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SHARPENING MILOVANOVIĆS' RELATIONS BETWEEN ENERGY AND DETERMINANT OF ADJACENCY MATRIX OF GRAPHS

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A b s t r a c t. The energy *of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. I. Milovanović, E. Milovanović et al.* [*Discr. Math. Algorithms Appl.* **11**(1) (2019) #1950001] *established several inequalities relating the graph energy to the determinant of the adjacency matrix. We now sharpen the proofs and formulations of some key results from that work.*

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In memory of Igor Milovanović, colleague and friend

1. *Introduction*

Let $G = (V, E)$ be a simple, undirected graph with vertex set

$$V = \{v_1, v_2, \dots, v_n\}$$

and edge set $E = E(G)$. The order and size of G are denoted by $|V(G)| = n$ and $|E(G)| = m$, respectively. Two vertices v_i and v_j are *adjacent* if the edge v_iv_j belongs to $E(G)$, which we denote by $v_iv_j \in E(G)$. The *degree* of a vertex v, written as d_v, is defined as $d_v = |N(v)|$, where $N(v)$ denotes the open neighborhood of v. The maximum and minimum degree of G are Δ and δ, respectively.

We adhere to standard graph-theoretic notation: K_n, $\overline{K}_n$, C_n, and P_n denote the complete graph, the complement of the complete graph (edgeless graph), the cycle graph, and the path graph on n vertices, respectively.

The *adjacency matrix* $A = A(G)$ of G is the $n \times n$ symmetric matrix defined by entries $a_{ij} = 1$ if $v_i v_j \in E(G)$, and $a_{ij} = 0$ otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of A. Furthermore, let the distinct absolute values of the non-zero eigenvalues be ordered as $|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*|$.

The following relations hold for the determinant of the adjacency matrix and its non-zero eigenvalues:

$$|\det A| = \prod_{i=1}^{n} |\lambda_i| \quad \text{and} \quad DA^* = \prod_{i=1}^{s} |\mu_i^*|$$

where, of course, DA^* is no determinant whatsoever, and is necessarily positive-valued.

The *energy* of a graph G is defined in terms of the eigenvalues of its adjacency matrix as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{i=1}^{s} |\mu_i^*| \,. \tag{1.1}$$

This concept was introduced by one of the present authors within an approximation of the total π-electron energy of conjugated hydrocarbons [3, 5, 7, 11]. Since its inception, graph energy has developed into a significant topic of research in spectral graph theory and found numerous, quite surprising applications; for comprehensive surveys and key results, we refer the reader to [4, 7–11].

2. *Preliminaries*

In this section, we present several lemmas that will be instrumental in the subsequent analysis. We begin by recalling two inequalities for sequences of real numbers.

Lemma 2.1 ([2]). *Let $a_1 \geq a_2 \geq \cdots \geq a_n > 0$ be a sequence of positive real numbers. Then*

$$\sum_{i=1}^{n} a_i \geq n \left(\prod_{i=1}^{n} a_i \right)^{1/n} + \left(\sqrt{a_1} - \sqrt{a_n}\right)^2 . \tag{2.1}$$

Equality holds in (2.1) if and only if $a_2 = a_3 = \cdots = a_{n-1} = \sqrt{a_1 a_n}$.

Lemma 2.2 ([1]). *Let* $\mathbf{a} = (a_i)$ *and* $\mathbf{b} = (b_i)$, $i = 1, 2, \ldots, n$, *be two sequences of positive real numbers satisfying*

$$0 < r_1 \le a_i \le R_1 < +\infty \quad \textit{and} \quad 0 < r_2 \le b_i \le R_2 < +\infty.$$

Then the following inequality holds:

$$\left| n \sum_{i=1}^{n} a_i\, b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \alpha(n)(R_1 - r_1)(R_2 - r_2), \tag{2.2}$$

where

$$\alpha(n) = n \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \right).$$

Lemma 2.3 ([17]). *Let* $a_1 \ge a_2 \ge \cdots \ge a_n > 0$ *be a sequence of positive real numbers. Then*

$$\left(\sum_{i=1}^{n} \sqrt{a_i} \right)^2 \le (n-1) \sum_{i=1}^{n} a_i + n \left(\prod_{i=1}^{n} \sqrt{a_i} \right)^{1/n}. \tag{2.3}$$

Equality holds in (2.3) if and only if $a_1 = a_2 = \cdots = a_n$.

