

Extremal Energies of Weighted Trees and Forests with Fixed Total Weight Sum

Jia-Yu Shao^{a*}, Fei Gong^{b†} and Zhi-bin Du^{c‡}

Department of Mathematics, Tongji University,
Shanghai, 200092, P. R. China

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Abstract

Let $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$ be, respectively, the set of positively weighted trees and forests, of order n with a (fixed) total weight sum K . In this paper we determine the minimal energy together with the unique extremal weighted graph achieving the minimal energy for both the classes $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$. We also determine the maximal energy together with all extremal weighted graphs achieving the maximal energy for the class $\mathcal{F}_{n,K}$, and show that there does not exist weighted graphs in the class $\mathcal{T}_{n,K}$ having the largest energy. Some related problems are also considered.

1 Introduction

Let A be a real matrix of order n and $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A . Then the energy of A , denoted by $\mathbb{E}(A)$, is defined as $\mathbb{E}(A) = \sum_{i=1}^n |\lambda_i|$. The energy of a graph

^{a*}jyshao@tongji.edu.cn. Research supported by National Natural Science Foundation of China 10731040

[†]gfmichelle@hotmail.com

[‡]zhibindu@126.com

G is defined to be the energy of its adjacency matrix [5]. For details of the theory of graph energy see the reviews [5, 7], the recent paper [10, 11, 13–18] and the references cited therein.

Nikiforov [12] first pointed out that the energy of the graph is equal to the sum of the singular values of its adjacency matrix. Let M be an $m \times n$ real matrix. Then MM^T is a positive semi-definite matrix of order m . If we denote the eigenvalues of MM^T by $\sigma_1^2, \dots, \sigma_m^2$ with $\sigma_i \geq 0$ for $i = 1, \dots, m$, then $\sigma_1, \dots, \sigma_m$ are called the singular values of the matrix M . For convenience, we call the sum $\sigma_1 + \dots + \sigma_m$ as the singular energy of M , denoted by $\sigma(M)$.

It is easy to see that if A is a real symmetric matrix with eigenvalues $\lambda_1, \dots, \lambda_n$, then $AA^T = A^2$ has eigenvalues $\lambda_1^2, \dots, \lambda_n^2$, and thus the singular values of A are just the absolute values of the eigenvalues of A . Consequently, the energy of A is the same as the singular energy of A , namely we have $\mathbb{E}(A) = \sigma(A)$ for real symmetric matrix A .

An (edge)-weighted graph is a graph G each of whose edges has a nonzero weight. In other words, there is a weight function w from the edge set $E(G)$ of G to the set of nonzero real numbers. Such weighted graph is usually denoted by (G, w) .

The (weighted) adjacency matrix $A_w(G)$ of the weighted graph (G, w) of order n is defined as the matrix $A(G) = A_w(G) = (a_{ij})$ of order n with

$$a_{ij} = \begin{cases} w(e) & \text{if } ij \text{ is an edge } e \text{ of } G \\ 0 & \text{otherwise.} \end{cases}$$

Similar to the unweighted graphs, the energy of a weighted graph (G, w) (sometimes simply denoted by G) is defined to be the energy of its (weighted) adjacency matrix $A(G)$ [9]. Since $A(G)$ is still a real symmetric matrix for weighted graph G , we see that the energy of G is also the same as the singular energy of $A(G)$. Namely, $\mathbb{E}(G) = \sigma(A(G))$ holds also for weighted graphs.

