Recent Development
In The Uniform Experimental Design

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Two Monographes

Fang, K.T., R. Li and A. Sudjianto (2005)

Design and Modeling for Computer Experiments

Chapman & Hall/CRC Press, London.

Fang, K.T. and F.J. Hickernell (2007)

Uniform Experimental Designs

Working now.

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1 Motivation and Philosophy

The orthogonal design has been widely applied in China since 1970. I joined many experiments during the Great Culture Revolution and found:

- Model uncertainty Most of experimenters do not know the underlying model.
- Multi-level Experiments with multi-factors each having several levels are mostly appreciate.
- Best level-combination Experimenters were urgent to find a 'best' level-combination.
- Simplicity of design and modeling The user more like orthogonal design tables and the profile analysis.

1.1. Knowledge learnt from a case study

- An example was a porcelain insulator factory in Nanjing in 1973.
- The factory had a team of staff assigned to conduct experiments continually to identify a satisfactory parameter-combination.
- In the past 10 years although they had achieved much in their experiments, they still failed to get one of the responses to meet the requirement.
- At that time, the factory received a large number of orders for glass insulators but was unable to deliver the products.
- In view of the complexity of the issue, I adhered to the principle of "big net catching big fish".

- I conducted an experiment with 25 runs and six factors each having six 5-levels by an orthogonal design $L_{25}(5^6)$. From a statistical point of view, the experiment model was inestimable and was therefore incorrect.

- However, in those 25 experiments, one had all the responses fulfilling the requirements. That was great news to the factory in-charge.

- In fact, the 25 runs conducted via the orthogonal design actually represented $15,625 = 5^6$ level-combinations, thus greatly increasing the likelihood of attaining an ideal technical/manufacturing condition. In my opinion, one power of fractional factorial design is that the experimental points have a good representation.

- Since then, I have used the same strategy to solve many of the "lasting, major and difficult" problems of many big projects. That is to employ orthogonal designs with 4 or 5 levels and to arrange all the columns of the design tables for significant factors.

- This success has also injected in me the necessary courage to initiate the uniform design philosophy and method.

- Experiments under Model uncertainty and Spread experimental points uniformly on the domain.

1.2. Three important projects in computer experiments

In 1978 three big projects in system engineering raised the same type of problems to me. It needs one day calculation in a computer to obtain the output y, the solution of a system of differential equations, from the given input under the true model.

$$y = g(x_1, \cdots, x_s) = g(\boldsymbol{x}).$$

We wish to find a simple and approximate model (metamodel)

$$\hat{y} = \hat{g}(x_1, \cdots, x_s) = \hat{g}(\boldsymbol{x})$$

such that the difference of $|y(\boldsymbol{x}) - \hat{y}(\boldsymbol{x})|$ is small in a certain sense.

The new concept: design of computer experiments was proposed.

1.3. Experiments with Model Uncertainty

I met many experiments with model uncertainty

$$y = g(x_1, \cdots, x_s) + \varepsilon,$$

where g is unknown and ε random error. We want to estimate g based on an experiment.

Both kinds of experiments need a design that spreads experimental points evenly on the experimental domain.

- Space-filling design: Uniform design
- Modeling

2 Approaches

The simplest approach is the overall mean model that wants to estimate the overall mean of y on the domain $C^s = [0, 1]^s$

$$\mathrm{Mean}(y) = \int_{C^s} g(\boldsymbol{x}) d\boldsymbol{x}$$

by the sample mean

$$\bar{y}(\mathcal{P}) = \frac{1}{n} \sum_{i=1}^{n} g(\boldsymbol{x}_i),$$

where $\mathcal{P} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\}$ is a set of experimental points.

How can we find a design such that $\bar{y}(\mathcal{P})$ has the best estimate of $\mathrm{Mean}(y)$ in a certain sense.

- Latin hypercube sampling (stochastic approach)

McKay, Beckaman, and Conover (1979)

They want to choose a design $\mathcal{P}$ such that $\bar{y}(\mathcal{P})$ is unbiased estimator of Mean(y) and has a smaller variance.

