

A New Class of Latin Hypercube for Computer Experiments

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Summary. Computer models can describe complicated physical phenomena. To use these models for scientific investigation, however, their generally long running times and mostly deterministic nature require a specially designed experiment. Standard factorial designs are inadequate; in the absence of one or more main effects, their replication cannot be used to estimate error but instead produces redundancy. A number of alternative designs have been proposed, but many can be burdensome computationally. This paper presents a class of Latin hypercube designs developed from the rotation of factorial designs. These rotated factorial designs are easy to construct and preserve many of the attractive properties of standard factorial designs: they have equally-spaced projections to univariate dimensions and yield uncorrelated regression effect estimates (orthogonality). They also rate comparably to maximin Latin hypercube designs by the minimum interpoint distance criterion used in the latter's construction.

Key words: Effect correlation, maximin distance, minimum interpoint distance, rotated factorial design

1 Introduction

Computer models are often used to describe complicated physical phenomena encountered in science and engineering. These phenomena are often governed by a set of equations, including linear, nonlinear, ordinary, and partial differential equations. The equations are often too difficult to be solved simultaneously by any person, but can be by a computer modeling program. These programs, due to the number and complexity of the equations, may have long running times, making their use difficult for comprehensive scientific investigation.

The SOLA-PTS algorithm described in Daly & Torrey (1984), for example, has been developed at the Los Alamos National Laboratory for modeling the rapid cooling of a nuclear reactor wall as a result of cold water injected into the reactor's downcomer for containment during a nuclear accident. The authors' three-pronged goal is to study the response of the reactor, to study the turbulent mixture of the cold water and the warm fluid already in the downcomer, and to predict the onset and growth of cracks in the reactor wall as a result of the rapid cooling. This algorithm simultaneously solves eight partial differential equations with eight inputs and takes approximately 90 minutes on a Cray supercomputer to run. It solves a large number of differential equations, is very computationally expensive in running time, and has a "black box" quality – one does not know in advance which factors have large effects and one would like to examine the response over a wide range of input combinations. This algorithm is typical of computer models needing designed experiments.

One goal in this setting is to build an approximating program which, although not as precise as the computer model, would run fast enough to study the phenomenon in detail. Construction of an adequate approximating function (or program) to the computer model requires the selection of design points (a designed experiment) at which the computer model will be run to build an approximating function. Because the computer models are mostly deterministic, these computer experiments require special designs. In physical experiments, if certain factors have no effect on the response and are taken out of the approximation function (linear model), then the replicated design points in the reduced design space can be used to estimate the random error present in the system. However, with computer experiments, there is no random error – only lack of fit. Replication of classical factorial designs cannot be used to estimate this error, but instead produces redundancy. That is, they are hindered by their non-unique projections to lower dimensions.

This paper presents a new and simple strategy for designs for computer experiments, developed from the rotation of the standard factorial design to yield a Latin hypercube. Section 2 discusses a number of alternative designs that have been proposed. The following sections develop the rationale for these new designs, using the two-dimensional case for illustration (Section 3), and compare them to other previously proposed designs (Section 4). Section 5 shows the high-dimensional rotation theorems and the concluding remarks are given in Section 6.

2 Design Criteria and Related Work

Selection of an appropriate designed experiment depends to an extent on the experimental region, the model to be fit, and the method of analysis. This paper assumes the following: the experimental region is cuboidal (each factor is bound between values of interest), the true model is unknown to the experimenter and that he will approximate it by a polynomial of some degree *a priori* unknown to him, and the method of analysis will be ordinary least squares regression,

although alternative methods are available (see Haaland, McMillan, Nychka & Welch (1994)).

In order to assess design criteria for computer experiments, it is valuable to study the progression of proposed designs. Koehler & Owen (1996) provide an overview of past and current approaches. The two main geometric designs are the standard (full or fractional) factorial designs and the Latin hypercube designs, but also include other traditional designs for physical experiments, such as central composite designs. Easterling (1989) points out that standard factorial designs have many attractive properties for physical experiments: balance (factor levels used an equal number of times), symmetry (permutation of design matrix columns yields same design), orthogonality (separability of main effects), collapsibility (projects to lower subspace as factorial design, sometimes redundantly), equally-spaced projections to each dimension, and straightforward measurability of main effects.

McKay, Beckman & Conover (1979) introduced the use of the Latin hypercube (LH) in computer experiments. A n -point LH design matrix is constructed by randomly permuting the integers $\{1, 2, \dots, n\}$ for each factor and rescaling to the experimental region, so that the points project uniquely and equally-spaced to each dimension. The unique projections of LHs allow for great flexibility in model fitting. Box & Draper (1959) showed that when the true model is a polynomial of unknown degree, the *best* design (in the sense of various criteria discussed in their paper) places its points evenly spaced over the design region. Thus, equally-spaced projections are also of value. For these reasons, the LH has become the standard for computer experiments. However, random LHs are susceptible to high correlations between factors, even complete confounding, and to omitting regions of the design space.

Computer-generated designs include those of Sacks, Schiller & Welch (1989) and Sacks, Welch, Mitchell & Wynn (1989) that try to minimize the integrated mean square error (IMSE) of prediction when prediction errors are taken as a realization of a spatial stochastic process. Johnson, Moore & Ylvisaker (1990) proposed similar designs to minimize the correlations between observations when responses are taken as a realization of a spatial stochastic process. The latter authors' design D^* they call a maximin distance design if

$$\min_{x_1, x_2 \in D^*} d(x_1, x_2) = \max_D \min_{x_1, x_2 \in D} d(x_1, x_2), \quad (1)$$

where d is a distance measure and $\min_{x_1, x_2 \in D} d(x_1, x_2)$ is the minimum interpoint distance (MID) of design D ; that is, its points are moved as far apart from one another as possible.

Attempts have been made to bridge the gap between geometric designs and computer-generated designs. Tang (1993) and Owen (1992) introduced orthogonal-array based LHs to guarantee coverage of all regions for every subset of r factors. Morris & Mitchell (1992) and Tang (1994) proposed LHs that attain the largest MID among all LHs, called maximin Latin hypercubes. Park (1994) tried to construct LHs that optimize the IMSE criterion. Owen (1994) attempted to control the correlations between design matrix columns of random LHs. These

methods are a step forward in merging the good properties of Latin hypercubes with the optimization of computer-generated designs. However, being themselves computer-generated designs leaves many susceptible to the aforementioned problems.

With this in mind, we seek a new design for computer experiments with these properties: the unique and equally-spaced projections to each dimension and flexibility in model selection provided by Latin hypercube designs and the orthogonality and ease of construction provided by standard factorial designs. In addition, these new designs should perform reasonably well in terms of other criteria mentioned, such as MID, correlation, and coverage of the design space.

3 Rotated Factorial Designs in Two Dimensions

The strategy taken here is to modify the standard factorial design by rotation so as to yield a Latin hypercube. To see how this is done, first consider the standard 3^2 factorial design, represented by the 3×3 square of points and how it can be rotated to yield equally-spaced projections (see Figure 1). The key to finding all such rotations is in the relationship between points A-D. We focus on nontrivial angles between 0 and 45 degrees clockwise due to the symmetry of the rotation problem.

