



Computer Experiments

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Where have all the Data gone?

- No need for data (Theoretical Development)
- Survey Sampling and Design of Experiment (Physical data collection)
- Computer Simulation (Experiment)
 - Statistical Simulation (Random Number generation)
 - Engineering Simulation
- Data from Internet
 - On-line auction
 - Search Engine



Statistics vs. Engineering Models

$$y = f(x, \theta) + \varepsilon$$

(Typical) Statistical Model

$$y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ij} x_i x_j + \varepsilon$$



A Typical Engineering Model (page 1 of 3, in Liao and Wang, 1995)

$$\begin{aligned}
 & \rho_1 A_1 \frac{\partial^2 w}{\partial t^2} + E_1 I_2 \frac{\partial^4 w}{\partial x^4} \\
 & + \left\{ (\rho_1 A_1 + \rho_1 A_2) \frac{\partial^2 w}{\partial t^2} - \rho_1 A_1 \left(\frac{t_2 + t_1}{2} \right) \left(\frac{\partial^3 u_2}{\partial x \partial t^2} - \frac{t_2 + t_1}{2} \frac{\partial^4 w}{\partial x^4} + \frac{t_1}{2} \frac{\partial^3 \beta}{\partial t^3} \right) \right. \\
 & + \rho_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x \partial t^2} - a \frac{\partial^4 w}{\partial x^4} + \frac{\partial^3 \beta}{\partial x \partial t^2} \right) + C_{11}^0 I_2 \frac{\partial^4 w}{\partial x^4} - E_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 w}{\partial x^4} + \frac{\partial^3 \beta}{\partial x^3} \right) \left[H(x-x_1) - H(x-x_2) \right] \left. \right\} \\
 & + \left\{ \rho_1 A_1 \left(\frac{t_2 + t_1}{2} \right) \left(\frac{\partial^3 u_2}{\partial t^3} - \frac{t_2 + t_1}{2} \frac{\partial^4 w}{\partial x^4} + \frac{t_1}{2} \frac{\partial^3 \beta}{\partial t^3} \right) + \rho_1 A_2 a \left(\frac{\partial^3 u_2}{\partial t^3} - a \frac{\partial^4 w}{\partial x^4} + \frac{\partial^3 \beta}{\partial t^3} \right) \right. \\
 & \left. + 2C_{11}^0 I_2 \frac{\partial^4 w}{\partial x^4} - 2E_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 w}{\partial x^4} + \frac{\partial^3 \beta}{\partial x^3} \right) \right\} [\delta(x-x_1) - \delta(x-x_2)] \\
 & + \left\{ C_{11}^0 I_2 \frac{\partial^4 w}{\partial x^4} - E_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 w}{\partial x^4} + \frac{\partial^3 \beta}{\partial x^3} \right) + b d_{11} E_1 a V(t) \right\} [\delta(x-x_1) - \delta(x-x_2)] = f(x, t)
 \end{aligned} \tag{1}$$

$$\begin{aligned}
 & \rho_1 A_1 \frac{\partial^2 u_2}{\partial t^2} - E_1 A_2 \frac{\partial^2 u_2}{\partial x^2} \\
 & + \left\{ \rho_1 A_1 \left(\frac{\partial^3 u_2}{\partial t^3} - \frac{t_2 + t_1}{2} \frac{\partial^4 u_2}{\partial x \partial t^2} + \frac{t_1}{2} \frac{\partial^3 \beta}{\partial t^3} \right) + \rho_1 A_2 a \left(\frac{\partial^3 u_2}{\partial t^3} - a \frac{\partial^4 u_2}{\partial x \partial t^2} + \frac{\partial^3 \beta}{\partial t^3} \right) \right. \\
 & \left. - E_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 u_2}{\partial x^4} + \frac{\partial^3 \beta}{\partial x^3} \right) \right\} [H(x-x_1) - H(x-x_2)] \\
 & + \left\{ -E_1 A_2 a \frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 u_2}{\partial x^4} - \frac{\partial^3 \beta}{\partial x^3} \right\} + b d_{11} E_1 a V(t) [\delta(x-x_1) - \delta(x-x_2)] = 0
 \end{aligned} \tag{2}$$

$$\begin{aligned}
 & \left\{ \rho_1 A_1 \left(\frac{\partial^3 u_2}{\partial t^3} - \frac{t_2 + t_1}{2} \frac{\partial^4 u_2}{\partial x \partial t^2} + \frac{t_1}{2} \frac{\partial^3 \beta}{\partial t^3} \right) + \rho_1 A_2 a \left(\frac{\partial^3 u_2}{\partial t^3} - a \frac{\partial^4 u_2}{\partial x \partial t^2} + \frac{\partial^3 \beta}{\partial t^3} \right) \right. \\
 & \left. + A_1 (G + \beta) - E_1 A_2 a \left(\frac{\partial^3 u_2}{\partial x^3} - a \frac{\partial^4 u_2}{\partial x^4} + \frac{\partial^3 \beta}{\partial x^3} \right) \right\} [H(x-x_1) - H(x-x_2)]
 \end{aligned} \tag{3}$$



“Statistical” Simulation Research

- Random Number Generators
 - Deng and Lin (1997, 2001)
- Robustness of transformation (Sensitivity Analysis)
 - From Uniform random numbers to other distributions



Goodness of Random Number Generators

- Period Length
- Efficiency
- Portability
- Theoretical Justification:
 - Uniformity
 - Independence
- Empirical Performance



LCG: Linear Congruential Generator Classical Random Number Generators

- $X_t = (B X_{t-1} + A) \text{ mod } m$
Length = m
Lehmer (1951); Knuth (1981)
- With proper choice of A & B
Length = $m = 2^{31} - 1 = 2147483647 (= 2.1 \times 10^9)$



Random Number Generation for the New Century

Lih-Yuan DENG and Dennis K. J. LIN

Use of empirical studies based on computer-generated random numbers has become a common practice in the development of statistical methods, particularly when the analytical study of a statistical procedure becomes intractable. The quality of any simulation study depends heavily on the quality of the random number generators. Classical uniform random number generators have some major defects—such as the (relatively) short period length and the lack of higher-dimension uniformity. Two recent uniform pseudo-random number generators (MRG and MCG) are reviewed. They are compared with the classical generator LCG. It is shown that MRG/MCG are much better random number generators than the popular LCG. Special forms of MRG/MCG are introduced and recommended as the random number generators for the new century. A step-by-step procedure for constructing such random number generators is also provided.

