A System of Experimental Design

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- System has four broad branches :

  (i) regular orthogonal designs,

  (ii) nonregular orthogonal designs,

  (iii) response surface designs,

  (iv) optimal designs.

- New opportunities in boarder areas.
  - Interface between (ii) <=> (iii), (iii) <=> (iv).
  - Space-filling designs.

New materials available in

“Experiments: Planning, Analysis and Parameter Design Optimization” by Wu - Hamada (2000)

- Regular orthogonal designs (Fisher, Yates, Finney, …): 2^{n-k}, 3^{n-k} designs, using minimum aberration criterion
- Nonregular orthogonal designs (Plackett-Burman, Rao, Bose): Plackett-Burman designs, orthogonal arrays

  ↕ (factor screening, projection)

- Response surface designs (Box) : fitting a parametric response surface
- Optimal designs (Kiefer): optimality driven by specific model/criterion

Fundamental Principles for Factorial Effects

- **Effect Hierarchy Principle**:
  - Lower order effects more important than higher order effects
  - Effects of same order equally important
- **Effect Sparsity Principle**: Number of relatively important effects is small
- **Effect Heredity Principle**: for an interaction to be significant, at least one of its parent factors should be significant

Fractional Factorial Designs

Run	1	2	3	12	13	23	123
1	-	-	-	+	+	+	-
2	-	-	+	+	-	-	+
3	-	+	-	-	+	-	+
4	-	+	+	-	-	+	-
5	+	-	-	-	-	+	+
6	+	-	+	-	+	-	-
7	+	+	-	+	-	-	-
8	+	+	+	+	+	+	+

col "12" = (col 1) $\times$ (col2), etc.

- 4 factors: 1, 2, 3, 4 =12
  (4 & 12 are said to be **aliased**)
  2^{4-1} design: I =124
- 5 factors: 1, 2, 3, 4 =12, 5 =13
  2^{5-2} design: I =124 =135 = 2345
  (defining contrast subgroup)

- Resolution = shortest wordlength in the defining contrast subgroup of a design
- Design of same resolution can be quite different

d_1 : **I=4567=12346=12357**

d_2 : **I=1236=1457=234567**

both are 2^{7-2} design of resolution IV

but d_1 is better (why?)

- Let $A_i(\mathrm{d})$= no. of words of length i in the defining contrast subgroup of design d
- **Minimum aberration criterion** (Fries-Hunter, 1980): sequentially minimizes the values A_3, A_4, A_5, …etc.
- Aberration criterion is an extension of resolution criterion
- Ready-to-use tables of minimum aberration (and related) 2^{k-p} designs in WH

Thirty-Two Run Fractional Factorial Designs

k	F&R	Design Generators	Clear Effects
6	2_{VI}^{6-1}	6 = 12345	all six main effects, all 15 2fi's
7	2_{IV}^{7-2}	6 = 123, 7 = 1245	all seven main effects, 14, 15, 17, 24, 25, 27, 34, 35, 37, 45, 46, 47, 56, 57, 67
8	2_{IV}^{8-3}	6 = 123, 7 = 124, 8 = 1345	all eight main effects, 15, 18, 25, 28, 35, 38, 45, 48, 56, 57, 58, 68, 78
9	2_{IV}^{9-4}	6 = 123, 7 = 124, 8 = 125, 9 = 1345	all nine main effects, 19, 29, 39, 49, 59, 69, 79, 89
9	2_{IV}^{9-4}	6 = 123, 7 = 124, 8 = 134, 9 = 2345	all nine main effects, 15, 19, 25, 29, 35, 39, 45, 49, 56, 57, 58, 59, 69, 79, 89
10	2_{IV}^{10-5}	6 = 123, 7 = 124, 8 = 125, 9 = 1345, t_0 = 2345	all 10 main effects
10	2_{III}^{10-5}	6 = 12, 7 = 134, 8 = 135, 9 = 145, t_0 = 345	3, 4, 5, 7, 8, 9, t_0, 23, 24, 25, 27, 28, 29, 2t_0, 36, 46, 56, 67, 68, 69, 6t_0

