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Combinatorial Patterns of D-Optimal Weighing Designs Using a Spring Balance

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Abstract

Given a spring balance that reports the true total weight of items plus a white noise of an unknown variance, which n subsets of n items will you weigh in order to estimate the true weights of each item with the highest possible precision?

For $n \leq 6$, we classify all D-optimal weighing designs according to the combinatorial patterns they exhibit (modulo permutation), we count the D-optimal designs exhibiting each pattern, and we explain how a D-optimal design for n items may arise out of a D-optimal design for $(n-1)$ items. For $n = 7, 11$ we exhibit D-optimal designs obtained from balanced incomplete block designs (BIBDs). We discuss some strategies to construct D-optimal designs of larger sizes, and pose some unsolved problems.

Key words: Design of experiments; Estimable parameter; Information matrix; Credibility region; Symmetric BIBD; Hadamard matrix.

AMS Subject Classifications: 62K05, 05B05

1. Introduction

This story has a humble beginning in a classroom activity, then a surprising discovery, and finally an unexpected entry into the fascinating world of combinatorial designs.

While teaching a master's level first course in *Design of Experiments*, one day we brought to class four books, A–D, and asked the students: "If you want to estimate the true weight of each book, but you will only receive the true weight of each subset plus a white noise of an unknown variance, which four subsets of books will you weigh?"

Once a student would make his/her choices of any 4 out of the 15 subsets A, B, C, D, AB, AC, AD, BC, BD, BC, ABC, ABD, ACD, BCD, $ABCD$, we would give him/her the true weight of each chosen subset plus a white noise. We wanted to demonstrate that a haphazard choice of four subsets may not yield an estimate of $\boldsymbol{\mu}_{4\times1}$, the vector of true weights of all four books; rather the subsets should be chosen with care, not only for estimating, but also for lowering the Euclidean volume of the estimated confidence region for $\boldsymbol{\mu}$. A more elaborate discussion on this classroom activity is given in the technical report, which we will happily share with the interested reader. Here we develop the main research ideas and their extensions to more general problems.

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Initially, we had thought that only one design is optimal in producing a confidence region for $\boldsymbol{\mu}$ having the smallest Euclidean volume. When we tried to establish this optimal property of our preconceived choice, we had hoped to show that no other design had the same property. So, we carried out a complete search of all $\binom{15}{4} = 1365$ viable binary designs that render $\boldsymbol{\mu}$ estimable. Although it was somewhat counter-intuitive to us at that time, we were pleasantly surprised to find several other optimal designs (to be revealed in Section 3)!

Naturally, curiosity took a hold of us and we wanted to study the problem not just for 4 books, but for any n books, allowing selection of n out of $(2^n - 1)$ possible non-empty subsets. The rest of the paper documents what we found. Not only did we find multiple optimal designs in most cases, but also we categorized the optimal designs into distinct patterns (modulo permutation) and counted the number of optimal designs within each pattern. Additionally, we discovered connections between the optimal designs for n books and the optimal designs for $(n-1)$ books, for some values of n.

The origin of this optimal design problem can be traced back to almost a century ago when Yates introduced the experiment in 1935, which lead to a precise formulation by Hotelling in 1944. Since then, weighing designs have been thoroughly studied for both the spring balance problem and the chemical balance problem, with and without bias. This paper focuses on the spring balance problem where the scale has no bias.

In Section 2, we summarize the mathematical basis to estimate the true weights of the n books based on the experimental design. Among several reasonable criteria for determining the optimal design, we adopt D-optimality for our problem. In Section 3, we count the number of D-optimal designs of size $n \leq 5$, and classify them into distinct patterns (modulo permutation). In Section 4, we describe how sometimes a D-optimal design of size n is related to that of size $(n-1)$, illustrating the feature for $n \leq 6$. In Section 5, we discuss D-optimal designs of size $n = 4k - 1$ (for $k > 1$) using balanced incomplete block designs (BIBDs), and illustrate the same for $n = 7, 11$. Section 6 gives some strategies to construct D-optimal designs of larger sizes, and poses some unsolved problems, hoping to inspire young researchers to study this fascinating topic. All computations are done using the freeware R.

2. Mathematical Background

Let μ_j denote the true weight of item $j \in S \equiv \{1, 2, \ldots, n\}$. When any subset of items $S_i \subset S$ is suspended from a spring balance, the reported weight y_i equals $\sum_{\{j \in S_i\}} \mu_j + \epsilon_i$, where ϵ_i is a white noise; that is, it is normally distributed with mean 0 and unknown variance σ^2. The white noises are assumed independent. For $1 \leq i \leq n$, let us write $x_{ij} = 1$ if $j \in S_i$ and $x_{ij} = 0$ if $j \notin S_i$. Then the linear model, in matrix notation, can be written as $\boldsymbol{y} = \mathbf{X}\boldsymbol{\mu} + \boldsymbol{\epsilon}$, where the binary matrix $\mathbf{X} = (x_{ij})$ is called the design matrix for weighing with a spring balance. Since each of the n^2 elements of $\mathbf{X}$ can be chosen to be either 0 or 1, there are altogether 2^{2n} possible design matrices, of which only a subset of $\binom{2^n - 1}{n}$ design matrices render $\boldsymbol{\mu}$ estimable. For details on the statistical model behind this estimation problem, see Banerjee (1975).

