Recent Advances in Computer Experiment

Dennis Lin
University Distinguished Professor
The Pennsylvania State University

University of Wisconsin-Madison
03 June, 2010

Happy 50th Birthday!!!

- What type of Jobs?
- *Agriculture*
- *Industry (Manufacturing)*
- *Service Industry*
- *Informatics*
- What's Next?

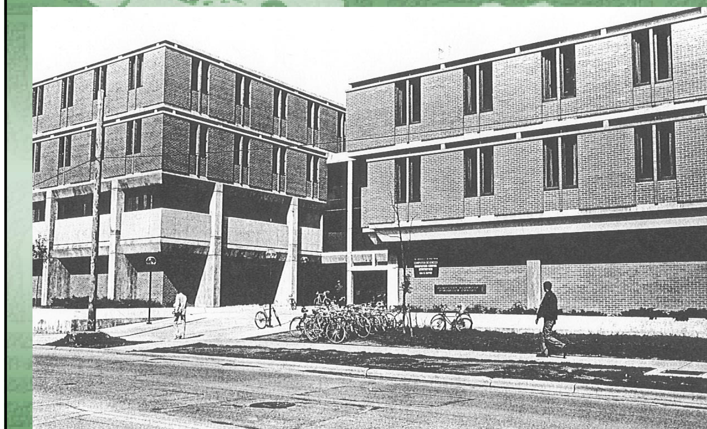
- What type of Designs?
- Treatment/BIBD …
- RSM, Factorials, OA Robust Design, …
- Design for Six Sigma etc
- Computer Experiment

UW-Madison

UW Department of Statistics Location

- 1960 Johnson Street (Zoology Building)
  Moving away from Van Vleck Hall (Math)
- then 710 University Avenue
- then 910 University Avenue
- 1967 1210 West Dayton Street
  - Unit-1 Sta Railroad
  - Unit-2 Computer Science
- 1987 Unit-3 Built
- 2003 1300 University Avenue
  (Medical Science Building)

1210 West Dayton Street



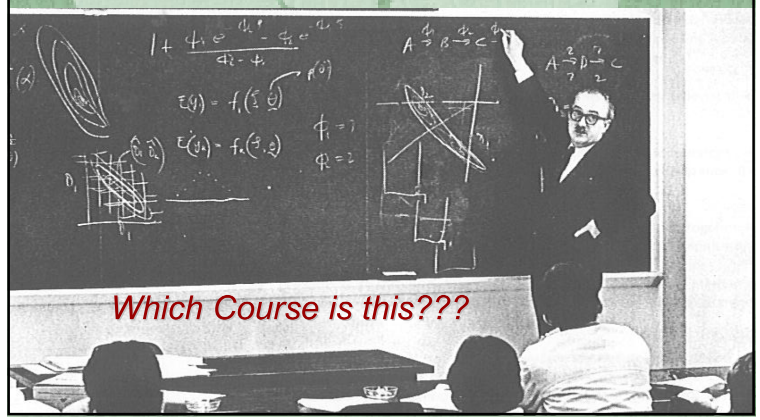
1210 W. Dayton Street Unit-3

Department of Statistics, UW-Madison, Medical Science Center, 1300 University Ave., Madison, WI 53706

UW-Madison Faculty in 1972

George E.P. Box

George Box in Classroom (1970s)



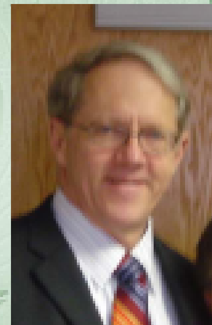
Which Course is this???

