Exceptional service in the national interest

Sandia National Laboratories

ESP700 Lecture 3: Sensitivity Analysis and Uncertainty Quantification

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

March 22, 2016

SAND Number: XXXXXXX

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Exceptional service in the national interest

Sandia National Laboratories

ESP700 Pre-Lecture 3: Crash Course on Probability and Dakota

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

March 22, 2016

Probability & Statistics

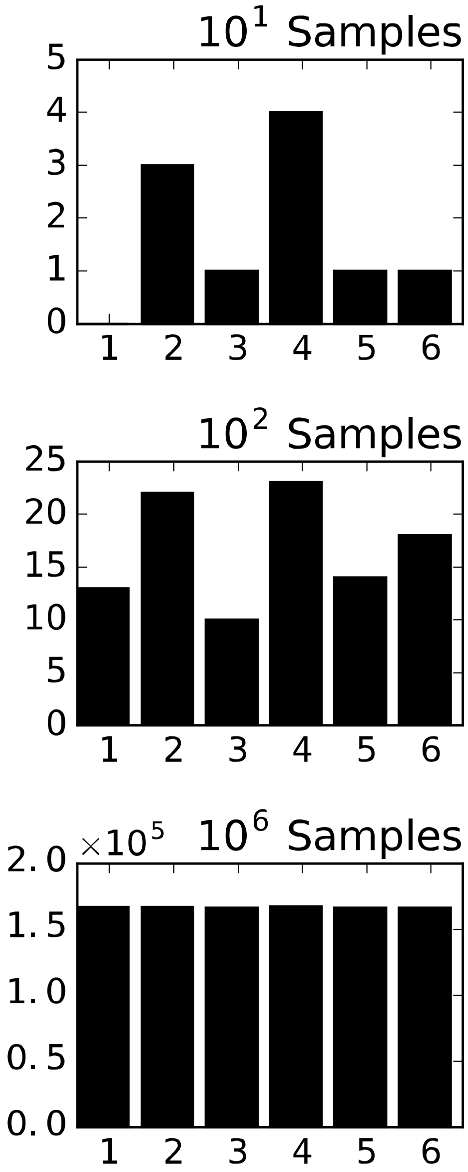
- Statistics = analysis of past events
  - **Observe** outcomes of events
  - **Build** & test statistical model **to explain outcomes**
- Probability = prediction of future events
  - **Assume** probability model
    - Often based on a statistical model
  - **Predict** outcomes **to make decisions**
- We are not going to go into probability theory

Statistics question: Is the Die fair?

- Observe data, find correlations

  → Hypothesize causation
- Statistics issues:
  - Inputs & Responses/ **Q**uantities **o**f **I**nterest (QoI)
    - What do we measure?
  - Quantity & Quality of data:
    - What can be said for 10 vs 1 million samples?
- Not a focus of this course

Histograms show frequencies of each *outcome* for the *response/QoI*: face number for a fair die



Probability Question: What is the next roll?

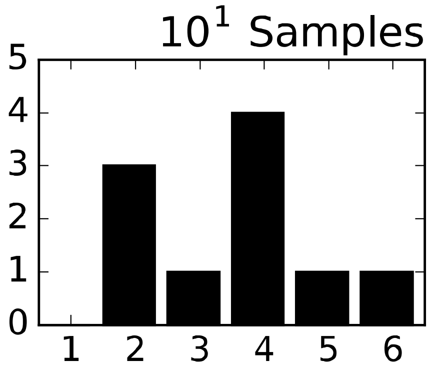
- Cannot be answered deterministically
- Identify **ALL possible outcomes** for the QoI
- Assume a model:
  Probability of occurrence of each outcome

→ Defines a probability distribution

- Use model to make predictions and decisions

(Were those predictions correct?)

Known unknowns, unknown unknowns?



- 10 rolls of a die
  - What is the statistical model?
- Probability: what is the probability mc
  - $P(face = 1) = 0$?
  - Expert opinion can help to improve a model
- Inherent weakness of models
  - Include only what you put in (including li
  - "Garbage in, garbage out"
  - "All models are wrong, some are useful"

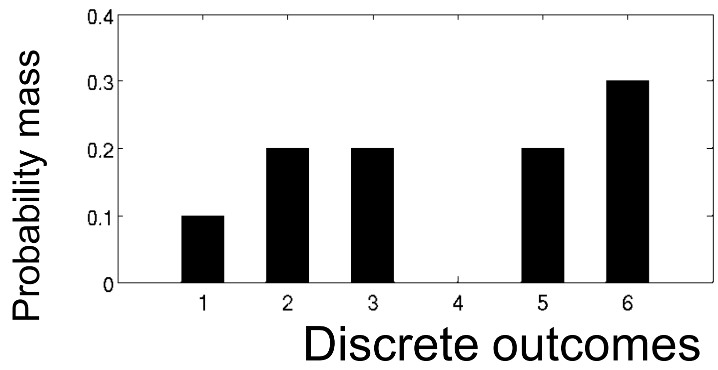
A bit of jargon

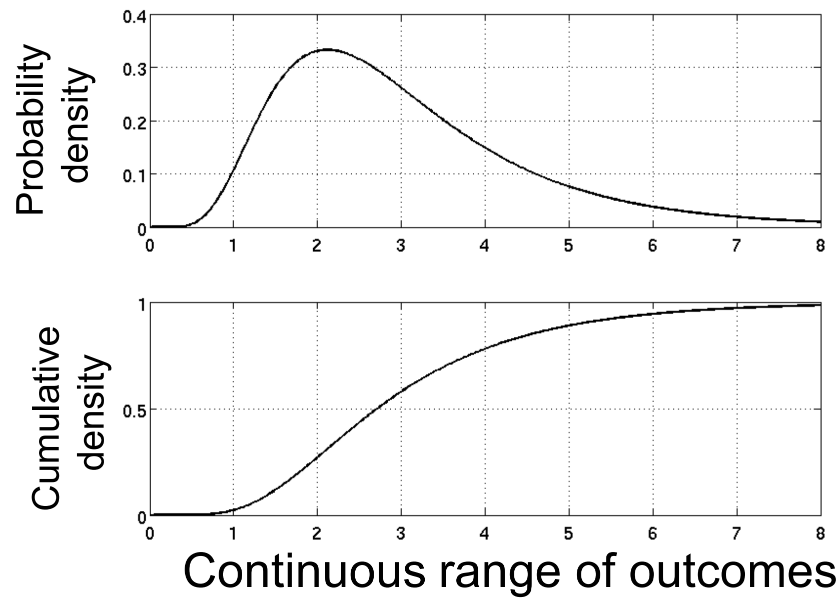
- (Real valued) Random Variable
  - A function that associates *outcomes* with *probabilities* of their occurrence
- Discrete:

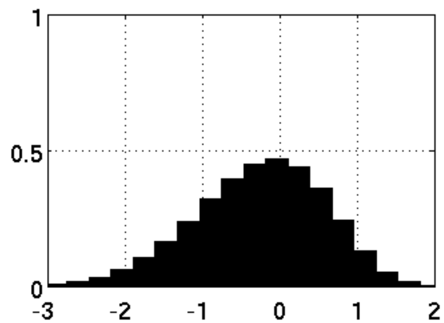
  Coin flip – *outcome* is heads, P(heads) = 1/2
- Continuous:

  Failure – *outcome* is that material will fail if subjected to impact at 1km/s, prob = ½
- Random variable ←→ probability distribution

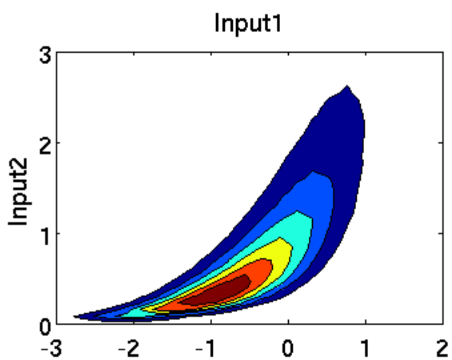
Probability distributions

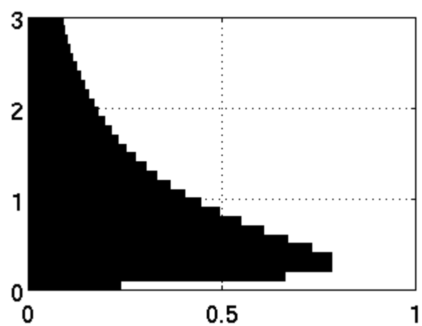






2+ dimensions project to 1D and 2D
→ See 2D correlation





Ways to summarize a distribution:

Mean, mode, median, standard deviation, etc.

Commonly used terms

- Statistics: based on data – N points
  - Sample Mean $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$
  - Sample Variance $\sigma_x^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2$
  - Coefficient of Variation (CoV) $\frac{\sigma_x}{\bar{x}}$

Estimates from data can have error

Standard Deviation is sqrt of variance

- Correlation

More samples → better estimates

  - Two random variables are correlated if the outcome of one changes the probabilities of the second
  - Example: Number of gate guards & Wait times at gate

UQ Tools

- Various tools exist internally and externally
  - UQLab (Matlab)
  - UQToolbox (Python)
  - PSUADE (from LLNL)
  - ...plus tons of home-grown tools and other statistics packages
- Sandia has it's own tools
  - UQ Toolkit (C++/Matlab)
  - Dakota (standalone and C++)
- We will focus on Dakota but this is **not** a Dakota training course!