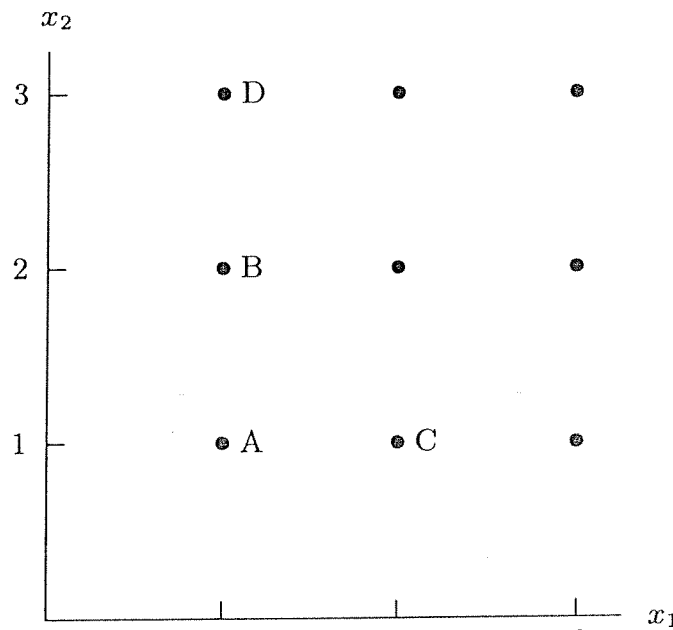


Fig. 1. Standard 3^2 factorial design before rotation

The matrix equation to rotate a set of points clockwise by an angle w about the origin is

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \times \begin{bmatrix} \cos(w) & -\sin(w) \\ \sin(w) & \cos(w) \end{bmatrix}, \quad (2)$$

so that if (x_1, x_2) are the coordinates of a design point in the standard factorial design, then the rotation moves the point to $(x_1 \cos(w) + x_2 \sin(w), -x_1 \sin(w) + x_2 \cos(w))$.

Notice first that as the points are rotated clockwise about the origin that A will have the smallest x_1 -coordinate for any angle between 0° and 45° . (A 45° rotation will place A directly on the x_1 -axis and A is the closest point to the origin.) Also notice that the x_1 -projections of points with the same initial x_1 -coordinate (like A, B, and D) will be equally spaced, by $\sin(w)$, regardless of the rotation angle. Likewise, the x_1 -projections of points with the same initial x_2 -coordinate (like A and C) will be equally spaced, by $\cos(w)$, regardless of the rotation angle. It suffices to find all angles that make the x_1 -projections of points A-D equally spaced. For the x_1 -coordinates of A-D, see the table below.

point	x_1 -coordinate
A	$\cos(w) + \sin(w)$
B	$\cos(w) + 2 \sin(w)$
C	$2 \cos(w) + \sin(w)$
D	$\cos(w) + 3 \sin(w)$

Between 0° and 45° , $\sin(w) \leq \cos(w)$, so the point with the next smallest x_1 -coordinate will always be B (although C will tie B when $w = 45^\circ$) and the distance between the smallest two x_1 -projections will always be $\sin(w)$. To achieve equally-spaced x_1 -projections, the distance between all x_1 -projections must equal $\sin(w)$. We've already seen that this is true when $w = 45^\circ$ (equivalently, $\tan^{-1}(1)$) and both C and B have the second smallest x_1 -coordinate (see Figures 2(b) and 2(c), for example).

Another possibility is that C will have the third smallest x_1 -coordinate, and that the " x_1 -distance" between B and C will be $\sin(w)$. However, the " x_1 -distance" between B and D is always $\sin(w)$. In this case, C and D will have the same x_1 -coordinate, hence

$$\cos(w) = 2 \sin(w) \implies w = \tan^{-1}(1/2).$$

Continuing in this manner, consider the case where C has the fourth smallest x_1 -coordinate – after A, B, and D – and the " x_1 -distance" between D and C is $\sin(w)$. Then

$$\cos(w) - 2 \sin(w) = \sin(w) \implies w = \tan^{-1}(1/3).$$

Point C cannot have the fifth smallest x_1 -coordinate, so these three rotations are the only ones (again, among nontrivial angles between 0° and 45°) that yield equally-spaced x_1 -projections from the 3^2 design. It is easily verified that these also yield equally-spaced x_2 -projections.

Figure 2 displays the standard 3^2 factorial design, shown in open circles, and the designs that result from these rotations, shown in solid circles. Boxes are drawn around the rotated designs to identify the design regions. In practice, one would then scale this design (by subtraction and division) to the experimental region of interest. Along each axis, we have provided dot plots of the projections from which it is plain to see the equally-spaced property.

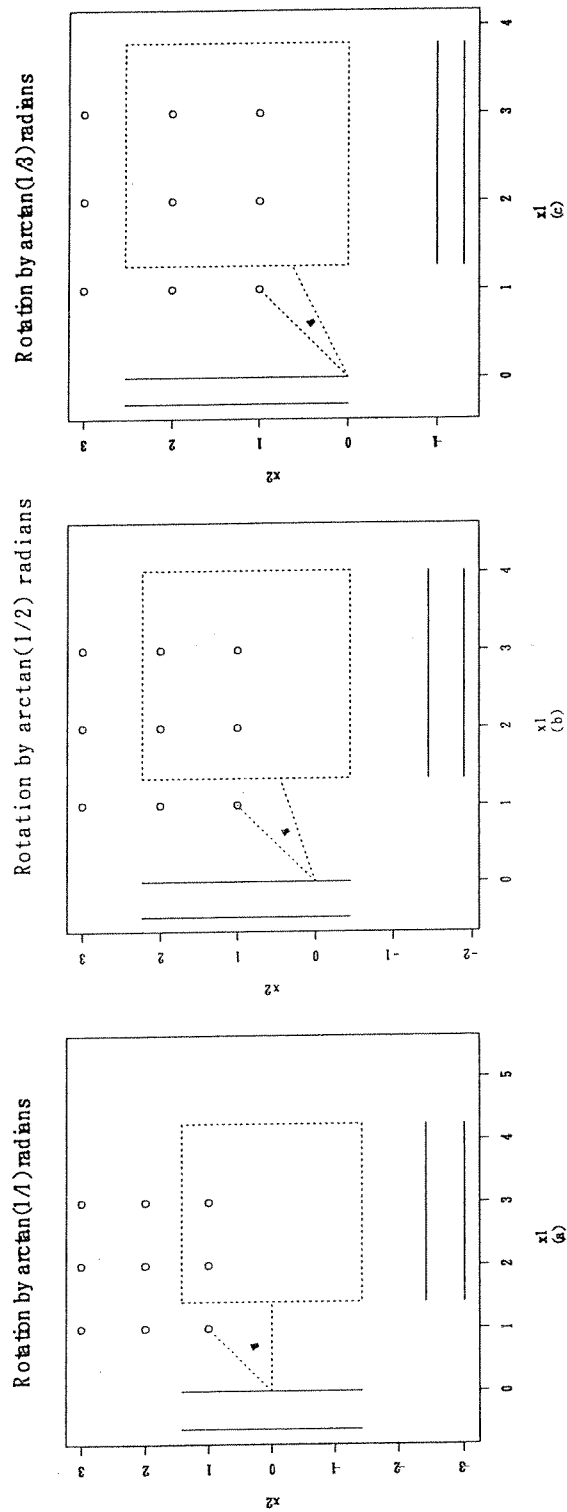


Fig. 2. Three rotations of a standard 3^2 factorial design:
 (a) $w = \tan^{-1}(1)$, (b) $w = \tan^{-1}(1/2)$, (c) $w = \tan^{-1}(1/3)$

Following the argument above, a general result for factorial designs can be stated. (The proofs of Theorems 1 and 2 are straightforward and are thus omitted here.)