KEY WORDS: Linear congruential generator (LCG); Matrix congruential generator (MCG); Multiple recursive generator (MRG); Portable and efficient generator.

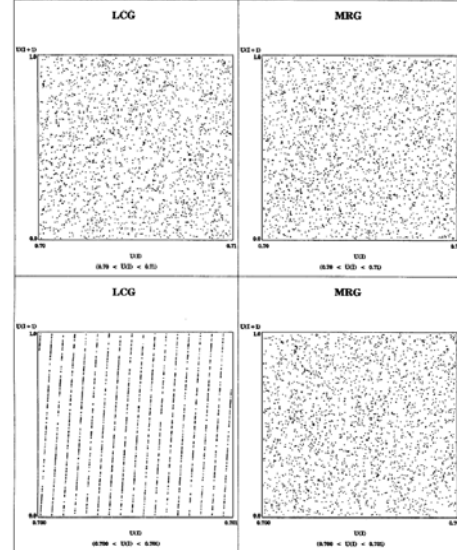
*Deng & Lin (2000)
The American Statistician*



MRG: Multiple Recursive Generators

Table 2. Listing of B_i in (10), $p = 2^{31} - 1$

		(a)				
k = 2	B_1	41546	32840	45670	13489	34601
	B_2	39606	35496	1853	22921	32207
Period = 4, 611, 686, 014, 132, 420, 608						
		(b)				
k = 3	B_1	24101	28876	21199	34577	4572
	B_2	13872	44515	34942	25100	25580
	B_3	11269	794	34546	20127	32253
Period = 9, 903, 520, 300, 447, 984, 150, 353, 281, 022						
		(c)				
k = 4	B_1	36421	18331	2995	19875	18799
	B_2	42276	32944	72	35787	24874
	B_3	28478	24787	5121	18825	25217
	B_4	42247	45231	18677	25443	24181
Period = 21267647892944572736998860269687930880						



Brief

- We have found a system of random number generators breaking the current world record. (Recall $p=2^{31}-1$ is about 10^9)
 - Old world record:
 - MT19937 (1998)
 - Period length $2^{19937}-1=10^{6001.6}$
 - New record with $p=2^{31}-1$:
 - DX-1597 [Deng, 2005]
 - Period length: $10^{14903.1}$
 - Longest Period found so far:



Normal Random Numbers: Examples

- Central Limit Theorem
 - $X_i \sim \text{iid } U(0,1) \rightarrow Z = \sum X_i - 6$
- Box-Muller Transformation
 - $X_i \sim \text{iid } U(0,1), i=1 \& 2 \rightarrow$

$$Z_1 = \sqrt{-2 \ln x_1} \cos(2\pi x_2)$$

$$Z_2 = \sqrt{-2 \ln x_1} \sin(2\pi x_2).$$
- Rejection Polar Method



Other Approaches

- Kinderman and Ramage (1976)
- Triangular Acceptance/Rejection Method
- Trapezoidal Method
 - (Ahrens, 1977)
- Ratio of Uniform
 - (Kinderman & Monahan, 1976)
- Rectangle/Wedge/Tail Method
 - (Marsaglia, Maclaren & Bray, 1964)



“Engineering” Computer Experiments

A Structured Roadmap for Verification and Validation-- Highlighting the Critical Role of Experiment Design

James J. Filliben

National Institute of Standards and Technology
Information Technology Division
Statistical Engineering Division

2004 Workshop on Verification & Validation of Computer
Models of High-Consequence Engineering Systems
NIST Administration Building
Lecture Room D
3:10-3:25, November 8, 2004



Computer Experiment

- Expensive simulation
- When Monte Carlo study is infeasible,
how to run simulation?
- Latin Hypercube



Irrelevant Issues

- Replicates
- Blocking
- Randomization

Question: How can a computer experiment be run in an efficient manner?

Lin (1997)



Why Latin Hypercube Designs?

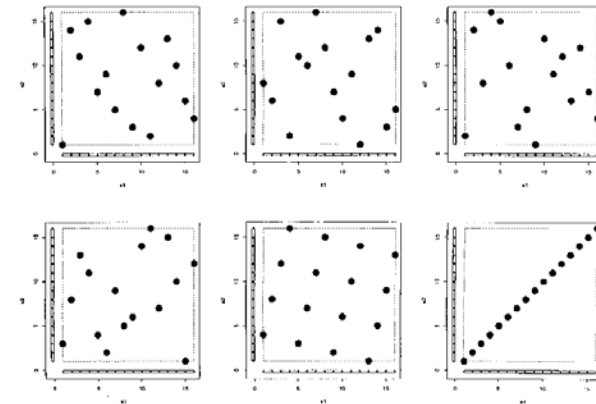
- Replication is worthless in CEs
- Factor levels are easily changed in CEs (not so in PEs)
- Suppose certain terms have little influence
 - Factorial designs produce replication when terms dropped
 - Can estimate high-order terms for other factors
- Provides pseudo-randomness since CEs are deterministic
- Smaller variance than random sampling or stratified random sampling (McKay, Beckman, and Conover (1979))