Extensions of Minimum Aberration to Designs with Factor Asymmetry

- 2^{n-k} designs in 2^q blocks: "treatment defining contrast subgroup", and "block defining contrast subgroup" are intertwined
- 2^{n-k} parameter designs, control and noise factors (control-by-noise interaction key to robustness): modified effect hierarchy principle: *c*, *n*, *cn* (1st group), *cc*, *ccn*, *nn* (2nd group), etc.
- 2^{n-k} split-plot designs, n_1 whole-plot factors, n_2 split-plot factors: *wp* effects, *wp* x *sp* effects, *sp* effects treated differently, two variance components

Two Types of Fractional Factorial Designs:

- Regular (2^{n-k}, 3^{n-k} designs):

  columns of the design matrix form a group over a finite field; the interaction between any two columns is among the columns

  $\Rightarrow$ any two factorial effects are either

  orthogonal or *fully aliased*

- Nonregular (mixed-level designs, orthogonal arrays)

  some pairs of factorial effects can be *partially* aliased

  $\Rightarrow$ more complex aliasing pattern

Orthogonal Arrays

- Two columns of a design matrix are orthogonal if all possible level combinations of the two columns appear equally often in the matrix
- An **orthogonal array** $OA(N, s_1^{m_1} \cdots s_k^{m_k})$ of strength two is an $N \times m$ matrix,

  $m = m_1 + \cdots + m_k$ in which m_i columns have s_i levels and any two columns are orthogonal
- 2^{n-k}, 3^{n-k} designs are OA's

Cast Fatigue Experiment

Factor		Level −	Level +
A.	initial structure	as received	β treat
B.	bead size	small	large
C.	pressure treat	none	HIP
D.	heat treat	anneal	solution treat/age
E.	cooling rate	slow	rapid
F.	polish	chemical	mechanical
G.	final treat	none	peen

Design Matrix OA(12, 2^7) and Lifetime Data

Full Matrix: $OA(12,2^{11})$

Run	Factor *A*	*B*	*C*	*D*	*E*	*F*	*G*	8	9	10	11	Logged Lifetime
1	+	+	−	+	+	+	−	−	−	+	−	6.058
2	+	−	+	+	+	−	−	−	+	−	+	4.733
3	−	+	+	+	−	−	−	+	−	+	+	4.625
4	+	+	+	−	−	−	+	−	+	+	−	5.899
5	+	+	−	−	−	+	−	+	+	−	+	7.000
6	+	−	−	−	+	−	+	+	−	+	+	5.752
7	−	−	−	+	−	+	+	−	+	+	+	5.682
8	−	−	+	−	+	+	−	+	+	+	−	6.607
9	−	+	−	+	+	−	+	+	+	−	−	5.818
10	+	−	+	+	−	+	+	+	−	−	−	5.917
11	−	+	+	−	+	+	+	−	−	−	+	5.863
12	−	−	−	−	−	−	−	−	−	−	−	4.809

Partial and Complex Aliasing

- For the 12-run Plackett-Burman design OA(12, 2^{11})

$$\mathrm{E}\hat{b}_i = b_i + \frac{1}{3} \sum_{j,k \neq i} \pm b_{jk}$$

partial aliasing: coefficient $\pm \frac{1}{3}$

complex aliasing: 45 (= $\binom{10}{2}$) partial aliases

- Traditionally complex aliasing was considered to be a disadvantage
- Standard texts pay little attention to this type of designs