Theorem 1. *For nontrivial rotations between 0° and 45° , a rotated standard p^2 factorial design will produce equally-spaced projections to each dimension if and only if the rotation angle is $\tan^{-1}(1/k)$, where $k \in \{1, \dots, p\}$.*

Among the rotated standard p^2 factorial designs with equally-spaced projections, only those obtained from rotation angles of $\tan^{-1}(1/p)$ contain no redundant projections. Therefore, we define a p^2 -point rotated full factorial design to be a rotated standard p^2 factorial design with unique, equally-spaced projections to each dimension (which is a Latin hypercube).

Theorem 2. *For a linear first-order regression model, any two-dimensional rotated factorial design has uncorrelated regression effects estimates.*

4 Two-Dimensional Subset Designs and Design Comparisons

Two-dimensional rotated full factorial designs can be easily modified to accommodate many design sizes other than p^2 . After rotating the standard factorial design, remove the four most extreme points - two for each factor - to get a new design. This process can be repeated to get any design with the number of points equal to $p^2 - 4j$ for $j \in \{0, 1, \dots, \max(p-2, 0)\}$. When points are removed through this deletion process, the resulting design will no longer have the equally-spaced projection property, although it will have unique projections. We will refer to designs created by applying the deletion process to a rotated full factorial design as *Type U rotated factorial designs*, where U emphasizes these *unique* projections. Figure 3 shows the 12-point Type U rotated factorial design that is created by removing the four most extreme design points of the 16-point rotated full factorial design.

After the deletion process, these new designs can be given equally-spaced projections by adjusting the angle of rotation, although this may have the simultaneous effect of creating some redundant projections. We will refer to designs created by modifying the rotation angle of a Type U design to yield the greatest number of unique, equally-spaced projections as *Type E rotated factorial designs*, where E emphasizes the *equally-spaced* projections. Figure 4 shows the 12-point Type E rotated factorial design which has been given equally-spaced projections by adjusting the rotation angle to $\tan^{-1}(2/3)$. Our preference is for Type E designs because of the equally-spaced projections, but others may choose Type U designs because of the unique projections. A complete illustration for the exact construction of $n = 16$, $n = 12$ Type U and Type E designs is given in the Appendix.

Table 1 presents the minimum interpoint distances calculated by scaling the designs to the unit square $[0, 1]^2$ and using Euclidean distance for these same

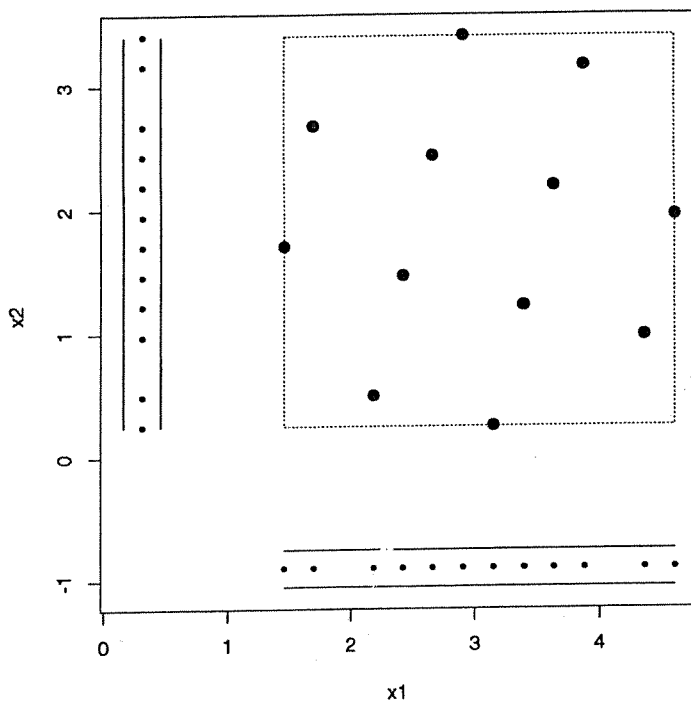


Fig. 3. 12-point $(4^2 - 4)$ Type U rotated factorial design

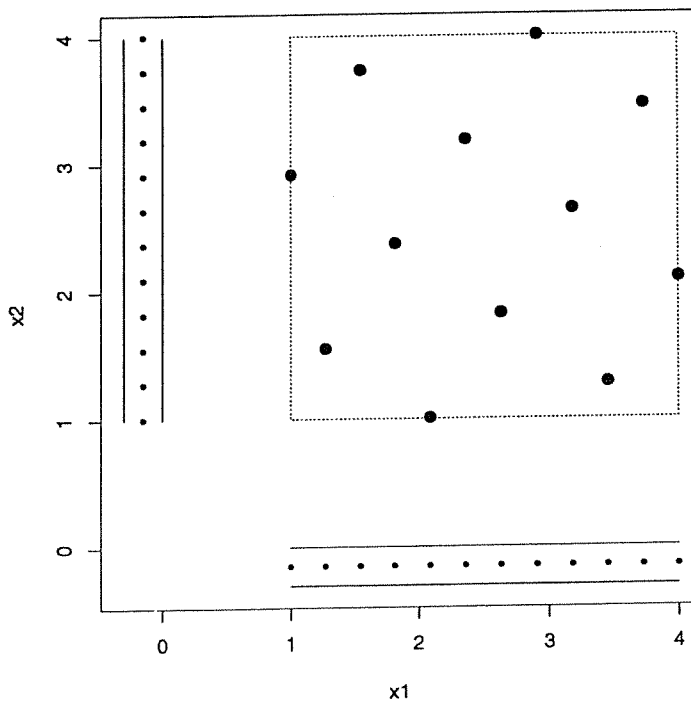


Fig. 4. 12-point $(4^2 - 4)$ Type E rotated factorial design

designs. Johnson, Moore & Ylvisaker (1990) gave ranges for the MIDs of maximin distance designs. These are listed merely as a reference for the other designs; no direct comparison will be made since maximin distance designs aren't necessarily appropriate for computer experiments (see, for example, Koehler & Owen (1996)). A few maximin distance designs were published in Johnson, Moore & Ylvisaker (1990) and in Koehler & Owen (1996) and the exact MIDs are listed for those designs.