A special class
of LHC

x_1	x_2
1	τ_1
2	τ_2
3	τ_3
4	τ_4
·	·
·	·
·	·
16	τ_{16}

τ_i : permutation of $\{1, \dots, 16\}$
 $16!$
 $n!$ for size n &
 $(n!)^{d-1}$ for d -dim

Some Latin Hypercube Designs

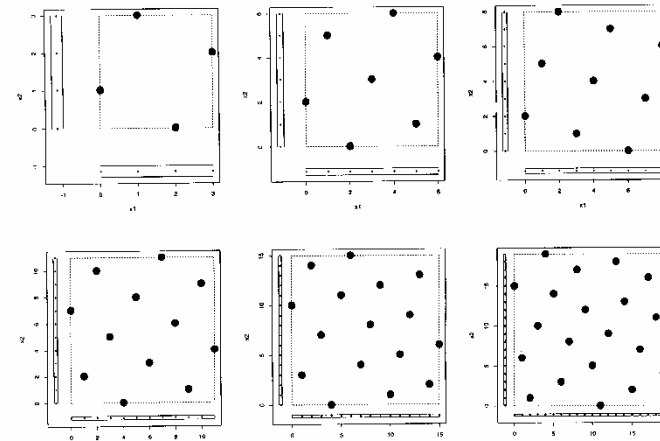




Bayesian Designs

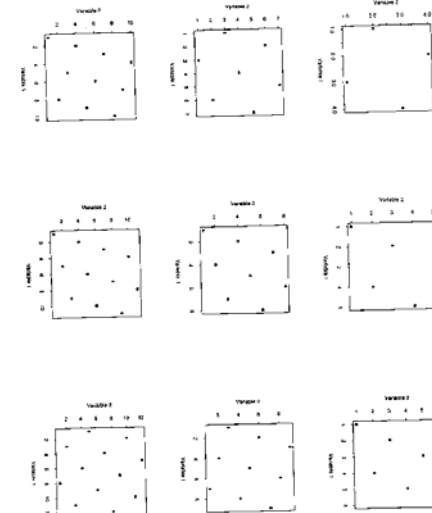
- Maximin Distance Designs, Johnson, Moore, and Ylvisaker (1990)
- Maximizes the Minimum Interpoint Distance (MID)
- Moves design points as far apart as possible in design space $MID = \min_{x_1, x_2 \in D} d(x_1, x_2)$
- D^* is a Maximin Distance Design if $MID = \min_{x_1, x_2 \in D^*} d(x_1, x_2) = \max_D \min_{x_1, x_2 \in D} d(x_1, x_2)$

Maximin Latin Hypercube Designs



Combination Designs

- Maximin Latin Hypercube Designs
 - Morris and Mitchell (1992)
 - Begin with Latin Hypercube
 - Iteratively permute
 - Stop when achieve largest MID
- Orthogonal Array-Based LH's
 - Owen (1992), Tang (1993)
 - Begin with Orthogonal Array
 - Construct Latin Hypercube from OA



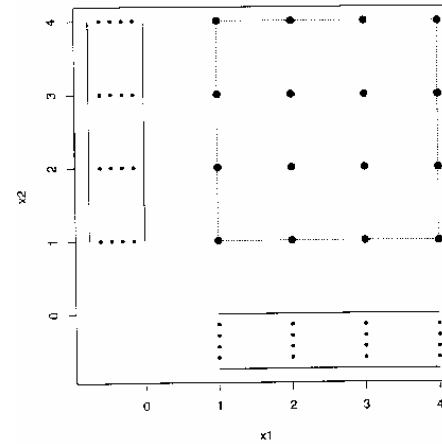


Rotated Factorial Designs

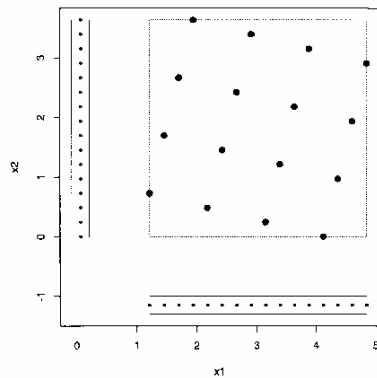
- Computer experiments are gaining in popularity
 - One main research area of the next 10 years
- Rotated factorial designs
 - good factorial design properties (orthogonality and structure)
 - good Latin hypercube properties (unique and equally-spaced projections)
 - easy to construct
 - comparable by Bayesian criteria
 - very suitable for computer experiments

Lin (1997)

16 point factorial design



Rotation by $\arctan(1/4)$ radians



- Rotation Theorem
- Orthogonality Theorem



$$D = X \cdot V$$

desirable design

factorial design

rotated matrix

$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ \vdots & \vdots \\ p & 1 \\ 1 & 2 \\ 2 & 2 \\ \vdots & \vdots \\ p & 2 \\ \vdots & \vdots \\ 1 & p \\ 2 & p \\ \vdots & \vdots \\ p & p \end{bmatrix}_{p^2 \times d}$$

$$\begin{bmatrix} u_1 & u_3 \\ u_2 & u_4 \end{bmatrix}_{d \times d}$$



For $d = 2$

$$V_1 = [v_1 \quad v_2] = \begin{bmatrix} +1 & +p \\ +p & -1 \end{bmatrix}$$

For $d = 2^c$

$$V_c = \begin{bmatrix} V_{c-1} & -(p^{2^{c-1}} V_{c-1})^* \\ p^{2^{c-1}} V_{c-1} & (V_{c-1})^* \end{bmatrix}$$

where the operator $(\bullet)^*$ works on any matrix with an even number of rows by multiplying the entries in the top half of the matrix by -1 and leaving those in the bottom half unchanged.