For our in-class book-weighing activity, intending to estimate each parameter μ_i with the highest possible precision, we prefer small values on the diagonal of the inverse of the information matrix $(\mathbf{X}^T\mathbf{X})^{-1}$, which correspond to the variances of the estimates $\hat{\mu}_i$. However, it may not be possible to minimize all diagonal elements simultaneously. We must thoughtfully choose an optimality criterion. Among the various notions of optimality discussed in Nishii (1993) and Pukelsheim (2006), we like D-optimality the most: It minimizes the determinant of $(\mathbf{X}^T\mathbf{X})^{-1}$; or equivalently, maximizes the determinant of $\mathbf{X}^T\mathbf{X}$. Moreover, when we adopt a Bayesian point of view, then under a non-informative prior distribution, the posterior credibility region of the *smallest Euclidean volume* turns out to be an ellipsoid with center $\hat{\boldsymbol{\mu}}$. Therefore, we adopt D-optimality as the criterion for choosing the best design.

3. Classifying D-optimal Designs into Patterns

Among the $\binom{2^n-1}{n}$ designs that render $\boldsymbol{\mu}$ estimable, many exhibit similar patterns. We will present these patterns by showing a characteristic illustrative design, along with its incidence matrix. However, before we construct and classify the different D-optimal weighing designs (DWDs) into patterns, it is helpful to know how many binary square matrices of degree n achieve the maximal determinant, and what is the value of that maximal determinant. Let us denote the determinant of $\mathbf{X}$ by $\det(\mathbf{X})$. Then $\det(\mathbf{X}^T\mathbf{X})^{-1} = |\det(\mathbf{X})|^{-2}$. Among the 2^{2n} binary matrices $\mathbf{X}$, what is $\delta = \max\det(\mathbf{X})$, and how many binary matrices achieve this maximum determinant δ?

In fact, the answers are well known for small n as summarized by Weisstein (no date) and presented in Table 1. Using this information, let us explain how to determine the number of DWDs (modulo permutation). Any binary design matrix $\mathbf{X}$ represents a weighing design, but a weighing design is invariant under row-permutation, since the order in which we weigh the subsets is irrelevant. As there are $n!$ permutations of the n rows, each weighing design can be represented by $n!$ binary matrices. Moreover, since the number of matrices achieving the maximal absolute value of determinant is twice the number of binary matrices achieving the maximal determinant, the total number of DWDs is given by the relation

$$\#\text{ D-optimal weighing designs} = \frac{\#\text{ D-optimal matrices}}{n!} = \frac{2\cdot\#\{\mathbf{X}:\det(\mathbf{X})=\delta\}}{n!},$$

where D-optimal matrices are those matrices $\mathbf{X}$ that attain the maximal determinant δ in absolute value. We summarize the information in Table 1, where $\mathbf{X}$ is a binary matrix of size n. Next, Table 2 shows the number of DWDs per pattern.

Table 1: The number of D-optimal matrices (DMs) and weighing designs

n	$\max\det(\mathbf{X})$	$\frac{1}{2}\#$ DMs	# DWDs	# patterns
2	1	3	3	2
3	2	3	1	1
4	3	60	5	2
5	5	3600	60	3
6	9	529200	1470	7
7	32	75600	30	1
8	56	195955200	9720	?*
9	144	13716864000	75600	??*

*The undisclosed # patterns for $n = 8, 9$ are offered as exercise to the interested reader.

Table 2: The number of D-optimal weighing designs per pattern

Pattern	# DWDs
$D_{2,1}$	1
$D_{2,2}$	2
$D_{3,1}$	1
$D_{4,1}$	1
$D_{4,2}$	4
$D_{5,1}$	20
$D_{5,2}$	10
$D_{5,3}$	30

Pattern	# DWDs
$D_{6,1}$	360
$D_{6,2}$	180
$D_{6,3}$	180
$D_{6,4}$	180
$D_{6,5}$	360
$D_{6,6}$	180
$D_{6,7}$	30
$D_{7,1}$	30

Table 3 shows an illustrative design characterizing each pattern for $n = 2, 3, 4$, along with its incidence matrix, information matrix and inverse of information matrix.

