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Designs from good Hadamard matrices

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Hadamard matrices are very useful mathematical objects for the construction of various statistical designs. Some Hadamard matrices are better than others in terms of the qualities of designs they produce. In this paper, we provide a theoretical investigation into such good Hadamard matrices and discuss their applications in the construction of nonregular factorial designs and supersaturated designs.

Keywords: generalized resolution; nonregular design; supersaturated design

1. Introduction

Hadamard matrices have wide-ranging applications in science and technology (Horadam [13]), and are particularly useful in the construction of statistical designs (Dey and Mukerjee [10]; Cheng [7]). They can be directly used as optimal weighing designs, and are also intimately related to balanced incomplete block designs. In this article, we concern ourselves with the use of Hadamard matrices for constructing nonregular factorial designs and supersaturated designs.

A Hadamard matrix H is an orthogonal square matrix of entries ± 1. Therefore, $H^T H = HH^T = nE$, where n is the order of H and E denotes the identity matrix. For a Hadamard matrix of order n to exist, n must be 1, 2 or a multiple of 4. Though not yet proven, it is widely believed that there exists a Hadamard matrix for every n that is a multiple of 4 – the famous Hadamard conjecture. Hadamard matrices of order $n \le 1000$ are all known to exist except these three unresolved cases $n = 668, 716$ and 892.

Two Hadamard matrices are said to be isomorphic or equivalent, if one can be obtained from the other by permuting the rows, permuting the columns, sign-switching a row or a column, or a combination of the above. If a complete list of all nonisomorphic Hadamard matrices for a given order is available, then all Hadamard matrices of the same order can be obtained. To date, Hadamard matrices of order $n \le 32$ have been completely enumerated (Kharaghani and Tayfeh-Rezaie [14]). For $n = 1, 2, 4, 8, 12$, there exists only one nonisomorphic Hadamard matrix. For $n = 16, 20, 24, 28$ and 32, the number of nonisomorphic Hadamard matrices is 5, 3, 60, 487 and 13 710 027, respectively.

There arises a natural question as to which Hadamard matrices to use when it comes to the construction of nonregular designs and supersaturated designs. In this paper, we provide an answer to this question by characterizing and identifying some "good" Hadamard matrices. This is done using a notion of *type* for Hadamard matrices, which was introduced by Kimura [15] and further explored by Kharaghani and Tayfeh-Rezaie [14]. We establish a theoretical result linking the type of a Hadamard matrix with its J-characteristics. Based on this result, it follows that the larger the type, the better a Hadamard matrix. We then embark on an investigation into Hadamard matrices of the largest type and their usefulness in the construction of nonregular designs with

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the maximum generalized resolutions and supersaturated designs that minimize the maximum correlations.

2. Good Hadamard matrices

2.1. Hadamard matrices of type *b*

Let H be a Hadamard matrix of order n. By permutation and negation of rows and columns, any four columns of H can be uniquely transformed into the following form

$$\begin{bmatrix} I_a & I_a & I_a & I_a \\ I_b & I_b & I_b & -I_b \\ I_b & I_b & -I_b & I_b \\ I_a & I_a & -I_a & -I_a \\ I_b & -I_b & I_b & I_b \\ I_a & -I_a & I_a & -I_a \\ I_a & -I_a & -I_a & I_a \\ I_b & -I_b & -I_b & -I_b \end{bmatrix}, \tag{1}$$

where $a + b = n/4$, $0 \leq b \leq [n/8]$ and I_a is an all-ones column vector of length a.

Following Kimura [15], a set of four columns that can be transformed to the above form is said to be of type b. A Hadamard matrix is of type b if it has a set of four columns of type b but has no set of four columns of type less than b. The type of a Hadamard matrix is invariant with respect to isomorphism operations, but it is generally not so for matrix transposition. Up to order 32, Hadamard matrices have also been enumerated according to their types. Kharaghani and Tayfeh-Rezaie [14] obtained Table 1.

Pondering this table, one cannot keep from hoping that Hadamard matrices of large types are good for design construction. This is indeed the case and its justification follows.