Impossibility Theorem

For $d = 3$

$$v_1 = \begin{bmatrix} \pm 1 \\ \pm p \\ \pm p^2 \end{bmatrix}, v_2 = \begin{bmatrix} \pm p \\ \pm p^2 \\ \pm 1 \end{bmatrix}, v_3 = \begin{bmatrix} \pm p^2 \\ \pm 1 \\ \pm p \end{bmatrix}$$

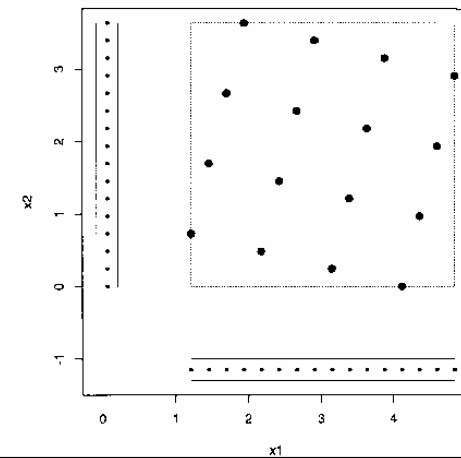
Conjecture 1:

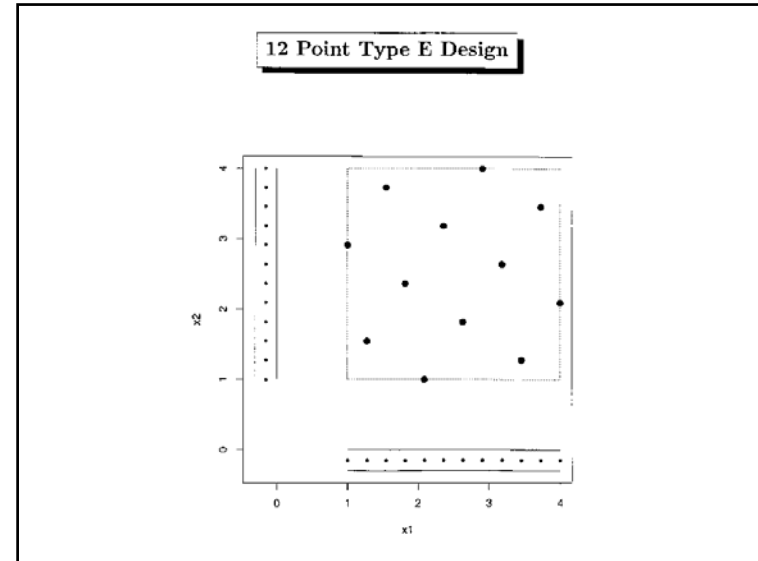
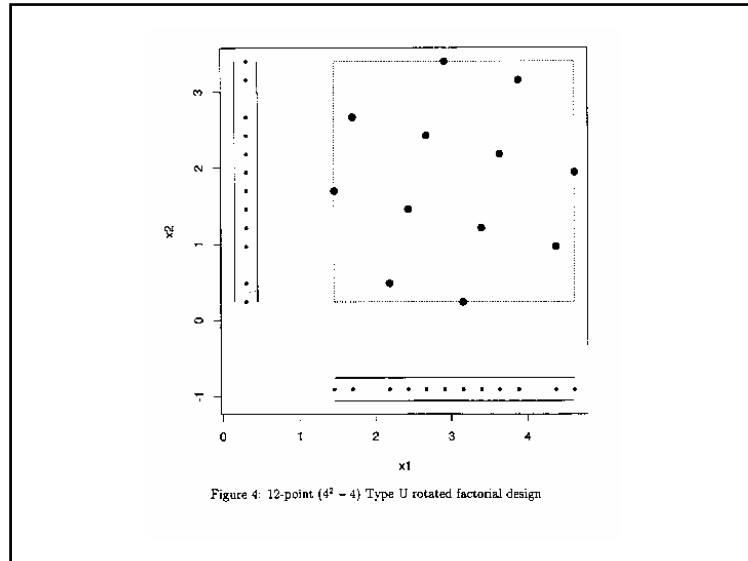
There does not exist a rotation matrix to rotate a d -factor, p -level full factorial design into a Latin Hypercube, unless d is a power of two, .