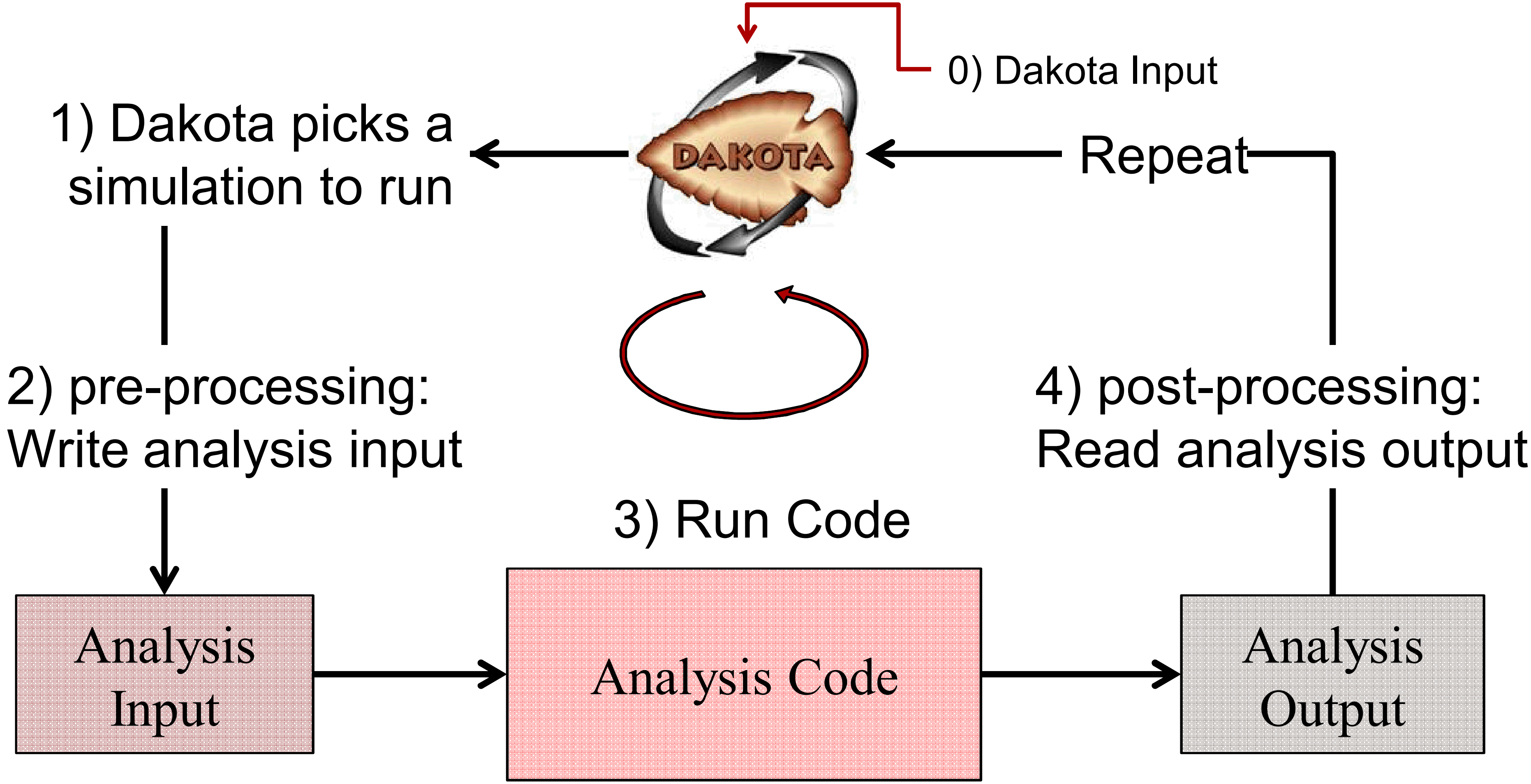
What is Dakota?

- **Automation** of model runs
  - Make it cheap to run simulations (user time, not CPU hrs)

+

- **Methods**
  - Make the runs more useful
  - Uncertainty Quantification, Surrogate Models, Optimization, Design of Experiments, Parameter Study, Sensitivity Analysis

How does it work?



Look familiar? Many analysts do this manually.
Many similar codes exist.

Comparisons

Manual

- Repetitive process
  - Costs add up
- Can make mistakes, lose track of data, simulations, etc.
- Hard to repeat. Poor data provenance

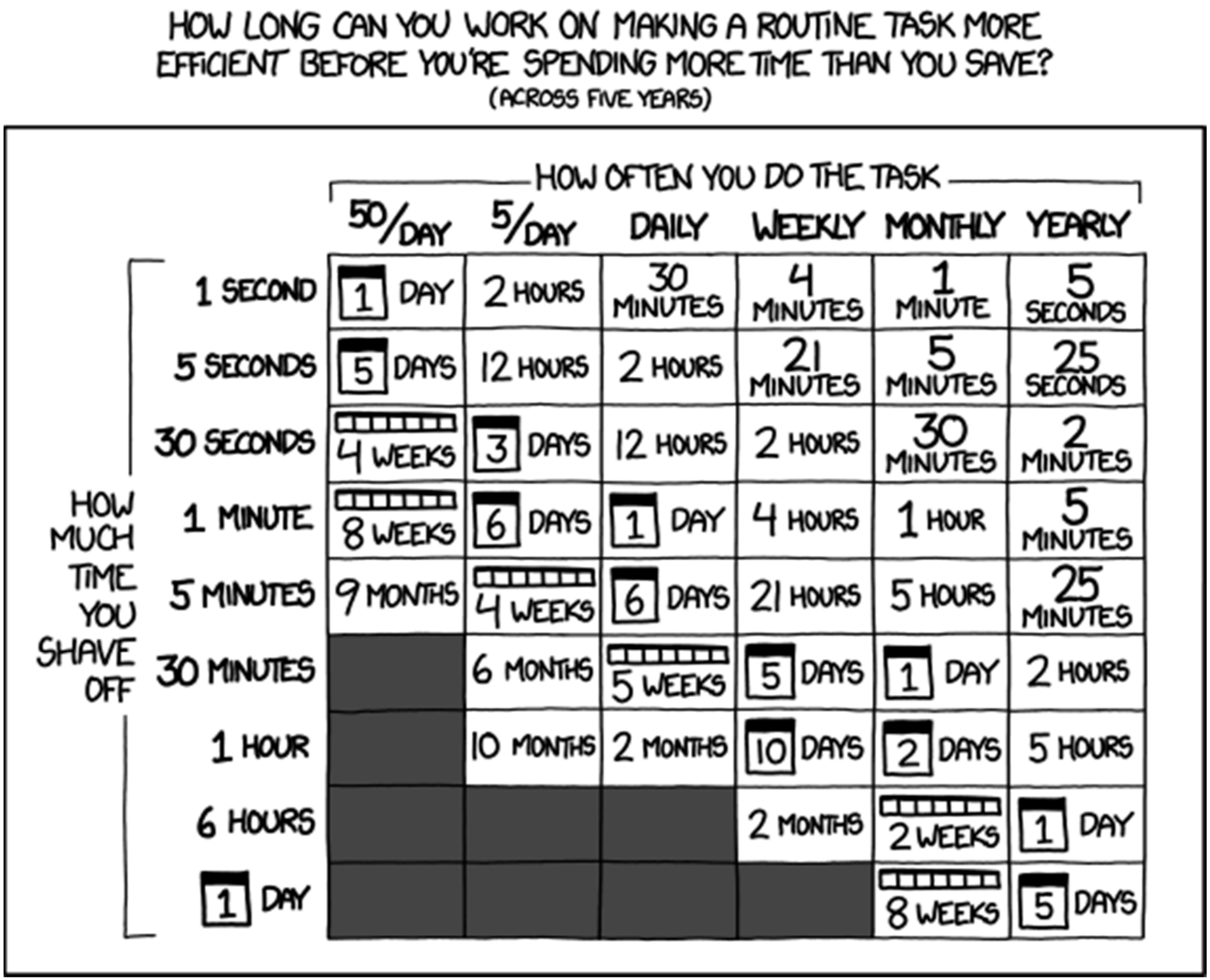
Automation

- Requires scripting
  - Larger up-front cost
  - Minimal additional cost
- Fewer errors
- Gain access to powerful methods

Rule 1: There is **always** a relevant XKCD

Sandia National Laboratories

http://xkcd.com/1205/



Automation is vital when analyzing many model evaluations

Typically:

- Bash
- Python
- (mix)

Dakota can do some of it

Tools in ESP700

- Simple Dakota Examples
  - Demonstrate capabilities/ methods
  - Simple workflow
- Learn about available resources
- What you won't see
  - Dakota tutorial
  - Scripting details
  - Complicated data analysis
- Today's examples use Bash, Matlab and Python
- Similar tools:
  - JMP
  - Minitab
  - R
  - Octave
  - Excel
  - Etc…

Questions?

- Dakota resources:
  - dakota.sandia.gov
  - Dakota Product Manager for 1500: George Orient
  - Dakota support: Adam Stephens

Exceptional service in the national interest

ESP700 Lecture 3: Methods and Tools for Sensitivity Analysis

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

March 22, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Models are wrong, but they can be useful

Questions to ask about the model:

What parts matter most?

- Sensitivity analysis: which inputs affect the response?

How well do we know the response value?

- UQ: how do uncertainties in inputs affect the response?

Do we know enough? ARE the models useful?

- V&V → how accurate / wrong is the response?

What are the costs and benefits? VALUE?

