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ROTATED FACTORIAL DESIGNS FOR COMPUTER EXPERIMENTS

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ABSTRACT

Computer models can describe complicated phenomena encountered in science and engineering fields. To use these models for scientific investigation, however, their generally long running times and mostly deterministic nature require a specially designed experiment. 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 uncorrelated regression effect estimates (orthogonality). A thorough application of the newly proposed design in mechanical engineering is presented. New results on the rotated mixed-level factorial designs are discussed.

Key words and phrases: Effect correlation, minimum interpoint distance, mixed level, rotated factorial design.

AMS 2000 subject classifications: Primary 62K15.

1. Introduction

When observations are scarce, one is faced with important issues at both the design and analysis stages of experimentation. The literature has addressed many of these problems, but one application has special requirements and deserve more attention. The selection of input combinations to a computer model, called a computer experiment, is unique because of the deterministic nature of the model.

Computer models can describe complicated phenomena encountered in science and engineering fields. However, their generally long running times make Monte Carlo simulation studies infeasible. An approximation can be constructed from a designed experiment, but the mostly deterministic nature of the computer model requires a special design. Standard factorial designs are inadequate; in the absence of one or more main effects, their replication produces redundancy. Traditional optimal designs also fail because they are based on variance considerations. New designs have been proposed, but many are computationally burdensome.

This paper presents a new class of designs obtained by rotating factorial designs into Latin hypercubes. The Latin hypercube projection property guarantees that these rotated factorial designs can be constructed for any number of factors. They are simple to construct and combine factorial design properties – equally-spaced projections to univariate dimensions and spatial dispersion – with Latin hypercube properties – unique projections and model flexibility. When p^d factorial designs are used, the rotated factorial designs possess orthogonality and are shown to be optimal by the minimum interpoint distance criterion in two dimensions. In other dimensions, the designs compare well to the optimal designs obtained in practice.

This paper is organized as follows. A brief summary of our previous work (Beattie and Lin, 1998) on rotated regular p^d full factorial designs is given in Section 2. Section 3 presents a thorough application on Mechanical Engineering. Section 4 discusses the rotation properties for mixed-level factorial design. Summary and concluding remarks are given in Section 5.

2. Rotated Factorial Designs

The use of rotated designs for experiments (not necessarily computer experiments) is not a new idea. DeFeo and Myers (1992), Crosier (1993) and Lucas (1996), for example, have suggested rotation for accomplishing various objectives. Their objectives are very different from our study here, however. The new strategy taken here is to modify the standard factorial design by rotation to yield a Latin hypercube (Mckay, Beckman and Conover, 1979). A general result for rotating two-dimensional factorial designs can be stated in this theorem (see, Beattie and Lin, 1998):

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* $k \in \{1, \ldots, p\}$. *These projections will be unique if and only if the rotation angle is* $\tan^{-1}(1/p)$.

For higher dimensions, consider a standard full factorial design consisting of d factors, each with p levels. A p-level, d-factor standard full factorial design can be represented by the $p^d \times d$ matrix with entries from $\{1, 2, \ldots, p\}$ and all p^d combinations present:

$$D = \begin{bmatrix} 1 & 1 & & \cdots & & 1 & \cdots & p & p & & \cdots & & & p \\ \vdots & & & & & \vdots & & & & & & & & \vdots \\ 1 & 1 & \cdots & 1 & \cdots & p & p & \cdots & p & \cdots & 1 & 1 & \cdots & 1 & \cdots & p & p & \cdots & p \\ 1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p & \cdots & 1 & 2 & \cdots & p \end{bmatrix}^{\mathrm{T}}. \tag{1}$$

For example, a 3^3 full factorial design can be presented as

$$D = \begin{bmatrix} 1&1&1&1&1&1&1&1&1&2&2&2&2&2&2&2&2&2&3&3&3&3&3&3&3&3&3 \\ 1&1&1&2&2&2&3&3&3&1&1&1&2&2&2&3&3&3&1&1&1&2&2&2&3&3&3 \\ 1&2&3&1&2&3&1&2&3&1&2&3&1&2&3&1&2&3&1&2&3&1&2&3&1&2&3 \end{bmatrix}^{\mathrm{T}}.$$

A rotation of this matrix is then accomplished by post-multiplication by a $d \times d$ matrix V with the property that $V^{\mathrm{T}}V = I_d$, where I_d is the $d \times d$ identity matrix. Let also d be a power of 2 and $c = \log_2 d$. Let

$$V_1 = [v_1 \quad v_2] = \begin{bmatrix} 1 & +p \\ +p & -1 \end{bmatrix}. \tag{2}$$

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

$$V_c = \begin{bmatrix} V_{c-1} & -(p^{2^{c-1}} V_{c-1})^* \\ p^{2^{c-1}} V_{c-1} & (V_{c-1})^* \end{bmatrix}, \tag{3}$$

where the operator $(\cdot)^*$ works on any matrix with an even number of rows by m ultiplying the entries in the top half of the matrix by -1 and leaving those in the bottom half unchanged. The higher dimensional rotation can be stated in the Theorem given in Beattie and Lin (2005).

