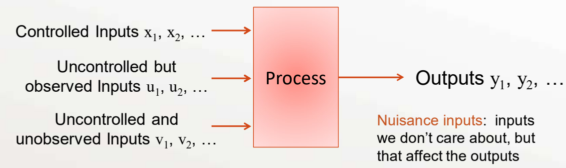
CHE384, From Data to Decisions: Measurement, Uncertainty, Analysis, and Modeling

Lecture 64
Introduction to Design of Experiments

Chris A. Mack

Adjunct Associate Professor

http://www.lithoguru.com/scientist/statistics/



Modeling (characterization): How do inputs affect the output?

Optimization: What input values produce the desired outputs (both mean and variance)?

Control: How do we adjust controlled inputs to maximize control of the outputs?

Dealing with the Three Types of Inputs

- Controlled Inputs (x)
  - Variation + repeats/replication: vary the inputs and repeat the experiments in a systematic way
- Uncontrolled but Observed Inputs (u)
  - Blocking: group experiments into blocks, each block having a fixed value of u
  - Analysis of covariance: Model the impact of u, then subtract it out from the model
- Uncontrolled and Unobserved Inputs (v)
  - Randomization: for sufficiently large sample sizes, let impact of v average out to zero

What is Experimental Design?

- We design our experiments to get the most information from the least data (that is, minimize time and cost)
- Experiment: the deliberate variation of one or more process variables while observing the effect on one or more response variables
- Design of Experiments (DOE): a procedure for planning experiments to efficiently provide valid conclusions
  - Does the experiment have enough statistical power to answer the research questions?

Uses of Design of Experiments

- DOE can be used for exploratory work
  - Choosing between alternatives (comparison)
  - Selecting the key factors that affect a response (screening)
- DOE can be used to optimize a given process (response surface modeling)
  - Hitting and controlling a target response with minimum variability
  - Maximize or minimize a response or goal
  - Increase process robustness
- DOE can be used for regression/modelling

DOE for Regression

- For a given n (number of data points), pick values of the predictor variables in the experiment to produce some desired statistical behavior
  - The smallest standard errors of the coefficients
  - The smallest standard errors of the predictions
  - Others
- Called Optimal Design
  - In general, this requires a numerical search

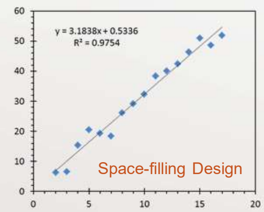
DOE for Simple Linear Regression

- Example: optimize for the smallest standard errors of the coefficients
- Consider a straight line model with one predictor variable

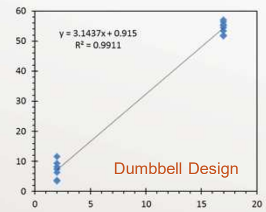
$$s_{b1}^2 = \frac{s_\varepsilon^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \qquad s_{b0}^2 = \frac{s_\varepsilon^2}{n} + s_{b1}^2 \bar{x}^2$$

- The lowest SE(b_1) is obtained by picking half of the data points to be at the lowest x-value, and half of the data points to be at the highest data value (dumbbell design)
  - We should space the x-values more evenly only if we wish to check whether the model is correct

DOE for Simple Linear Regression



SE(b_1) = 0.135



SE(b_1) = 0.080

DOE for Regression

- For a straight line model with one predictor

Dumbbell Design: $SE(b_1) = \frac{\sigma_\varepsilon}{\sqrt{n}(x_{max} - x_{min})/2}$
(1/2 at each extreme)

Space-filling Design: $SE(b_1) = SE_{dumbbell}\sqrt{3\left(\frac{n-1}{n+1}\right)}$
(data spaced evenly apart)

Quadratic Design: $SE(b_1) = S_{dumbbell}\sqrt{3/2}$
(1/3 at each end, 1/3 in middle)

Experimental Design Leverage

- An important goal of Design of Experiments (DoE) is to equalize the leverage of every point during multiple regression
  - We want to make $h_{ii} = \overline{h_{ii}} = \frac{p}{n}$ for every i
- For the case of only one predictor variable,

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{2}{n}$$

We want: $(x_i - \bar{x})^2 = same\ for\ each\ i$

Six Principles for Regression Design

(NIST/SEMATECH e-Handbook of Statistical Methods, section 4.3.3)

- Capacity for the primary model
- Capacity for the alternate model
- Minimum variance of estimated coefficients or predicted values
  - Except for simple cases, must search for optimal design
- Sample where the variation is
- Repeats and replication
  - To compute a model-independent estimate of the process standard deviation
- Randomization and blocking
  - Allows the detection of drift, reduces influence of known/unknown but unimportant variations

Lecture 64: What have we learned?

- Name the three types of inputs to a process
- Define design of experiments
- What are the three uses of experimental design?
- For regression to a straight line, what is the most efficient design?
- For regression to a straight line, what design produces uniform leverage?