**Recent Advances on Computer Experiment**

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**All Chinese Look Alike? Why?**

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

You must simulate under the “correct” (right subject/model).

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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

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**Computer Experiment**

What is Computer Simulation?  
What for?  
And How?
Simulation

A device that enables the operator to reproduce under test conditions phenomena likely to occur in actual performance —Webster

Under $H_0$ is true

Computer Experiment

- Stochastic
  Deterministic

- Expensive (really expensive)
  Inexpensive (really cheap)

What to Simulate???

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

You Could
- Simulate $y$
- Simulate $f$
- Simulate $x$
- Simulate $\theta$
- Simulate $\varepsilon$
What do you mean by simulation??

- A sequence of points that follows
  - a specific desirable distribution $\pi$
    - Simple $\pi$
    - Complicated $\pi$
  - geometrical properties
    - Equal spacing (Uniform)
    - orthogonal
- Independent?
- Conditional Independent?

What to Simulate?? More

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

You could also

- Simulate $y|x$,
- Simulate $\theta|x$, ...
- Simulate $\{u_1, u_2, \ldots, u_m\}$
  - Take them all,
  - or use reject-accept strategy;
- Simulate $u_i|u_{i-1}$, ... etc

Did you use the correct simulation??

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

Statistics vs. Engineering Models
In this Talk

- Distribution Theory: Coin Example
- Distribution Theory: \( R^2 \) Story
- Distribution Theory: Significance
- Bootstrapping
- MCMC (Markov Chain Monte Carlo)
- Random Number Generation
- Orthogonal Latin Hypercube Design and more
- Uniform Design
- Strategy for Computer Experiments
- Special Topics

If time permits...

- Bootstrapping (Re-sampling)
  - Sampling from the “samples”
  - Treat “Samples” as “Population”
  - Alternatively, delete some data from the “samples”
  - Evaluate “statistic” from the current sample—obtain one value
  - Repeat this many times
  - Average these “statistics” as the estimate
- MCMC (Markov Chain Monte Carlo)
- OR-seminar by Dr. Murali Haran (Nov 2007)
Distribution Theory

Coin Example
R² Story
Significance in Regression Model

Statistical Hypothesis Testing

H₀: Null Hypothesis
vs
H₁: Alternative Hypothesis

Statistical Hypothesis Testing

Does Not Prove anything, but
Could be powerful to
Disapprove “something” (H₀)

1. Under the Null Hypothesis H₀ (typically implies the white noise), what will the test statistics behave?
   - what is “typical” and what is “abnormal”?
2. Now, compare your “observed” test statistic to the distribution in (1)
   - If it is “typical” → accept Null Hypothesis (H₀)
   - If it is “abnormal” → Reject H₀
Throw a fair coin 200 times and the results were recorded: One sequence is real and the other one is fake.

(A) 111100000000001011000001000000101001111001100011111101001001011101100111011100111100110001101110110000010001001111110100100010110010111011011100010100100110011111100011100101001011010011101011001110011100010100111

(B) 0111001001001010001001111001010001001101011100111011110110100100111010110101011010010010100111011010010000111010110110100111010110011001110011010111001110011110010100111

Potential Indexes/Statistics
- Number of Heads (1’s)
- Number of Sign Changes
- Maximal Length

Computer Simulation
- Assumption: For a fair coin (50-50)
- Do the followings
  - Toss the coin 200 times
  - From this 200 “0-1” sequence, evaluate its statistic (say, number of 1’s)
  - Now, repeat this process for 1000 times (say), and you will have 1000 statistics.
  - Put these statistics in a histogram (this is the distribution of such a statistic)
Number of 1’s in 1000 Simulations (97 vs 109)

Histogram of Success

Numbers of Change in 1000 Simulations

Max-Length in 1000 Simulations

Regression Model: JMP Demo

Significance

$R^2$
“Statistical” Simulation Research

- Random Number Generators

- Robustness of transformation
  - From Uniform random numbers to other distributions

Goodness of Random Number Generators

- Period Length
- Efficiency
- Portability
- Theoretical Justification:
  - Uniformity
  - Independence
- Empirical Performance
  - Small & Big Crash Tests

LCG: Linear Congruential Generator
Classic Random Number Generators

- \( X_t = (B \cdot X_{t-1} + A) \mod m \)
- 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
Dependence: $y_t$ vs $y_{t-1}$

Range: (0.70, 0.71)

