

Article

Exact variance-energy relations and optimal spectral bounds for graphs

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Abstract: Let G be a graph of order n and size m , with adjacency matrix eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. The *energy* of G , denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of its eigenvalues. A classical upper bound on the energy, originally established by McClelland [1], states that $\mathcal{E}(G) \leq \sqrt{2mn}$. In this paper, we refine the spectral analysis of graph energy by deriving an exact analytical expression relating $\mathcal{E}(G)$ to the variance of the vector of absolute eigenvalues $x = (|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|)$. Specifically, we prove that $\mathcal{E}(G) = \sqrt{2mn - n^2 \text{Var}(x)}$, providing a more precise and quantitative spectral characterization of graph energy. As an application, this identity allows us to derive improved lower bounds for $\mathcal{E}(G)$, thereby strengthening and generalizing previously known inequalities. Furthermore we conjecture that for any non-singular graph G of order n , $\mathcal{E}(G) \geq 2\sqrt{\langle d \rangle(n-1)}$, where $\langle d \rangle = 2m/n$ is the average vertex degree of G . Equality holds if and only if $G \cong K_n$.

Keywords: graph energy, McClelland bound, spectral graph theory, spectral variance

MSC: 05C50, 05C35.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph with order $n = |V|$ and size $m = |E|$. The *adjacency matrix* $A = [a_{ij}]$ of G is an $n \times n$ symmetric matrix defined by

$$a_{ij} = \begin{cases} 1 & \text{if } \{i, j\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Since A is a real symmetric matrix, all its eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ are real.

The *energy* of G , denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of the eigenvalues of A :

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

This notion, introduced by one of the present authors [2], has important applications in chemistry and spectral graph theory [3–5]. Among various known bounds on graph energy, a classical upper bound due to McClelland [1] states that

$$\mathcal{E}(G) \leq \sqrt{2mn}.$$

In the past, it has been much investigated, mainly aiming at its sharpening, see for instance [6–12].

Let $x = (|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|)$ be the vector of absolute values of the eigenvalues. The *variance* of x , denoted by $\text{Var}(x)$, is

$$\text{Var}(x) = \frac{1}{n} \sum_{i=1}^n (|\lambda_i| - \mu)^2, \quad \text{where} \quad \mu = \frac{1}{n} \sum_{i=1}^n |\lambda_i|.$$

In this paper, we explore a deeper connection between the energy of a graph and the variance of its absolute eigenvalues. This approach yields new insights and improved lower bounds on graph energy.

2. An exact formula for graph energy based on variance

In this section, we establish an exact analytical relation between the energy of a graph G and the variance of the absolute values of its adjacency eigenvalues. This identity sharpens the classical upper bound $\mathcal{E}(G) \leq \sqrt{2mn}$ by explicitly expressing the energy in terms of both the number of edges and the eigenvalue distribution.

The following result highlights the role of variance as a measure of deviation from maximal energy and provides a refined spectral insight. It also may serve as a foundation for deriving improved bounds in subsequent discussions.

Theorem 1. *Let G be a graph with n vertices, m edges, and energy $\mathcal{E}(G)$. Then*

$$\mathcal{E}(G) = \sqrt{2mn - n^2 \operatorname{Var}(|\lambda|)}.$$

Proof. Recall that from the trace of A^2 ,

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

The variance of the absolute eigenvalues is given by

$$\operatorname{Var}(|\lambda|) = \frac{1}{n} \sum_{i=1}^n |\lambda_i|^2 - \left(\frac{1}{n} \sum_{i=1}^n |\lambda_i| \right)^2 = \frac{2m}{n} - \left(\frac{\mathcal{E}(G)}{n} \right)^2.$$

Rearranging this expression completes the proof. $\square$

Remark 1. Applying Popoviciu's inequality,

$$\operatorname{Var}(x) \leq \frac{(\lambda_1 - |\lambda_n|)^2}{4},$$

to Theorem 1 yields the known lower bound

$$\mathcal{E}(G) \geq \sqrt{2mn - \frac{n^2}{4}(\lambda_1 - |\lambda_n|)^2},$$

relating the energy to the spectral span $\lambda_1 - |\lambda_n|$, as previously observed in [10].

Remark 2. Using the von Székelyfalvi–Nagy inequality

$$\operatorname{Var}(x) \geq \frac{(\lambda_1 - |\lambda_n|)^2}{2n},$$

together with Theorem 1, we obtain the improved upper bound

$$\mathcal{E}(G) \leq \sqrt{2mn - \frac{n}{2}(\lambda_1 - |\lambda_n|)^2},$$

which was the key result in [9].

3. A spectral inequality for the energy of a graph

In this section, we establish new inequalities for the energy of graphs and compare them with some existing bounds in the literature.

