## Youden Square to George Box to Latin Hypercube: <br> The Evolution of Experimental Design

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tecuber 6-9, 20010




## The Evolution of Science

Observational Science
Scientist gathers data by direct observation Scientist analyzes data
Analytical Science
$)_{2}$ Scientist builds analytical model
a Makes predictions

- Computational Science $\propto$ Simulate analytical model $\propto$ Q Validate model and makes predictions
- Data Exploration Science Data-driven science
Data captured by instruments or data generated by simulation
c Processed by software
© Placed in a database / files
Scientist(s) analyze(s) database / files Access crucial



## Statistics based upon data

EDA: Exploratory Data Analysis (Tukey)

- Learning from Data
- What can the data tell you?
- Show me your problems?
- Show me your data?
- Tell me how were the data collected?



## Likelihood Principle

- Full Likelihood
- Partial Likelihood
- Empirical Likelihood
- Pseudo Likelihood
- Quasi Likelihood
- Penalized Likelihood
- Posterior Likelihood
- Composite Likelihood
- Profile Likelihood



## Design of Experiment-I

- Treatment Comparison
- Complete Randomized Block Design
- Greco-Latin Square
- Youden Square
- Balanced Incomplete Block Design
- Split-Plot Design
- Nested Designs

Row-Column Design
etc


## Design of Experiment-II

- Response Surface Design ${ }_{a}$ Central Composite Design $\cdots$ Box-Behenken Design
- Robust Design
- Fractional Factorial Design
- Orthogonal Arrays
- Supersaturated Design

Design for Six-Sigma

- Multi-Stage Design

- What type of Jobs?
- What type of Designs?
- Agricultu: (ivuderia
- BIBD/Split/Treatment ..
- Industry
- RSM, Factorials, OA Robust Design,
- Design for Six Sigma etc
- Computer Experiment


## Classroom vs. Reality

Classroom
as Theoretical
${ }_{3}$ Pure Knowledge
a Orderly
${ }_{c}$ Pristine
${ }_{2}$ Controlled
${ }_{3}$ General
${ }^{2}$ Covering Laws
${ }_{2}$ Predictions
Certain

## Reality

${ }_{2}$ Practical
© Applied to problems
${ }_{2}$ Disorderly ${ }_{\infty}$ Contaminated
${ }_{\infty}$ Chaotic
©Specific
approximations ${ }^{2}$ Conjectures ${ }_{2}$ Uncertain

```
Will Computer Model be another version of Ivory Tower?
```

| Latin Square |  |  |  |
| :--- | :--- | :---: | :---: |
| $\qquad$$\alpha$ $\beta$ $\gamma$ $\delta$ <br> $\gamma$ $\delta$ $\alpha$ $\beta$ <br> $\delta$ $\gamma$ $\beta$ $\alpha$ <br> $\beta$ $\alpha$ $\delta$ $\gamma$ |  |  |  |

## Greco-Latin Square

| $A$ | $B$ | $C$ | $D$ |
| :--- | :--- | :--- | :--- |
| C | D | A | B |
| D | C | $B$ | $A$ |
| $B$ | $A$ | $D$ | $C$ |


| 1 | 2 | 3 | 4 |
| :--- | :--- | :--- | :--- |
| 4 | 3 | 2 | 1 |
| 2 | 1 | 4 | 3 |
| 3 | 4 | 1 | 2 |


| $1 A$ | $2 B$ | $3 C$ | $4 D$ |
| :--- | :--- | :--- | :--- |
| $4 C$ | $3 D$ | $2 A$ | $1 B$ |
| $2 D$ | $1 C$ | $4 B$ | $3 A$ |
| $3 B$ | $4 A$ | $1 D$ | $2 C$ |

## A $4 \times 4$ Greco-Latin Square

## Latin Square \& Youden Square

(doubly balanced incompleted block design)

| $\checkmark$ A | $\pm \mathrm{K}$ | $\div$ Q | + J |
| :---: | :---: | :---: | :---: |
| $\bigcirc \mathrm{J}$ | - Q | - K | $\pm$ A |
| - K | $\div$ A | $\pm$ J | - Q |
| Q | $\bullet J$ | - A | $\therefore \mathrm{K}$ |