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

3. A Practical Application to Mechanical Engineering

Liao and Wang (1996) used a computer model to study the effects of an "active constrained layer" on damping the vibrations in a beam induced by a varying (over time and location) force on one of the beam's ends. This active constrained layer consisted of two parts: a viscoelastic material (VEM), which acts as a shock absorber, attached to the top of the beam and a piezoelectric material (PZT), which by way of a control voltage produces a counter-force, on top of the VEM.

The current project studies the effects of an "enhanced active constrained layer," similar to that in Liao and Wang (1996) but incorporating two edge elements which are able to transmit the force of the PZT directly to the beam without being dampened by the VEM. Figure 1 illustrates this system. In it we see the stationary beam, fixed to a wall on one end, with the VEM and PZT (controlled by input voltage V) layers on its top side. Because the counter-effects of the PZT are dampened by the VEM, two edge elements (k_1 and k_2) are incorporated to transfer the force of the PZT directly to the beam.

The effects of four factors can be studied via the computer model using the MATLAB software package: the stiffness of each of the edge elements, which can be adjusted between 0 (no edge element) and 10 units, and the thicknesses of the VEM and the PZT, which can be adjusted between 0 (no VEM or no PZT) and 100% of the beam thickness. The program, which solves several partial differential equations, provides as output two measures of the performance of the Enhanced Active Constrained Layer (EACL): the performance index of the system and the control voltage (V) of the PZT, both of which are ideal when minimized. The performance index is the researcher's primary concern.

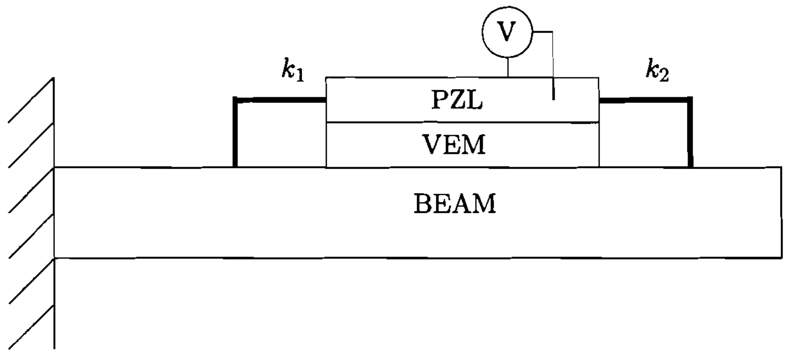

Figure 1 Beam with Enhanced Active Constrained Layer (EACL) including viscoelastic material (VEM), piezoelectric material (PZT) controlled by voltage V, and edge elements (k_1 and k_2)

To investigate the effects of the four input variables on the performance index, the traditional approach in this field of engineering would be one of the following: incorporate a full factorial design in all four variables or fix two of the factors at a time and use a full factorial design in the remaining two variables. The latter approach, as is well known, is unable to estimate three-way or higher interactions among the variables, although it would require fewer experimental runs than the former. The former method, while able to determine these high-order interactions, may require an inordinate number of runs, depending on the degree to which the experimenter wants to estimate the response surface.

Using the Penn State Center for Academic Computing PC network, the time to obtain a single observation from the computer model was approximately 2 minutes, 50 seconds on an IBM computer with 486 processor and 32 MB RAM. Using such equipment, incorporating a 3^4 factorial design would require almost 4 hours of computing time, while a 4^4 or larger design would require over 12 hours. Running the set of all 6 pairwise 4^2 factorial designs (that is, holding two variables constant and letting two vary) would require 4 and a half hours, while the 6×5^2 design would require 7 hours. Due to the large requirements in computer time, one can see that a typical Monte Carlo type study is not possible.

An 81-point, 4-dimensional rotated factorial design was employed for this computer experiment. After multiplying the standard 3^4 factorial design by the rotation matrix of Equation (3), the design matrix was scaled to the actual design region: $[0, 10]^2 \times [0, 1]^2$. The factor levels used with their resulting performance index values are shown in Table 1. Two types of three-dimensional plots are used to study the response surface over bivariate margins. Figure 2 shows S-Plus perspective plots, which provide a very eye-pleasing surface. These graphs, however, require linear interpolation between points and may exaggerate certain features of the distribution. Some other three-dimensional plots are shown in Figure 3. These graphs display the responses as circles of varying diameters. Points with larger circles had larger responses at those coordinates in projected two-dimensional space.

Table 1:

Data from 81-point Rotated Factorial Design for EACL study

k_1 stiffness	k_2 stiffness	VEM thickness	PZL thickness	Performance Index
0	1	0.703	0.2575	0.00093924
1.125	0.875	0.368875	0.294625	0.00057009
2.25	0.75	0.03475	0.33175	0.00064918
0.375	4.375	0.690625	0.146125	0.00051996
1.5	4.25	0.3565	0.18325	0.00049537
2.625	4.125	0.022375	0.220375	0.00057361
0.75	7.75	0.67825	0.03475	0.00042830
1.875	7.625	0.344125	0.071875	0.00046549
3	7.5	0.01	0.109	0.00056944
3.375	0.625	0.814375	0.245125	0.00049967
4.5	0.5	0.48025	0.28225	0.00055685
5.625	0.375	0.146125	0.319375	0.00066222
3.75	4	0.802	0.13375	0.00040415
4.875	3.875	0.467875	0.170875	0.00044878
6	3.75	0.13375	0.208	0.00052095
4.125	7.375	0.789625	0.022375	0.00035029
5.25	7.25	0.4555	0.0595	0.00041486
6.375	7.125	0.121375	0.096625	0.00050837
6.75	0.25	0.92575	0.23275	0.00055769
7.875	0.125	0.591625	0.269875	0.00072333
9	0	0.2575	0.307	0.00113730