UW-Madison Faculty in 1972

Norman R. Draper

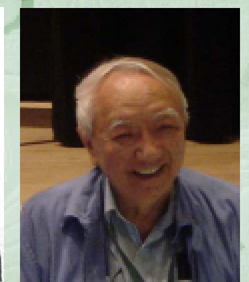
Draper's Major Contribution in Statistics

UW-Madison Faculty in 1972



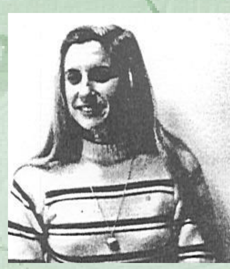
Stephen Stigler

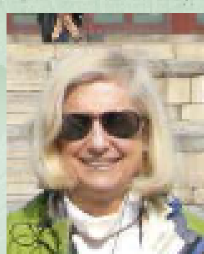
UW-Madison Faculty in 1972



George C. Tiao

UW-Madison Faculty (Others)





Grace Wahba

Dick Johnson: Now (Observed) and Not too long ago (Simulation)

Coming to USA!!!

Dennis Lin in 1984
(1984—1988 @ Madison)

I am not an USA President,

but
I was a "C" student all right!!!

Dream Team: Courses Taken

- 709/710 Math Stat
- 731 Probability
- 998 Stat Consulting
- 701/702 Time Series
- 840 Time Series
- 749 Response Surface
- 611 Sampling
- 824 Design/Nonlin
- 826 Reliability
- 775 Bayesian
- 803 Design Theory
- 992 Quality Improvement

- Dennis Cox
- B. Harris
- R. Nordheim
- G. Reinsel
- G. Wahba
- NR Draper
- Kam Tsui
- D. Bates
- G. Bhattacharya
- T. Leonard
- Jeff Wu
- GEP Box

Something Special by then (1984-1988)

- Monday Night Box's Beer and Seminar
- Christmas Party at Box's House

All Chinese Look Alike

All Chinese Look Alike? Why?

- (US) criteria for people classification (as used in the driver license):
  - Height — *Short*
  - Weight — *Light*
  - Hair Color — *Black*
  - Eye Color — *Black*

You must study under the "correct" (right statistics/subject/variable/model).

Computer Experiment

What is Computer Simulation?

What for?

And How?

What to Simulate???

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

You Could

Simulate y

Simulate f

Simulate x

Simulate θ

Simulate ε

What to Simulate??? More

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

You could also

- Simulate $y\,|x$, $x\,|y$, …
- *Simulate* $\theta\,|x$, …
- Simulate $\{u_1, u_2, \ldots, u_m\}$
  - Take them all,
  - or use reject-accept strategy;
- Simulate $u_t|u_{t-1}$, … etc

All simulations look alike

Did you use the correct simulation???

How Should the Data be collected/simulated?

Randomly

or

Systematically

There is no accident!

— *Master WuGuei*

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

Statistics vs. Engineering Models

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

Statistical Model, f

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

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

$$\begin{aligned}
&\rho_b A_b \frac{\partial^2 w}{\partial t^2} + E_b I_b \frac{\partial^4 w}{\partial x^4} \\
&+\{(\rho_s A_s + \rho_c A_c)\frac{\partial^2 w}{\partial t^2} + \rho_s A_s (\frac{t_b+t_s}{2})(\frac{\partial^3 u_b}{\partial x \partial t^2} - \frac{t_b+t_s}{2}\frac{\partial^4 w}{\partial x^2 \partial t^2} + \frac{t_s}{2}\frac{\partial^3 \beta}{\partial x \partial t^2}) \\
&+\rho_c A_c a(\frac{\partial^3 u_b}{\partial x \partial t^2} - a\frac{\partial^4 w}{\partial x^2 \partial t^2} + t_s \frac{\partial^3 \beta}{\partial x \partial t^2}) + C_{11}^0 I_c \frac{\partial^4 w}{\partial x^4} - E_c A_c a(\frac{\partial^3 u_b}{\partial x^3} - a\frac{\partial^4 w}{\partial x^4} + t_s \frac{\partial^3 \beta}{\partial x^3})\}[H(x-x_1) - H(x-x_2)] \qquad (1) \\
&+\{\rho_s A_s (\frac{t_b+t_s}{2})(\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b+t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c a(\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \\
&+2C_{11}^0 I_c \frac{\partial^3 w}{\partial x^3} - 2E_c A_c a(\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})\}[\delta(x-x_1) - \delta(x-x_2)] \\
&+\{C_{11}^0 I_c \frac{\partial^2 w}{\partial x^2} - E_c A_c a(\frac{\partial u_b}{\partial x} - a\frac{\partial^2 w}{\partial x^2} - t_s \frac{\partial \beta}{\partial x}) + b d_{31} E_c a V(t)\}[\delta'(x-x_1) - \delta'(x-x_2)] = f(x,t)
\end{aligned}$$

