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Bounds for Energy of Matrices and Energy of Graphs

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Abstract

For any square complex matrix A the energy of A, denoted by $\mathcal{E}(A)$, is defined as the sum of the absolute values of the eigenvalues of A. In this paper we investigate the energy of matrices and find some bounds for $\mathcal{E}(A)$. As a consequence we obtain some bounds for energy of graphs.

1 Introduction

In this paper the matrices are complex and the graphs are simple (that is graphs are finite and undirected, without loops and multiple edges). The *conjugate transpose* of a complex matrix A is denoted by A^*. A *Hermitian* matrix (or *self-adjoint* matrix) is a complex square matrix that is equal to its own *conjugate transpose*. We note that when A is a real matrix, then A is Hermitian if and only if A is symmetric. It is well known that the eigenvalues of Hermitian matrices (in particular, the eigenvalues of real symmetric matrices) are real. A complex square matrix A is called *normal* if it commutes with its conjugate transpose, that is $AA^* = A^*A$. For example, every real symmetric matrix is normal. Let B be a square complex matrix. The *trace* and the *determinant* of B are denoted by $tr(B)$ and $det(B)$, respectively. The *energy* of B, denoted by $\mathcal{E}(B)$, is defined as the sum of the absolute values of its eigenvalues. In other words, if B is an $n \times n$ complex matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$, then

$$\mathcal{E}(B) = |\lambda_1| + \cdots + |\lambda_n|. \tag{1}$$

Nikiforov [9] defined the energy of any complex matrix A by considering the *singular values*. This definition of energy of matrices coincides with the previous definition of energy of matrices if and only if the matrix is normal [1].

Let $G = (V(G), E(G))$ be a simple graph. The *order* of G denotes the number of vertices of G. For a vertex v of G, the *degree* of v is the number of edges incident with v. An *isolated* vertex of G is a vertex of G with degree zero. The *complete graph* of order n is denoted by K_n. Let $t \geq 2$ and $n_1, \ldots, n_t$ be some positive integers. By $K_{n_1,\ldots,n_t}$ we mean the *complete multipartite graph* with parts size $n_1, \ldots, n_t$. In particular, the *complete bipartite graph* with part sizes m and n is denoted by $K_{m,n}$.

Let G be a simple graph with vertex set $\{v_1, \ldots, v_n\}$. The *adjacency matrix* of G, denoted by $A(G)$, is the $n \times n$ matrix such that the (i, j)-entry is 1 if v_i and v_j are adjacent, and is 0 otherwise. Since $A(G)$ is symmetric, all of its eigenvalues are real. By the eigenvalues of G we mean those of its adjacency matrix. By $Spec(G)$ we mean the multiset of all eigenvalues of G. The *energy* of G, denoted by $\mathcal{E}(G)$, is defined as the energy of the adjacency matrix of G. In other words, the energy of G is the sum of the absolute values of all eigenvalues of G. More precisely, $\mathcal{E}(G) = |\lambda_1| + \cdots + |\lambda_n|$, where $Spec(G) = \{\lambda_1, \ldots, \lambda_n\}$. For instance, since the eigenvalues of the complete graph K_n are $n-1$ (with multiplicity 1) and -1 (with multiplicity $n-1$), so $\mathcal{E}(K_n) = 2n-2$. The energy of graphs was defined by Ivan Gutman [7]. Many papers are devoted to studying the properties of the spectra of adjacency matrix, in particular studying the energy of graphs. For instance see [1]– [20] and the references therein. There are many other matrices associated to graphs such as *Laplacian matrix*, *signless Laplacian matrix*. We recall that the Laplacian matrix and the signless Laplacian matrix of a graph G are defined as $D(G) - A(G)$ and $D(G) + A(G)$, respectively, where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees of G.

In this paper first we obtain some bounds for energy of complex matrices and real symmetric matrices with trace zero. Finally by using the bounds related to energy of matrices, we obtain some bounds for energy of graphs.

2 Energy of matrices

In this section we obtain some bounds for the energy of matrices. First we recall some inequalities. The following is well known.

Theorem 1. *Let $n \geq 2$ and $x_1, x_2, \ldots, x_n$ be some non-negative real numbers. Let α and β be the arithmetic average and geometric average of $x_1, x_2, \ldots, x_n$, respectively, that is*

$$\alpha = \frac{x_1 + x_2 + \cdots + x_n}{n} \text{ and } \beta = \sqrt[n]{x_1 x_2 \cdots x_n}.$$

Then $\alpha \geq \beta$ and the equality holds if and only if $x_1 = x_2 = \cdots = x_n$.

In [8] Kober generalizes the above inequality as the following.

Theorem 2. [8] *Let $n \geq 2$ and $x_1, x_2, \ldots, x_n$ be some non-negative real numbers. Let α and β be the arithmetic average and geometric average of $x_1, x_2, \ldots, x_n$, respectively. Then*

$$\frac{1}{n} \sum_{1 \leq i < j \leq n} (\sqrt{x_i} - \sqrt{x_j})^2 \geq \alpha - \beta \geq \frac{1}{n(n-1)} \sum_{1 \leq i < j \leq n} (\sqrt{x_i} - \sqrt{x_j})^2.$$

Moreover the equality holds if and only if $x_1 = x_2 = \cdots = x_n$.

