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Proofs of a Few Special Cases of a Conjecture on Energy of Non-Singular Graphs☆

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Abstract

Akbari and Hosseinzadeh [MATCH Commun. Math. Comput. Chem. 83 (2020), 631–633] conjectured that the energy of a non-singular graph G is bounded from below by the sum of the maximum and the minimum vertex degree of G, with equality if and only if G is a complete graph. We discuss this conjecture here and provide a few lower bounds on the energy which prove this conjecture in several special cases.

1 Introduction

Let $G = (V, E)$, with $|V| = n$ and $|E| = m$, be a simple graph with adjacency matrix A, and let $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of A. The energy of a graph G is given by $E(G) = \sum_{i=1}^{n} |\lambda_i|$, as defined by Ivan Gutman [10] back in 1978. With some delay for initial acceptance, graph energy became one of the most studied topological indices since the 2000s—see, e.g., [15] for an in-depth monograph covering the development of graph energy and [12, 13] for overviews of recent research on graph energies.

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Let Δ, δ and $\bar{d} = \frac{2m}{n}$, respectively, represent the maximum, the minimum and the average vertex degree of G. Motivated by an unnecessarily lengthy proof of the lower bound

$$E(G) \geq 2\delta \tag{1}$$

from [16], both Oboudi [18] and Akbari and Hosseinzadeh [2] improved this lower bound to

$$E(G) \geq 2\lambda_1 \geq 2\bar{d} \geq 2\delta \tag{2}$$

using very short proofs. For the sake of thoroughness, we shortly rephrase the Oboudi's proof [18]: Assume that for some $1 \leq p < n$, we have $\lambda_p > 0 \geq \lambda_{p+1}$. Then $\mathrm{Tr}(A) = 0$ leads to $\sum_{j=p+1}^{n} \lambda_j = -\sum_{i=1}^{p} \lambda_i$, so that

$$E(G) = \sum_{i=1}^{n} |\lambda_i| = 2\sum_{i=1}^{p} \lambda_i \geq 2\lambda_1.$$

The inequality $\lambda_1 \geq \bar{d}$ is well-known in spectral graph theory [6], and the cases of equality can be easily characterized in the above inequalities [2, 18].

However, after obtaining the corollary $E(G) \geq 2\delta$, Akbari and Hosseinzadeh [2] posed the following conjecture.

Conjecture 1 ([2]) *If the adjacency matrix of G is non-singular then $E(G) \geq \Delta + \delta$, with the equality if and only if G is a complete graph.*

Apart from an obvious attempt at generalizing the lower bound (1), Akbari and Hosseinzadeh [2] did not provide any further motivation or computational evidence for this conjecture. Moreover, the sudden appearance of the additional condition that (the adjacency matrix of) G is non-singular is somewhat frustrating, as there are obvious counterexamples for this lower bound among the graphs that have zero eigenvalues. For example, the complete bipartite graph $K_{\Delta,\delta}$ has the adjacency spectrum $[\sqrt{\Delta\delta}, 0^{(\Delta+\delta-2)}, -\sqrt{\Delta\delta}]$ (where the exponent $(\Delta + \delta - 2)$ denotes the multiplicity of the zero eigenvalue), so that

$$E(K_{\Delta,\delta}) = 2\sqrt{\Delta\delta} < \Delta + \delta$$

whenever $\Delta > \delta$.

Nevertheless, the exclusion of singular graphs appears to make Conjecture 1 correct. In the next section, we build upon some of the existing energy bounds and we additionally provide a few new lower bounds on energy of non-singular graphs to show that Conjecture 1 holds in a number of special cases.

2 Lower bounds on the energy of non-singular graphs

Probably the simplest class of graphs for which Conjecture 1 holds are regular graphs for which $\lambda_1 = \Delta = \delta$ [5]. Hence from (1) and (2) we have $E(G) \geq 2\lambda_1 = \Delta + \delta$, regardless of whether the regular graph G is singular or not.

Let us revisit the Gutman's lower bound on the energy of non-singular graphs [11].