- Uniform design (deterministic approach)

Wang and Fang (Fang (1980), Wang and Fang (1981))

To find a design such that $|\text{Mean}(y) - \bar{y}(\mathcal{P})|$ is as small as possible.

Of course, the overall mean model is far not enough in practice, but it is surprising that

- The overall mean model provides a simple way to develop methodology and theory on computer experiments and experiments under model uncertainty.

- The overall mean model created LHS/UD that have a excellent performance for more complex models (nonlinear, multi-extreme values, etc) as the true model can be in a large class of functions

Advantages of LHS

- ♠ Easy to generate
- ♠ Can be efficiently work for high dimensions

Disadvantages of LHS

- ♠ Some designs have a poor quality
- ♠ There is a large space to reduce variance of $\bar{y}(\mathcal{P})$
- ♠ The convergence rate is slow, $O_p(\frac{1}{\sqrt{n}})$

Modified versions of LHS

- ♠ centered (midpoint) Latin hypercube sampling
- ♠ randomized orthogonal array
- ♠ symmetric and orthogonal column Latin hypercubes
- ♠ optimal Latin hypercube designs in the following criteria:
  - † mean squared error
  - † entropy
  - † minimax and maximin distance
  - † ϕ_p-criterion

Uniform Design

The uniform design put experimental points uniformly scattered on the experimental domain.

The Koksma-Hlawka inequality in quasi-Monte carlo theory provides an upper bound of

$$\text{diff-mean} = |\text{Mean}(y) - \bar{y}(\mathcal{P})| \leq V(g)D(\mathcal{P}),$$

where $D(\mathcal{P})$ is the star discrepancy of the design $\mathcal{P}$, not depending on g, and $V(g)$ is the total variation of the function g in the sense of Hardy and Krause.

The K-H inequality still holds when the star discrepancy is replaced by many other discrepancies.

Uniform Design

- For construction of uniform designs it is not tractable to find a set of n points, $\mathcal{P} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\} \subset C^s$, such that it has the minimum discrepancy.

- We need concept of U-type designs.

A U-type design with n runs and s factors each having respective $q_1, \cdots, q_s$ levels is an $n \times s$ matrix such that the q_j levels in the jth column appear equally often and is denoted by $U(n, q_1 \times \cdots \times q_s)$. When some q_j's are equal, we denote it by $U(n, q^{r_1} \times \cdots \times q_m^{r_m})$ where $r_1 + \cdots + r_m = s$. If all the q_j's are equal, denoted by $U(n, q^s)$, it is said to be symmetrical, otherwise asymmetrical.

- Denote the design space by $\mathcal{U}$, all the $U(n, q_1 \times \cdots \times q_s)$. We want to find one with minimum discrepancy on $\mathcal{U}$.

Common aspects between LHS and UD

♡ space-filling designs

♡ motivated by the overall mean model

♡ robust against model specification

♡ construction of the design may be based on U-type designs

♡ Have been widely applied to computer experiments and experiments under model uncertainty.

3 New Development: Discrepancy and Design Construction

Difficulty and complexity

- The uniformity is a geometrical criterion, it needs some justification in statistical sense

- The overall mean model is far from the request of modeling

- Initially, the uniform design theory is based on the quasi-Monte Carlo methods. The useful tool is the number theory. Most statisticians are lack of knowledge of the number theory.

- Numerical search of uniform design is a NP hard problem. It needs some powerful algorithms in optimization.