Applying the above inequality we obtain the following result for energy of square complex matrices. See also [5] for some applications of Kober's inequality.

Theorem 3. *Let $n \geq 3$ and A be an $n \times n$ complex matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Then*

$$\mathcal{E}(A) \geq \frac{2}{n-2} \sum_{1 \leq i < j \leq n} \sqrt{|\lambda_i \lambda_j|} - \frac{n}{n-2} \sqrt[n]{|det(A)|}.$$

Proof. Let $x_i = |\lambda_i|$, for $i = 1, 2, \ldots, n$. Since $det(A) = \lambda_1 \lambda_2 \cdots \lambda_n$, we find that $|det(A)| = x_1 x_2 \cdots x_n$. In addition, since $\mathcal{E}(A) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$, we conclude that $\mathcal{E}(A) = x_1 + x_2 + \cdots + x_n$. Using Theorem 2 we find that

$$\frac{1}{n} \sum_{1 \leq i < j \leq n} (\sqrt{x_i} - \sqrt{x_j})^2 \geq \frac{\mathcal{E}(A)}{n} - \sqrt[n]{|det(A)|}. \tag{2}$$

On the other hand one can see that

$$\sum_{1 \leq i < j \leq n} (\sqrt{x_i} - \sqrt{x_j})^2 = (n-1) \sum_{i=1}^{n} x_i - 2 \sum_{1 \leq i < j \leq n} \sqrt{x_i x_j}. \tag{3}$$

By combining Equations (2) and (3) and some computations we conclude that

$$\mathcal{E}(A) \geq \frac{2}{n-2} \sum_{1 \leq i < j \leq n} \sqrt{x_i x_j} - \frac{n}{n-2} \sqrt[n]{|det(A)|}. \tag{4}$$

Thus the result follows. ■

In sequel we obtain some bounds for energy of real symmetric matrices in terms of their positive eigenvalues.

Theorem 4. *Let A be a square real symmetric matrix such that $tr(A) = 0$. Assume that A has at least two positive eigenvalues and $\lambda_1, \lambda_2, \ldots, \lambda_p$ are all positive eigenvalues of A. Then*

$$\mathcal{E}(A) \geq \frac{4}{p-1} \sum_{1\leq i<j\leq p} \sqrt{\lambda_i \lambda_j},$$

and the equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_p$.

Proof. First we note that the eigenvalues of every real symmetric matrix are real. Suppose that $\lambda_{p+1}, \ldots, \lambda_n$ are all non-positive eigenvalues of A. Thus

$$\mathcal{E}(A) = \lambda_1 + \cdots + \lambda_p - \lambda_{p+1} - \cdots - \lambda_n.$$

On the other hand $\lambda_1 + \cdots + \lambda_p + \lambda_{p+1} + \cdots + \lambda_n = 0$ (since $tr(A) = 0$). Therefore we obtain that (for every integer $p \geq 0$)

$$\mathcal{E}(A) = 2(\lambda_1 + \cdots + \lambda_p). \tag{5}$$

It is not hard to see that

$$\sum_{1\leq i<j\leq p} (\sqrt{\lambda_i} - \sqrt{\lambda_j})^2 = (p-1)\sum_{i=1}^{p} \lambda_i - 2 \sum_{1\leq i<j\leq p} \sqrt{\lambda_i \lambda_j}. \tag{6}$$

This shows that (since $p \geq 2$)

$$\sum_{i=1}^{p} \lambda_i \geq \frac{2}{p-1} \sum_{1\leq i<j\leq p} \sqrt{\lambda_i \lambda_j}, \tag{7}$$

and the equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_p$. Now by combining Equations (5) and (7) we find that

$$\mathcal{E}(A) \geq \frac{4}{p-1} \sum_{1\leq i<j\leq p} \sqrt{\lambda_i \lambda_j},$$

and the equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_p$. ∎

We note that if A is a square zero matrix, then every eigenvalue of A is equal to zero and so $\mathcal{E}(A) = 0$. Now we obtain some bounds for the energy of non-zero matrices in terms of the positive eigenvalues.

Theorem 5. *Let $A \neq 0$ be a square real symmetric matrix such that $tr(A) = 0$. Assume that $\lambda_1, \ldots, \lambda_p$ are all positive eigenvalues of A. Then*

$$\sqrt{2}\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big) \geq \sqrt{\mathcal{E}(A)} \geq \sqrt{\frac{2}{p}}\,\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big).$$

Moreover in the left hand side the equality holds if and only if $p = 1$ and in the right hand side the equality holds if and only if $p = 1$ or $p \geq 2$ and $\lambda_1 = \cdots = \lambda_p$.