Useful Orthogonal Arrays

- Collection in WH

$OA(12,2^{11})$ $OA(12,3^1 2^4)$ $OA(18,2^1 3^7)$

$OA(18,6^1 2^6)$ $OA(20,2^{19})$ $OA(24,3^1 2^{16})$

$OA(24,6^1 2^{14})$ $OA(36,2^{11} 3^{12})$ $OA(36,3^7 6^3)$

$OA(36,2^8 6^3)$ $OA(48,2^{11} 4^{12})$ $OA(50,2^1 5^{11})$

$OA(54,2^1 3^{25})$

- Run Size Economy

$OA(12,2^{11})$ vs.16-run 2^{k-p} designs, $8 \le k \le 11$

$OA(18,3^7)$ vs. 27-run 3^{k-p} designs, $5 \le k \le 7$

- Flexibility in level combinations

Blood Glucose Experiment

$OA(18.2^1 3^7)$

Run	Factor A	G	B	C	D	E	F	H	Mean Reading
1	0	0	0	0	0	0	0	0	97.94
2	0	0	1	1	1	1	1	1	83.40
3	0	0	2	2	2	2	2	2	95.88
4	0	1	0	0	1	1	2	2	88.86
5	0	1	1	1	2	2	0	0	106.58
6	0	1	2	2	0	0	1	1	89.57
7	0	2	0	1	0	2	1	2	91.98
8	0	2	1	2	1	0	2	0	98.41
9	0	2	2	0	2	1	0	1	87.56
10	1	0	0	2	2	1	1	0	88.11
11	1	0	1	0	0	2	2	1	83.81
12	1	0	2	1	1	0	0	2	98.27
13	1	1	0	1	2	0	2	1	115.52
14	1	1	1	2	0	1	0	2	94.89
15	1	1	2	0	1	2	1	0	94.70
16	1	2	0	2	1	2	0	1	121.62
17	1	2	1	0	2	0	1	2	93.86
18	1	2	2	1	0	1	2	0	96.10

Analysis Strategies

- Traditionally experiments with **complex aliasing** were used for **screening** purpose, i.e., estimating main effects only
- A paradigm shift: using effect sparsity/heredity, Hamada-Wu (1992) recognized that complex aliasing can be turned into an advantage for studying interactions
- Analysis methods (frequentist and Bayesian) allow two-factor interactions to be entertained (in addition to main effects). Effective if the number of significant interactions is small

Examples

- Cast Fatigue Experiment:

Main effect analysis:	F	(R^2=0.45)
	F, D	(R^2=0.59)
HW analysis:	F, FG	(R^2=0.89)
	F, FG, D	(R^2=0.92)

- Blood Glucose Experiment:

Main effect analysis:	E_q, F_q	(R^2=0.36)
HW analysis:	B_l, $(BH)_{lq}$, $(BH)_{qq}$	(R^2=0.89)

Bayesian analysis also identifies B_l, $(BH)_{ll}$, $(BH)_{lq}$, $(BH)_{qq}$ as having the highest posterior model probability

Further Analysis

- Success in the HW analysis strategy led to research on the *hidden projection* properties of nonregular designs. Commonly used arrays like $OA(12, 2^{11})$, $OA(18, 3^{7})$, $OA(36, 2^{11}3^{12})$ have desirable projection properties (i.e., for 4 - 8 factors, a number of interactions can be estimated with good efficiency)
- This is achieved *without* adding new runs
- It has also inspired a new approach to response surface methodologyFurther Analysis

A Poorman's Response Surface Methodology

- Consider an experiment to study three quantitative factors with up to 5 levels.

Factors and Levels, Ranitidine Experiment

Factor	Levels
A. pH	2, 3.42, 5.5, 7.58, 9
B. voltage (kV)	9.9, 14, 20, 26, 30.1
C. α-CD (mM)	0, 2, 5, 8, 10

- The design matrix and the data are given on the next page. The design differs from 2^{k-p} design in two respects :
  - 6 replicates at the center,
  - 6 runs along the three axes.

  It belongs to the class of *central composite designs*.

