On the energy of $(0,1)$-matrices

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Abstract

The energy of a matrix is the sum of its singular values. We study the energy of $(0,1)$-matrices and present two methods for constructing balanced incomplete block designs whose incidence matrices have the maximum possible energy amongst the family of all $(0,1)$-matrices of given order and total number of ones. We also find a new upper bound for the energy of (p,q)-bipartite graphs.

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1 Introduction

The energy of a graph is defined to be the sum of the absolute values of its eigenvalues. This notion was introduced by Gutman and is related to the concept of the total π-electron

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energy of a molecule in chemistry, see [3, 6, 7]. Recently, Nikiforov studied the energy of matrices in [13, 14]. Let M be a $p \times q$ real matrix, $2 \le p \le q$. Then all the eigenvalues of MM^t are non-negative. Let λ_i^2 $(1 \le i \le p)$ be the eigenvalues of MM^t. The *energy* of M is defined as $\mathcal{E}(M) = \sum_{i=1}^{p} |\lambda_i|$.

A *Balanced Incomplete Block Design BIBD*(v, b, r, k, λ) is a pair $(V, \mathcal{B})$, where V is a v-set of *points* and $\mathcal{B}$ is a collection of k-subsets of V called *blocks* such that any pair of distinct points occurs in exactly λ blocks. Here b denotes the number of blocks and r is the number of blocks containing each point. The incidence matrix of a BIBD is a $(0, 1)$-matrix whose rows and columns are indexed by the points and the blocks, respectively, and the entry (p, B) is 1 if and only if $p \in B$.

Koolen and Moulton obtained an upper bound in [11] for the energy of graphs and proved that the upper bound is achieved only by strongly regular graphs. The same authors studied the energy of bipartite graphs in [10]. The upper bound was extended by Nikiforov in [14] to matrices. In this paper we study $(0, 1)$-matrices and show that the upper bound given by Nikiforov is attained only by the incidence matrices of balanced incomplete block designs. We also present two methods to construct balanced incomplete block designs with maximum possible energy. As an application we improve Koolen and Moulton's upper bound for the energy of bipartite graphs.

We refer the reader to [1, 8, 12, 15, 16] for other works related to the maximum energy of matrices and graphs.

2 The energy of matrices

Koolen and Moulton [11] gave an upper bound for the energy of graphs which was then extended by Nikiforov [14] to matrices. In the following theorem we present Nikiforov's bound for $(0, 1)$-matrices and provide a characterization of matrices attaining the bound.

Theorem 1 *Let M be a $p \times q$ $(0, 1)$-matrix with m ones, where $m \ge q \ge p$. Then*

$$\mathcal{E}(M) \le \frac{m}{\sqrt{pq}} + \sqrt{(p-1)(m - \frac{m^2}{pq})}. \qquad (1)$$

The equality is attained if and only if M is the incidence matrix of a BIBD.

Proof. We adapt the proofs in [11, 14]. Let $\lambda_1^2 \geq \lambda_2^2 \geq \cdots \geq \lambda_p^2$ ($\lambda_i \geq 0$) be the eigenvalues of MM^t. Then, by the Cauchy-Schwartz inequality

$$\begin{aligned}
\mathcal{E}(M) &= \sum_{i=1}^{p} \lambda_i \\
&= \lambda_1 + \sum_{i=2}^{p} \lambda_i \\
&\leq \lambda_1 + \sqrt{(p-1)\sum_{i=2}^{p} \lambda_i^2} \qquad (2)\\
&= \lambda_1 + \sqrt{(p-1)(m-\lambda_1^2)}.
\end{aligned}$$