3. *Sharpening Some Milovanovićs' Results*

The research group of Igor and Emina Milovanović published scores of papers on various graph energies, including several concerned with the energy of the adjacency matrix [6, 12–16]. To our knowledge, only in a single paper [15], they examined the relations between graph energy and the determinant of the adjacency matrix.

In this section, we comment and sharpen several results of the paper [15].

In [15], the authors denote by $|\lambda_1^*| \ge |\lambda_2^*| \ge \cdots \ge |\lambda_n^*|$ the absolute values of the eigenvalues of a graph G, arranged in non-increasing order. Their first result on graph energy is stated as follows.

Theorem 3.1 ([15]). *Let* G *be a simple graph with* $n \ge 2$ *vertices. Then*

$$\left(\sqrt{|\lambda_1^*|} - \sqrt{|\lambda_n^*|} \right)^2 \le \mathcal{E}(G) - n\left(|\det A|\right)^{1/n} \le n^2\, \alpha(n) \left(\sqrt{|\lambda_1^*|} - \sqrt{|\lambda_n^*|} \right)^2.$$

The equalities hold if $G \cong \frac{n}{2} K_2$ *(for even* n*) or* $G \cong \overline{K}_n$.

Remark 3.1. The proof of Theorem 3.1 in [15] contains several imprecise applications of Lemmas 2.1, 2.2, and 2.3. The issues are as follows.

First, the authors set $a_i = b_i = \sqrt{|\lambda_i^*|}$ for $i = 1, 2, \ldots, n$ in inequality (2.2). Consider the cycle graph C_4, whose spectrum is $\{2, -2, 0, 0\}$. Then $\sqrt{|\lambda_1^*|} =$

$\sqrt{|\lambda_2^*|} = \sqrt{2}$ and $\sqrt{|\lambda_3^*|} = \sqrt{|\lambda_4^*|} = 0$. For inequality (2.2), this yields $R_1 = R_2 = \sqrt{2}$ and $r_1 = r_2 = 0$, which violates the condition $0 < r_1, r_2$ required by Lemma 2.2.

Second, setting $a_i = |\lambda_i^*|$ in inequality (2.3) leads to a similar contradiction for C_4, as $a_1 = a_2 = 2$ and $a_3 = a_4 = 0$, again violating the positivity condition.

Third, the same issue arises when applying inequality (2.1) with $a_i = |\lambda_i^*|$.

Analogous counterexamples can be constructed for other graphs, including odd paths P_n ($n \geq 3$), star graphs S_n, and complete bipartite graphs $K_{n,m}$, demonstrating that the inequalities are not applicable as used.

Moreover, the characterization of extremal graphs is incorrect. For $G \cong \overline{K}_n$, all eigenvalues are zero. Equality in (2.3) requires $a_1 = a_2 = \cdots = a_n > 0$, while equality in (2.1) requires $a_2 = \cdots = a_{n-1} = \sqrt{a_1 a_n} > 0$. Both conditions are violated when all eigenvalues are zero.

We now present a corrected version of Theorem 3.1. The proof follows a similar structure but replaces the absolute values of the eigenvalues $|\lambda_i^*|$ with the absolute values of the non-zero eigenvalues $|\mu_i^*|$, and uses DA^* instead of $|\det A|$. Consequently, the proof is omitted.