Lemma 1.1. *Let G be a graph and e be a cut edge of G with $G - e = G_1 \dot{\cup} G_2$. Let $H_1 = (G, w_1)$ and $H_2 = (G, w_2)$ be two weighted graphs on G such that $w_2(e) = -w_1(e)$, and they have the same weights on all other edges of G . Then we have $\mathbb{E}(H_1) = \mathbb{E}(H_2)$.*

Proof. By suitably ordering the vertices of G , we may write the weighted adjacency matrices of H_1 and H_2 as:

$$A(H_1) = \begin{pmatrix} A_1 & X \\ X^T & A_2 \end{pmatrix} \quad \text{and} \quad A(H_2) = \begin{pmatrix} A_1 & -X \\ -X^T & A_2 \end{pmatrix}$$

where A_i is the weighted adjacency matrix of G_i ($i = 1, 2$), and X contains exactly one nonzero entry corresponding to the cut edge e . Now it is easy to verify that

$$\begin{pmatrix} I_{n_1} & 0 \\ 0 & -I_{n_2} \end{pmatrix} \begin{pmatrix} A_1 & X \\ X^T & A_2 \end{pmatrix} \begin{pmatrix} I_{n_1} & 0 \\ 0 & -I_{n_2} \end{pmatrix}^{-1} = \begin{pmatrix} A_1 & -X \\ -X^T & A_2 \end{pmatrix}$$

which means that $A(H_1)$ and $A(H_2)$ are similar. Thus $A(H_1)$ and $A(H_2)$ have the same spectrum, and therefore $\mathbb{E}(H_1) = \mathbb{E}(H_2)$. \square

From Lemma 1.1 we can see that when we study the energy of weighted trees or forests (each of their edges is a cut edge), we can always assume that they are positively weighted.

Let $K > 0$ be a fixed number and n be a fixed positive integer. Let $\mathcal{T}_{n,K}$, and $\mathcal{F}_{n,K}$, be the set of positively weighted trees, and forests, of order n with the fixed total weight sum K , respectively. In this paper, we study the extremal energy together with the corresponding extremal weighted graphs for the classes $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$, and we will also study some further related problems.

In §3, we determine the minimal energy together with the unique extremal weighted graph achieving this minimal value for both the classes $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$. In §4, we use the continuity property of the energy as a function of the weights to prove that there do not exist weighted graphs in $\mathcal{T}_{n,K}$ (and $\mathcal{F}_{n,K}$) having the second smallest energy. In §5, we study the maximal energy problem. We determine the maximal energy together with all the extremal weighted graphs achieving this maximal value for the class $\mathcal{F}_{n,K}$, and also show that there do not exist weighted graphs in the class $\mathcal{T}_{n,K}$ having the maximal energy. We also answer the analogous maximal energy problems for the class of all weighted connected graphs of order n with the total weight sum K , as well as the class of all weighted graphs of order n with the total weight sum K .

2 The quasi order of weighted bipartite graphs

Lemma 2.1. [8] *Let G be a weighted bipartite graph on n vertices. Then its characteristic polynomial can be written as:*

$$\phi(G, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G, k) x^{n-2k} \tag{2.1}$$

where $b(G, k) \geq 0$ for all k .

From the Coulson integral formula for the energy of graphs [8], we can see that if G is a weighted bipartite graph with the characteristic polynomial as in (2.1), then:

$$\mathbb{E}(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{k=0}^{\lfloor n/2 \rfloor} b(G, k) x^{2k} \right) dx . \tag{2.2}$$

Formula (2.2) holds for both simple and weighted bipartite graphs. It is much used in the study of the energy of bipartite graphs (see [11] and the references cited therein).

It follows that $\mathbb{E}(G)$ is a strictly monotonically increasing function of those numbers $b(G, k)$ ($k = 0, 1, \dots, \lfloor \frac{n}{2} \rfloor$) for weighted bipartite graphs. Thus we can also define the quasi-ordering relation " \preceq " for weighted bipartite graphs as the following. (The analogous quasi ordering of simple graphs, first conceived in [4], is nowadays much used in the theory of graph energy, see [10,13-16,18] and the references cited therein.)

Let G_1 and G_2 be two weighted bipartite graphs of order n . If $b(G_1, k) \leq b(G_2, k)$ for all k with $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$, then we write $G_1 \preceq G_2$. (Note that $b(G, 0) = 1$ for all weighted bipartite graphs G). Furthermore, if $G_1 \preceq G_2$ and there exists at least one index j such that $b(G_1, j) < b(G_2, j)$, then we write $G_1 \prec G_2$. If $b(G_1, k) = b(G_2, k)$ for all k , we write $G_1 \approx G_2$.