Outline

- A day in the life of a 1544 analyst
- Examples
- Sensitivity analysis
- Uncertainty quantification
- Surrogate models
- Advanced methods

Basic methods, demonstrations, interpretation, value proposition

Lecture 3 Goals

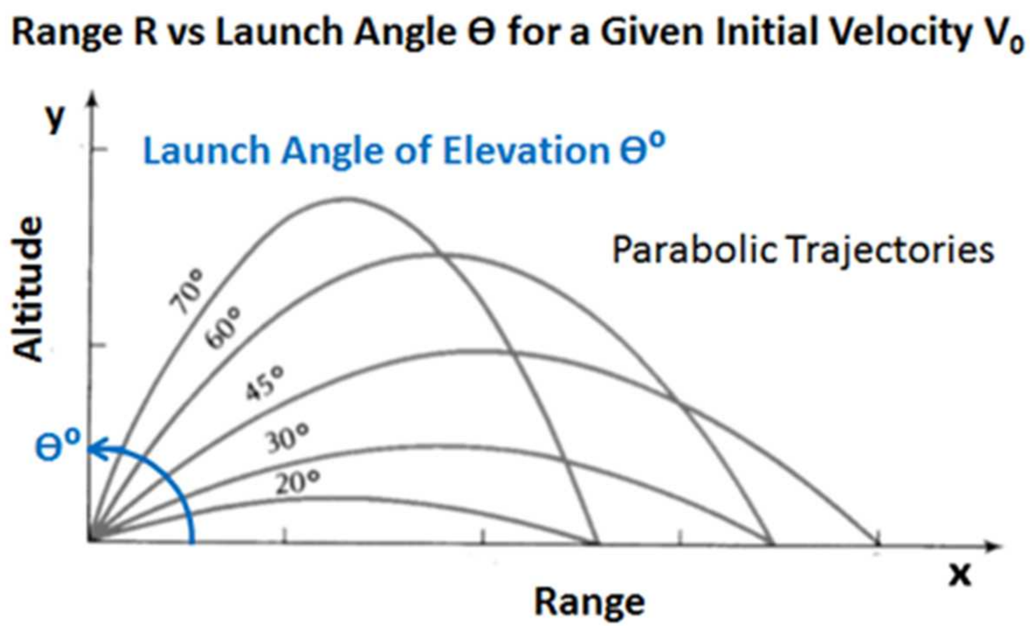
- Introduce topics at a high level
- Describe the basic methods
- Promote Dakota usage
- Demonstrate methods and tools
  - Simple example – compute ballistic trajectory
  - Case study – 3 leg structural dynamics problem
- **Leave with a basic knowledge of methods, tools, context – there is much more**

What does 1544 do?

- Project work
  - Supporting other analysts (1500 and others)
  - Sensitivity analysis, UQ, V&V, optimization
  - Tailoring methods for each project
  - Interpreting results
- Methods research & development
- Creating resources/ tools

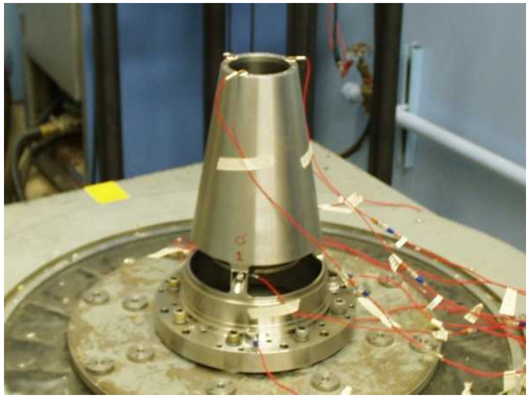
  → Enable other analysts to do what we do

Example: Ballistic Trajectory



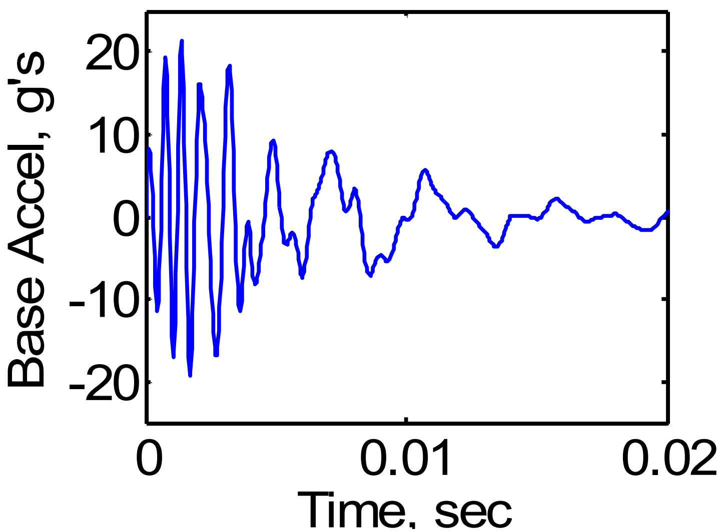
- Inputs
  - Angle, θ
  - Initial Velocity,
  - Gravity
- Quantities of Interest
  - Max Height, H
  - Range, R

Case Study: 3leg model

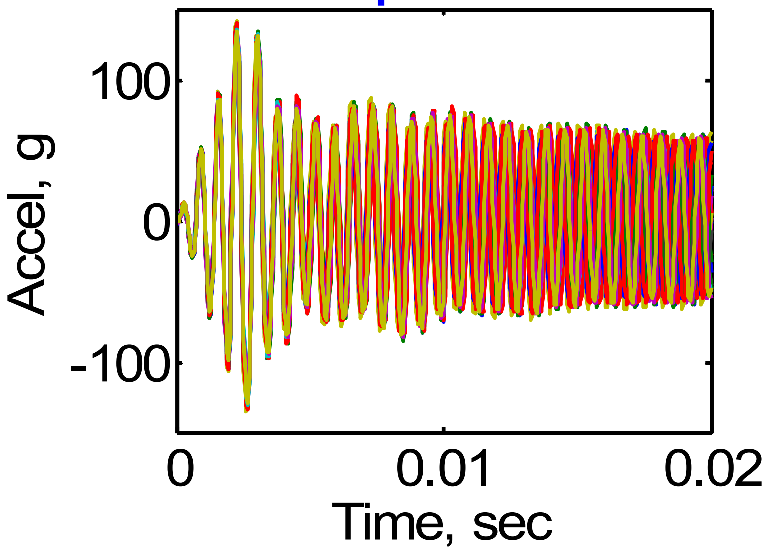


- Hardware consists of 3 top conic sections and 3 bottom sections
- 9 total combinations of top/bottoms

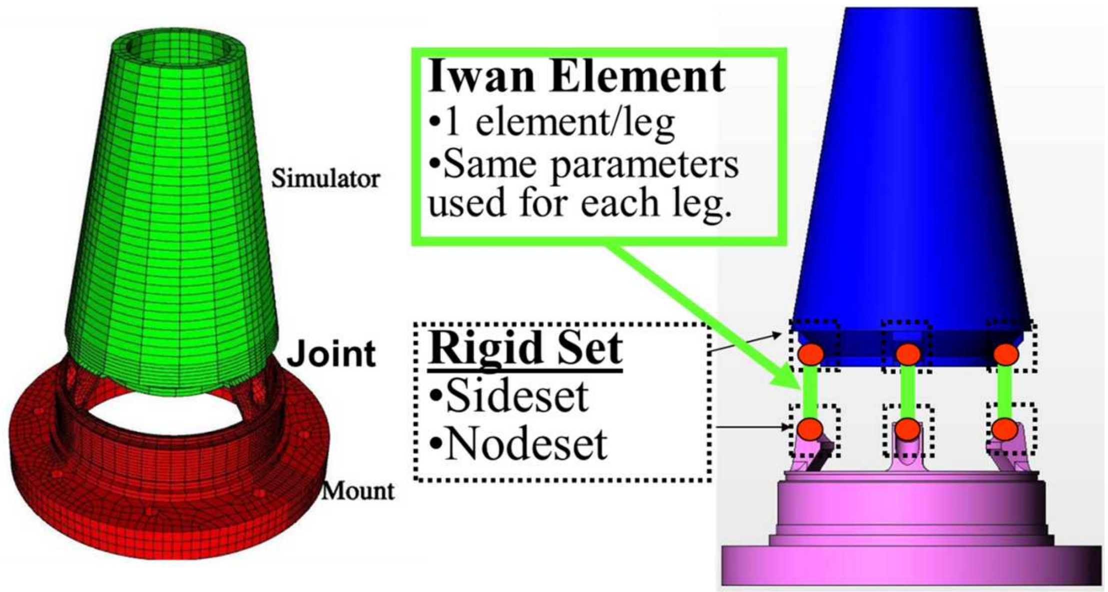
Acceleration input

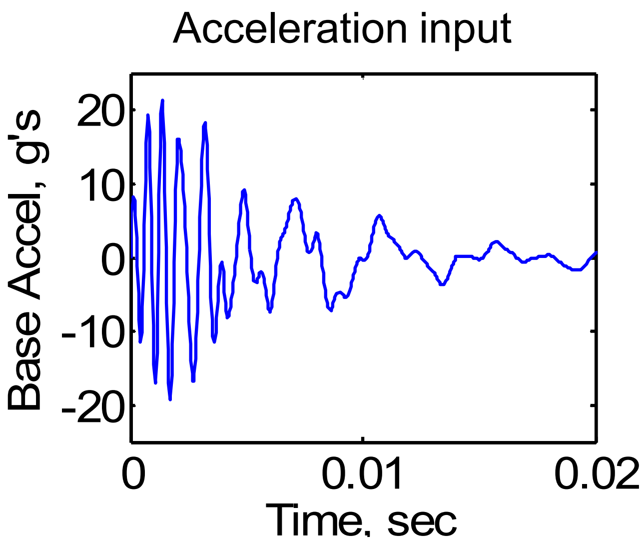


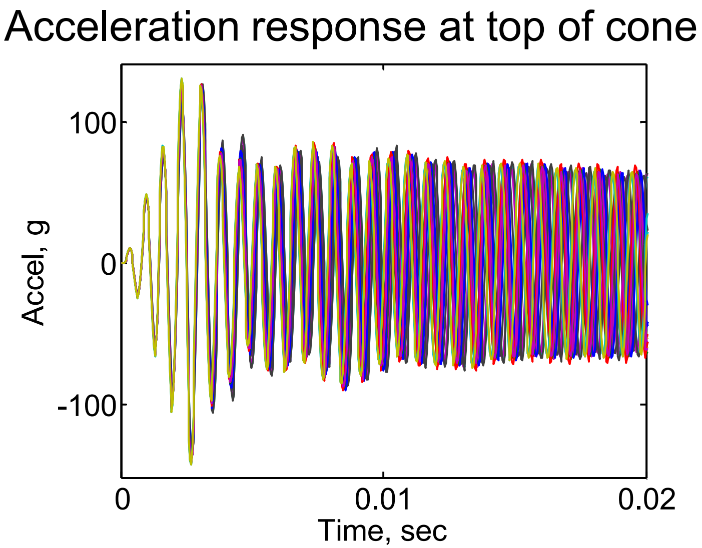
Average acceleration response at top of conic



