Maximin Strong Orthogonal Arrays

by

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Abstract

As space-filling designs, orthogonal arrays have been widely used either directly or via OA-based Latin hypercubes in computer experiments. He and Tang (2013) introduced and constructed a new class of arrays, strong orthogonal arrays, for computer experiments. Strong orthogonal arrays of strength t enjoy better space-filling properties than comparable orthogonal arrays of strength t in all dimensions lower than t. Given a single orthogonal array, many strong orthogonal arrays can be generated using the method of He and Tang (2013). We examine the selection of better strong orthogonal arrays using the maximin distance, which is a criterion attempting to place points in a design region so that no two points are too close. In this project, we focus on maximin strong orthogonal arrays of strength three. For small designs, we apply the method of complete search. For large designs, the complete search is infeasible and we propose a search algorithm, which greatly reduces the computation time compared with the complete search approach. The performance of the algorithm is examined and it is found that the algorithm performs almost as well as the complete search.

Key words: Strong Orthogonal Array; Maximin Distance; Search Algorithm

To my family.

“And medicine, law, business, engineering, these are noble pursuits and necessary to sustain life.

But poetry, beauty, romance, love, these are what we stay alive for”

— John Keating, DEAD POETS SOCIETY*, 1989*

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Chapter 1

Introduction

In scientific and engineering research, it is common that systems of interest are often very complicated. Conducting real experiments on such complicated systems can be too expensive or simply infeasible. These systems can be generally approximated by computer models, on which we can run computer experiments. Various models can be built using different methods to emulate the system of interest. We are interested in the relationship between the input and the output of this system. Many input variables can be manipulated over plausible ranges. Constrained by time and resources, we can only run very limited experimental trials. Before running a computer experiment, a key step is to determine what subset of the full input space should be considered, that is, how to select values of input variables for the experiments.

In this chapter, we discuss a general design approach to planning computer experiments and then review relevant concepts such as space-filling designs, Latin hypercubes, OA-based Latin hypercubes and SOA-based Latin hypercubes. A variety of optimality criteria are available to evaluate the space-filling properties of designs. We review the distance-based criteria and in particular the maximin distance criterion in Chapter 2. There are many strong orthogonal arrays available for the experimenter to use but they are not equally space-filling. We use the maximin distance criterion to select preferable strong orthogonal arrays and present the results based on a complete search

in Chapter 3. A complete search for maximin strong orthogonal arrays is feasible for small examples of strong orthogonal arrays. However, when the number of factors and the run size increase, conducting a complete search becomes impractical due to limited computational capabilities under time constraints, hence the need for developing a computationally efficient algorithm. In Chapter 4, we introduce the algorithm and evaluate its performance via comparing with the complete search. In Chapter 5, we conclude this project, provide suggestions for similar studies and also mention possible future work.

1.1 Computer Experiments

A **computer experiment** is used to study a computer model and is conducted by running computer codes that take a set of inputs and produce outputs. The output is usually referred to as the response. Computer models can be either stochastic or deterministic. We limit our discussion to deterministic models. For deterministic computer models, the three basic design principles, randomization, replication and blocking, do not apply. Given the same inputs, the computer code yields identical responses. In computer experiments, the uncertainty comes from the fact that we do not know the exact relationship between the inputs and the response. Computer models built to describe this relationship are just approximations. Two principles for selecting designs are:

1. There should not be more than one observation at any set of inputs. This principle assumes the computer code remains unchanged over time.

2. Designs should allow one to fit various models and should provide information about all portions of the experimental region.

1.2 Space-Filling Designs

Designing a computer experiment is to select values of input variables before running the experiment. Due to the lack of knowledge of the relationship between inputs and outputs, there exist differences between the approximate computer models and the mathematical function representing

the physical experiments. To detect such differences, designs should provide information about all portions of the experimental region. So the approach is to spread the design points throughout the experimental region as evenly as possible. Such designs are referred to as **space-filling designs**. There are a number of ways to define what it means by ”spread points evenly” throughout a region, which corresponds to different criteria for assessing space-filling designs. More will be discussed in Chapter 2.

1.3 Latin Hypercube Designs

One most commonly used class of space-filling designs is that of Latin hypercubes. Latin hypercube designs were introduced in McKay, Beckman and Conover (1979), and achieve uniformity in all one-dimensional projections. In practice, an experiment usually involves a large number of input variables. Due to the curse of dimensionality, it is rather difficult for design points to cover a large portion of a high dimensional design region. Thus, it is more reasonable to consider designs that are space-filling in lower dimensional projections of the input space. We now review the definition of Latin hypercubes.

Definition 1.1. A **Latin hypercube** is a design for m factors in n runs and is represented by an $n \times m$ matrix, where each column is a permutation of n equally spaced levels $x = 0, 1, 2, ..., n-1$.

Example 1.2. Two random Latin hypercubes X_1 and X_2, for three factors in five runs are given below:

$$X_1 = \begin{pmatrix} 1 & 1 & 2 \\ 2 & 2 & 3 \\ 3 & 4 & 1 \\ 4 & 0 & 4 \\ 0 & 3 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 3 & 2 & 4 \\ 2 & 4 & 1 \\ 4 & 0 & 3 \\ 0 & 1 & 2 \\ 1 & 3 & 0 \end{pmatrix}.$$

1.4 Orthogonal Array-Based Latin Hypercubes

Orthogonal arrays were originally developed by Rao (1947). Orthogonal array-based Latin hypercube designs, also known as U designs, were proposed by Tang (1993). We will review the concept of orthogonal arrays and the construction of OA-based Latin hypercubes.

Definition 1.3. An $n \times m$ matrix is an n-run **orthogonal array** of strength t and index λ with m factors each at s levels if all possible t-tuples appear in each $n \times t$ submatrix with the same frequency λ satisfying $n = \lambda s^t$. This orthogonal array is denoted by $OA(n, m, s, t)$.

A Latin hypercube is an orthogonal array of strength 1. An orthogonal array with mixed levels can be similarly defined, and is denoted by $OA(n, m, s_1 \times ... \times s_m, t)$.

Definition 1.4. Let A be an $OA(n, m, s, t)$. For each column of A with entry $k = 0, 1, ..., s-1$, replace the λs^{t-1} entries for level k with a random permutation of $k\lambda s^{t-1}$, $k\lambda s^{t-1}+1$, ..., $k\lambda s^{t-1}+\lambda s^{t-1}-1 = (k+1)\lambda s^{t-1} - 1$. After the replacement, the design is an **OA-based Latin hypercube**.

Example 1.5. A strength two orthogonal array A is given below, which is an $OA(4, 2, 2, 2)$. Based on this orthogonal array A, many Latin hypercubes can be generated. Designs D_1, D_2, D_3, D_4 and D_5 are just some randomly generated Latin hypercubes based on the orthogonal array A.

$$A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}, \; D_1 = \begin{pmatrix} 0 & 1 \\ 1 & 3 \\ 2 & 0 \\ 3 & 2 \end{pmatrix}, \; D_2 = \begin{pmatrix} 0 & 0 \\ 1 & 3 \\ 3 & 1 \\ 2 & 2 \end{pmatrix}, \; D_3 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \\ 3 & 1 \\ 2 & 3 \end{pmatrix}, \; D_4 = \begin{pmatrix} 1 & 1 \\ 0 & 3 \\ 2 & 0 \\ 3 & 2 \end{pmatrix}, \; D_5 = \begin{pmatrix} 1 & 0 \\ 0 & 3 \\ 2 & 1 \\ 3 & 2 \end{pmatrix}.$$

Latin hypercubes achieve uniformity in all one-dimensional projections. A random Latin hypercube design is not guaranteed to achieve uniformity in multi-dimensional projections, but an OA-based Latin hypercube enjoys a multi-dimensional space-filling property. OA-based Latin hypercubes achieve uniformity in t-dimensional projections when orthogonal arrays of strength t are used.

1.5 Strong Orthogonal Array-Based Latin Hypercubes

Definition 1.6. An $n \times m$ matrix with entries from levels $\{0, 1, ..., s^t - 1\}$ is a **strong orthogonal array** of n runs, m factors, s^t levels and strength t if any subarray of g columns for any g with $1 \leq g \leq t$ can be collapsed into an $OA(n, g, s^{u_1} \times s^{u_2} \times ... \times s^{u_g}, g)$ for any positive integers $u_1, ..., u_g$ with $u_1 + ... + u_g = t$, where collapsing into s^{u_j} levels is done by dividing the entries by s^{t-u_j} and then taking the largest integer not exceeding the resulting entries, equivalently $[a/s^{t-u_j}]$. We denote such a strong orthogonal array as $SOA(n, m, s^t, t)$.

Example 1.7. A strength three strong orthogonal array D is given below, which is an $SOA(8, 3, 2^3, 3)$. Collapsing the first two columns into 2×4 and 4×2 levels gives C_1 and C_2. Similarly, C_3 and C_4 are obtained from the first and the last columns. We see that C_1, C_3 are $OA(8, 2, 2 \times 2^2, 2)$ and C_2, C_4 are $OA(8, 2, 2^2 \times 2, 2)$.