According to the Coulson integral formula (2.2), we see that if G_1 and G_2 are two weighted bipartite graphs of order n , then $G_1 \preceq G_2$ implies $\mathbb{E}(G_1) \leq \mathbb{E}(G_2)$ and $G_1 \prec G_2$ implies $\mathbb{E}(G_1) < \mathbb{E}(G_2)$.

3 The minimal energy problems for $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$

Lemma 3.1. *Let G be a weighted bipartite graph. Then we have*

$$b(G, 1) = \sum_{e \in E(G)} w(e)^2 .$$

Proof. By the symmetry of the spectrum of G with respect to the origin, we see that the characteristic polynomial of G can be written as

$$\phi(G, \lambda) = \lambda^{n-2r}(\lambda^2 - c_1) \cdots (\lambda^2 - c_r) \quad (c_i > 0, i = 1, \dots, r) . \tag{3.1}$$

Thus in this form we have $b(G, 1) = \sum_{i=1}^r c_i$.

Let $\lambda_1, \dots, \lambda_n$ be all the eigenvalues of G . Then from (3.1) we also have

$$\text{tr}(A(G)^2) = \sum_{j=1}^n \lambda_j^2 = 2 \sum_{i=1}^r c_i = 2b(G, 1) . \tag{3.2}$$

On the other hand, since $A(G)$ is symmetric, we have

$$\text{tr}(A(G)^2) = \sum_{i=1}^n \sum_{j=1}^n a_{ij}^2 = 2 \sum_{e \in E(G)} w(e)^2 . \tag{3.3}$$

Comparing (3.2) and (3.3) we get the result. □

Lemma 3.2. *Let x_1, \dots, x_k and y_1, \dots, y_k be real numbers satisfying:*

(1) $x_1 + \cdots + x_k = y_1 + \cdots + y_k$

(2) $y_1 = \cdots = y_k$

(3) $(x_1, \dots, x_k) \neq (y_1, \dots, y_k)$.

Then $x_1^2 + \cdots + x_k^2 > y_1^2 + \cdots + y_k^2$.

Proof. First we have

$$(x_1 + \cdots + x_k)^2 + \sum_{1 \leq i < j \leq k} (x_i - x_j)^2 = k(x_1^2 + \cdots + x_k^2) .$$

So

$$\begin{aligned} & k(x_1^2 + \cdots + x_k^2) - k(y_1^2 + \cdots + y_k^2) \\ &= \sum_{1 \leq i < j \leq k} (x_i - x_j)^2 - \sum_{1 \leq i < j \leq k} (y_i - y_j)^2 = \sum_{1 \leq i < j \leq k} (x_i - x_j)^2 > 0 . \end{aligned}$$

□

An equally weighted star S in $\mathcal{T}_{n,K}$ is a weighted star $S = (K_{1,n-1}, w)$ of order n each of whose edges has the weight $\frac{K}{n-1}$.

Lemma 3.3. *Let S be the equally weighted star in $\mathcal{T}_{n,K}$. Then $b(S, 1) = \frac{K^2}{n-1}$, and $b(S, k) = 0$ for all $k \geq 2$.*

Proof. First, by Lemma 3.1 we have $b(S, 1) = \sum_{e \in E(S)} w(e)^2 = \frac{K^2}{n-1}$.

Second, it is easy to see that the rank of the adjacency matrix $A(S)$ of S is 2. So S has $n - 2$ zero eigenvalues, and thus $b(S, k) = 0$ for all $k \geq 2$. □

Theorem 3.1. *Let S be the equally weighted star in $\mathcal{T}_{n,K}$, and T be any weighted tree in $\mathcal{T}_{n,K}$ with $T \neq S$ (as weighted graphs). Then $S \prec T$.*

Proof. First we always have $b(S, 0) = b(T, 0) = 1$. Also by Lemma 3.3 we have

$$b(S, k) = 0 \leq b(T, k) \quad (\text{for all } k \geq 2).$$

We now consider the case $k = 1$.