Case Study: 3leg model

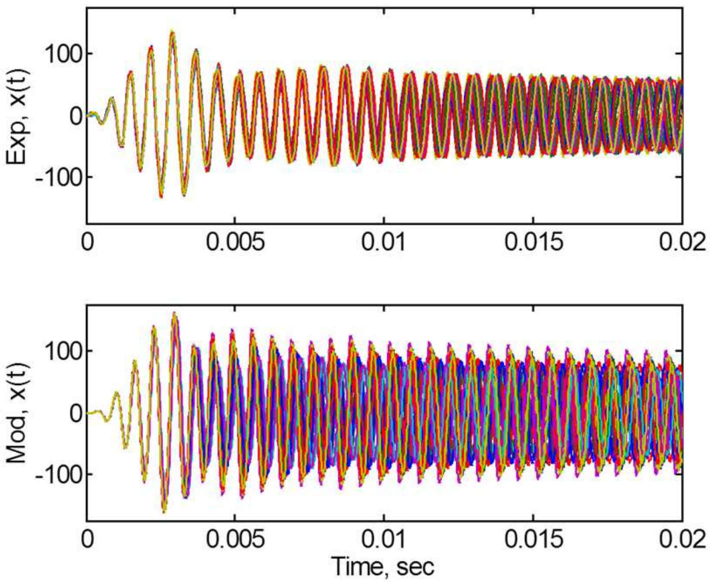


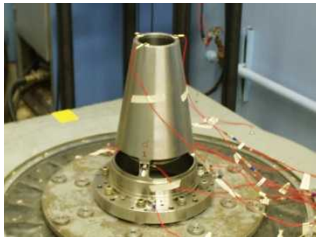


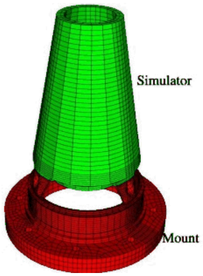


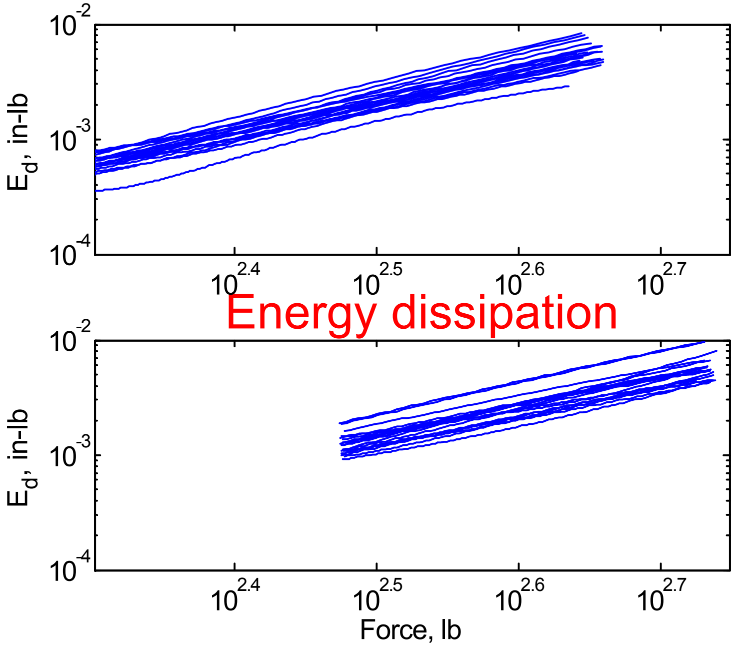
- 3D finite element model representing 3 leg hardware was created
- Bolted joints are modeled using an Iwan element
- Non linear transient analysis was performed using Sierra-SD (structural dynamics)

Quantities of interest

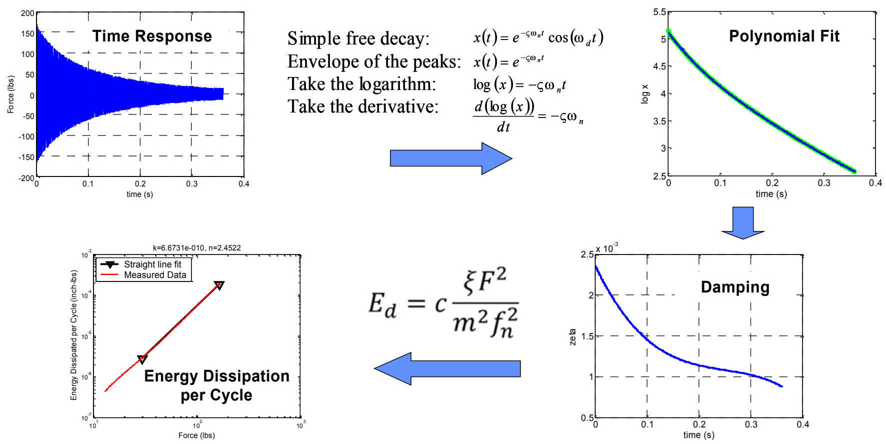








Energy dissipation per cycle from transient responses



QoIs:

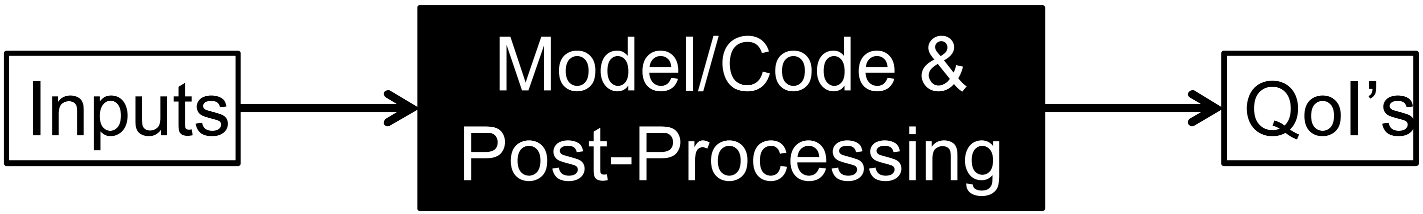
- **Slope**
- **Peak Force**
- **Max Acceleration**

3leg Simulations

- Sierra SD, a.k.a Salinas
- Ran on CEE platforms, 8cores, ~20 min
- Salinas results file
- Dakota “drives” the simulations
- Automation
  - Bash scripting, Linux utilities
  - Matlab post-processing

Abstract View of Simulation

- Think of models / code as a black box
  - Inputs go in, QoI’s come out

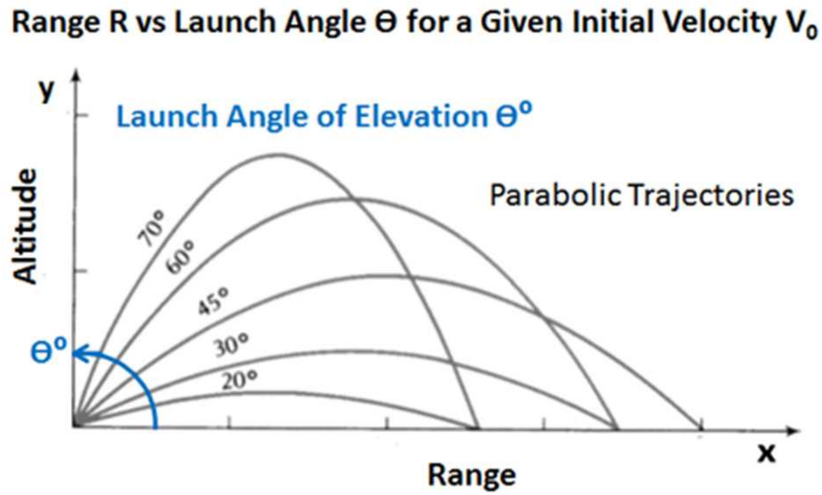


- Input = ANYTHING that changes the QoI’s
  - Model parameter, code setting (solvers, tolerances)
  - Boundary conditions, external forcing, etc.
  - mesh, geometry
  - model form a.k.a model structure
  - Computational hardware

Sensitivity Analysis

- How do changes to inputs affect the response?
  - How “sensitive” is the response to each input?
  - Direction and magnitude
  - Which inputs matter the most?
- Typically focus on model parameters
  OR other inputs
  - **Today – focus on quantitative inputs (parameters)**
  - Lecture 2: verification – Sensitivity analysis and uncertainty quantification for meshes/ codes

Example 1: Ballistic Trajectory



- Qualitative Sensitivity, a.k.a. “Expert Opinion”
  - V↑ → Height ↑ & Range ↑
  - Gravity ↑ → Height ↓ & Range ↓
  - θ↑ → Height ↑ & Range ??
  - V↑, θ↓ → Height ?? & Range ??