Table 3: The patterns of D-optimal weighing designs for $n = 2, 3, 4$ illustrated

Pattern	Illustrative Design	Corresponding $\mathbf{X}$	$\mathbf{X}^T\mathbf{X}$	$(\mathbf{X}^T\mathbf{X})^{-1}$
$D_{2,1}$	$\{P_1, P_2\}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$
$D_{2,2}$	$\{P_1P_2, P_1\}$	$\begin{pmatrix}1 & 1\\ 1 & 0\end{pmatrix}$	$\begin{pmatrix}2 & 1\\ 1 & 1\end{pmatrix}$	$\begin{pmatrix}1 & -1\\ -1 & 2\end{pmatrix}$
$D_{3,1}$	$\{P_1P_2, P_1S_1, P_2S_1\}$	$\begin{pmatrix}1 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 1\end{pmatrix}$	$\begin{pmatrix}2 & 1 & 1\\ 1 & 2 & 1\\ 1 & 1 & 2\end{pmatrix}$	$\frac{1}{4}\begin{pmatrix}3 & -1 & -1\\ -1 & 3 & -1\\ -1 & -1 & 3\end{pmatrix}$
$D_{4,1}$	$\{P_1P_2Q_1,\ P_1P_2Q_2,$ $P_1Q_1Q_2,\ P_2Q_1Q_2\}$	$\begin{pmatrix}1 & 1 & 1 & 0\\ 1 & 1 & 0 & 1\\ 1 & 0 & 1 & 1\\ 0 & 1 & 1 & 1\end{pmatrix}$	$\begin{pmatrix}3 & 2 & 2 & 2\\ & 3 & 2 & 2\\ & & 3 & 2\\ & & & 3\end{pmatrix}$	$\frac{1}{9}\begin{pmatrix}7 & -2 & -2 & -2\\ & 7 & -2 & -2\\ & & 7 & -2\\ & & & 7\end{pmatrix}$
$D_{4,2}$	$\{Q_1Q_2Q_3,\ Q_1S_1,$ $Q_2S_1,\ Q_3S_1\}$	$\begin{pmatrix}1 & 1 & 1 & 0\\ 1 & 0 & 0 & 1\\ 0 & 1 & 0 & 1\\ 0 & 0 & 1 & 1\end{pmatrix}$	$\begin{pmatrix}2 & 1 & 1 & 1\\ & 2 & 1 & 1\\ & & 2 & 1\\ & & & 3\end{pmatrix}$	$\frac{1}{9}\begin{pmatrix}7 & -2 & -2 & -1\\ & 7 & -2 & -1\\ & & 7 & -1\\ & & & 4\end{pmatrix}$

Returning to our classroom book-weighing activity, we note that there are exactly five DWD's. The first pattern $D_{4,1}$ represents only one DWD, namely $\{ABC, ABD, ACD, BCD\}$, which we had anticipated beforehand; and the second pattern $D_{4,2}$ represents the following four DWD's whose discovery surprised us and propelled us into this research:

$$\{ABC, AD, BD, CD\}, \{ABD, AC, BC, CD\}, \{ACD, AB, BC, BD\}, \{BCD, AB, AC, AD\}.$$

For $n = 5$ and 6, we simply present the incidence matrices, the information matrices and the inverse information matrices in Table 4 below and in Table B1 in Annexure B, respectively, leaving the reader to find the corresponding illustrative designs. Details of these designs, along with ways to construct them, can be found in the technical report, which we will be happy to share with the interested reader, if needed.

Table 4: The three patterns of D-optimal designs for $n = 5$ illustrated

Pattern	Corresponding $\mathbf{X}$	$\mathbf{X}^T\mathbf{X}$	$25(\mathbf{X}^T\mathbf{X})^{-1}$
$D_{5,1}$	$\begin{pmatrix} 1&0&0&0&1\\ 1&1&1&0&0\\ 1&1&0&1&0\\ 1&0&1&1&0\\ 0&1&1&1&1 \end{pmatrix}$	$\begin{pmatrix} 4&2&2&2&1\\ &3&2&2&1\\ &&3&2&1\\ &&&3&1\\ &&&&2 \end{pmatrix}$	$\begin{pmatrix} 11&-3&-3&-3&-1\\ &19&-6&-6&-2\\ &&19&-6&-2\\ &&&19&-2\\ &&&&16 \end{pmatrix}$
$D_{5,2}$	$\begin{pmatrix} 1&1&1&0&0\\ 1&1&0&1&0\\ 1&1&0&0&1\\ 1&0&1&1&1\\ 0&1&1&1&1 \end{pmatrix}$	$\begin{pmatrix} 4&3&2&2&2\\ &4&2&2&2\\ &&3&2&2\\ &&&3&2\\ &&&&3 \end{pmatrix}$	$\begin{pmatrix} 16&-9&-2&-2&-2\\ &16&-2&-2&-2\\ &&19&-6&-6\\ &&&19&-6\\ &&&&19 \end{pmatrix}$
$D_{5,3}$	$\begin{pmatrix} 1&1&1&0&0\\ 0&1&0&1&0\\ 0&1&0&0&1\\ 0&0&1&1&1\\ 1&0&0&1&1 \end{pmatrix}$	$\begin{pmatrix} 3&1&1&1&1\\ &2&1&1&1\\ &&2&1&1\\ &&&3&2\\ &&&&3 \end{pmatrix}$	$\begin{pmatrix} 11&-3&-3&-1&-1\\ &19&-6&-2&-2\\ &&19&-2&-2\\ &&&16&-9\\ &&&&16 \end{pmatrix}$

4. Interrelations Between DWD's of Sizes $(n-1)$ and n

As n gets larger, patterns become more complicated. However, we have found that all designs of size n for $n = 2, \ldots, 6$ are related to at least one pattern of size $(n-1)$, and thus, can be constructed by simply adding a new letter to some words of a design of size $(n-1)$, and then adding a new word (or equivalently, by adding a row and column to a binary matrix representing the design of size $(n-1)$). Alternatively, we can think of a pattern or design of size n to have a D-optimal design of size $(n-1)$ embedded in it; or in terms of matrices, a D-optimal matrix of order n to have a minor of order $(n-1)$ which attains the maximal determinant for that order. However, this feature fails for $n = 7$ and $n = 11$.

