Designs for computer experiments constructed from block-circulant matrices

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In this presentation, we propose procedures for constructing orthogonal or low-correlation block-circulant designs for computer experiments. Emphasis is given on the construction of block-circulant Latin hypercube designs. The basic concept of these methods is to use vectors with a constant periodic autocorrelation function to obtain suitable block-circulant orthogonal matrices. Using these matrices in a construction, including their full fold-over design, orthogonal Latin hypercube designs are obtained. In addition, an expansion of the method is provided for constructing Latin hypercube designs with low correlation. This expansion is useful when orthogonal Latin hypercube designs do not exist. The properties of the generated designs are further investigated. Some examples of the new designs, as generated by the proposed procedures, are tabulated. In addition, a brief comparison with the designs that appear in the literature is given.

An experimental design $D(n,s^m)$ with n runs, m factors and s levels will be denoted by an $n\times m$ matrix $X=[x_1,\dots,x_m]$, where x_j, is the jth factor (column vector) and d_{ij} is the level of factor j on the ith experimental run. The levels of a design X are selected to be centered, equally spaced and for simplicity integer-valued. This class of designs includes the well known and commonly used family of Latin hypercube designs where in this case s is equal to n. There are several variations on how to space the levels 'uniformly' for each factor. The simplest scheme, and the one that we will employ in this paper, is to take the levels to be $(-(s-1)/2,\ \dots,\ -1,\ 0,\ 1,\ \dots,(s-1)/2)$ when s is odd and $(-s/2,\ \dots,\ -1,\ 1,\ \dots,s/2)$ when s is even. All levels (except zero; if exist) should be equally replicated in each column so that the design will be mean orthogonal.

In regression analysis, it is desirable to include orthogonal independent variables in a regression model, so that the estimates of the factors and interactions coefficients would be uncorrelated. Usually, a polynomial model, of degree k with m factors, is fitted. This model is of the form

$$Y=\beta_0+\sum_{i\le m}\beta_i x_i+\sum_{i_1\le i_2\le m}\beta_{i_1i_2}x_{i_1}x_{i_2}+\dots+\sum_{i_1\le\dots\le i_k\le m}\beta_{i_1\dots i_k}x_{i_1}\dots x_{i_k}+\varepsilon,$$

where x_i are the independent variables, β_i are the linear effects of x_i, $\beta_{i_1,\dots,i_t}$ is the effect of the t-order interaction of $x_{i_1}\dots,x_{i_t}$. Obviously β_{ii} corresponds to the quadratic effect of factor x_i while $\beta_{i_1i_2}$, for $i_1\neq i_2$, is the second order interaction of factors $x_{i_1}x_{i_2}$.

Let $A=\{A_j : A_j=(a_{j,0},a_{j,1},\dots,a_{j,n-1}),\ j=1,\dots,\ell\}$, be a set of ℓ row vectors of length n. The *periodic autocorrelation function* $P_A(s)$ (abbreviated as PAF), is defined, reducing $i+s$ modulo n, as

$$P_A(s)=\sum_{j=1}^{\ell}\sum_{i=0}^{n-1}a_{j,i}a_{j,i+s},\quad s=0,1,\dots,n-1,$$

Construction of orthogonal matrices :

[Geramita&Seberry(1979)] The Goethals-Seidel array

$$GS=\begin{pmatrix} A & BR_n & CR_n & DR_n\\ -BR_n & A & D^TR_n & -C^TR_n\\ -CR_n & -D^TR_n & A & B^TR_n\\ -DR_n & C^TR_n & -B^TR_n & A\end{pmatrix}$$

$$AA^T+BB^T+CC^T+DD^T=fI_n.$$

is an orthogonal matrix of order $4n$.

The Kharaghani array [Kharaghani(2000)]

$$H=\begin{pmatrix} A_1 & A_2 & A_4R_n & A_3R_n & A_6R_n & A_5R_n & A_8R_n & A_7R_n\\ -A_2 & A_1 & A_3R_n & -A_4R_n & A_5R_n & -A_6R_n & A_7R_n & -A_8R_n\\ -A_4R_n & -A_3R_n & A_1 & A_2 & -A_8^TR_n & A_7^TR_n & A_6^TR_n & -A_5^TR_n\\ -A_3R_n & A_4R_n & -A_2 & A_1 & A_7^TR_n & A_8^TR_n & -A_5^TR_n & -A_6^TR_n\\ -A_6R_n & -A_5R_n & A_8^TR_n & -A_7^TR_n & A_1 & A_2 & -A_4^TR_n & A_3^TR_n\\ -A_5R_n & A_6R_n & -A_7^TR_n & -A_8^TR_n & -A_2 & A_1 & A_3^TR_n & A_4^TR_n\\ -A_8R_n & -A_7R_n & -A_6^TR_n & A_5^TR_n & A_4^TR_n & -A_3^TR_n & A_1 & A_2\\ -A_7R_n & A_8R_n & A_5^TR_n & A_6^TR_n & -A_3^TR_n & -A_4^TR_n & -A_2 & A_1\end{pmatrix}$$

$$\sum_{i=1}^{8}A_iA_i^T=fI_n,\qquad \sum_{i=1}\left(A_{2i-1}A_{2i}^T-A_{2i}A_{2i-1}^T\right)=0.$$

is an orthogonal matrix of order $8n$.