Is this enough information?

Why Do Sensitivity Analysis?

- Identify trends in responses – exploration
  - Bonus information: smoothness, robustness
- Provide a focus for future work
  - Model development
  - New experiments
  - Characterization of input uncertainty & UQ

Goal: spend resources to understand the **significant inputs** for the **important responses**

Summary

1. Vary the inputs
2. Run the model
3. See if QoI's change, compute metrics

- More samples → more information
- Methods – efficiently compute metrics
  - Efficiently gather information

Basic Quantitative Sensitivity Analysis

- Local sensitivity:
  - Metric: Partial derivative
  - Method: [Relative] Finite differences

$$\left.\frac{\partial R}{\partial \theta}\right|_{nom} = \frac{\left(R(\widetilde{\theta}+\delta\theta) - R(\widetilde{\theta}-\delta\theta)\right)/R(\widetilde{\theta})}{2\delta\theta/\widetilde{\theta}}$$

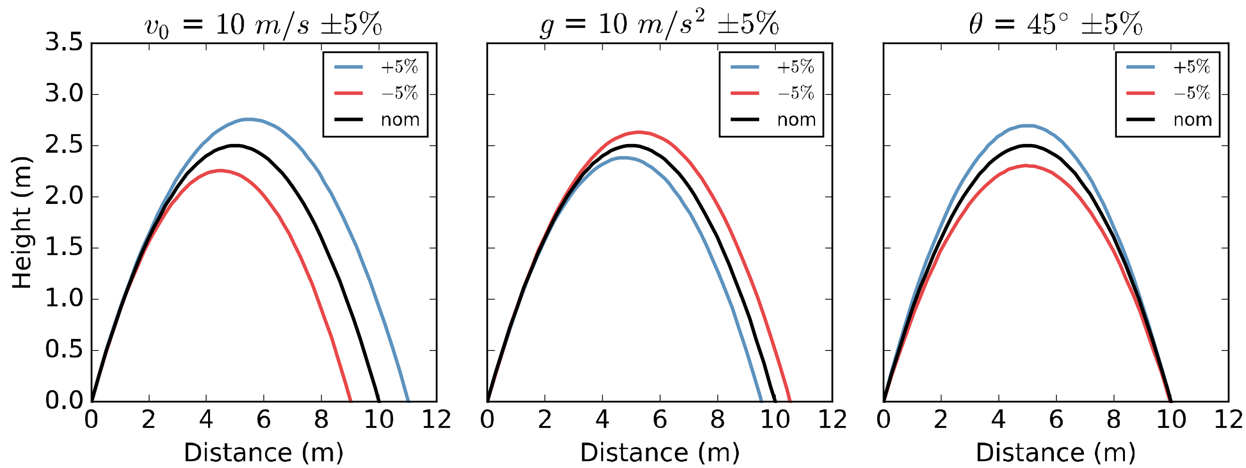
- Must pick nominal point and step sizes

Example: Ballistic Trajectory

Nominal $\widetilde{\theta} = 45^\circ,\ \widetilde{V_0} = 10m/s,\ \widetilde{g} = 10m/s^2$

Step size = ±5%

Results: $\left[\frac{\partial R}{\partial \theta}, \frac{\partial R}{\partial V_0}, \frac{\partial R}{\partial g}\right]_{nom} = [0.00, 1.00, -0.50]$ $\left[\frac{\partial H}{\partial \theta}, \frac{\partial H}{\partial V_0}, \frac{\partial H}{\partial g}\right]_{nom} = [0.78, 1.00, -0.50]$



Lessons

- Sensitivities: $V_0 > g > \theta$ (But depends on QoI)
  - On Earth: how much does gravity vary?
  - **Most sensitive ≠ most significant**
  - Must consider possible range of values (CoV[g] ≈0.001)
- Compare sensitivity of height and range
  - Depends on the QoI
- Repeat at: $\theta = 1^0, V_0 = 10m/s, g = 10m/s^2$
  - Sensitivities: $\theta > V_0 > g$
  - Nominal value matters

Cheap – bare minimum of model evaluations

Limited – Estimate of main effects, no interactions

Case Study: 3leg

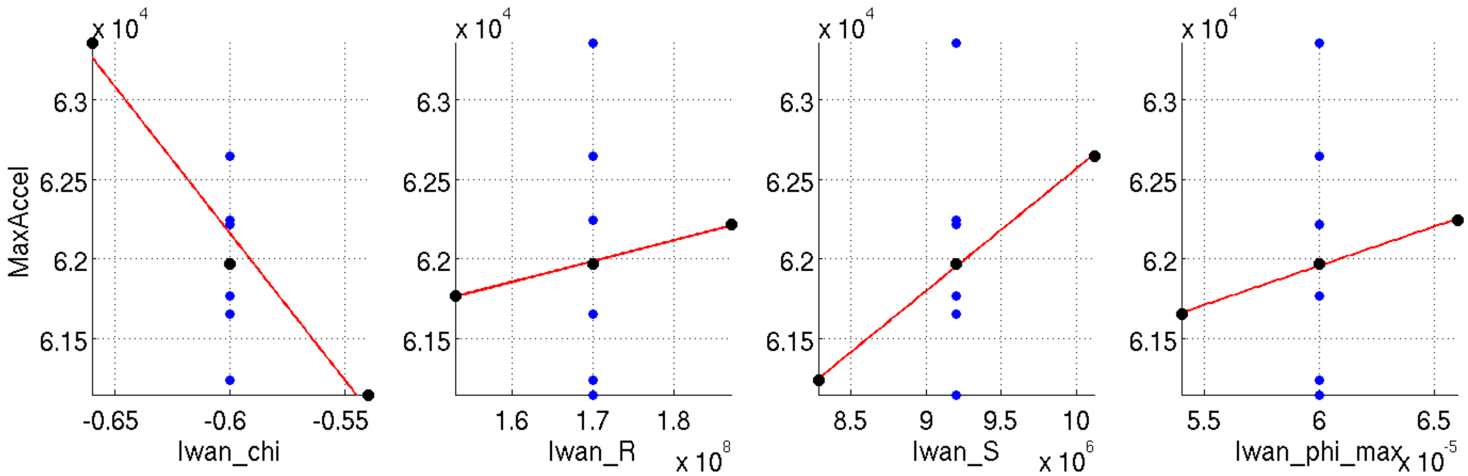
- Local sensitivity
  - Pick nominal values for 4 Iwan parameters
  - Pick range & step size = 10%
  - QoI’s are most sensitive to Phi_max
- Absolute change in response over whole range
  - chi and S are most significant

Forward differences :	'chi'	'R'	'S‘	'phi_max'
MaxAccelSensitivity	-2e-2	2e-10	1e-8	8e2
MaxAccelDiffOverRange	1400	250	680	280

'chi‘ >> 'S‘ >> 'phi_max‘ ≈ 'R‘

"Projection" Plots

- 5D space – 4 parameters, 1 response
- Project onto 2D – collapse 4 parameters into 1D



Central differences

- Visualize change over ranges (2x step size)
- Absolute changes of QoI are an indicator of significance
- Limited # of runs → receive minimal information

Basic Method 2 – Sampling "LHS"

1. Define ranges for each input
2. Sample uniformly within the ranges for all inputs
3. Run model at samples
4. Analysis: plotting + correlation coefficients

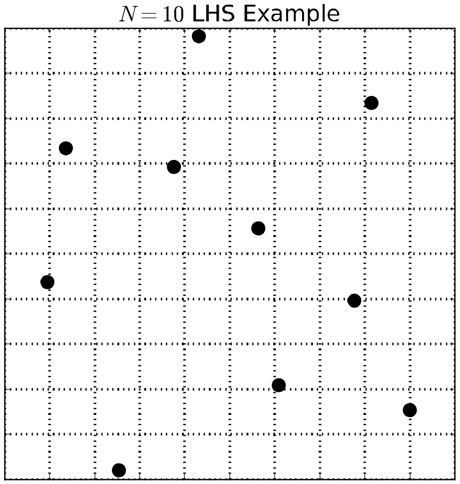
Concept – local sensitivity at many nominal values