2.2. Statistical properties

A Hadamard matrix of type b can be *normalized* so that its first column consists of all ones. The resulting Hadamard matrix H is still of type b. Deleting the column of all ones gives a saturated

Table 1. Number of nonisomorphic Hadamard matrices by type

	Order	12	16	20	24	28	32
Type	0	0	5	0	58	0	13 680 757
	1	1	0	3	1	486	26 369
	2	0	0	0	1	1	2900
	3	0	0	0	0	0	1
	Total	1	5	3	60	487	13 710 027

orthogonal array D of n runs for $n-1$ factors. Let $D=(d_1,\ldots,d_{n-1})=(d_{ij})$, where d_j is the jth column of D and d_{ij} is the ith entry of d_j. A key result of this paper is Theorem 1 below, which links the type of H to the J-characteristics of D.

Theorem 1. *Let $D=(d_1,\ldots,d_{n-1})$ be a saturated orthogonal array obtained by deleting the all-ones column from a Hadamard matrix H. Then H is of type b if and only if*

$$\max_{|t|=3,4} |J_t| = n-8b,$$

where t denotes a subset of column indices $1,2,\ldots,n-1$ and J_t is the J-characteristic $J_t=\sum_{i=1}^{n}\prod_{j\in t} d_{ij}$ of the corresponding columns.

The proofs of Theorem 1 and later results are all deferred to Appendix A. One consequence of Theorem 1 is Corollary 1 below.

Corollary 1. *Let H_1 be any Hadamard matrix. Then*

$$H_2=\begin{bmatrix} H_1 & H_1 \\ H_1 & -H_1 \end{bmatrix}$$

is a Hadamard matrix of type 0.

A theory for J-characteristics was fully developed in Tang [20]. It was used earlier in Deng and Tang [9] and Tang and Deng [22] to define minimum G and G_2 aberration and later in Stufken and Tang [19] to enumerate orthogonal arrays. Recent applications of J-characteristics include Bulutoglu and Kaziska [2], Bulutoglu and Ryan [3], Evangelaras [11] and Bulutoglu and Ryan [4].

As small $|J_t|$ values represent less aliasing, Theorem 1 implies that the larger the type, the better a Hadamard matrix.

2.3. Hadamard matrices of type $b_{\max}$

Let $b_{\max}$ denote the largest b for a Hadamard matrix of order n. Table 1 says that $b_{\max}=1,0,1,2,2$ and 3 for $n=12,16,20,24,28$ and 32, respectively. From the definition, we must have $b_{\max}\le[n/8]$. In fact, the following bound can be established.

Lemma 1. *For any $n\ge 4$, we have that*

$$b_{\max}\le\left[\frac{n}{8}\left(1-\frac{1}{\sqrt{n-3}}\right)\right].$$

A much simpler, yet almost equally useful, result is in the next lemma.

Lemma 2. *We have that*

$$b_{\max} \le [n/8] - 1 \qquad \text{for all } n \ge 20.$$

This simple bound is attained for all currently known cases $n = 20$, 24, 28 and 32. The bound, say B_1, in Lemma 1 improves that, say B_2, in Lemma 2 only for large n. It can be shown that $B_1 < B_2$ for $n \ge 64$ when n is a multiple of 8 and for $n \ge 148$ when n is not a multiple of 8, and $B_1 = B_2$ for all other cases with $n \ge 20$.

For $n = 16$ and 20, all Hadamard matrices are of the same type. For $n = 24$, only one Hadamard matrix has type $b_{\max} = 2$ and we find that it is given by Paley's first construction [18]. For $n = 28$, the unique Hadamard matrix of type $b_{\max} = 2$ is from Paley's first construction (Kimura [15]). We find that the Hadamard matrix of order 28 from Paley's second construction is of type 1. For $n = 32$, again there is only one Hadamard matrix of type $b_{\max} = 3$, which is given by Paley's first construction (Kharaghani and Tayfeh-Rezaie [14]). For details on various constructions of Hadamard matrices, we refer to Hedayat, Sloane and Stufken [12].

Hadamard matrices of order 36 have not been completely enumerated although millions of them have been found. By examining the 235 Hadamard matrices of order 36 available at http://www.indiana.edu/~maxdet/had_36all.can.gz, we find that two of them have type $b = 3$. Lemma 2 gives $b_{\max} \le [36/8] - 1 = 3$. Thus, $b_{\max} = 3$ for $n = 36$. These two Hadamard matrices of type $b_{\max} = 3$ are presented in Appendix B.

