Experimental Design for Simulation

[Law, Ch. 12][Sanchez et al.[1]]

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CS 590M: Simulation
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[1] S. M. Sanchez, P. J. Sanchez, and H. Wan. "Work smarter, not harder: a tutorial on designing and conducting simulation experiments". *Proc. Winter Simulation Conf.*, 2018, p. 237–251.

Overview

Goal: Understand the behavior of your simulation model

- Gain general understanding (today's focus)
- What factors are important?
- What choices of controllable factors are robust to uncontrollable factors?
- Which choice of controllable factors optimizes some performance measure?

Overview, Continued

Challenge: Exploring the parameter space

- Ex: 100 parameters, each “high” or “low”
- Number of combinations to simulate: $2^{100} \approx 10^{30}$
- Say each simulation consists of one floating point operation(!)
- Use world’s fastest computer: Summit (148.6 petaflops)
- Required time for simulation: approximately 271,000 years

Experimental Design for Simulation

Basic Concepts: Factors

Factors (simulation inputs)

- Have impact on responses (simulation outputs)
- Levels: Values of a factor used in experiments
- Factor taxonomy:
  - Quantitative vs qualitative (can encode qualitative)
  - Discrete vs continuous
  - Binary or not
  - Controllable vs uncontrollable
- Factors must be carefully defined
  - Ex: (s, S)-inventory model
  - Use (s, S) or $(s, S - s)$ as the factors?

"parameter sweep"
try all combinations

$s = 6$
$S = 3$ ✗

$s = \{1, 2, 3, 4, 5, 6, 7\}$

$S = \{3, 4, 5, 6, 7, 8, 9\}$

Factor type	Example
quantitative (cont.)	Poisson arrival rate
quantitative (discr.)	# of machines
qualitative	service policy (FIFO, LIFO, ...)
binary	(open,closed), (high,low),...
controllable	# of servers
uncontrollable	weather (sun, rain, fog)

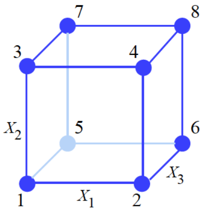
Basic Concepts: Designs

Design matrix

- One column per factor
- Each row is a design point
  - Contains a level for each factor
  - Level values determined by a domain expert
  - Natural or coded design levels
- Can have multiple replications of the design
  - Especially in simulation!

Design point	Factor settings x_1	x_2	x_3
1	-1	-1	-1
2	$+1$	-1	-1
3	-1	$+1$	-1
4	$+1$	$+1$	-1
5	-1	-1	$+1$
6	$+1$	-1	$+1$
7	-1	$+1$	$+1$
8	$+1$	$+1$	$+1$

2^3 factorial design

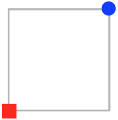


Experimental Design for Simulation

Some Bad Designs: Capture the Flag

Confounded effects

Speed	Stealth	Success?
Low	Low	No
High	High	Yes

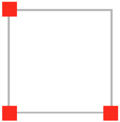


- Claim: Speed is the most important
- Claim: Stealth is the most important
- Claim: Both are equally important
- There is no way to determine who is right without more data
- Moral: haphazardly choosing design points can use up a lot of time while not providing insight

One-factor-at-a-time (OFAT) sampling

- Claim: Neither speed nor stealth is important
- Problem: an interaction between two factors is being missed

Speed	Stealth	Success?
Low	Low	No
High	Low	No
Low	High	No



Understanding Simulation Behavior: Metamodels

Simulation metamodels approximate true response

- Simplified representation for greater insight
- Allows "simulation on demand"
- Allows factor screening and optimization

Main-effects metamodel (quantitative factors)

$R(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \epsilon$

Metamodel with second-order interaction effects

$R(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \sum_i \sum_j \beta_{ij} x_i x_j + \epsilon$

- $R =$ simulation model output (i.e., response)
- Factors $x = (x_1, \ldots, x_k)$
- $\epsilon =$ mean-zero noise term, often assumed to be $N(0, \sigma^2)$

A Classical Design: 2^k Factorial Design

Basic setup: k factors with two levels each $(-1, +1)$

- Metamodel for $k = 2$: $R(x) = \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$
- So $r(x) = E[R(x)] = \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$

Estimating "main effects"

- Avg. change in r when x_1 goes from -1 to $+1$ (x_2 fixed):
  - $\frac{(r_3 - r_1) + (r_4 - r_2)}{2} = \frac{-r_1 - r_2 + r_3 + r_4}{2} = \frac{\mathbf{r} \cdot \mathbf{x_1}}{2} = 2\beta_1$
- Similarly, $\frac{\mathbf{r} \cdot \mathbf{x_2}}{2} = 2\beta_2$
- Method-of-moments estimators: $2\hat{\beta}_1 = \frac{\mathbf{R} \cdot \mathbf{x_1}}{2}$ and $2\hat{\beta}_2 = \frac{\mathbf{R} \cdot \mathbf{x_2}}{2}$

