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On the Conjecture Related to the Energy of Graphs with Self–Loops

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Abstract

Let G_σ be a graph obtained by attaching a self-loop, or just a loop, for short, at each of σ chosen vertices of a given graph G. Gutman et al. have recently introduced the concept of the energy of graphs with self-loops, and conjectured that the energy $E(G)$ of a graph G of order n is always strictly less than the energy $E(G_\sigma)$ of a corresponding graph G_σ, for $1 \leq \sigma \leq n-1$. In this paper, a simple set of graphs which disproves this conjecture is exposed, together with some remarks regarding the standard deviations of the (adjacency) eigenvalues of G and G_σ, respectively.

1 Introduction

Let $G = (V(G), E(G))$ be a simple graph on n vertices and m edges, where $V(G)$ stands for the set of vertices of G, while $E(G)$ is the set of its edges. The degree of a vertex $v \in V(G)$ will be denoted by $\deg(v)$, while for the maximum degree of G, the label $\Delta(G)$ will be used.

Let $A(G)$ be the *adjacency matrix* of G. The *characteristic polynomial* $P_G(x) = \det(xI - A(G))$ of G is the characteristic polynomial of its adjacency matrix $A(G)$. The *(adjacency) eigenvalues* $\lambda_1(G) \geq \cdots \geq \lambda_n(G)$

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of G are actually the eigenvalues of $A(G)$, and we say that they form the *(adjacency) spectrum* of G. The largest eigenvalue $\lambda_1(G)$ is usually called the *index* of G. If $\lambda_i(G)$, for some i, is the eigenvalue of the multiplicity k, we will write $[\lambda_i(G)]^k$. It is well known that $\sum_{i=1}^{n} \lambda_i(G) = 0$, while $\sum_{i=1}^{n} \lambda_i^2(G) = 2m$.

The *energy* $E(G)$ of G was defined by Ivan Gutman in [3]:

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

This graph invariant has been intensively studied in the last two decades, and plenty of research papers on this subject can be found in the literature in the field of applied mathematics and mathematical chemistry. For more details about graph energy, we refer the reader to the monographs [6] and [8], and the review papers [4] and [5].

Let us denote by G_σ a graph obtained by attaching a self-loop, or just a loop, for short, at each of σ chosen vertices of G. Precisely, if S is a subset of $V(G)$ whose cardinality is equal to σ, then G_σ is formed by adding a loop at each vertex from the set S. Notice that a loop at $v \in V(G)$ contributes to its degree in G_σ with 1.

The adjacency matrix $A(G_\sigma)$ of G_σ is of the form $A(G_\sigma) = A(G) + \mathcal{I}_\sigma$, where $\mathcal{I}_\sigma$ is the "almost" identity matrix, with exactly σ ones on the main diagonal and all other entries equal to zero. The non-zero entries correspond to the vertices with a loop attached from the set S. Since $A(G_\sigma)$ is a square and symmetric matrix, its (adjacency) eigenvalues $\lambda_1(G_\sigma) \geq \lambda_2(G_\sigma) \geq \cdots \geq \lambda_n(G_\sigma)$ are reals. In [7], it has been proved that $\sum_{i=1}^{n} \lambda_i(G_\sigma) = \sigma$ and $\sum_{i=1}^{n} \lambda_i^2(G_\sigma) = 2m + \sigma$.

Because of its importance and significance in chemistry, the energy $E(G_\sigma)$ of G_σ has been recently introduced in [7]:

$$E(G_\sigma) = \sum_{i=1}^{n} \left| \lambda_i(G_\sigma) - \frac{\sigma}{n} \right|.$$

It can be noticed that the average value of $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ is equal to 0, while the average value of $\lambda_1(G_\sigma), \lambda_2(G_\sigma), \ldots, \lambda_n(G_\sigma)$ is equal to $\frac{\sigma}{n}$, so $E(G)$ and $E(G_\sigma)$ can be interpreted as the *absolute deviation* of the corresponding eigenvalues. In that sense, the *standard deviation* Σ_G of the eigenvalues $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ is

$$\Sigma_G = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \lambda_i^2(G)} = \sqrt{\frac{2m}{n}}, \tag{1}$$

while the standard deviation Σ_{G_σ} of the eigenvalues $\lambda_1(G_\sigma), \ldots, \lambda_n(G_\sigma)$ is equal to:

$$\Sigma_{G_\sigma} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \left(\lambda_i(G_\sigma) - \frac{\sigma}{n}\right)^2} = \sqrt{\frac{1}{n}\left(2m + \sigma - \frac{\sigma^2}{n}\right)}. \tag{2}$$

In [7], some properties of $E(G_\sigma)$ are exposed, together with the following conjecture

Conjecture 1. *Let $G = (V(G), E(G))$ be a simple graph of order n, and let $S \subset V(G)$ be a subset of cardinality σ, where $1 \le \sigma \le n-1$. Then $E(G_\sigma) > E(G)$.*

In the section that follows, we give a simple set of graphs that disproves this conjecture.