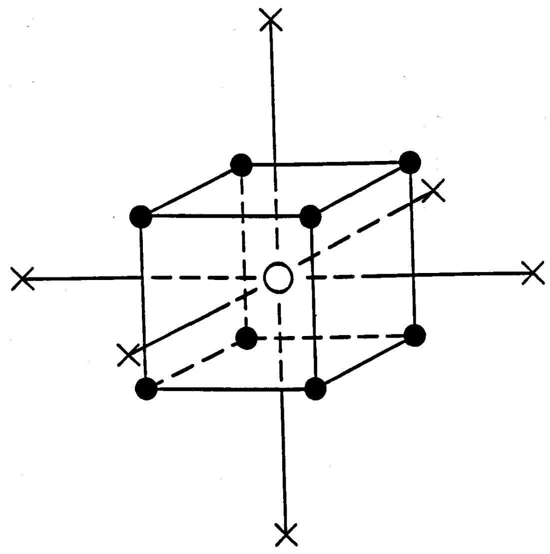
Ranitidine Experiment

Design Matrix and Response Data

Run	Factor *A*	*B*	*C*	CEF	ln CEF
1	−1	−1	−1	17.293	2.850
2	1	−1	−1	45.488	3.817
3	−1	1	−1	10.311	2.333
4	1	1	−1	11757.084	9.372
5	−1	−1	1	16.942	2.830
6	1	−1	1	25.400	3.235
7	−1	1	1	31697.199	10.364
8	1	1	1	12039.201	9.396
9	0	0	−1.67	7.474	2.011
10	0	0	1.67	6.312	1.842
11	0	−1.68	0	11.145	2.411
12	0	1.68	0	6.664	1.897
13	−1.68	0	0	16548.749	9.714
14	1.68	0	0	26351.811	10.179
15	0	0	0	9.854	2.288
16	0	0	0	9.606	2.262
17	0	0	0	8.863	2.182
18	0	0	0	8.783	2.173
19	0	0	0	8.013	2.081
20	0	0	0	8.059	2.087