Table 1. Minimum Interpoint Distance (MID) Comparisons for $d = 2$ Dimensional Designs

No. of Pts.	Maximin Distance Design †	Maximin Latin Hypercube †	Rotated Factorial Design ‡	
			Type U	Type E
4	1.0000	.7454	.7454	.7454
5	.7071	.5590	.5270	.5590
8	.5000-1.0000	.4041	.3748	.4472
9	.5000	.3953	.3953	.3953
12	.3333-.5000	.3278	.3172	.3278
13	.3333-.5000	.3005	.2833	.3162
16	.3333	.2749	.2749	.2749
17	.2500-.3333	.2652	.2550	.2577
20	.2500-.3333	.2233	.2253	.2425

† Obtained via Johnson, Moore and Ylvisaker (1991).
 ‡ Obtained via Koehler and Owen (1996).
 § Obtained by authors' algorithm.

In certain cases, the minimum interpoint distances of maximin LH and rotated factorial designs are equal – most notably when there are p^2 design points, but also when $n = 5, 12$. For $n = 8, 13, 20$, the MIDs are better for RFDs, while maximin LH designs are superior in the other listed case ($n = 17$). Maximin LH designs were constructed to have large MIDs while preserving the unique, equally-spaced projections of LHs, while RFDs were constructed to be LHs with a factorial design structure. The gains in MID from using maximin LH designs over rotated factorial designs, despite the significant increase in computer effort, are never very large when compared alongside maximin distance designs, the ideal according to minimum interpoint distance.

5 High-Dimensional Rotation Theory

Consider a standard full factorial design consisting of d factors, each with p levels. The goal is to rotate this design to convert it into a LH design, so that the p^d

points create unique and equally-spaced projections to each individual factor. For certain values of d (notably when d is a power of 2) such a rotation exists, but not for general d . The following proof proceeds in three parts: identification of the required form of the rotation matrix, construction of the power-of-2 rotation matrix, and failure of the transformation matrix to be a rotation matrix when d is not a power of two.

A p -level, d -factor standard full factorial design can be represented by a $p^d \times d$ matrix, D , with entries from $\{1, 2, \dots, p\}$ and all p^d combinations represented.

$$D = \begin{bmatrix} 1 & 1 & \dots & 1 & \dots & p & p & \dots & p \\ \vdots & & & \vdots & & & & & \vdots \\ 1 & 1 & \dots & 1 & \dots & p & p & \dots & p \\ 1 & 2 & \dots & p & \dots & 1 & 2 & \dots & p \end{bmatrix}^T$$

A rotation of this matrix is accomplished by post-multiplication by a $d \times d$ matrix R with the property that $R^T R = I_d$ where I_d is the $d \times d$ identity matrix. (In this section, we relax the definition of rotation to be a matrix R that satisfies $R^T R = kI_d$ for some scalar k , since the true rotation can be obtained as $(1/\sqrt{k})R$.) Let the multiplication matrix R have entries denoted as $r_{[i,j]}$, which is the entry from the i th row and j th column. Lemma 1 below will not be concerned with whether the multiplication matrix is indeed a rotation matrix, but with how such a matrix would yield unique and equally-spaced projections to each dimension.

Lemma 1. *The entries of each column of the transformation matrix R must be unique from the set $\{p^t | t = 0, 1, \dots, d - 1\}$ in order to yield unique and equally-spaced projections.*

The proof of Lemma 1 and all following lemmas and theorems are given in the Appendix.

The previous lemma shows that every column of the transformation matrix must be a permutation of the set $\{1, p, \dots, p^{d-1}\}$ (allowing sign changes to elements and multiplication of entire columns by a constant). However, every rotation matrix R satisfies $R^T R = kI_d$, so that the sum of squares for all columns of R must be equal. Then, WLOG, every column of the transformation matrix must be a permutation of the set $\{1, p, \dots, p^{d-1}\}$ (allowing only sign changes to elements).

It is obvious that the columns of the transformation matrix cannot be identical, for otherwise the columns of the transformed matrix would be identical. The following lemma shows that the i th entries for the d columns must be unique in magnitude in order for the transformation to be a rotation.

Lemma 2. *For a rotation matrix R , the i th entries of the d columns are unique in magnitude for all i .*

Lemmas 1 and 2 proved that all the rows and columns of the transformation matrix must be permutations of the set $\{1, p, \dots, p^{d-1}\}$ (up to sign changes). However, this is not sufficient to guarantee that the matrix will also be a rotation.

Another requirement implied by the rotation condition $R^T R = kI_d$ is that the columns of R must be orthogonal. Any matrix satisfying the requirements of the lemmas and this last condition will rotate factorial designs into Latin hypercubes. The remainder of this section shows how to create these matrices for d that are powers of two and illustrates why other choices of d , in general, have no such rotation matrix.

Let d be a power of 2. Let $c = \log_2 d$. Let

$$V_1 = [v_1 \quad v_2] = \begin{bmatrix} +1 & -p \\ +p & +1 \end{bmatrix}. \tag{3}$$

Now, for $c > 1$, let V_c be defined inductively from V_{c-1} as follows:

$$V_c = \begin{bmatrix} V_{c-1} & -(p^{2^{c-1}} V_{c-1})^* \\ p^{2^{c-1}} V_{c-1} & (V_{c-1})^* \end{bmatrix}, \tag{4}$$

where the operator $(\cdot)^*$ works on any matrix with an even number of rows by multiplying the entries in the top half of the matrix by -1 and leaving those in the bottom half unchanged.

Theorem 3. *The matrix V_c is a rotation of the d -factor ($d = 2^c$), p -level standard full factorial design which yields unique and equally-spaced projections to each dimension.*

Reviewing the two-dimensional result from section 3, when $d = 2 = 2^1$, equation (2) with $w = \tan^{-1}(1/p)$ can be re-expressed as

$$V_1 = \begin{bmatrix} \cos(\tan^{-1}(1/p)) & -\sin(\tan^{-1}(1/p)) \\ \sin(\tan^{-1}(1/p)) & \cos(\tan^{-1}(1/p)) \end{bmatrix} = \frac{1}{\sqrt{1+p^2}} \begin{bmatrix} +1 & -p \\ +p & +1 \end{bmatrix}, \tag{5}$$

which is the correctly scaled rotation matrix V_1 given in equation (3).

Other scaled rotation matrices for cases of interest ($d = 4, 8$ corresponding to $c = 2, 3$) are

$$V_2 = \sqrt{\frac{p^2 - 1}{p^8 - 1}} \begin{bmatrix} +1 & -p & +p^2 & -p^3 \\ +p & +1 & -p^3 & -p^2 \\ +p^2 & -p^3 & -1 & +p \\ +p^3 & +p^2 & +p & +1 \end{bmatrix} \tag{6}$$

and

$$V_3 = \sqrt{\frac{p^2 - 1}{p^{16} - 1}} \begin{bmatrix} +1 & -p & +p^2 & -p^3 & +p^4 & -p^5 & +p^6 & -p^7 \\ +p & +1 & -p^3 & -p^2 & +p^5 & +p^4 & -p^7 & -p^6 \\ +p^2 & -p^3 & -1 & +p & -p^6 & +p^7 & +p^4 & -p^5 \\ +p^3 & +p^2 & +p & +1 & -p^7 & -p^6 & -p^5 & -p^4 \\ +p^4 & -p^5 & +p^6 & -p^7 & -1 & +p & -p^2 & +p^3 \\ +p^5 & +p^4 & -p^7 & -p^6 & -p & -1 & +p^3 & +p^2 \\ +p^6 & -p^7 & -p^4 & +p^5 & +p^2 & -p^3 & -1 & +p \\ +p^7 & +p^6 & +p^5 & +p^4 & +p^3 & +p^2 & +p & +1 \end{bmatrix}, \tag{7}$$

respectively.