Design point	Factor settings x_1	x_2	$x_1 x_2$	Observed response (R)	Predicted expected value (r)
1	-1	-1	$+1$	R_1	$r_1 = -\beta_1 - \beta_2 + \beta_{12}$
2	-1	$+1$	-1	R_2	$r_2 = -\beta_1 + \beta_2 - \beta_{12}$
3	$+1$	-1	-1	R_3	$r_3 = \beta_1 - \beta_2 - \beta_{12}$
4	$+1$	$+1$	$+1$	R_4	$r_4 = \beta_1 + \beta_2 + \beta_{12}$

2^k Factorial Design, Continued

Estimating "interaction effect"

- (Effect of $\uparrow x_1$ with x_2 high minus effect with x_2 low) / 2
  - $\frac{(r_4 - r_2) - (r_3 - r_1)}{2} = \frac{\mathbf{r} \cdot (\mathbf{x_1 x_2})}{2} = 2\beta_{12}$
- Method of moments estimator: $2\hat{\beta}_{12} = \frac{\mathbf{R} \cdot (\mathbf{x_1 x_2})}{2}$

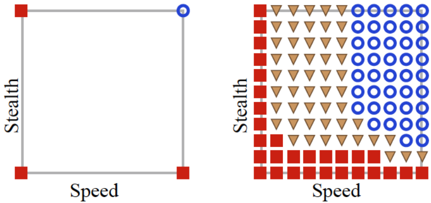
Observations:

- Can replicate design to get (Student-t) CI's for coefficients
- Estimating effects $\Leftrightarrow$ estimating regression coefficients
- Above analysis generalizes to more factors, e.g.,

$$R(x) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \epsilon$$

Design point	Factor settings x_1	x_2	$x_1 x_2$	Observed response (R)	Predicted expected value (r)
1	-1	-1	$+1$	R_1	$r_1 = -\beta_1 - \beta_2 + \beta_{12}$
2	-1	$+1$	-1	R_2	$r_2 = -\beta_1 + \beta_2 - \beta_{12}$
3	$+1$	-1	-1	R_3	$r_3 = \beta_1 - \beta_2 - \beta_{12}$
4	$+1$	$+1$	$+1$	R_4	$r_4 = \beta_1 + \beta_2 + \beta_{12}$

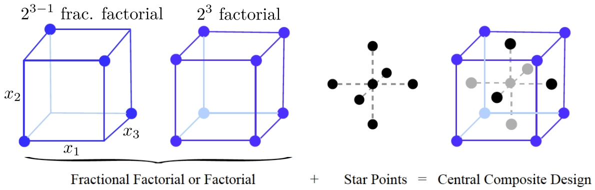
m^k Designs



Using more than two levels gives more detail

- E.g., capture the flag with 2^2 versus 11^2 designs
  - After achieving a minimal level of stealth, speed is more important
- Only possible for very small number of factors

2^{k-p} Fractional Factorial and Central Composite Designs

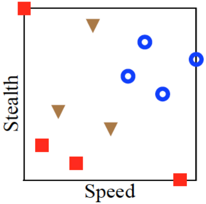


2^{k-p} fractional factorial designs

- Fewer design points, carefully chosen (see Law, Table 12.17)
  - E.g., 2^{3-1} design with 4 design points
  - Left/right faces: 1 val. of x_2 at each level, 1 val. of x_3 at each level (can isolate x_1 effect)
  - Similarly for other face pairs
- The degree of confounding is specified by the resolution
  - No m-way and n-way effect are confounded if $m + n <$ resolution
  - So for Resolution V design, no main effect or 2-way interaction are confounded

Space-Filling Designs

DP	Speed	Stealth	DP	Speed	Stealth
1	1	11	7	10	1
2	3	5	8	4	2
3	7	7	9	11	8
4	2	3	10	8	9
5	5	10	11	9	6
6	6	4			



Random Latin Hypercube design

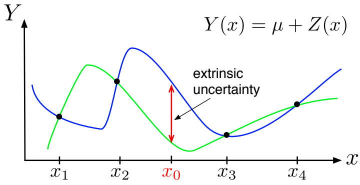
- Based on random permutations of levels for each factor
- Good coverage of param. space w. relatively few design points
- Carefully crafted LH designs are needed in practice

Experimental Design for Simulation

Gaussian Metamodeling (Kriging)

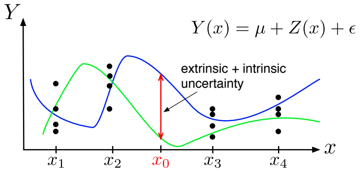
Ordinary kriging (deterministic simulations)