Surely, all DWDs of size 2 embed in them a DWD of size 1. We illustrate how new designs are constructed from a lower order design for $n = 3, \ldots, 6$, by taking matrices of the previous order displayed in Section 3 and adding a new row and a new column to them.

4.1. From $n = 2$ to $n = 3$

Recall that for $n = 2$ and $n = 3$ some of the D-optimal matrices we found were

$$\mathbf{X}_{2,1} = \begin{pmatrix} 1&0\\ 0&1 \end{pmatrix}, \qquad \mathbf{X}_{2,2} = \begin{pmatrix} 1&1\\ 1&0 \end{pmatrix}, \qquad \mathbf{X}_{3,1} = \begin{pmatrix} 1&1&0\\ 1&0&1\\ 0&1&1 \end{pmatrix}$$

Note that $\mathbf{X}_{2,1}$ and $\mathbf{X}_{2,2}$ are both embedded in $\mathbf{X}_{3,1}$, as shown below:

$$\mathbf{X}_{3,1} = \left(\begin{array}{c:cc} 1 & 1 & 0 \\ 1 & 0 & 1 \\ \hdashline 0 & 1 & 1 \end{array}\right) = \left(\begin{array}{cc:c} 1 & 1 & 0 \\ 1 & 0 & 1 \\ \hdashline 0 & 1 & 1 \end{array}\right)$$

4.2. From $n = 3$ to $n = 4$

From $D_{3,1}$, we can construct both, $D_{4,1}$ and $D_{4,2}$. Below we give an illustrative matrix for each pattern (permute the rows/columns to see $D_{3,1}$ embedded in $D_{4,2}$):

$$\mathbf{X}_{4,1} = \left(\begin{array}{ccc:c} 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ \hdashline 1 & 1 & 1 & 0 \end{array}\right) \qquad \mathbf{X}_{4,2} = \left(\begin{array}{ccc:c} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ \hdashline 1 & 0 & 0 & 1 \end{array}\right)$$

4.3. From $n = 4$ to $n = 5$

Patterns $D_{5,1}$ and $D_{5,2}$ are constructed from either $D_{4,1}$ or $D_{4,2}$; but $D_{5,3}$ comes only from $D_{4,2}$. Refer to the technical report for details about how to construct these patterns. Below are illustrative matrices for each of these cases. Within the first two cases, permute the rows/columns to see that the two incidence matrices represent the same pattern.

1) Illustrative matrices for $D_{5,1}$ coming from $\mathbf{X}_{4,1}$ and $\mathbf{X}_{4,2}$, respectively:

$$\left(\begin{array}{cccc:c} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ \hdashline 1 & 0 & 0 & 0 & 1 \end{array}\right) \qquad \left(\begin{array}{cccc:c} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ \hdashline 1 & 1 & 1 & 0 & 1 \end{array}\right)$$

2) Illustrative matrices for $D_{5,2}$ coming from $\mathbf{X}_{4,1}$ and $\mathbf{X}_{4,2}$, respectively:

$$\left(\begin{array}{cccc:c} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ \hdashline 1 & 1 & 0 & 0 & 1 \end{array}\right) \qquad \left(\begin{array}{cccc:c} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 \\ \hdashline 1 & 1 & 1 & 1 & 0 \end{array}\right)$$

3) An illustrative matrix for $D_{5,3}$ coming from $D_{4,2}$:

$$\left(\begin{array}{cccc:c} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ \hdashline 0 & 1 & 1 & 0 & 1 \end{array}\right)$$

4.4. From $n = 5$ to $n = 6$

Patterns $D_{6,1}$ and $D_{6,2}$ come from $D_{5,1}$, patterns $D_{6,3}$ and $D_{6,4}$ come from $D_{5,2}$, and patterns $D_{6,5}$, $D_{6,6}$ and $D_{6,7}$ come from $D_{5,3}$. The matrices representing these designs can be found in Table B1 in Annexure B. We invite the astute reader to contemplate how to obtain these extensions from size 5 to size 6, how to count the number of DWDs, and how to construct the different patterns. All of these topics and more are thoroughly addressed in the technical report, which we will gladly share, if needed.

What we found absolutely delightful, we offer as a gift to our dear readers: We present a D-optimal matrix of size 6, coming from a D-optimal matrix of size 5, coming from a D-optimal matrix of size 4, coming from ... you get the idea. Here it is:

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Without first memorizing it, can you reconstruct this DWD?

