2/n} \\ &+ \frac{4}{(n+1)(n-2)} \sum_{i < j \leq k < \ell} \left(\sqrt{|\lambda_i||\lambda_j|} - \sqrt{|\lambda_k||\lambda_\ell|} \right)^2. \end{aligned}$$

By Lemma 2.4,

$$\lambda_{n/2} \leq \sqrt{\frac{2m}{n}} \quad \text{and} \quad \lambda_{(n+1)/2} \leq \sqrt{\frac{2m(n-1)}{n(n+1)}} < \sqrt{\frac{2m}{n}}$$

for even and odd n , respectively.

From Lemma 2.5 and also from the above, we get for $n \geq 3$,

$$(3.7) \quad \lambda_1 \geq \frac{2m}{n} \quad \text{and} \quad \lambda_{\lceil \frac{n}{2} \rceil} \leq \sqrt{\frac{2m}{n}}.$$

Since $m \geq 1$, by Lemma 2.1,

$$\lambda_n \leq \lambda_2(\mathbf{A}_2) = -1.$$

From the above, we have that $|\lambda_n| \geq 1$. Since $n \geq 3$ and $m_1 \geq 2$, we further have

$$\begin{aligned} &\sum_{i < j \leq k < \ell} \left(\sqrt{|\lambda_i||\lambda_j|} - \sqrt{|\lambda_k||\lambda_\ell|} \right)^2 \geq \left(\sqrt{|\lambda_1||\lambda_n|} - \sqrt{|\lambda_{\lceil \frac{n}{2} \rceil}||\lambda_n|} \right)^2 \\ &+ \sum_{\substack{i < j \leq k < \ell \\ (i, j) \neq (1, n), \\ (k, \ell) \neq (\lceil \frac{n}{2} \rceil, n)}} \left(\sqrt{|\lambda_i||\lambda_j|} - \sqrt{|\lambda_k||\lambda_\ell|} \right)^2 > |\lambda_n| \left(\sqrt{|\lambda_1|} - \sqrt{|\lambda_{\lceil \frac{n}{2} \rceil}|} \right)^2 \\ &\geq \left[\sqrt{\frac{2m}{n}} - \left(\frac{2m}{n} \right)^{1/4} \right]^2. \end{aligned}$$

Combining the above result with (3.6), we get

$$2 \sum_{1 \leq i < j \leq n} |\lambda_i||\lambda_j| > n(n-1) |\det \mathbf{A}|^{2/n} + \frac{4}{(n+1)(n-2)} \left[\sqrt{\frac{2m}{n}} - \left(\frac{2m}{n} \right)^{1/4} \right]^2.$$

Adding to both sides $\sum_{i=1}^n \lambda_i^2 (= 2m)$, we get

$$E(G)^2 > 2m + n(n-1) |\det \mathbf{A}|^{2/n} + \frac{4}{(n+1)(n-2)} \left[\sqrt{\frac{2m}{n}} - \left(\frac{2m}{n}\right)^{1/4} \right]^2$$

which straightforwardly implies (3.4). \square

Inequality (3.4), as well as (4.1), was mentioned in [9], but without details and without the characterization of the equality cases.

3.2. Remark. Our lower bound (3.4) is better than the lower bound (3.2).

3.3. Remark. In [5], it has been mentioned that sometimes the lower bound in (3.3) is better than the lower bounds in (3.1) and (3.2), but the lower bound in (3.3) is applicable for non-singular graphs.

4. Upper bound on graph energy

In this section we give an upper bound on energy $E(G)$ in terms of n , m , and $\det \mathbf{A}$. Other upper bounds on graph energy are discussed in the book [14] and the recent papers [4, 9, 19].

4.1. Theorem. *Let G be a connected non-singular graph of order n with m edges. Then*

$$(4.1) \quad E(G) \leq 2m - \frac{2m}{n} \left(\frac{2m}{n} - 1 \right) - \ln \left(\frac{n |\det \mathbf{A}|}{2m} \right)$$

where $\det \mathbf{A} (\neq 0)$ is the determinant of the adjacency matrix. Equality holds in (4.1) if and only if $G \cong K_n$.