The choice of rotation matrices for higher dimensions ($d > 2$) is not unique. Other inductive definitions for V_c in equation (4) are possible, namely

$$\begin{bmatrix} V_{c-1} & -p^{2^{c-1}}V_{c-1} \\ p^{2^{c-1}}V_{c-1} & V_{c-1} \end{bmatrix}. \quad (8)$$

However, the point is still clear, such rotations do exist.

Owen (1994) showed why orthogonality of design matrix columns is important in the estimation of Monte Carlo integrals and attempted to control the column correlations within Latin hypercubes. Theorem 4 will prove that all designs obtained by rotation of standard factorial designs, specifically rotated full factorial designs, will also be orthogonal. Let k be the sum of squares of the first column of X . As X is an orthogonal matrix with equal sum of squares for every column, $X^T X = kI_d$. So $(XR)^T(XR) = R^T X^T X R = R^T kI_d R = kR^T R = kI_d$, a diagonal matrix. Therefore, the rotated design matrix XR is an orthogonal design.

Theorem 4. *Let X be an orthogonal design matrix of n rows and d columns in which the sums of squares for columns are equal. Let R be a $d \times d$ rotation matrix. The design resulting from the matrix product XR is also an orthogonal design.*

Since computation of Monte Carlo integrals is, in effect, a computer experiment, it is beneficial for designs for computer experiments to have uncorrelated regression estimates of main effects. The following theorem shows this to be true for all designs obtained by rotation of standard full factorial designs, specifically rotated factorial designs.

Theorem 5. *Any p^d -point rotated factorial design has uncorrelated regression estimates of main effects.*

Recall that Johnson *et al.* (1990) introduced the use of minimum interpoint distance (MID) as an important design criterion (see equation (1)). It can be shown that the MID using Euclidean distance for a p^d -point rotated factorial design scaled to the unit hypercube, $[0, 1]^d$, is $\sqrt{1 + p^2 + \dots + p^{d+1}} / (p - 1) = \sqrt{(p^{2d} - 1) / ((p^2 - 1)(p - 1)^2)}$. Additionally, it can be shown this is the maximal MID for $d = 2$. We are unable to obtain a formal proof for higher dimensions, however.

Table 2 lists the MIDs for several of the four-dimensional RFDs requiring fewer than 100 points and for the respective MmLH and MmU designs. Due to the computational requirements of obtaining designs from other methods, some were results not available (N/A). It is clear that the easily-constructed RFDs have similar (if not equal) MIDs to other computing-extensive constructed designs.

6 Concluding Remarks

This paper has presented a new class of experimental designs for computer experiments: the rotated factorial designs. Developed from a rotation of the standard

Table 2. MID Comparisons of Four-Dimensional MmLH, RFD, and MmU Designs

No. of Pts	Maximin Latin H-cube	Rotated Design Type U	Factorial Design Type E#	Maximin U Design
8	0.9258 †	0.8692	0.7071 (3)	0.7954 ◁
9	0.8101 †	0.5762	1.0000 (3)	0.6960 ◁
10	0.7857 †	*	*	*
11	0.7416 †	*	*	*
12	0.7216 †	*	*	*
16	0.6218 ◊	0.6146	0.6146 (16)	0.5292 ◁
24	0.5325 ◊	0.3963	0.3963 (24)	N/A
28	N/A	0.3951	0.4167 (7)	*
36	N/A	0.3725	0.3725 (36)	N/A
40	N/A	0.5192	0.5192 (40)	N/A
41	0.4507 ◊	0.5062	0.5062 (41)	*
54	N/A	0.3641	0.3641 (54)	N/A
67	N/A	0.3825	0.3825 (67)	*
68	N/A	0.3751	0.3751 (68)	*
81	N/A	0.3579	0.3579 (81)	N/A

The number in parenthesis means the number of unique projected points.
 * No design can be constructed as defined.
 † Published in Morris & Mitchell (1992).
 ◊ Obtained via Morris & Mitchell (1992) algorithm by the author.
 ◁ Obtained by author's algorithm.

factorial design to produce a Latin hypercube, these designs have qualities that make them excellent candidates for use in today's computer experiments. The rotated full factorial designs possess the orthogonality of factorial designs and the unique and equally-spaced projections of Latin hypercubes, while maintaining a high spatial dispersion according to minimum interpoint distance. The Type U and E RFDs possess the orthogonality of factorial designs and either the unique or equally-spaced projections of Latin hypercubes, again while maintaining high spatial dispersion. All of the rotated factorial designs are extremely simple to construct, in contrast to the computer-intensive nature of most other recent designs, and perform well in terms of the minimum interpoint distance criterion used in the construction of a competing design. In terms of orthogonality, these RFDs perform even better. We have developed software to construct the rotated factorial designs presented in this paper. Users of S-Plus or C who are interested in obtaining this, please contact the authors.

Directions for future research in this area include finding alternative procedures for dimensions that are not powers of two, considering rotation of fractional factorial designs (or some other method to reduce the number of required points as d increases), and investigating the possibility of rotating mixed-level designs (perhaps as an alternative for the other dimensions). Johnson *et al.* (1990) also defined the index of a design - the number of pairs separated by the MID - as a second criterion to distinguish among several designs with identical MIDs. The performance of these designs may be investigated or modifications suggested, if and when this criterion becomes relevant. Some related recent work can be found in Bursztyn and Steinberg (2001, 2002).

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Appendices

6.1 A Sample Construction

(1) A $4^2=16$ -run rotated factorial design.
Start with a 4^2 standard factorial design.