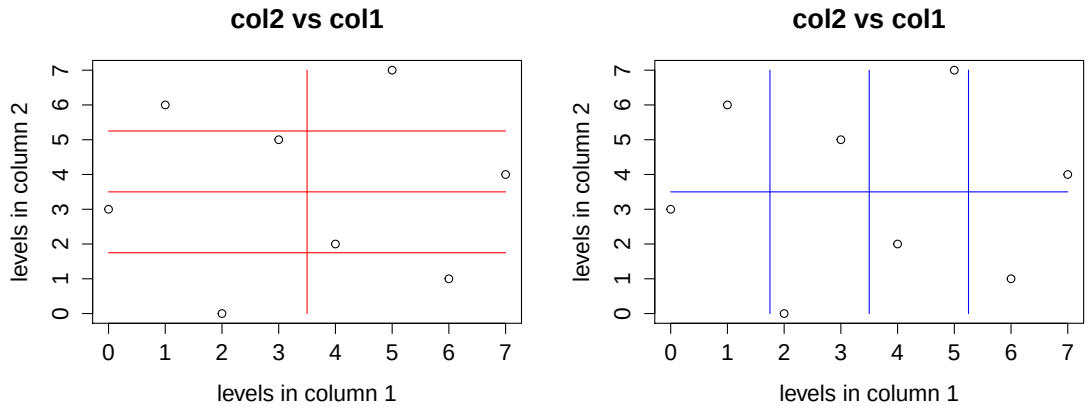
$$D = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 6 \\ 1 & 6 & 2 \\ 3 & 5 & 4 \\ 4 & 2 & 3 \\ 6 & 1 & 5 \\ 7 & 4 & 1 \\ 5 & 7 & 7 \end{pmatrix}, \; C_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 0 & 3 \\ 0 & 2 \\ 1 & 1 \\ 1 & 0 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}, \; C_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 1 & 1 \\ 2 & 0 \\ 3 & 0 \\ 3 & 1 \\ 2 & 1 \end{pmatrix}, \; C_3 = \begin{pmatrix} 0 & 0 \\ 0 & 3 \\ 0 & 1 \\ 0 & 2 \\ 1 & 1 \\ 1 & 2 \\ 1 & 0 \\ 1 & 3 \end{pmatrix}, \; C_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 1 & 1 \\ 2 & 0 \\ 3 & 1 \\ 3 & 0 \\ 2 & 1 \end{pmatrix}.$$

Definition 1.8. Recall that a Latin hypercube of n runs for m factors is an $n \times m$ matrix where each column is a permutation of $0, 1, ..., n - 1$. The index of the strong orthogonal array λ is defined the same way as that of an orthogonal array. Since the index satisfies $n = \lambda s^t$, an $SOA(n, m, s^t, t)$ itself is a Latin hypercube when $\lambda = 1$. When $\lambda \geq 2$, the SOA is not a Latin hypercube but can be converted into one by expanding the s^t levels into $n = \lambda s^t$ levels. For each column of the SOA, this is done by replacing the λ entries for level j by any permutation of $j\lambda, j\lambda + 1, ..., (j + 1)\lambda - 1$ for $j = 0, 1, ..., s^t - 1$. The Latin hypercubes generated this way is called **SOA-based Latin hypercubes**.

Strong orthogonal arrays (SOAs) were introduced and constructed by He and Tang (2013). An $SOA(n, m, s^t, t)$ promises a stratification of design points on an $s^{u_1} \times ... \times s^{u_g}$ grid for any positive u_j with $u_1 + ... + u_g = t$ on any g-variate margins, where $g \leq t$. In addition to retaining all the projection space-filling properties of an SOA, a Latin hypercube based on an $SOA(n, m, s^t, t)$ maximizes the stratification for one-dimensional projections.

Both a Latin hypercube based on an $SOA(n, m, s^2, 2)$ and one based on an $OA(n, m, s, 2)$ achieve a stratification on an $s \times s$ grid in any two-dimensional projection. Hence, Latin hypercubes based on the $OA(n, m, s, 2)$ are as space-filling in two-dimensional projections as Latin hypercubes based on the $SOA(n, m, s^2, 2)$. For strength three or higher, SOA-based Latin hypercubes are more space-filling than OA-based Latin hypercubes when projected on g dimensions, where $1 < g < t$. For two Latin hyperubes of strength three, one is based on an $OA(n, m, s, 3)$ and the other based on an $SOA(n, m, s^3, 3)$. Both achieve a stratification on an $s \times s \times s$ grid on any trivariate margin. But the Latin hypercube based on the $SOA(n, m, s^3, 3)$ achieves stratifications on $s^2 \times s$ and $s \times s^2$ grids on any bivariate margin, while that based on the $OA(n, m, s, 3)$ ensures a stratification on an $s \times s$ grid on any bivariate margin.

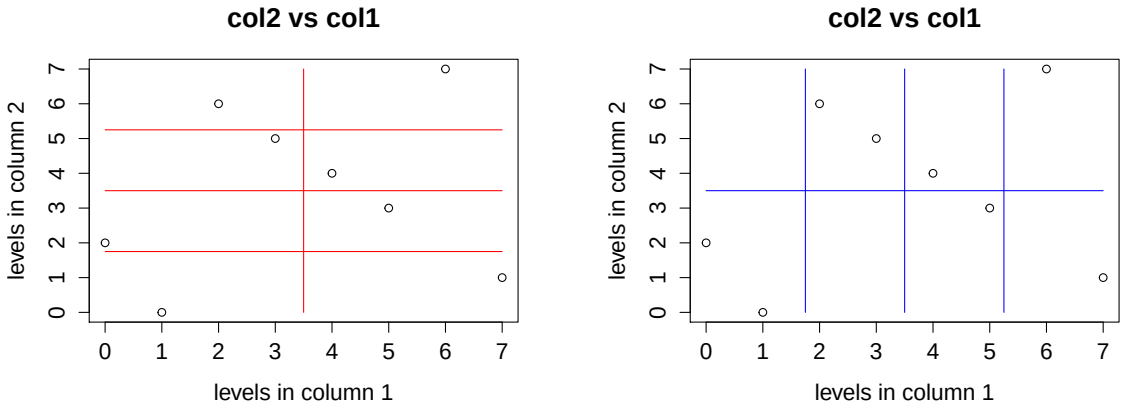
Figure 1.1 shows the two-dimensional projections of an $SOA(8, 3, 2^3, 3)$, design D from Example 1.7, which is also a Latin hypercube since $\lambda = 1$. For first two columns, stratifications are achieved on 2×4 grids as in (a) and 4×2 grids as in (b); such stratifications also hold for any other two columns, 3 vs.1 and 3 vs. 2. Figure 1.2 provides the two-dimensional projections for a Latin hypercube based on an $OA(8, 3, 2, 3)$. This OA-based Latin hypercube achieves a stratification on 2×2 grid as in (c). But stratifications on finer grids are not promised as in (b). Stratification on 2×4 grids is achieved, but this is not guaranteed for all OA-based Latin hypercubes.



(a) SOA: 2 × 4 grid

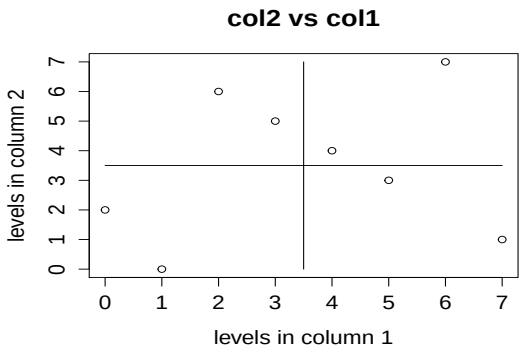
(b) SOA: 4 × 2 grid

Figure 1.1: 2D projection of an SOA (also a Latin hypercube)



(a) OALH: 2 × 4 grid

(b) OALH: 4 × 2 grid



(c) OALH: 2 × 2 grid

$$\begin{pmatrix} 0 & 2 & 1 \\ 1 & 0 & 5 \\ 3 & 5 & 2 \\ 2 & 6 & 6 \\ 5 & 3 & 0 \\ 7 & 1 & 7 \\ 4 & 4 & 3 \\ 6 & 7 & 4 \end{pmatrix}$$

(d) The OA-based Latin hypercube

Figure 1.2: 2D projection of an OA-based Latin hypercube

Chapter 2

Distance-Based Design Selection Criteria

There is a large number of strong orthogonal arrays available and we suspect that they are not equally space-filling. To choose strong orthogonal arrays that have better space-filling properties, we need to adopt some optimality criteria. In Section 2.1, we give a general introduction to these criteria. In Sections 2.2, 2.3 and 2.4, we review distance-based criteria and discuss the minimax and maximin criteria. We will use the maximin criterion to select preferable arrays among a family of strong orthogonal arrays.

2.1 Space-Filling Criteria

One idea of finding more space-filling designs is to apply some optimality criteria to the available designs and select those with desirable space-filling properties. To evaluate the space-filling property of a design, several criteria have been developed in the literature. Some select points in the experimental region using certain sampling methods, others are based on a measure of distance between points, and still more look at how uniformly distributed the points are throughout a region. For a detailed discussion, see Santner, Williams and Notz (2003).

2.2 Distance-Based Criteria

We consider the criteria for selecting a design based on a measure that quantifies how "spread out" a set of points is. One way in which design points may be considered "spread out" is to avoid two design points that are "too" close together; another way in which designs points may be regarded as "spread out" is to make every point in the design space close to some point in the design. These are the fundamental ideas of maximin and minimax distance criteria, which were originally introduced in Johnson, Moore and Ylvisaker (1990).

More precisely, consider a design consisting of n distinct design points $\{ \vec{x_1}, \vec{x_2},...,\vec{x_n} \}$ in a d-dimensional space. The location of design points in the experimental region represents the site of chosen inputs in the plausible space for input variables. An important distance measure is the pth-order distance between two points $\vec{x}$ and $\vec{y}$ in the design region. We use the Euclidean and rectangular distances between two points, which is d_p for $p = 2$ and $p = 1$ respectively:

$$d_p(\vec{x}, \vec{y}) = [\sum_{i=1}^{d} |x_i - y_i|^p]^{1/p} \ , \ p \geq 1.$$

2.3 Minimax Distance Criterion

Suppose the firefighting department will be setting up new fire stations in a new region. The following considerations must be made when choosing the sites. Given that there is a fire, it should be obvious that a fire truck will be dispatched from the closest fire station to the scene of the fire. However, not all locations will be equidistant from its closest fire station, leaving those furthest from the nearest station to be in the worst case scenario should a fire occur there. Taking this into consideration, the department must now consider optimizing (minimizing) the longest (maximum) distance to travel from the closest (minimum) fire station for every location in the region so that the firefighting services are more evenly distributed throughout the region. This is in essence what the minimax distance criterion is aiming for.

The minimax criterion considers the distance from a given point in the design region to the closest design point. This is just the distance from a place to its closest fire station. We regard this distance as the distance between a point $\vec{x}$ and a design D:

$$d_p(\vec{x}, D) = \min_{\vec{x_i} \in D} d_p(\vec{x}, \vec{x_i}).$$

For any design D, the worst place will have a maximum distance to its closest fire station. Different designs will have different maximum distances to its closest fire stations, $\max_{\vec{x}}\ d_p(\vec{x}, D)$. A design is a **minimax distance design** if the maximum distance between arbitrary points $\vec{x}$ in the experimental region and the design is a minimum among all designs, i.e., D^* is a minimax distance design if

$$\max_{\vec{x}}\ d_p(\vec{x}, D^*) = \min_{all\ D}\ \max_{\vec{x}}\ d_p(\vec{x}, D).$$

2.4 Maximin Distance Criterion and Φ_p Criterion

A **maximin distance design** is a design that maximizes the minimum inter-site distance $d_p(\vec{x_i}, \vec{x_j})$ for $1 \leq i, j \leq n$ and $i \neq j$, equivalently

$$\max_{all\ D}\ \min_{\vec{x_i}, \vec{x_j} \in D} d_p(\vec{x_i}, \vec{x_j}).$$

It is undesirable to have design points that are too close, so the maximin criterion tries to avoid such cases. Maximin designs guarantee that no two points in the design are ”too close”, which makes design points spread out over the experimental region.