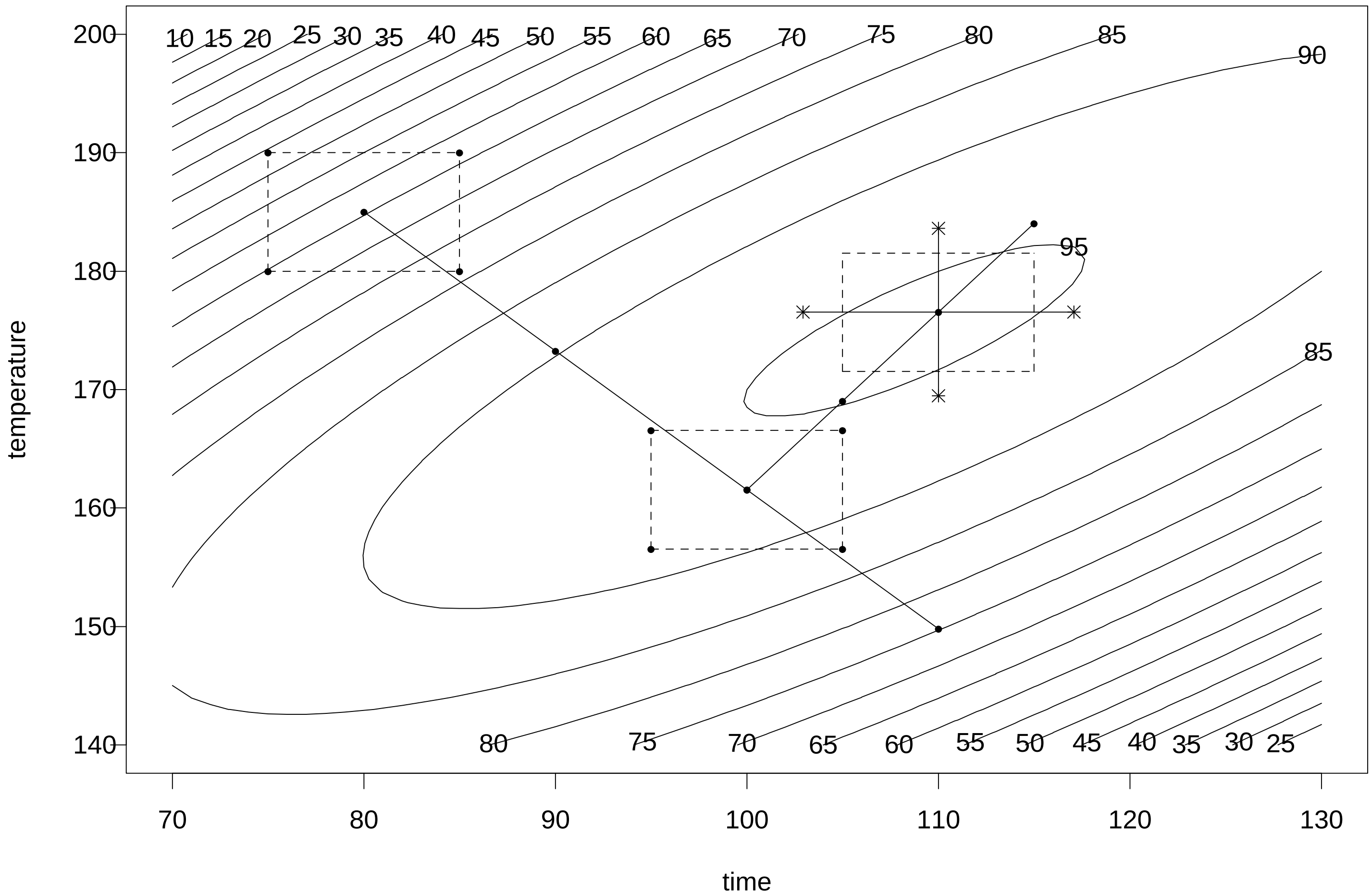
Central Composite Designs

A simple CCD is shown graphically below. It has three parts (1) *cube* (or corner) points, (2) *axial* (or star) points, (3) *center* points.



A Central Composite Design in Three Dimensions (cube point (dot), star point(cross), center point (circle))

Sequential Exploration of Response Surface



An Alternative to Standard Response Surface Methodology

- Standard RSM employs a 2-stage experimentation strategy; this can be time consuming and expensive.
- S. W. Cheng - Wu (2001) proposed a new strategy to perform factor screening (1^{st} order model) and response surface exploration (2^{nd} order model) on the *same* experiment using *one* design, based on new optimality criteria called *projection - aberration*

Optimal Designs

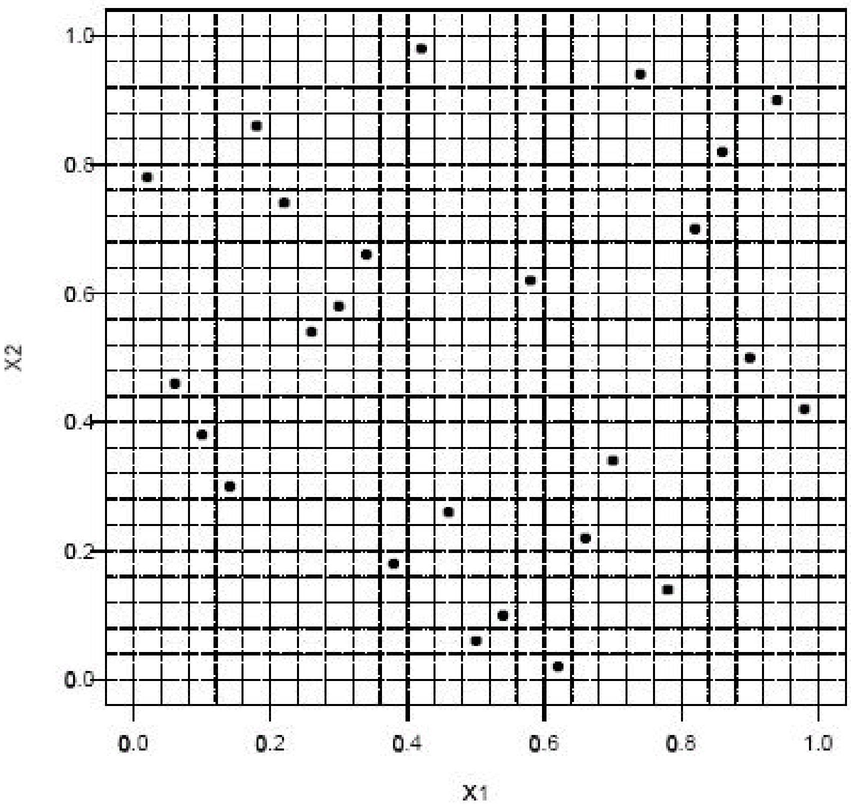
- *D*-,*G*-,*I*-optimality based on a *single* model, performance not guaranteed over a variety of models. Performance is highly *model-dependent*.
- Exact optimality more interesting than approximate (continuous) optimality. Algorithms make more impact than theory; generally *applicable to any models*.
- Bigger impact when used in conjunction with or as a supplement to a combinatorial or reasonably uniform design (irregular design, follow-up experiment, sequential designs).
- Generally useful as a benchmark.