3.1. Characteristics of UD

Maximin and Minimax

Wiens, D. P. (1991), *Stat. & Prob. Letters*

Admissibility and minimax

Xie, M.Y. and Fang, K.T. (2000), *JSPI*

Robustness and efficiency

Hickernell, F.J. (1999), *Stat. & Prob. Letters*

Hickernell, F.J. and Yue, R.X. (1999), *Statistica Sinica*

Hickernell, F.J. and Liu, M.Q. (2002), *Biometrika*

3.2. Measures of uniformity

The star L_p-discrepancy has been widely used in number-theoretic methods (quasi-Monte Carlo methods) and is defined by

$$D_p(\mathcal{P})^p = \int_{C^s} \left| \frac{N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))}{n} - \mathrm{Vol}([\mathbf{0}, \boldsymbol{x}))\right|^p d\boldsymbol{x}$$

that is the most popular measure from quasi-Monte Carlo methods, where

- ‡ $[\mathbf{0}, \boldsymbol{x}) = [0, x_1) \times \cdots \times [0, x_s)$,
- ‡ $N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))$ the number of points of $\mathcal{P}$ falling in $[\mathbf{0}, \boldsymbol{x})$,
- ‡ $\mathrm{Vol}(A)$ the volume of A.

3.2. Measures of uniformity

The star L_p-discrepancy has some shortcomings:

‡ the star discrepancy (L_∞-discrepancy) is not easy to compute and is not sensitive enough for construction of UDs

‡ the star L_2-discrepancy ignores discrepancy in any low-dimensional subspace.

‡ the star L_p-discrepancy is not invariant under the coordinates rotations.

3.2. Measures of uniformity

Hickernell (1998) proposed several new discrepancies:

- Centered L_2-discrepancy (CD)
- Wrap-around L_2-discrepancy (WD)
- Discrete discrepancy (DD)

A unified approach to the discrepancy

Let $\mathcal{X}$ be the experimental domain that is a measurable set of R^s and $K(\boldsymbol{x}, \boldsymbol{w})$ be a symmetric and positive definite function on $\mathcal{X} \times \mathcal{X}$, i.e.,

$$\begin{aligned} K(\boldsymbol{x}, \boldsymbol{w}) &= K(\boldsymbol{w}, \boldsymbol{x}), \text{ for any } \boldsymbol{x}, \boldsymbol{w} \in \mathcal{X}, \\ \sum_{i,j=1}^{n} a_i a_j K(\boldsymbol{x}_i, \boldsymbol{x}_j) &> 0, \text{ for any } a_i \in R, \boldsymbol{x}_i \in \mathcal{X}, i = 1, \cdots, n, \end{aligned}$$

Let F be the uniform distribution on $\mathcal{X}$ and $F_n(\boldsymbol{x})$ be the empirical distribution of $\mathcal{P}$. The L_2-discrepancy is defined by

$$D_K^2(\mathcal{P}) = ||F - F_n||_K^2 = \int_{\mathcal{X}\times\mathcal{X}} K(\boldsymbol{x}, \boldsymbol{w}) d(F - F_n)(\boldsymbol{x}) d(F - F_n)(\boldsymbol{w}).$$

It can be expressed

$$
\begin{aligned}
D_K^2(\mathcal{P}) \;&=\; \int_{\mathcal{X}\times\mathcal{X}} K(\boldsymbol{x},\boldsymbol{w})dF(\boldsymbol{x})dF(\boldsymbol{w}) \\
&\quad -\frac{2}{n}\sum_{i=1}^{n} K(\boldsymbol{x},\boldsymbol{x}_i)dF(\boldsymbol{x}) + \frac{1}{n^2}\sum_{i,j=1}^{n} K(\boldsymbol{x}_i,\boldsymbol{x}_j),
\end{aligned}
$$

Different kernel K's imply different discrepancies.

The new measures of uniformity satisfying:

- [C1] Invariant under permuting factors and/or runs
- [C2] It is invariant under the coordinates rotation
- [C3] It can measure not only uniformity over C^s, but also projection uniformity over C^u, where u is a non-empty subset of $\{1, \cdots, s\}$.
- [C4] There have some reasonable geometric meaning
- [C5] Easy to compute
- [C6] Satisfy Koksma-Hlawka-like inequality
- [C7] It consists with other criteria in experimental designs

3.3. Construction of Uniform Designs

- For one-factor experiment, the unique UD on [0,1] is $\left\{\frac{1}{2n}, \frac{3}{2n}, \cdots, \frac{2n-1}{2n}\right\}$ with $CD_2^2 = \frac{1}{12n^2}$.