## BIBD with

The number of block
is equal to
The number of treatment


## Sudoku

| 9 |  |  | 1 |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  | 5 |  | 9 |  | 2 |  |
| 8 |  |  | 4 |  |  |  |  |
|  |  |  |  | 8 |  |  |  |
|  |  |  | 7 |  |  |  |  |
|  |  |  |  | 2 | 6 |  |  |
| 2 |  | 3 |  |  |  |  |  |
|  |  |  | 2 |  |  | 9 |  |
|  |  | 1 | 9 |  | 4 | 5 | 7 |



## What to Simulate??? More

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

You could also
Simulate $y|x, x| y, \ldots$
Simulate $\theta \mid x, \ldots$
Simulate $\left\{u_{1}, u_{2}, \ldots, u_{m}\right\}$
Did you use the correct simulation???


$$
\begin{aligned}
& \text { A Typical Engineering Model } f \text { (page } 1 \text { of } 3 \text {, in Liao and Wang, 1995) }
\end{aligned}
$$

$$
\begin{aligned}
& \rho_{0} x_{1} \frac{\partial^{2} v_{y_{1}}}{\alpha^{2}}-\varepsilon_{1} \alpha_{1} \frac{\partial^{2} v_{v_{1}}}{\frac{x^{2}}{2}}
\end{aligned}
$$

## "Statistical" Simulation Research

- Random Number Generators

๙Deng and Lin $(1997,2001,2007)$

- Robustness of transformation
(Sensitivity Analysis)
${ }_{c}$ From Uniform random numbers to other distributions



## Analysis of Computer Experiments

- Complicate mean model, with relatively simple error structure
caPolynomial model for mean model $\propto \varepsilon \sim N\left(0, \sigma^{2}\right)$ for error
- Simple mean model, with relatively complicated error structure
caGaussian 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?


## How to estimate $\pi$ ?

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

$$
2 r \quad \begin{array}{cc}
\because \because & \frac{\pi}{4}=\frac{\pi r^{2}}{4 r^{2}}=\frac{a}{n} \\
\because \because & \pi=\frac{4 a}{n}
\end{array}
$$

Now, suppose I do know $\pi$ ( $=3.14159 \ldots$ ), how could I know how uniform are these points?

## 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?



- $[0, \mathrm{x})=\left[0, x_{1}\right) \times\left[0, x_{2}\right) \times \cdots \times\left[0, x_{s}\right)$;
- $P \cap[0, \mathbf{x}) \mid$ the number of points of $P$ falling in $[0, \mathbf{x})$;
- $d_{P}([0, \mathbf{x}))=\left|\frac{|P \cap[0, \mathbf{x})|}{n}-\operatorname{Vol}([0, \mathbf{x}))\right|$ is called the discrepancy of $P$ over the rectangular $[0, x)$;
$D_{p}(P)$ is called the $L_{p}$-star discrepancy of the set $P$.


## 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 $M I D=\min _{x_{1}, x_{2} \in D} d\left(x_{1}, x_{2}\right)$
- $\mathrm{D}^{*}$ is a Maximin Distance Design if

$$
M I D=\min _{x_{1}, x_{2} \in D^{*}} d\left(x_{1}, x_{2}\right)=\max _{D} \min _{x_{1}, x_{2} \in D} d\left(x_{1}, x_{2}\right)
$$



## Theorem 1

Rotation Theorem For nontrivial rotations between 0 and 45 degrees, a rotated standardp ${ }^{2}$ 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

$$
D=X \cdot V
$$ factorial design

$\left[\begin{array}{ll}1 & 1 \\ 2\end{array}\right]$
desirable
design

## rotated matrix

$\left[\begin{array}{ll}v_{1} & v_{3} \\ v_{2} & v_{4}\end{array}\right]_{d \times d}$


## LHD's as Rotated Factorial Designs

Steinberg and Lin:

$$
\begin{aligned}
D R & =\left[D_{1}|\cdots| D_{t}\right]\left[\begin{array}{ccc}
R & 0 & 0 \\
0 & \ddots & 0 \\
0 & 0 & R
\end{array}\right] \\
& =\left[D_{1} R|\cdots| D_{t} R\right]
\end{aligned}
$$