Morris and Mitchell (1995) further discussed the maximin distance criterion for computer experiments and introduced a more elaborate version of the criterion. For a given design, consider the list of distinct distances between design points (d_1, d_2, ... , d_q) sorted in ascending order. Let J_j denote the number of pairs of design points separated by distance d_j. The index list (J_1, J_2, ... J_q) can be obtained. A design is maximin if

- among available designs, it maximizes d_1;
- among those, it also minimizes J_1;
- among those, it maximizes d_2;
- among those, it minimizes J_2;

  ...

- among those, it maximizes d_q;
- among those it minimizes J_q.

Going through this selection process, we can select preferable designs according to the maximin criterion. We consider not only maximizing the shortest distance but also minimizing the number of pairs reaching this distance. This criterion further maximizes subsequent shorter distances and minimizes the number of pairs reaching these distances. This more elaborate version further distinguishes designs when they have the same minimum distance and the same number of pairs reaching the minimum distance.

However, this procedure is not efficient, so a computationally convenient surrogate is used instead. A scalar-value criterion function can be used to rank competing designs,

$$\Phi_p(D) = [\sum_{j=1}^{q}(J_j d_j^{-p})]^{1/p} = (\sum_{j=1}^{m} d_j^{-p})^{1/p},$$

where p is a positive integer. Here q represents the number of distinct distances between two design points while m is the total number of point pairs, and clearly $m = \binom{n}{2}$. For large enough p, each term in the sum dominates subsequent terms; in other words, term d_1^{-p} dominates that of d_2^{-p}; also d_2^{-p} term dominates that of d_3^{-p}; ... ; and d_{q-1}^{-p} term dominates that of d_q^{-p}. For any given sets of designs, the designs that minimize the Φ_p value are preferable designs. With a very large p, the Φ_p criterion is equivalent to the maximin distance criterion.

Chapter 3

Maximin Strong Orthogonal Arrays by Complete Search

In this chapter, we search for preferable arrays among a class of strong orthogonal arrays (SOAs). The focus is on the case of strength three. The reason is as follows: strength two SOAs are no more space-filling than strength two OAs; SOAs of strength four or higher are too expensive to use in practice because two or more columns have to be sacrificed to obtain SOAs from an OA. Constructing strength three SOAs only sacrifices one column in an OA, which is a reasonable price to pay for obtaining more space-filling SOA-based Latin hypercubes.

3.1 Method of Complete Search and an Illustrative Example

Based on a given orthogonal array, we can produce a family of strong orthogonal arrays as proposed in He and Tang (2013). For a given ordinary orthogonal array $OA(n, m, s, 3)$, we denote the ith column of the array as a_i. Let $A = OA(n, m, s, 3) = (a_1, a_2, ..., a_m)$. Given A, an $n \times 3m'$ array B can be constructed with b_{ij}'s obtained by (3.1)-(3.3). Here $m' = m - 1$.

$$B = \{(b_{11}\ b_{12}\ b_{13}); ...; ((b_{m'1}\ b_{m'2}\ b_{m'3})\}$$

$$(b_{11}, ..., b_{m'1}) = (a_1, ..., a_{m'}) \quad (3.1)$$

$$(b_{12}, ..., b_{m'2}) = (a_m, ..., a_m) \quad (3.2)$$

$$(b_{13}, ..., b_{m'3}) = (a_2, ..., a'_m, a_1). \quad (3.3)$$

Then a strong orthogonal array $D = (d_1, ..., d_{m'}) = SOA(n, m', s^3, 3)$ can be generated by

$$d_i = \sum_{j=1}^{3} b_{ij} s^{3-j}. \quad (3.4)$$

We give an example to illustrate how to construct SOAs based on an OA. Consider $A = OA(8, 4, 2, 3) = (a_1, a_2, a_3, a_4)$, we obtain an array $B = \{(a_1\ a_4\ a_2); (a_2\ a_4\ a_3); (a_3\ a_4\ a_1)\}$. Then we generate $D = SOA(8, 3, 2^3, 3) = (d_1, d_2, d_3)$ by

$$d_1 = 4a_1 + 2a_4 + a_2, \quad (3.5)$$

$$d_2 = 4a_2 + 2a_4 + a_3, \quad (3.6)$$

$$d_3 = 4a_3 + 2a_4 + a_1. \quad (3.7)$$

In this example, various permutations of levels (symbols) within a_i's in (3.5)-(3.7) can generate different corresponding SOAs. For example, based on A given below, we generate two SOAs D_1 and D_2. The first array is obtained by using (3.5)-(3.7). The only difference for the second is by permuting the symbols 0,1 in a_1 in (3.5).

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad D_1 = \begin{pmatrix} 0 & 0 & 0 \\ 2 & 3 & 6 \\ 3 & 6 & 2 \\ 1 & 5 & 4 \\ 6 & 2 & 3 \\ 4 & 1 & 5 \\ 5 & 4 & 1 \\ 7 & 7 & 7 \end{pmatrix}, \quad D_2 = \begin{pmatrix} 4 & 0 & 0 \\ 6 & 3 & 6 \\ 7 & 6 & 2 \\ 5 & 5 & 4 \\ 2 & 2 & 3 \\ 0 & 1 & 5 \\ 1 & 4 & 1 \\ 3 & 7 & 7 \end{pmatrix}$$

After generating a family of SOAs, we apply the maximin distance criterion to select preferable SOAs. We call such preferable arrays **maximin SOAs**. The basic idea of complete search for maximin SOAs is to rank the set of SOAs using the Φ_p criterion introduced in Section 2.4. The designs with minimal Φ_p are optimal designs. We can tune the value of p depending on the size of designs to ensure this criterion selects the maximin designs.

The complete search method has the following steps:

Step I Given an $OA(n, m, s, 3)$ with symbols $0, 1, ..., s-1$, generate an $SOA(n, m', s^3, 3)$ using (3.4) with b_{ij}'s defined as (3.1) - (3.3).

Step II Generate different SOAs by permuting symbols for the columns of A, a_i's, within the formula for d_j. There are $s!$ permutations of symbols for each column of A and there are $3m'$ positions of a_i where we can permute symbols. So in total, $(s!)^{3m'}$ SOAs can be generated.

Step III a List $\binom{n}{2}$ distances between point pairs. Given a p value, compute Φ_p for each SOA.

Step IV a Find the SOAs with the minimal Φ_p value and suppose there are q such SOAs.

These resulting q SOAs are the maximin SOAs for an appropriately chosen p.

3.2 Search Results and Discussion

Using the complete search method, we have obtained the maximin SOAs of strength three for 8 runs, 16 runs and 27 runs. Based on the Φ_p value, it is difficult to understand how diverse the designs are in terms of their distance properties. To have a better understanding of how the generated SOAs vary, we provide the results using the variants b of Steps III and IV instead.

Step III b Compute the minimal distance and record the number of pairs reaching this distance.

Step IV b Find SOAs with the maximized minimal distance, and among these candidate SOAs, find those with the smallest number of point pairs reaching this distance.

Table 3.1: Complete search results for maximin SOAs

	Euclidean distance				Rectangular distance				
Runs	MinDist	Pairs	%	Designs	MinDist	Pairs	%	Designs	Note
8	4.12	6	6.25	32	7	6	6.25	32	same[a]
	3	2	37.5	192	5	2	18.75	96	-
	3	4	37.5	192	5	3	18.75	96	-
	...				...				-
	1.73	1	6.25	32	3	1	6.25	32	-
				512				512	
16	7.141	2	0.0488	128	16	14	0.0488	128	same
	7.141	4	0.1465	384	15	2	0.3418	896	-
	7.141	8	0.0977	256	15	4	0.4395	1152	-
	...				...				-
	2.646	1	0.0488	128	7	1	0.0488	128	-
				262144 [b]				262144	
27	8.775	24	0.0064	3	14	3	0.0043	2	-
	8.367	18	0.0064	3	14	6	0.0021	1	-
	8.062	3	0.0386	18	14	18	0.00643	3	-
	...				...				-
	1.732	1	0.0450	21	3	1	0.0450	21	-
				46656				46656	

[a] The maximin SOAs are the same using the Euclidean or rectangular distance

[b] For 16 runs, $2^{21} = 2097152$ SOAs can be generated. The search result, however, shows that permuting the leading columns, a_1 in (3.5), a_2 in (3.6) and a_3 in (3.7), won't change the distribution of distances, leaving only $2^{18} = 262144$ SOAs; Similarly, we can reduce $6^9 = 10077696$ to $6^6 = 46656$ SOAs for 27 runs.

Using the method above, we present a summary of the complete search results. For each size, the distance between point pairs is either the Euclidean distance or the rectangular distance. Among all SOAs generated, only a small portion are maximin SOAs: 32 out of 512 for 8 runs; 128 out of 262144 for 16 runs; 3 out of 46656 using the Euclidean distance and 2 out of 46656 using the rectangular distance for 27 runs. The generated SOAs seem to differ by much when comparing their minimal distances between point pairs. The minimal Euclidean distances between point pairs range from 1.73 to 4.12 for 8 runs, 2.65 to 7.14 for 16 runs, 1.73 to 8.77 for 27 runs; the minimal rectangular distances between point pairs range from 3 to 7 for 8 runs, 7 to 16 for 16 runs, 3 to 14 for 27 runs. If you generate an SOA randomly, it is most likely not maximin. From the complete search, the percentage of the SOAs that are maximin is around 6.25% for 8 runs, 0.05% for 16 runs and 0.006% for 27 runs.

Some of the maximin SOAs found may be geometrically isomorphic (Cheng and Ye, 2004). Two designs are **geometrically isomorphic** if one can be obtained from the other by reordering the runs, relabelling the factors and/or reversing the level order of one or more factors. For 8 runs, all the 32 maximin SOAs are found to be geometrically isomorphic; For 27 runs, there are in total two non-isomorphic maximin SOAs; For 16 runs, it is too time-consuming to check for geometrical isomorphism among the 128 maximin SOAs.