Proposition 2 ([11]) *If the adjacency matrix of G is non-singular, then $E(G) \geq n$.*

This proposition follows easily from the inequality of arithmetic and geometric means. First note that the adjacency matrix A is integer-valued, so that $\det(A) = \lambda_1\lambda_2\cdots\lambda_n$ is also an integer. Hence if A is non-singular, then $|\det(A)| \geq 1$. Now we have

$$E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n| \geq n\sqrt[n]{|\lambda_1||\lambda_2|\cdots|\lambda_n|} = n\sqrt[n]{|\det(A)|} \geq n. \tag{3}$$

From this proposition we immediately have the following corollary.

Corollary 3 *If G is a non-singular graph with $n \geq \Delta + \delta$, then $E(G) \geq \Delta + \delta$.*

A particular example of such non-singular graphs are trees with perfect matchings. They are non-singular by the Sachs' theorem for the coefficients of the characteristic polynomial of A [6, Theorem 1.3, Proposition 1.1]. For trees we have $n - 1 \geq \Delta$ and $1 \geq \delta$ (including the 1-vertex tree in the second inequality), so that $n \geq \Delta + \delta$. As a matter of fact, Ashraf [4] recently improved Proposition 2 when G is a tree on n vertices with a perfect matching and maximum vertex degree at most 3, by showing that

$$E(G) > 1.21n - 3.23.$$

Another example of graphs that satisfy $n \geq \Delta + \delta$ are triangle-free graphs. Namely, if G does not contain a triangle, then the sets of neighbors of any two adjacent vertices u and v are disjoint, so that $d(u) + d(v) \leq n$. If we suppose that u has the maximum vertex degree $d(u) = \Delta$, then $d(v) \geq \delta$, so that $\Delta + \delta \leq n$. Hence Corollary 3 is applicable to non-singular triangle-free graphs as well.

We can tweak the Gutman's bound (3) in a few ways. For example, we may assume that we know upfront the number of positive and negative eigenvalues of a non-singular graph G. Suppose that

$$\lambda_1 \geq \cdots \geq \lambda_k > 0 > \lambda_{k+1} \geq \cdots \geq \lambda_n.$$

From $\mathrm{Tr}(A) = 0 = (\lambda_1 + \cdots + \lambda_k) + (\lambda_{k+1} + \cdots + \lambda_n)$, we have

$$\frac{E(G)}{2} = \lambda_1 + \cdots + \lambda_k = |\lambda_{k+1}| + \cdots + |\lambda_n|.$$

Applying the arithmetic-geometric mean inequality separately to the first and the second sum above, we get

$$\frac{E(G)}{2} \geq k \sqrt[k]{\lambda_1 \cdots \lambda_k} \qquad \text{and} \qquad \frac{E(G)}{2} \geq (n-k) \sqrt[n-k]{|\lambda_{k+1}| \cdots |\lambda_n|}.$$

Then

$$\frac{E(G)^k E(G)^{n-k}}{2^n} \geq k^k (n-k)^{n-k} \lambda_1 \cdots \lambda_k |\lambda_{k+1}| \cdots |\lambda_n|,$$

so that after taking the n-th root, we obtain

$$E(G) \geq 2 \sqrt[n]{k^k (n-k)^{n-k}} \sqrt[n]{|\det(A)|}. \tag{4}$$

The minimum of $\sqrt[n]{k^k (n-k)^{n-k}}$ is obtained for $k = n/2$, in which case (4) reduces to the Gutman's lower bound $E(G) \geq n \sqrt[n]{|\det(A)|}$. However, if we know that, say, the number of positive eigenvalues k is much smaller than n, i.e., $k = o(n)$, then

$$\lim_{n \to \infty} \frac{\sqrt[n]{k^k (n-k)^{n-k}}}{n} = 1.$$

In such case, we have that for each $\varepsilon > 0$, there exists n_0 such that for all $n \geq n_0$, we obtain

$$E(G) \geq 2n(1-\varepsilon) \sqrt[n]{|\det(A)|} \geq 2n(1-\varepsilon),$$

that satisfies Conjecture 1, unless both Δ and δ are too close to n.

On the other hand, discarding λ_1 when applying the arithmetic-geometric mean inequality in the Gutman's lower bound (3) leads to:

$$|\lambda_2| + \cdots + |\lambda_n| \geq (n-1) \sqrt[n-1]{|\lambda_2| \cdots |\lambda_n|} = (n-1) \sqrt[n-1]{|\det(A)|/\lambda_1}.$$

This inequality leads us to the following proposition.

