Experimental Design for Simulation

[Law, Ch. 12][Sanchez et al.\textsuperscript{1}]

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CS 590M: Simulation
Spring Semester 2020

Experimental Design for Simulation

Overview
Basic Concepts and Terminology
Pitfalls
Regression Metamodels and Classical Designs
Other Metamodels
Data Farming
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

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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?

<table>
<thead>
<tr>
<th>Factor type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>quantitative (cont.)</td>
<td>Poisson arrival rate</td>
</tr>
<tr>
<td>quantitative (discr.)</td>
<td># of machines</td>
</tr>
<tr>
<td>qualitative</td>
<td>service policy (FIFO, LIFO, ...)</td>
</tr>
<tr>
<td>binary</td>
<td>(open,closed), (high,low),...</td>
</tr>
<tr>
<td>controllable</td>
<td># of servers</td>
</tr>
<tr>
<td>uncontrollable</td>
<td>weather (sun, rain, fog)</td>
</tr>
</tbody>
</table>

\[ S = \{ 1, 2, 3, 4, 5, 6, 7 \} \]
\[ s = \{ 3, 4, 5, 6, 7, 4, 9 \} \]
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!

<table>
<thead>
<tr>
<th>Design point</th>
<th>Factor settings $x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$-1$</td>
<td>$-1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>2</td>
<td>$+1$</td>
<td>$-1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>3</td>
<td>$-1$</td>
<td>$+1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>4</td>
<td>$+1$</td>
<td>$+1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>5</td>
<td>$-1$</td>
<td>$-1$</td>
<td>$+1$</td>
</tr>
<tr>
<td>6</td>
<td>$+1$</td>
<td>$-1$</td>
<td>$+1$</td>
</tr>
<tr>
<td>7</td>
<td>$-1$</td>
<td>$+1$</td>
<td>$+1$</td>
</tr>
<tr>
<td>8</td>
<td>$+1$</td>
<td>$+1$</td>
<td>$+1$</td>
</tr>
</tbody>
</table>

$2^3$ factorial design
Experimental Design for Simulation

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Some Bad Designs: Capture the Flag

Confounded effects

- 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
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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):
  - $\frac{(r_3-r_1)+(r_4-r_2)}{2} = \frac{-r_1-r_2+r_3+r_4}{2} = \frac{r \cdot x_1}{2} = 2\beta_1$
  - Similarly, $\frac{r \cdot x_2}{2} = 2\beta_2$
- Method-of-moments estimators: $2\hat{\beta}_1 = \frac{R \cdot x_1}{2}$ and $2\hat{\beta}_2 = \frac{R \cdot x_2}{2}$

<table>
<thead>
<tr>
<th>Design point</th>
<th>Factor settings</th>
<th>Observed response ($R$)</th>
<th>Predicted expected value ($r$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$-1$ $-1$ $+1$</td>
<td>$R_1$</td>
<td>$r_1 = -\beta_1 - \beta_2 + \beta_{12}$</td>
</tr>
<tr>
<td>2</td>
<td>$-1$ $+1$ $-1$</td>
<td>$R_2$</td>
<td>$r_2 = -\beta_1 + \beta_2 - \beta_{12}$</td>
</tr>
<tr>
<td>3</td>
<td>$+1$ $-1$ $-1$</td>
<td>$R_3$</td>
<td>$r_3 = \beta_1 - \beta_2 - \beta_{12}$</td>
</tr>
<tr>
<td>4</td>
<td>$+1$ $+1$ $+1$</td>
<td>$R_4$</td>
<td>$r_4 = \beta_1 + \beta_2 + \beta_{12}$</td>
</tr>
</tbody>
</table>
Estimating “interaction effect”

- (Effect of $x_1$ high minus $x_2$ low) / 2
  - $\frac{(r_4-r_2)-(r_3-r_1)}{2} = \frac{r(x_1x_2)}{2} = 2\beta_{12}$
- Method of moments estimator: $2\hat{\beta}_{12} = \frac{R(x_1x_2)}{2}$

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.,

$$R(x) = \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{23}x_2x_3 + \beta_{123}x_1x_2x_3 + \epsilon$$

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<th>Factor settings $x_1$</th>
<th>$x_2$</th>
<th>$x_1x_2$</th>
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<tbody>
<tr>
<td>1</td>
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<td>+1</td>
<td>$R_1$</td>
<td>$r_1 = -\beta_1 - \beta_2 + \beta_{12}$</td>
</tr>
<tr>
<td>2</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>$R_2$</td>
<td>$r_2 = -\beta_1 + \beta_2 - \beta_{12}$</td>
</tr>
<tr>
<td>3</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>$R_3$</td>
<td>$r_3 = \beta_1 - \beta_2 - \beta_{12}$</td>
</tr>
<tr>
<td>4</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>$R_4$</td>
<td>$r_4 = \beta_1 + \beta_2 + \beta_{12}$</td>
</tr>
</tbody>
</table>
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 \(m + n < \text{resolution}\)
  - So for Resolution V design, no main effect or 2-way interaction are confounded
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
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Gaussian Metamodeling (Kriging)

**Ordinary kriging (deterministic simulations)**

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

**Stochastic kriging (stochastic simulations)**

- \( \epsilon \) is \( \mathcal{N}(0, \sigma^2) \) ("the nugget")
- Captures simulation variability
- Many other variants
  - Fitted derivatives
  - Varying \( \sigma^2 \)
  - Non-constant mean function
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
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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

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.
Graphical Methods

Figure 7: Capture-the-flag contour plots. (a) displays the actual response based on an $11 \times 11$ 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