A collection of obtained maximin SOAs is provided in Appendix A, giving the experimenter the flexibility to apply a secondary criterion to select even more preferable arrays. For larger size SOAs, this complete search algorithm still works but is rather time consuming. To find maximin SOA of run size n, m constraints each with s levels, $SOA(n, m, s^3, 3)$, $(s!)^{3m}$ SOAs can be generated by permuting the symbols in each column of A in the formula. Complete search for maximin $SOA(64, 3, 4^3, 3)$ requires calculating 2016 distances for each design, evaluating the Φ_p values for 2,641,807,540,224 designs. The amount of evaluations increases exponentially every time m increases by 1. As the number of factors and the run size increase, the complete search can take an insurmountable amount of time. This justifies a need for a much more efficient method to search for larger maximin SOAs. So we will propose a computationally efficient algorithm to search for maximin SOAs in the next chapter.

Chapter 4

Maximin Strong Orthogonal Arrays by Algorithmic Search

In the previous chapter, we have found maximin SOA designs of strength three for 3 factors in 8 runs, 7 factors in 16 runs and 3 factors in 27 runs. When the run size n $>$ 27 or the number of factors m $>$ 7, the complete search method requires a huge amount of computation. The proposed algorithm in this chapter takes much shorter time to obtain the optimal designs under the maximin criterion.

4.1 Basic Idea

Suppose a group of scientists wants to find the point with the lowest elevation in an area. They start with measuring the elevations of a chosen location S_0 and nine other locations $S_1, S_2, ..., S_9$ evenly spaced in the neighbourhood of S_0 with the same distance (1km) away from S_0. If the current location S_0 does not have the lowest elevation among the nine neighbouring locations, then the scientists will move to the new location that is the lowest among the nine. If there happens to be more than one neighbour having the lowest elevation, then just randomly choose one of these neighbours to move to. The idea is that as one moves towards lower and lower elevations, it becomes more and more likely to reach the lowest point in the area. The search will continue until the current location

is the lowest among its neighbours. Given that there is no new lowest location from the nine 1km away neighbours, the search will be expanded to the 2km away neighbourhood. If a new lowest location is detected, the scientists will move to this new location and search in a neighbourhood starting from 1km radius. Again, the scientists will keep moving to the new lowest location until no neighbour with lower elevation is found within 2km-radius neighbourhood. This final location is the lowest point found when starting from location S_0.

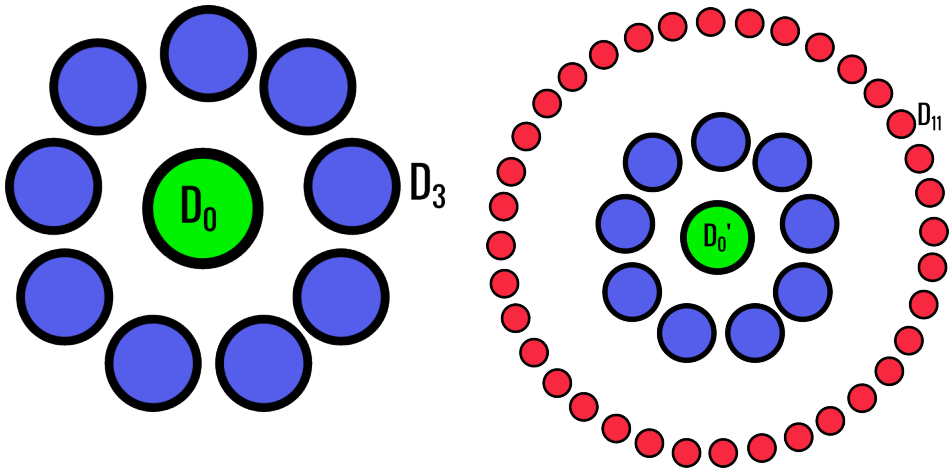
A useful strategy to increase the chance of finding the lowest point in an area is to start the search at different locations. Navigation starting from different points may lead to discovering other better local optimal points or the global optimal point. The example here limits the local search within a radius of 2km; one may expand the maximum search radius to 4km or even 6km. The radius is restricted because as you increase the maximum search radius, more candidate neighbours will be scanned and it can become increasingly computationally expensive. So it will be wise to flexibly modify this maximum search radius depending on the size of the radius relative to the whole area.

4.2 An Illustrative Example

The idea of the algorithm is fairly similar to the method of exploring the lowest point in an area. Consider the problem of searching for maximin SOAs of strength three in 8 runs, $SOA(8, 3, 2^3, 3)$. Following Step I in Chapter 3, we start with a randomly generated SOA, D_0, obtained from an OA. The one-unit away neighbours around D_0 can be obtained by permuting symbols in just one column of the OA, a_i, in the formulas (3.5)-(3.7). Compute the distances between any two points of D_0 and also those for the nine neighbours, which gives a sequence of $\binom{8}{2} = 28$ distances $d_1, d_2, ..., d_{28}$ for each design. Then compute the Φ_p value for each design. In this illustrative example, we use rectangular distance and $p = 4$ in Table 4.1.

	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9
$\Phi_4(D)$	0.3193	0.3196	0.3332	**0.2993**	0.3196	0.3332	**0.2993**	0.3196	0.3332	**0.2993**

Table 4.1: Φ values for the starting design and its neighbours



(a) One-unit away neighbours (b) One and two-unit away neighbours

Figure 4.1: Illustrative pictures of designs and their neighbours

	D_0'	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9
$\Phi_4(D)$	**0.2993**	0.3193	0.3332	0.3196	0.3193	0.3332	0.3196	0.3193	0.3332	0.3196

Table 4.2: Φ values for the current design and its one-unit away neighbours

We see that the neighbours D_3, D_6 and D_9 have the smallest Φ_4 value. Here we just move to one of these neighbours. Suppose that D_3 is randomly selected among the three best neighbours. See Figure 4.1 (a) for the illustrative picture: the large center circle (green) represents the initial design D_0 and surrounding smaller circle (blue) represent the one-unit away neighbours of D_0, with D_3 minimizing the Φ_4 value. We then treat D_3 as our current optimal design, new D_0, denoted by D_0' and obtain its nine new neighbours. Again, we compute the corresponding Φ_4 values for this current design and its neighbours, as seen in Table 4.2. Comparing D_0' with its one-unit away neighbours, it is still our current optimal design, which minimizes the Φ_4 value. We have found the optimal design among its one-unit away neighbours, D_0'. But we cannot claim it as the optimal design yet.

To avoid searching within "too" small a neighbourhood for the lowest point in an area, we need to look into further away neighbourhood. Similarly, we need to check neighbours that are two units away from D_0'. So we expand the search from one-unit away neighbourhood (medium-size blue circle) to two-unit away neighbourhood (small red circle) as in Figure 4.1 (b). In other words, obtain 36, i.e. $\binom{3m}{2}$ when $m = 3$, neighbouring designs and calculate their Φ_4 values. From Table 4.3,

	D_0'	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9
$\Phi_4(D)$	0.2993	0.3196	0.333	0.3346	0.3196	0.3110	0.3196	0.2993	0.3657	0.3657
		D_{10} D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}
$\Phi_4(D)$	0.2993	**0.2748**	0.311	0.3346	0.3196	0.311	0.3193	0.311	0.3196	0.3193
	D_{20}	D_{21}	D_{22}	D_{23}	D_{24}	D_{25}	D_{26}	D_{27}	D_{28}	D_{29}
$\Phi_4(D)$	0.333	0.3196	0.3196	0.311	**0.2748**	0.2993	0.3193	0.3193	0.2993	0.3193
	D_{30}	D_{31}	D_{32}	D_{33}	D_{34}	D_{35}	D_{36}			
$\Phi_4(D)$	0.311	0.3193	0.333	0.3196	0.3196	0.333	0.3193			

Table 4.3: Φ values for the current design and its two-unit away neighbours

	D_0'	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9
$\Phi_4(D)$	**0.2748**	0.3110	0.3193	0.2993	0.3110	0.3193	0.2993	0.3110	0.3193	0.2993

Table 4.4: Φ values for the current design and its one-unit away neighbours

D_{11} and D_{24} minimize the Φ_4 value among its two-unit away neighbours. Suppose D_{11} is randomly selected among the two best neighbours. Since D_{11} is treated as the current optimal design, we replace D_0' by D_{11}. Then we move to D_0'. For the current design D_0', we checked all of its one-unit and two-unit away neighbours and found that D_0' is the optimal design compared to one-unit and two-unit away neighbours (Tables 4.4 and 4.5) and we denote it as D_L.

4.3 Algorithm and Search Results

The algorithm for finding maximin $SOA(n, m, s^3, 3)$ can be summarized as follows:

	D_0'	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9
$\Phi_4(D)$	**0.2748**	0.2993	0.3193	0.3196	0.3346	0.3193	0.2748	0.2993	0.3193	0.3193
	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}
$\Phi_4(D)$	0.2993	0.3196	0.3332	0.2993	0.3196	0.3332	0.3657	0.3110	0.3196	0.3193
	D_{20}	D_{21}	D_{22}	D_{23}	D_{24}	D_{25}	D_{26}	D_{27}	D_{28}	D_{29}
$\Phi_4(D)$	0.3110	0.3196	0.3196	0.311	0.3196	0.2993	0.3657	0.3657	0.2993	**0.2748**
	D_{30}	D_{31}	D_{32}	D_{33}	D_{34}	D_{35}	D_{36}			
$\Phi_4(D)$	0.3110	0.3193	0.3110	0.3196	0.3196	0.3110	0.3193			

Table 4.5: Φ values for the current design and its two-unit away neighbours

STEP A For given n, m, s, obtain an $OA(n, m+1, s, 3)$ using symbols $0, 1, ..., s-1$. For the $(m+1)$ columns, keep all the possible symbol permutations of each column in a list. Each column has $s!$ symbol permutations. If $s = 2$, only two permutations are available, which is 01 and 10. If $s = 3$, there are six permutations available, that is 012, 021, 102, 120 ,201, and 210.

STEP B Construct an initial SOA using (3.1) - (3.4) with a random choice of symbol permutation for the $3m$ a_i's. Denote this initial SOA as D_0.