Proposition 4 *If G is a non-singular graph, then $E(G) \geq \lambda_1 + (n-1) \sqrt[n-1]{|\det(A)|/\lambda_1}$.*

This proposition leads to another case when Conjecture 1 holds.

Corollary 5 *If G is a non-singular graph with $|\det(A)| \geq \lambda_1$, then $E(G) \geq \Delta + \delta$.*

The assumption $|\det(A)| \geq \lambda_1$ (as well as a relaxed condition $|\det(A)| \geq n-1$) yields $\sqrt[n-1]{|\det(A)|/\lambda_1} \geq 1$, so that from Proposition 4 we have $E(G) \geq \lambda_1 + (n-1) \geq \Delta + \delta$.

Small graphs with up to nine vertices have been classified according to the values of the determinants of their adjacency matrices by Abdollahi in [1]. From the table in [1, Proposition 2.5] we can see, for example, that only 12.7% of all non-singular graphs on eight vertices and only 16.6% of all non-singular graphs on nine vertices satisfy $|\det(A)| \geq n-1$. Hence even if it turns out that this percentage continues to grow with increasing numbers of vertices, it may very well be expected that it will be far from covering all non-singular graphs.

On the other hand, Deift and Tomei [9] proved that $\det(A) \in \{-1, 0, +1\}$ for any simply connected, finite subgraph G of the lattice $\mathbb{Z} \times \mathbb{Z}$. By [9], the vertex $v \in \mathbb{Z} \times \mathbb{Z}$ is *not enclosed* by G if, for any integer n, there exists a sequence of distinct vertices $v_0, v_1, \dots, v_n$, where $v_0 = v$, $v_i \notin G$, and each segment $v_i v_{i+1}$ is either a horizontal or vertical line of (Euclidean) length one, or a diagonal line of (Euclidean) length $\sqrt{2}$. Then, G is *simply connected* in $\mathbb{Z} \times \mathbb{Z}$ if each vertex $v \notin G$ is not enclosed by G. Particular cases of such graphs are polyominos (finite, 2-connected plane graphs, with each interior face a quadrangle) whose inner dual is a tree. For nonsingular polyominos we have $|\det(A)| = 1$, so that for these graphs we have

$$|\lambda_2| \cdots |\lambda_n| = \frac{1}{\lambda_1}.$$

Building upon the results of Deift and Tomei [9], Huang and Yan [14] provided further examples of plane graphs with $\det(A) \in \{-1, 0, +1\}$.

As a short digression and a quick excursion into the graphs satisfying $|\det(A)| = 1$, we prove here a slight improvement of the McClelland's upper bound [17] $E(G) \leq \sqrt{2mn}$ for such graphs.

Proposition 6 *If G is a graph with $|\det(A)| = 1$, then*

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

Proof. Assume for the purpose of this proof that the eigenvalues of A are now ordered by their absolute values:

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n| > 0.$$

The inequality (5) is equivalent to

$$(E(G)-1)^2 \leq (2m-1)(n-1),$$

which is equivalent to

$$(|\lambda_1|+|\lambda_2|+\ldots+|\lambda_n|-1)^2 \leq (n-1)(\lambda_1^2+\lambda_2^2+\ldots+\lambda_n^2-1),$$

because $2m = \mathrm{Tr}(A^2) = \sum_{i=1}^{n} \lambda_i^2$.

Since $|\det(A)| = 1$, we have $|\lambda_1| \geq 1 \geq |\lambda_n|$, so that we can set $\mu_1 = \sqrt{\lambda_1^2+\lambda_n^2-1}$. The inequality between arithmetic and quadratic means applied to $|\mu_1|, |\lambda_2|, \ldots, |\lambda_{n-1}|$ yields

$$(|\mu_1|+|\lambda_2|+\ldots+|\lambda_{n-1}|)^2 \leq (n-1)(\mu_1^2+\lambda_2^2+\ldots+\lambda_{n-1}^2) = (n-1)(\lambda_1^2+\lambda_2^2+\ldots+\lambda_n^2-1).$$