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 & 4 & 4 & 4 & 4 \\ 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \end{bmatrix}^T$$

Rotate by $\tan^{-1}(1/4)$. This yields a 16-point rotated factorial design.

$$\begin{bmatrix} 1 \cos(\tan^{-1}(1/4)) + 1 \sin(\tan^{-1}(1/4)) & -1 \sin(\tan^{-1}(1/4)) + 1 \cos(\tan^{-1}(1/4)) \\ 1 \cos(\tan^{-1}(1/4)) + 2 \sin(\tan^{-1}(1/4)) & -1 \sin(\tan^{-1}(1/4)) + 2 \cos(\tan^{-1}(1/4)) \\ 1 \cos(\tan^{-1}(1/4)) + 3 \sin(\tan^{-1}(1/4)) & -1 \sin(\tan^{-1}(1/4)) + 3 \cos(\tan^{-1}(1/4)) \\ 1 \cos(\tan^{-1}(1/4)) + 4 \sin(\tan^{-1}(1/4)) & -1 \sin(\tan^{-1}(1/4)) + 4 \cos(\tan^{-1}(1/4)) \\ 2 \cos(\tan^{-1}(1/4)) + 1 \sin(\tan^{-1}(1/4)) & -2 \sin(\tan^{-1}(1/4)) + 1 \cos(\tan^{-1}(1/4)) \\ 2 \cos(\tan^{-1}(1/4)) + 2 \sin(\tan^{-1}(1/4)) & -2 \sin(\tan^{-1}(1/4)) + 2 \cos(\tan^{-1}(1/4)) \\ 2 \cos(\tan^{-1}(1/4)) + 3 \sin(\tan^{-1}(1/4)) & -2 \sin(\tan^{-1}(1/4)) + 3 \cos(\tan^{-1}(1/4)) \\ 2 \cos(\tan^{-1}(1/4)) + 4 \sin(\tan^{-1}(1/4)) & -2 \sin(\tan^{-1}(1/4)) + 4 \cos(\tan^{-1}(1/4)) \\ 3 \cos(\tan^{-1}(1/4)) + 1 \sin(\tan^{-1}(1/4)) & -3 \sin(\tan^{-1}(1/4)) + 1 \cos(\tan^{-1}(1/4)) \\ 3 \cos(\tan^{-1}(1/4)) + 2 \sin(\tan^{-1}(1/4)) & -3 \sin(\tan^{-1}(1/4)) + 2 \cos(\tan^{-1}(1/4)) \\ 3 \cos(\tan^{-1}(1/4)) + 3 \sin(\tan^{-1}(1/4)) & -3 \sin(\tan^{-1}(1/4)) + 3 \cos(\tan^{-1}(1/4)) \\ 3 \cos(\tan^{-1}(1/4)) + 4 \sin(\tan^{-1}(1/4)) & -3 \sin(\tan^{-1}(1/4)) + 4 \cos(\tan^{-1}(1/4)) \\ 4 \cos(\tan^{-1}(1/4)) + 1 \sin(\tan^{-1}(1/4)) & -4 \sin(\tan^{-1}(1/4)) + 1 \cos(\tan^{-1}(1/4)) \\ 4 \cos(\tan^{-1}(1/4)) + 2 \sin(\tan^{-1}(1/4)) & -4 \sin(\tan^{-1}(1/4)) + 2 \cos(\tan^{-1}(1/4)) \\ 4 \cos(\tan^{-1}(1/4)) + 3 \sin(\tan^{-1}(1/4)) & -4 \sin(\tan^{-1}(1/4)) + 3 \cos(\tan^{-1}(1/4)) \\ 4 \cos(\tan^{-1}(1/4)) + 4 \sin(\tan^{-1}(1/4)) & -4 \sin(\tan^{-1}(1/4)) + 4 \cos(\tan^{-1}(1/4)) \end{bmatrix}$$

$$= \begin{bmatrix} 1.21 & 0.73 \\ 1.46 & 1.70 \\ 1.70 & 2.67 \\ 1.94 & 3.64 \\ 2.18 & 0.49 \\ 2.43 & 1.46 \\ 2.67 & 2.43 \\ 2.91 & 3.40 \\ 3.15 & 0.24 \\ 3.40 & 1.21 \\ 3.64 & 2.18 \\ 3.88 & 3.15 \\ 4.12 & 0.00 \\ 4.37 & 0.97 \\ 4.61 & 1.94 \\ 4.85 & 2.91 \end{bmatrix}$$

This can be rescaled to be a 16-point Latin hypercube by multiplying by 15/3.64 then subtracting 3.99 from the first column and adding 1.00 to the second column.

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\ 4 & 8 & 12 & 16 & 3 & 7 & 11 & 15 & 2 & 6 & 10 & 14 & 1 & 5 & 9 & 13 \end{bmatrix}^T$$

(2) A 12-run Type U design.

To construct a 12-point Type U design, remove the 4 most extreme design points (from the prescaled matrix): the 1st, 4th, 13th, and 16th.

(3) A 12-run Type E design.

To get a 12-point Type E rotated factorial design, adjust the rotation angle to $\tan^{-1}(2/3)$. Figuring out the correct rotation angle is easy. If the original design has p^2 points, then the angle is unadjusted if 0 points are removed and is adjusted to $\tan^{-1}(1/(p-1))$ if $\{2, 4, \dots, 2p-2\}$ points are removed or to $\tan^{-1}(1/(p-2))$

if $\{2p, 2p + 2, \dots, 4p - 8\}$ points are removed. However, there is one exception to this rule: if the new design has an even number of points which exceed a square by 3, then the angle is adjusted to $\tan^{-1}(2/(p - 1))$. (Note that 12 is such a number, making the rotation angle $\tan^{-1}(2/3)$.)

$$\begin{aligned}
 & \begin{bmatrix} 1 \cos(\tan^{-1}(2/3)) + 2 \sin(\tan^{-1}(2/3)) & -1 \sin(\tan^{-1}(2/3)) + 2 \cos(\tan^{-1}(2/3)) \\ 1 \cos(\tan^{-1}(2/3)) + 3 \sin(\tan^{-1}(2/3)) & -1 \sin(\tan^{-1}(2/3)) + 3 \cos(\tan^{-1}(2/3)) \\ 2 \cos(\tan^{-1}(2/3)) + 1 \sin(\tan^{-1}(2/3)) & -2 \sin(\tan^{-1}(2/3)) + 1 \cos(\tan^{-1}(2/3)) \\ 2 \cos(\tan^{-1}(2/3)) + 2 \sin(\tan^{-1}(2/3)) & -2 \sin(\tan^{-1}(2/3)) + 2 \cos(\tan^{-1}(2/3)) \\ 2 \cos(\tan^{-1}(2/3)) + 3 \sin(\tan^{-1}(2/3)) & -2 \sin(\tan^{-1}(2/3)) + 3 \cos(\tan^{-1}(2/3)) \\ 2 \cos(\tan^{-1}(2/3)) + 4 \sin(\tan^{-1}(2/3)) & -2 \sin(\tan^{-1}(2/3)) + 4 \cos(\tan^{-1}(2/3)) \\ 3 \cos(\tan^{-1}(2/3)) + 1 \sin(\tan^{-1}(2/3)) & -3 \sin(\tan^{-1}(2/3)) + 1 \cos(\tan^{-1}(2/3)) \\ 3 \cos(\tan^{-1}(2/3)) + 2 \sin(\tan^{-1}(2/3)) & -3 \sin(\tan^{-1}(2/3)) + 2 \cos(\tan^{-1}(2/3)) \\ 3 \cos(\tan^{-1}(2/3)) + 3 \sin(\tan^{-1}(2/3)) & -3 \sin(\tan^{-1}(2/3)) + 3 \cos(\tan^{-1}(2/3)) \\ 3 \cos(\tan^{-1}(2/3)) + 4 \sin(\tan^{-1}(2/3)) & -3 \sin(\tan^{-1}(2/3)) + 4 \cos(\tan^{-1}(2/3)) \\ 4 \cos(\tan^{-1}(2/3)) + 2 \sin(\tan^{-1}(2/3)) & -4 \sin(\tan^{-1}(2/3)) + 2 \cos(\tan^{-1}(2/3)) \\ 4 \cos(\tan^{-1}(2/3)) + 3 \sin(\tan^{-1}(2/3)) & -4 \sin(\tan^{-1}(2/3)) + 3 \cos(\tan^{-1}(2/3)) \end{bmatrix} \\
 = & \begin{bmatrix} 1.94 & 1.11 \\ 2.50 & 1.94 \\ 2.22 & -0.28 \\ 2.77 & 0.55 \\ 3.33 & 1.39 \\ 3.88 & 2.22 \\ 3.05 & -0.83 \\ 3.61 & 0.00 \\ 4.16 & 0.83 \\ 4.71 & 1.66 \\ 4.44 & -0.55 \\ 4.99 & 0.28 \end{bmatrix}
 \end{aligned}$$