To finding a $U_n(q^s)$ with $s > 2$ is a very difficult problem. There are two approaches:

† by the theory

† by numerical search

‡ Reduce of design space (quasi-Monte Carlo methods)

‡ Lower bounds of the criterion

3.3. Construction: quasi-Monte Carlo methods

Good lattice point method

Fang (1980), Wang and Fang (1981), Fang and Li (1994)

Latin square method

Fang, Shiu and Pan (1999), *Statistica Sinica*

Cutting method

Ma and Fang (2004), *International Journal of Materials and Product Technology*

Collapsing method

Fang and Qin (2003), *Statist. & Prob. Letters*

3.3. Construction: quasi-Monte Carlo methods

Digit net method

Hickernell (2004), submitted

Extensible uniform designs

Wang, X.Q. and Fang, K. T. (2003)

3.3. Construction: Combinatorial method:

- ‡ Lu, X and Meng, Y. (2000), *JSPI*
- ‡ Fang,K.T. Ge, G. and Liu, M.Q. (2002), *CSA Bulletin*
- ‡ Fang,K.T. Ge, G. and Liu, M.Q. (2002, 2003), *Science in China*
- ‡ Fang,K.T. Ge, G., Liu, M.Q. and Qin, H.
  (2004), *Discrete Math.* (2005), *Utilitas Math.*
- ‡ Fang, K.T., Lu, X., Tang, Y. and Yin, J. (2004), *Discrete Math.*

3.4. Construction: Numerical search

To finding a $U_n(q^s)$ with $s > 2$ is a NP hard problem in the sense of computation complexity.

◇ Optimization

- ‡ Local search algorithm
- ‡ simulated annealing algorithm
- ‡ stochastic evolutionary algorithm
- ‡ threshold accepting algorithm
  - ♯ Winker and Fang (1997), *SIAM J. Numer. Anal.*
  - ♯ Fang and Ma (2001), *J. Complexity*
  - ♯ Fang, Ma and Winker (2002), *Math. Computation*

- ♯ Fang, Lu and Winker (2003), *J. Complexity*
- ♯ Fang, Tang and Yin (2005), *J. Complexity*
- ♯ Fang,, Maringer, D., Tang, Y. and Winker, P. (2006), *Math. Computation*

◇ Key points in optimization aogorithms

- ♯ Neighborhood
- ♯ Replacement rule
- ♯ Jumping rule and iteration formula
- ♯ Lower bound of the criterion

4 New Development: Relationships among Factorial, Supersaturated and Uniform Designs

4.1. Classification

They are constructed based on U-type designs.

A U-type design, $U(n, q_1 \times \cdots \times q_s)$, can be classified as

$\sharp$ unsaturated if $n - 1 > q_1 + \cdots + q_s$

$\sharp$ saturated if $n - 1 = q_1 + \cdots + q_s$

$\sharp$ supersaturated if $n - 1 < q_1 + \cdots + q_s$

$\sharp$ uniform design if it has the smallest pre-decided discrepancy.

4.2. More condition on U-type designs

♯ Balance of level-combinations. orthogonal array of strength t

♯ statistical inference. word-length pattern, maximum estimation capacity, Q and Q_B criteria (Tasi et al. (2000, 2005))

♯ uniformity. uniform design

♯ projection uniformity pattern.

4.3. Criteria for competing fractional designs

♯ word-length pattern.

resolution (Box and Hunter, 1961)

minimum aberration (Fries and Hunter, 1980)

♯ Generalized word-length pattern. Xu and Wu (2001) and Ma and Fang (2001)

Minimum G_2-aberration, Tang and Deng (1999)

β-aberration, Cheng and Ye (2004)

Minimum moment aberration, Xu (2003)

4.4. Projection Criteria for competing fractional designs

$\sharp$ The projection discrepancy pattern.