Theorem 3.2. *Let G be a simple graph with $n \geq s \geq 2$ vertices, and let*

$$|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*|\,,\ (s \leq n),$$

be the absolute values of the non-zero eigenvalues of G. Then

$$\left(\sqrt{|\mu_1^*|} - \sqrt{|\mu_s^*|}\right)^2 \leq \mathcal{E}(G) - s\,(DA^*)^{1/s} \leq s^2\,\alpha(s)\left(\sqrt{|\mu_1^*|} - \sqrt{|\mu_s^*|}\right)^2.$$

Equality holds if $G \cong \frac{s}{2}K_2$ (for even s).

Another result from [15] is the following:

Theorem 3.3 ([15]). *Let G be a simple graph of order $n \geq 3$ without isolated vertices. For any real number γ satisfying $\gamma \geq \lambda_1$, it holds that*

$$\mathcal{E}(G) \geq \gamma + (n-1)\left(\frac{|\det A|}{\gamma}\right)^{\frac{1}{n-1}} + (n-1)^2\,\alpha(n-1)\left(\sqrt{|\mu_2^*|} - \sqrt{|\mu_n^*|}\right)^2. \quad (3.1)$$

Remark 3.2. The proof of Theorem 3.3 in [15] is not precise enough. The authors set $n := n-1$, $a_i = \sqrt{|\lambda_{i+1}^*|}$ for $i = 1, 2, \ldots, n-1$, and take $R_1 = R_2 = \sqrt{|\lambda_2^*|}$, $r_1 = r_2 = \sqrt{|\lambda_n^*|}$ in inequality (2.2). For the path graph P_5 with spectrum $\{\pm\sqrt{3}, \pm 1, 0\}$, we have $\sqrt{|\lambda_2^*|} = \sqrt[4]{3}$, $\sqrt{|\lambda_3^*|} = \sqrt{|\lambda_4^*|} = 1$, and $\sqrt{|\lambda_5^*|} = 0$. This gives $R_1 = R_2 = \sqrt[4]{3}$ and $r_1 = r_2 = 0$, contradicting the positivity condition of Lemma 2.2.

Furthermore, the proof considers the function

$$f(x) = x + (n-1)\left(\frac{|\det A|}{x}\right)^{\frac{1}{n-1}}$$

and claims that it is increasing for $|\mu_1^*| \geq x \geq (|\det A|)^{\frac{1}{n}}$. However, for graphs like P_5, $|\det A| = 0$, making $f(x)$ undefined at $x = 0$.

The corrected version of Theorem 3.3 is given below. The proof is analogous but uses non-zero eigenvalues and DA^* instead of $|\det A|$.

Theorem 3.4. *Let G be a simple graph of order ≥ 3 without isolated vertices, and let*

$$|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*| \quad (s \leq n)$$

be the absolute values of the non-zero eigenvalues of G. For any real number γ satisfying $\gamma \geq \lambda_1 = |\mu_1^*|$, it holds that

$$\mathcal{E}(G) \geq \gamma + (s-1)\left(\frac{DA^*}{\gamma}\right)^{\frac{1}{s-1}} + (s-1)^2\,\alpha(s-1)\left(\sqrt{|\mu_2^*|} - \sqrt{|\mu_s^*|}\right)^2. \quad (3.2)$$

The following result is also stated in [15].

Theorem 3.5 ([15]). *Let G be a simple graph of order $n \geq 3$ without isolated vertices. For any real number k satisfying*

$$\lambda_1 \geq k \geq (|\det A|)^{\frac{1}{n-1}},$$

it holds that

$$\mathcal{E}(G) \geq k + (n-1)\left(\frac{|\det A|}{k}\right)^{\frac{1}{n-1}} + \left(\sqrt{|\lambda_2^*|} - \sqrt{|\lambda_n^*|}\right)^2. \quad (3.3)$$

Remark 3.3. *In the proof of Theorem 3.5, Lemma 2.1 is imprecisely applied. Setting $n := n-1$ and $a_i = |\lambda_{i+1}^*|$ for $i = 1, 2, \ldots, n-1$, leads to a violation of the positivity condition for graphs like P_5, where $|\lambda_2^*| = \sqrt{3}$, $|\lambda_3^*| = |\lambda_4^*| = 1$, and $|\lambda_5^*| = 0$.*

We now present an improved version of Theorem 3.5.