Case 1: T is not equally weighted.

Then by Lemma 3.1 and Lemma 3.2 we have

$$b(T, 1) = \sum_{e \in E(T)} w(e)^2 > \sum_{e \in E(S)} w(e)^2 = b(S, 1).$$

Thus we have $S \prec T$.

Case 2: T is equally weighted.

Then the underlying unweighted graph of T (say, denoted by H) is not a star.

By the well-known quasi-ordering fact for unweighted trees we have $K_{1,n-1} \prec H$, since H is not a star. It follows from this that $S \prec T$ since S and T are both equally weighted. □

It is not difficult to verify that the equally weighted star $S \in \mathcal{T}_{n,K}$ has the energy $\frac{2K}{\sqrt{n-1}}$.

Next we show that this S is also the unique weighted forest with the minimal energy in $\mathcal{F}_{n,K}$.

Theorem 3.2. *Let S be the equally weighted star in $\mathcal{T}_{n,K}$ and F be a weighted forest in $\mathcal{F}_{n,K}$. If $F \neq S$, then $\mathbb{E}(F) > \mathbb{E}(S)$.*

Proof. Case 1: F is connected (i.e., F is a tree). Then the result follows from Theorem 3.1.

Case 2: F is not connected. Suppose T_1, \dots, T_r ($r \geq 2$) are all the components of F , where T_i has order n_i and total weight sum K_i . Then $\sum_{i=1}^r n_i = n$ and $\sum_{i=1}^r K_i = K$.

Let S_i be the equally weighted star of order n_i with the total weight sum K_i , then by Theorem 3.1 we have $\mathbb{E}(S_i) \leq \mathbb{E}(T_i)$. Thus

$$\mathbb{E}(F) = \sum_{i=1}^r \mathbb{E}(T_i) \geq \sum_{i=1}^r \mathbb{E}(S_i) = \sum_{i=1}^r \frac{2K_i}{\sqrt{n_i - 1}} > \sum_{i=1}^r \frac{2K_i}{\sqrt{n - 1}} = \frac{2K}{\sqrt{n - 1}} = \mathbb{E}(S) .$$

□

4 The non-existence of the second smallest energy in $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$

The following inequality about the singular energy for the sum of two matrices is due to Ky Fan [3], for details see [17]:

Lemma 4.1. [3] (*The Ky Fan inequality*): *Suppose the matrices A, B, C satisfy $C = A + B$. Then*

$$\sigma(C) \leq \sigma(A) + \sigma(B) .$$

Equality holds if and only if there exists a unitary matrix P , such that both PA and PB are positive semi-definite.

The following lemma is a simple generalization of the Ky Fan inequality.

Lemma 4.2. (*a variation of Ky Fan inequality*): *Suppose the matrices A, B, C satisfy $C = A + B$. Then*

$$|\sigma(C) - \sigma(A)| \leq \sigma(B) . \tag{4.1}$$

Proof. $\sigma(C) - \sigma(A) \leq \sigma(B)$ is the Ky Fan inequality. On the other hand, we have $A = C + (-B)$, so

$$\sigma(A) \leq \sigma(C) + \sigma(-B) = \sigma(C) + \sigma(B)$$

which implies that $\sigma(C) - \sigma(A) \geq -\sigma(B)$. □

Using Lemma 4.2, we can show that $\mathbb{E}(G)$ is a continuous function of the weights of all edges (supposing that the weight of each edge is an independent variable).