Bursztyn \& Steinberg Lin \& Beattie

## Grouping Example (16 runs)

- Full $\left(2^{4}=16\right)$ Factorial Design
esBasic factors: $a, b, c, d$
- Fractional Factorial
œBasic Factors: a, b, c, d
aGenerators:
$a b, a c, a d, b c, b d, c d, a b c, a b d, a c d, b c d, a b c d$
- Grouping into three: each form a full factorial
c® $(a, b, c, d)$,
«( $a b, a c, a d, a b c d)$, and
ç(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


```
M
A construction method for orthogonal Latin hypercube designs
By DAVID M. STEINBERG
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dk15@psu.edu
```

Pang, Liu and Lin (Statistica Sinica, 2009)
Statisticas Sliniea $10(2000), 1721-172 s$

A CONSTRUCTION METHOD FOR ORTHOGONAL LATIN HYPERCUBE DESIGNS WITH PRIME POWER LEVELS

Fang Pang ${ }^{1}$, Min-Qian Liu ${ }^{1}$ and Dennis K. J. Lin ${ }^{2}$
${ }^{1}$ Nankai University and ${ }^{2}$ The Pennsyluania State University
Astract Latin hypercube deeige (LHD) is poppularly ued in desgiging compute experimens. This paper explorexe how to construet LHDD with $\left.p^{4}(d=2)^{2}\right)$ rum

 attrective properties of standard fuctorial deesigss . The propposd methoo woves orthogoonal LifDs with nttractive propertios. Theseretical propertise as well as the construction algorithr are discussod, witi ar exmple or inserion

$D=X \cdot V$
desirable design
fractional factorial design
rotated matrix
$\left[\begin{array}{ll}s_{1} & \\ & s_{2}\end{array}\right.$


## Miscellanea

THEOREM 1. (i) The $T_{c}$ in (2) consists of rows and columns of permutations of the $2^{c}$ elements

Construction of orthogonal Latin hypercube designs
..., $2^{c}$, up to sign changes.
(ii) The $L_{c}$ in (3) is a Latin hypercube design $L\left(2^{c+1}+1,2^{c}\right)$ with properties (a) and (b).

By FASHENG SUN, MIN-QIAN LIU
The Key Laboratory of Pure Mathematics and Combinatorics, School of Mathematical
(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 column
are orthogonal to all columns in the design. seiences, Nankai University, Tanjin 3000n, Chin

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THEOREM 3. If $L(n, k)=\left(l_{i j}\right)$ is a centered Latin hypercube design with properties (a) and (b), then $k \leq|n / 2|$, where $\lfloor x \mid$ is the integer part of $x$

Orthogonal Latin Hypercube ( $\mathrm{n}=2^{\mathrm{c}}+1$ or $2^{\mathrm{c}}$ )

| Design | Ye (1998) JASA | C\&L <br> (2007) <br> Technometrics | S\&L <br> (2006) <br> Biometrika | PLL (2009) Sinica | SLL <br> (2009) <br> Biometrika |
| :---: | :---: | :---: | :---: | :---: | :---: |
| No. of Factor | 2(c-1) | $\mathrm{c}(\mathrm{c}-1) / 2+1$ | $c[(n-1) / c]$ | $c[(n-1) / \mathrm{c} /(\mathrm{q}-1)]$ | $2^{\text {c-1 }}$ |
| $\mathrm{c}=4$ | 6 | 7 | 12 | 12 | 8 |
| $\begin{aligned} & \text { c=8 } \\ & \text { c large } \end{aligned}$ | 14 | 29 | - | - | 256 |
| Main Orthog | Yes | Yes | Yes | Yes | Yes |
| SecondOrder Othog | Yes | yes | No | No | Yes |

## Sun, Liu and Lin (2009, Biometrika)

(1) Let $M_{1}=\left(\begin{array}{ll}1 & 2 \\ 2 & 1\end{array}\right), \quad S_{1}=\left(\begin{array}{rr}1 & 1 \\ 1 & -1\end{array}\right)$
(2) Let $M_{c}=\left(\begin{array}{cc}M_{c-1} & M_{c-1}+2^{c-1} J_{2^{c-1}} \\ M_{c-1}+2^{c-1} J_{2^{c-1}} & M_{c-1}\end{array}\right)$,
$S_{c}=\left(\begin{array}{cc}S_{c-1} & -S_{c-1}^{*} \\ S_{c-1} & S_{c-1}^{*}\end{array}\right)$
$M_{2}=\left(\begin{array}{ll|ll}1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \\ \hline 3 & 4 & 1 & 2 \\ 4 & 3 & 2 & 1\end{array}\right), \quad S_{2}=\left(\begin{array}{rr|rr}1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ \hline 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1\end{array}\right)$