Once constructed, these designs can be rescaled to the experimental region. For example, to convert the 12-point Type E design matrix to LH notation, multiply by 11/3.05 then subtract 6.00 from the first column and add 3.99 to the second column.

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ 8 & 11 & 3 & 6 & 9 & 12 & 1 & 4 & 7 & 10 & 2 & 5 \end{bmatrix}^T$$

6.2 Proofs

Lemma 1: *The entries of each column of the transformation matrix R must be unique from the set $\{p^t | t = 0, 1, \dots, d - 1\}$ in order to yield unique and equally-spaced projections.*

Proof: The multiplication of the factorial design by R yields a new $p^d \times d$ matrix X with entries labeled $x_{[i,j]}$:

$$X = D \times R$$

Note that the values of the j th column of X depend on the j th column of matrix R , but on none of its other columns. Without loss of generality (WLOG), consider only the first column of these matrices and examine how the choices of $r_{[1,1]}, \dots, r_{[d,1]}$ affect the values of $x_{[1,1]}, \dots, x_{[p^d,1]}$.

The rows of the factorial design matrix can be arranged into p^{d-1} groups of rows where the rows in each group are identical in $d-1$ columns but unique in one column. They can be arranged, WLOG, as above with the first $d-1$ columns identical and the last column unique. Within each group the transformed coordinates differ only in respect to the value of $r_{[d,1]}$:

$$\begin{aligned} x_{[(i_1-1)p^{d-1}+(i_2-1)p^{d-2}+\dots+(i_{d-1}-1)p+1,1]} &= i_1r_{[1,1]} + i_2r_{[2,1]} + \dots + i_{d-1}r_{[d-1,1]} \\ &\quad + 1r_{[d,1]} \\ x_{[(i_1-1)p^{d-1}+(i_2-1)p^{d-2}+\dots+(i_{d-1}-1)p+2,1]} &= i_1r_{[1,1]} + i_2r_{[2,1]} + \dots + i_{d-1}r_{[d-1,1]} \\ &\quad + 2r_{[d,1]} \\ &\quad \vdots \\ x_{[(i_1-1)p^{d-1}+(i_2-1)p^{d-2}+\dots+(i_{d-1}-1)p+p,1]} &= i_1r_{[1,1]} + i_2r_{[2,1]} + \dots + i_{d-1}r_{[d-1,1]} \\ &\quad + pr_{[d,1]} \end{aligned}$$

where $i_1, \dots, i_{d-1} \in \{1, \dots, p\}$. For these points to be unique and equally-spaced requires only that $r_{[d,1]} \neq 0$. Let $r_{[d,1]} = 1$ (or -1), WLOG, so that the transformed points within any group differ by one unit and there are p^{d-1} such groups.

Now arrange the factorial design matrix into p^{d-2} groups of p^2 rows so that the rows within each group are identical in the first $d-2$ columns, subgrouped as before by the last column, and unique (by subgroups) in the $(d-1)$ th column. For any group, examine the j th transformed point within each subgroup. Then their transformed coordinates differ only in respect to the value of $r_{[d-1,1]}$:

$$\begin{aligned} x_{[(i_1-1)p^{d-1}+\dots+(i_{d-2}-1)p^2+j,1]} &= i_1r_{[1,1]} + \dots + i_{d-2}r_{[d-2,1]} + 1r_{[d-1,1]} \\ &\quad + jr_{[d,1]} \\ x_{[(i_1-1)p^{d-1}+\dots+(i_{d-2}-1)p^2+p+j,1]} &= i_1r_{[1,1]} + \dots + i_{d-2}r_{[d-2,1]} + 2r_{[d-1,1]} \\ &\quad + jr_{[d,1]} \\ &\quad \vdots \\ x_{[(i_1-1)p^{d-1}+\dots+(i_{d-2}-1)p^2+(p-1)p+j,1]} &= i_1r_{[1,1]} + \dots + i_{d-2}r_{[d-2,1]} + pr_{[d-1,1]} \\ &\quad + jr_{[d,1]} \end{aligned}$$

where $i_1, \dots, i_{d-2}, j \in \{1, \dots, p\}$. For these p points to be unique and equally-spaced requires only that $r_{[d-1,1]} \neq 0$. However, for all p^2 points within the group to be unique and equally-spaced requires that $r_{[d-1,1]} = \pm p$, since each of the p listed points represents one subgroup of p points differing by one unit. (Note that $r_{[d-1,1]} = \pm 1/p$ also satisfies the requirement; but then the entire matrix R could be multiplied by p to obtain $r_{[d-1,1]} = \pm 1$ and $r_{[d,1]} = \pm p$, essentially the

same transformation.) This strategy yields p^{d-2} groups of p^2 points where the transformed points within any group differ by one unit.

Continuing in this manner, it is clear that to yield unique and equally-spaced points in the transformed space, the values of $r_{[1,1]}, \dots, r_{[d,1]}$ must be unique from the set $\{1, p, \dots, p^{d-1}\}$ (up to sign changes and multiplication by a constant). As the choice of columns to examine was arbitrary, so must the entries from each column of the transformation matrix be of this form.

□

Lemma 2: *For a rotation matrix R , the i th entries of the d columns are unique in magnitude for all i .*

Proof: Assume that R is a rotation matrix. Then $R^T R = kI_d$, which implies that $RR^T = kI_d$. This says that the sum of squares for all rows (in addition to columns) of R must be equal to

$$\sum_{j=0}^{d-1} p^{2j} = (p^{2d} - 1)/(p^2 - 1).$$

Suppose that one row has two (or more) entries with magnitude equal to p^{d-1} . Then its sum of squares is greater than

$$2p^{2(d-1)} > (2(p^2 - 1)/p^2)((p^{2d} - 1)/(p^2 - 1)).$$

Note that, since $p \geq 2$, we have $2(p^2 - 1)/p^2 > 1$. Thus its sum of squares is greater than $(p^{2d} - 1)/(p^2 - 1)$, and this row has greater sum of squares than is possible. Thus each row has exactly one entry with magnitude equal to p^{d-1} .

Now, suppose that one row has two (or more) entries with magnitude equal to p^{d-2} . Examining the sum of squares of that row shows that it too is larger than is possible. Therefore each row has exactly one entry with magnitude equal to p^{d-2} . Continuing in this manner, since d is finite, proves the lemma.