Space-Filling Designs

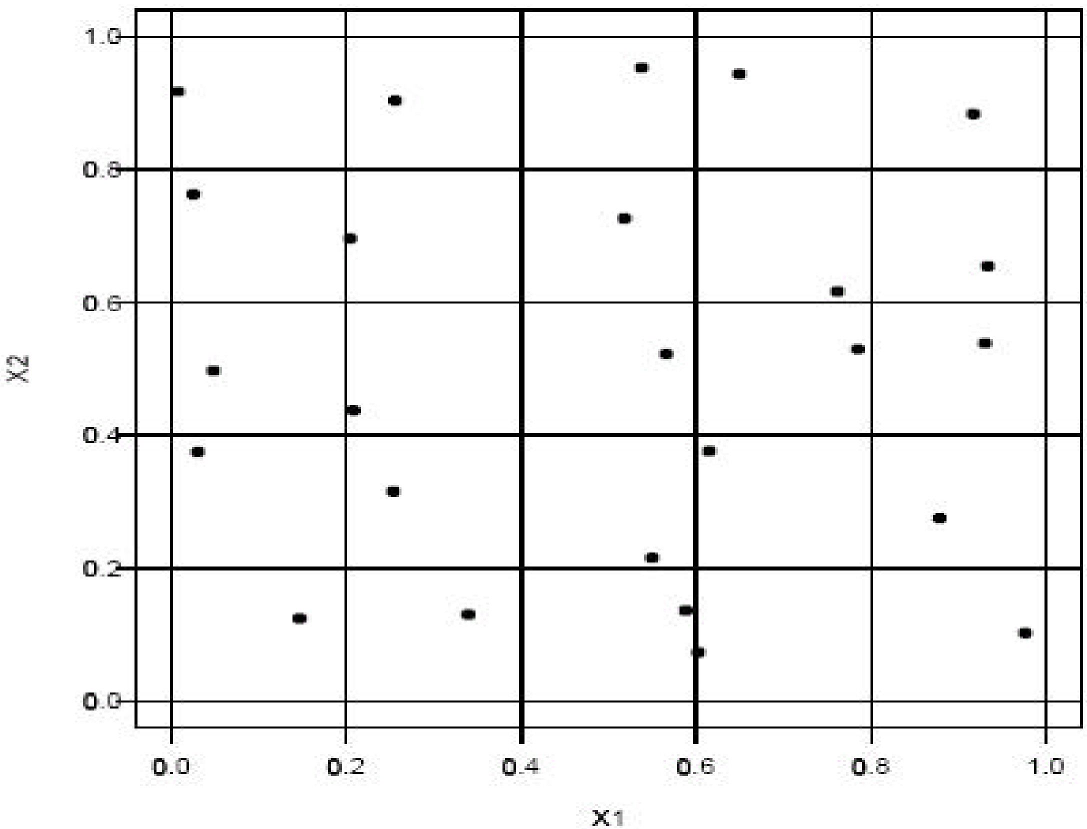
- Latin Hypercube in s^d (McKay, Beckman, Conover, 1979): *one-dimensional balance* for each of the d dimensions with s levels. Various extensions available: OA-based LHS (Tang, 1993) achieves 2- or higher-dimensional balance by combining LHS and OA.

- Uniform designs (Fang): based on wrapping around a sequence in high dimensions using number-theoretic justifications. More generally, *good lattice points*: work by Niederreiter etc.

