Module 1: What is a Computer Experiment?

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Adapted from materials prepared by Jerry Sacks and Will Welch for various short courses

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Outline of Topics

1 Examples of Computer Models

2 Computer codes

3 Role of Statistics

4 Next Steps
**Computer Models**

- **Scientific / engineering / ... phenomenon**
  - car crash
  - vehicle suspension system meets pothole

- **Theory and mathematical formulation**
  - mechanical deformation
  - dynamic stress-strain

- **Computational implementation (computer model, numerical model, computer code)**
  - finite element code; vehicle represented by as many as 300,000 elements; 1+ days per run per work station
  - suspension system less, but 1 hour/run
Car Crash
Vehicle Suspension

Pothole Data: 1st pothole

Distance (m)

Tension (N)
Vehicle Suspension Experiment

- Implementation, generally complex
  - characteristics of restraint systems and components
  - inputs for geometry, materials properties
  - inputs for numerical parameters (time-step, mesh size)
- assessment of validity of the code
  - physical data needed
- Objectives
  - prediction (e.g., peak stress); answer what if questions
  - optimize time to deploy air bag
  - validate code against physical data
- Iterative feedback at all stages
Arctic Sea-Ice (Chapman, Welch, Bowman, Sacks, Walsh 1994)

- **Objective:** estimate sensitivities to input parameters
- **Computer model:** dynamic formulation based on a momentum balance for a mass of ice within a grid cell
- **Model run:** daily time step 1960-1988; 110 km grid covering Arctic Ocean and nearby bodies of water
- **Inputs (13 variables):** drag coefficients (ocean, atmosphere), albedo (snow, ice, open water), surface sensible heat, etc.
- **Output(s):** Ice mass, ice area, mean drift velocity, range of ice area
Arctic Ocean
Arctic Sea-Ice Code

See icecode.pdf
Characteristics of Computer Codes

- Numerical solution of differential equations
- Science is complex, codes are complex
- Codes often costly to run
- Deterministic: repeating the inputs produces the same outputs
- Black-box: codes can be proprietary or scientifically/mathematically impenetrable; sometimes partially transparent (gray-box)
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Computer Code

Inputs
\[ x_1, \ldots, x_d \]

Black box
\[ \frac{\partial y}{\partial x_1} = \ldots \]
\[ \vdots \]

Output(s)
\[ y(x_1, \ldots, x_d) \]
Role of Statistics

Deterministic Codes: Why Statistics?

- Need for statistical approximation of computer output
  - limited number of runs (few data)
  - many inputs (high dimension)
  - predict model output at untried inputs based on limited data
  - there will be uncertainty in predictions

- Some other sources of uncertainty
  - propagation of variation: variability in inputs induces uncertainty in outputs
  - assess the fidelity of the model to reality (validation); needs field/experimental data which will be measured with error

- Design
  - where to make the runs (selection of inputs)
What’s Different?

- The pillars of classical design of experiments are blocking, randomization, and replication.
- The codes we will look at are (nearly) deterministic: blocking, randomization, and replication (with the same input values) are largely irrelevant.
- Bias dominates in variance-bias trade-offs.
- Less concerned with balanced (symmetric) designs for minimizing variance; more with spatial coverage (space filling).
- Experimenters will often have wide ranges for inputs, hence highly nonlinear relationships are often found.
- With many input variables and limited computer runs, polynomial regression, neural nets, common nonparametric smoothers are difficult to use.
Plan for the Next Few Weeks

- **Analysis**: Approximation / prediction / emulation of a computer code, mainly via Gaussian process (GP) statistical models, along with a measure of uncertainty
- **Design of computer experiments**: space-filling designs, sequential designs
- **Scientific and engineering objectives**
- **Combining computer model runs and physical data**: calibration, assessment of validity
- **See course outline for more details**
- **Task for Thursday**: Write down and bring to class 10 properties of the normal distribution, multivariate normal distribution, or conditional multivariate normal distribution. They will be collected and we will compile a list of such properties.