□

Theorem 1: *The matrix V_c is a rotation of the d -factor ($d = 2^c$), p -level standard full factorial design which yields unique and equally-spaced projections to each dimension.*

Proof: It suffices to show for each $c \geq 1$ that V_c is comprised of rows and columns of permutations of the set $\{1, p, p^2, \dots, p^{d-1}\}$ (up to sign changes) and that the columns are all orthogonal. The proof proceeds by induction.

First, consider the simplest case where $d = 2$ and $c = 1$. Clearly V_1 meets these criteria and is therefore a rotation satisfying the projection criteria.

Suppose now that V_{c-1} is a rotation satisfying the projection criteria. If this implies that V_c is also such a rotation, the proof is completed.

Note these observations:

1. V_{c-1} is comprised of rows and columns of permutations of $\{1, p, p^2, \dots, p^{2^{c-1}-1}\}$ (up to sign changes).

2. $V_{c-1}^T V_{c-1} = k' I_{2^{c-1}}$, where $k' = 1 + p^2 + \dots + p^{2^{c-1}}$.
3. The rows and columns of $p^{2^{c-1}} V_{c-1}$ are permutations (up to sign changes) of $\{p^{2^{c-1}}, p^{2^{c-1}+1}, \dots, p^{2^c-1}\}$.
4. The operator $(\cdot)^*$ does not affect the magnitudes of entries in a matrix, only their signs.

From these 4 observations it follows that V_c is comprised of rows and columns of permutations of $\{1, p, p^2, \dots, p^{2^c-1}\}$ (up to sign changes). All that remains to show is that the columns of V_c are orthogonal.

Recall that for an arbitrary matrix subdivided into 4 submatrices A ($n_1 \times p_1$), B ($n_2 \times p_1$), C ($n_1 \times p_2$), and D ($n_2 \times p_2$),

$$\begin{bmatrix} A & C \\ B & D \end{bmatrix}^T \begin{bmatrix} A & C \\ B & D \end{bmatrix} = \begin{bmatrix} A^T & B^T \\ C^T & D^T \end{bmatrix} \begin{bmatrix} A & C \\ B & D \end{bmatrix} = \begin{bmatrix} A^T A + B^T B & A^T C + B^T D \\ C^T A + D^T B & C^T C + D^T D \end{bmatrix}. \quad (9)$$

Letting $A = V_{c-1}$, $B = p^{2^{c-1}} V_{c-1}$, $C = -(p^{2^{c-1}} V_{c-1})^*$, and $D = (V_{c-1})^*$, it suffices to show that $A^T A + B^T B = C^T C + D^T D = k I_{2^{c-1}}$ for some k and that $A^T C + B^T D = 0$.

First,

$$A^T A = V_{c-1}^T V_{c-1} = k' I_{2^{c-1}} \quad (10)$$

and

$$B^T B = p^{2^{c-1}} V_{c-1}^T p^{2^{c-1}} V_{c-1} = p^{2^c} V_{c-1}^T V_{c-1} = p^{2^c} k' I_{2^{c-1}}. \quad (11)$$

Thus $A^T A + B^T B = (1 + p^{2^c}) k' I_{2^{c-1}}$. Now for simplicity let for any matrix M with even number of rows

$$(M)^* = \begin{bmatrix} -M^{(1)} \\ M^{(2)} \end{bmatrix}, \quad (12)$$

where $M^{(1)}$ and $M^{(2)}$ are the top and bottom half of M , respectively. Then

$$\begin{aligned} D^T D &= (V_{c-1})^{*T} (V_{c-1})^* \\ &= \begin{bmatrix} -V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix}^T \begin{bmatrix} -V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix} \\ &= \begin{bmatrix} -V_{c-1}^{(1)T} & V_{c-1}^{(2)T} \end{bmatrix} \begin{bmatrix} -V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix} \\ &= V_{c-1}^{(1)T} V_{c-1}^{(1)} + V_{c-1}^{(2)T} V_{c-1}^{(2)} \\ &= \begin{bmatrix} V_{c-1}^{(1)T} & V_{c-1}^{(2)T} \end{bmatrix} \begin{bmatrix} V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix} \\ &= \begin{bmatrix} V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix}^T \begin{bmatrix} V_{c-1}^{(1)} \\ V_{c-1}^{(2)} \end{bmatrix} \\ &= V_{c-1}^T V_{c-1} \\ &= k' I_{2^{c-1}} \end{aligned} \quad (13)$$

and

$$\begin{aligned} C^T C &= [-(p^{2^{c-1}} V_{c-1})^*]^T [-(p^{2^{c-1}} V_{c-1})^*] \\ &= p^{2^c} [(V_{c-1})^*]^T (V_{c-1})^* \\ &= p^{2^c} k' I_{2^{c-1}}. \end{aligned} \tag{14}$$

Thus $C^T C + D^T D = (1 + p^{2^c})k' I_{2^{c-1}} = A^T A + B^T B$. Finally,

$$A^T C = V_{c-1}^T [-(p^{2^{c-1}} V_{c-1})^*] = -p^{2^{c-1}} V_{c-1}^T (V_{c-1})^* \tag{15}$$

and

$$B^T D = [p^{2^{c-1}} V_{c-1}]^T (V_{c-1})^* = p^{2^{c-1}} V_{c-1}^T (V_{c-1})^*. \tag{16}$$

Thus $A^T C + B^T D = 0$, and the columns of V_c are orthogonal. By the principle of mathematical induction, for all $c \geq 1$, V_c is a rotation of the d -factor ($d = 2^c$), p -level standard full factorial design which yields unique and equally-spaced projections to each dimension. That is, V_c turns standard factorial designs into Latin hypercubes.

Theorem 5: *Any p^d -point rotated factorial design has uncorrelated regression estimates of main effects.*

Proof: Let N be the model matrix with p^d rows and $d + 1$ columns: a first column (x_0) of 1s for an intercept and d centered and scaled columns (x_1, \dots, x_d) representing the standard p^d full factorial design. The columns are centered so that $x_0^T x_i = \sum_{j=1}^{p^d} x_{ij} = 0$ for all $i = 1, \dots, d$ and scaled so that $x_i^T x_i = \sum_{j=1}^{p^d} x_{ij}^2 = p^d$. Since each level of any one factor is used in combination with all other levels of any other factor, we have $x_0^T x_i = 0$ for all $i \neq k$. That is the matrix $X^T X = p^d I_{d+1}$.

Let R be the $D \times d$ rotation matrix which transforms the factorial design into a rotated factorial design. Since the rotation matrix does not affect the intercept, the associated transformation matrix on the model matrix X is the $(d+1) \times (d+1)$ matrix

$$R^* = \begin{bmatrix} 1 & 0 \\ 0 & R \end{bmatrix}.$$

Then

$$(XR^*)^T (XR^*) = p^d R^{*T} R^* = p^d \begin{bmatrix} 1 & 0 \\ 0 & I_d \end{bmatrix} p^d I_{d+1}.$$

It follows that the regression estimates of the main effects are uncorrelated.

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