Sun, Liu and Lin (2009, Biometrika)
(3) Let $T_{c}=M_{c} \odot S_{c}$, i.e., $\left(T_{c}\right)_{i j}=\left(M_{c}\right)_{i j} \cdot\left(S_{c}\right)_{i j}$.

$$
T_{2}=M_{2} \odot S_{2}=\left(\begin{array}{rrrr}
1 & 2 & 3 & 4 \\
2 & -1 & -4 & 3 \\
3 & 4 & -1 & -2 \\
4 & -3 & 2 & -1
\end{array}\right)
$$

(0. $L_{c}=\left(\begin{array}{c}T_{c} \\ 0_{2^{c}}^{\prime} \\ -T_{c}\end{array}\right)$ is an OLHD with $n=2^{c+1}+1$ runs and $m=2^{c}$
factors.

$$
L_{2}=\left(\begin{array}{c}
T_{2} \\
0_{4}^{\prime} \\
-T_{2}
\end{array}\right) \text { is an OLHD with } n=9 \text { runs and } m=4 \text { factors. }
$$

$$
\begin{gathered}
M_{2}=\left(\begin{array}{ll|ll}
1 & 2 & 3 & 4 \\
2 & 1 & 4 & 3 \\
\hline 3 & 4 & 1 & 2 \\
4 & 3 & 2 & 1
\end{array}\right), \quad S_{2}=\left(\begin{array}{rr|rr}
1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
\hline 1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1
\end{array}\right) \\
T_{2}=M_{2} \odot S_{2}=\left(\begin{array}{rrrr}
1 & 2 & 3 & 4 \\
2 & -1 & -4 & 3 \\
3 & 4 & -1 & -2 \\
4 & -3 & 2 & -1
\end{array}\right) \quad L_{2}=\left(\begin{array}{c}
T_{2} \\
0_{4}^{\prime} \\
-T_{2}
\end{array}\right)
\end{gathered}
$$

$n \times k$ matrix $L(n, k): n$ runs, $k$ factors, each factor includes $n$ uniformly spaced levels.

$$
L_{2}=\left(\begin{array}{c}
T_{2} \\
0_{4}^{\prime} \\
-T_{2}
\end{array}\right) \quad L(9,4)=\left(\begin{array}{rrrr}
1 & 2 & 3 & 4 \\
2 & -1 & -4 & 3 \\
3 & 4 & -1 & -2 \\
4 & -3 & 2 & -1 \\
0 & 0 & 0 & 0 \\
-1 & -2 & -3 & -4 \\
-2 & 1 & 4 & -3 \\
-3 & -4 & 1 & 2 \\
-4 & 3 & -2 & 1
\end{array}\right)
$$

## Beyond

Orthogonal Latin Hypercube

Near-Orthogonal Latin Hypercube \&

Orthogonal near-Latin Hypercube
(Nguyen, Steinberg and Lin, 2010)


Good for "description,"
But
Not necessary good for a solid proof!

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


## Future Design \& Analysis

## Number

Text


Vek deda: acebook. Google Video (YouTube)
etc




## Youden-Squear, George Box and Latin Hypercube: Conclusion

- Youden Square is not a Square cait's in fact a rectangle!
- George Box is not a box asAND he did not invent Box plot!
- Latin Hypercube is not a Latin œAlthough it is indeed a hypercube!
- New design (data collection) concept is needed for the informatic/computational age.


## What is this?




## Remembering Box (1910- )

- All Modes are wrong, some are useful.
- Statistician, like artist, has the bad habit of easily falling in love with his model.


## Remember Today (Lin)

- 1997—Rotated Full Factorials (to form a new class of Latin Hypercube)
- Orthogonal Latin Hypercube
- Second-Order Orthogonal Latin Hypercube ${ }_{\infty}$ Steinberger and Lin (Biometrika, 2006)
$\propto_{3}$ Pang, Liu and Lin (Statistica Sinica, 2009)
$\propto$ Sun, Liu and Lin (Biometrika, 2009)
- Nearly Orthogonal Latin Hypercube (for flexible run sizes)
- New design (data collection) concept is needed for the informatic/computational age.