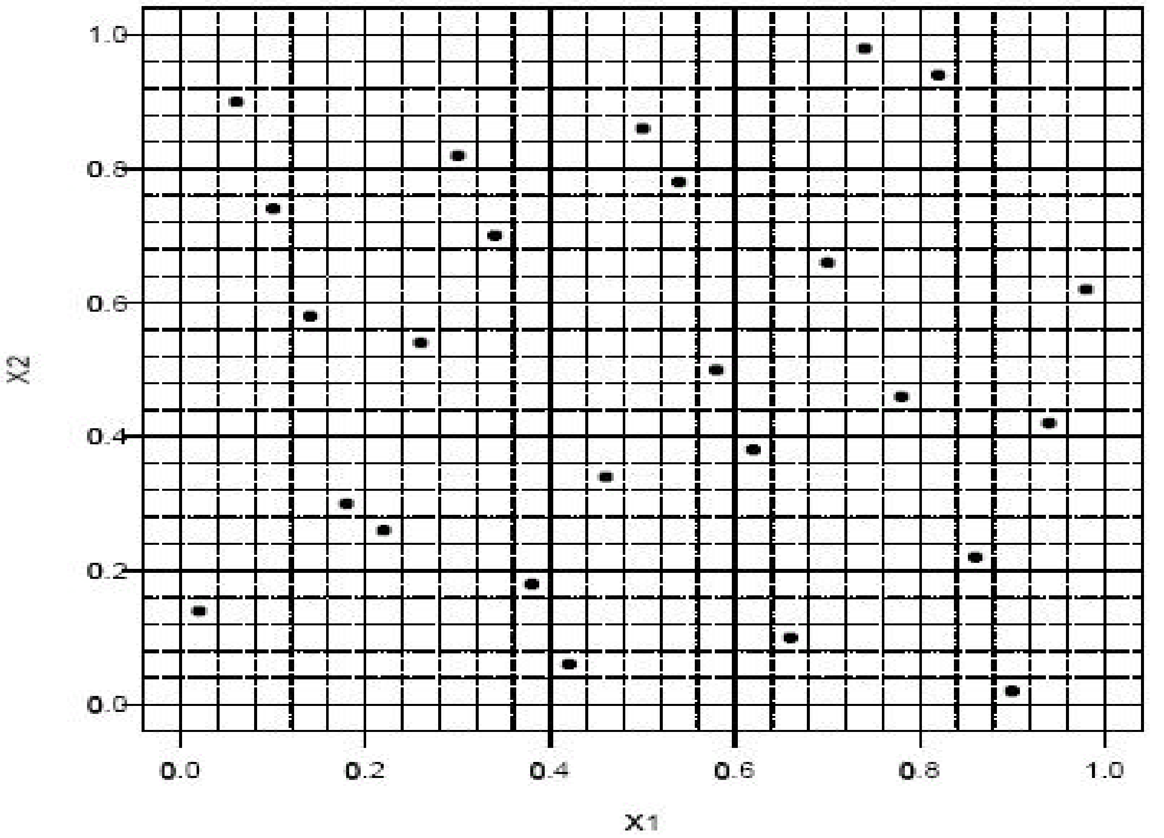
- Design criteria and modeling are drastically *different* from all the previous approaches: space-filling, minimax or maximin distance; use of semi-parametric modeling or Gaussian process modeling that allows highly *nonlinear* fitting.



25 points of a Latin hypercube sample



25 points of a randomly centered randomized orthogonal array. For any two variables, there is one point in each reference square.



25 points of an OA-based Latin hypercube sample

Innovations in Bayesian Analysis for Designed Experiments

- Choice of priors reflects the three principles (hierarchy, sparsity, heredity)
- Model search strategy depends on nature of design (much easier for regular designs; not so for nonregular designs); strategy should exploit the effect aliasing pattern
- Convenient for computer experiments.

A Summary of Layout Techniques

A flexible strategy for selecting a suitable design from among

(i) 2^{k-p} designs : 8, 16, 32, 64, 128-run designs.

(ii) 3^{k-p} designs : 9, 27, 81-run designs (optimal selection of factor columns by minimum aberration criterion).

(iii) Plackett-Burman designs : $OA(12,2^{11})$, $OA(20,2^{19})$,...

(iv) Mixed-level designs : $OA(8,4^1 2^4)$,$OA(16,4^m 2^n)$ (derived from 2^{k-p} designs), $OA(18,2^1 3^7)$, $OA(36,2^{11} 3^{12})$, $OA(12,3^1 2^4)$, $OA(24,3^1 2^{16})$, ...

(allowing main effects and a flexible choice of interactions to be estimated; hidden-projection property).

(v) Central Composite designs.

(vi) Optimal Designs (SAS/QC).

(vii) Space-filling designs (Latin hypercube designs).