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From Ultimate Energy to Graph Energies

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Abstract

A lower bound is given for the ultimate energy, which is applicable to all graph energies. The extremal characterization is provided for the energy and Laplacian energy when the graph is connected.

1 Introduction

Let $\mathbf{x} = (x_1, \dots, x_n)$ be an arbitrary n-tuple of real numbers, and let $\overline{x}$ be their arithmetic mean, where n is a positive integer. Then the ultimate energy associated with $\mathbf{x}$ is defined as

$$UE = UE(\mathbf{x}) = \sum_{i=1}^{n} |x_i - \overline{x}|.$$

UE was defined by Gutman [3] without any relation to a graph, to a matrix, or even to a polynomial.

We consider simple graphs. Let G be a graph of order n with vertex set $V(G)$. Let $M(G)$ be an $n \times n$ real symmetric matrix associated to G. Let $\lambda_1(M) \geq \cdots \geq \lambda_n(M)$ be the eigenvalues of $M(G)$. Then the M-energy of G is defined as $UE((\lambda_1(M), \dots, \lambda_n(M)))$. For $u, v \in V(G)$, $u \sim v$ means

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that u and v are adjacent in G. The adjacency matrix of G is the $n \times n$ symmetric matrix $A(G) = (a_{uv})_{u,v \in V(G)}$, where

$$a_{uv} = \begin{cases} 1 & \text{if } u \sim v, \\ 0 & \text{otherwise.} \end{cases}$$

The spectrum of G is the spectrum of $A(G)$. Denote by $\rho_1 \geq \cdots \geq \rho_n$ the eigenvalues of G. For $u \in V(G)$, denote by $d_G(u)$ the degree of u in G. The Laplacian matrix of G is the $n \times n$ symmetric matrix $L(G) = (\ell_{uv})_{u,v \in V(G)}$, where

$$\ell_{uv} = \begin{cases} d_u & \text{if } u = v, \\ -1 & \text{if } u \sim v, \\ 0 & \text{otherwise.} \end{cases}$$

The Laplacian matrix of a graph is positive semi-definite. The Laplacian spectrum of a graph G is just the spectrum of $L(G)$. Denote by $\mu_1 \geq \cdots \geq \mu_n$ the Laplacian eigenvalues of G. It is known that $\mu_n = 0$. The energy of a graph G, denoted by $E(G)$, is defined as the A-energy of G, see [7]. That is,

$$E(G) = \sum_{k=1}^{n} |\rho_k|.$$

The Laplacian energy of G, denoted by $LE(G)$, is defined as the L-energy of G, see [5]. That is,

$$LE(G) = \sum_{i=1}^{n} |\mu_i - d|,$$

where d is the average degree of G, i.e., $d = \frac{2m}{n}$ with $m = |E(G)|$. Both energy and Laplacian energy have been studied extensively, see Gutman and Furtula [4].

Denote by $\mathrm{Var}(\mathbf{x})$ the variance of the numbers $x_1, \ldots, x_n$ and by $P(x)$ the polynomial $\prod_{i=1}^{n}(x - x_i)$. Gutman established the following bounds for UE,

$$\sqrt{n\mathrm{Var}(\mathbf{x}) + n(n-1)|P(\overline{x})|^{2/n}} \le UE(\mathbf{x}) \le \sqrt{n(n-1)\mathrm{Var}(\mathbf{x}) + n|P(\overline{x})|^{2/n}},$$

which then hold for any other energy as well.

In this paper, we give a lower on UE, its special forms for energy and Laplacian energy are known. However, there is no complete characterization for connected graphs that attain the respective bound. We fill this gap by giving a complete characterization.

2 Preliminaries

We need some lemmas in the proofs.

Lemma 1. *[11] A connected graph has exactly one positive eigenvalue if and only if it is a complete multipartite graph.*

Denote by $K_{n_1,\dots,n_s}$ the complete s-partite graph whose partite sizes are $n_1,\dots,n_s$, where $s \ge 2$. It is easy to see that there are exactly s different rows in $A(K_{n_1,\dots,n_s})$, so its rank is s. Thus, if $n > s$, then 0 is a A-eigenvalue of $K_{n_1,\dots,n_s}$ with multiplicity $n-s$. This follows also from the characteristic polynomial of $K_{n_1,\dots,n_s}$ given in [1].