Hickernell and Liu (2002), *Biometrika*

$\sharp$ The uniformity pattern

Fang and Qin (2004), *Science in China*

$\sharp$ The minimum aberration majorization

Fang and Zhang (2004), *JSPI*

4.5 Criteria for competing supersaturated designs

♯ Correlation coefficients $E(s^2)$. Booth and Cox (1962)

Lin (1993, 1995), Wu (1993), Tang and Wu (1997), Cheng (1997), Yamada and Lin (1997), Lu and Meng (2000) Liu and Hickernell (2002), indicated that the $E(s^2)$ criterion and the discrete discrepancy share the same optimal designs.

4.5 Criteria for competing supersaturated designs

♯ Balance pattern

Consider a U-type design $U(n, q_1 \times \ldots \times q_s)$ with the design matrix $\boldsymbol{U} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_s)$, where $\boldsymbol{u}_j$ is the j-th column of $\boldsymbol{U}$. Define

$$B_{l_1,\ldots,l_m}(\boldsymbol{U}) = \sum_{1 \le \alpha_1,\ldots,\alpha_m \le q} \left(n_{\alpha_1,\ldots,\alpha_m}^{(l_1,\ldots,l_m)} - \frac{n}{q_{l_1} \ldots q_{l_m}} \right)^2,$$

where $n_{\alpha_1,\ldots,\alpha_m}^{(l_1,\ldots,l_m)}$ is the number of rows in which the column group $\{\boldsymbol{u}_{l_1}, \ldots, \boldsymbol{u}_{l_m}\}$ takes the level combination $\{\alpha_1, \ldots, \alpha_m\}$, and the summation is taken over all possible level combinations. Let

$$B_m(\boldsymbol{U}) = \frac{1}{\binom{s}{m}} \sum_{1 \le l_1 < \ldots < l_m \le s} B_{l_1,\ldots,l_m}(\boldsymbol{U}).$$

♯ Balance pattern

$$B(\boldsymbol{U}) = (B_1(\boldsymbol{U}), B_2(\boldsymbol{U}), \ldots, B_s(\boldsymbol{U}))$$

1. $B_1(\boldsymbol{U}) = 0$ if and only if $\boldsymbol{U}$ is U-type design.
2. The fact $B_m(\boldsymbol{U}) = 0$ implies $B_j(\boldsymbol{U}) = 0, j < m$.
3. $B_m(\boldsymbol{U}) = 0$ for some $m \geq 2$ if and only if the design is orthogonal array with strength m.
4. Ave(χ^2) proposed by Yamada and Lin (1999) is a special case of $B_2(\boldsymbol{U})$.
5. Ave(f_{NOD}) studied by Fang, Lin and Liu (2003) is just $B_2(\boldsymbol{U})$.

4.6. Relationships among various criteria

For two-level U-type design CD and WD can be expressed as a function of the balance pattern of word length pattern

$$[CD_2(\boldsymbol{U})]^2 = \left(\frac{13}{12}\right)^s - 2\left(\frac{35}{32}\right)^s + \left(\frac{9}{8}\right)^s + \frac{1}{n^2}\sum_{m=1}^{s} 4^{-m} \left(\begin{array}{c} s \\ m \end{array}\right) B_m(\boldsymbol{U})$$

$$[CD_2(\boldsymbol{U})]^2 = \left(\frac{13}{12}\right)^s - 2\left(\frac{35}{32}\right)^s + \left(\frac{8}{9}\right)^s \left\{1 + \sum_{i=1}^{s} \frac{A_i(\boldsymbol{U})}{9^i}\right\}.$$

These relationships can be extended to WD for two- or three-level designs.

4.6. Relationships among various criteria

$\sharp$ For any design matrix $U(n, q^s)$, the three design criteria $E(f_{NOD})$, $E(s^2)$ and $Ave(\chi^2)$ satisfy the following relations:

$$
\begin{aligned}
E(f_{NOD}) &= \frac{n}{9} Ave(\chi^2), \text{ when } q = 3, \text{ and} \\
E(f_{NOD}) &= \frac{1}{4} E(s^2), \text{ when } q = 2, \text{ with two levels } -1 \text{ and } 1.
\end{aligned}
$$

$\sharp$ A design $U(n; q_1 \times \ldots \times q_s)$ is a uniform design under the discrete discrepancy if and only it is $E(f_{NOD})$-optimal.

