Recent Development on Designs for Computer Experiments with Mixed Inputs

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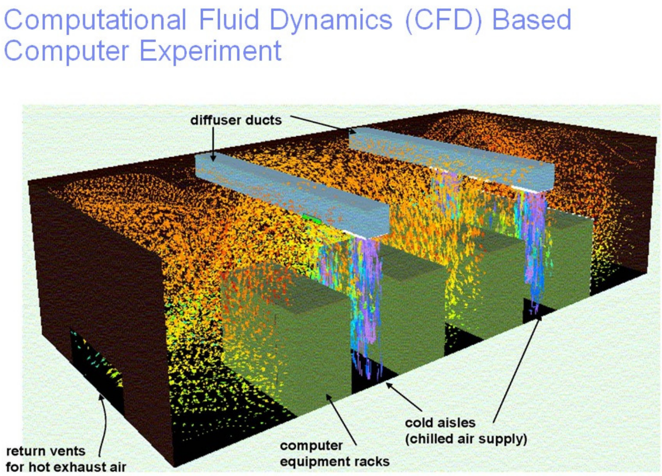
Workshop on Design of Experiments: New Challenges

CIRM Marseilles 2018

Motivating Example 1



Data Center Thermal Management @2007 IBM Corporation

Configuration Variables

Goal: Predict the highest temperature spot with different inputs of configuration variables

Variable	Description	Values
X_1	CRAC unit 1 flow rate (cfm)	0 7000 8500 10000 11500 13000
X_2	CRAC unit 2 flow rate (cfm)	0 7000 8500 10000 11500 13000
X_3	CRAC unit 3 flow rate (cfm)	0 2500 4000 5500
X_4	CRAC unit 4 flow rate (cfm)	0 2500 4000 5500
X_5	Room temperature (F)	65 67 69 71 73 75
X_6	Tile distribution (location)	Layout1 Layout2 Layout3
X_7	Tile percentage open area	$(0, 1)$

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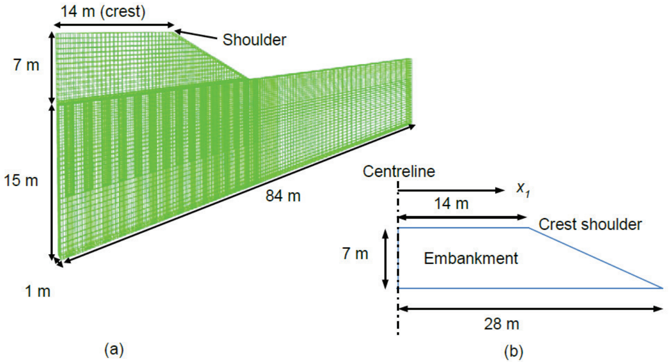
Motivating Example 2



A fully 3D coupled finite element model is calibrated and verified by successfully modeling the performance of a full-scale embankment constructed on soft soil (Rowe and Liu, 2015).

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    - Uniform designs
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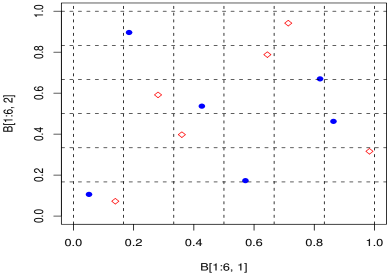
- Designs with good or guaranteed low-dimensional projection properties (Sun and Tang, 2017; Joseph, Gul and Ba, 2015)
- Sequential designs (for optimization, sensitivity analysis, contour estimation, quantile estimation, global fitting)

Sliced Latin Hypercube Designs

A special Latin hypercube design that can be partitioned into slices of smaller Latin hypercube designs (Qian, 2012)

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} = \begin{bmatrix} 6 & 7 \\ 1 & 2 \\ 10 & 9 \\ 11 & 6 \\ 7 & 3 \\ 3 & 11 \\ \hdashline 9 & 12 \\ 8 & 10 \\ 4 & 8 \\ 12 & 4 \\ 2 & 1 \\ 5 & 5 \end{bmatrix} \Longrightarrow \begin{bmatrix} 0.42 & 0.53 \\ 0.05 & 0.10 \\ 0.81 & 0.66 \\ 0.86 & 0.46 \\ 0.57 & 0.17 \\ 0.18 & 0.89 \\ \hdashline 0.71 & 0.94 \\ 0.64 & 0.78 \\ 0.28 & 0.59 \\ 0.98 & 0.31 \\ 0.13 & 0.07 \\ 0.36 & 0.39 \end{bmatrix}$$



Sliced Latin Hypercube Designs

- More flexible structures
  - General sliced Latin hypercubes (Xie, Xiong, Qian and Wu, 2013)
  - Bi-directional sliced Latin hypercubes (Zhou, Jin, Qian and Zhou, 2016)
  - Clustered-sliced Latin hypercubes (Huang, Lin, Liu and Yang, 2016)

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- Sampling property, central limit theorem, applications (He and Qian, 2016; Zhang and Qian, 2013)

Using SLHD for CE with QQ Variables

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- Each slice of a sliced Latin hypercube design corresponds to each level combination of qualitative variables.