Lemma 2. *[1, Interlacing Theorem for Complete Multipartite Graphs] Suppose that $G = K_{n_1,\dots,n_s}$ with $s \ge 2$ and $\sum_{k=1}^{s} n_k = n$.*

(i) G has exactly $s-1$ negative integers $\rho_{n-s+2},\dots,\rho_n$ such that

$$n_1 \le -\rho_{n-s+2} \le n_2 \le -\rho_{n-s+3} \le n_3 \le \cdots \le n_{s-1} \le -\rho_n \le n_s$$

(ii) If the sequence $n_1,\dots,n_s$ contains t different numbers $n_1 = p_1 < \cdots < p_t$, then G has a negative eigenvalue in each of the internals of $(p_1,p_2),\dots,(p_{t-1},p_t)$.

Lemma 3. *[8] Let G be a connected graph with diameter D. Suppose that G has exactly k distinct Laplacian eigenvalues. Then $D+1 \le k$.*

Lemma 4. *[2, 8] Let G be a graph of order n with minimum degree δ. If G is not a complete graph, then $\mu_{n-1} \leq \delta$.*

3 A lower bound for ultimate energy

The inequality in the following lemma has been given in the book [10, p. 346], but it was not mentioned when the equality holds there. For completeness, we give a proof here.

Lemma 5. *If $y_1, \ldots, y_n$ are real numbers such that*

$$\sum_{k=1}^{n} |y_k| = 1 \text{ and } \sum_{k=1}^{n} y_k = 0,$$

then for real numbers $a_1, \ldots, a_n$,

$$\left|\sum_{k=1}^{n} a_k y_k\right| \leq \frac{1}{2}\left(\max_{1\leq i\leq n} a_k - \min_{1\leq i\leq n} a_k\right) \tag{1}$$

with equality if and only if $a_k = \max_{1\leq i\leq n} a_i, \min_{1\leq i\leq n} a_i$ whenever $y_k \neq 0$.

Proof. Assume that $a_1 \geq \cdots \geq a_n$. As $\sum_{k=1}^{n} y_k = 0$, one has

$$\left|\sum_{k=1}^{n} a_k y_k\right| = \frac{1}{2}\left|\sum_{k=1}^{n}(2a_k - a_1 - a_n)y_k\right| \leq \frac{1}{2}\sum_{k=1}^{n}|2a_k - a_1 - a_n||y_k|$$

with equality if and only if $(2a_k - a_1 - a_n)y_k$ and $(2a_j - a_1 - a_n)y_j$ have the same sign for all k and j with $1 \leq k < j \leq n$. As $a_n \leq a_k \leq a_1$, we have $|2a_k - a_1 - a_n| \leq a_1 - a_n$ with equality if and only if $a_k = a_1$ or $a_k = a_n$. As $\sum_{k=1}^{n} |y_k| = 1$, one has

$$\left|\sum_{k=1}^{n} a_k y_k\right| \leq \frac{1}{2}\sum_{k=1}^{n}(a_1 - a_n)|y_k| = \frac{1}{2}(a_1 - a_n)$$

with equality if and only if $a_k = a_1$ or $a_k = a_n$ whenever $y_k \neq 0$, and $(2a_k - a_1 - a_n)y_k$ and $(2a_j - a_1 - a_n)y_j$ have the same sign whenever

$y_k, y_j \neq 0$ with $1 \leq k < j \leq n$. Note that if $a_k = a_1$ or $a_k = a_n$ whenever $y_k \neq 0$, then $2a_k - a_1 - a_n = a_1 - a_n, a_n - a_1$, so $(2a_k - a_1 - a_n)y_k$ and $(2a_j - a_1 - a_n)y_j$ have the same sign whenever $y_k, y_j \neq 0$ with $1 \leq k < j \leq n$. Thus, (1) follows and equality holds in (1) if and only if $a_k = a_1$ or $a_k = a_n$ whenever $y_k \neq 0$ with $2 \leq k \leq n-1$. ■

Theorem 1. *Let* $\mathbf{x} = (x_1, \ldots, x_n)$*, where not all* $x_1, \ldots, x_n$ *are equal. Then*

$$UE(\mathbf{x}) \geq \frac{2n\,Var(\mathbf{x})}{\max_{1\leq k\leq n} x_k - \min_{1\leq k\leq n} x_k}, \tag{2}$$

with equality if and only if $x_k = \max_{1\leq i\leq n} x_i$ *when* $x_k > \overline{x}$ *and* $x_k = \min_{1\leq i\leq n} x_i$ *when* $x_k < \overline{x}$.