$$\begin{aligned}
&\rho_b A_b \frac{\partial^2 u_b}{\partial t^2} - E_b A_b \frac{\partial^2 u_b}{\partial x^2} \\
&+\{\rho_s A_s(\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b+t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c(\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \qquad (2) \\
&-E_c A_c(\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})\}[H(x-x_1) - H(x-x_2)] \\
&+\{-E_c A_c(\frac{\partial u_b}{\partial x} - a\frac{\partial^2 w}{\partial x^2} + t_s \frac{\partial \beta}{\partial x}) + b d_{31} E_c V(t)\}[\delta(x-x_1) - \delta(x-x_2)] = 0
\end{aligned}$$

$$\begin{aligned}
&[\rho_s A_s \frac{t_s}{2}(\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b+t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c t_s(\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \\
&+A_s(G \circ \beta) - E_c A_c t_s(\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})][H(x-x_1) - H(x-x_2)] \qquad (3)
\end{aligned}$$

"Statistical" Simulation Research

- Random Number Generators
  - Deng and Lin (1997, 2001, 2007)
- Robustness of transformation (Sensitivity Analysis)
  - From Uniform random numbers to other distributions

Briefings & Update

- 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:
  - Deng and Lin (2007)—A Penn State Patent
  - Period= 10^{69980}.
  - Survived from all (Small & Big Crash) Tests

Many theorems to transform U(0,1) to N(0,1)

They are all correct (in principle)!

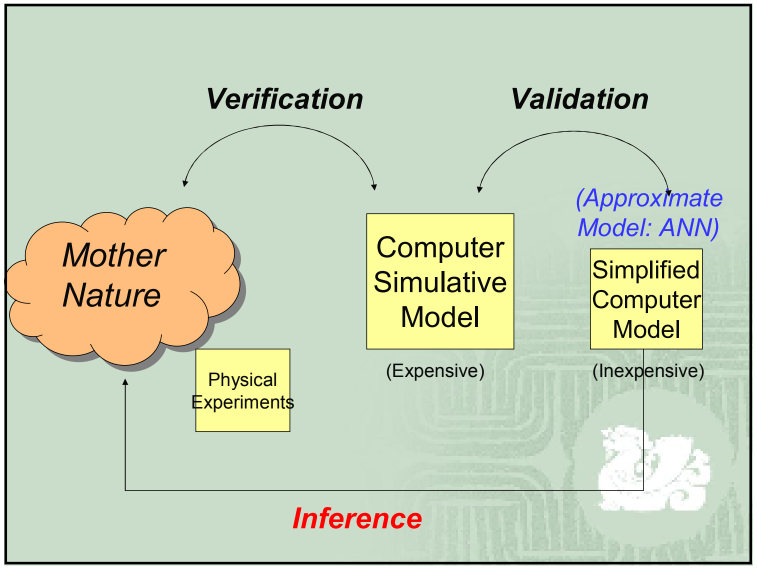
However, when the input is not a perfect U(0,1), some methods are more "robust" (insensitive/stable) than others

"Engineering" Computer Experiments

Mostly deterministic
Many input variables
Time consuming
Grid Search is not feasible

Analysis of Computer Experiments

- Complicate mean model, with relatively simple error structure
  - Polynomial model for mean model
  - $\varepsilon \sim N(0,\sigma^2)$ for error
- Simple mean model, with relatively complicated error structure
  - Gaussian Process Model
    - Intercept model for mean
    - Matern Covariance for error
- Comparisons on pros & cons: Theoretically and Empirically.