The notation common for spectral graph theory is used in the paper. In that way, K_n is the complete graph on n vertices, while P_n is the n-vertex path. The graph $G \cup H$ means the *disjoint union* of the graphs G and H, while the *coalescence* $G \circ H$ of these two graphs, is a graph obtained from their disjoint union by identifying a vertex u of G with a vertex v of H. For the remaining terminology and additional details, the reader is referred to [1] and [2].

Below, we shall list some previously known results that will be needed in the next section.

Corollary 1 (Corollary 1.3.12. from [2]). *Let G be a graph with n vertices and eigenvalues $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$, and let H be an induced subgraph of G with m vertices. If the eigenvalues of H are $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_m$, then $\lambda_{n-m+i} \le \mu_i \le \lambda_i$, $i = 1, 2, \ldots, m$.*

Theorem 1 (Theorem 1.3.15. from [2]). *Let A and B be $n \times n$ Hermitian matrices. Then*

$$\lambda_i(A+B) \leq \lambda_j(A) + \lambda_{i-j+1}(B), n \geq i \geq j \geq 1; \quad (3)$$

$$\lambda_i(A+B) \geq \lambda_j(A) + \lambda_{i-j+n}(B), 1 \leq i \leq j \leq n. \quad (4)$$

Theorem 2 (Theorem 2.2.1. from [2]). *Let G_j denote the graph obtained from G by adding a pendant edge at the vertex j. Then*

$$P_{G_j}(x) = xP_G(x) - P_{G-j}(x).$$

Theorem 3 (Theorem 3.2.1. from [2]). *Let λ_1 be the index of the graph G, and let $\overline{d}$ and Δ be its average degree and maximum degree, respectively. Then*

$$\overline{d} \leq \lambda_1 \leq \Delta.$$

Moreover, $\overline{d} = \lambda_1$ if and only if G is regular. For a connected graph G, $\lambda_1 = \Delta$ if and only if G is regular.

2 A counterexample

Let $\mathcal{G} = K_n \circ K_2$ be the graph obtained by coalescing K_n, for $n \geq 4$, with K_2. Precisely, a vertex of K_n is identified with a vertex of K_2.

Lemma 1. *The adjacency spectrum of $\mathcal{G}$ consists of an eigenvalue -1 with multiplicity $n-2$, and three simple eigenvalues $\lambda_1 \in [n-1, n]$, $\lambda_2 \in (0,1)$ and $\lambda_3 \in (-2, -1.5)$.*

Proof. The characteristic polynomial of $\mathcal{G}$, according to Theorem 2, is:

$$\begin{aligned} P_{\mathcal{G}}(x) &= x\, P_{K_n}(x) - P_{K_{n-1}}(x) \\ &= x\,(x-n+1)\,(x+1)^{n-1} - (x-n+2)\,(x+1)^{n-2} \\ &= (x+1)^{n-2}\,(x^3 - (n-2)x^2 - nx + n - 2), \end{aligned}$$

wherefrom it is obvious that the spectrum of $\mathcal{G}$ has an eigenvalue -1 with multiplicity $n-2$.

Let us denote $r(x) = x^3 - (n-2)x^2 - nx + n - 2$, and let λ_1, λ_2 and λ_3 be the roots of the polynomial $r(x)$. For $n \geq 4$, the following holds:

$$\begin{aligned} &r(0) = n - 2 > 0; \\ &r(1) = -n + 1 < 0; \\ &r(-1.5) = 0.25\,n - 0.875 > 0; \\ &r(-2) = -n - 2 < 0. \end{aligned}$$

Therefore, the polynomial $r(x)$ has one positive root, say λ_2, in the interval $(0,1)$, and one negative root, say λ_3, in the interval $(-2,-1.5)$.

Since K_n is an induced subgraph of $\mathcal{G}$, from Corollary 1, we find that the largest eigenvalue of $\mathcal{G}$ must be greater than or equal to $n-1$, while from Theorem 3, we obtain that this eigenvalue is not greater than $\Delta(\mathcal{G}) = n$, i.e. $\lambda_1 = \lambda_1(\mathcal{G}) \in [n-1, n]$. ■

Let $\mathcal{G}_\sigma$ be the graph obtained by adding a loop at each vertex of $\mathcal{G}$, except at the vertex whose degree is equal to one. The graph $\mathcal{G}_\sigma$ for $n = 4$ is depicted in Figure 1. The adjacency matrix $A(\mathcal{G}_\sigma)$ of $\mathcal{G}_\sigma$ is of the following form

$$A(\mathcal{G}_\sigma) = \begin{pmatrix} J_n & M \\ M^T & 0 \end{pmatrix},$$

where J_n is the $n \times n$ all-ones matrix, while M denotes the vector (of appropriate size) whose all but one of the coordinates are equal to zero. Without loss of generality, we may assume that $M = (\underbrace{0, 0, \ldots, 0}_{n-1}, 1)^T$.