Theorem 4.1. *Let G be a weighted graph with m edges e_1, \dots, e_m , where $w(e_i) = x_i$ ($i = 1, \dots, m$), and x_1, \dots, x_m are viewed as independent variables. Let $f(x_1, \dots, x_m) = \mathbb{E}(G)$. Then $f(x_1, \dots, x_m)$ is (multi-variables) continuous.*

Proof. Let $A(G(x_1, \dots, x_m))$ be the weighted adjacency matrix of G . Let G_e be the spanning (unweighted) subgraph of G containing a single edge e . Then we have:

$$A(G(x_1 + \Delta x_1, \dots, x_m + \Delta x_m)) - A(G(x_1, \dots, x_m)) = \sum_{i=1}^m \Delta x_i A(G_{e_i}) .$$

Thus from Lemma 4.2 and Ky Fan inequality we have:

$$\begin{aligned} & |f(x_1 + \Delta x_1, \dots, x_m + \Delta x_m) - f(x_1, \dots, x_m)| \\ &= |\sigma(A(G(x_1 + \Delta x_1, \dots, x_m + \Delta x_m))) - \sigma(A(G(x_1, \dots, x_m)))| \\ &\leq \sigma\left(\sum_{i=1}^m \Delta x_i A(G_{e_i})\right) \leq \sum_{i=1}^m \sigma(\Delta x_i A(G_{e_i})) = 2 \sum_{i=1}^m |\Delta x_i| . \end{aligned}$$

□

From Theorem 4.1 we have:

Theorem 4.2. *Let S be the equally weighted star in $\mathcal{T}_{n,K}$. For any $\varepsilon > 0$, there exists some weighted star $T \neq S$ of order n in $\mathcal{T}_{n,K}$ such that*

$$\mathbb{E}(S) < \mathbb{E}(T) < \mathbb{E}(S) + \varepsilon . \tag{4.2}$$

Proof. Take any two edges e_1 and e_2 of the star $K_{1,n-1}$, define weights $w(e_1) = \frac{K}{n-1} + \delta$ and $w(e_2) = \frac{K}{n-1} - \delta$, and $w(e) = \frac{K}{n-1}$ for all other edges of $K_{1,n-1}$. Take T to be such a weighted star. Then by the continuity of $\mathbb{E}(T)$ with respect to δ we see that T will satisfy (4.2) if $\delta > 0$ is sufficiently small. □

From Theorem 4.2 we can immediately see that among all weighted graphs in $\mathcal{T}_{n,K}$ (or in $\mathcal{F}_{n,K}$), there do not exist graphs with the second smallest energy.

5 The maximal energy problems for $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$

To study the maximal energy problems for $\mathcal{T}_{n,K}$ and $\mathcal{F}_{n,K}$, we first need the following matrix version of a result by Day and So [2, Theorem 2.6(i)]:

Lemma 5.1. [2] *Let A be a symmetric real matrix of the form $A = \begin{pmatrix} A_1 & X \\ X^T & A_2 \end{pmatrix}$, where A_1 is a non-singular square matrix. Let $B = \begin{pmatrix} O & X \\ X^T & A_2 \end{pmatrix}$. Then we have $\sigma(A) \leq \sigma(B) + \sigma(A_1)$, where equality holds if and only if $X = O$.*

From Lemma 5.1 we have:

Corollary 5.1. *Let G be a connected weighted graph of order $n \geq 3$, and e be an edge of G with $w(e) \neq 0$. Then $\mathbb{E}(G) < \mathbb{E}(G - e) + 2|w(e)|$.*

Proof. Without loss of generality, we may assume that $e = v_1v_2$. Then we can write $A(G)$ as:

$$A(G) = \begin{pmatrix} H & X \\ X^T & A_2 \end{pmatrix}$$

where $H = \begin{pmatrix} 0 & w(e) \\ w(e) & 0 \end{pmatrix}$ is non-singular since $w(e) \neq 0$, and $A(G - e) = \begin{pmatrix} O & X \\ X^T & A_2 \end{pmatrix}$. Since G is connected of order $n \geq 3$, we have $X \neq O$. Thus by Lemma 5.1 we have $\sigma(A(G)) < \sigma(A(G - e)) + \sigma(H)$ which is equivalent to (5.1). \square

Theorem 5.1. *Let G be a weighted graph of order n each of whose edges has nonzero weight, and e_1, \dots, e_m be all the edges of G . Then*

$$\mathbb{E}(G) \leq 2 \sum_{i=1}^m |w(e_i)|$$

where equality holds if and only if each connected component of G has at most two vertices.