It remains to show that $|\lambda_1|+|\lambda_n|-1 \leq \mu_1$, i.e., $(|\lambda_1|+|\lambda_n|-1)^2 \leq \lambda_1^2+\lambda_n^2-1$. But this is equivalent to $(|\lambda_1|-1)(|\lambda_n|-1) \leq 0$, which holds because of $|\lambda_1| \geq 1 \geq |\lambda_n|$. ■

It is easy to verify that the bound (5) is slightly stronger than the McClelland's bound $E(G) \leq \sqrt{2mn}$. Squaring the inequality

$$1+\sqrt{(2m-1)(n-1)} \leq \sqrt{2mn}$$

we conclude that it is equivalent to $2\sqrt{(2m-1)(n-1)} \leq (2m-1)+(n-1)$, which is correct by the arithmetic-geometric mean inequality.

Back to discussing Conjecture 1, we can obtain corollaries analogous to Corollaries 3 and 5 from other familiar lower bounds on energy. Consider, for example, the McClelland's lower bound [17]:

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

In the case of non-singular graphs with $|\det(A)| \geq 1$, the McClelland's bound reduces to

$$E(G) \geq \sqrt{2m+n(n-1)}.$$

Hence we have the following corollary.

Corollary 7 *If G is a non-singular graph with $2m+n(n-1) \geq (\Delta+\delta)^2$, then $E(G) \geq \Delta+\delta$.*

However, one should note that many graphs actually satisfy the opposite inequality $2m + n(n-1) < (\Delta+\delta)^2$. Prominent examples of such graphs are the complete graphs K_n for which $m = n(n-1)/2$ and $\Delta = \delta = n-1$, so that whenever $n \geq 3$, we have

$$2m + n(n-1) = 2n(n-1) < 4(n-1)^2 = (\Delta+\delta)^2.$$

Das, Mojallal, and Gutman [8] provided another lower bound on energy of non-singular graphs:

$$E(G) \geq \frac{2m}{n} + n - 1 + \ln|\det(A)| - \ln\frac{2m}{n}. \tag{6}$$

Within their proof, they relied on the monotonicity of the function $f(x) = x - 1 - \ln x$ for $x \geq 1$, and their interim result is as follows

$$E(G) \geq \lambda_1 + n - 1 + \ln|\det(A)| - \ln\lambda_1. \tag{7}$$

Since $\ln|\det(A)| \geq 0$ and $n-1 \geq \Delta$, this further reduces to $E(G) \geq \lambda_1 - \ln\lambda_1 + \Delta$. Hence we obtain the following corollary.

Corollary 8 *If G is a non-singular graph with $\lambda_1 - \ln\lambda_1 \geq \delta$, then $E(G) \geq \Delta + \delta$.*

Since $\lambda_1 \geq \bar{d} = \frac{2m}{n}$, a more relaxed condition for this corollary to be valid is when δ is sufficiently smaller than the average vertex degree $\frac{2m}{n}$, i.e., if $\frac{2m}{n} - \ln\frac{2m}{n} \geq \delta$. However, we note that there exist nonsingular graphs for which

$$\Delta + \delta > \lambda_1 + n - 1 + \ln|\det(A)| - \ln\lambda_1,$$

so that neither Corollary 8 nor the lower bound (7) implies Conjecture 1 for them. One example of such a graph is shown in Fig. 1.

It is worth mentioning here that the lower bound (6) was further improved both by Das and Gutman [7] and by Andrade et al. [3]. However, the expressions obtained in [3,7] do not lend themselves to easy corollaries that would imply the validity of Conjecture 1, so we skip them here.

Another case in which Conjecture 1 holds can be obtained from Proposition 4 by using the condition $|\det(A)| \geq 1$ for non-singular graphs. In such a case, Proposition 4 implies

$$E(G) \geq \lambda_1 + \frac{n-1}{\sqrt[n-1]{\lambda_1}},$$

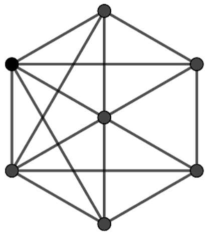

Figure 1. A non-singular graph with $\Delta + \delta > \lambda_1 + n - 1 + \ln|\det(A)| - \ln\lambda_1$. It has $\Delta = 6$, $\delta = 4$, and its adjacency eigenvalues are $[4.6619, 0.8019, 0.2124, -0.5550, -1.2240, -1.6502, -2.2470]$, so that $\det(A) = 2$, while $E(G) \approx 11.3524$.