5. DWD's for Cases $n = 4k - 1$ where $k = 2, 3, \ldots$

These special cases are related to a well-studied group of chemical balance weighing designs. A square sign matrix (all whose elements are -1 and 1) of size n that attains the maximal determinant is known as a Hadamard matrix. The order of a Hadamard matrix is $n = 1, 2$ or $n = 4k$ for $k \geq 1$, and its determinant is $n^{n/2}$ (see Brenner, 1972). Mood (1946) and Banerjee (1975) show that there is a one-to-one correspondence between Hadamard matrices of size n and square binary matrices of size $(n - 1)$ with maximal determinant. Thus, the number of inequivalent Hadamard matrices of size n is also the number of patterns for DWD's of size $(n - 1)$.

The existence of Hadamard matrices is known for all n divisible by 4 up to $n < 668$, thereby implying the existance of D-optimal binary matrices of size $n = 4k - 1 < 667$. Moreover, Raghavarao (1971) provides methods for constructing Hadamard matrices of order $n \leq 100$, and the number of inequivalent Hadamard matrices is known for orders $n \leq 32$, as given in the On-Line Encyclopedia of Integer Sequences (OEIS).

Since square binary matrices with maximal determinants can be constructed from Hadamard matrices, as shown by Mood (1946) and as found in Stinson (2004), we can construct DWDs of size $n = 4k - 1$, $k = 1, 2, \ldots$ starting from Hadamard matrices of size $n = 4k$. Here, we illustrate two of them, $n = 7$ and $n = 11$, leaving the rest to the reader.

5.1. Case $n = 7$

There are more reasons that make this case very, very special. First, there is only one possible pattern, yielding 30 possible DWDs. Note that both the number of patterns and the number of DWDs is much smaller than the previous case of $n = 6$. Moreover, the only pattern for $n = 7$ does not come from any of the patterns for $n = 6$, as proven by Williamson (1946). Surprisingly, that single pattern for $n = 7$ is rather easy to construct: First, find the incidence matrix of the symmetric BIBD$(7, 3, 1)$ associated with the Hadamard matrix of size 8, and then take its complement, which gives a symmetric BIBD$(7, 4, 2)$.

Recall that the symmetric BIBD$(7, 3, 1)$ can be found from the Fano plane shown below. To construct a particular design, we label the vertices of the Fano plane with distinct letters and make words consisting of the three letters on each line on the graph. (Here, the central circle also counts as a line.) There are 30 distinct ways to label of the Fano plane, not counting rotation and reflection symmetries. By taking the complements of each such labelled symmetric BIBD$(7, 3, 1)$, we obtain 30 possible DWDs of size $n = 7$.

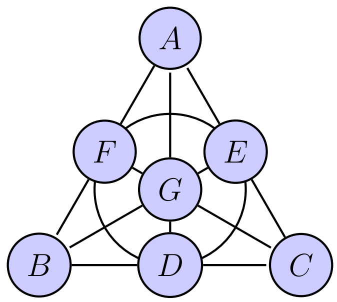

Figure 1: The Fano plane yields the symmetric BIBD$(7, 3, 1)$.

For example, using the labeling shown in Figure 1 above, we obtain the symmetric BIBD $\{ABF, ACE, ADG, BCD, BEG, CFG, DEF\}$. Thereafter, its complement yields the following DWD of size $n = 7$:

$$\{CDEG, BDFG, BCEF, AEFG, ACDF, ABDE, ABCG\}.$$

Another DWD is given below along with its corresponding matrix. Can you find the labeling of the Fano plane that leads to this DWD?

Illustrative Design: $\{ABCD, ABEF, ACEG, ADFG, BCFG, BDEG, CDEF\}$.

$$\mathbf{X}_7 = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}, \qquad \mathbf{X}_7^T\mathbf{X}_7 = \begin{pmatrix} 4 & 2 & 2 & 2 & 2 & 2 & 2 \\ & 4 & 2 & 2 & 2 & 2 & 2 \\ & & 4 & 2 & 2 & 2 & 2 \\ & & & 4 & 2 & 2 & 2 \\ & & & & 4 & 2 & 2 \\ & & & & & 4 & 2 \\ & & & & & & 4 \end{pmatrix},$$

$$(\mathbf{X}_7^T\mathbf{X}_7)^{-1} = \frac{1}{16}\begin{pmatrix} 7 & -1 & -1 & -1 & -1 & -1 & -1 \\ & 7 & -1 & -1 & -1 & -1 & -1 \\ & & 7 & -1 & -1 & -1 & -1 \\ & & & 7 & -1 & -1 & -1 \\ & & & & 7 & -1 & -1 \\ & & & & & 7 & -1 \\ & & & & & & 7 \end{pmatrix}.$$

5.2. Case $n = 11$

According to the OEIS, there is only one distinct (up to permutation of rows and columns) Hadamard matrix of order 12, implying that there is only one possible pattern of DWDs for $n = 11$. This pattern can be found by using the Paley biplane (shown below), which leads to a symmetric BIBD$(11, 5, 2)$, as explained in the next paragraph. The Paley biplane can be labelled in 60,480 distinct ways not counting symmetries.

