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Strongly regular graphs with maximal energy

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Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. Koolen and Moulton have proved that the energy of a graph on n vertices is at most $n(1 + \sqrt{n})/2$, and that equality holds if and only if the graph is strongly regular with parameters $(n, (n + \sqrt{n})/2, (n + 2\sqrt{n})/4, (n + 2\sqrt{n})/4)$. Such graphs are equivalent to a certain type of Hadamard matrices. Here we survey constructions of these Hadamard matrices and the related strongly regular graphs.

Keywords: Graph energy; Strongly regular graph; Hadamard matrix. JEL code C0.

1 Introduction

Throughout G will denote a graph on n vertices with adjacency matrix A and eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$. The energy \mathcal{E} of G is defined by

$$\mathcal{E} = \sum_{i=1}^{n} |\lambda_i|.$$

The energy of a graph was introduced by Gutman (see [3]). The name and the motivation come from chemistry. A graph G is strongly regular with parameters (n, k, λ, μ) whenever G is regular of degree k, every pair of adjacent vertices has λ common neighbors, and every pair of distinct nonadjacent vertices has μ common neighbors. Although it is standard to exclude the complete graph (and its complement) from being strongly regular, we will not do so in this paper. In terms of the adjacency matrix A, the definition translates into:

$$A^2 = kI + \lambda A + \mu (J - A - I)$$

(as usual, I is the identity matrix, and J denotes the all-ones matrix, so J - A - I is the adjacency matrix of the complement of G). Koolen and Moulton [7] proved the following:

Theorem 1 The energy of a graph G on n vertices is at most $n(1+\sqrt{n})/2$. Equality holds if and only if G is a strongly regular graph with parameters

$$(n, (n + \sqrt{n})/2, (n + 2\sqrt{n})/4, (n + 2\sqrt{n})/4).$$

We will call a strongly regular graph with the above parameters, a max energy graph of order n. From the theory of strongly regular graphs (see for example [4]), it follows that a max energy graph has eigenvalues

$$[(n+\sqrt{n})/2]^1, \ [\sqrt{n}/2]^{(n-\sqrt{n})/2-1}, \ [-\sqrt{n}/2]^{(n+\sqrt{n})/2}$$

(with multiplicities written as exponents). So the energy equals $(n+\sqrt{n})/2+(n-1)\sqrt{n}/2 = n(1+\sqrt{n})/2$, which is indeed maximal. In [7] a family of max energy graphs (coming from finite geometries) with n a power of 4 is given. However, many more max energy graphs exist, as we shall see in the coming sections. Since the parameters are integer, n must be an even square, and the author conjectures that this necessary condition for existence is also sufficient.

2 Hadamard matrices

We recall some results of Hadamard matrices (see for example [2]). A square (+1, -1)matrix H of order n is a Hadamard matrix whenever $HH^{\top} = nI$. For example

$$H_{+} = \begin{bmatrix} 1 & 1 & 1 & - \\ 1 & 1 & - & 1 \\ 1 & - & 1 & 1 \\ - & 1 & 1 & 1 \end{bmatrix} \text{ and } H_{-} = \begin{bmatrix} 1 & - & - & - \\ - & 1 & - & - \\ - & - & 1 & - \\ - & - & - & 1 \end{bmatrix}$$