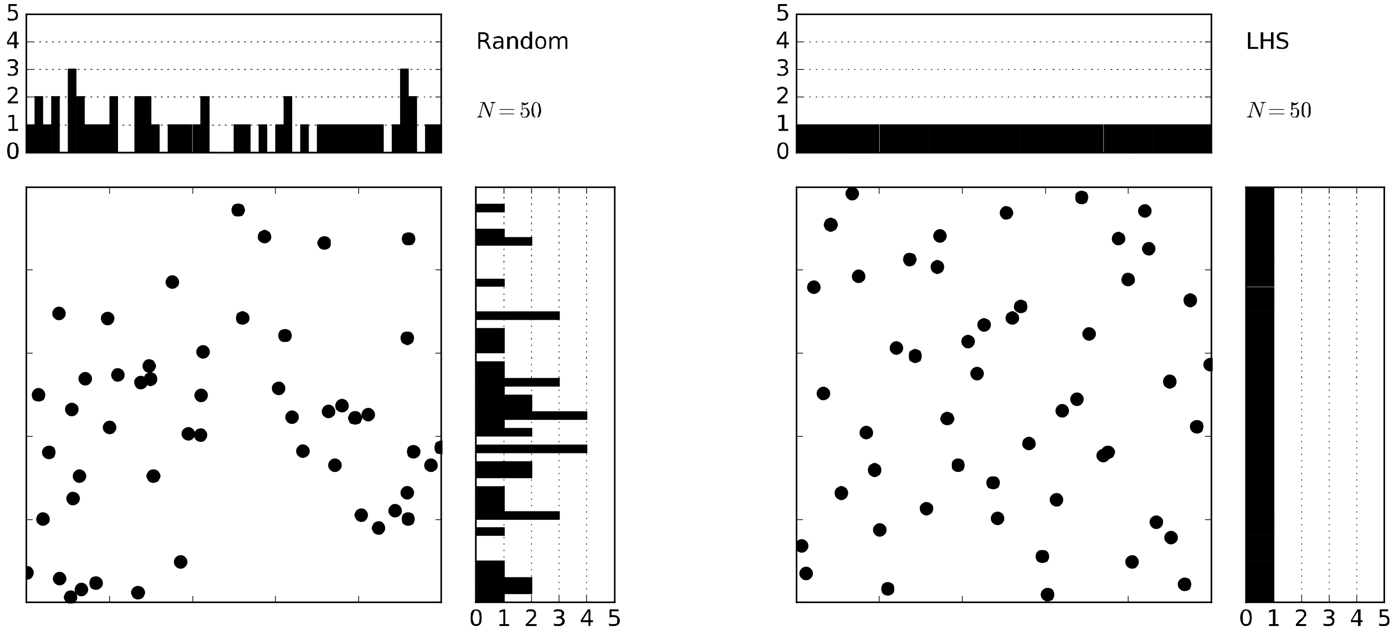
- Average the sensitivities "globally" over parameter space
- Need a lot of samples

No connotations of probability

Aside: Latin Hypercube Sampling (LHS)

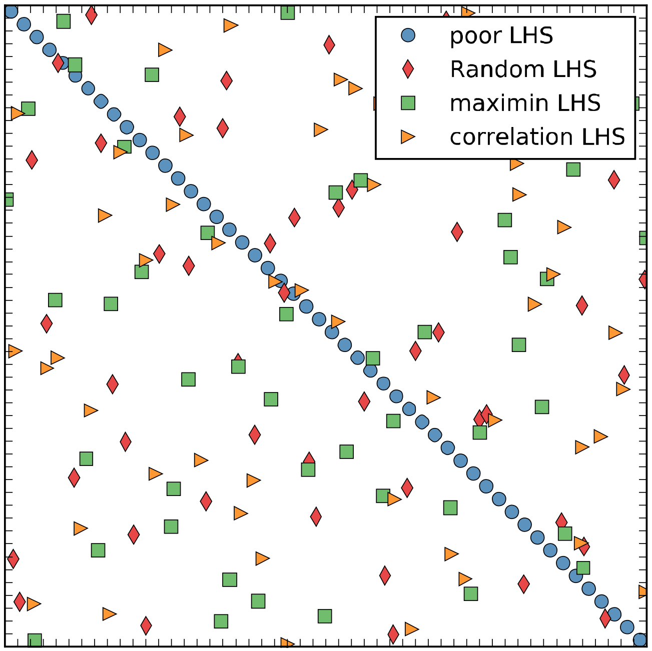
- LHS seeks to maximizes the spread of the samples by:
  - Subdividing the space
  - Selecting “active” regions to be the only one in each row/column/...
  - Placing points randomly in regions





LHS Continued

- More advanced algorithms also optimize properties of the LHS
  - Maximin – Maximize minimum distance
  - Correlation – Minimize correlation
  - Random – No further improvements
- Note: Not all LHS samples are "good"
- Key advantage of LHS sampling:
  - Dimensionally independent



Python: pyDOE

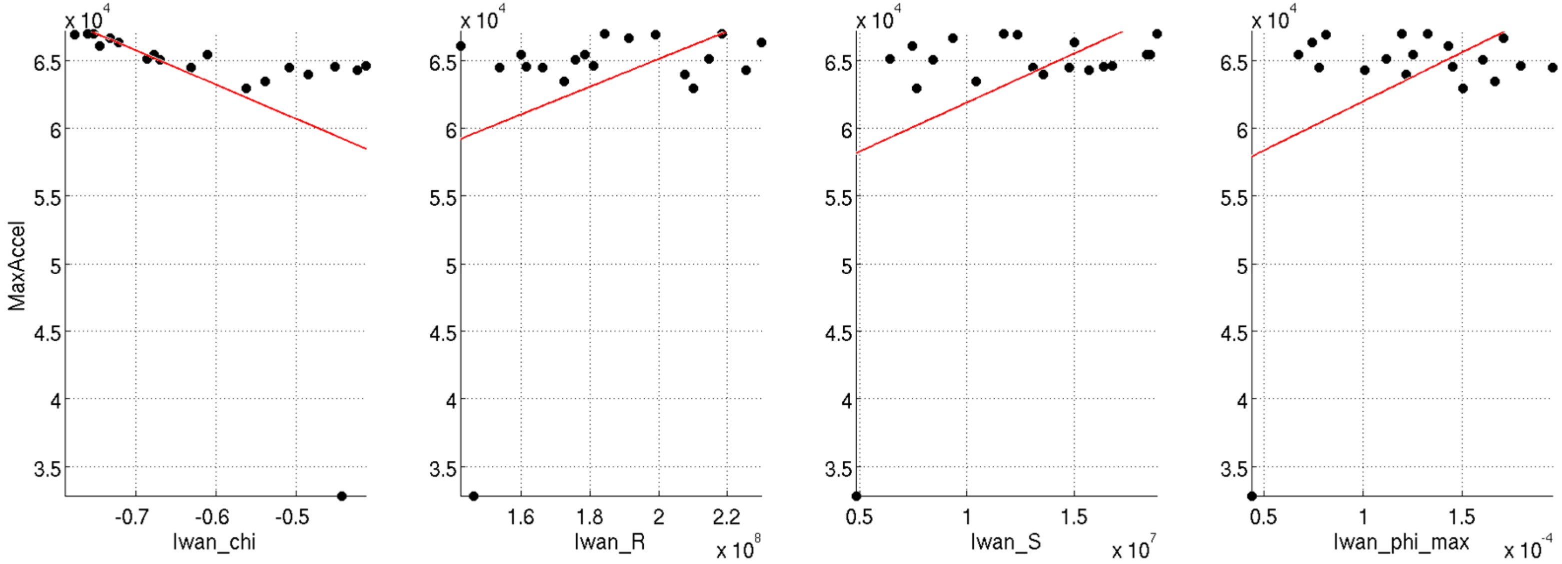
Matlab: `lhsdesign`

Dakota:

```
method
  sampling
    sample_type lhs
```

Qualitative LHS Analysis

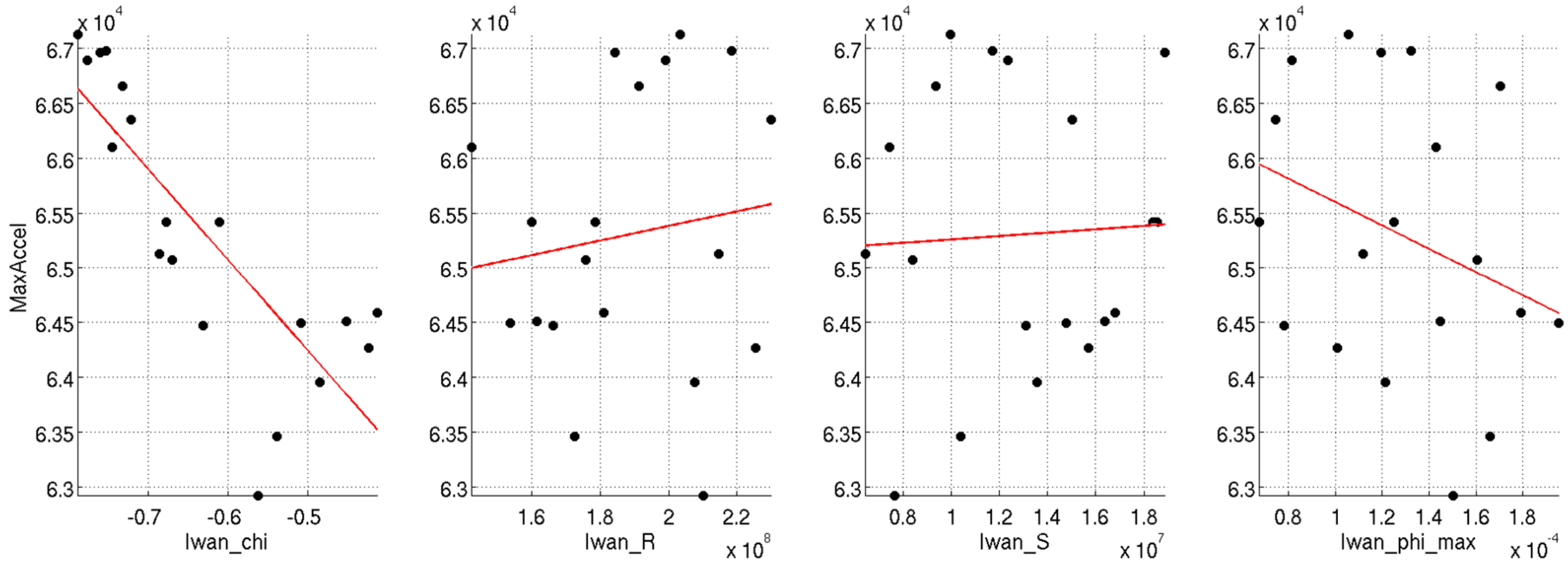
- Projection, scatterplot see nonlinear trends
- Compare vertical spread vs. trendline
  - Qualitative indicator of significance