Proof. Let G_e be the spanning (weighted) subgraph of G containing a single edge e . Then $A(G) = \sum_{i=1}^m A(G_{e_i})$. Thus by the Ky Fan inequality,

$$\mathbb{E}(G) = \sigma(A(G)) \leq \sum_{i=1}^m \sigma(A(G_{e_i})) = 2 \sum_{i=1}^m |w(e_i)| .$$

Next we prove the equality case. For sufficiency, let G_i be the component of G containing the (single) edge e_i . Then

$$\mathbb{E}(G) = \sum_{i=1}^m \mathbb{E}(G_i) = 2 \sum_{i=1}^m |w(e_i)| .$$

For the necessity part, suppose that some component H_1 of G contains at least three vertices (thus at least two edges). Assume that e_1 is an edge of H_1 , and H_2, \dots, H_r are all the other components of G . Then by Corollary 5.1 we have $\mathbb{E}(H_1) < \mathbb{E}(H_1 - e_1) + 2|w(e_1)|$, implying

$$\begin{aligned} \mathbb{E}(G) &= \sum_{i=2}^r \mathbb{E}(H_i) + \mathbb{E}(H_1) < \sum_{i=2}^r \mathbb{E}(H_i) + \mathbb{E}(H_1 - e_1) + 2|w(e_1)| \\ &= \mathbb{E}(G - e_1) + 2|w(e_1)| \leq 2 \sum_{i=2}^m |w(e_i)| + 2|w(e_1)| = 2 \sum_{i=1}^m |w(e_i)| . \end{aligned}$$

□

From Theorem 5.1 we have:

Theorem 5.2. *Let $n \geq 3$ and $K > 0$ be fixed. Let $\mathcal{C}_{n,K}$, and $\mathcal{G}_{n,K}$, be the set of all positively weighted connected graphs, and all positively weighted graphs, of order n with the total weight sum K , respectively. Then we have:*

(1) *A weighted graph G in $\mathcal{F}_{n,K}$, or in $\mathcal{G}_{n,K}$, has the maximal energy in $\mathcal{F}_{n,K}$, or in $\mathcal{G}_{n,K}$, if and only if each component of G is K_1 or K_2 . And the value of the maximal energy in $\mathcal{F}_{n,K}$, or in $\mathcal{G}_{n,K}$, is $2K$.*

(2) *There do not exist weighted graphs in $\mathcal{T}_{n,K}$ (or $\mathcal{C}_{n,K}$) having the maximal energy in $\mathcal{T}_{n,K}$ (or $\mathcal{C}_{n,K}$).*

Proof. We have now $\sum_{e \in E(G)} |w(e)| = \sum_{e \in E(G)} w(e) = K$.

(1) follows directly from Theorem 5.1.

For (2), from Theorem 5.1 and $n \geq 3$, we see that $\mathbb{E}(T) < 2K$ for all $T \in \mathcal{T}_{n,K}$ (or $\mathcal{C}_{n,K}$) since T is now connected of order $n \geq 3$. On the other hand, for each $\varepsilon > 0$, take sufficiently small $\delta > 0$ and take $T_\delta \in \mathcal{T}_{n,K}$ such that one edge of T_δ has weight $K - (m - 1)\delta$, and all the other $(m - 1)$ edges have weight δ . Then by the continuity of the energy function (Theorem 4.1), we have

$$2K - \varepsilon < \mathbb{E}(T_\delta) < 2K \quad (\text{if } \delta > 0 \text{ is sufficiently small}) .$$

This shows that no weighted graph in $\mathcal{T}_{n,K}$ (or $\mathcal{C}_{n,K}$) has the largest energy in $\mathcal{T}_{n,K}$ (or $\mathcal{C}_{n,K}$). \square

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