The rest of this subsection is devoted to a study on the types of Hadamard matrices given by Paley's first construction. For convenience, we will simply call them Paley matrices, which is available for every order n that is a multiple of 4 such that $n - 1$ is a prime power. The next result provides a lower bound on the type of a Paley matrix.

Lemma 3. *Let b_{Paley} denote the type of a Paley matrix of order n. Then*

$$b_{\text{Paley}} \ge l_{\text{Paley}} = \begin{cases} n/8 - \left[(2 + \sqrt{n-1})/4\right] & \text{if } n = 0 \ (\text{mod}\, 8), \\ (n-4)/8 - [\sqrt{n-1}/4] & \text{if } n = 4 \ (\text{mod}\, 8). \end{cases}$$

The lower bound l_{Paley} on b_{Paley} in Lemma 3 appears quite sharp, as we have verified that for all $n \le 5000$ where Paley matrices are available, the bound is attained. We therefore conjecture that $b_{\text{Paley}} = l_{\text{Paley}}$ for all Paley matrices.

Combining Lemmas 1 and 3, we have

$$l_{\text{Paley}} \le b_{\text{Paley}} \le b_{\max} \le \left[(n/8)(1 - 1/\sqrt{n-3}\,)\right].$$

Thus, if

$$l_{\text{Paley}} = \left[(n/8)(1 - 1/\sqrt{n-3}\,)\right], \tag{2}$$

then $b_{\text{Paley}} = b_{\max}$. We have checked that (2) holds for $n = 24, 28, 32, 44, 60, 72$ and 80, and l_{Paley} is strictly smaller than the right-hand side of (2) for every other $n \ge 48$ that is a multiple of 4 such that $n - 1$ is a prime power. This provides several more Hadamard matrices of type $b_{\max}$ as summarized in Corollary 2.

Corollary 2. *The Paley matrix of order n has type* $b_{\max}$ *for* $n = 44, 60, 72$ *and* 80, *in addition to* $n = 24, 28$ *and* 32.

3. Designs from good Hadamard matrices

3.1. Generalized resolution

Let D be a two-level fractional factorial design of n runs. Suppose r is the smallest integer such that $\max_{|t|=r} |J_t| > 0$. Then the generalized resolution of design D is defined as

$$R(D) = r + \Bigl(1 - \max_{|t|=r} |J_t|/n\Bigr),$$

which extends the notion of resolution for regular designs to all factorial designs and enjoys some attractive properties (Deng and Tang [9]). Let $H = (I, D_1)$ be a Hadamard matrix of order n and type $b_{\max}$, and $D_2 = (H^{\mathrm{T}}, -H^{\mathrm{T}})^{\mathrm{T}}$. Proposition 1 below is immediate from Theorem 1.

Proposition 1.

(i) *For design* D_2, *we have that* $R(D_2) = 4 + 8b_{\max}/n$. *Thus*, D_2 *has the maximum generalized resolution.*

(ii) *For design* D_1, *we have that* $R(D_1) \geq 3 + 8b_{\max}/n$. *If* $b_{\max}$ *attains the bound in Lemma* 1, *then* $R(D_1) = 3 + 8b_{\max}/n$, *in which case*, D_1 *must have the maximum generalized resolution.*

Some illustrations of Proposition 1 follow. For $n = 24$, D_1 is a design of 24 runs for 23 factors and has a generalized resolution of 3.67 and D_2 is a design of 48 runs for 24 factors and has $R(D_2) = 4.67$. For $n = 32$, D_1 has $R(D_1) = 3.75$ and D_2 has $R(D_2) = 4.75$. That D_1 has $R(D_1) = 3.75$ was noted earlier in Xu and Wong [24] but their quaternary code designs have a generalized resolution of 3.5. For $n = 36$, $R(D_1) = 3.67$ and $R(D_2) = 4.67$, where D_1 is a design of 36 runs for 35 factors and D_2 a design of 72 runs for 36 factors. All these designs have the maximum generalized resolutions.