Theorem 2. Let G be a graph of order n and size m , with adjacency matrix eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ such that $\lambda_1 = |\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$. Then the energy of G satisfies the inequality

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1}. \quad (1)$$

Equality holds if and only if either $|\lambda_1| = |\lambda_2| = \dots = |\lambda_n|$, or $|\lambda_1| = |\lambda_s|$ for some $2 \leq s \leq n$ and $|\lambda_k| = 0$ for all $k \neq s$, with $2 \leq k \leq n$.

Proof. Since for each $1 \leq i \leq n$ we have

$$|\lambda_i| \leq \lambda_1,$$

it follows that

$$\lambda_1 |\lambda_i| \geq |\lambda_i|^2 = \lambda_i^2.$$

Summing over all i gives

$$\lambda_1 \sum_{i=1}^n |\lambda_i| \geq \sum_{i=1}^n \lambda_i^2.$$

Recalling that $\mathcal{E}(G) = \sum_{i=1}^n |\lambda_i|$ and $\sum_{i=1}^n \lambda_i^2 = \text{trace}(A^2) = 2m$, we obtain

$$\lambda_1 \mathcal{E}(G) \geq 2m,$$

which implies inequality (1).

Equality holds if and only if all inequalities above are equalities, which requires that for each i ,

$$\lambda_1 |\lambda_i| = \lambda_i^2.$$

This condition is satisfied precisely when either all absolute eigenvalues coincide, or when there exists a single eigenvalue λ_s with the same absolute value as λ_1 , and all other eigenvalues (except possibly the first and the s -th) are zero in absolute value. $\square$

4. Comparison with earlier obtained bounds

In order to demonstrate the strength of Theorem 2, we compare it with the lower bound for the energy of graphs given by Filipovski [13].

Remark 3. Filipovski [13] proved that if G is a connected graph with n vertices, m edges, and maximum vertex degree Δ , then

$$\mathcal{E}(G) \geq \frac{2m}{\Delta}. \quad (2)$$

Note that $\lambda_1 \leq \Delta$, and therefore,

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq \frac{2m}{\Delta}.$$

This implies that the inequality in Theorem 2 is a refinement of inequality (2).

The following result is well known [4,5]

$$\mathcal{E}(G) \geq 2\sqrt{n-1}, \quad (3)$$

representing the best possible lower bound for connected graphs of order n . Equality holds if and only if G is the n -vertex star.

We now observe that for certain classes of graphs, Theorem 2 provides a sharper lower bound than the inequality (3). In particular, it gives a better bound for (i) trees and (ii) connected cyclic graphs with girth $g \geq 5$.

Remark 4. (i) From [14], we know that if G is a tree of order n , then $\lambda_1 \leq \sqrt{n-1}$. Since $m = n - 1$ for any tree, applying Theorem 2 yields

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq \frac{2(n-1)}{\sqrt{n-1}} = 2\sqrt{n-1}.$$

(ii) From [15], for any graph with girth $g \geq 5$, we have $\lambda_1 \leq \sqrt{n-1}$. Since $m \geq n - 1$ for connected graphs, we get

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq \frac{2(n-1)}{\sqrt{n-1}} = 2\sqrt{n-1}.$$

Therefore, Theorem 2 implies a stronger inequality than (3) for both trees and graphs with girth at least 5.

We now compare our bound with another earlier known lower bound for graph energy, and show that Theorem 2 improves it for K_3 -free graphs.

Remark 5. From [4,5], for any graph G of size m , it holds

$$\mathcal{E}(G) \geq 2\sqrt{m}. \quad (4)$$

In addition, from [15], we know that for any K_3 -free graph, $\lambda_1 \leq \sqrt{m}$. Applying Theorem 2, we then get

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq \frac{2m}{\sqrt{m}} = 2\sqrt{m}.$$

Therefore, the inequality in Theorem 2 is stronger than inequality (4) for any K_3 -free graph.

In the following remark, we show that our bound is stronger than the classical estimate (4) for all graphs whose largest eigenvalue satisfies $\lambda_1 \leq \sqrt{m}$. This includes all triangle-free graphs such as trees and cycles.

Remark 6. Let G be a graph of size m such that its largest eigenvalue satisfies $\lambda_1 \leq \sqrt{m}$. Then, by applying Theorem 2, we obtain

$$\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq 2\sqrt{m}.$$

Therefore, the bound in Theorem 2 is stronger than the inequality (4), for any graph with $\lambda_1 \leq \sqrt{m}$, including all K_3 -free graphs.

Next, we compare our bound in Theorem 2 with the lower bound obtained by Ma [16], namely with

$$\mathcal{E}(G) \geq 2\delta, \quad (5)$$

where δ is the minimum vertex degree of G .

Remark 7. We compare our bound in Theorem 2 with the inequality (5) in the following cases:

(i) If G is any graph with $\lambda_1 \leq \sqrt{m}$, then $\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq 2\lambda_1 \geq 2\delta$. Thus, Theorem 2 provides a better lower bound than (5) for this class of graphs.