are two Hadamard matrices of order 4 (we write - instead of -1). It follows that n = 1, 2, or a multiple of 4. A Hadamard matrix is called graphical if it is symmetric with constant diagonal. If H is a graphical Hadamard matrix with δ on the diagonal, then $A = \frac{1}{2}(J - \delta H)$ is the adjacency matrix of a graph G. A Hadamard matrix is called regular if all its row and column sums are constant, that is, $H\mathbf{1} = H^{\mathsf{T}}\mathbf{1} = \ell\mathbf{1}$ for some integer ℓ ($\mathbf{1}$ is the allones vector). For example, the two Hadamard matrices, given above, are both regular and graphical. Note that $H\mathbf{1} = H^{\mathsf{T}}\mathbf{1} = \ell\mathbf{1}$ and $HH^{\mathsf{T}} = nI$ imply that $\ell^2\mathbf{1} = n\mathbf{1}$. So $\ell^2 = n$. Suppose H is a regular graphical Hadamard matrix with row sum ℓ , and δ on the diagonal. We call H of type +1, or positive type if $\delta\ell > 0$, and of type -1, or negative type if $\delta\ell < 0$. Let ε be the type of H, then $\delta\ell = \varepsilon\sqrt{n}$, and the associated graph G of H is regular of degree $(n - \delta\ell)/2 = (n - \varepsilon\sqrt{n})/2$. Moreover, $HH^{\mathsf{T}} = H^2 = nI$, $H\mathbf{1} = \ell\mathbf{1}$ and $J - \delta H = 2A$, imply

$$A^2 = \frac{n-\delta\ell}{2}I + \frac{n-2\delta\ell}{4}(J-I).$$

Therefore G is a strongly regular graph with parameter set

$$(n, (n - \varepsilon \sqrt{n})/2, (n - 2\varepsilon \sqrt{n})/4, (n - 2\varepsilon \sqrt{n})/4).$$
 (1)

And conversely, if A is the adjacency matrix of a strongly regular graph with one of the above parameters then J - 2A is a regular graphical Hadamard matrix. So, the regular graphical Hadamard matrices of negative type give max energy graphs. Note that the complement of a max energy graph is a strongly regular graphs with parameter set

$$(n, (n - \sqrt{n})/2 - 1, (n - 2\sqrt{n})/4 - 2, (n - 2\sqrt{n})/4),$$

which is only slightly different from the parameter set (1) with $\varepsilon = 1$.

In the example above, H_+ is of positive type and the corresponding graph is $2K_2$ (two disjoint edges), and H_- is of negative type, and the corresponding graph is K_4 , the complete graph on 4 vertices. And indeed, K_4 is the max energy graph for n = 4.

It is well known (and easily verified) that if H_1 is a Hadamard matrix of order n_1 , and H_2 is a Hadamard matrix of order n_2 , then the Kronecker product $H_1 \otimes H_2$ is a Hadamard matrix of order n_1n_2 . In addition, if H_1 and H_2 are regular and graphical, then so is $H_1 \otimes H_2$, and the type of $H_1 \otimes H_2$ is just the product of the types of H_1 and H_2 . Because regular graphical Hadamard matrices of order 4 of both types exist, we have the following result.

Lemma 1 If there exist a regular graphical Hadamard matrix of order n of positive, or negative type, then there exist regular graphical Hadamard matrices of order 4n of both types.

In particular, we can make regular graphical Hadamard matrices of order 4^k of any type for all positive integers k. Hence, for n a power of 4, there exist strongly regular graphs with parameters (1) for $\varepsilon = 1$ and for $\varepsilon = -1$. So we can conclude that max energy graphs exist for all orders $n = 4^k$.

3 Bush type Hadamard matrices

A Hadamard matrix H of order $n = \ell^2$ is said to be of *Bush type* if H is partitioned into $\ell \times \ell$ blocks of size $\ell \times \ell$ such that all diagonal blocks are all-ones matrices, and each offdiagonal block has all its row and column sums equal to 0. For example H_+ is of Bush type, but H_- is not. It is easily seen that a symmetric Bush type Hadamard matrix is regular graphical of positive type. Bush type Hadamard matrices did get much attention in recent years. An important construction method is due to Muzychuk and Xiang [9]. They construct symmetric Bush type Hadamard matrices of order $4m^4$ for all odd m. Together with Lemma 1 this gives: **Proposition 1** Regular graphical Hadamard matrices of negative type, and max energy graphs of order $n = 4^{k+1}m^4$ exist for all positive integers k and m.