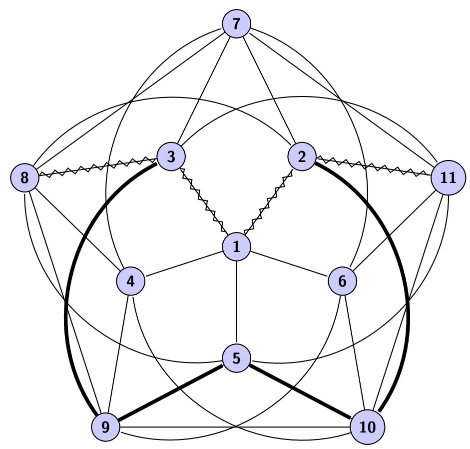

Figure 2: The Paley biplane yields the symmetric BIBD$(11, 5, 2)$**.**

After the Paley biplane is labelled, Brown (2004) explains that each of the 11 subsets (rows of the incidence matrix of the BIBD) can be found by traveling on three types of paths in the graph: The first type, shown in bold line gives rise to 5 subsets, via a 1/5 rotation about the center. Similarly, the second type of path, shown with the zigzag lines gives rise to 5 more subsets, via a 1/5 rotation about the center. Finally, any four edges of the outer pentagon constitute the last subset needed to construct the symmetric BIBD$(11, 5, 2)$.

Thereafter, we take its complement, a symmetric BIBD$(11, 6, 3)$, to obtain the pattern of DWDs for $n = 11$. We give the incidence matrix of one such DWD; but leave to the avid reader the task of finding other such designs by relabelling the Paley biplane.

$$\mathbf{X}_{11} = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \end{pmatrix}$$

Note that the above matrix has determinant 1458, which means that it achieves the maximal determinant for a square binary matrix of order 11. Alternatively, a matrix for this design can be found by using the standardized Hadamard matrix of order 12 and deleting its first row and column, or by using the Paley construction. Moreover, we know from Williamson (1946) that this pattern cannot be constructed using a DWD of size $n = 10$. In fact, there is no DWD of order $n = 8, 9$ or 10 embedded in this design.

We constructed DWDs of sizes $n = 7$ and $n = 11$ using symmetric BIBDs. This is no coincidence: Raghavarao (1971) proves that when estimating the weights of $n = 4k - 1$ objects using exactly n weighings, the incidence matrix of a symmetric BIBD$(4k - 1, 2k, k)$ is D-optimal as a spring balance weighing design of size $n = 4k - 1$.

This result can be strengthened. Mood (1946) proves that there is a one-to-one correspondence between D-optimal binary matrices and Hadamard matrices. Additionally, Stinson (2004) states that for $k > 1$, there exists a Hadamard matrix of order $4k$ if and only if there exists a symmetric BIBD$(4k - 1, 2k - 1, k - 1)$. Hence, the following lemma holds.

Lemma 1. For $k > 1$, there exists a D-optimal binary matrix of size $n = 4k - 1$ if and only if there exists a symmetric BIBD$(4k - 1, 2k, k)$.

Lemma 1 aids us in counting DWDs associated with each pattern (or equivalently, with each symmetric BIBD). For $n = 4k - 1$, the number of DWDs associated with a particular symmetric BIBD is given by $n!$ divided by the number of symmetries of the symmetric BIBD(v, k, λ); that is, the number of permutations of the v treatments (columns) that simultaneously permute the blocks (rows). (This number is also known as the order of the automorphism group of the design). This explains our counting of DWDs for $n = 7$ and $n = 11$:

$$\frac{7!}{168} = 30 \text{ DWDs} \qquad\qquad \frac{11!}{660} = 60480 \text{ DWDs}$$

In other words, there were 7! and 11! ways to relabel the Fano plane and the Paley biplane, respectively; but to remove all duplicates, we divided by 168 and 660—the number of symmetries of the plane/biplane.

6. Future Work

We have found, classified and counted all D-optimal weighing designs of sizes $n = 2, \ldots 7$. One may now consider other types of optimality, such as A-optimality and E-optimality, mentioned in Nishii (1993) and Pukelsheim (2006), to choose a preferred design depending on the research goal. We leave this task to the interested reader, aiding them with the following table of traces of the $(\mathbf{X}^T\mathbf{X})^{-1}$ matrices that we used in Sections 3 and 4. The reader can also find a thorough discussion of this topic in Shah and Sinha (1989).

A natural extension of this work is to study designs of sizes $n > 7$. As mentioned in Section 5, designs of sizes $n = 4k - 1$ are very well studied, given the study of Hadamard matrices and the association between Hadamard matrices and D-optimal binary matrices.