0	0	B_1
0	1	B_2
1	0	B_3
1	1	B_4

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  - Each level combination of qualitative variable is replicated with the same number as the run size of B_i.
  - It is useful when the number of qualitative factors is small.

Marginally Coupled Design

- Consider a computer experiment with q qualitative factors and p quantitative variables. Suppose that the ith qualitative factor has s_i levels, $1 \leq i \leq q$.

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- Consider a computer experiment with q qualitative factors and p quantitative variables. Suppose that the ith qualitative factor has s_i levels, $1 \leq i \leq q$.

- Let D_1 and D_2 be the design matrices for qualitative variables and quantitative variables, respectively.

- A design $D = (D_1, D_2)$ is called a marginally coupled design if D_2 is a Latin hypercube design and the rows in D_2 corresponding to each level of any factor in D_1 form a small Latin hypercube design. In this work, we focus on using orthogonal arrays for D_1.

D_1	
z_1	z_2
0	0
0	1
0	2
1	0
1	1
1	2
2	0
2	1
2	2

D_2	
x_1	x_2
−2	−2
−1	4
3	−1
0	1
2	−3
−3	2
4	3
−4	0
1	−4

(1)

An example of MCD

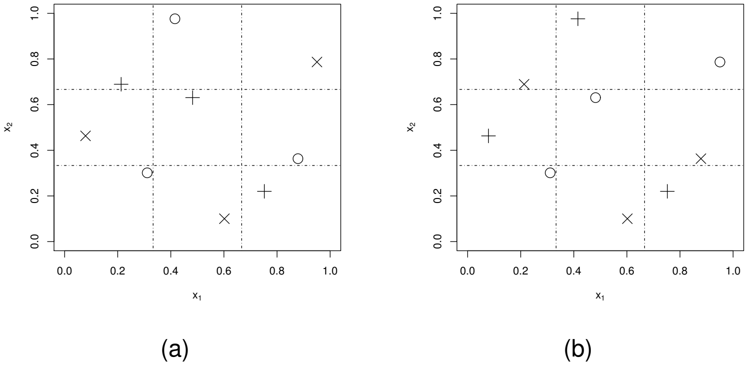

Figure: Scatter plots of x_1 versus x_2 where rows of D_2 corresponding to levels 0,1,2 of z_i are marked by $\times$, $\circ$, and $+$: (a) the levels of z_1; (b) the levels of z_2.

Orthogonal Array

An orthogonal array D of strength t, denoted by $\mathrm{OA}(n, s_1 \cdots s_k, t)$, is an $n \times k$ matrix of which the ith column has s_i levels $0, \ldots, s_i - 1$ and for every $n \times t$ submatrix of D, each of all possible level combinations appears equally often. If not all s_i's are equal, an orthogonal array is mixed. Otherwise it is called symmetric. (Hedayat, Sloane and Stufken, 1999)

$\mathrm{OA}(9, 3^4, 2)$

0	0	0	0
0	1	1	2
0	2	2	1
1	0	1	1
1	1	2	0
1	2	0	2
2	0	2	2
2	1	0	1
2	2	1	0

$\mathrm{OA}(8, 2^4 3^1, 2)$

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

Resolvable Orthogonal Arrays

An $OA(n, s_1^{q_1} \cdots s_k^{q_k}, 2)$ is said to be $(\alpha_1 \times \alpha_2 \times \cdots \times \alpha_k)$ resolvable if for $1 \leq j \leq k$, its rows can be partitioned into $n/(\alpha_j s_j)$ subarrays $A_1, \ldots, A_{n/(\alpha_j s_j)}$ of $\alpha_j s_j$ rows each such that each of $A_1, \ldots, A_{n/(\alpha_j s_j)}$ is an $OA(\alpha_j s_j, s_1^{q_1} \cdots s_k^{q_k}, 1)$. If $\alpha_1 = \cdots = \alpha_k = 1$, the orthogonal array is called completely resolvable.

Resolvable Orthogonal Arrays

$CROA(9, 3^3, 2)$

0	0	0
1	1	2
2	2	1
0	1	1
1	2	0
2	0	2
0	2	2
1	0	1
2	1	0

$\alpha = 1$

$CROA(16, 4^2 2^3, 2)$

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

$\alpha_1 = 1, \alpha_2 = 2$

Characterization

Proposition

Given $D_1 = OA(n, s^q, 2)$, a marginally coupled design exists if and only if D_1 is a completely resolvable orthogonal array.