Proof. For $k = 1, \ldots, n$, let $a_k = x_k - \overline{x}$. Then $UE(\mathbf{x}) = \sum_{k=1}^n |a_k|$. Now, for $k = 1, \ldots, n$, let $y_k = \frac{a_k}{UE(\mathbf{x})}$. Note that

$$\sum_{k=1}^n |y_k| = 1 \text{ and } \sum_{k=1}^n y_k = 0.$$

By Lemma 5,

$$\sum_{k=1}^n (x_k - \overline{x})\frac{x_k - \overline{x}}{UE(\mathbf{x})} \leq \frac{1}{2}\left(\max_{1\leq k\leq n} x_k - \min_{1\leq k\leq n} x_k\right),$$

or

$$\begin{aligned} UE(\mathbf{x}) &\geq \frac{2\sum_{k=1}^n (x_k - \overline{x})^2}{\max_{1\leq k\leq n} x_k - \min_{1\leq k\leq n} x_k} \\ &= \frac{2n\mathrm{Var}(\mathbf{x})}{\max_{1\leq k\leq n} x_k - \min_{1\leq k\leq n} x_k}, \end{aligned}$$

so (2) follows and equality holds if and only if $x_k = \max_{1\leq i\leq n} x_i$ when $x_k > \overline{x}$ and $x_k = \min_{1\leq i\leq n} x_i$ when $x_k < \overline{x}$. ■

4 Lower bounds for energy

Apply Theorem 1 to the energy of a graph, we have

Theorem 2. *Let G be a graph on n vertices with $m \geq 1$ edges. Then*

$$E(G) \geq \frac{4m}{\rho_1 - \rho_n} \tag{3}$$

with equality when G is connected if and only if G is a complete bipartite graph or a regular complete multipartite graph.

Inequality (3) was recently reported in [6], where a sufficient condition (i.e. G is a complete graph or a regular complete bipartite graph) is given for which the equality is attained. Here, a different proof is given with a complete characterization of the equality when G is connected.

Proof of Theorem 2. By Theorem 1,

$$E(G) \geq \frac{2\sum_{k=1}^{n} \rho_k^2}{\rho_1 - \rho_n} = \frac{4m}{\rho_1 - \rho_n}$$

with equality if and only if

$$\rho_k = \rho_1 \text{ if } \rho_k > 0 \tag{4}$$

and

$$\rho_k = \rho_n \text{ if } \rho_k < 0. \tag{5}$$

Suppose that G is connected.

Suppose that the equality holds in (3). Then, by Perron-Frobenius theorem, ρ_1 is simple. From (4), G possesses exactly one positive eigenvalue, so G is a complete s-partite graph for some s with $2 \leq s \leq n$ by Lemma 1.

If $s = n$, then G is regular. Suppose that $3 \leq s \leq n-1$. It follows from (5) that all negative eigenvalues are equal. So G possesses exactly three distinct eigenvalues, apart from the largest eigenvalue and 0 of multiplicity $n - s$, the $s - 1$ negative eigenvalues $\rho_{n-s+2}, \ldots, \rho_n$ are all equal, which we denote by ρ. Assume that $G = K_{n_1,\ldots,n_s}$, where $n_1 \leq \cdots \leq n_s$ and $n = \sum_{k=1}^{s} n_k$. By Lemma 2(i),

$$n_1 \leq -\rho \leq n_2 \leq -\rho \leq n_3 \leq \cdots \leq n_{s-1} \leq -\rho \leq n_s. \tag{6}$$

If $n_i < n_{i+1}$ for $i = 1$ or $i = s - 1$, then Lemma 2(ii) implies there is an eigenvalue in the interval (n_i, n_{i+1}), contradicting (6). Therefore, $n_1 = n_2$, $n_{s-1} = n_s$ and from (6), $n_1 = \cdots = n_s$. That is, G is regular.

Conversely, suppose that G is a complete bipartite graph or a regular complete s-partite graph with $s \geq 3$. If G is a complete bipartite graph, then $\rho_1 = -\rho_n$ and $\rho_i = 0$ for $i = 2, \ldots, n-1$, so we have (4) and (5), implying that equality holds in (3). Suppose that G is a regular complete s-partite graph with $s \geq 3$. Then the largest eigenvalue of G is the degree of any vertex, that is $n - \frac{n}{s}$, and 0 is an eigenvalue of G with multiplicity $n - s$, and the least eigenvalue of G is $-\frac{n-\frac{n}{s}}{s-1} = -\frac{n}{s}$ of multiplicity $s - 1$. Thus, (4) and (5) hold, so (3) becomes an equality. ■

Theorem 3. *Let G be a bipartite graph on n vertices with m edges, where $n \geq 4$ and $m \geq 1$. Suppose that $\rho_2 > 0$. Then*

$$E(G) \geq 2\rho_1 + \frac{2m - \rho_1^2}{\rho_2} \tag{7}$$

with equality when G is connected if and only if G has four or five distinct eigenvalues.