STEP C Obtain a list of the current SOA and its one-unit away neighbours. The length of this list is $(3m+1)$. The one-unit away neighbours are obtained by permuting symbols in one column of OA, i.e. a_i in (3.1) - (3.4). After obtaining the $3m$ such neighbours, compute the Φ_p values for the designs in this list using the Φ criterion function for a specified p value as given below.

$$\Phi_p(D) = (\sum_{j=1}^{m} d_j^{-p})^{1/p}.$$

If there is more than one design that minimizes the Φ_p value and the current one is not one of them, then replace the current design D_0 by one of the designs minimizing Φ_p.

STEP D Repeat STEP C until the current SOA D_0 is one of the designs with the smallest Φ_p value among the one-unit away neighbours. Denote the current design as D_0 when the repeat stops.

STEP E Obtain a list of the current SOA and its two-unit away neighbours, the length of this list is $\binom{3m}{2}+1$. The two-unit away neighbours are obtained by permuting symbols in any two columns of OA, i.e. a_i and a_j in (3.1) - (3.4). After obtaining the $\binom{3m}{2}$ such neighbours, compute the Φ_p values for the designs in this list.

STEP F If the current design D_0 does not minimize the Φ_p value among its two-unit away neighbours, set D_0 to one of the designs minimizing Φ_p and start from STEP C again. Otherwise, the current design D_0 is the optimal design found by the algorithm.

The complete search approach requires comparing $(s!)^{3m}$ designs. In contrast, the algorithm developed in this chapter requires comparing D_0 with $3m$ designs for Step C and $\binom{3m}{2}$ designs for Step E. The algorithmic search requires 2 to 7 iterations for 8-run SOAs, 3 to 12 iterations for 16-run SOAs and 3 to 16 iterations for 27-run SOAs, showing a great reduction in the amount of computation.

There is no guarantee that the proposed algorithm will produce a maximin SOA (global optimal design) since the algorithm is based on a local search. As shown in the next section, our algorithm actually performs quite well, at least for the cases we have examined.

4.4 Performance of Algorithm

In Chapter 3, we have found the maximin SOA designs for 8 run, 16 runs, and 27 runs using the complete search. We will compare these results with those found using our algorithm. The comparison is based on the Φ_p values. For 8-run SOAs for three factors, there are 512 SOAs that can be generated using the method in Chapter 3. Using our algorithm we can always find a maximin SOA for 8 runs. For 16-run SOAs for 7 factors, there are 262144 SOA designs in total. For each 16-run design, there are 21 one-unit away neighbours and 210 two-unit away neighbours. For 27-run SOAs for 3 factors, there are 46656 SOA designs that can be generated.

For each run size, we use the histogram of the Φ_p values of all the generated SOAs to assess the performance of our algorithm. The vertical lines are the first quartile (green), median (blue), and the third quartile (orange) from left to right. We run our algorithm 100 times for each p value and the large red and the small brown triangles mark the positions of the design found with the largest Φ_p (the worst case) and the smallest Φ_p (the best case) among the hundred trials. We present the histograms for $p = 1, 3, 6, 9$ (16-run SOAs) in Figure 4.2, and $p = 1, 3, 5, 7$ (27-run SOAs) in Figure 4.3. We have also investigated other p values. All these results show that although our algorithm may not find the maximin design all the time, it always generates designs very close to the maximin.

Euclidean:	Φ_1	Frequency	Position
	21.517	50	1
	21.528	9	2
	21.580	34	7
	21.589	5	9
	21.593	1	10
	21.605	1	12

Euclidean:	Φ_3	Frequency	Position
	0.4912	33	1
	0.4928	12	2
	0.4947	48	5
	0.4952	6	6
	0.4955	1	9

Euclidean:	Φ_5	Frequency	Position
	0.4912	33	1
	0.4928	12	2
	0.4947	48	5
	0.4953	6	6
	0.4955	1	9

Euclidean:	Φ_7	Frequency	Position
	0.193	20	1
	0.195	79	3
	0.196	1	5

Rectangular:	Φ_1	Frequency	Position
	14.238	49	1
	14.245	7	2
	14.283	40	6
	14.287	1	8
	14.293	1	10
	14.294	2	11

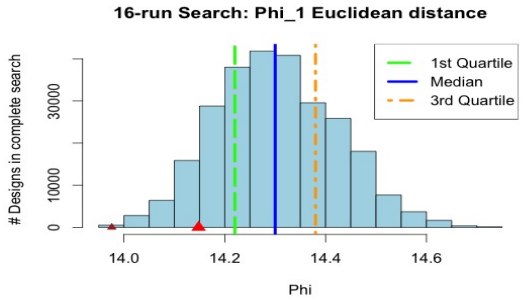
Rectangular:	Φ_3	Frequency	Position
	0.320	33	1
	0.321	8	2
	0.323	58	6
	0.324	1	7

Rectangular:	Φ_5	Frequency	Position
	0.1592	33	1
	0.1604	16	2
	0.1619	47	6
	0.1620	4	7

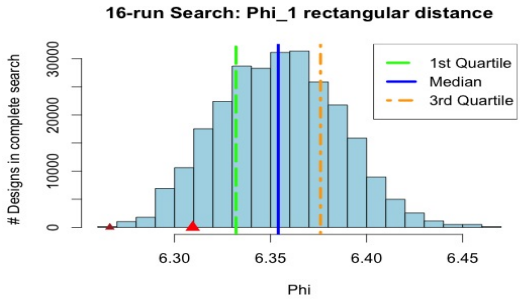
Rectangular:	Φ_7	Frequency	Position
	0.1205	33	1
	0.1217	3	2
	0.1220	7	3
	0.1232	53	4
	0.1233	4	5

Table 4.6: Distribution of Φ_p values for 27-run algorithmic search

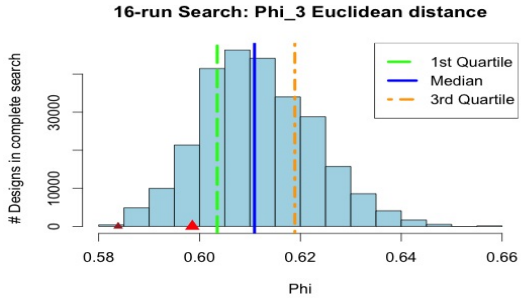
To get a closer look at the performance of the algorithm, for SOAs of 27 runs, we run our algorithm 100 times and present the resulting distribution of Φ_p and their positions among the 46656 designs in Table 4.6. For almost all p values investigated, designs at the first position (minimizing the Φ_p value) are found 20 out of 100 times in the worst case and 50 out of 100 times in the best case. It is also seen that the algorithm outputs the top-ranked designs in all cases.



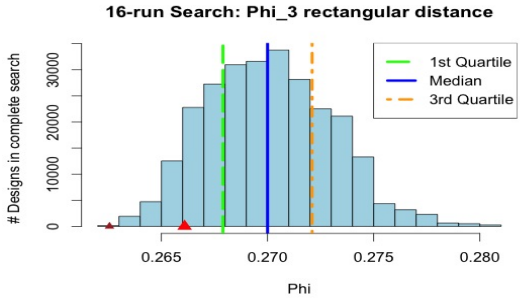
(a) Euclidean distance, p=1



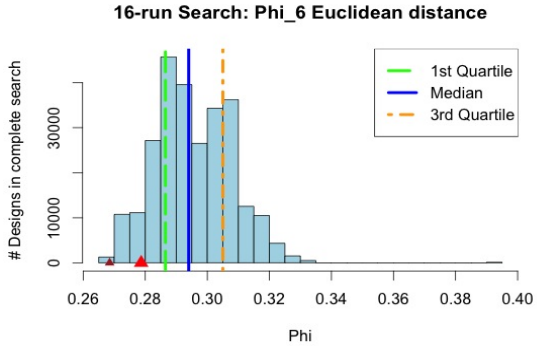
(b) Rectangular distance, p=1



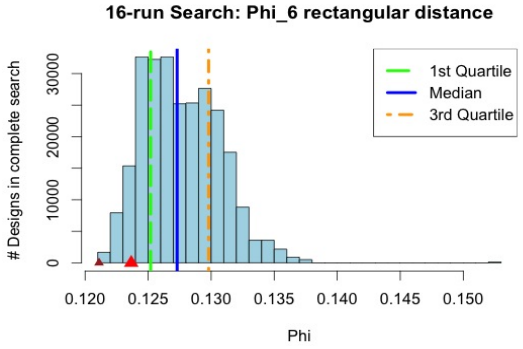
(c) Euclidean distance, p=3



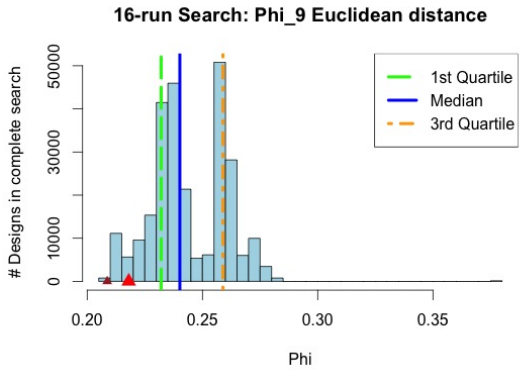
(d) Rectangular distance, p=3



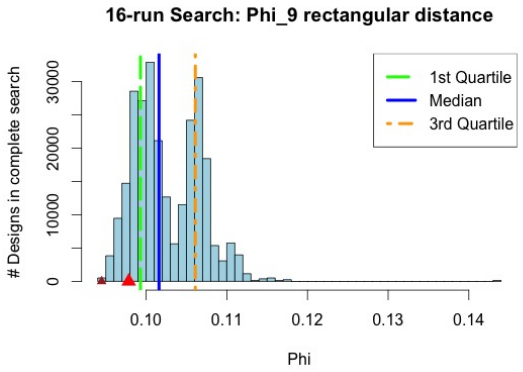
(e) Euclidean distance, p=6



(f) Rectangular distance, p=6

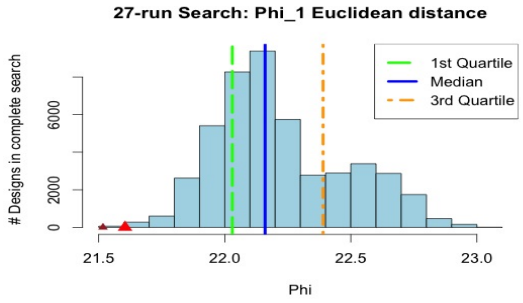


(g) Euclidean distance, p=9

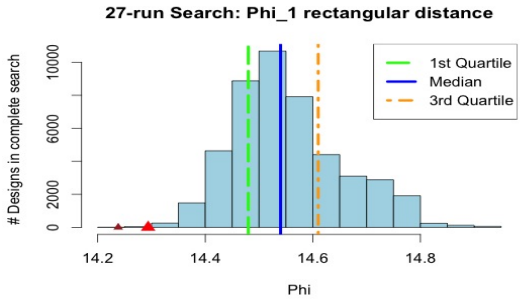


(h) Rectangular distance, p=9

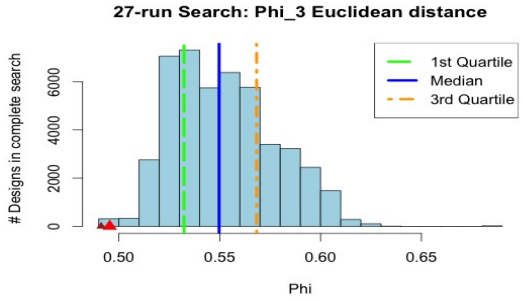
Figure 4.2: Histograms of Φ values for 16-run search



