MORE ON THE RELATION BETWEEN ENERGY
AND LAPLACIAN ENERGY OF GRAPHS

Dragan Stevanović\textsuperscript{a}, Ivan Stanković\textsuperscript{b}, Marko Milošević\textsuperscript{b}

\textsuperscript{a} PMF, University of Niš, Niš, Serbia and
FAMNIT/PINT, University of Primorska, Koper, Slovenia
e-mail: dragance106@yahoo.com

\textsuperscript{b} PMF, University of Niš, Niš, Serbia
e-mails: ivanstankovic76@gmail.com, ninja643@gmail.com

(Received January 30, 2008)

Abstract

I. Gutman et al. have recently conjectured that the energy of a graph does
not exceed its Laplacian energy. We disprove this conjecture by giving a few small
counterexamples and, in addition, an infinite set of counterexamples. Nevertheless,
we do show that the standard deviation of eigenvalues of the adjacency matrix of
every graph does not exceed the standard deviation of eigenvalues of its Laplacian
matrix.

1 Introduction

Let \( G = (V, E) \) be a finite, simple and undirected graph with vertices \( V = \{1, \ldots, n\} \) and
\( m = |E| \) edges. The degree of a vertex \( u \in V \) will be denoted by \( d_u \). Let \( G \) have the
adjacency matrix \( A \) with eigenvalues \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \), and the Laplacian matrix \( L \)
with eigenvalues \( \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0 \).

\textsuperscript{1}This work was supported by the research grant 144015G of the Serbian Ministry of Science and
Environmental Protection and the research program P1-0285 of the Slovenian Agency for Research.
These eigenvalues obey the following well-known relations:

\[
\sum_{i=1}^{n} \lambda_i = 0, \quad \sum_{i=1}^{n} \lambda_i^2 = 2m, \\
\sum_{i=1}^{n} \mu_i = 2m, \quad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2.
\]

Further details on the spectral graph theory can be found in [1].

The energy and the Laplacian energy of \(G\) are defined as follows

\[
E = E(G) = \sum_{i=1}^{n} |\lambda_i|, \quad LE = LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|.
\]

Having in mind that 0 is the average value of \(\lambda_1, \ldots, \lambda_n\), while \(\frac{2m}{n}\) is the average value of \(\mu_1, \ldots, \mu_n\), we may think of \(E(G)\) and \(LE(G)\) as the absolute deviation of corresponding eigenvalues.

The energy of a graph was defined by Ivan Gutman in [2] and it has a long known chemical applications; for details see the surveys [3, 4, 5]. Much work has appeared in the literature in the last decade, and, in particular, in this journal (see, for instance, [6]-[19]). On the other hand, the Laplacian energy has been recently defined in [20], with some further properties given in [21].

Ivan Gutman et al. have conjectured in [22] that \(E(G) \leq LE(G)\) holds for any graph. We have checked this conjecture on all connected graphs up to ten vertices, and we have found two counterexamples on 9 vertices and 115 counterexamples on 10 vertices. The two counterexamples on 9 vertices and the two counterexamples with fewest number of edges on 10 vertices are shown in Fig. 1. Note that the graphs on 10 vertices in this figure are chemical graphs as well.

2 A negative result

There is a simple infinite set of counterexamples. Let \(KK_n\) be the graph obtained from two copies of the complete graph \(K_n\) by joining a vertex from one copy of \(K_n\) to two vertices from the other copy of \(K_n\). For example, the graph \(KK_8\) is shown in Fig. 2. It turns out that \(KK_n\) is a counterexample for all other values of \(n \geq 9\) as well.

Proposition 1 \(E(KK_n) > LE(KK_n)\) for every \(n \geq 8\).
Proof. The adjacency matrix of $K K_n$ has an eigenvalue $-1$ with multiplicity $2n - 4$, and four simple eigenvalues $\lambda_1, \ldots, \lambda_4$ which are the roots of the characteristic polynomial of the obvious four-vertex divisor of $K K_n$ (see, e.g., [1, Chapter 4] to learn more about the concept of the divisor of a graph)

$$p(\lambda) = \lambda^4 - 2(n - 2)\lambda^3 + (n^2 - 6n + 4)\lambda^2 + 2(n^2 - n - 3)\lambda - (n^2 - 8n + 11).$$

Proposition may be verified directly for $n = 8$.