The needed squared matrices can be circularly constructed from generating vectors of length n with zero periodic autocorrelation function.

The construction methods:

$$X_a=\begin{pmatrix} D\\ -D\end{pmatrix}\qquad X_b=\begin{pmatrix} D\\ 0_n\\ -D\end{pmatrix}\qquad X_c=\begin{pmatrix} D\\ 1_n\\ -1_n\\ -D\end{pmatrix}\qquad X_d=\begin{pmatrix} D\\ 1_n\\ 0_n\\ -1_n\\ -D\end{pmatrix}$$

1. Let D be an orthogonal matrix of order n. D can be constructed by GS or H- array using circ matrices. If each column of $abs(D)$ is a permutation of

- $(1,\dots,2n-3,2n-1)$, then there exists an **orthogonal** Latin hypercube design $L(2n,n)$ with $2n$ **runs and** n **factors** (Use X_a). [Georgiou&Stylianou (2011)]
- $(1,\dots,n-1,n)$, then there exists an **orthogonal** Latin hypercube design $L(2n+1,n)$ with $2n+1$ **runs and** n **factors** (Use X_b).
- $(2,\dots,2n-1,2n+1)$, then there exists a Latin hypercube design $L(2n+2,n)$ with $2n+2$ **runs and** n **factors with low correlation** (Use X_c).
- $(2,\dots,n,n+1)$, then there exists a Latin hypercube design $L(2n+3,n)$ with $2n+3$ **runs and** n **factors with low correlation** (Use X_d).

2. Let $A=(a_1,a_2,\dots,a_n)$ be a row vector of length n and $P_A(s)=\gamma$, $\forall s=1,2,\dots,n-1$. Set D=circ(A). If the $1\times 2n$ row vector $[A,-A]$ is a permutation of

- $(1,3,\dots,2n-1,-2n+1,\dots,-3,-1)$ then X_a is Latin hypercube design $L(2n,n)$ **with correlation** $r_{xy}=3\gamma/\{n(4n^2-1)\}$ of columns x and y.
- $(1,2,\dots,n,-n,\dots,-2,-1)$ then X_b is **Latin hypercube design** $L(2n+1,n)$ **with correlation** $r_{xy}=6\gamma/\{n(n+1)(2n+1)\}$ of columns x and y.

Example:

The following four vectors $A=(5,11,-7)$, $B=(9,13,15)$, $C=(-17,-19,21)$ and $D=(-23,1,-3)$ of length $n=3$ have zero periodic autocorrelation function. Thus, a 12×12 suitable orthogonal matrix D is constructed using the GS-array. By X_a we obtain an orthogonal LHD $L(24,12)$. Note that this orthogonal Latin hypercube design is new and cannot be constructed by the methods proposed in Steinberg and Lin(2006), Lin etal. (2009) or Georgiou(2009).

Important Properties: 1. Any quadratic effect of a factor is orthogonal to all the main effects in the constructed orthogonal design. 2. Any two-factor interaction is orthogonal to all the main effects in the constructed orthogonal design.

More Examples:

$$\left.\begin{aligned} A_1&=(b+21,b+5,-(b+27),b+29,b+23)\\ A_2&=(b+25,b+31,b+33,b+35,-(b+37))\\ A_3&=(b+39,b+1,-(b+3),-(b+7),-(b+9))\\ A_4&=(b+11,b+13,-(b+15),b+17,-(b+19))\end{aligned}\right\}(*)$$

Using (*) in GS-array, suitably chosen integer numbers b and the construction X_a we obtain an OLHD(40m,20) for m=1,2,....

$$\left.\begin{aligned} A_1&=(b+15,-(b+5),b+19)\quad A_2=(b+17,-(b+21),b+23)\\ A_3&=(b+1,b+3,-(b+7))\quad A_4=(b+9,b+11,b+13)\end{aligned}\right\}(**)$$

Using (**) as above we obtain an OLHD(24m,12) for m=1,2,...

Theorem (Lin et al. [2010]): *Suppose that an OLH(n,m) is available where n is a multiple of 4 such that a Hadamard matrix of order n exists. Then* an OLHD(2an,am) and an OLHD(2an + 1,am) for $a=1,2,4,8$ can all be constructed.

We extent this result to construct the above designs for $a=1,2,4,8,12,16,20,24$.

Runs	*Factors*	*LBST Factors*	*SLL Factors*	*Runs*	*Factors*	*LBST Factors*	*SLL Factors*
24	12	8	4	256	64	192	128
32	16	12	16	320	80	48	32
40	20	_	4	384	144	48	64
48	24	12	8	512	128	_	256
64	16	32	32	576	144	_	32
80	20	12	8	640	160	96	64
96	24	24	16	768	192	96	128
128	32	48	64	768	288	96	128
160	40	24	16	960	240	24	32
192	48	48	32	1024	256	384	512

In columns "LBST Factors" and "SLL Factors" we present the number of factor of the designs constructed by Lin et al. (2010) and Sun et al. (2010), respectively

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