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k_1 stiffness	k_2 stiffness	VEM thickness	PZL thickness	Performance Index
7.125	3.625	0.913375	0.121375	0.00038577
8.25	3.5	0.57925	0.1585	0.00042808
9.375	3.375	0.245125	0.195625	0.00048914
7.5	7	0.901	0.01	0.00032207
8.625	6.875	0.566875	0.047125	0.00038603
9.75	6.75	0.23275	0.08425	0.00046671
0.125	2.125	0.740125	0.591625	0.00070623
1.25	2	0.406	0.62875	0.00059986
2.375	1.875	0.071875	0.665875	0.00061133
0.5	5.5	0.72775	0.48025	0.00057804
1.625	5.375	0.393625	0.517375	0.00055743
2.75	5.25	0.0595	0.5545	0.00057613
0.875	8.875	0.715375	0.368875	0.00052122
2	8.75	0.38125	0.406	0.00052421
3.125	8.625	0.047125	0.443125	0.00055937
3.5	1.75	0.8515	0.57925	0.00057622
4.625	1.625	0.517375	0.616375	0.00058212
5.75	1.5	0.18325	0.6535	0.00059987
3.875	5.125	0.839125	0.467875	0.00052931
5	5	0.505	0.505	0.00053742
6.125	4.875	0.170875	0.542125	0.00055764
4.25	8.5	0.82675	0.3565	0.00048609
5.375	8.375	0.492625	0.393625	0.00050200
6.5	8.25	0.1585	0.43075	0.00053395
6.875	1.375	0.962875	0.566875	0.00057586
8	1.25	0.62875	0.604	0.00058230
9.125	1.125	0.294625	0.641125	0.00059870
7.25	4.75	0.9505	0.4555	0.00052459
8.375	4.625	0.616375	0.492625	0.00053137
9.5	4.5	0.28225	0.52975	0.00054689
7.625	8.125	0.938125	0.344125	0.00047870
8.75	8	0.604	0.38125	0.00049253
9.875	7.875	0.269875	0.418375	0.00051781
0.25	3.25	0.77725	0.92575	0.00070878
1.375	3.125	0.443125	0.962875	0.00066371
2.5	3	0.109	1	0.00063985
0.625	6.625	0.764875	0.814375	0.00065063
1.75	6.5	0.43075	0.8515	0.00063136
2.875	6.375	0.096625	0.888625	0.00061380
1	10	0.7525	0.703	0.00061145
2.125	9.875	0.418375	0.740125	0.00060175

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k_1 stiffness	k_2 stiffness	VEM thickness	PZL thickness	Performance Index
3.25	9.75	0.08425	0.77725	0.00059436
3.625	2.875	0.888625	0.913375	0.00066282
4.75	2.75	0.5545	0.9505	0.00065707
5.875	2.625	0.220375	0.987625	0.00064767
4	6.25	0.87625	0.802	0.00062946
5.125	6.125	0.542125	0.839125	0.00062453
6.25	6	0.208	0.87625	0.00061789
4.375	9.625	0.863875	0.690625	0.00059665
5.5	9.5	0.52975	0.72775	0.00059418
6.625	9.375	0.195625	0.764875	0.00059362
7	2.5	1	0.901	0.00066329
8.125	2.375	0.665875	0.938125	0.00065894
9.25	2.25	0.33175	0.97525	0.00065256
7.375	5.875	0.987625	0.789625	0.00062901
8.5	5.75	0.6535	0.82675	0.00062472
9.625	5.625	0.319375	0.863875	0.00061959
7.75	9.25	0.97525	0.67825	0.00059559
8.875	9.125	0.641125	0.715375	0.00059307
10	9	0.307	0.7525	0.00059222