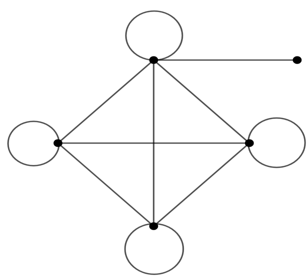

Figure 1. Graph $\mathcal{G}_\sigma$, where $\mathcal{G} = K_4 \circ K_2$

Lemma 2. *The adjacency spectrum of $\mathcal{G}_\sigma$ consists of an eigenvalue* 0, *whose multiplicity is* $n-2$, *and three simple eigenvalues* $\lambda_1^\sigma \in [n-1, n+1]$, $\lambda_2^\sigma \in \left(\frac{n}{n+1}, 1\right)$ *and* $\lambda_3^\sigma \in (-1, 0)$.

Proof. The adjacency matrix $A(\mathcal{G}_\sigma)$ of $\mathcal{G}_\sigma$ has $n-1$ identical rows, which means that $\operatorname{rank}(A(\mathcal{G}_\sigma)) \leq 3$, and therefore the characteristic polynomial $P_{\mathcal{G}_\sigma}(x)$ of $\mathcal{G}_\sigma$ has a factor x^{n-2}.

Let $V_1 = \{v \in V(\mathcal{G}_\sigma) : \deg(v) = 1\}$, $V_2 = \{v \in V(\mathcal{G}_\sigma) : \deg(v) = n+1\}$ and $V_3 = \{v \in V(\mathcal{G}_\sigma) : \deg(v) = n\}$. It is obvious that the partition $V(\mathcal{G}_\sigma) = V_1 \sqcup V_2 \sqcup V_3$, where $\sqcup$ stands for the disjoint union, is an equitable partition (for more details related to equitable partitions, as well as graph divisors, see Chapter 3 in [2] or Chapter 4 in [1]), with the following quotient matrix

$$Q = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & n-1 \\ 0 & 1 & n-1 \end{pmatrix}.$$

The characteristic polynomial $q(x)$ of Q equals: $q(x) = \det(xI - Q) = x^3 - nx^2 - x + n - 1$. Since $q(x)$ is a divisor of $P_{\mathcal{G}_\sigma}(x)$, we may conclude that the roots λ_1^σ, λ_2^σ and λ_3^σ of $q(x)$ are the remaining three eigenvalues of $\mathcal{G}_\sigma$.

For $n \geq 4$, we have

$$\begin{aligned}
&q(1) = -1 < 0;\\
&q\left(\frac{n}{n+1}\right) = \frac{n^3 - 2n^2 - 3n - 1}{(n+1)^3} > 0;\\
&q(0) = n - 1 > 0;\\
&q(-1) = -1 < 0.
\end{aligned}$$

Therefore, the polynomial $q(x)$ has one positive root, say λ_2^σ, in the interval $\left(\frac{n}{n+1}, 1\right)$, and one negative root, say λ_3^σ, in the interval $(-1, 0)$.

Let us apply Theorem 1 to the matrices $A(\mathcal{G})$ and $\mathcal{I}_\sigma$, where $A(\mathcal{G})$ is the adjacency matrix of $\mathcal{G}$, while $\mathcal{I}_\sigma$ is the $(n+1) \times (n+1)$ "almost" identity matrix, with n diagonal entries equal to 1. Given the previous, we may assume that

$$\mathcal{I}_\sigma = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

By setting $i = j = 1$ in (3) and (4), we obtain $\lambda_1(\mathcal{G}) \leq \lambda_1(\mathcal{G}_\sigma) \leq \lambda_1(\mathcal{G})+1$, i.e. $\lambda_1^\sigma \in [n-1, n+1]$. ∎

Proposition 4. *For every $n \geq 3$, $E(\mathcal{G}) > E(\mathcal{G}_\sigma)$.*

Proof. For $n = 3$, by direct computation, we find that the spectrum of $\mathcal{G}$ is: 2.17, 0.31, -1, -1.48, while the spectrum of $\mathcal{G}_\sigma$ consists of the following eigenvalues: 3.11, 0.75, 0, -0.86. Therefore, $4.96 = E(\mathcal{G}) > E(\mathcal{G}_\sigma) = 4.72$.