Rotated Factorial with other n ($\neq p^k$) Points

Rotation by $\arctan(1/4)$ radians






Available Design Sizes of 100 Points or Fewer for Rotated Factorial Designs

Dimensions	Available Design Sizes
2	4 [†] , 5 [†] , 6 [†] , 7 [†] , 8 [†] , 9 [†] , 11 [†] , 12 [†] , 13 [†] , 14 [†] , 15 [†] , 16 [†] , 17 [†] , 18 [†] , 19 [†] , 20 [†] , 21 [†] , 22 [†] , 23 [†] , 24 [†] , 25 [†] , 26 [†] , 27 [†] , 28 [†] , 29 [†] , 30 [†] , 31 [†] , 32 [†] , 33 [†] , 34 [†] , 35 [†] , 36 [†] , 37 [†] , 38 [†] , 39 [†] , 40 [†] , 41 [†] , 42 [†] , 44 [†] , 45 [†] , 46 [†] , 48 [†] , 49 [†] , 50 [†] , 52 [†] , 54 [†] , 55 [†] , 56 [†] , 57 [†] , 58 [†] , 59 [†] , 60 [†] , 61 [†] , 62 [†] , 63 [†] , 64 [†] , 65 [†] , 66 [†] , 67 [†] , 68 [†] , 69 [†] , 70 [†] , 71 [†] , 72 [†] , 73 [†] , 76 [†] , 77 [†] , 78 [†] , 79 [†] , 80 [†] , 81 [†] , 82 [†] , 83 [†] , 84 [†] , 85 [†] , 86 [†] , 87 [†] , 88 [†] , 89 [†] , 90 [†] , 91 [†] , 92 [†] , 93 [†] , 94 [†] , 95 [†] , 96 [†] , 97 [†] , 98 [†] , 99 [†] , 100 [†]
3-4	8 [†] , 9 [†] , 12 [†] , 16 [†] , 20 [†] , 24 [†] , 25 [†] , 28 [†] , 29 [†] , 32 [†] , 33 [†] , 36 [†] , 37 [†] , 38 [†] , 40 [†] , 41 [†] , 42 [†] , 46 [†] , 50 [†] , 51 [†] , 52 [†] , 54 [†] , 55 [†] , 56 [†] , 59 [†] , 60 [†] , 63 [†] , 64 [†] , 65 [†] , 67 [†] , 68 [†] , 73 [†] , 77 [†] , 81 [†]
5-8	8 [†] , 12 [†] , 16 [†] , 20 [†] , 24 [†] , 28 [†] , 32 [†] , 36 [†] , 40 [†] , 44 [†] , 48 [†] , 52 [†] , 56 [†] , 60 [†] , 64 [†] , 68 [†] , 72 [†] , 76 [†] , 80 [†] , 84 [†] , 88 [†] , 92 [†] , 96 [†] , 100 [†]

- † - Rotated p^d full factorial design
- ‡ - "Half-fraction" of rotated p^d full factorial design
- ◊ - Rotated mixed-level factorial design
- ◄ - "Half-fraction" (-1) of rotated mixed-level factorial design
- - "Half-fraction" (+1) of rotated mixed-level factorial design
- - Rotated full factorial design
- - Obtained via subtraction algorithm



MID Comparisons (2-dim)

No. of Pts.	Maximin Distance Design	Maximin Latin Hypercube Design	Rotated Factorial Type U Design	Rotated Factorial Type E Design
4	1.0000	.7454	.7454	.7454
5	.7071	.5590	.5270	.5590
8	.5000-1.0000	.4041	.3748	.4472
9	.5000	.3953	.3953	.3953
12	.3333-.5000	.3278	.3172	.3278
13	.3333-5000	.3005	.2833	.3162
16	.3333	.2749	.2749	.2749
17	.2500-.3333	.2652	.2550	.2577
20	.2500-.3333	.2233	.2253	.2425

† Obtained via Johnson, Moore and Ylvisaker (1991).
 ◊ Obtained via Koehler and Owen (1996).
 ◄ Obtained by authors' algorithm.



MID Comparison (4-dim)

No. of Pts	Maximin Latin H-cube	Rotated Design Type U	Factorial Design Type E	Maximin U Design
8	0.9258 †	0.8692	0.7071 (3)	0.7954 ◁
9	0.8101 †	0.5762	1.0000 (3)	0.6960 ◁
10	0.7857 †	*	*	*
11	0.7416 †	*	*	*
12	0.7216 †	*	*	*
16	0.6218 ◊	0.6146	0.6146 (16)	0.5292 ◁
24	0.5325 ◊	0.3963	0.3963 (24)	N/A
28	N/A	0.3951	0.4167 (7)	*
36	N/A	0.3725	0.3725 (36)	N/A
40	N/A	0.5192	0.5192 (40)	N/A
41	0.4507 ◊	0.5062	0.5062 (41)	*
54	N/A	0.3641	0.3641 (54)	N/A
67	N/A	0.3825	0.3825 (67)	*
68	N/A	0.3751	0.3751 (68)	*
81	N/A	0.3579	0.3579 (81)	N/A

* No design can be constructed as defined.
 † Published in Morris & Mitchell (1992).
 ◊ Obtained via Morris & Mitchell (1992) algorithm by the author.
 ◁ Obtained by author's algorithm.



Further Design Comparisons

No. Of Pts.	Minimum Interpoint Distance				Effect Correlation			
	Maximin Design Distance	Maximin Latin Hypercube	Rotated Factorial Design		Maximin Latin Hypercube	Rotated Factorial Design		
			Type U	Type E		Type U	Type E	
3	1.0000-1.4142	.7071	*	*	-.5000	*	*	
4	1.0000	.7454	.7454	.7454	0	0	0	
5	.7071	.5590	.5270	.5590	0	0	0	
6	.6009	.4472	*	*	-.0286	*	*	
7	.5314	.4714	.4518	.4472	-.1429	.0462	.0616	
8	.5000-1.0000	.4041	.3748	.4472	-.1429	0	0	
9	.5000	.3953	.3953	.3953	0	0	0	
10	.3333-.5000	.3514	.3436	.3514	-.20000	.0299	.0303	
11	.3333-.5000	.3162	*	*	-.0091	*	*	
12	.3333-.5000	.3278	.3172	.3278	0	0	0	
13	.3333-.5000	.3005	.2833	.3162	.2143	0	0	
14	.3333-.5000	.3172	.2945	.2875	.2088	.0100	.0127	
15	.3333-.5000	.2945	.2684	.2875	.0143	.0125	.0108	
16	.3333	.2749	.2749	.2749	.1265	0	0	
17	.2500-.3333	.2652	.2550	.2577	.0588	0	0	
18	.2500-.3333	.2496	*	*	.0588	0	0	
19	.2500-.3333	.2357	.2428	.2425	-.1263	.0079	.0083	
20	.2500-.3333	.2233	.2253	.2425	.0617	0	0	