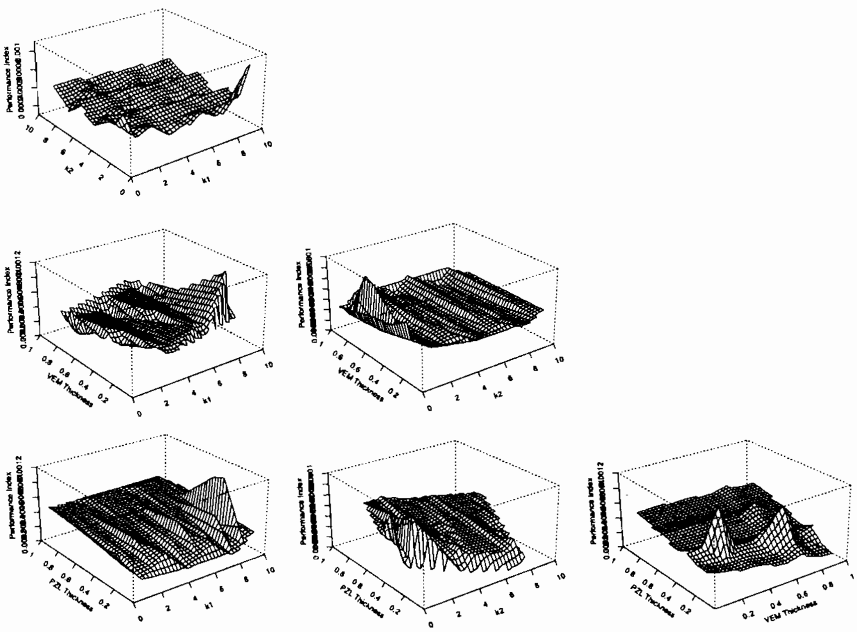

Figure 2 Bivariate 3-dimensional perspective plots of the Performance Index

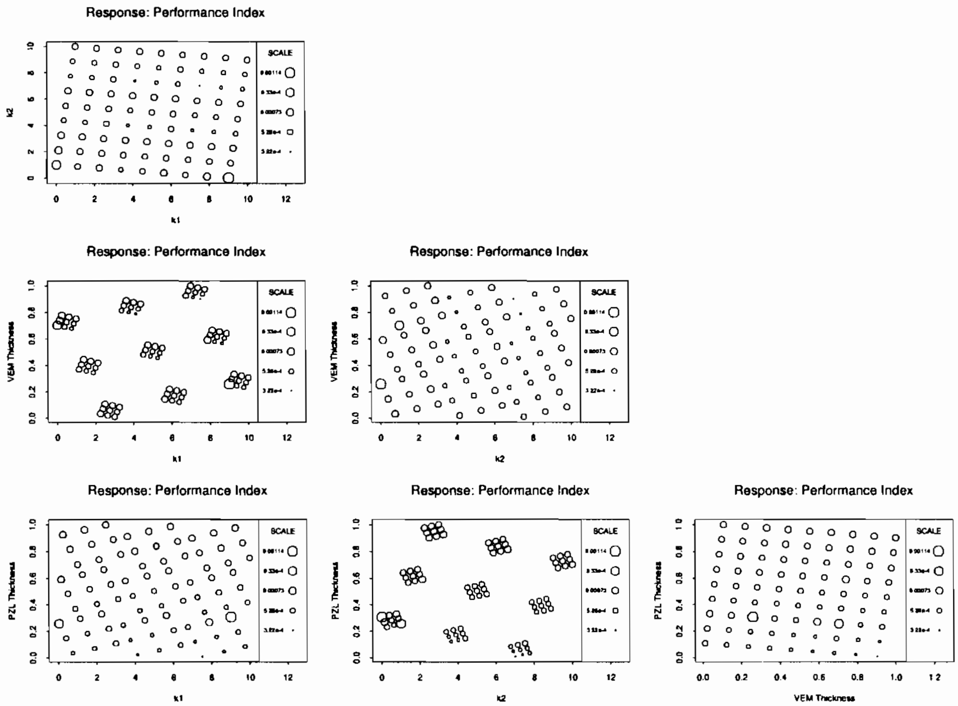

Figure 3 Bivariate 3-dimensional circle plots of the Performance Index

Then stepwise regression in S-Plus, which utilizes the AIC criterion (Statistical Sciences 1995), was used to choose a well-fitting model for the performance index. The stepwise procedure began with the intercept-only model, rewarded those terms which lowered AIC the most and fit only hierarchical models. Although in practice one might utilize more intelligent regression schemes for this complicated response surface, the goal here is to demonstrate that a simple methodology based on approximation by the Taylor series expansion applied to data from a rotated factorial design results in a model that verifies basic physical laws. To keep the number of terms moderate for this demonstration, the stepwise procedure was stopped when the best candidate term for inclusion had a non-significant p-value (greater than .05). The results are shown in Table 2 and include both sequential (in the order selected by the stepwise procedure) and partial (as if last term included) 2-sided p-values.

Table 2 Significant EACL effects identified via stepwise regression

		Sequential		Partial	
Source	df	MS	p-value	t	p-value
PZL thickness	1	2.516819×10^{-7}	0.00000000	-3.0592	0.0031
k2 stiffness (linear)	1	1.388989×10^{-7}	0.00000139	-5.3621	0.0000
VEM thickness	1	1.529360×10^{-8}	0.08520369	-3.8873	0.0002
k2 stiffness (quadratic)	1	1.111523×10^{-7}	0.00001177	4.2680	0.0001
VEM thickness / PZL thickness	1	5.576510×10^{-8}	0.00135561	3.3987	0.0011
k2 stiffness (L) / PZL thickness	1	1.867760×10^{-8}	0.05770075	3.5085	0.0008
k2 stiffness (Q) / PZL thickness	1	4.963070×10^{-8}	0.00241421	-3.1434	0.0024
Residuals	73	5.022800×10^{-9}			

Residual standard error: 7.087×10^{-5} on 73 degrees of freedom

Multiple R-Squared: 0.6362

The stepwise regression procedure identified several effects as important: linear effects of VEM and PZL thickness plus their interaction and also linear and quadratic effects of k_2 stiffness plus their interactions with PZL thickness. Although this model could have been fit using a standard 3^4 factorial design, the rotated factorial design offered greater model flexibility plus the advantage of being able to test for univariate cubic effects. Additionally, the model with all main effects, two-factor interactions, and univariate quadratic effects – the second order model – was fit to the data. This model agreed well with the stepwise model, except that the second order model identified a significant quadratic effect of k_1 stiffness.