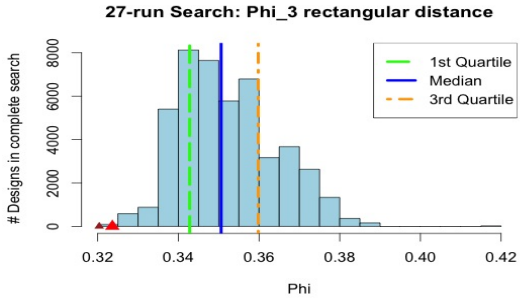
(a) Euclidean distance, p=1



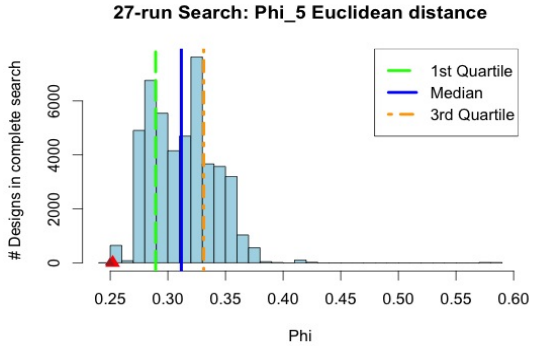
(b) Rectangular distance, p=1



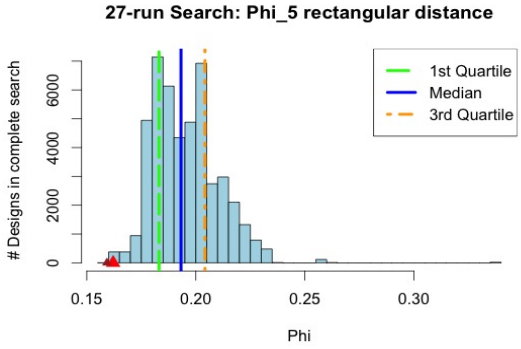
(c) Euclidean distance, p=3



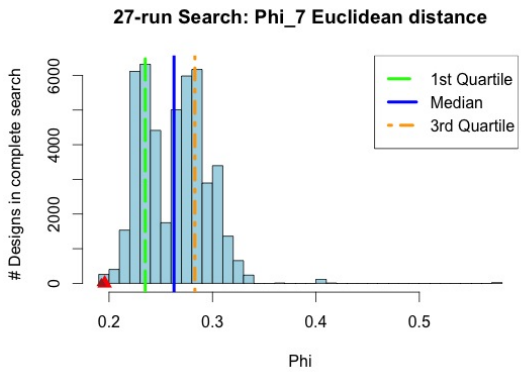
(d) Rectangular distance, p=3



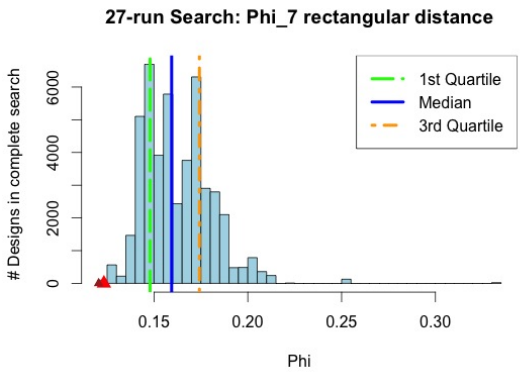
(e) Euclidean distance, p=5



(f) Rectangular distance, p=5



(g) Euclidean distance, p=7



(h) Rectangular distance, p=7

Figure 4.3: Histograms of Φ values for 27-run search

Chapter 5

Concluding Remarks

This project considers searching for maximin strong orthogonal arrays of strength three. When the number of factors is seven or less and the run size is twenty-seven or less, we have conducted a complete search. For designs of larger sizes, the complete search requires too large an amount of computation. We have proposed a search algorithm to reduce computation time. The performance of our search algorithm has been examined and we have found that the algorithm performs quite well when compared with the complete search. We have applied the algorithm to search for larger maximin SOAs. See the 54-run SOAs found in Appendix B.

To improve the algorithm, one can simply consider neighbourhoods of larger than two units. An even better algorithm can be developed by allowing the size of neighbourhoods to vary, giving the flexibility to travel to potentially larger neighbourhood and scan more diverse neighbours. This can be done by assigning a probability p_j to size j, where $j = 1, 2..., g$, $p_1 > p_2 > ... > p_g$, and $\sum_{i=1}^{g} p_j = 1$ if neighbourhoods of size g or less are considered. Rather than considering one-unit away neighbours before expanding to two-unit away neighbours, we randomly select a size before each iteration using $p_1, p_2, ..., p_g$. This search approach will be considered in future studies.

As the number m of factors and the number s of symbols increase, the number of neighbours increases: $3m \times (s! - 1)$ one-unit away neighbours, $\binom{3m}{2} \times (s! - 1)^2$ for size two neighbours. When

$m = 10$ and $s = 3$, the total number of two-unit away neighbours, 10875, may be too large to be all examined. One may choose a portion of the totality. For example, we may randomly select 100 two-unit away neighbours to examine. A threshold may be set to decide when to stop the search. For example, for a threshold of 10, the search will claim it has found the optimal design if no movement is made for 10 iterations.

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Appendix A

A Collection of Maximin Strong Orthogonal Arrays

A.1 Maximin SOAs in 8 Runs - Maximin $SOA(8, 3, 2^3, 3)$

$$\begin{pmatrix} 4 & 2 & 0 \\ 6 & 1 & 6 \\ 7 & 4 & 2 \\ 5 & 7 & 4 \\ 2 & 0 & 3 \\ 0 & 3 & 5 \\ 1 & 6 & 1 \\ 3 & 5 & 7 \end{pmatrix}, \begin{pmatrix} 3 & 2 & 0 \\ 1 & 1 & 6 \\ 0 & 4 & 2 \\ 2 & 7 & 4 \\ 5 & 0 & 3 \\ 7 & 3 & 5 \\ 6 & 6 & 1 \\ 4 & 5 & 7 \end{pmatrix}, \begin{pmatrix} 4 & 5 & 0 \\ 6 & 6 & 6 \\ 7 & 3 & 2 \\ 5 & 0 & 4 \\ 2 & 7 & 3 \\ 0 & 4 & 5 \\ 1 & 1 & 1 \\ 3 & 2 & 7 \end{pmatrix}, \begin{pmatrix} 3 & 5 & 0 \\ 1 & 6 & 6 \\ 0 & 3 & 2 \\ 2 & 0 & 4 \\ 5 & 7 & 3 \\ 7 & 4 & 5 \\ 6 & 1 & 1 \\ 4 & 2 & 7 \end{pmatrix}, \begin{pmatrix} 2 & 0 & 4 \\ 0 & 3 & 2 \\ 1 & 6 & 6 \\ 3 & 5 & 0 \\ 4 & 2 & 7 \\ 6 & 1 & 1 \\ 7 & 4 & 5 \\ 5 & 7 & 3 \end{pmatrix}, \begin{pmatrix} 5 & 0 & 4 \\ 7 & 3 & 2 \\ 6 & 6 & 6 \\ 4 & 5 & 0 \\ 3 & 2 & 7 \\ 1 & 1 & 1 \\ 0 & 4 & 5 \\ 2 & 7 & 3 \end{pmatrix}, \begin{pmatrix} 2 & 7 & 4 \\ 0 & 4 & 2 \\ 1 & 1 & 6 \\ 3 & 2 & 0 \\ 4 & 5 & 7 \\ 6 & 6 & 1 \\ 7 & 3 & 5 \\ 5 & 0 & 3 \end{pmatrix}$$