$\sharp$ For any design matrix $U(n, q^s)$, the discrete discrepancy, MMA, GMA and $E(f_{NOD})$ criterion are equivalent in a certain sense.

4.7. Relationships among various criteria via majorization

Zhang, Fang, Li and Sudjianto (2005) *Annuals of Statistics* consider the pairwise coincidence (PC) vector, denoted by $\delta(\boldsymbol{U})$, among any two rows of a U-type design $\boldsymbol{U}$.

Admissibility: we say design $\boldsymbol{U}_1$ is better than $\boldsymbol{U}_2$ if $\delta(\boldsymbol{U}_1) \prec \delta(\boldsymbol{U}_2)$. A design $\boldsymbol{U}$ is inadmissible if there exists $\boldsymbol{U}^*$ such that $\delta(\boldsymbol{U}^*) \prec \delta(\boldsymbol{U})$. A design which is not inadmissible is called admissible.

Majorant: If there exists $\boldsymbol{U}$ such that

$$\delta(\boldsymbol{U}) \preceq \delta(\boldsymbol{U}^*), \text{ for any } \boldsymbol{U}^*$$

we call $\boldsymbol{U}$ a majorum design in the design space.

Schur-convex optimality: For a predefined Schur-convex kernel function $\Psi(\cdot)$ on R_+^m, $m = n(n-1)/2$, a design $\boldsymbol{U}$ is called Schur-Ψ-optimal with respect to (w.r.t.) $\Psi(\cdot)$

$$\Psi(\delta(\boldsymbol{U})) \leq \Psi(\delta(\boldsymbol{U}^*)), \text{ for any } \boldsymbol{U}^*.$$

A Schur-convex function $\Psi(\cdot)$ is called a separable convex function if $\Psi(\boldsymbol{x}) = \sum_{r=1}^m \psi(x_r)$, where ψ is convex function on R_+.

The criteria $E(s^2)$, $Ave(\chi^2)$, Ave(f^2), A_2^g, A_3^g in the generalized word length pattern, DD, WD for the case of $q = 2, 3$ and CD for the case of $q = 2$, can be expressed as a separable convex function.

By the majorization theory and Lemma 5.2.1 of Dey and Mukerjee (1999) Zhang et al. (2005) proposed a united way to find tight lower bounds for the above criteria.

4 Applications

Advantages of The Uniform Design

- Flexibility in design and modeling
- Easy to understand and use
- Good for nonlinear models
- Can be applied on complicated system
- Can be used for several occasions:
  - fractional factorial experiments with unknown model
  - computer experiments
  - experiments with mixtures

- There are more than 500 hundreds case studies published in more than one hundred journals.
- More than one hundred theoretic research papers have been published in various journals.
- Ford Motor Company has been used UD for car development and “Design for Six Sigma”.
- A nationwide society “The Uniform Design Association of China” was established in 1994.

Performance of Uniform Designs

- W.I. Notz (2003) gave a comprehensive comparisons among maximin Latin hypercube design, uniform design, Sobol sequence, scrambled net, Niederreiter design, maximum entropy designs and others and found that the uniform design has a good performance.

- Ling, Fang and Xu (2001) gave a comprehensive review on applications of UD in chemistry and chemical engineering.

Performance of Uniform Designs

- The Ford Motor Company has used the UD for developing new engines. Agus Sudjianto, Engineering Manager in FORD invited me to visit the FORD in 2002. His letter of invitation wrote: “In the past few years, we have tremendous in using Uniform Design for computer experiments. The technique has become a critical enabler for us to execute ‘design for Six Sigma’ to support new product development, in particular, automotive engine design. Today, computer experiments using uniform design have become standard practices at Ford Motor Company to support early stage of product design before hardware is available.” It shows that there is a big potential applications of the uniform design in Six Sigma development.

Thank you for your attention