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Given $D_1 = OA(n, s_1^{q_1} s_2^{q_2}, 2)$ with $s_1 = \alpha_2 s_2$, a marginally coupled design exists if and only if D_1 is a $(1 \times \alpha_2)$-resolvable orthogonal array that can be expressed as

$$\begin{pmatrix} A_{11} & A_{12} \\ \vdots & \vdots \\ A_{m1} & A_{m2} \end{pmatrix} \tag{2}$$

such that (A_{i1}, A_{i2}) is an $OA(s_1, s_1^{q_1} s_2^{q_2}, 1)$, where $m = n/s_1$, and for $1 \le i \le m$, the A_{i2} is completely resolvable.

Characterization

Define a matrix $\tilde{D}_2$, let

$$\tilde{D}_{2,ij} = \left\lfloor \frac{D_{2,ij}}{s} \right\rfloor, \quad (3)$$

where $D_{2,ij}$ and $\tilde{D}_{2,ij}$ are the (i,j)th entry of D_2 and $\tilde{D}_2$, and $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x.

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Proposition

Given D_1 is an $OA(n,q,s,2)$, D_2 is an $LHD(n,p)$ and $\tilde{D}_2$ is defined via (3), then (D_1, D_2) is a marginally coupled design if and only if for $j = 1, \ldots, p$, $(D_1, \tilde{d}_j)$ is an $MOA(n, s^q(n/s), 2)$, where $\tilde{d}_j$ is the jth column of $\tilde{D}_2$.

Maximum Number q of Columns

Lemma

(Suen, 1989) If a resolvable $OA(n, s^q, 2)$ *can be partitioned into* r $OA(n/r, s^q, 1)$*'s, then* $q \leq (n-r)/(s-1)$.

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Corollary

Let $q*$ be the maximum value of q such that a marginally coupled design $D = (D_1, D_2)$ with $D_1 = OA(n, s^q, 2)$ exists. We have $q^* \leq n/s$.

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Subspace Theory

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- Let S_u consist of s-level column vectors of length u. All of its column vectors form a space of dimension u.
- For a nonzero element $\mathbf{x} \in S_u$, define

$$O(\mathbf{x}) = \{\mathbf{y} \in S_u \mid \mathbf{y}^T\mathbf{x} = 0\}. \quad (4)$$

It can be seen that $O(\mathbf{x})$ is a $(u-1)$-dimensional subspace of S_u.

Construction

Suppose we choose $q+p$ vectors $\mathbf{z}_1,\ldots,\mathbf{z}_q,\mathbf{x}_1,\ldots,\mathbf{x}_p$ from S_u, such that $\mathbf{z}_i$ is not in any of $O(\mathbf{x}_j)$. We propose the following three-step construction.

Step 1. Obtain $D_1=(\mathbf{a}_1,\ldots,\mathbf{a}_q)$ by taking all linear combinations of the rows of $(\mathbf{z}_1,\ldots,\mathbf{z}_q)$, where $\mathbf{a}_i$ is the ith column of D_1;

Step 2. For each $\mathbf{x}_j$, choose $u-1$ independent columns from $O(\mathbf{x}_j)$ in (4) to form a generator matrix $G(\mathbf{x}_j)$. Obtain $A(\mathbf{x}_j)$ by taking all linear combinations of the rows of $G(\mathbf{x}_j)$. Apply the *method of replacement* to obtain an s^{u-1}-level column vector $\mathbf{d}_j$ from $A(\mathbf{x}_j)$. Denote the resulting design by $\tilde{D}_2=(\mathbf{d}_1,\ldots,\mathbf{d}_p)$;

Step 3. Obtain D_2 from $\tilde{D}_2$ via the *level replacement-based Latin hypercube* approach (Tang, 1993)

Notations

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- The set of vectors $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\} \subset S_u$, where $\mathbf{e}_i$ is a vector of S_u with the ith entry equal to 1 and the other entries equal to 0, and $1 \leq u_1 \leq u$.

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-
$$\mathcal{A} = \{\mathbf{x} \in S_u \setminus (\cup_{i=1}^{u_1} O(\mathbf{e}_i)) \mid \text{the first entry of } \mathbf{x} \text{ is } 1\}, \qquad (5)$$

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- $$\mathcal{A} = \{\mathbf{x} \in S_u \setminus (\cup_{i=1}^{u_1} O(\mathbf{e}_i)) \mid \text{the first entry of } \mathbf{x} \text{ is } 1\}, \qquad (5)$$
- $n_A = (s-1)^{u_1-1} s^{u-u_1}$ column vectors in $\mathcal{A}$ in (5).