* No rotated factorial design can be constructed



Rotation Theorem for Mixed Level Design

d = 2

$$R = \begin{bmatrix} 1 & \sqrt{pq} \\ -\sqrt{pq} & 1 \end{bmatrix}$$

d = 4

$$R = \begin{bmatrix} \frac{1}{\sqrt{1+pq}\sqrt{1+pqr}} & \frac{\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+q^2r^2}} & \frac{\sqrt{pqrs}}{\sqrt{1+pq}\sqrt{1+pqr}} & \frac{qr\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+q^2r^2}} \\ \frac{-\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+pqr}} & \frac{1}{\sqrt{1+pq}\sqrt{1+q^2r^2}} & \frac{-\sqrt{pqrs}\sqrt{pq}}{\sqrt{1+pq}\sqrt{1+pqr}} & \frac{qr}{\sqrt{1+pq}\sqrt{1+q^2r^2}} \\ \frac{-\sqrt{pqrs}}{\sqrt{1+rs}\sqrt{1+pqr}} & \frac{-qr\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+q^2r^2}} & \frac{1}{\sqrt{1+rs}\sqrt{1+pqr}} & \frac{\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+q^2r^2}} \\ \frac{\sqrt{pqrs}\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+pqr}} & \frac{-qr}{\sqrt{1+rs}\sqrt{1+q^2r^2}} & \frac{-\sqrt{rs}}{\sqrt{1+rs}\sqrt{1+pqr}} & \frac{1}{\sqrt{1+rs}\sqrt{1+q^2r^2}} \end{bmatrix}$$

d = 8

d = 2^c

Beattie & Lin (2004)



Beam Example

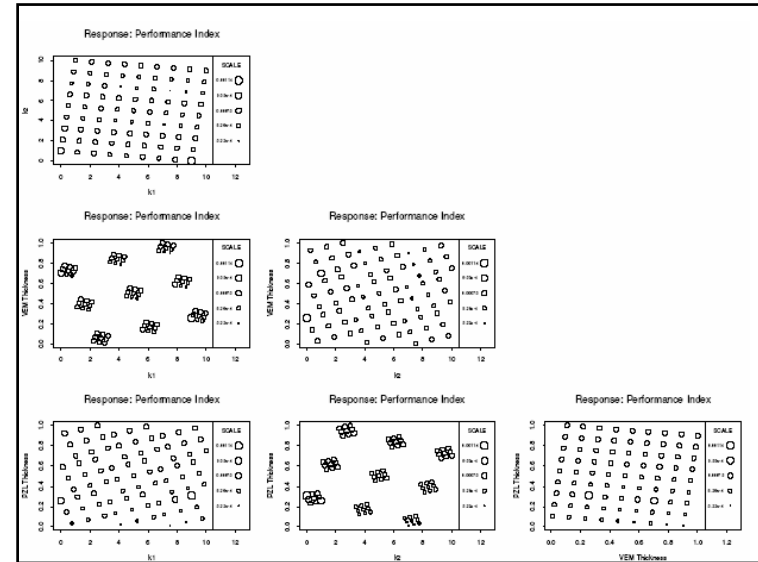
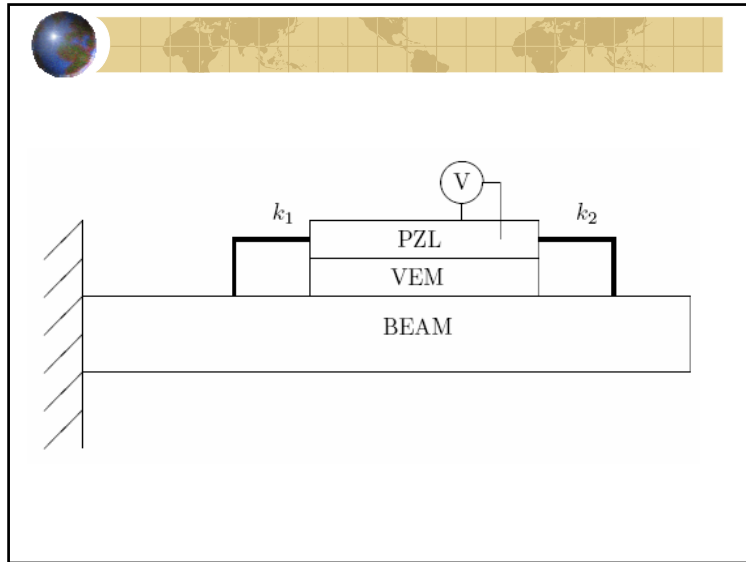


Table 2 Significant EACL effects identified via stepwise regression

Source	df	Sequential		Partial	
		MS	p-value	t	p-value
PZL thickness	1	2.516819×10^{-7}	0.00000000	-3.0592	0.0031
k2 stiffness (linear)	1	1.388989×10^{-7}	0.00000139	-5.3621	0.0000
VEM thickness	1	1.529360×10^{-8}	0.08520369	-3.8873	0.0002
k2 stiffness (quadratic)	1	1.111523×10^{-7}	0.00001177	4.2680	0.0001
VEM thickness / PZL thickness	1	5.576510×10^{-8}	0.00135561	3.3987	0.0011
k2 stiffness (L) / PZL thickness	1	1.867760×10^{-8}	0.05770075	3.5085	0.0008
k2 stiffness (Q) / PZL thickness	1	4.963070×10^{-8}	0.00241421	-3.1434	0.0024
Residuals	73	5.022800×10^{-9}			

Residual standard error: 7.087×10^{-5} on 73 degrees of freedom
Multiple R-Squared: 0.6362

- ### Some Comments
- Computer experiments are gaining in popularity
 - main research area of the next 10 years
 - Rotated factorial designs
 - good factorial design properties
 - (orthogonality and structure)
 - good Latin hypercube properties
 - (unique and equally-spaced projections)
 - easy to construct
 - comparable by Bayesian criteria
 - very suitable for computer experiments
 - Extensions
 - Type U and Type E designs
 - extension to sizes other than p^2
 - higher dimensional extension promising



Uniform Designs

Fang, Lin, Winker & Yang
 (*Technometrics*, 1999)
 Fang and Lin
 (Handbook of Statistics, Vol 22, 2003)



Uniform Design

A uniform design provides uniformly scatter design points in the experimental domain.