Proof. Since G is non-singular, we have $|\lambda_i| > 0$, $i = 1, 2, \dots, n$. Thus

$$|\det \mathbf{A}| = \prod_{i=1}^n |\lambda_i| > 0.$$

Moreover, since G has no isolated vertices,

$$2m = \sum_{i=1}^n d_i \geq n \quad \text{i.e.,} \quad \frac{2m}{n} \geq 1.$$

Consider now the function

$$f(x) = x^2 - x - \ln x, \quad x > 0$$

for which

$$f'(x) = 2x - 1 - \frac{1}{x}.$$

Thus $f(x)$ is an increasing function on $x \geq 1$ and a decreasing function on $0 < x \leq 1$. Thus, $f(x) \geq f(1) = 0$ implying $x \leq x^2 - \ln x$ for $x > 0$, with equality holding if and

only if $x = 1$. Using this result, we get

$$\begin{aligned}
 E(G) &= \lambda_1 + \sum_{i=2}^n |\lambda_i| \\
 (4.2) \quad &\leq \lambda_1 + \sum_{i=2}^n (\lambda_i^2 - \ln |\lambda_i|) \\
 &= \lambda_1 + 2m - \lambda_1^2 - \ln \prod_{i=1}^n |\lambda_i| + \ln \lambda_1 \\
 (4.3) \quad &= 2m + \lambda_1 - \lambda_1^2 - \ln |\det \mathbf{A}| + \ln \lambda_1 .
 \end{aligned}$$

From Lemma 2.5 we know that $\lambda_1 \geq 2m/n$. Since

$$g(x) = 2m + x - x^2 - \ln |\det \mathbf{A}| + \ln x$$

is an increasing function on $0 < x \leq 1$ and a decreasing function on $x \geq 1$, and since $x \geq \frac{2m}{n} \geq 1$, we have

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

Combining this with (4.3), we arrive at (4.1). By this, the first part of the proof is done.

Suppose now that the equality holds in (4.1). Then all the inequalities in the above consideration must be equalities. From equality in (4.2), we get

$$(4.4) \quad |\lambda_2| = |\lambda_3| = \cdots = |\lambda_n| = 1 .$$

Since G is connected, condition (4.4) is satisfied if and only if $G \cong K_n$ [3].

Conversely, one can see easily that the equality holds in (4.1) for K_n . □

Concluding this section, it should be mentioned that similar techniques (based on the inequalities stated in Section 2) have been used in estimating other spectrum-based graph indices, especially the Estrada index $EE(G)$ [7, 12, 15, 16, 21, 22]. Recall that this index is defined as

$$EE(G) = \sum_{i=1}^n e^{\lambda_i}$$

and that details of its theory can be found in the survey [10].

5. Nordhaus–Gaddum–type results for graph energy

Motivated by the seminal work of Nordhaus and Gaddum [20], we report here analogous results for graph energy. As usual, \overline{G} denotes the complement of the graph G .

5.1. Theorem. *Let G and \overline{G} be both connected non-singular graphs. If G has n vertices and m edges, then*

$$\begin{aligned}
 (5.1) \quad &3(n-1) + \ln\left(\frac{n^2 |\det(A\overline{A})|}{2m(n(n-1)-2m)}\right) \leq E(G) + E(\overline{G}) \leq 2(n-1) \\
 &+ \frac{4m(n(n-1)-2m)}{n^2} - \ln\left(\frac{n^2 |\det(\mathbf{A}\overline{\mathbf{A}})|}{2m(n(n-1)-2m)}\right)
 \end{aligned}$$

where $\det \mathbf{A} (\neq 0)$ and $\det \bar{\mathbf{A}} (\neq 0)$ are the determinants of the adjacency matrices of G and \bar{G} , respectively.

Proof. By (3.3),

$$E(G) + E(\bar{G}) \geq \frac{2m + 2\bar{m}}{n} + 2(n-1) + \ln \left(\frac{n |\det \mathbf{A}|}{2m} \right) + \ln \left(\frac{n |\det \bar{\mathbf{A}}|}{2\bar{m}} \right)$$

where \bar{m} and $\bar{\mathbf{A}}$ are the number of edges and the adjacency matrix of \bar{G} .