Theorem

For given $\{\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}\}$, $\mathcal{A}$ *and* n_A, *if in the general construction we*

(i) *choose* $\mathbf{z}_i = \mathbf{e}_i$ *and* $\mathbf{x}_j \in \mathcal{A}$ *for* $1 \leq i \leq u_1$ *and* $1 \leq j \leq n_A$, *an* $MCD(D_1, D_2)$ *with* $D_1 = OA(s^u, u_1, s, u_1), D_2 = LHD(s^u, n_A)$ *can be obtained, or,*

(ii) *choose* $\mathbf{z}_i \in \mathcal{A}$ *and* $\mathbf{x}_j = \mathbf{e}_j$ *for* $1 \leq i \leq n_A$ *and* $1 \leq j \leq u_1$, *an* $MCD(D_1, D_2)$ *with* $D_1 = OA(s^u, n_A, s, 2), D_2 = LHD(s^u, u_1)$ *can be obtained,*

where both D_2*'s are non-cascading Latin hypercubes.*

Subspace Construction

- The first u_1 entries of $\mathbf{x} \in \mathcal{A}$ can take $n_B = (s-1)^{u_1-1}$ distinct values, say $\{(1, b_{i2}, \ldots, b_{iu_1}) \mid i = 1, \ldots, n_B\}$. Let $\mathbf{b}_i = (1, b_{i2}, \ldots, b_{iu_1}, 0, \ldots, 0)^T$.
- Let $E = \{\sum_{j=1}^{u_1} \lambda_j \mathbf{e}_j \mid \lambda_j \in GF(s)\}$ consist of all linear combinations of $\mathbf{e}_1, \ldots, \mathbf{e}_{u_1}$. For fixed i, $\mathbf{b}_i$ and $\mathcal{A}_i$, $1 \le i \le n_B$, define

$$E_i = \{\, \mathbf{z} \in E \mid \mathbf{z}^T \mathbf{b}_i = 0 \,\} \text{ and } \overline{E}_i = E \setminus E_i.$$

  If $\mathbf{z} \in \overline{E}_i$, then $\mathbf{z} \notin O(\mathbf{b}_i)$, which implies $\mathbf{z} \notin O(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{A}_i$ since the last $u - u_1$ entries of $\mathbf{z}$ are zeros.
- Define E_v^* to be the subset of $\cap_{j=1}^{v} \overline{E}_{i_j}$ in which the first nonzero entry of each element is equal to 1. The value $g(v) = f(v)/(s-1)$ is the number of elements of E_v^*. Define $\mathcal{A}_v^* = \cup_{j=1}^{v} \mathcal{A}_{i_j}$.

Proposition

For $\{\mathbf{b}_1,\ldots,\mathbf{b}_{n_B}\}$ *defined above, suppose that there exists a subset* $\{\mathbf{b}_{i_1},\ldots,\mathbf{b}_{i_{n^*}}\}$ *such that any* u_1 *elements of the set are independent, for* $n^* \leq n_B$*. We have that for* $1 \leq v \leq n^*$ *and* $1 \leq i_1 < i_2 \ldots < i_v \leq n_B$*, the set* $\cap_{j=1}^{v} \overline{E}_{i_j}$ *contains* $f(v)$ *elements with*

$$f(v) = \begin{cases} (s-1)^v s^{u_1-v}, & 1 \leq v \leq u_1, \\ m^*, & u_1+1 \leq v \leq n^*, \end{cases} \tag{6}$$

where

$$m^* = s^{u_1}\left[1-\binom{v}{1}s^{-1}+\cdots+(-1)^{u_1}\binom{v}{u_1}s^{-u_1}\right]+\sum_{i=u_1+1}^{v}(-1)^i\binom{v}{i}.$$

Theorem

For E_v^*, $\mathcal{A}_v^*$ and $g(v)$ defined above, if in the general construction, we

(i) *choose $\mathbf{z}_i \in E_v^*$ and $\mathbf{x}_j \in \mathcal{A}_v^*$, $i = 1, \ldots, g(v)$ and $j = 1, \ldots, vs^{u-u_1}$, an $MCD(D_1, D_2)$ with $D_1 = OA(s^u, g(v), s, 2), D_2 = LHD(s^u, vs^{u-u_1})$ can be obtained, or*

(ii) *choose $\mathbf{z}_i \in \mathcal{A}_v^*$ and $\mathbf{x}_j \in E_v^*$, $i = 1, \ldots, vs^{u-u_1}$ and $j = 1, \ldots, g(v)$, an $MCD(D_1, D_2)$ with $D_1 = OA(s^u, vs^{u-u_1}, s, 2), D_2 = LHD(s^u, g(v))$ can be obtained,*

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Conclusion

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- Constructions for designs with better the overall space-filling property and the low-dimensional projection property, and flexible run sizes

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- Big data

Thank you! Q&A.