An older construction is due to Kharaghani [6]. He constructs symmetric Bush type Hadamard matrices of order n^2 from an ordinary Hadamard matrix of order n. Like above, we can apply Lemma 1 and find max energy graphs of order $4n^2$, but it turned that Kharaghani's construction can be modified, such that the outcome is a regular graphical Hadamard matrix of negative type of order n^2 .

Theorem 2 If n is the order of a Hadamard matrix, then there exist regular graphical Hadamard matrices of negative type, and max energy graphs of order n^2 .

Proof. Let H be a Hadamard matrix of order n such the last column of H equals 1 (this can always be achieved by multiplying rows by -1). Write $H = [\mathbf{c}_1, \ldots, \mathbf{c}_n]$, define $C_i = \mathbf{c}_i \mathbf{c}_i^{\mathsf{T}}$ for $i = 1, \ldots, n-1$, and put $C_n = -J$. Then it is easily verified that:

- 1. C_i is symmetric with constant diagonal 1 for $i = 1, \ldots, n-1$,
- 2. $C_i \mathbf{1} = C_i^{\top} \mathbf{1} = \mathbf{0}$ for i = 1, ..., n 1,
- 3. $C_i C_j = O$ for $i \neq j, 1 \leq i, j \leq n$,
- 4. $\sum_{i=1}^{n} C_i^2 = n \sum_{i=1}^{n} \mathbf{c}_i \mathbf{c}_i^{\top} = n H H^{\top} = n^2 I.$

Next, take a symmetric Latin square with entries $1, \ldots, n$ with constant diagonal 1 (such a Latin square can be constructed easily from a back-circulant Latin square of order n-1). Make the $n^2 \times n^2$ matrix \widetilde{H} by replacing each entry i of the Latin square by C_i . Then properties 3 and 4 above show that \widetilde{H} is a Hadamard matrix, property 1 implies that \widetilde{H} is graphical with diagonal 1, and property 2 gives that \widetilde{H} has constant row sum -n. So \widetilde{H} is regular graphical of negative type.

The famous Hadamard conjecture states that Hadamard matrices of order n = 4m exist for all positive integers m. The conjecture has been confirmed for many values of m. For example if 4m - 1 or 2m - 1 is a prime power. The smallest open case is m = 167. With the above results this leads to:

Corollary 1 There exist regular graphical Hadamard matrices of negative type and max energy graphs of order $n = 4^{k+1}m^2$ for all positive integers k, if 4m - 1 is a prime power, if 2m - 1 is a prime power, if m is a square, and if m < 167.

4 Small cases

The smallest example of a max energy graph is the complete graph K_4 . The second case is a strongly regular graph with parameters (16, 10, 6, 6). There is a unique such graph (see [10]), which is known as the Clebsch graph. Its adjacency matrix can be obtained easily from the corresponding graphical Hadamard matrix $H = H_+ \otimes H_-$ (with H_+ and H_- as in the example above). The next case is the parameter set (36, 21, 12, 12). McKay and Spence [8] have enumerated all these strongly regular graphs by computer, and found exactly 180 such max energy graphs. Also for the orders 64, 100, and 144 constructions exist. Max energy graphs for n = 64 and n = 144 can be constructed by taking Kronecker products, or by the method of Theorem 2. Since there is much freedom in these constructions there exist many max energy graphs for these orders. Max energy graphs for n = 100 have been constructed by Jørgenson and Klin [5]. They found five such graphs. The first open case is n = 196. There does exist a regular graphical Hadamard matrix of positive type for this order. But the negative type is still open (see [1]). In fact, if m is odd, only for m = 1, 3and 5 existence of a max energy graph of order $n = 4m^2$ has been established.

It would be interesting if it were possible to adjust the construction of Muzychuk and Xiang for Bush-type Hadamard matrices in a way similar to what was done with Kharaghani's construction (Theorem 2). This would give max energy graphs of order $n = 4m^4$ for all odd m.

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