As Hadamard matrices of type $b_{\max}$ are only available for small orders, it will be very useful to have a result that can construct large designs with large generalized resolutions. The next proposition does just that.

Proposition 2. *Let* D_1 *be as in Proposition* 1 *and* H' *be any Hadamard matrix of order* n'. *Then* $D_1 \otimes H'$, *a design of* nn' *runs for* $(n-1)n'$ *factors, has* $R(D_1 \otimes H') = 3 + 8b_{\max}/n$.

The validity of Proposition 2 can be verified routinely using Lemma 2 in Tang [21]. For $n = 24$, Proposition 2 gives a design of $24n'$ runs for $23n'$ factors with a generalized resolution of 3.67. For $n = 32$, we obtain a design of $32n'$ runs for $31n'$ factors with a generalized resolution of 3.75. Here $n' = 1, 2$ or a multiple of 4 so long as a Hadamard matrix of order n' exists.

3.2. Supersaturated designs

Using half fractions of Hadamard matrices, Lin [16] provided a construction of supersaturated designs, which are $E(s^2)$-optimal according to Nguyen [17]. Let $H = (I, d_1, \ldots, d_{n-1})$ be a Hadamard matrix of order n and type $b_{\max}$. Then Lin's method [16] constructs a supersaturated design of $n/2$ runs for $n-2$ factors by selecting the $n/2$ rows of matrix $(d_1, \ldots, d_{n-2})$ that have an entry of $+1$ in column d_{n-1}. Let $C = (c_1, \ldots, c_{n-2})$ denote this design with c_j being its jth column. Further let $s_{jk} = c_j^{\mathrm{T}} c_k$. The next result establishes a connection between $\max_{j<k} |s_{jk}|$ and type $b_{\max}$.

Proposition 3. *Design C satisfies that* $\max_{j<k} |s_{jk}| \le (n - 8b_{\max})/2$. *If $b_{\max}$ reaches the bound in Lemma 1, then* $\max_{j<k} |s_{jk}| = (n - 8b_{\max})/2$, *which means that no other Hadamard matrix of the same order can produce a better supersaturated design in terms of minimizing* $\max_{j<k} |s_{jk}|$ *using the method of half-fractioning Hadamard matrices.*

For $n = 20, 24, 28, 32$ and 36, Proposition 3 gives supersaturated designs of 10, 12, 14, 16 and 18 runs, respectively for 18, 22, 26, 30 and 34 factors, respectively. Proposition 3 also says $\max_{j<k} |s_{jk}| = 4$ for $n = 24$ and 32 and $\max_{j<k} |s_{jk}| = 6$ for $n = 20, 28$ and 36. These designs minimize $\max_{j<k} |s_{jk}|$ among all designs that can be constructed using Lin's method [16]. By the results of Cheng and Tang [8], they actually minimize $\max_{j<k} |s_{jk}|$ among all supersaturated designs of the same sizes. Thus, these designs are also $\max_{j<k} |s_{jk}|$ optimal in addition to being $E(s^2)$ optimal.

Wu [23] proposed a method of constructing a supersaturated design by adding the interaction columns to a Hadamard matrix. This design is $E(s^2)$ optimal according to Bulutoglu and Cheng [1]. Let $H = (d_0, d_1, \ldots, d_{n-1})$ be a Hadamard matrix of order n and type $b_{\max}$ where $d_0 = I$, the all-ones column. Then Wu's design [23] is given by collecting all the columns $d_j d_k$ for $0 \le j < k \le n-1$, where for example $d_1 d_2$ denotes the componentwise product of columns d_1 and d_2. Let C_2 denote this supersaturated design of n runs for $n(n-1)/2$ factors. The next result is immediate from Theorem 1.

Proposition 4. *Design C_2 has that* $\max_{j<k} |s_{jk}| = (n - 8b_{\max})$ *and thus minimizes* $\max_{j<k} |s_{jk}|$ *among all designs that can be constructed using Wu's method* [23].

For $n = 24$, Proposition 4 gives a supersaturated design of 24 runs for 276 factors with $\max_{j<k} |s_{jk}| = 8$. For $n = 32$, we obtain a supersaturated design of 32 runs for 496 factors with $\max_{j<k} |s_{jk}| = 8$.