so that Conjecture 1 holds if $\dfrac{n-1}{\sqrt[n-1]{\lambda_1}} \geq \Delta$, i.e., if

$$\lambda_1 \leq \left(\frac{n-1}{\Delta}\right)^{n-1}. \tag{8}$$

Having in mind that $\lambda_1 \leq \Delta$ [5], the condition (8) necessarily holds if $\Delta \leq \left(\dfrac{n-1}{\Delta}\right)^{(n-1)}$, i.e., if

$$\Delta \leq (n-1)^{1-\frac{1}{n}}.$$

This gives rise to the following corollary.

Corollary 9 *If G is a non-singular graph with $\Delta \leq (n-1)^{1-\frac{1}{n}}$, then $E(G) \geq \Delta + \delta$.*

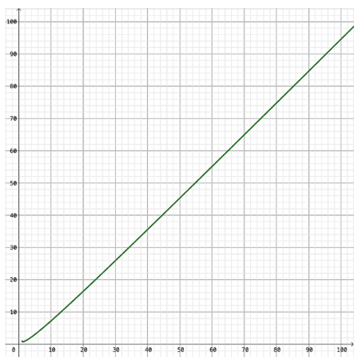

Figure 2. Graph of the function $f(n) = (n-1)^{1-\frac{1}{n}}$ for $1 \leq n \leq 100$.

This corollary covers a much larger spectrum of non-singular graphs, simply because

$$\lim_{n\to\infty} \frac{(n-1)^{1-\frac{1}{n}}}{n-1} = \lim_{n\to\infty} \frac{1}{\sqrt[n]{n-1}} = 1,$$

which is also clearly visible from the graph of $(n-1)^{1-\frac{1}{n}}$ depicted in Fig. 2. Hence the validity of Conjecture 1 remains to be studied only for non-singular graphs with high values of the maximum vertex degree Δ that satisfy

$$(n-1)^{1-\frac{1}{n}} < \Delta \leq n-1.$$

3 Conclusion

We have seen from the previous section that Conjecture 1 is valid for a number of non-singular graphs, in particular, for those that satisfy either $n \geq \Delta + \delta$ (Corollary 3) or $|\det(A)| \geq \lambda_1$ (Corollary 5) or $\sqrt{2m + n(n-1)} \geq \Delta + \delta$ (Corollary 7) or $\lambda_1 - \ln \lambda_1 \geq \delta$ (Corollary 8) or $\Delta \leq (n-1)^{1-\frac{1}{n}}$ (Corollary 9). While these corollaries cover the majority of small non-singular graphs, there exist non-singular graphs that do not satisfy either of these corollaries, yet they still satisfy $E(G) \geq \Delta + \delta$. In addition to the 7-vertex graph shown in Fig. 1, further examples of such graphs on 8 vertices are shown in Fig. 3.

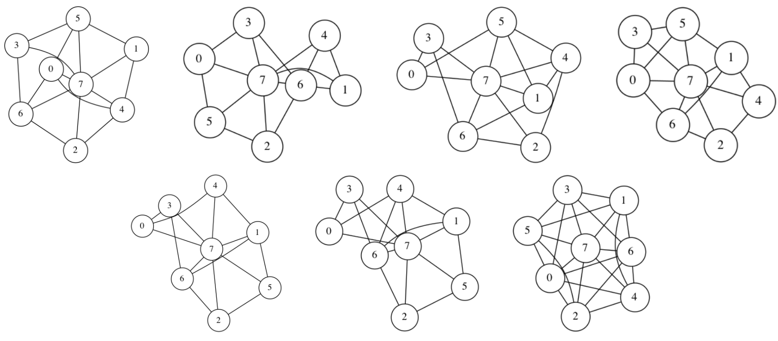

Figure 3. Examples of graphs on 8 vertices that satisfy Conjecture 1, but do not satisfy any of Corollaries 3, 5, 7, 8 and 9.

To conclude, the main problem with Conjecture 1 appears to be the absence of results in the literature which relate $\det(A)$, λ_1, and Δ for non-singular graphs. As a result, we cordially invite fellow researchers to investigate such relations.

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