The effects identified by the stepwise procedure make sense physically. One would guess that VEM thickness has a negative effect on the performance index – more VEM will dampen the system more – as well as PZT thickness – more PZT can generate a larger counter-force. One would also expect to see a strong VEM/PZT interaction – since the counter-force of the PZT travels primarily through the VEM, a larger layer of VEM would restrict the amount of counter-force generated on the beam by the PZT. The negative linear effect due to k_2 stiffness (plus some small quadratic effect) and the PZL/k_2 interaction are reasonable – again, the effects of PZL travel partially through k_2 to the beam. On the other hand, the stepwise procedure did not identify a significant effect due to k_1 stiffness. Though this may or may not be surprising, one would agree that the effect of k_1 stiffness is less than that of k_2. After all, the lever arm (component of torque) is smaller for k_1. Finally, one might take special notice that no VEM/k_2 or VEM/k_1 interactions were found, logical since those two components are not directly connected in the system.

To evaluate the appropriateness of the rotated factorial design strategy for this application, an 81-point standard factorial design was also employed on the data set. Second order models were fit to both the rotated factorial design and standard factorial design data. Thirty points were selected at random uniformly over the design region and actual responses obtained and compared to model predictions. Table 3 lists the data obtained from this follow-up computer experiment, along with the predicted values from the two models. At the bottom of the table is the estimated bias from each design, measured by observed sums of squares for bias and mean square bias. The estimated bias using the rotated factorial design was approximately one-fifth that from employing the standard factorial design.

4. Mixed-Level Rotated Factorial Designs

Focus until this point has been on the use of factorial designs with the same number of levels for each factor. However, the arguments for the existence of rotations converting these designs into Latin hypercubes can be extended to mixed-level factorial designs, where the numbers of levels for factors may be distinct. The form of the rotation matrix will be shown to agree with that found for p^2 factorial designs. Recognition of this agreement leads naturally to rotations for designs in which the dimension is any power of two. Specifically, the four-dimensional rotation matrix for mixed-level factorial designs will be obtained.

First, consider the two-dimensional setting using a factorial design of pq points, where one factor is set to p levels and another to q levels. A key step is the rescaling of the second column of the factorial design by a constant, α, as

$$D = \begin{bmatrix} 1 & 1 & 1 & 2 & 2 & 2 & \dots & p & p & p \\ 1\alpha & \dots & q\alpha & 1\alpha & \dots & q\alpha & \dots & 1\alpha & \dots & q\alpha \end{bmatrix}^{\mathrm{T}}. \tag{4}$$

Table 3 Empirical comparison of Rotated Factorial and Standard Factorial Designs using 30 randomly selected points of observation

Factor Settings				Performance Index (times 10^8)		
k_1	k_2	VEM	PZL	Actual	Predicted	
stiffness	stiffness	thickness	thickness		RFD	3^4 FD
6.87965	1.49429	0.24219	0.55273	57620	63985	80357
6.29913	2.94720	0.62782	0.56775	55908	54643	79423
4.46316	3.47452	0.38456	0.99386	65650	60727	74693
1.47957	7.57190	0.61610	0.23336	46807	47481	58399
9.95273	3.01604	0.06337	0.09407	54764	69771	48970
7.09213	3.05195	0.47020	0.99439	66057	63260	76887
1.86722	9.13514	0.65839	0.11443	41766	44042	49775
2.36317	7.99654	0.69916	0.65626	58619	58361	70840
3.84331	6.85965	0.65839	0.38038	49756	45805	59187
5.77096	5.98134	0.72508	0.15855	41122	38693	41743
1.54342	9.05181	0.17163	0.36722	54735	54317	64523
7.21732	6.54021	0.72045	0.78647	61692	56950	64349
0.94097	9.97976	0.67023	0.65004	59772	67002	76898
6.64037	6.00297	0.47995	0.28754	47205	44289	52451
5.24531	5.87590	0.15650	0.74958	59421	55047	58221
0.24121	8.37977	0.42827	0.29549	62786	54037	67374
5.92850	7.51320	0.44569	0.47747	52703	47763	59730
9.39484	5.44347	0.67972	0.76755	61043	59219	68194
2.37518	3.57215	0.67238	0.57743	56779	56688	87831
9.42977	0.70129	0.21077	0.31865	58005	74620	76938
0.75551	5.78426	0.68025	0.57058	58540	58566	82178
9.70392	6.02336	0.10585	0.93759	61669	66606	55539
4.66313	8.90121	0.53800	0.66778	57977	55320	64883
9.19884	5.23249	0.92034	0.17002	40334	40482	37299
5.86649	3.74807	0.55385	0.19946	44524	46802	54284
7.74653	8.13527	0.93594	0.31718	46743	41740	43104
8.51586	2.10426	0.10339	0.58974	58407	67664	72201
2.09206	1.98344	0.62740	0.02453	41873	55265	61748
6.93150	1.78096	0.31887	0.73003	60573	62989	83831
8.58616	8.59875	0.27621	0.83926	61064	62406	61374
				Observed SS Bias	1.144×10^{-7}	5.497×10^{-7}
				Observed MS Bias	3.813×10^{-9}	1.832×10^{-8}