Moreover, to construct designs of sizes $n > 7$ where $n \neq 4k - 1$, Bose and Nair (1939) and Banerjee (1952) use some partial BIBDs as weighing designs. Also, one can try to extend designs of size $(n - 1)$, following strategies used in Section 4, and further explained in the technical report. For instance, starting with the matrix $\mathbf{X}_7$ in Section 5 illustrating the case

Table 5: Traces of $(\mathbf{X}^T\mathbf{X})^{-1}$ matrices for D-optimal weighing designs

Pattern	$tr((\mathbf{X}^T\mathbf{X})^{-1})$	Pattern	$tr((\mathbf{X}^T X)^{-1})$
$D_{2,1}$	2	$D_{6,1}$	298/81
$D_{2,2}$	3	$D_{6,2}$	310/81
$D_{3,1}$	9/4	$D_{6,3}$	309/81
$D_{4,1}$	28/9	$D_{6,4}$	309/81
$D_{4,2}$	25/9	$D_{6,5}$	295/81
$D_{5,1}$	84/25	$D_{6,6}$	319/81
$D_{5,2}$	89/25	$D_{6,7}$	306/81
$D_{5,3}$	81/25	$D_{7,1}$	49/16

for $n = 7$, and adding an extra row and column leads to a matrix of order $n = 8$ with determinant 56, which, as reported in Table 1, is the largest determinant a binary matrix of this size can attain.

$$\mathbf{X}_8 = \left(\begin{array}{ccccccc:c} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\ \hdashline 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{array}\right)$$

As mentioned in Section 3, we leave to the reader the task of finding all patterns and counting all DWDs for cases $n = 8, 9$. We empower them with yet another potent idea described below. But first let us explain a geometric representation of a design matrix: We construct an $n \times n$ grid of unit squares; color a unit square if the corresponding matrix entry is 1, but leave the unit square colorless if the entry is 0. We may also partition the grid suitably to enhance the pattern. For example, designs $D_{6,3}$ and $D_{6,4}$, after suitable rearrangements of rows and columns, are represented as shown in Figure 3.

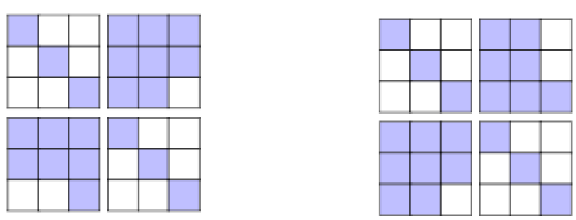

Figure 3: These geometric patterns for $D_{6,3}$ and $D_{6,4}$ are obtained by coloring and spacing unit squares.

Having given such a geometric representation of a design matrix, let us describe another type of extension from a smaller size design to a larger size design that is worth exploring: Carefully observe the patterns themselves, and replicate them for a larger n. For example, the geometric representation of $\mathbf{X}_7$, shown in Figure 4, reveals a visual pattern, which may be time-consuming to express verbally. Instead, we invite the astute reader to imitate the same pattern for a 9×9 grid. The resulting picture is shown in Figure 5 in Annexure A. Please do not peek at it too early, lest you miss the joy of discovery.

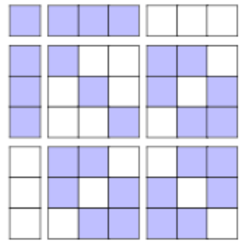

Figure 4: Here is a geometric pattern for $n = 7$. Can you imitate it for $n = 9$?

Figure 5 serves as a design matrix for the case $n = 9$, and it has determinant 144, which is the largest determinant a binary matrix of this size can attain. Although performing such extensions multiple times may not result in D-optimal matrices of larger orders (for example, this pattern does not work for $n = 11$ or $n = 13$), the idea is worth testing with other patterns of different sizes.

Let us briefly mention yet another avenue of research involving designs that do not necessarily involve square matrices. In this case, to estimate all parameters, we allow *more weighings* than objects to weigh (see Mood, 1946, Banerjee 1975, or Neubauer *et al.*, 1998 for designs corresponding to four and five objects). While the investment is higher than absolutely necessary in terms of increased number of weighings, the added benefit is that the estimates have smaller standard errors and one can also estimate the error variance σ^2. For an introduction to a very general description of weighing designs in this direction and related results, we refer to Raghavarao (1971) and Shah and Sinha (1989).

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ANNEXURE A

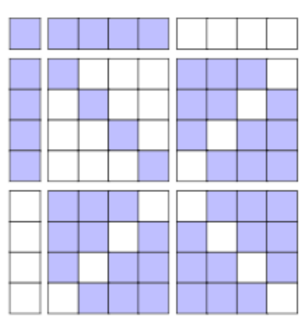

Figure 5: This geometric pattern for $n = 9$ imitates the pattern shown in Figure 4.