<http://www.math.hkbu.edu.hk/UniformDesign>



Uniform Design

$\hat{F}_n(x)$ = **Empirical** Cumulative Distribution Function

$F(x)$ = Uniform Cumulative Distribution Function

Find $x = (x_1, x_2, \dots, x_n)$

such that $\hat{F}_n(x)$ is closest to $F(x)$.

Discrepancy

$$D = \left[\int_{\Omega} \|\hat{F}_n(x) - F(x)\|^p dx \right]^{1/p}$$

● Wang & Fang (1980)



The centered L_p -discrepancy is invariant under exchanging coordinates from x to $1-x$. Especially, the centered L_2 -discrepancy, denoted by CL_2 , has the following computation formula:

$$(CL_2(P))^2$$

$$= \binom{13}{12}^s - \frac{2}{n} \sum_{k=1}^n \prod_{i=1}^s \left(1 + \frac{1}{2} |x_{ki} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - \frac{1}{2}|^2 \right) + \frac{1}{n^2} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^s \left[1 + \frac{1}{2} |x_{ki} - \frac{1}{2}| + \frac{1}{2} |x_{ji} - \frac{1}{2}| - \frac{1}{2} |x_{ki} - x_{ji}| \right]$$

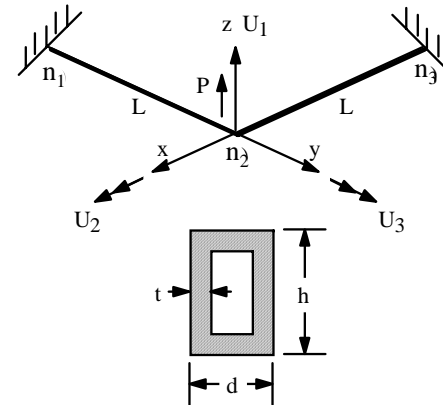


Sampling Strategies for Computer Experiments: Design and Analysis

Simpson, T.W., Lin, D.K.J., and Chen,
W. (2001)



Two-Member Frame Example



$2.5 \text{ in.} \leq d \leq 10 \text{ in.}$
 $2.5 \text{ in.} \leq h \leq 10 \text{ in.}$
 $0.1 \text{ in.} \leq t \leq 1.0 \text{ in.}$



- DOE 5 experimental design type
(i.e., hss, lhd, rnd, oay, rnd, uni)
- APPROX 4 approximation model type
(i.e., krg, mar, rbf, rs2)
- SAMP 6 number of sample points in an
experimental design (9,16,25,32,49,64)
- FCN 3 response functions
- A total of $5 \times 4 \times 6 \times 3 = 360$ cases



- MAX maximum absolute error
- RMSE root mean square error

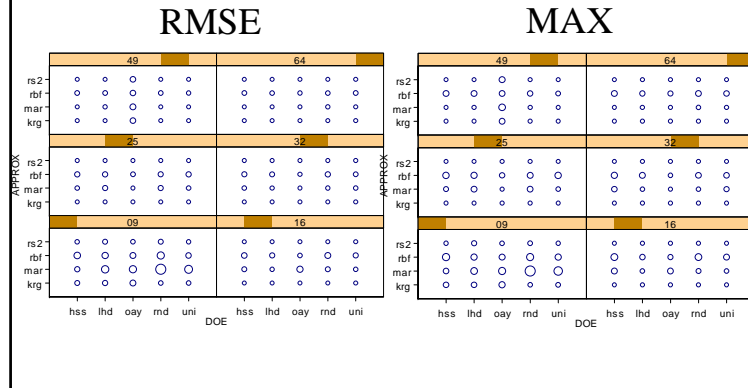
$$\text{MAX} = \max \{ |y_i - \hat{y}_i| \}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n_{\text{error}}} (y_i - \hat{y}_i)^2}{n_{\text{error}}}}$$