The function $f(x) = x + \sqrt{(p-1)(m-x^2)}$ is decreasing on the interval $\sqrt{m/p} \leq x \leq \sqrt{m}$. Using the Rayleigh quotient and the Cauchy-Schwartz inequality, we have

$$\begin{aligned}
\lambda_1^2 &\geq \frac{\mathbf{j}^t MM^t \mathbf{j}}{\mathbf{j}^t \mathbf{j}} \qquad (3)\\
&\geq \frac{\sum_{i=1}^{q} c_i^2}{p} \\
&\geq \frac{(\sum_{i=1}^{q} c_i)^2}{pq} \qquad (4)\\
&= \frac{m^2}{pq} \\
&\geq \frac{m}{p},
\end{aligned}$$

where c_i is the ith column sum of M and $\mathbf{j}$ is the column vector of all one. Thus $m \geq \lambda_1 \geq m/\sqrt{pq} \geq \sqrt{m/p}$. From this we conclude that

$$\mathcal{E}(M) \leq f(\lambda_1) \leq f(\frac{m}{\sqrt{pq}}) = \frac{m}{\sqrt{pq}} + \sqrt{(p-1)(m - \frac{m^2}{pq})}.$$

We now pay attention to the case when the equality happens in (1). In order to have equality it is necessary and sufficient to have the following three conditions:

(i) M has constant column sums,

(ii) MM^t has constant row sums,

(iii) MM^t has at most two distinct eigenvalues.

(i) follows from the fact that equality occurs in (4). (ii) is a consequence of the occurrence of the equality in (3). Finally, (iii) follows from the equality in (2). Now we deduce from (ii) and (iii) that $MM^t = \alpha I + \beta J$, for some positive integers α and β. Noting (i) it is easy to see that M is the incidence matrix of a BIBD (for convenience, we assume that the identity matrix represents a BIBD). □

Theorem 2 *Let M be a $p \times q$ $(0,1)$-matrix, where $q \geq p$. Then*

$$\mathcal{E}(M) \leq \frac{(\sqrt{p}+1)\sqrt{pq}}{2}.$$

The equality is attained if and only if M is the incidence matrix of a

$$\text{\textit{BIBD}}(p, q, q(p+\sqrt{p})/2p, (p+\sqrt{p})/2, q(p+2\sqrt{p})/4p).$$

Proof. The maximum value of the upper bound given in Theorem 1 is attained at $m = q(p+\sqrt{p})/2$. Hence the inequality holds. The rest also follows from the same Theorem.□

Remark 1 Since the parameters of a BIBD$(p, q, q(p+\sqrt{p})/2p, (p+\sqrt{p})/2, q(p+2\sqrt{p})/4p)$ must be all integers, there are two possible subclasses of these designs, namely,

$$\text{BIBD}(a^2, 2ab, b(a+1), (a^2+a)/2, b(a+2)/2),$$

if a is even and

$$\text{BIBD}(a^2, 4ab, 2b(a+1), (a^2+a)/2, b(a+2)),$$

if a is odd.

We now show how one can construct many infinite classes with the above parameters for a a multiple of 4 and b even. We need a couple of definitions first. A $(-1,1)$-matrix H of order $m \times n$, $m \leq n$ for which $HH^t = I_m$ is called a *partial Hadamard* matrix. A square partial Hadamard matrix is a Hadamard matrix. Many infinite classes of Hadamard matrices are known and 668 is the smallest order for which the existence of such matrices is in question, see [9] for details.

Theorem 3 *If there is a partial Hadamard matrix of order* $m \times n$*,* $m \leq n$*, and a Hadamard matrix of order* m*, then there is a*

$$BIBD(m^2, mn, n(m+1)/2, m(m+1)/2, n(m+2)/4).$$

Proof. Let r_i, $i = 1, 2, \ldots, m$ be the rows of a partial Hadamard matrix of order $m \times n$ and assume that r_1 is the all one vector. Let c_i, $i = 1, 2, \ldots, m$ be the m columns of a Hadamard matrix of order m and assume that c_1 is the all one vector. Let $E_i = c_i r_i$, $i = 1, 2, \ldots, m$. Then we have

(i) $E_1 = J$,

(ii) $E_i E_j^t = 0$, $i \neq j$,

(iii) $\sum_{i=1}^{m} E_i E_i^t = mnI$.