(ii) If G is a graph with $\lambda_1 \leq \frac{n}{2}$, then $\mathcal{E}(G) \geq \frac{2m}{\lambda_1} \geq \frac{2\delta n}{\lambda_1} \geq 2\delta$. Therefore, also in this case Theorem 2 improves upon inequality (5).

Now, we compare our bound with a recently established lower bound involving the Sombor index, obtained by Ülker et al. [17]. In [17] the following result was obtained:

$$\mathcal{E}(G) \geq \frac{SO(G)}{\Delta^3}, \quad (6)$$

where $SO(G)$ is the Sombor index of G .

Remark 8. Since $SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \leq \sqrt{2m\Delta}$, and noting that

$$\sqrt{2\Delta^2} \geq \lambda_1 \implies \frac{2m}{\lambda_1} \geq \frac{\sqrt{2}m}{\Delta^2} = \frac{\sqrt{2}m\Delta}{\Delta^3} \geq \frac{SO(G)}{\Delta^3},$$

it follows that the inequality in Theorem 2 is stronger than inequality (6).

Next, we compare our bound with another result pertaining to the Sombor index, obtained by Reja et al. [18] as

$$\mathcal{E}(G) \geq \frac{SO(G)^2}{m\Delta^5}, \quad (7)$$

where $SO(G)$ is the Sombor index of G .

Remark 9. Since

$$SO(G)^2 = \left(\sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \right)^2 \leq 2m^2 \Delta^2,$$

we have:

$$\Delta^3 \geq \lambda_1 \implies \frac{2m}{\lambda_1} \geq \frac{2m}{\Delta^3} = \frac{2m^2\Delta^2}{m\Delta^5} \geq \frac{SO(G)^2}{m\Delta^5}.$$

Therefore, the inequality in Theorem 2 is stronger than inequality (7), for any graph.

Finally, we compare our bound with two results for regular graphs involving the Sombor index.

For regular graph, Ülker et al. [17] obtained

$$\mathcal{E}(G) \geq \frac{SO(G)}{\Delta^2},$$

whereas Reja et al. [18] improved it as

$$\mathcal{E}(G) \geq \frac{\sqrt{2}SO(G)}{\Delta^2}. \quad (8)$$

Remark 10. Notice that

$$\Delta \geq \lambda_1 \Leftrightarrow \frac{2m}{\lambda_1} \geq \frac{2m}{\Delta} = \frac{2m\Delta}{\Delta^2} \geq \frac{\sqrt{2}SO(G)}{\Delta^2}.$$

Therefore, the inequality in Theorem 2 is stronger than the inequality inequality (8).

5. A conjecture

One of the present authors has earlier extensively studied lower bounds for graph energy, see for instance [19–21]. Based on his experience in this area, and the above demonstration that Theorem 2 consistently yields stronger lower bounds than a wide range of earlier discovered results, we ventured to state the below Conjecture 1.

In the above considerations, we observed that for several graphs *satisfying the non-singularity condition* the bound from Theorem 2 is close to the actual value of $\mathcal{E}(G)$, and in some tested cases it coincides with it. For example, for the complete graph K_n one has

$$\mathcal{E}(K_n) = 2(n-1) = 2\sqrt{\frac{2m(n-1)}{n}},$$

so the expression, stated below as Conjecture 1, is sharp for K_n .

We emphasize that many commonly studied graph families are *generally singular* and so were excluded from these tests unless the particular parameter choices made them non-singular. For example, a complete bipartite graph $K_{p,q}$ has eigenvalues $\sqrt{pq}$, $-\sqrt{pq}$, and 0 with multiplicity $p+q-2$, implying that $K_{p,q}$ is singular whenever $p+q > 2$ (thus, among such graphs, only $K_{1,1}$ is non-singular).

For instance, as well known, the energy of the complete bipartite graph $K_{p,q}$ is

$$\mathcal{E}(K_{p,q}) = 2\sqrt{pq},$$

whereas the right-hand side of the conjectured inequality evaluates to

$$2\sqrt{\frac{2m(n-1)}{n}} = 2\sqrt{\frac{2pq(p+q-1)}{p+q}},$$

which is strictly greater than $2\sqrt{pq}$ whenever $p, q > 1$. This shows that the conjecture does not hold for $K_{p,q}$ with $p+q > 2$, in agreement with the fact that such graphs are singular due to the multiplicity of the zero eigenvalue.

Given the sharpness for K_n and the empirical evidence on non-singular examples, we formulate the following conjecture.

Conjecture 1. Let G be a non-singular graph of order n and size m . Then

$$\mathcal{E}(G) \geq 2\sqrt{\frac{2m(n-1)}{n}} \quad \text{i.e.,} \quad \mathcal{E}(G) \geq 2\sqrt{\langle d \rangle (n-1)},$$

where $\langle d \rangle = 2m/n$ is the average vertex degree. Moreover, equality holds if and only if $G \cong K_n$.

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