Proof. It is well known that every real non-zero square real symmetric matrix has at least one non-zero eigenvalue. Thus A has at least one non-zero eigenvalue. Since $tr(A) = 0$, we obtain that A has at least one positive eigenvalue and one negative eigenvalue. We recall that for every integer $p \geq 0$ (see Equation (5))

$$\mathcal{E}(A) = 2(\lambda_1 + \cdots + \lambda_p). \tag{8}$$

First assume that A has exactly one positive eigenvalue, that is $p = 1$. Thus by Equation (8) we obtain that $\mathcal{E}(A) = 2\lambda_1$ and so there is nothing to prove.

Now assume that A has at least two positive eigenvalues. In other words, assume that $p \geq 2$. By Theorem 4 we find that

$$\mathcal{E}(A) \geq \frac{4}{p-1} \sum_{1 \leq i < j \leq p} \sqrt{\lambda_i \lambda_j} \tag{9}$$

and the equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_p$. By Equation (8) and the fact that

$$\left(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\right)^2 = \sum_{i=1}^{p} \lambda_i + 2 \sum_{1 \leq i < j \leq p} \sqrt{\lambda_i \lambda_j},$$

we obtain that

$$\sum_{1 \leq i < j \leq p} \sqrt{\lambda_i \lambda_j} = \frac{\left(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\right)^2}{2} - \frac{\mathcal{E}(A)}{4}. \tag{10}$$

Using Equations (9) and (10) we conclude that

$$\mathcal{E}(A) \geq \frac{2}{p}\left(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\right)^2,$$

and the equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_p$. This completes the right hand side part.

Now we prove the other part. It is obvious that $\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p} \geq \sqrt{\lambda_1 + \cdots + \lambda_p}$ and the equality holds if and only if $p = 1$. Since $\mathcal{E}(A) = 2(\lambda_1 + \lambda_2 + \cdots + \lambda_p)$, the latter inequality shows that

$$\sqrt{2}\left(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\right) \geq \sqrt{\mathcal{E}(A)}$$

and the equality holds if and only if $p = 1$. This completes the proof. ∎

3 Energy of graphs

In this section as some applications of the previous theorems we find some bounds for energy of graphs. First we recall some results.

Theorem 6. [2] *Let G be a graph and $\rho(G)$ be the largest eigenvalue (the spectral radius) of G. Then the following hold:*

(*i*) *If G is connected, then the multiplicity of $\rho(G)$ is one.*

(*ii*) *For every eigenvalue λ of G, $|\lambda| \leq \rho(G)$.*

Theorem 7. [20] *A graph has exactly one positive eigenvalue if and only if its non-isolated vertices form a complete multipartite graph.*

By applying Theorem 3 for the adjacency matrices of graphs we obtain the following result immediately. For every graph G, by $det(G)$ we mean the determinant of the adjacency matrix of G.

Theorem 8. *Let G be a graph of order $n \geq 3$. Assume that $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. Then*

$$\mathcal{E}(G) \geq \frac{2}{n-2} \sum_{1 \leq i < j \leq n} \sqrt{|\lambda_i \lambda_j|} - \frac{n}{n-2} \sqrt[n]{|det(G)|}.$$

Theorem 9. *Let G be a connected graph of order n. Assume that G has at least two positive eigenvalues and $\lambda_1, \lambda_2, \ldots, \lambda_p$ are all positive eigenvalues of G. Then*

$$\mathcal{E}(G) > \frac{4}{p-1} \sum_{1 \leq i < j \leq p} \sqrt{\lambda_i \lambda_j}.$$

Proof. Without losing the generality assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$. Since G is connected by the first part of Theorem 6, we conclude that $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_p$. Now, by applying Theorem 4 for $A = A(G)$ we obtain that

$$\mathcal{E}(G) > \frac{4}{p-1} \sum_{1 \leq i < j \leq p} \sqrt{\lambda_i \lambda_j}.$$

■

We finish the paper by obtaining a lower bound and an upper bound for the energy of graphs in terms of the positive eigenvalue of graphs. We note that if G is a graph with at least one edge, then G has at least one positive eigenvalue.

Theorem 10. *Let G be a connected graph of order $n \geq 2$. Assume that $\lambda_1, \ldots, \lambda_p$ are all positive eigenvalues of A. Then*

$$\sqrt{2}\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big) \geq \sqrt{\mathcal{E}(A)} \geq \sqrt{\frac{2}{p}}\,\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big).$$

Moreover in the left hand side the equality holds if and only if G is a complete multipartite graph. Similarly, in the right hand side the equality holds if and only if G is a complete multipartite graph.

Proof. First assume that G is a complete multipartite graph. Thus by Theorem 7 we find that $p = 1$. Hence by applying Theorem 5 we conclude that

$$\sqrt{2}\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big) = \sqrt{\mathcal{E}(G)} = \sqrt{\frac{2}{p}}\,\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big).$$

Now assume that G is not a complete multipartite graph. Thus by Theorem 7, $p \geq 2$. Without losing the generality suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$. Since G is connected, by the first part of Theorem 6, we find that $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_p$. Using Theorem 5 for $A = A(G)$ we deduce that

$$\sqrt{2}\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big) > \sqrt{\mathcal{E}(G)} > \sqrt{\frac{2}{p}}\,\Big(\sqrt{\lambda_1} + \cdots + \sqrt{\lambda_p}\Big).$$

This completes the proof. ■

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