Irrelevant Issues

- Replicates
- Blocking
- Randomization

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

Lin (1997)

Space Filling Design

How to (optimally) put n points in d dimensional space?

Optimal=cover as much space as possible

Space Filling Design

- Original Problem Setup
- Uniform Design
  - Fang and Wang (1982)
  - Fang, Lin, Winker & Yang (*Technometrics*, 1999)
  - Fang and Lin (Handbook of Statistics, Vol 22, 2003)
- Latin Hypercube Design
  - McKay, Beckman & Conover (1979)
- Orthogonal Latin Hypercube
  - Beattie and Lin (1997)
  - Steinberg and Lin (2006, *Biometrika*)
  - Sun, Liu and Lin (2009, *Biometrika*)

Uniform Design

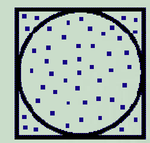
A uniform design provides uniformly scatter design points in the experimental domain.

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

How to estimate π ?

- Randomly (uniformly) drop n points into the square, suppose that there are a points fell in the circle. Then…

2r

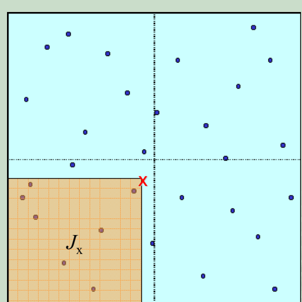


$$\frac{\pi}{4} = \frac{\pi r^2}{4r^2} = \frac{a}{n}$$

$$\pi = \frac{4a}{n}$$

Now, suppose I do know π (=3.14159…), how could I know how uniform are these points?

The Discrepancy at [0,x)



L_p-star Discrepancy

$$D_p(P) = \left[\int_{C^s} \left| \frac{|P \cap [0,\mathbf{x})|}{n} - \mathrm{Vol}([0,\mathbf{x})) \right|^p dx \right]^{1/p}$$

where

- $[0,\mathbf{x}) = [0,x_1)\times[0,x_2)\times\cdots\times[0,x_s)$;
- $|P \cap [0,\mathbf{x})|$: **the number of points of** P **falling in** $[0,\mathbf{x})$;
- $d_P([0,\mathbf{x})) = \left| \frac{|P \cap [0,\mathbf{x})|}{n} - \mathbf{Vol}([0,\mathbf{x})) \right|$ is called the discrepancy of $\mathcal{P}$ over the rectangular [0,x);

$D_p(\mathcal{P})$ is called the L_p -star discrepancy of the set $\mathcal{P}$.

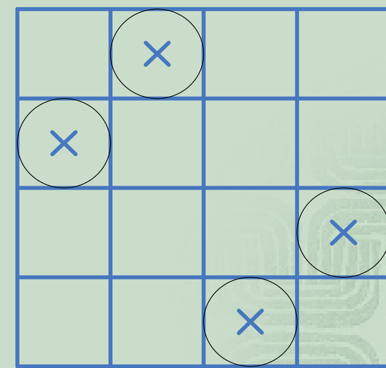
Uniform Design: Summary

- Uniformity
- Model Robustness
- Flexibility in experimental runs
- Flexibility in the number of levels

References

- Fang and Lin (2003)
  Handbook of Statistics, Statistics in Industry (Vol.22).
- Fang, Lin, Winker and Zhang
  (Technometrics, 2000)
- Website
  www.math.hkbu.edu.hk/UniformDesign

What is a Latin Hypercube?