Dependence: $y_t$ vs $y_{t-1}$

Range: (0.700, 0.701)

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

Normal Random Numbers: Examples

- Central Limit Theorem
  - $X_i \sim \text{iid } U(0,1)$ \rightarrow $Z=\Sigma X_i-6$

- Box-Muller Transformation
  - $X_i \sim \text{ind } U(0,1), \ i=1 \& 2$ \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)

Box-Muller Transformation

\[
Z_1 = \sqrt{-2 \ln x_1 \cos(2\pi x_2)} \quad Z_2 = \sqrt{-2 \ln x_1 \sin(2\pi x_2)}
\]

\[
x_1 = e^{-\frac{1}{2}}/\sqrt{\pi} \quad x_2 = \frac{1}{\sqrt{2}} \tan^{-1}\left(\frac{1}{x_1}\right)
\]

\[
\frac{\partial (x_1, x_2)}{\partial (x_1, x_2)} = \begin{bmatrix}
\frac{\partial x_1}{\partial x_1} & \frac{\partial x_1}{\partial x_2} \\
\frac{\partial x_2}{\partial x_1} & \frac{\partial x_2}{\partial x_2}
\end{bmatrix} = -\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}} \begin{bmatrix}
\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}}
\end{bmatrix}
\]

Goals—Computer Experiment

- Confirmation
- Sensitivity Analysis
- Empirical Model Building
- Optimization
- Model Validation
- High Dimension Integration

“Engineering” Computer Experiments

Mostly deterministic
Many input variables
Time consuming
Space Filling Design

How to (optimally) put n points in d dimensional space?
Optimal=cover as much space as possible

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

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))

What is a Latin Hypercube?

![Diagram of a Latin Hypercube]

A special class of LHC

\[
\begin{pmatrix}
  x_1 \\
  x_2 \\
  1 \\
  2 \\
  3 \\
  4 \\
  \vdots \\
  16
\end{pmatrix}
\]

\[\tau_i: \text{permutation of } \{1, \ldots, 16\}, \quad 16! \text{ for size } n \& \quad (n!)^{d-1} \text{ for } d\text{-dim}\]
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
  \[ \text{MID} = \min_{x_1, x_2 \in D} d(x_1, x_2) \]
- \( D^* \) is a Maximin Distance Design if
  \[ \text{MID} = \min_{x_1, x_2 \in D^*} d(x_1, x_2) = \max_{D} \min_{x_1, x_2 \in D} d(x_1, x_2) \]

Rotated Factorial Designs

- 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)
For $d = 2$

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

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

Rotation Theorem for Mixed Level Design

\[ R = \begin{bmatrix} \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{1} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} \end{bmatrix} \]

\[ R = \begin{bmatrix} \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} \\ \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{\sqrt{pq}}{\sqrt{pq}} & \frac{1}{\sqrt{pq}} \end{bmatrix} \]

\[ d = 2 \]
\[ d = 4 \]
\[ d = 8 \]
\[ d = 2^c \]  

Beattie & Lin (2004)

Beam Example
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

\[ D = X \cdot V \]

Basic Idea-1
- Rotating Full Factorials
- Basic Idea-2
- Two-level fractional factorial design
- Beattie & Lin (1998): Rotating Full Factorials
- Basic Idea-3
- 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).
Uniform Design

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

Fang, Lin, Winker & Yang
(Technometrics, 1999)
Fang and Lin

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

\( \hat{F}_n(x) = \text{Empirical Cumulative Distribution Function} \)
\( F(x) = \text{Uniform Cumulative Distribution Function} \)

Find \( x = (x_1, x_2, ..., x_n) \) such that \( \hat{F}_n(x) \) is closest to \( F(x) \).

Discrepancy

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


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:

\[
(CL_2(P))^2 = \left( \frac{13}{12} \right)^x - \frac{2}{n} \sum_{k=1}^{n} \left( \frac{1}{2} \right)^k \prod_{i=1}^{k} \left( x_i - \frac{1}{2} \right)^2
\]

Sampling Strategies for Computer Experiments: Design and Analysis


Recent Research on

- Obtaining information which are not possible, without modern technology
  - Censor
  - RFID
  - Simulation

- How to (optimally) design these devices?
- How to analyze the outcomes (data)?
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!

This talk is based on

<http://www.personal.psu.edu/users/j/x/jxz203/lin/Lin_pub/>

STILL QUESTION?

Send $500 to

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