Orthogonal Latin Hypercube Designs for Computer Experiments

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This talk is based on two papers:

- Lin, Mukerjee and Tang (2009 *Biometrika*)
- Lin, Bingham, Sitter and Tang (2010 *Annals of Statistics*)

Outline

Introduction

Designs for Computer Experiments

1. Model-dependent criteria (Santner, Williams and Notz 2003)
2. Space-filling designs
   - Maximin distance designs
     (Johnson, Moore and Ylvisaker 1990)
   - OA based designs (Owen 1992; Tang 1993)
   - (t, m, s)-nets from quasi Monte Carlo (Niederreiter 1992)
3. **Orthogonal Latin hypercubes** (Ye 1998; Butler 2001)

Introduction

Orthogonal Latin Hypercube Designs

1. Why Latin hypercube designs?
   - guarantee one-dimensional stratification
   - a simple structure for finding good designs
2. Why orthogonality?
   - directly useful for regression type modeling
   - provides a stepping stone to space-filling

Introduction

Latin Hypercube Designs

1. An $n \times m$ matrix $D = (d_{ij})$ is called a *Latin hypercube* if each column of D is a permutation of $1, \ldots, n$.
2. Two ways of generating design points within $[0,1]^m$
   - $x_{ij} = (d_{ij} - 0.5)/n$, $x_{ij} = (d_{ij} - u_{ij})/n$
   - the n points given by $(x_{i1}, \ldots, x_{im})$ with $i = 1, \ldots, n$

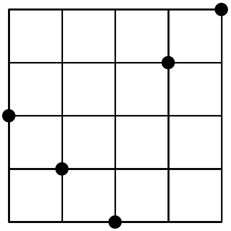
Introduction

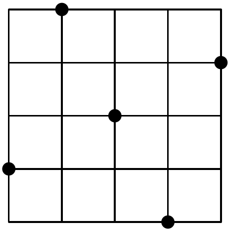
D_1

1	3
2	2
3	1
4	4
5	5

D_2

1	2
2	5
3	3
4	1
5	4





Lin, Mukerjee and Tang (2009)

- Use the idea of rotation. Early work includes Steinberg and Lin (2006) and Pang, Liu and Lin (2009).
- Let $B = (b_{ij})$ be a Latin hypercube of n runs for p factors with each column being a permutation of $-(n-1)/2$, $-(n-3)/2, \ldots, (n-3)/2$, $(n-1)/2$.
- Let A be an $OA(n^2, 2f, n, 2)$. Denote the symbols in A by $1, 2, \ldots, n$.

Lin, Mukerjee and Tang (2009)

The construction has three steps.

Step 1. For each j, obtain A_j from A by replacing $1, 2, \ldots, n$ by $b_{1j}, b_{2j}, \ldots, b_{nj}$ respectively, and then partition A_j as $A_j = [A_{j1}, \ldots, A_{jf}]$, where each of $A_{j1}, \ldots, A_{jf}$ has two columns.

Step 2. For each j, obtain $M_j = [A_{j1}V, \ldots, A_{jf}V]$, where

$$V = \begin{bmatrix} 1 & -n \\ n & 1 \end{bmatrix}.$$

Step 3. Finally, obtain $M = [M_1, \ldots, M_p]$, of order $N \times q$, where $N = n^2$ and $q = 2pf$.

Lin, Mukerjee and Tang (2009)

If $p = 1$, the above construction is equivalent to that in Steinberg & Lin (2006) and Pang et al. (2009). The power of our method is derived from allowing $p \geq 2$.

Theorem 1. *We have that*

- *M is a Latin hypercube;*
- *M is orthogonal if B is orthogonal.*
- *M is nearly orthogonal if B is nearly orthogonal.*

Lin, Mukerjee and Tang (2009)

Some example

We use $OLH(n, p)$ to denote an orthogonal Latin hypercube with n rows and p columns.

The orthogonal Latin hypercubes shown in Table 1 were obtained by a computer search. To the best of our knowledge, these are new.