Local Sensitivity Result:
'chi' >> 'S' >> 'R' > 'phi_max'

Qualitative LHS Analysis

- Identify outliers w/ major effect on quantitative indicators
- Investigate discrepancy between visualizations and quantitative results



Local Sensitivity Result:
'chi‘ >> 'S‘ >> 'R‘ > 'phi_max'

Quantitative LHS Analysis

Simple Correlation Matrix

	MaxAccel
chi	-0.43
R	0.25
S	0.52
phi_max	0.45

Partial Correlation Matrix

	MaxAccel	slope
chi	-0.56	0.46
R	0.18	0.34
S	0.64	0.25
phi_max	0.57	-0.21

- Correlation Coefficients
- Regression slope ∝ simple correlation
- Linear assumptions!
- Compare simple vs. partial
  - Difference indicates significance of interactions between inputs

most data analysis software will compute these also

Dakota Output

Simple Correlation Matrix among all inputs and outputs:

	Iwan_chi	Iwan_R	Iwan_S	Iwan_phi_max	MaxAccel	slope	peakf
Iwan_chi	1.00000e+00						
Iwan_R	-2.43445e-01	1.00000e+00					
Iwan_S	-1.36501e-02	2.08260e-03	1.00000e+00				
Iwan_phi_max	3.74511e-02	9.00157e-02	7.24891e-02	1.00000e+00			
MaxAccel	-4.33950e-01	2.54036e-01	5.24557e-01	4.46247e-01	1.00000e+00		
slope	3.61841e-01	1.89368e-01	1.95584e-01	-1.25004e-01	-3.46778e-01	1.00000e+00	
peakf	-3.48324e-01	2.08969e-01	5.30246e-01	4.77021e-01	9.91092e-01	-3.74105e-01	1.00000e+00

Partial Correlation Matrix between input and output:

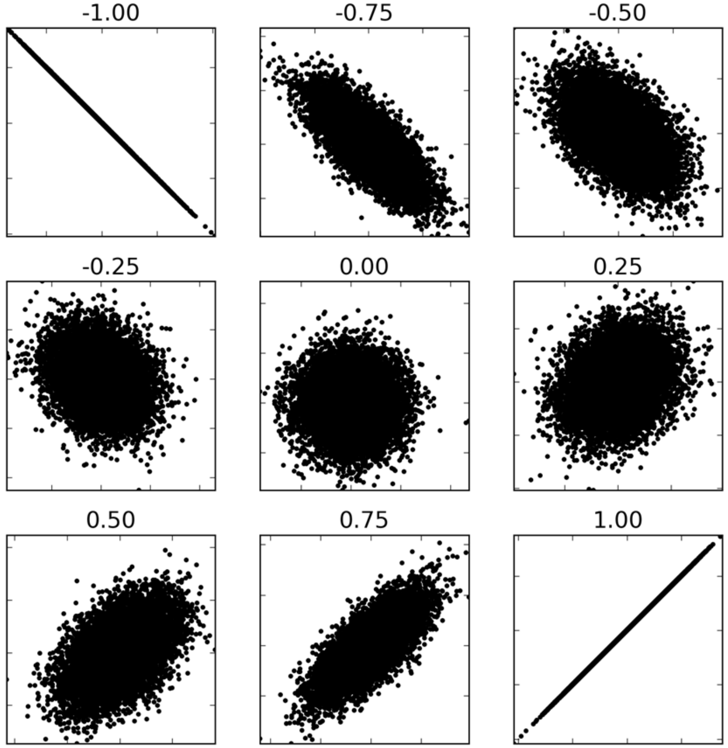
	MaxAccel	slope	peakf
Iwan_chi	-5.62312e-01	4.57113e-01	-4.63355e-01
Iwan_R	1.83893e-01	3.38446e-01	1.31099e-01
Iwan_S	6.36234e-01	2.45571e-01	6.18525e-01
Iwan_phi_max	5.72524e-01	-2.12998e-01	5.77898e-01

Quantitative LHS Analysis

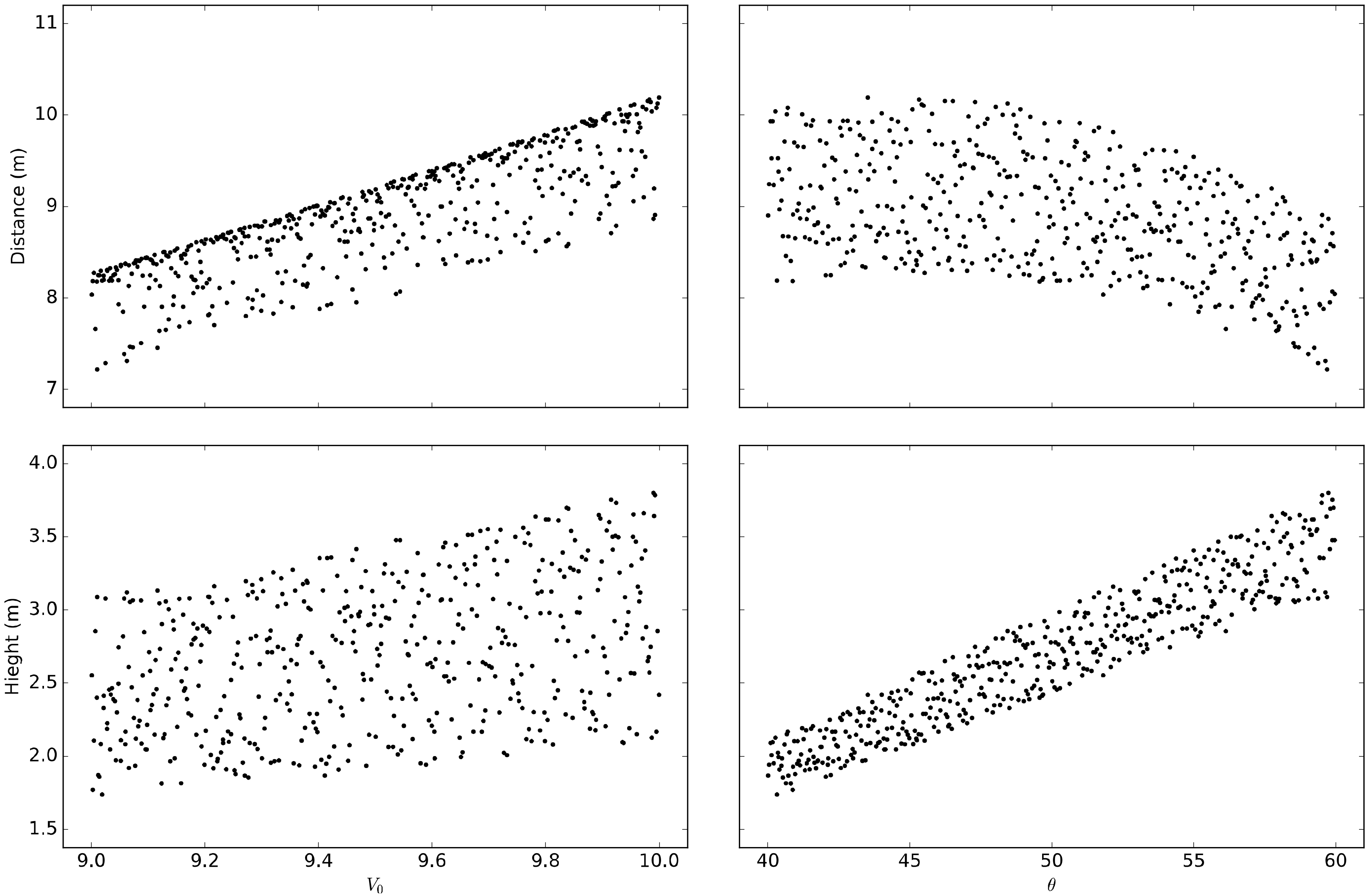
- Simple correlation:
  measures the strength and direction of a linear relationship between variables
- Partial correlation:
  like simple correlation but adjusts for the effects of the other variables

Correlation coefficients have range [-1 , 1]

0, no relationship
+1, strong positive relationship
-1, strong negative relationship



Back to Ballistics Example



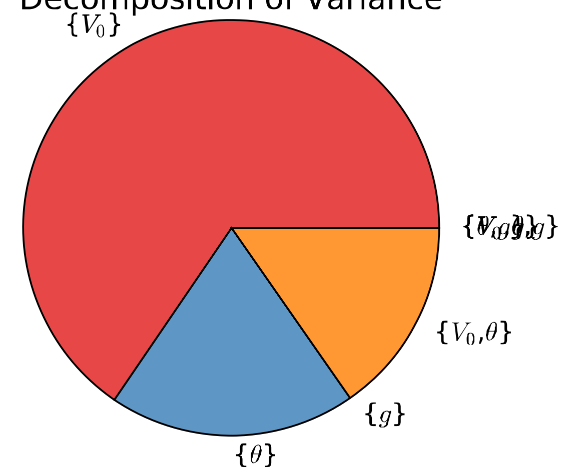
Variance Based Methods

- Another method is to decompose the variance:

$$\mathbb{V} = \mathbb{V}_{\{V_0\}} + \mathbb{V}_{\{g\}} + \mathbb{V}\}_{\{\theta\}} + \mathbb{V}_{\{V_0,g\}} + \mathbb{V}_{\{V_0,\theta\}} + \mathbb{V}_{\{g,\theta\}} + \mathbb{V}_{\{V_0,g,\theta\}}$$