Then a rotation matrix

$$R = \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \tag{5}$$

satisfying the equations implied by $D \times R$ is then obtained. It can be shown via a straightforward algebra that the matrix R becomes

$$\begin{bmatrix} 1 & p/\alpha \\ -p/\alpha & 1 \end{bmatrix}. \tag{6}$$

It suffices to find the value of α. To do so, consider the other set of equations implied by $D \times R$. That is, the q equations

$$\begin{array}{c} x_1 b_1 + 1\alpha b_2 \\ x_1 b_1 + 2\alpha b_2 \\ \vdots \\ x_1 b_1 + q\alpha b_2 \end{array} \tag{7}$$

(for all $x_1 \in \{1, \ldots, p\}$) are separated by the amount $\alpha b_2 = \alpha$, and the p equations

$$\begin{array}{c} 1b_1 + x_2 \alpha b_2 \\ 2b_1 + x_2 \alpha b_2 \\ \vdots \\ pb_1 + x_2 \alpha b_2 \end{array} \tag{8}$$

(for all $x_2 \in \{1, \ldots, q\}$) are separated by the amount $b_1 = \pm q\alpha$, implying that $\alpha = \sqrt{p/q}$. Therefore, the matrix R,

$$R = \begin{bmatrix} 1 & \sqrt{pq} \\ -\sqrt{pq} & 1 \end{bmatrix}, \tag{9}$$

is a rotation (one it's scaled) transforming the $p \times q$ factorial design into a pq-point Latin hypercube design for two factors. When the numbers of levels for the two factors in the factorial design are equal (say, p), $\alpha = \sqrt{p/p} = 1$ (so the factorial design is unscaled) and the rotation agrees with that previously obtained in Equation (2).

An extension to higher dimensions for mixed-level factorial designs is based on the form of the rotation matrix for p^d designs given in Equation (3), by which V_2 can be written (before scaling)

$$V_2 = \begin{bmatrix} 1 & +p & +p^2 & +p^3 \\ -p & 1 & -p^3 & +p^2 \\ -p^2 & -p^3 & 1 & +p \\ +p^3 & -p^2 & -p & 1 \end{bmatrix} = \begin{bmatrix} 1 & +p & 0 & 0 \\ -p & 1 & 0 & 0 \\ 0 & 0 & 1 & +p \\ 0 & 0 & -p & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & +p^2 & 0 \\ 0 & 1 & 0 & +p^2 \\ -p^2 & 0 & 1 & 0 \\ 0 & -p^2 & 0 & 1 \end{bmatrix}, \tag{10}$$

so that the four-dimensional rotation matrix is the product of rotation matrices. Let the four factors be labeled as A, B, C, and D. Then the rotation can be interpreted as a sequence of rotations occuring in the AB-, CD-, AC-, and BD-planes, respectively.

If factors A and C have p levels and factors B and D have q levels, then a four-dimensional rotation matrix to convert the $p^2 \times q^2$ mixed-level factorial design into a Latin hypercube can be found by considering the product

$$\begin{bmatrix} 1 & +\sqrt{pq} & 0 & 0 \\ -\sqrt{pq} & 1 & 0 & 0 \\ 0 & 0 & 1 & +\sqrt{pq} \\ 0 & 0 & -\sqrt{pq} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & +\alpha & 0 \\ 0 & 1 & 0 & +\alpha \\ -\alpha & 0 & 1 & 0 \\ 0 & -\alpha & 0 & 1 \end{bmatrix} \tag{11}$$

and obtaining α and the necessary factorial design scaling constants. It can be shown that $\alpha = pq$, that the rotation matrix is

$$\begin{bmatrix} 1 & \sqrt{pq} & 0 & 0 \\ -\sqrt{pq} & 1 & 0 & 0 \\ 0 & 0 & 1 & \sqrt{pq} \\ 0 & 0 & -\sqrt{pq} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & pq & 0 \\ 0 & 1 & 0 & pq \\ -pq & 0 & 1 & 0 \\ 0 & -pq & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{pq} & pq & pq\sqrt{pq} \\ -\sqrt{pq} & 1 & -pq\sqrt{pq} & pq \\ -pq & -pq\sqrt{pq} & 1 & \sqrt{pq} \\ pq\sqrt{pq} & -pq & -\sqrt{pq} & 1 \end{bmatrix}, \tag{12}$$

and that the scaling constants are $\sqrt{q}$ for factors A and C and $\sqrt{p}$ for factors B and D. (Letting $p = q$ shows the agreement with Equation (10).)