Lin, Mukerjee and Tang (2009)

Table 1. *Small Orthogonal Latin hypercubes*

OLH(7, 3)

-3	3	2
-2	0	-3
-1	-2	-1
0	-3	1
1	-1	3
2	1	-2
3	2	0

OLH(9, 5)

-4	-2	0	-3	3
-3	4	2	1	-2
-2	-3	-4	-1	-3
-1	3	-2	3	4
0	-4	4	4	0
1	2	-1	0	-4
2	0	3	-2	-1
3	1	1	-4	2
4	-1	-3	2	1

OLH(11, 7)

-5	-4	-5	-5
-4	2	-1	3
-3	-2	4	5
-2	3	-3	4
-1	4	2	-4
0	-5	5	-2
1	5	3	-3
2	-1	1	1
3	0	0	-1
4	1	-4	0
5	-3	-2	2

In addition to the above, we will also use the $OLH(5, 2)$ and $OLH(8, 4)$ constructed by Ye (1998).

Lin, Mukerjee and Tang (2009)

- Let B be $OLH(5,2)$, $OLH(7,3)$, $OLH(8,4)$, $OLH(9,5)$ and $OLH(11,7)$
- Let A be $OA(25,6,5,2)$, $OA(49,8,7,2)$, $OA(64,8,8,2)$, $OA(81,10,9,2)$ and $OA(121,12,11,2)$.
- We obtain $OLH(25,12)$, $OLH(49,24)$, $OLH(64,32)$, $OLH(81,50)$, and $OLH(121,84)$.

Lin, Bingham, Sitter and Tang (2010)

Consider the following construction:

$$L = A \otimes B + n_2 C \otimes D,$$

- $A = (a_{ij})_{n_1 \times m_1}$, with $a_{ij} = \pm 1$,
- $B_{n_2 \times m_2}$ is a Latin hypercube
- $C_{n_1 \times m_1}$ is a Latin hypercube,
- $D = (d_{ij})_{n_2 \times m_2}$, with $d_{ij} = \pm 1$.

Design L has $n = n_1 n_2$ runs and $m = m_1 m_2$ factors.

Lin, Bingham, Sitter and Tang (2010)

Theorem 2. *Design L is an orthogonal Latin hypercube if*

(i) A and D are orthogonal matrices of ± 1,

(ii) B and C are orthogonal Latin hypercubes,

(iii) $A^T C = 0$ *or* $B^T D = 0$,

(iv) there does not exist i such that $a_{pi} = -a_{p'i}$ *where p and* p' *are determined by* $c_{pi} = -c_{p'i}$.

(L is nearly orthogonal if B and C are nearly orthogonal)

Lin, Bingham, Sitter and Tang (2010)

Theorem 3. 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 we can construct

OLH$(2n, m)$, OLH$(4n, 2m)$, OLH$(8n, 4m)$, OLH$(16n, 8m)$.

Lin, Bingham, Sitter and Tang (2010)

Theorem 3 is a very powerful result. By repeated application, one can obtain many infinite series of orthogonal Latin hypercubes.

For example, starting with an $\mathrm{OLH}(12, 6)$, we can obtain an $\mathrm{OLH}(192, 48)$, which can be used in turn to construct an $\mathrm{OLH}(768, 96)$ and so on.

For another example, an $\mathrm{OLH}(256, 248)$ in Steinberg and Lin (2006) can be used to construct an $\mathrm{OLH}(1024, 496)$, an $\mathrm{OLH}(4096, 1984)$ and so on.

Lin, Bingham, Sitter and Tang (2010)

For any run size n, what is the maximum number m^* of factors for an OLH(n, m^*) to exist?

Theorem 4. *Let $n = 16k + j$. Then we have that:*

(i) $m^* = 1$ if $j = 2, 6, 10, 14$;

(ii) $m^* \geq 6$ for all n where $k \geq 1$ and $j \neq 2, 6, 10, 14$;

(iii) $m^* \geq 7$ for $n = 16k + 11$ where $k \geq 0$;

(iv) $m^* \geq 12$ for $n = 16k, 16k + 1$ where $k \geq 2$;

(v) $m^* \geq 24$ for $n = 32k, 32k + 1$ where $k \geq 2$;

(vi) $m^* \geq 48$ for $n = 64k, 64k + 1$ where $k \geq 2$.

Lin, Bingham, Sitter and Tang (2010)

Note that

1. Part (i) is a non-existence result.
2. Other parts of the theorem make use of a stacking method in combination with Table 2.

   Table 2. The maximum number m of columns in OLH(n, m) *by the algorithm for* $4 \le n \le 21$

n	4	5	7	8	9	11	12	13	15	16	17	19	20	21
m	2	2	3	4	5	7	6	6	6	12	6	6	6	6

Concluding remarks

- Discussed two general methods for constructing orthogonal or nearly orthogonal Latin hypercubes.
- Powerful methods both in terms of the large ratio m/n and the flexibility of the run size.
- Future work?