Using Lemma 1, and the fact $\sum\limits_{i=1}^{n+1} \lambda_i(\mathcal{G}) = 0$, i.e. $\lambda_1 + \lambda_2 + \lambda_3 = n-2$, for $n \geq 4$, we calculate

$$\begin{aligned} E(\mathcal{G}) &= \lambda_1 + \lambda_2 - \lambda_3 + n - 2 \\ &= 2(n-2) - 2\lambda_3 \\ &> 2n - 1. \end{aligned}$$

By using Lemma 2, since $\sum\limits_{i=1}^{n+1} \lambda_i(\mathcal{G}_\sigma) = n$, i.e. $\lambda_1^\sigma + \lambda_2^\sigma + \lambda_3^\sigma = n$, for $n \geq 4$, we compute

$$\begin{aligned} E(\mathcal{G}_\sigma) &= \lambda_1^\sigma + \lambda_2^\sigma - \lambda_3^\sigma + \frac{n\,(n-3)}{n+1} \\ &= n - 2\lambda_3^\sigma + \frac{n\,(n-3)}{n+1} \\ &< n + 2 + \frac{n\,(n-3)}{n+1}. \end{aligned}$$

For $n \geq 4$, $2n-1 > n+2+\frac{n\,(n-3)}{n+1}$. Indeed, this inequality is equivalent to

$$(2n-1)(n+1) > (n+2)(n+1) + n(n-3),$$

i.e. $n > 3$. Therefore,

$$E(\mathcal{G}) > 2n-1 > n+2+\frac{n(n-3)}{n+1} > E(\mathcal{G}_\sigma).$$

■

3 Concluding remarks

Considering the given counterexample, the absolute deviations of the adjacency eigenvalues of G and G_σ, respectively, do not seem to be comparable. But, in a similar way as it is elaborated in [9], from (1) and (2), and using the fact that the function $f(\sigma) = \sigma - \frac{\sigma^2}{n}$ is non-negative and concave in the interval $[0, n]$, we obtain that the standard deviations of the adjacency eigenvalues of G and G_σ, respectively, satisfy the following inequality:

Proposition 5. *The standard deviation of the adjacency eigenvalues of an arbitrary graph G is not greater than the standard deviation of the adjacency eigenvalues of the corresponding graph G_σ, i.e. $\Sigma_G \leq \Sigma_{G_\sigma}$.*

In order to possibly find some more counterexamples for the conjectured inequality $E(G_\sigma) > E(G)$, n-vertex graphs G_σ for which the value of $f(\sigma)$ is small, i.e. n-vertex graphs G with $\sigma = 1$ or $\sigma = n-1$ loops attached, as in the exposed example, should be considered. However, it is interesting to mention that the conjectured inequality will not be valid even for large values of $f(\sigma)$, for example if $\sigma = [\frac{n}{2}]$. Indeed, let us consider the graph $\mathcal{H} = K_6 \circ P_7$ and the graph $\mathcal{H}_\sigma$, presented in Figure 2, which is obtained by attaching a loop at all vertices of $\mathcal{H}$ whose degree is equal to 5 and 6. The spectrum of $\mathcal{H}$ consists of the following eigenvalues: 5.04, 1.82, 1.31, 0.58, -0.23, $[-1]^5$, -1.59, -1.92, while the adjacency eigenvalues of $\mathcal{H}_\sigma$ are: 6.03, 1.83, 1.38, 0.73, $[0]^5$, -0.74, -1.39, -1.84. Therefore, $17.49 = E(\mathcal{H}) > E(\mathcal{H}_\sigma) = 15.94$.

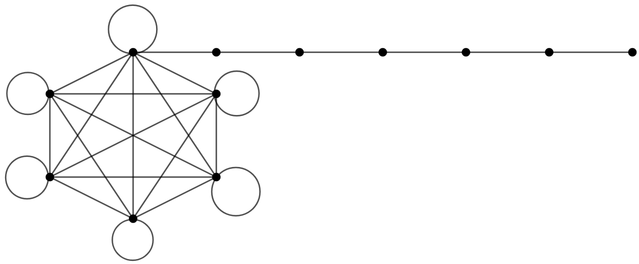

Figure 2. Graph $\mathcal{H}_\sigma$, where $\mathcal{H} = K_6 \circ P_7$

It is worth mentioning that according to some computational results,

$$E(K_n \circ P_m) > E((K_n \circ P_m)_\sigma),$$

for $n \geq 3$ and $m > 2$, where $(K_n \circ P_m)_\sigma$ is the graph obtained by adding a loop at all vertices of $K_n \circ P_m$ whose degree is equal to $n - 1$ and n.

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