4. Discussion

Good Hadamard matrices are those of largest types as they produce least aliasing among their three and four columns. We have investigated the usefulness of such good Hadamard matrices in the construction of nonregular designs and supersaturated designs. From Section 2.3, we know that Paley's first construction gives rise to Hadamard matrices of type $b_{\max}$ for

$n = 24, 28, 32, 44, 60, 72$ and 80. It will be of great interest to examine if this holds in general. A counterexample would settle the issue. Otherwise, we would need a sharper bound on $b_{\max}$ than that given in Lemma 1. Another research direction is to explore other possible applications. For example, Butler [5] obtained some theoretical constructions of minimum G_2 aberration designs using Hadamard matrices. One would expect that if good Hadamard matrices are used in his constructions, the resulting designs should also do well in terms of minimum G aberration. We leave these problems for future research.

Appendix A: Proofs

Proof of Theorem 1. Let H be of type b. We will prove that $\max_{|t|=3,4} |J_t| = n - 8b$. From the proof, it is obvious that the converse is also true. For convenience, our notation for J-characteristics will be slightly different but quite self-explanatory. Consider the four columns in (1) of Section 2. Obviously, their J-characteristic is $4(a-b) = n - 8b \geq 0$ as $a + b = n/4$ and $b \leq [n/8]$. For any four columns of type b, their J-characteristic must be equal to $\pm(n - 8b)$. This is because permutation of rows and columns and negation of rows have no effect on the J value, and only negation of columns can possibly change the sign of the J value.

Now let us look at design $D = (d_1, \ldots, d_{n-1})$ as in Theorem 1, which is obtained from a Hadamard matrix $H = (I, d_1, \ldots, d_{n-1})$ of type b by deleting the all-ones column I. Then any set of four different columns $d_{j_1}, d_{j_2}, d_{j_3}, d_{j_4}$ must be of type $b' \geq b$. Thus $|J(d_{j_1}, d_{j_2}, d_{j_3}, d_{j_4})| = n - 8b' \leq n - 8b$. Since the set of four columns $I, d_{j_1}, d_{j_2}, d_{j_3}$ is also of type $b' \geq b$, we obtain $|J(d_{j_1}, d_{j_2}, d_{j_3})| = |J(I, d_{j_1}, d_{j_2}, d_{j_3})| = n - 8b' \leq n - 8b$. That $H = (I, d_1, \ldots, d_{n-1})$ has a set of four columns of type b implies that equality must be attained for at least one of the above $|J|$ values. □

Proof of Corollary 1. Let c, d be two columns of H_1. Then H_2 has the following set of four columns

$$\begin{bmatrix} c & d & c & d \\ c & d & -c & -d \end{bmatrix}$$

which has a J value equal to n, and is thus of type 0. □

Proof of Lemmas 1 and 2. Noting that $I/\sqrt{n}, d_1/\sqrt{n}, \ldots, d_{n-1}/\sqrt{n}$ form an orthonormal basis, we obtain $\sum_{j=3}^{n-1} \{J(d_1, d_2, d_j)\}^2 = n^2$. This leads to $n^2 \leq (n-3)(n - 8b_{\max})^2$ by Theorem 1. Solving the above inequality we obtain Lemma 1. To prove Lemma 2, we only need to show that

$$\left[\frac{n}{8}\left(1 - \frac{1}{\sqrt{n-3}}\right)\right] \leq [n/8] - 1 \tag{3}$$

holds for $n \geq 20$. The inequality in (3) is obvious if n is a multiple of 8. Let n be a multiple of 4 but not a multiple of 8. Then (3) holds if $n/(8\sqrt{n-3}) > 0.5$, which is true when $n \geq 20$. □