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

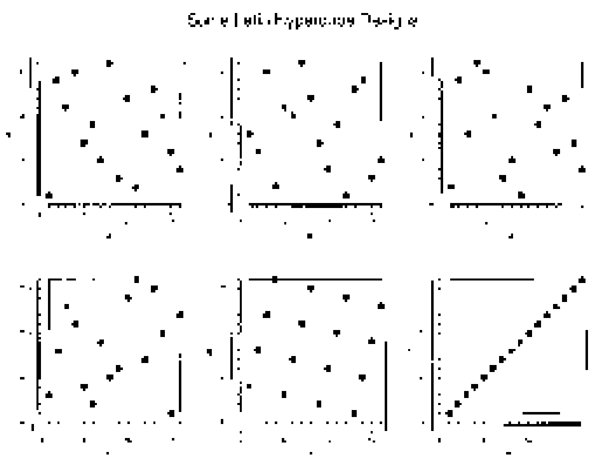
$$\begin{array}{cc} x_1 & x_2 \end{array}$$
$$\begin{bmatrix} 1 & \tau_1 \\ 2 & \tau_2 \\ 3 & \tau_3 \\ 4 & \tau_4 \\ . & . \\ . & . \\ . & . \\ 16 & \tau_{16} \end{bmatrix}$$

τ_i: permutation of $\{1, \ldots, 16\}$

16!

n! for size n &

$(n!)^{d-1}$ for d-dim



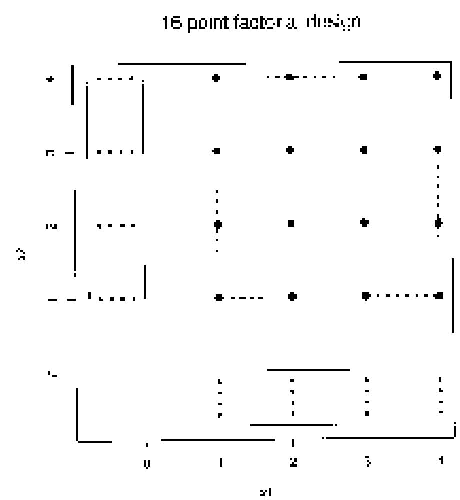
Bayesian Designs

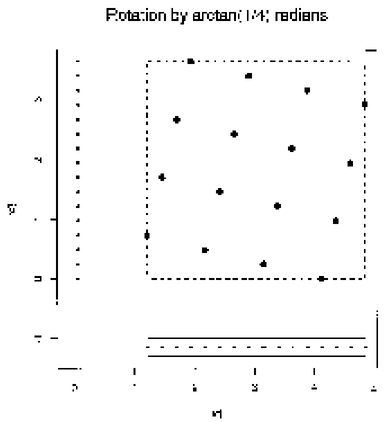
- Maximin Distance Designs, Johnson, Moore,and Ylvisaker (1990)
- Maximizes the Minimum Interpoint Distance (MID)
- Moves design points as far apart as possible in design space $MID = \min_{x_1, x_2 \in D} d(x_1, x_2)$
- D* is a Maximin Distance Design if

$$MID = \min_{x_1, x_2 \in D^*} d(x_1, x_2) = \max_{D} \min_{x_1, x_2 \in D} d(x_1, x_2)$$

Rotated Factorial Designs

Beattie and Lin (1997)





- Rotation Theorem
- Orthogonality Theorem

Theorem 1

Rotation Theorem *For nontrivial rotations between 0 and 45 degrees, a rotated standard p^2 factorial design will produce equally-spaced projections to each dimension if and only if the rotation angle is* $\tan^{-1}(1/k)$ *where* $k \in \{1,\ldots,p\}$. *These equally-spaced projections will be unique if and only if the rotation angle is* $\tan^{-1}(1/p)$.