Suppose that factors A, B, C, and D have p, q, r, and s levels, respectively. Let the scaling constant for factor A be one, and denote the other three scaling constants by β, γ, and δ, for factors B, C, and D, respectively. Consider a transformation matrix from the product of rotation matrices

$$R = \begin{bmatrix} \frac{1}{\sqrt{1+pq}} & \frac{\sqrt{pq}}{\sqrt{1+pq}} & 0 & 0 \\ \frac{-\sqrt{pq}}{\sqrt{1+pq}} & \frac{1}{\sqrt{1+pq}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+rs}} & \frac{\sqrt{rs}}{\sqrt{1+rs}} \\ 0 & 0 & \frac{-\sqrt{rs}}{\sqrt{1+rs}} & \frac{1}{\sqrt{1+rs}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+\alpha^2}} & 0 & \frac{\alpha}{\sqrt{1+\alpha^2}} & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon^2}} & 0 & \frac{\epsilon}{\sqrt{1+\epsilon^2}} \\ \frac{-\alpha}{\sqrt{1+\alpha^2}} & 0 & \frac{1}{\sqrt{1+\alpha^2}} & 0 \\ 0 & \frac{-\epsilon}{\sqrt{1+\epsilon^2}} & 0 & \frac{1}{\sqrt{1+\epsilon^2}} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{\sqrt{1+pq}\sqrt{1+\alpha^2}} & \frac{\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} & \frac{\alpha}{\sqrt{1+pq}\sqrt{1+\alpha^2}} & \frac{\epsilon\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \\ \frac{-\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\alpha^2}} & \frac{1}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} & \frac{-\alpha\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\alpha^2}} & \frac{\epsilon}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \\ \frac{-\alpha}{\sqrt{1+rs}\sqrt{1+\alpha^2}} & \frac{-\epsilon\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} & \frac{1}{\sqrt{1+rs}\sqrt{1+\alpha^2}} & \frac{\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} \\ \frac{\alpha\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\alpha^2}} & \frac{-\epsilon}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} & \frac{-\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\alpha^2}} & \frac{1}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} \end{bmatrix}, \tag{13}$$

where here the matrices are appropriately scaled to ensure that they are rotations.

Consider first the effect in multiplication of the first column of R on the factorial design. Following the idea used to derive the two-dimensional rotation, there are

$$p \text{ points separated by } \Delta_A = \frac{1}{\sqrt{1+pq}\sqrt{1+\alpha^2}} \tag{14}$$
$$q \text{ points separated by } \Delta_B = \frac{\beta\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\alpha^2}} \tag{15}$$
$$r \text{ points separated by } \Delta_C = \frac{\gamma\alpha}{\sqrt{1+rs}\sqrt{1+\alpha^2}} \tag{16}$$
$$s \text{ points separated by } \Delta_D = \frac{\delta\alpha\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\alpha^2}}. \tag{17}$$

Letting $\Delta_B = p\Delta_A$, $\Delta_C = pq\Delta_A$, and $\Delta_D = pqr\Delta_A$ implies that

$$\beta = \sqrt{p/q} \tag{18}$$
$$\gamma = \frac{pq\sqrt{1+rs}}{\alpha\sqrt{1+pq}} \tag{19}$$
$$\delta = \frac{pq\sqrt{r}\sqrt{1+rs}}{\alpha\sqrt{s}\sqrt{1+pq}}. \tag{20}$$

Next, consider the effect of the second column of R on the factorial design. There are

$$p \text{ points separated by } \Delta_A = \frac{\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \tag{21}$$
$$q \text{ points separated by } \Delta_B = \frac{\beta}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \tag{22}$$
$$r \text{ points separated by } \Delta_C = \frac{\gamma\epsilon\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} \tag{23}$$
$$s \text{ points separated by } \Delta_D = \frac{\delta\epsilon}{\sqrt{1+rs}\sqrt{1+\epsilon^2}}, \tag{24}$$

where the Δs are distinct from those in Equations (14 - 17) regarding the first column's effect. It is easily verified that $\Delta_A = q\Delta_B$. Letting $\Delta_D = qp\Delta_B$ results in

$$\frac{\epsilon}{\alpha} = \frac{\sqrt{ps}}{\sqrt{qr}}. \tag{25}$$

From this it follows that $\Delta_C = s\Delta_D = qps\Delta_B$.

The effect of the third column of R is then determined. There are

$$p \text{ points separated by } \Delta_A = \frac{\alpha}{\sqrt{1+pq}\sqrt{1+\alpha^2}} \tag{26}$$

$$q \text{ points separated by } \Delta_B = \frac{\beta\alpha\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\alpha^2}} \tag{27}$$

$$r \text{ points separated by } \Delta_C = \frac{\gamma}{\sqrt{1+rs}\sqrt{1+\alpha^2}} \tag{28}$$

$$s \text{ points separated by } \Delta_D = \frac{\delta\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\alpha^2}}. \tag{29}$$

Again, it is easily verified that $\Delta_D = r\Delta_C$. Setting $\Delta_A = rs\Delta_C$ yields

$$\alpha = \sqrt{pqrs}. \tag{30}$$

Then it follows directly that $\Delta_B = p\Delta_A = rsp\Delta_C$.