Let L be any Latin square on the elements of $\{1, 2, \ldots, m\}$. Replacing each i by E_i for $i = 1, 2, \ldots, m$, we obtain a matrix of order $m^2 \times mn$. Replacing all minus ones with zeros gives the desired BIBD. □

Remark 2 It is conjectured that Hadamard matrices of all orders $4n$, n a positive integer exist. While the validity of this conjecture is yet to be established, there has been a number of constructions for partial Hadamard matrices. We refer the reader to [4, 5] for details.

For $a = 4n - 1$ and $b = n$ we have the following construction. A Hadamard matrix H is called to be *skew-type* if $H = I + P$ and $P^t = -P$.

Theorem 4 *Let* $4n$ *be the order of a skew-type Hadamard matrix. Then there is a*

$$BIBD((4n-1)^2, 4n(4n-1), 8n^2, 2n(4n-1), n(4n+1)).$$

Proof. Let $H = [h_{ij}]$ be a skew-type Hadamard matrix of order $4n$. We may assume that $h_{11} = -1$, $h_{1j} = h_{i1} = 1$ for $i, j = 2, 3, \ldots, 4n$. Let C be the matrix remaining after removing the first row and column of H. Then $C = I + Q$, $Q^t = -Q$ and Q has zero row and column sums. Deleting the first row of H we have the following matrix:

$$\left(\begin{array}{cc} \mathbf{j} & Q+I \end{array} \right).$$

Consider the matrix

$$\left(\begin{array}{cc} \mathbf{j} \otimes C & Q \otimes C + I \otimes J \end{array} \right),$$

and change -1 to zero to get the incidence matrix of the required BIBD. $\square$

Remark 3 It is conjectured that there is a skew-type Hadamard matrix of order $4n$ for every positive integer n. One of the known classes of these matrices includes all orders $4n = q^k + 1$, where $q \equiv 3 \pmod 4$ is a prime power and k is an odd integer, see [2].

3 Application to bipartite graphs

We now apply Theorems 1 and 2 to obtain a new upper bound for the energy of bipartite graphs. A (p, q)-bipartite graph is a graph with the vertex set $U \cup V$, $|U| = p$, $|V| = q$, and the edges only between U and V. The *incidence graph* of a BIBD is a bipartite graph whose vertices are the points and the blocks of the BIBD and there is an edge between a point and a block, if the point belongs to the block.

Theorem 5 *Let G be a (p, q)-bipartite graph with m edges, $m \geq q \geq p$. Then*

$$\mathcal{E}(G) \leq \frac{2m}{\sqrt{pq}} + 2\sqrt{(p-1)(m - \frac{m^2}{pq})}.$$

The equality is attained if and only if G is the incidence graph of a BIBD.

Proof. Let

$$A = \left(\begin{array}{cc} 0 & M \\ M^t & 0 \end{array} \right),$$

be the adjacency matrix of G, where M is a $p \times q$ $(0, 1)$ matrix. Then

$$AA^t = \left(\begin{array}{cc} MM^t & 0 \\ 0 & M^tM \end{array} \right).$$

Since MM^t and M^tM have the same non-zero eigenvalues, it follows that $\mathcal{E}(G) = \mathcal{E}(A) = 2\mathcal{E}(M)$ and so the inequality is a consequence of Theorem 1. The rest also follows from the same Theorem. $\square$

Theorem 6 *Let G be a (p, q)-bipartite graph. Then*

$$\mathcal{E}(G) \leq (\sqrt{p} + 1)\sqrt{pq}. \tag{5}$$

The equality is attained if and only if G is the incidence graph of a

$$\mathit{BIBD}(p, q, q(p + \sqrt{p})/2p, (p + \sqrt{p})/2, q(p + 2\sqrt{p})/4p).$$

Proof. This follows from the previous theorem and Theorem 2. $\square$

Remark 4 Koolen and Moulton [10] have proven that if G is a bipartite graph of order n, then $\mathcal{E}(G) \leq n(\sqrt{n/2}+1)/2$. This bound follows from the bound in Theorem 6 by noting that $p \leq n/2$ and $\sqrt{pq} \leq n/2$. The constructions given in Theorems 3 and 4 can be used to find many infinite classes of bipartite graphs meeting the upper bound (5).

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