Proof of Lemma 3. Theorem 2.1 of Bulutoglu and Cheng [1] states that $|J_t| \leq k + 1 + (k - 1)\sqrt{n-1}$ if $|t| = k$ is odd, which leads to $|J_t| \leq 4 + 2\sqrt{n-1}$ for $|t| = 3$. Their same theorem says that $|J_t+1| \le k+1+(k-2)\sqrt{n-1}$ if $|t|=k$ is even. But with a simple modification to their proof, one can actually show that $|J_t| \le k+(k-2)\sqrt{n-1}$ if $|t|=k$ is even. This gives $|J_t| \le 4+2\sqrt{n-1}$ for $|t|=4$. Thus $|J_t| \le 4+2\sqrt{n-1}$ for $|t|=3,4$. Let $J_{\max}=\max_{|t|=3,4}|J_t|$. Invoking Lemma 3 in Stufken and Tang [19], we obtain that $J_{\max}=8\alpha \le 4+2\sqrt{n-1}$ if $n=0 \pmod 8$ and $J_{\max}=8\alpha+4 \le 4+2\sqrt{n-1}$ if $n=4 \pmod 8$ for some integer α. This gives $\alpha \le [(1/4)(2+\sqrt{n-1})]$ for $n=0 \pmod 8$ and $\alpha \le [(1/4)\sqrt{n-1}]$ for $n=4 \pmod 8$. Thus, $J_{\max} \le 8[(1/4)(2+\sqrt{n-1})]$ for $n=0 \pmod 8$ and $J_{\max} \le 4+8[(1/4)\sqrt{n-1}]$ for $n=4 \pmod 8$. Finally by Theorem 1, we obtain Lemma 3. □

Proof of Proposition 1. Part (i) follows from Theorem 1 and a result of Butler [6], Theorem 3. From the proof of Lemma 1, we see that if $b_{\max}$ attains the bound in Lemma 1, then there must exist three columns in D_1 that have $|J_t|=n-8b_{\max}$. This implies that $R(D_1)=3+8b_{\max}/n$. The same idea can also be used to show that if $b_{\max}$ reaches the bound in Lemma 1, any other Hadamard matrix will not produce a D_1 that has a generalized resolution greater than $3+8b_{\max}/n$. This proves part (ii). □

Proof of Proposition 3. We have that

$$J(d_j,d_k,d_{n-1})=\sum_{i=1}^{n} d_{ij}d_{ik}d_{i(n-1)}=\sum_{d_{i(n-1)}=+1} d_{ij}d_{ik}d_{i(n-1)}+\sum_{d_{i(n-1)}=-1} d_{ij}d_{ik}d_{i(n-1)}$$

which simplifies to $\sum_{d_{i(n-1)}=+1} d_{ij}d_{ik}-\sum_{d_{i(n-1)}=-1} d_{ij}d_{ik}$. Noting that

$$s_{jk}=c_j^{\mathrm{T}}c_k=\sum_{d_{i(n-1)}=+1} d_{ij}d_{ik}$$

and that

$$\sum_{d_{i(n-1)}=+1} d_{ij}d_{ik}+\sum_{d_{i(n-1)}=-1} d_{ij}d_{ik}=\sum_{i=1}^{n} d_{ij}d_{ik}=0 \qquad \text{for } j<k,$$

we obtain $J(d_j,d_k,d_{n-1})=2s_{jk}$, which leads to $\max_{j<k}|s_{jk}| \le (n-8b_{\max})/2$ by invoking Theorem 1. If $b_{\max}$ reaches the bound in Lemma 1, then there must exist three columns d_j, d_k, d_{n-1} that have $|J(d_j,d_k,d_{n-1})|=n-8b_{\max}$. This proves Proposition 3. □

Proof of Proposition 4. For $j_1<k_1$ and $j_2<k_2$ where $(j_1,k_1)\ne(j_2,k_2)$, we have

$$\left|(d_{j_1}d_{k_1})^{\mathrm{T}}(d_{j_2}d_{k_2})\right|=\left|J(d_{j_1},d_{k_1},d_{j_2},d_{k_2})\right|=\begin{cases}(n-8b') & \text{if } j_1,k_1,j_2,k_2 \text{ are all distinct,}\\ 0 & \text{otherwise,}\end{cases}$$

where $b' \ge b_{\max}$ is the type of the four columns $(d_{j_1},d_{k_1},d_{j_2},d_{k_2})$ when they are all distinct. Proposition 4 then follows from Theorem 1. □

Appendix B: Two Hadamard matrices of order 36 and type $b_{max} = 3$

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