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MORE ON THE RELATION BETWEEN ENERGY AND LAPLACIAN ENERGY OF GRAPHS[1]

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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 $V = \{1, \dots, n\}$ 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 $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$.

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These eigenvalues obey the following well-known relations:

$$\sum_{i=1}^{n} \lambda_i = 0, \qquad \sum_{i=1}^{n} \lambda_i^2 = 2m,$$

$$\sum_{i=1}^{n} \mu_i = 2m, \qquad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2.$$

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

The energy and the Laplacian energy of G are defined as follows

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|, \qquad LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

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.

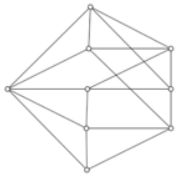
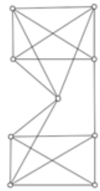
The energy of a graph was defined by Ivan Gutman in [2] and it has a long known chemical applications; for details see the surveys [3, 4, 5]. Much work has appeared in the literature in the last decade, and, in particular, in this journal (see, for instance, [6]-[19]). On the other hand, the Laplacian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

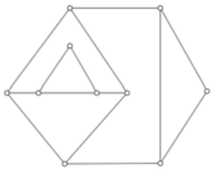
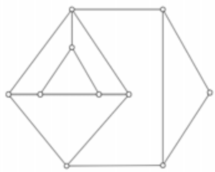
2 A negative result

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 $n \geq 8$.*

$E \approx 15.03468, LE \approx 14.97990$ $\quad$ $E \approx 15.22982, LE \approx 14.96961$

$E \approx 15.03045, LE \approx 14.76604$ $\quad$ $E \approx 15.18101, LE \approx 14.96204$

Figure 1: A few small counterexamples.

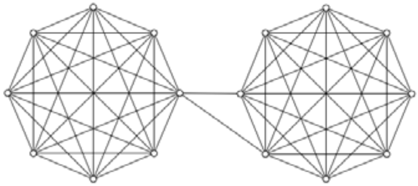
Proof. The adjacency matrix of KK_n has an eigenvalue -1 with multiplicity $2n-4$, and four simple eigenvalues $\lambda_1, \ldots, \lambda_4$ which are the roots of the characteristic polynomial of the obvious four-vertex divisor of KK_n (see, e.g., [1, Chapter 4] to learn more about the concept of the 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:

$$\begin{aligned}
p(n) &= n^2 + 2n - 11 > 0 \\
p(n-1) &= -4 < 0 \\
p(n-2) &= (n-1)^2 > 0 \\
p(1) &= 2(n^2 - n - 4) > 0 \\
p(0) &= -n^2 + 8n - 11 < 0 \\
p(-2.2) &= -0.56n^2 + 4.656n + 2.3936 < 0 \\
p(-3) &= 2(n^2 + 7n + 8) > 0
\end{aligned}$$



$E \approx 28.36128, LE \approx 28.24695$

Figure 2: Graph KK_8.

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,

$$\begin{aligned} E(KK_n) &= |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_4| + (2n-4)|-1| \\ &= \lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 + 2n - 4 \\ &= 2(n-2) - 2\lambda_4 + 2n - 4 \\ &> 4n - 3.6. \end{aligned}$$

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* σ 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

[1] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs—Theory and Application, 3rd edition, Johann Ambrosius Barth Verlag, 1995.

[2] I. Gutman, *The energy of a graph*, Ber. Math.–Statist. Sekt. Forschungsz. Graz 103 (1978) 1–22.

[3] I. Gutman, *Total π-electron energy of benzenoid hydrocarbons*, Topics Curr. Chem. 162 (1992) 29–63.

[4] I. Gutman, *The energy of a graph: old and new results*, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (eds.), Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 2001, pp. 196–211.

[5] I. Gutman, *Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology*, J. Serb. Chem. Soc. 70 (2005) 441–456.

[6] J.A. de la Peña, L. Mendoza, *Moments and π-electron energy of hexagonal systems in 3-space*, MATCH Commun. Math. Comput. Chem. 56 (2006) 113–129.

[7] B. Zhou, I. Gutman, J.A. de la Peña, J. Rada, L. Mendoza, *On spectral moments and energy of graphs*, MATCH Commun. Math. Comput. Chem. 57 (2007) 183–191.

[8] L. Ye, X. Yuan, *On the minimal energy of trees with a given number of pendent vertices*, MATCH Commun. Math. Comput. Chem. 57 (2007) 193–201.

[9] H.S. Ramane, H.B. Walikar, *Construction of equienergetic graphs*, MATCH Commun. Math. Comput. Chem. 57 (2007) 203–210.

[10] Y. Hou, Z. Teng, C. Woo, *On the spectral radius, k-degree and the upper bound of energy in a graph*, MATCH Commun. Math. Comput. Chem. 57 (2007) 341–350.

[11] M. Mateljević, I. Gutman, *Note on the Coulson and Coulson-Jacobs Integral Formulas*, MATCH Commun. Math. Comput. Chem. 59 (2008) 257–268.

[12] G. Indulal, A. Vijayakumar, *A Note on Energy of Some Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008) 269–274.

[13] J. Liu, B. Liu, *Note on a Pair of Equienergetic Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008) 275–278.

[14] H. Liu, M. Lu, *Sharp Bounds on the Spectral Radius and the Energy of Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008) 279–290.

[15] N. Li, S. Li, *On the Extremal Energies of Trees*, MATCH Commun. Math. Comput. Chem. 59 (2008) 291–314.

[16] I. Gutman, S. Radenković, N. Li, S. Li, *Extremal Energy Trees*, MATCH Commun. Math. Comput. Chem. 59 (2008) 315–320.

[17] Y. Yang, B. Zhou, *Minimal Energy of Bicyclic Graphs of a Given Diameter*, MATCH Commun. Math. Comput. Chem. 59 (2008) 321–342.

[18] Z. Liu, B. Zhou, *Minimal Energies of Bipartite Bicyclic Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008) 381–396.

[19] S. Li, X. Li, Z. Zhu, *On Tricyclic Graphs with Minimal Energy*, MATCH Commun. Math. Comput. Chem. 59 (2008) 397–419.

[20] I. Gutman, B. Zhou, *Laplacian energy of a graph*, Linear Algebra Appl. 414 (2006) 29–37.

[21] H. Wang, H. Hua, *Note on Laplacian Energy of Graphs*, MATCH Commun. Math. Comput. Chem. 59 (2008) 373–380.

[22] I. Gutman, N.M.M. de Abreu, C.T.M. Vinagre, A.S. Bonifácio, S. Radenković, *Relation between Energy and Laplacian Energy*, MATCH Commun. Math. Comput. Chem. 59 (2008) 343–354.

[23] D. Stevanović, V. Brankov, D. Cvetković, S. Simić, *newGRAPH*, a system for visualization and interactive modification of graphs and automatic recalculation of graph invariants, available for download from `http://www.mi.sanu.ac.yu/newgraph/`