$$\begin{pmatrix} 5 & 7 & 4 \\ 7 & 4 & 2 \\ 6 & 1 & 6 \\ 4 & 2 & 0 \\ 3 & 5 & 7 \\ 1 & 6 & 1 \\ 0 & 3 & 5 \\ 2 & 0 & 3 \end{pmatrix}, \begin{pmatrix} 0 & 4 & 2 \\ 2 & 7 & 4 \\ 3 & 2 & 0 \\ 1 & 1 & 6 \\ 6 & 6 & 1 \\ 4 & 5 & 7 \\ 5 & 0 & 3 \\ 7 & 3 & 5 \end{pmatrix}, \begin{pmatrix} 7 & 4 & 2 \\ 5 & 7 & 4 \\ 4 & 2 & 0 \\ 6 & 1 & 6 \\ 1 & 6 & 1 \\ 3 & 5 & 7 \\ 2 & 0 & 3 \\ 0 & 3 & 5 \end{pmatrix}, \begin{pmatrix} 0 & 3 & 2 \\ 2 & 0 & 4 \\ 3 & 5 & 0 \\ 1 & 6 & 6 \\ 6 & 1 & 1 \\ 4 & 2 & 7 \\ 5 & 7 & 3 \\ 7 & 4 & 5 \end{pmatrix}, \begin{pmatrix} 7 & 3 & 2 \\ 5 & 0 & 4 \\ 4 & 5 & 0 \\ 6 & 6 & 6 \\ 1 & 1 & 1 \\ 3 & 2 & 7 \\ 2 & 7 & 3 \\ 0 & 4 & 5 \end{pmatrix}, \begin{pmatrix} 6 & 6 & 6 \\ 4 & 5 & 0 \\ 5 & 0 & 4 \\ 7 & 3 & 2 \\ 0 & 4 & 5 \\ 2 & 7 & 3 \\ 3 & 2 & 7 \\ 1 & 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 6 & 6 \\ 3 & 5 & 0 \\ 2 & 0 & 4 \\ 0 & 3 & 2 \\ 7 & 4 & 5 \\ 5 & 7 & 3 \\ 4 & 2 & 7 \\ 6 & 1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 6 & 1 & 6 \\ 4 & 2 & 0 \\ 5 & 7 & 4 \\ 7 & 4 & 2 \\ 0 & 3 & 5 \\ 2 & 0 & 3 \\ 3 & 5 & 7 \\ 1 & 6 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 6 \\ 3 & 2 & 0 \\ 2 & 7 & 4 \\ 0 & 4 & 2 \\ 7 & 3 & 5 \\ 5 & 0 & 3 \\ 4 & 5 & 7 \\ 6 & 6 & 1 \end{pmatrix}, \begin{pmatrix} 6 & 6 & 1 \\ 4 & 5 & 7 \\ 5 & 0 & 3 \\ 7 & 3 & 5 \\ 0 & 4 & 2 \\ 2 & 7 & 4 \\ 3 & 2 & 0 \\ 1 & 1 & 6 \end{pmatrix}, \begin{pmatrix} 1 & 6 & 1 \\ 3 & 5 & 7 \\ 2 & 0 & 3 \\ 0 & 3 & 5 \\ 7 & 4 & 2 \\ 5 & 7 & 4 \\ 4 & 2 & 0 \\ 6 & 1 & 6 \end{pmatrix}, \begin{pmatrix} 6 & 1 & 1 \\ 4 & 2 & 7 \\ 5 & 7 & 3 \\ 7 & 4 & 5 \\ 0 & 3 & 2 \\ 2 & 0 & 4 \\ 3 & 5 & 0 \\ 1 & 6 & 6 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 1 \\ 3 & 2 & 7 \\ 2 & 7 & 3 \\ 0 & 4 & 5 \\ 7 & 3 & 2 \\ 5 & 0 & 4 \\ 4 & 5 & 0 \\ 6 & 6 & 6 \end{pmatrix}, \begin{pmatrix} 0 & 4 & 5 \\ 2 & 7 & 3 \\ 3 & 2 & 7 \\ 1 & 1 & 1 \\ 6 & 6 & 6 \\ 4 & 5 & 0 \\ 5 & 0 & 4 \\ 7 & 3 & 2 \end{pmatrix}$$

$$\begin{pmatrix} 7 & 4 & 5 \\ 5 & 7 & 3 \\ 4 & 2 & 7 \\ 6 & 1 & 1 \\ 1 & 6 & 6 \\ 3 & 5 & 0 \\ 2 & 0 & 4 \\ 0 & 3 & 2 \end{pmatrix}, \begin{pmatrix} 0 & 3 & 5 \\ 2 & 0 & 3 \\ 3 & 5 & 7 \\ 1 & 6 & 1 \\ 6 & 1 & 6 \\ 4 & 2 & 0 \\ 5 & 7 & 4 \\ 7 & 4 & 2 \end{pmatrix}, \begin{pmatrix} 7 & 3 & 5 \\ 5 & 0 & 3 \\ 4 & 5 & 7 \\ 6 & 6 & 1 \\ 1 & 1 & 6 \\ 3 & 2 & 0 \\ 2 & 7 & 4 \\ 0 & 4 & 2 \end{pmatrix}, \begin{pmatrix} 2 & 0 & 3 \\ 0 & 3 & 5 \\ 1 & 6 & 1 \\ 3 & 5 & 7 \\ 4 & 2 & 0 \\ 6 & 1 & 6 \\ 7 & 4 & 2 \\ 5 & 7 & 4 \end{pmatrix}, \begin{pmatrix} 5 & 0 & 3 \\ 7 & 3 & 5 \\ 6 & 6 & 1 \\ 4 & 5 & 7 \\ 3 & 2 & 0 \\ 1 & 1 & 6 \\ 0 & 4 & 2 \\ 2 & 7 & 4 \end{pmatrix}, \begin{pmatrix} 2 & 7 & 3 \\ 0 & 4 & 5 \\ 1 & 1 & 1 \\ 3 & 2 & 7 \\ 4 & 5 & 0 \\ 6 & 6 & 6 \\ 7 & 3 & 2 \\ 5 & 0 & 4 \end{pmatrix}, \begin{pmatrix} 5 & 7 & 3 \\ 7 & 4 & 5 \\ 6 & 1 & 1 \\ 4 & 2 & 7 \\ 3 & 5 & 0 \\ 1 & 6 & 6 \\ 0 & 3 & 2 \\ 2 & 0 & 4 \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & 7 \\ 6 & 1 & 1 \\ 7 & 4 & 5 \\ 5 & 7 & 3 \\ 2 & 0 & 4 \\ 0 & 3 & 2 \\ 1 & 6 & 6 \\ 3 & 5 & 0 \end{pmatrix}, \begin{pmatrix} 3 & 2 & 7 \\ 1 & 1 & 1 \\ 0 & 4 & 5 \\ 2 & 7 & 3 \\ 5 & 0 & 4 \\ 7 & 3 & 2 \\ 6 & 6 & 6 \\ 4 & 5 & 0 \end{pmatrix}, \begin{pmatrix} 4 & 5 & 7 \\ 6 & 6 & 1 \\ 7 & 3 & 5 \\ 5 & 0 & 3 \\ 2 & 7 & 4 \\ 0 & 4 & 2 \\ 1 & 1 & 6 \\ 3 & 2 & 0 \end{pmatrix}, \begin{pmatrix} 3 & 5 & 7 \\ 1 & 6 & 1 \\ 0 & 3 & 5 \\ 2 & 0 & 3 \\ 5 & 7 & 4 \\ 7 & 4 & 2 \\ 6 & 1 & 6 \\ 4 & 2 & 0 \end{pmatrix}$$

A.2 Maximin SOAs in 16 Runs - Maximin $SOA(16, 7, 2^3, 3)$

Due to the limited space, only a subset of 128 maximin SOAs found is given here.

$$\begin{pmatrix} 4 & 0 & 0 & 1 & 5 & 5 & 5 \\ 6 & 2 & 3 & 7 & 6 & 2 & 3 \\ 6 & 3 & 6 & 2 & 3 & 6 & 3 \\ 4 & 1 & 5 & 4 & 0 & 1 & 5 \\ 7 & 6 & 2 & 2 & 2 & 3 & 7 \\ 5 & 4 & 1 & 4 & 1 & 4 & 1 \\ 5 & 5 & 4 & 1 & 4 & 0 & 1 \\ 7 & 7 & 7 & 7 & 7 & 7 & 7 \\ 3 & 7 & 7 & 6 & 2 & 2 & 2 \\ 1 & 5 & 4 & 0 & 1 & 5 & 4 \\ 1 & 4 & 1 & 5 & 4 & 1 & 4 \\ 3 & 6 & 2 & 3 & 7 & 6 & 2 \\ 0 & 1 & 5 & 5 & 5 & 4 & 0 \\ 2 & 3 & 6 & 3 & 6 & 3 & 6 \\ 2 & 2 & 3 & 6 & 3 & 7 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 4 & 0 & 0 & 5 & 5 & 5 & 5 \\ 6 & 2 & 3 & 3 & 6 & 2 & 3 \\ 6 & 3 & 6 & 6 & 3 & 6 & 3 \\ 4 & 1 & 5 & 0 & 0 & 1 & 5 \\ 7 & 6 & 2 & 6 & 2 & 3 & 7 \\ 5 & 4 & 1 & 0 & 1 & 4 & 1 \\ 5 & 5 & 4 & 5 & 4 & 0 & 1 \\ 7 & 7 & 7 & 3 & 7 & 7 & 7 \\ 3 & 7 & 7 & 2 & 2 & 2 & 2 \\ 1 & 5 & 4 & 4 & 1 & 5 & 4 \\ 1 & 4 & 1 & 1 & 4 & 1 & 4 \\ 3 & 6 & 2 & 7 & 7 & 6 & 2 \\ 0 & 1 & 5 & 1 & 5 & 4 & 0 \\ 2 & 3 & 6 & 7 & 6 & 3 & 6 \\ 2 & 2 & 3 & 2 & 3 & 7 & 6 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 4 & 0 & 0 & 1 & 3 & 5 & 5 \\ 6 & 2 & 3 & 7 & 0 & 2 & 3 \\ 6 & 3 & 6 & 2 & 5 & 6 & 3 \\ 4 & 1 & 5 & 4 & 6 & 1 & 5 \\ 7 & 6 & 2 & 2 & 4 & 3 & 7 \\ 5 & 4 & 1 & 4 & 7 & 4 & 1 \\ 5 & 5 & 4 & 1 & 2 & 0 & 1 \\ 7 & 7 & 7 & 7 & 1 & 7 & 7 \\ 3 & 7 & 7 & 6 & 4 & 2 & 2 \\ 1 & 5 & 4 & 0 & 7 & 5 & 4 \\ 1 & 4 & 1 & 5 & 2 & 1 & 4 \\ 3 & 6 & 2 & 3 & 1 & 6 & 2 \\ 0 & 1 & 5 & 5 & 3 & 4 & 0 \\ 2 & 3 & 6 & 3 & 0 & 3 & 6 \\ 2 & 2 & 3 & 6 & 5 & 7 & 6 \\ 0 & 0 & 0 & 0 & 6 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix}
4 & 0 & 0 & 7 & 7 & 1 & 5 \\
6 & 2 & 3 & 1 & 4 & 6 & 3 \\
6 & 3 & 6 & 4 & 1 & 2 & 3 \\
4 & 1 & 5 & 2 & 2 & 5 & 5 \\
7 & 6 & 2 & 4 & 0 & 7 & 7 \\
5 & 4 & 1 & 2 & 3 & 0 & 1 \\
5 & 5 & 4 & 7 & 6 & 4 & 1 \\
7 & 7 & 7 & 1 & 5 & 3 & 7 \\
3 & 7 & 7 & 0 & 0 & 6 & 2 \\
1 & 5 & 4 & 6 & 3 & 1 & 4 \\
1 & 4 & 1 & 3 & 6 & 5 & 4 \\
3 & 6 & 2 & 5 & 5 & 2 & 2 \\
0 & 1 & 5 & 3 & 7 & 0 & 0 \\
2 & 3 & 6 & 5 & 4 & 7 & 6 \\
2 & 2 & 3 & 0 & 1 & 3 & 6 \\
0 & 0 & 0 & 6 & 2 & 4 & 0
\end{pmatrix},
\begin{pmatrix}
4 & 0 & 0 & 0 & 5 & 5 & 5 \\
6 & 2 & 3 & 6 & 6 & 2 & 3 \\
6 & 3 & 6 & 3 & 3 & 6 & 3 \\
4 & 1 & 5 & 5 & 0 & 1 & 5 \\
7 & 6 & 2 & 3 & 2 & 3 & 7 \\
5 & 4 & 1 & 5 & 1 & 4 & 1 \\
5 & 5 & 4 & 0 & 4 & 0 & 1 \\
7 & 7 & 7 & 6 & 7 & 7 & 7 \\
3 & 7 & 7 & 7 & 2 & 2 & 2 \\
1 & 5 & 4 & 1 & 1 & 5 & 4 \\
1 & 4 & 1 & 4 & 4 & 1 & 4 \\
3 & 6 & 2 & 2 & 7 & 6 & 2 \\
0 & 1 & 5 & 4 & 5 & 4 & 0 \\
2 & 3 & 6 & 2 & 6 & 3 & 6 \\
2 & 2 & 3 & 7 & 3 & 7 & 6 \\
0 & 0 & 0 & 1 & 0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
4 & 0 & 0 & 3 & 1 & 5 & 5 \\
6 & 2 & 3 & 5 & 2 & 2 & 3 \\
6 & 3 & 6 & 0 & 7 & 6 & 3 \\
4 & 1 & 5 & 6 & 4 & 1 & 5 \\
7 & 6 & 2 & 0 & 6 & 3 & 7 \\
5 & 4 & 1 & 6 & 5 & 4 & 1 \\
5 & 5 & 4 & 3 & 0 & 0 & 1 \\
7 & 7 & 7 & 5 & 3 & 7 & 7 \\
3 & 7 & 7 & 4 & 6 & 2 & 2 \\
1 & 5 & 4 & 2 & 5 & 5 & 4 \\
1 & 4 & 1 & 7 & 0 & 1 & 4 \\
3 & 6 & 2 & 1 & 3 & 6 & 2 \\
0 & 1 & 5 & 7 & 1 & 4 & 0 \\
2 & 3 & 6 & 1 & 2 & 3 & 6 \\
2 & 2 & 3 & 4 & 7 & 7 & 6 \\
0 & 0 & 0 & 2 & 4 & 0 & 0
\end{pmatrix}$$