Theorem 3.6. *Let G be a simple graph of order $n \geq s \geq 3$ without isolated vertices, and let*

$$|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*| \quad (s \leq n),$$

be the absolute values of the non-zero eigenvalues of G. For any real number k, satisfying $\lambda_1 \geq k \geq (DA^*)^{\frac{1}{s-1}}$, it holds that

$$\mathcal{E}(G) \geq k + (s-1)\left(\frac{DA^*}{k}\right)^{\frac{1}{s-1}} + \left(\sqrt{|\mu_2^*|} - \sqrt{|\mu_s^*|}\right)^2.$$

The next two results from [15] pertain to bipartite graphs.

Theorem 3.7 ([15]). *Let G be a simple bipartite graph of order $n \geq 4$ without isolated vertices. For any real number γ satisfying $\gamma \geq \lambda_1$, it holds that*

$$\begin{aligned}\mathcal{E}(G) \geq & 2\gamma + (n-2)\left(\frac{|\det A|}{\gamma^2}\right)^{\frac{1}{n-2}} \\ & + (n-2)^2\,\alpha(n-2)\left(\sqrt{|\lambda_3^*|} - \sqrt{|\lambda_n^*|}\right)^2 . \end{aligned} \tag{3.4}$$

Theorem 3.8 ([15]). *Let G be a simple bipartite graph of order $n \geq 4$ without isolated vertices. For any real number k satisfying $\lambda_1 \geq k \geq (|\det A|)^{\frac{1}{n}}$, it holds that*

$$\mathcal{E}(G) \geq 2k + (n-2)\left(\frac{|\det A|}{k^2}\right)^{\frac{1}{n-2}} + \left(\sqrt{|\lambda_3^*|} - \sqrt{|\lambda_n^*|}\right)^2 .$$

Using arguments similar to those in Remarks 3.1 and 3.2, it can be shown that the sharpened version of Theorems 3.7 and 3.8 read as follows:

Theorem 3.9. *Let G be a simple bipartite graph of order $n \geq s \geq 4$ without isolated vertices, and let*

$$|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*| \quad (s \leq n),$$

be same as before. For any real number γ, satisfying $\gamma \geq \lambda_1 = |\mu_1^*|$, it holds that

$$\mathcal{E}(G) \geq 2\gamma + (s-2)\left(\frac{DA^*}{\gamma^2}\right)^{\frac{1}{s-2}} + (s-2)^2\,\alpha(s-2)\left(\sqrt{|\mu_3^*|} - \sqrt{|\mu_s^*|}\right)^2 .$$

Theorem 3.10. *Let G be a simple bipartite graph of order $n \geq s \geq 4$ without isolated vertices, and let*

$$|\mu_1^*| \geq |\mu_2^*| \geq \cdots \geq |\mu_s^*| \quad (s \leq n),$$

be same as before. For any real number k, satisfying $|\mu_1^*| = \lambda_1 \geq k \geq (DA^*)^{\frac{1}{s}}$, it holds that

$$\mathcal{E}(G) \geq 2k + (s-2)\left(\frac{DA^*}{k^2}\right)^{\frac{1}{s-2}} + \left(\sqrt{|\mu_3^*|} - \sqrt{|\mu_s^*|}\right)^2 .$$

4. *Concluding Remarks*

All the results reported in the paper [15] are correct if the underlying graph is non-singular, i.e., if all its eigenvalues are non-zero. In the case of singular graphs, the above indicated amendments are needed.

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