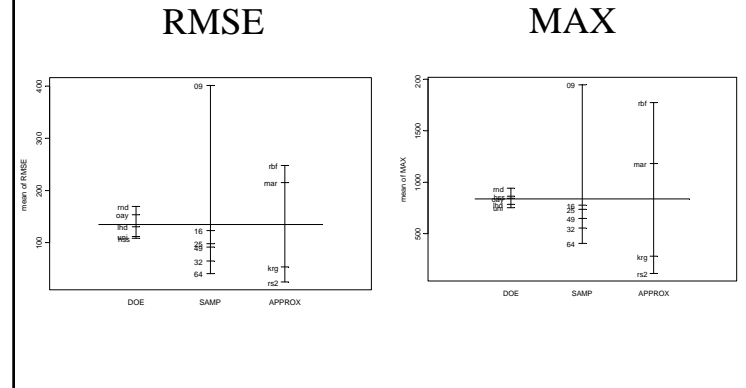
Effects of DOE, APPROX, and SAMP

Response-1



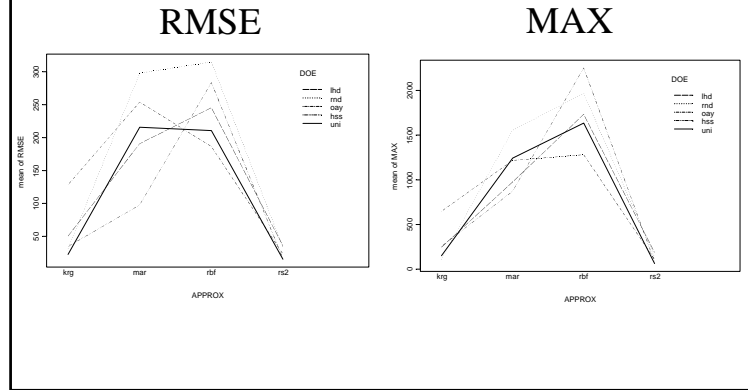
Individual Factor Contributions

Response-1



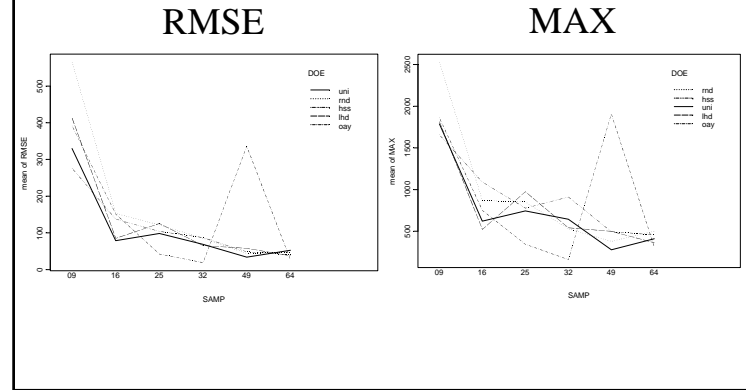
Interaction of DOE and APPROX

Response-1



Interaction of DOE and SAMP

Response-1

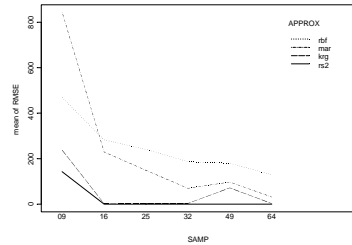




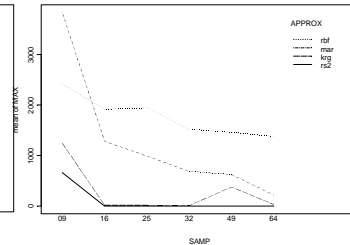
Interaction of SAMP and APPROX

Response-1

RMSE

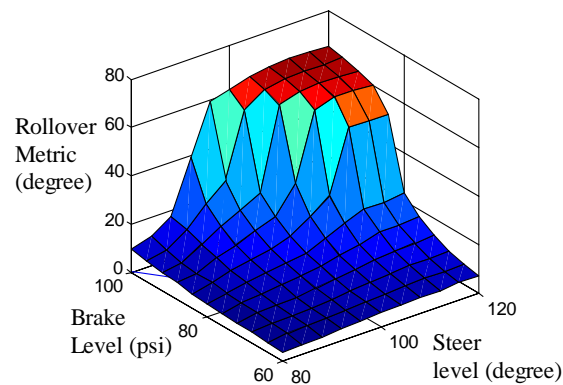


MAX



ArcSim Variables and Ranges of Interest (k=14)

Design Variable	Description	Lower Bound	Upper Bound
HH1	Height of Hitch above ground	51.2 in	76.8 in
KHX1	Hitch roll torsional stiffness	8e5 in-lb/deg	1.2e6 in-lb/deg
LTS11	Distance between springs on Axle 1	30.4 in	45.6 in
LTS123	Distance between springs on Axles 2 & 3	30.4 in	45.6 in
LTS2123	Distance between springs on Axles 4,5 & 6	30.4 in	45.6 in
M11	Laden load for Axle 1	11540 lbn	17310 lbn
M2123	Laden load for Axles 4, 5 and 6	16274.4 lbn	24411.6 lbn
KT2123	Axles 4, 5 & 6 tire stiffness	4139.20 lb/in	6208.80 lb/in
SCFS11	Axle 1 spring stiffness scale factor	0.8	1.2
Noise Variables	Description	Lower Bound	Upper Bound
brake_start	Time at which braking is applied	1.02 sec	1.38 sec
brake_level	Level of braking that is applied	70 psi	100 psi
brake_end	Time after which braking is no longer applied	1.53 sec	2.07sec
steer_level	Level of steering that is applied	60 deg	100 deg
steer_end	Time after which steering is no longer applied	2.16 sec	3.24 sec



- Experimental Design (DOE): 5 types
Hammersley sequence (hss), Latin hypercube design (lhd), orthogonal array (oay), random set of points (rnd), uniform design (uni)
- Sample size (SAMP): 4 sizes – 128, 169, 256, 361
- Approximation Model (APPROX): 4 types
kriging model (krg), radial basis function (rbf), second-order response surface (rs2), multivariate adaptive regression splines (mar)
- Function (FCN): 1 type – roll-over metric



Some Observations

- uniform designs and Hammersley sampling sequences tend to yield more accurate approximations
- uniform designs tend to perform well at low sample sizes while the Hammersley sampling sequences tend to fair better when large sample sizes
- both offer improvements over standard Latin hypercube designs and random sets of points



More Observations

- kriging (krig) and radial basis function (rbf) tend to offer more accurate approximations.
- the multivariate adaptive regression splines (mar) is the least stable.
- second-order response surfaces yield average results and also perform well, particularly well when approximating the low-order non-linearity.
- larger sizes generally improve the accuracy



Orthogonal Latin Hypercube Designs

Steinberg and Lin (*Biometrika*, 2006)

If time permits!!!



Send \$500 to

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