ANNEXURE B

Table B1: The seven patterns of D-optimal designs for $n = 6$ illustrated

Pattern	Illustrative $\mathbf{X}$	$\mathbf{X}^T\mathbf{X}$	$81(\mathbf{X}^T\mathbf{X})^{-1}$
$D_{6,1}$	$\left(\begin{array}{ccccc:c} 1&1&1&0&0&0\\ 1&1&0&1&0&0\\ 1&0&1&1&0&1\\ 0&1&1&1&1&0\\ 1&0&0&0&1&1\\ \hdashline 0&1&0&0&0&1 \end{array}\right)$	$\begin{pmatrix} 4&2&2&2&1&2\\ &4&2&2&1&1\\ &&3&2&1&1\\ &&&3&1&1\\ &&&&2&1\\ &&&&&3 \end{pmatrix}$	$\begin{pmatrix} 45&-6&-12&-12&3&-21\\ &35&-11&-11&-4&1\\ &&59&-22&-8&2\\ &&&59&-8&2\\ &&&&56&-14\\ &&&&&44 \end{pmatrix}$
$D_{6,2}$	$\left(\begin{array}{ccccc:c} 1&1&1&0&0&0\\ 1&1&0&1&0&0\\ 1&0&1&1&0&1\\ 0&1&1&1&1&1\\ 1&0&0&0&1&1\\ \hdashline 1&0&1&1&1&0 \end{array}\right)$	$\begin{pmatrix} 5&2&3&3&2&2\\ &3&2&2&1&1\\ &&4&3&2&2\\ &&&4&2&2\\ &&&&3&2\\ &&&&&3 \end{pmatrix}$	$\begin{pmatrix} 35&-6&-11&-11&-4&-4\\ &45&-12&-12&3&3\\ &&59&-22&-8&-8\\ &&&59&-8&-8\\ &&&&56&-25\\ &&&&&56 \end{pmatrix}$
$D_{6,3}$	$\left(\begin{array}{ccccc:c} 1&1&0&0&1&1\\ 1&0&1&0&1&1\\ 1&0&0&1&1&0\\ 0&1&1&1&1&0\\ 1&1&1&1&0&0\\ \hdashline 0&0&0&1&0&1 \end{array}\right)$	$\begin{pmatrix} 4&2&2&2&3&2\\ &3&2&2&2&1\\ &&3&2&2&1\\ &&&4&2&1\\ &&&&4&2\\ &&&&&3 \end{pmatrix}$	$\begin{pmatrix} 56&-8&-8&-4&-25&-14\\ &59&-22&-11&-8&2\\ &&59&-11&-8&2\\ &&&35&-4&1\\ &&&&56&-14\\ &&&&&44 \end{pmatrix}$
$D_{6,4}$	$\left(\begin{array}{ccccc:c} 1&1&0&0&1&0\\ 1&0&1&0&1&0\\ 1&0&0&1&1&1\\ 0&1&1&1&1&0\\ 1&1&1&1&0&0\\ \hdashline 0&1&1&0&0&1 \end{array}\right)$	$\begin{pmatrix} 4&2&2&2&3&1\\ &4&3&2&2&1\\ &&4&2&2&1\\ &&&3&2&1\\ &&&&4&1\\ &&&&&2 \end{pmatrix}$	$3\begin{pmatrix} 17&-1&-1&-3&-10&-1\\ &17&-10&-3&-1&-1\\ &&17&-3&-1&-1\\ &&&18&-3&-3\\ &&&&17&-1\\ &&&&&17 \end{pmatrix}$
$D_{6,5}$	$\left(\begin{array}{ccccc:c} 1&1&0&0&1&0\\ 1&0&1&0&0&0\\ 1&0&0&1&0&1\\ 0&1&1&1&0&0\\ 0&0&1&1&1&0\\ \hdashline 0&1&1&0&1&1 \end{array}\right)$	$\begin{pmatrix} 3&1&1&1&1&1\\ &3&2&1&2&1\\ &&4&2&2&1\\ &&&3&1&1\\ &&&&3&1\\ &&&&&2 \end{pmatrix}$	$\begin{pmatrix} 35&-4&1&-6&-4&-11\\ &56&-14&3&-25&-8\\ &&44&-21&-14&2\\ &&&45&3&-12\\ &&&&56&-8\\ &&&&&59 \end{pmatrix}$
$D_{6,6}$	$\left(\begin{array}{ccccc:c} 1&1&0&0&1&1\\ 1&0&1&0&0&1\\ 1&0&0&1&0&1\\ 0&1&1&1&0&1\\ 0&0&1&1&1&1\\ \hdashline 1&1&1&1&1&0 \end{array}\right)$	$\begin{pmatrix} 4&2&2&2&2&3\\ &3&2&2&2&2\\ &&4&3&2&3\\ &&&4&2&3\\ &&&&3&2\\ &&&&&5 \end{pmatrix}$	$\begin{pmatrix} 45&-12&3&3&-12&-21\\ &59&-8&-8&-22&2\\ &&56&-25&-8&-14\\ &&&56&-8&-14\\ &&&&59&2\\ &&&&&44 \end{pmatrix}$
$D_{6,7}$	$\left(\begin{array}{ccccc:c} 1&1&0&0&1&0\\ 1&0&1&0&0&1\\ 1&0&0&1&0&1\\ 0&1&1&1&0&0\\ 0&0&1&1&1&0\\ \hdashline 0&1&0&0&1&1 \end{array}\right)$	$\begin{pmatrix} 3&1&1&1&1&2\\ &3&1&1&2&1\\ &&3&2&1&1\\ &&&3&1&1\\ &&&&3&1\\ &&&&&3 \end{pmatrix}$	$3\begin{pmatrix} 17&-1&-1&-1&-1&-10\\ &17&-1&-1&-10&-1\\ &&17&-10&-1&-1\\ &&&17&-1&-1\\ &&&&17&-1\\ &&&&&17 \end{pmatrix}$