Theorem 2

Orthogonality Theorem *Any rotated standard factorial design, regardless of the rotation angle, has uncorrelated regression effect estimates (that is, orthogonal design matrix columns).*

Orthogonal Latin Hypercube Designs

$$D = X \cdot V$$

desirable design

factorial design

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

rotated matrix

$$\begin{bmatrix} \upsilon_1 & \upsilon_3 \\ \upsilon_2 & \upsilon_4 \end{bmatrix}_{d \times d}$$

Beattie & Lin (1998): Rotating Full Factorials

$$D = X \cdot V$$

desirable design

Two-level fractional factorial design

rotated matrix

$$\begin{bmatrix} S_1 & & & & & \\ & S_2 & & & & \\ & & \ddots & & & \\ & & & S_i & & \\ & & & & \ddots & \\ & & & & & S_m \end{bmatrix}_{n \times n}$$

Bursztyn & Steinberg (2002): Rotating in Groups

Now,
Put these two ideas together!

- Grouping all design columns into groups,
- each forms a full factorial design,
- then rotate each group (in block).

LHD's as Rotated Factorial Designs

Steinberg and Lin:

$$DR = [D_1 | \cdots | D_t] \begin{bmatrix} R & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & R \end{bmatrix}$$

Bursztyn & Steinberg

$$= [D_1 R | \cdots | D_t R]$$

Lin & Beattie

The resulting design is an orthogonal Latin hypercube.

Grouping Example (16 runs)

- Full (2^4=16) Factorial Design
  - Basic factors: *a, b, c, d*
- Fractional Factorial
  - Basic Factors: *a, b, c, d*
  - Generators:
    ab, ac, ad, bc, bd, cd, abc, abd, acd, bcd, abcd
- Grouping into three: each form a full factorial
  - (*a,b,c,d*),
  - (*ab,ac,ad,abcd*), and
  - (*abc, abd, acd, bcd*)

Steinberg & Lin (2006, *Biometrika*)

Table 1: *Example 1. An orthogonal Latin hypercube design for 12 input factors in 16 runs. The numbers in the table should be divided by 15 to scale the design to the unit hypercube*

1	2	3	4	5	6	7	8	9	10	11	12
−15	5	9	−3	7	11	−11	7	−9	3	−15	5
−13	1	1	13	−7	−11	11	−7	−1	−13	−13	1
−11	7	−7	−11	13	−1	−1	−13	9	−3	15	−5
−9	3	−15	5	−13	1	1	13	1	13	13	−1
−7	−11	11	−7	11	−7	7	11	5	15	−3	−9
−5	−15	3	9	−11	7	−7	−11	13	−1	−1	−13
−3	−9	−5	−15	1	13	13	−1	−5	−15	3	9
−1	−13	−13	1	−1	−13	−13	1	−13	1	1	13
1	13	13	−1	−9	3	−15	5	11	−7	7	11
3	9	5	15	9	−3	15	−5	3	9	5	15
5	15	−3	−9	−3	−9	−5	−15	−11	7	−7	−11
7	11	−11	7	3	9	5	15	−3	−9	−5	−15
9	−3	15	−5	−5	−15	3	9	−7	−11	11	−7
11	−7	7	11	5	15	−3	−9	−15	5	9	−3
13	−1	−1	−13	−15	5	9	−3	7	11	−11	7
15	−5	−9	3	15	−5	−9	3	15	−5	−9	3

Steinberg and Lin (2006, *Biometrika*)

Biometrika (2006), 93, 2, *pp.* 279–288

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A construction method for orthogonal Latin hypercube designs

By DAVID M. STEINBERG
Department of Statistics and Operations Research, Tel-Aviv University, Tel-Aviv 69978, Israel
dms@post.tau.ac.il

AND DENNIS K. J. LIN
Department of Supply Chain & Information Systems, The Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.
dkl5@psu.edu

Pang, Liu and Lin (*Statistica Sinica*, 2009)

[illegible]

Ye (1998, JASA)

Table 1. A 5 × 2 Orthogonal Latin Hypercube

1	−2
2	1
0	0
−1	2
−2	−1

Table 2. A 9 × 4 Orthogonal Latin Hypercube

1	−2	4	3
2	1	3	−4
3	−4	−2	−1
4	3	−1	2
0	0	0	0
−4	−3	1	−2
−3	4	2	1
−2	−1	−3	4
−1	2	−4	−3

Second-Order Orthogonality

(a) All main effects are orthogonal, and

(b) All main effects are orthogonal to all quadratic & two factor interactions.