Since $2m + 2\bar{m} = n(n-1)$ and $\det \mathbf{A}\bar{\mathbf{A}} = \det \mathbf{A} \det \bar{\mathbf{A}}$, the lower bound in (5.1) follows.

By (4.1),

$$\begin{aligned} E(G) + E(\bar{G}) &\leq 2m + 2\bar{m} + \frac{2m + 2\bar{m}}{n} - \frac{4m^2 + 4\bar{m}^2}{n^2} \\ &\quad - \ln \left(\frac{n |\det \mathbf{A}|}{2m} \right) - \ln \left(\frac{n |\det \bar{\mathbf{A}}|}{2\bar{m}} \right). \end{aligned}$$

This straightforwardly leads to the upper bound in (5.1). \square

5.2. Theorem. *Let G be a graph of order n with m edges. Then*

$$\begin{aligned} (5.2) \quad E(G) + E(\bar{G}) &\leq n + \Delta - \delta - 1 \\ &\quad + \left[(n-1) \left(n-1 + \frac{4m(n(n-1) - 2m)}{n^2} \right. \right. \\ &\quad \left. \left. + \frac{2}{n^2} \sqrt{2m(2m+n)(n^2-2m)(n^2-2m-n)} \right) \right]^{1/2} \end{aligned}$$

where Δ and δ are the maximum degree and minimum degree of G , respectively.

Proof. By Lemma 2.3,

$$\left(\sum_{i=2}^n (|\lambda_i| + |\bar{\lambda}_i|)^2 \right)^{1/2} \leq \left(\sum_{i=2}^n \lambda_i^2 \right)^{1/2} + \left(\sum_{i=2}^n \bar{\lambda}_i^2 \right)^{1/2}$$

where λ_i and $\bar{\lambda}_i$ are eigenvalues of G and \bar{G} , respectively. Since

$$\sum_{i=1}^n \lambda_i^2 = 2m \quad \text{and} \quad \sum_{i=1}^n \bar{\lambda}_i^2 = 2\bar{m}$$

we get

$$\begin{aligned}
 \sum_{i=2}^n (|\lambda_i| + |\bar{\lambda}_i|)^2 &\leq \sum_{i=2}^n \lambda_i^2 + \sum_{i=2}^n \bar{\lambda}_i^2 + 2\sqrt{\sum_{i=2}^n \lambda_i^2 \sum_{i=2}^n \bar{\lambda}_i^2} \\
 &= 2m - \lambda_1^2 + 2\bar{m} - \bar{\lambda}_1^2 + 2\sqrt{(2m - \lambda_1^2)(2\bar{m} - \bar{\lambda}_1^2)} \\
 &\leq n(n-1) - \frac{4m^2 + 4\bar{m}^2}{n^2} + 2\sqrt{\frac{4m\bar{m}}{n^4}(n^2 - 2m)(2m + n)} \\
 &= n - 1 + \frac{4m(n(n-1) - 2m)}{n^2} \\
 (5.3) \quad &+ \frac{2}{n^2} \sqrt{2m(n^2 - 2m - n)(n^2 - 2m)(2m + n)}.
 \end{aligned}$$

Since $\lambda_1 \leq \Delta$, using the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}
 E(G) + E(\bar{G}) &= |\lambda_1| + |\bar{\lambda}_1| + \sum_{i=2}^n (|\lambda_i| + |\bar{\lambda}_i|) \\
 &\leq \Delta + n - \delta - 1 + \sqrt{(n-1) \sum_{i=2}^n (|\lambda_i| + |\bar{\lambda}_i|)^2}.
 \end{aligned}$$

Together with (5.3) this yields (5.2). \square

6. Concluding remarks

Studies of the structure–dependence of the total π -electron energy has a long history. Beginning with McClelland’s seminal work [18] in the early 1970s, most of the researches along these lines were done by means of estimates (upper and lower bounds); for details see the surveys [8, 9]. Eventually, the concept of total π -electron energy was extended and redefined to the mathematically more general and more convenient concept of graph energy, Eq. (1.1), see [14].

In the present work we offer a few more estimates for graph energy, in terms of parameters that have direct and straightforward structural interpretation. By this, we deem to have somewhat improved the understanding of how graph energy (and thus total π -electron energy) are influenced by the respective structural features of the underlying graph.

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