Proof. Note that $E(G) = 2\rho_1 + \sum_{k=2}^{n-1} |\rho_k|$. For $k = 2, \ldots, n-1$, let $y_k = \frac{\rho_k}{E(G) - 2\rho_1}$. Then

$$\sum_{k=2}^{n-1} |y_k| = 1 \text{ and } \sum_{k=2}^{n-1} y_k = 0.$$

By Theorem 1,

$$E(G) \geq 2\rho_1 + \frac{2m - \rho_1^2}{\rho_2}$$

with equality if and only if $\rho_k = \rho_2$ when $\rho_k > 0$ with $k \geq 2$ and $\rho_k = -\rho_2$ when $\rho_k < 0$ with $k \leq n-1$.

If G is connected, then $\rho_1 > \rho_2$, so equality holds in (7) if and only if G has four or five distinct eigenvalues. ■

5 Lower bounds for Laplacian energy

The (first) Zagreb index of a graph G is defined as $Z(G) = \sum_{u \in V(G)} d_G^2(u)$. Apply Theorem 1 to the Laplacian energy of a graph, we have

Theorem 4. *Let G be a graph with n vertices and $m \geq 1$ edges. Then*

$$LE(G) \geq \frac{2}{\mu_1}\left(Z(G) + 2m - \frac{4m^2}{n}\right) \tag{8}$$

with equality when G is connected if and only if G is a regular complete multipartite graph.

Inequality (8) has been already given by Milovanović et al. [9], where it was pointed out that equality holds if G is a complete graph or a regular complete bipartite graph. For completeness, a proof is included with a characterization for the equality case when G is connected.

Proof of Theorem 4. By Theorem 1, (8) follows and equality holds in (8) if and only if $\mu_k = \mu_1$ if $\mu_k > \frac{2m}{n}$ and $\mu_k = \mu_n$ if $\mu_k < \frac{2m}{n}$.

Suppose that G is connected. Then $\mu_{n-1} > \mu_n = 0$.

Suppose that the equality holds in (8). If $\frac{2m}{n}$ is not a Laplacian eigenvalue of G, then G has exactly two distinct Laplacian eigenvalues μ_1 and 0, so we have by Lemma 3 that G is a complete graph. Suppose that $\frac{2m}{n}$ is a Laplacian eigenvalue of G. Then G is not a complete graph and $\mu_{n-1} = \frac{2m}{n}$. By Lemma 4, G is regular of degree $\rho_1 = \frac{2m}{n}$. The Laplacian eigenvalues are

$$\rho_1 - \rho_n \geq \cdots \geq \rho_1 - \rho_2 > \rho_1 - \rho_1 = 0.$$

So $\rho_1 - \rho_2 = \frac{2m}{n}$, i.e., $\rho_2 = 0$. By Lemma 1, G is a complete s-partite graph with $2 \leq s \leq n-1$.

Conversely, suppose that G is a regular complete multipartite graph. If G is a complete graph, then $\mu_k = n$ for $k = 1, \ldots, n-1$, so equality holds in (8). Otherwise, G is a complete s-partite graph for some s with $2 \leq s \leq n-1$. As G is regular, its spectrum consists ρ_1, 0 with multiplicity $n-s$, and a negative eigenvalue say a with multiplicity $s-1$. So $\mu_k = \rho - a$

for $k = 1, \ldots, s-1$ and $\mu_k = \rho_1$ for $k = s, \ldots, n-1$. Thus, equality holds in (8). ■

For a graph G with n vertices, it is known that $\mu_1 \le n$ with equality if and only if the complement of G is not connected. So from Theorem 4 we arrive at the following conclusion: If G a graph with n vertices and $m \ge 1$ edges, then

$$LE(G) \ge \frac{2}{n}\left(Z(G) + 2m - \frac{4m^2}{n}\right)$$

with equality when G is connected if and only if G is a regular complete multipartite graph.

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