Finally, using the fourth column of R, there are

$$p \text{ points separated by } \Delta_A = \frac{\epsilon\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \tag{31}$$

$$q \text{ points separated by } \Delta_B = \frac{\beta\epsilon}{\sqrt{1+pq}\sqrt{1+\epsilon^2}} \tag{32}$$

$$r \text{ points separated by } \Delta_C = \frac{\gamma\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+\epsilon^2}} \tag{33}$$

$$s \text{ points separated by } \Delta_D = \frac{\delta}{\sqrt{1+rs}\sqrt{1+\epsilon^2}}. \tag{34}$$

From previously obtained results, $\Delta_C = s\Delta_D$. Setting $\Delta_B = sr\Delta_D$ gives

$$\epsilon = rq, \tag{35}$$

and thus $\Delta_A = q\Delta_B = srq\Delta_D$ follows immediately.

All constants having been obtained, the rotation matrix to convert a four-dimensional mixed-level factorial design into a Latin hypercube is R,

$$R = \begin{bmatrix} \frac{1}{\sqrt{1+pq}\sqrt{1+pqrs}} & \frac{\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+q^2r^2}} & \frac{\sqrt{pqrs}}{\sqrt{1+pq}\sqrt{1+pqrs}} & \frac{qr\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+q^2r^2}} \\ \frac{-\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+pqrs}} & \frac{1}{\sqrt{1+pq}\sqrt{1+q^2r^2}} & \frac{-\sqrt{pqrs}\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+pqrs}} & \frac{qr}{\sqrt{1+pq}\sqrt{1+q^2r^2}} \\ \frac{-\sqrt{pqrs}}{\sqrt{1+rs}\sqrt{1+pqrs}} & \frac{-qr\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+q^2r^2}} & \frac{1}{\sqrt{1+rs}\sqrt{1+pqrs}} & \frac{\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+q^2r^2}} \\ \frac{\sqrt{pqrs}\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+pqrs}} & \frac{-qr}{\sqrt{1+rs}\sqrt{1+q^2r^2}} & \frac{-\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+pqrs}} & \frac{1}{\sqrt{1+rs}\sqrt{1+q^2r^2}} \end{bmatrix}, \quad (36)$$

and the associated scaling constants are given in Equations (18 - 20).

Rotation matrices for other dimensions (8, 16, etc.) can be obtained in a similar fashion, by observing the form of the matrix for the associated p^d rotation matrix.

5. Summary and Concluding Remarks

This paper has proposed a new class of experimental designs for computer experiments: the rotated factorial designs (RFD). Specifically, it demonstrates how to create Latin hypercubes from factorial designs through rotations. These designs have qualities that make them excellent candidates for use in today's computer experiments. The rotated p^d factorial designs possess the orthogonality of traditional factorial designs and the unique and equally-spaced projections of Latin hypercubes, all while maintaining a nearly optimal spatial dispersion according to minimum interpoint distance.

The use of optimal designs for computer experiments, especially when the criteria are well-accepted and consistent with other measures of design quality, has strong merit. However, the extreme computational requirements of these designs are a serious deficiency in the bid to make them everyday tools for the practicing scientist. Certainly in the two-dimensional case, the computational time is not infeasible, although one should be wary of certain inabilities of search algorithms to converge to the correct answer. However, in this simplest case the rotated p^d factorial designs obtain optimal results, at least in terms of maximizing minimum interpoint distance. This, in addition to the fact that these designs are so easy to obtain that they may be constructed by hand make RFDs a viable alternative. The gains from using optimal-search designs are never very large when measured by the significant increase in effort. The use of rotated factorial designs seems to be ideal for today's computer experiment.

Directions for future research include the search for alternative rotated designs when the number of factors is not of power of two and for other construction methods that would yield even greater choice of available design sizes. Beattie (1999) illustrated that no three-dimensional rotation exists to convert the p^3 factorial design into a Latin hypercube. In fact, it is believed that no rotation exists for p^d designs unless the dimension is a power of two. Future work will attempt to prove this conjecture. If it is true, research in this area will focus on alternative rotation schemes, such as the use of mixed-level factorial designs or scaling constants for p^d designs.

Another area of future research is in the extension of fractional and subset designs. The existence of "half-fraction" rotated factorial designs (see Beattie, 1999, Chapter 8) leads one to ponder the existence of other so-called fractional designs of this nature. Is it possible to obtain Latin hypercubes by using every third projected point, say, instead of every second for any rotated full factorial designs? If so, what are the requirements on p and the sparsity of design rows used? Preliminary research indicates that other fractions are, unfortunately, not Latin hypercubes and supports the following conjecture. Additional work will show that the "half-fractions" of odd-point mixed-level designs are Latin hypercubes and will attempt to determine the existence of any other "fractions."

Most importantly, new applications of rotated factorial designs to scientific research will be explored, with an emphasis on real-life examples under a variety of analysis methods. Recent related work in this area includes uniform design (Fang and Lin, 2003; Fang et. al., 2000) and rotated fractional factorial design (Bursztyn and Steinberg, 2001 & 2002).

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