For $n \geq 9$, the following holds:

- $p(n) = n^2 + 2n - 11 > 0$
- $p(n - 1) = -4 < 0$
- $p(n - 2) = (n - 1)^2 > 0$
- $p(1) = 2(n^2 - n - 4) > 0$
- $p(0) = -n^2 + 8n - 11 < 0$
- $p(-2.2) = -0.56n^2 + 4.656n + 2.3936 < 0$
- $p(-3) = 2(n^2 + 7n + 8) > 0$
Therefore, $p(\lambda)$ has three positive roots, one in each of the intervals $(0, 1)$, $(n - 2, n - 1)$ and $(n - 1, n)$, and a single negative root in the interval $(-3, -2.2)$. We can assume $\lambda_1, \lambda_2, \lambda_3 > 0$ and $\lambda_4 < 0$. We have

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 2(n - 2),$$

and thus,

$$E(KK_n) = |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_4| + (2n - 4)| - 1|$$

$$= \lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 + 2n - 4$$

$$= 2(n - 2) - 2\lambda_4 + 2n - 4$$

$$> 4n - 3.6.$$

Similarly, the Laplacian matrix of $KK_n$ has an eigenvalue $n$ with multiplicity $2n - 5$, a simple eigenvalue $n + 1$, and four additional eigenvalues

$$0, n, (n + 3 + \sqrt{n^2 + 6n - 7})/2, (n + 3 - \sqrt{n^2 + 6n - 7})/2$$

which are the roots of the Laplacian characteristic polynomial of the divisor of $KK_n$ (see Theorem 4.7 and remark after Theorem 4.5 of [1])

$$\mu^4 - (2n + 3)\mu^3 + (n^2 + 3n + 4)\mu^2 - 4n\mu.$$ 

Since the average of these eigenvalues is $n - 1 + 2/n$, we obtain that for $n \geq 3$

$$LE(KK_n) = 3n - 7 + \frac{8}{n} + \sqrt{n^2 + 6n - 7}.$$ 

Then for $n \geq 9$ we have

$$E(KK_n) - LE(KK_n) > n + 3.4 - \frac{8}{n} - \sqrt{n^2 + 6n - 7} = g(n).$$
The first derivative of \( g(n) \) is positive for \( n \geq \frac{1}{2} \). Since further \( g(9) \approx 0.1974 > 0 \), we conclude that \( E(KK_n) > LE(KK_n) \) for all \( n \geq 9 \).

3 A positive result

Let us recall that the standard deviation \( \sigma \) of a set of data \( P = \{p_1, \ldots, p_n\} \), having average value \( p \), is defined as

\[
\sigma = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (p_i - p)^2}.
\]

While absolute deviations of adjacency and Laplacian eigenvalues of a graph turn out to be incomparable, their standard deviations behave in a much more predictable manner.

**Theorem 2** The standard deviation of the adjacency eigenvalues of any graph does not exceed the standard deviation of its Laplacian eigenvalues.

**Proof.** The statement of the theorem reduces to the inequality

\[
\sum_{i=1}^{n} \lambda_i^2 \leq \sum_{i=1}^{n} \left( \mu_i - \frac{2m}{n} \right)^2.
\]

On the left-hand side we have

\[
\sum_{i=1}^{n} \lambda_i^2 = 2m,
\]

while on the right-hand side we have

\[
\sum_{i=1}^{n} \left( \mu_i - \frac{2m}{n} \right)^2 = 2m + \sum_{i=1}^{n} d_i^2 - \frac{4m^2}{n}.
\]

Our theorem is now a consequence of the inequality \( 4m^2 \leq n \sum_{i=1}^{n} d_i^2 \), which is obtained by applying the Cauchy-Schwartz inequality to the vertex degree vector \((d_1, d_2, \ldots, d_n)\) and \((1, 1, \ldots, 1)\).

4 Conclusion

It is natural to expect that the standard deviation and the absolute deviation are relatively close to each other. Hence, if the standard deviation of Laplacian eigenvalues of a graph is much larger than the standard deviation of adjacency eigenvalues, then the Laplacian energy of a graph should be larger than its energy, as conjectured. Therefore, further
counterexamples for the conjectured inequality \( E(G) \leq LE(G) \) should be sought among graphs for which the value \( \sum_i d_i^2 - \frac{4m^2}{n} \) is rather small, or, in other words, among graphs that are almost regular. This is a common feature of all counterexamples presented here, and it was a starting point in our search for the structure of the infinite set of counterexamples using the system *newGRAPH* [23].

References