$$\begin{pmatrix}
4 & 0 & 0 & 1 & 4 & 5 & 5 \\
6 & 2 & 3 & 7 & 7 & 2 & 3 \\
6 & 3 & 6 & 2 & 2 & 6 & 3 \\
4 & 1 & 5 & 4 & 1 & 1 & 5 \\
7 & 6 & 2 & 2 & 3 & 3 & 7 \\
5 & 4 & 1 & 4 & 0 & 4 & 1 \\
5 & 5 & 4 & 1 & 5 & 0 & 1 \\
7 & 7 & 7 & 7 & 6 & 7 & 7 \\
3 & 7 & 7 & 6 & 3 & 2 & 2 \\
1 & 5 & 4 & 0 & 0 & 5 & 4 \\
1 & 4 & 1 & 5 & 5 & 1 & 4 \\
3 & 6 & 2 & 3 & 6 & 6 & 2 \\
0 & 1 & 5 & 5 & 4 & 4 & 0 \\
2 & 3 & 6 & 3 & 7 & 3 & 6 \\
2 & 2 & 3 & 6 & 2 & 7 & 6 \\
0 & 0 & 0 & 0 & 1 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
4 & 0 & 0 & 2 & 5 & 1 & 5 \\
6 & 2 & 3 & 4 & 6 & 6 & 3 \\
6 & 3 & 6 & 1 & 3 & 2 & 3 \\
4 & 1 & 5 & 7 & 0 & 5 & 5 \\
7 & 6 & 2 & 1 & 2 & 7 & 7 \\
5 & 4 & 1 & 7 & 1 & 0 & 1 \\
5 & 5 & 4 & 2 & 4 & 4 & 1 \\
7 & 7 & 7 & 4 & 7 & 3 & 7 \\
3 & 7 & 7 & 5 & 2 & 6 & 2 \\
1 & 5 & 4 & 3 & 1 & 1 & 4 \\
1 & 4 & 1 & 6 & 4 & 5 & 4 \\
3 & 6 & 2 & 0 & 7 & 2 & 2 \\
0 & 1 & 5 & 6 & 5 & 0 & 0 \\
2 & 3 & 6 & 0 & 6 & 7 & 6 \\
2 & 2 & 3 & 5 & 3 & 3 & 6 \\
0 & 0 & 0 & 3 & 0 & 4 & 0
\end{pmatrix}$$

A.3 Maximin SOAs in 27 Runs - Maximin $SOA(27, 3, 3^3, 3)$

Maximin SOAs: D_1, D_2, D_3 using Euclidean distance; D_1 and D_3 using rectangular.

$$D_1 = \begin{pmatrix}
8 & 8 & 8 \\
2 & 1 & 11 \\
1 & 11 & 2 \\
11 & 2 & 1 \\
5 & 3 & 23 \\
3 & 23 & 5 \\
23 & 5 & 3 \\
4 & 13 & 14 \\
14 & 4 & 13 \\
13 & 14 & 4 \\
16 & 16 & 16 \\
0 & 18 & 20 \\
20 & 0 & 18 \\
18 & 20 & 0 \\
24 & 24 & 24 \\
15 & 26 & 7 \\
17 & 6 & 25 \\
7 & 15 & 26 \\
25 & 17 & 6 \\
26 & 7 & 15 \\
6 & 25 & 17 \\
10 & 9 & 19 \\
9 & 19 & 10 \\
19 & 10 & 9 \\
12 & 21 & 22 \\
22 & 12 & 21 \\
21 & 22 & 12
\end{pmatrix}, D_2 = \begin{pmatrix}
5 & 5 & 5 \\
8 & 7 & 17 \\
7 & 17 & 8 \\
17 & 8 & 7 \\
2 & 0 & 20 \\
0 & 20 & 2 \\
20 & 2 & 0 \\
1 & 10 & 11 \\
11 & 1 & 10 \\
10 & 11 & 1 \\
13 & 13 & 13 \\
6 & 24 & 26 \\
26 & 6 & 24 \\
24 & 26 & 6 \\
21 & 21 & 21 \\
12 & 23 & 4 \\
14 & 3 & 22 \\
4 & 12 & 23 \\
22 & 14 & 3 \\
23 & 4 & 12 \\
3 & 22 & 14 \\
16 & 15 & 25 \\
15 & 25 & 16 \\
25 & 16 & 15 \\
9 & 18 & 19 \\
19 & 9 & 18 \\
18 & 19 & 9
\end{pmatrix}, D_3 = \begin{pmatrix}
2 & 2 & 2 \\
5 & 4 & 14 \\
4 & 14 & 5 \\
14 & 5 & 4 \\
8 & 6 & 26 \\
6 & 26 & 8 \\
26 & 8 & 6 \\
7 & 16 & 17 \\
17 & 7 & 16 \\
16 & 17 & 7 \\
10 & 10 & 10 \\
3 & 21 & 23 \\
23 & 3 & 21 \\
21 & 23 & 3 \\
18 & 18 & 18 \\
9 & 20 & 1 \\
11 & 0 & 19 \\
1 & 9 & 20 \\
19 & 11 & 0 \\
20 & 1 & 9 \\
0 & 19 & 11 \\
13 & 12 & 22 \\
12 & 22 & 13 \\
22 & 13 & 12 \\
15 & 24 & 25 \\
25 & 15 & 24 \\
24 & 25 & 15
\end{pmatrix}$$

Appendix B

Maximin Strong Orthogonal Arrays from Algorithmic Search

B.1 Maximin SOAs in 54 Runs - Maximin $SOA(54, 4, 3^3, 3)$

The transpose of the designs are as follows:

D_1^T	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	9	12	9	10	10	18	18	2	12	14	14	3	3	22	15	15	17	16	17	16
2	7	4	8	16	15	7	6	25	3	22	23	4	5	13	2	0	19	10	18	11
3	16	10	6	17	25	17	25	16	20	9	1	9	1	10	3	23	14	12	22	4
4	13	10	22	4	13	5	14	12	1	19	10	18	9	11	25	7	7	25	16	16

	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
1	6	24	6	24	8	25	11	11	0	0	1	20	1	20	13	13	21	21	23	4
2	1	1	0	2	19	10	26	24	8	6	16	25	17	26	12	14	3	5	22	13
3	14	12	22	4	13	13	8	24	8	24	15	15	7	7	18	2	18	2	11	11
4	6	26	15	17	15	17	4	22	3	21	21	23	12	14	19	1	20	2	2	0

	41	42	43	44	45	46	47	48	49	50	51	52	53	54
1	23	4	2	19	19	22	5	5	8	7	7	25	26	26
2	21	12	24	15	17	14	23	21	20	11	9	9	18	20
3	19	19	26	26	6	0	0	20	3	5	21	23	21	5
4	11	9	3	5	23	20	18	0	24	6	24	8	26	8

D_2^T	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	19	25	19	18	18	10	10	2	25	26	26	7	7	15	22	22	23	21	23	21
2	11	17	9	20	19	11	10	2	16	8	6	17	15	26	12	13	5	23	4	21
3	0	3	20	1	9	1	9	0	13	5	21	5	21	3	26	16	7	8	15	24
4	21	18	3	12	21	13	22	23	9	0	18	2	20	19	6	15	15	6	24	24

	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
1	4	13	4	13	5	12	20	20	1	1	0	11	0	11	24	24	16	16	17	6
2	14	14	13	12	5	23	0	1	9	10	20	2	18	0	25	24	16	15	8	26
3	7	8	15	24	6	6	19	11	19	11	2	2	18	18	14	22	14	22	4	4
4	17	7	26	25	26	25	12	3	14	5	5	4	23	22	0	9	1	10	10	11

	41	42	43	44	45	46	47	48	49	50	51	52	53	54
1	17	6	2	9	9	15	8	8	5	3	3	12	14	14
2	7	25	1	19	18	24	6	7	3	21	22	22	4	3
3	12	12	10	10	20	23	23	13	26	25	17	16	17	25
4	19	20	14	13	4	1	2	11	8	17	8	16	7	16