- $Z(x)$ is a Gaussian process
- $\big(Z(v_1), Z(v_2), \ldots, Z(v_n)\big) \sim N(\mathbf{0}, \mathbf{R}(\theta))$
- $r(v_i, v_j) = e^{-\theta(v_i - v_j)^2}$
- $\hat{Y}(x_0) = \hat{\mu} + \mathbf{r}^\top(x_0)\mathbf{R}(\hat{\theta})^{-1}(\mathbf{Y} - \mathbf{1}\hat{\mu})$
  - $\hat{\mu}$ and $\hat{\theta}$ are MLE estimates
  - $\mathbf{Y} = (Y_1, \ldots, Y_m)$ and $\mathbf{1} = (1, 1, \ldots, 1)$
  - $\mathbf{r} = \big(r(x_0, x_1), r(x_0, x_2), \ldots, r(x_0, x_m)\big)$

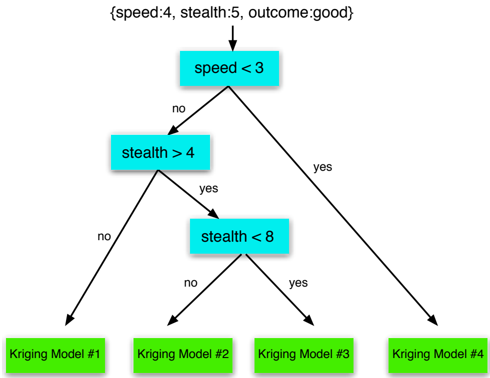


Stochastic kriging (stochastic simulations)

- ϵ is $N(0, \sigma^2)$ ("the nugget")
- Captures simulation variability
- Many other variants
  - Fitted derivatives
  - Varying σ^2
  - Non-constant mean function



Kriging + Trees



Idea: Build multiple models on subsets of homogeneous data

- Recursively split data to
  - Maximize heterogeneity (e.g., Gini index)
  - Maximize goodness of fit statistic (e.g., R^2)
- Build model on each subset

Experimental Design for Simulation

Data Farming

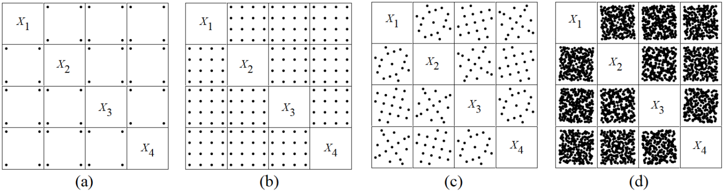


Figure 4: Scatterplot matrices for selected factorial and nearly orthogonal Latin hypercube (NOLH) designs: (a) 2^4 factorial with 16 design points, (b) 4^4 factorial with 256 design points, (c) NOLH with 17 design points, and (d) NOLH with 257 design points.

Modern "big data" approach

- Unlike real-world experiments, easier to generate a lot of simulation data
- Most effort usually spent building model, so work it hard!
- Use analytical, graphical, and data mining techniques on generated data

Graphical Methods

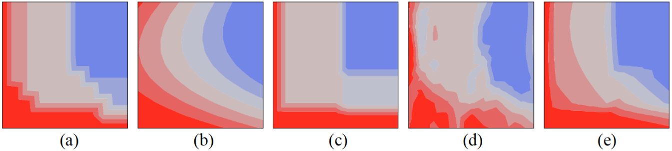
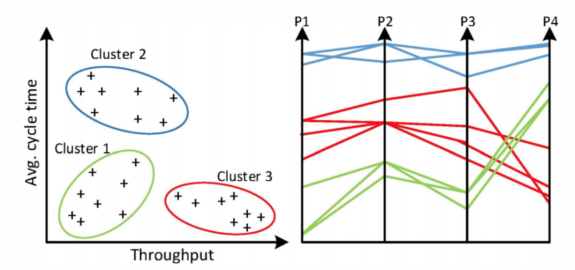


Figure 7: Capture-the-flag contour plots. (a) displays the actual response based on an 11×11 grid. The remaining contours are metamodels following a 65-dp NOLH: (b) 2nd-order regression metamodel, (c) partition tree with five splits, (d) Gaussian process metamodel, and (e) regression/partition metamodel.

Gaining insight through visualizations

- More sophisticated methods than simple regression
- Analyze flat areas (robustness)
- Other characteristics of interest

Data Mining and Visual Analytics



Visual analytics

- Experiments are clustered based on system performance
- Parallel-coordinate plot relates performance to factor levels
- Ex: Manufacturing model with parameters P1, P2, P3, P4

N. Feldkamp, S. Bergmann, and S. Strassburger. Visual analytics of manufacturing simulation data. *Proc. Winter Simulation Conference*, 2015, pp. 779–790.