Biometrika (2009), 96, 4, pp. [illegible]
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Miscellanea

Construction of orthogonal Latin hypercube designs

BY FASHENG SUN, MIN-QIAN LIU
The Key Laboratory of Pure Mathematics and Combinatorics, School of Mathematical Sciences, Nankai University, Tianjin 300071, China
sfasfs2008@mail.nankai.edu.cn mqliu@nankai.edu.cn

AND DENNIS K. J. LIN
Department of Statistics, The Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.
dkl5@psu.edu

Second-Order Orthogonality

Sun, Liu & Lin (2009, Biometrika)

THEOREM 1. (i) *The T_c in* (2) *consists of rows and columns of permutations of the 2^c elements $1, \ldots, 2^c$, up to sign changes.*

(ii) *The L_c in* (3) *is a Latin hypercube design $L(2^{c+1}+1, 2^c)$ with properties* (a) *and* (b).

(a) each column is orthogonal to the others in the design;

(b) the elementwise square of each column and the elementwise product of every two columns are orthogonal to all columns in the design.

THEOREM 3. *If $L(n,k) = (l_{ij})$ is a centered Latin hypercube design with properties* (a) *and* (b), *then $k \le \lfloor n/2 \rfloor$, where $\lfloor x \rfloor$ is the integer part of x.*

Orthogonal Latin Hypercube ($n=2^c+1$ or 2^c)

Design	Ye (1998) *JASA*	C&L (2007) *Technometrics*	S&L (2006) *Biometrika*	PLL (2009) *Sinica*	SLL (2009) *Biometrika*
No. of Factor	2(c-1)	c(c-1)/2+1	c[(n-1)/c]	c[(n-1)/c/(q-1)]	2^{c-1}
c=4 c=8 c large	6 14	7 29	12 -	12 -	8 256
Main Orthog	Yes	Yes	Yes	Yes	Yes
Second-Order Othog	**Yes**	yes	No	No	**Yes**

Relaxing Run Size Restriction

$2^c \rightarrow r\, 2^{c-1}$

Second-Order orthogonal Latin Hypercube designs with flexible run sizes

Sun, Liu and Lin (JSPI, 2010)

Beyond Orthogonal Latin Hypercube

Near-Orthogonal Latin Hypercube

&

Orthogonal near-Latin Hypercube

(Nguyen, Steinberg and Lin, 2010)

After all, simulation means "not real"

Good for "description,"

But

Not necessary good for a solid proof!

There are many types of simulations, they must be used with care!

What is real?

Motherhood in Animal Kingdom

&

Yoga and Drinking

What Am I Doing These Days???

STATISTICS DEPARTMENT COLLOQUIUM

MONDAY, APRIL 6, 2009
Talk: 4:00 PM – *Science Center 309*
Reception: 5:15 PM – Science Center, 7th Floor

"BIG Statistics"

Dennis K. J. Lin
Department of Supply Chain and Information Systems
The Pennsylvania State University

Looking Ahead:

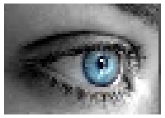
Design and Analysis

Future Design & Analysis

Number
Text
Image
Voice
Film
Web data: Facebook. Google
Video (YouTube)
etc

All-In-One Data

I Love UW-Statistics



UNIVERSITY OF WISCONSIN
Statistics

Dennis Lin

STILL QUESTION?

Send $500 to

- Dennis Lin
  University Distinguished Professor
  317 Thomas Building
  Department of Statistics
  Penn State University

- +1 814 865-0377 (phone)
- +1 814 863-7114 (fax)
- DKL5@psu.edu

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