  - Each $\mathbb{V}_{\{\cdot\}}$ is the variance *only* due to that parameter or group of parameters
  - Requires bounds (or distributions) on the inputs

$$0m/s \leq V_0 \leq 20m/s$$
$$0^\circ \leq \theta \leq 90^\circ$$
$$9.7m/s^2 \leq g \leq 9.9m/s^2$$



- Sensitivity:
  - First Order $\mathcal{S}_\theta = \dfrac{\mathbb{V}_{\{\theta\}}}{\mathbb{V}}$
  - Total Order $\mathcal{T}_\theta = \dfrac{\mathbb{V}_{\{\theta\}} + \mathbb{V}_{\{V_0,\theta\}} + \mathbb{V}_{\{g,\theta\}} + \mathbb{V}_{\{V_0,g,\theta\}}}{\mathbb{V}}$

$$[\mathcal{S}_{V_0}, \mathcal{S}_\theta, \mathcal{S}_g] = [0.66, 0.19, 0.00] \qquad [\mathcal{T}_{V_0}, \mathcal{T}_\theta, \mathcal{T}_g] = [0.81, 0.34, 0.00]$$

Sensitivity Methods

- Expert Opinion
- Local methods
  - **Finite differences**
  - Design of Computer Experiments
- Global methods
  - Sampling
    - Monte Carlo, Quasi-Monte Carlo
    - **Latin Hypercube Sampling (LHS)**
  - Variance Based

Low expense but not the full picture

More expensive.

Very expensive with sampling. Use alternative tools

Costs & benefits: you get what you pay for

- For N parameters
- Local sensitivities
  - Finite differences: N+1, 2N+1 model runs
  - Local estimates, no interactions
- Design of Computer Experiments
  - Full Factorial: 3^N (grows FAST) — Curse of Dimensionality
  - Other special designs → reduced cost, need to think
  - Use ANOVA – get "main effects" a.k.a sensitivity in each dimension, plus sensitivities for 2D interactions

What about sampling

Local Sensitivities

- Known cost
- Very easy to implement
- Limited information
  - Local analysis

Sampling

- Scales better with dimensions, N > 4
- Global, nonlinear effects
- Benefit is hard to predict

Warnings on Sampling

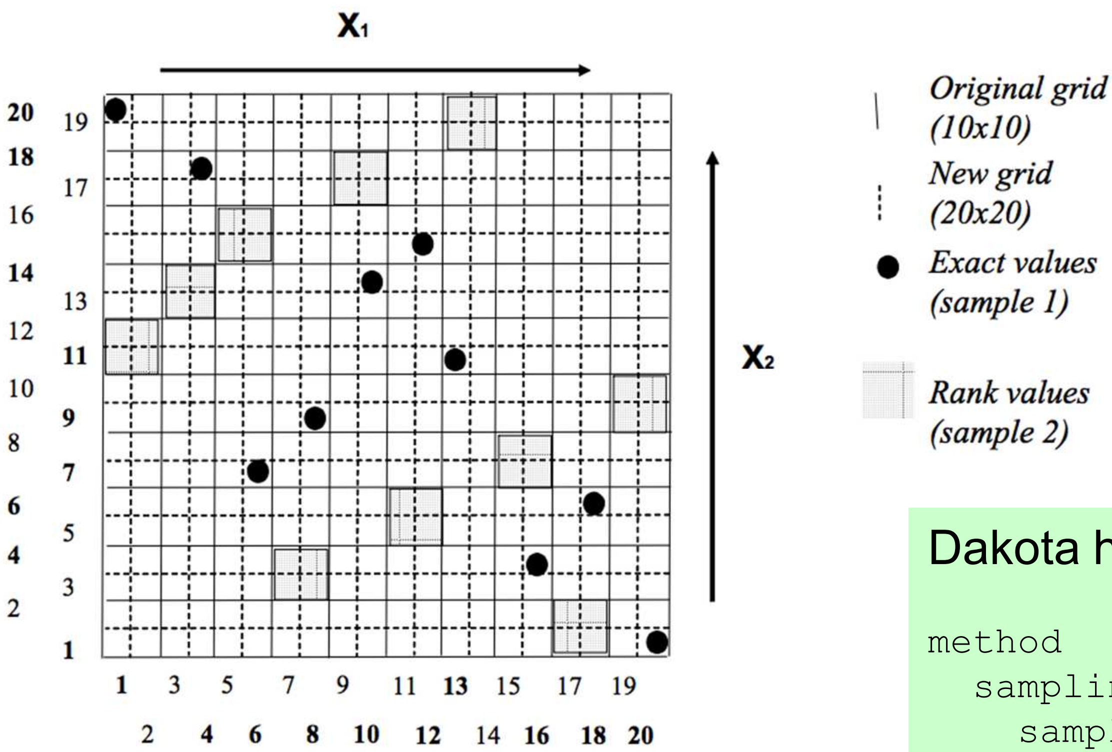
- Quality of statistics
  - Known convergence of statistics
  - Absolute accuracy of statistics is NOT KNOWN a priori
- Do not know whether the qualitative or quantitative results will help to downselect parameters

Some Guidance

- Which method?
  - Trade off simplicity and cost vs. amount of information
  - How much info do you need for sensitivity analysis?
  - **Why choose just one?**
  - Start w/ cheap local sensitivity method, add LHS
- How many LHS samples?
  - **Rule of thumb**: 10*N → get trends, mean, variance
- Use incremental studies – N, 2N, 4N, 8N, 16N …
  - Can predict computational cost
  - When benefit stops increasing, stop analysis

Incremental LHS Samples

- Advanced methods allow incremental LHS
  - Reuse previous sample for the new one



Source:
C. M. Sallaberry and J. C. Helton. *A method for extending the size of latin hypercube sample*. SAND2004-5092C, Sandia National Laboratories, 2004.UUR

Dakota has this build in

```
method
  sampling
    sample_type incremental_lhs
    previous_samples 10
    samples 20
```

3leg Sampling

- Ran 10, 20, 40 LHS samples
- See if metrics change

Simple Correlation Matrix MaxAccel

# samples	10	20	40
chi	-0.33	-0.43	-0.46
R	-0.14	0.25	0.17
S	0.62	0.52	0.49
phi_max	0.39	0.45	0.39

Partial Correlation Matrix MaxAccel

# samples	10	20	40
chi	-0.68	-0.56	-0.59
R	-0.59	0.18	0.15
S	0.78	0.64	0.61
phi_max	0.62	0.57	0.52

- Outlier has BIG effect w/ only 10 samples
- Check against local sensitivity result
- Check assumptions: are parameter ranges sensible?

Sensitivity Analysis Conclusion

- How many samples are needed to assess significance?
- **Recall goal: learn model, prioritize future analysis**
- Risks – will this impact the project, decision?
  - Miss significant parameters
  - Run future analysis on the wrong parameters
  - Future analyses is too expensive
- But remember…
  - This is exploratory work
  - Don’t spend too much time/effort

Questions?

- "Sensitivity Analysis in Practice A Guide to Assessing Scientific Models" by Saltelli, A. and Tarantola, Stefano and Campolongo, Francesca and Ratto, Marco. John Wiley & Sons, Chichester. 2004.

Exceptional service in the national interest

Sandia National Laboratories

ESP700 Lecture 3: Methods and Tools for Uncertainty Quantification

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

March 22, 2016

Models are wrong, but they can be useful

Questions to ask about the model:

What parts do we need to understand?

- Sensitivity analysis: which inputs affect the response?

How well do we know the response value?

- UQ: how do uncertainties in inputs affect the response?

Do we know enough? ARE the models useful?

- V&V → how accurate / wrong is the response?

What are the costs and benefits? VALUE?

Uncertainty Quantification

- What is uncertainty? Lack of information
- Uncertainty quantification = information quantification
  - Have a model, know the significant inputs, etc…
  - How much information do you have about QoI’s?
  - What are the significant sources of uncertainty?

1. Characterize the uncertainty in significant inputs
2. Propagate
3. Interpret

Characterization of Uncertainty

- Sources of Uncertainty
  - Model parameter, code setting (solvers), mesh, geometry, model form a.k.a model structure

Focus on parameters

- Types of uncertainty
  - Epistemic and Aleatoric
  - Provide more insight into the information we have

Very confusing!
We'll return to this later

- Quantitative methods

  → parameters require mathematical description

Mathematical Description of Uncertainty

Increasing cost, complexity, information content

- None – deterministic
- Intervals
  Lower Bound |-------------| Upper bound
- Probability distributions
  - Discrete – probability mass function (pmf)
  - Continuous – probability density function (pdf)
  - Uncertainty context
    Higher mass/density → value is more probable
- Fuzzy Probability, P-boxes, Evidence Theory

Sweet spot… (opinion)

Bounds, pdf's… Where do these come from???

- Experimental Data
- Expert Opinion/ Assumptions
- Theory/ Models

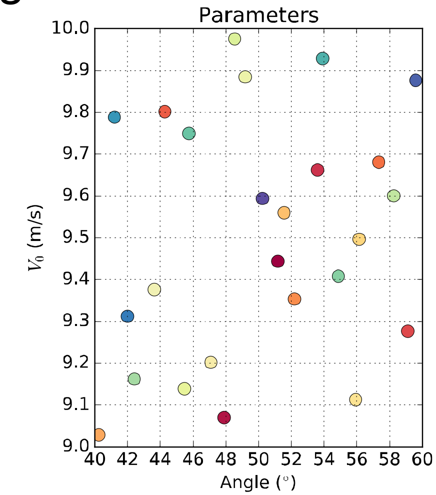
Statistics: Construct models from data and assumptions

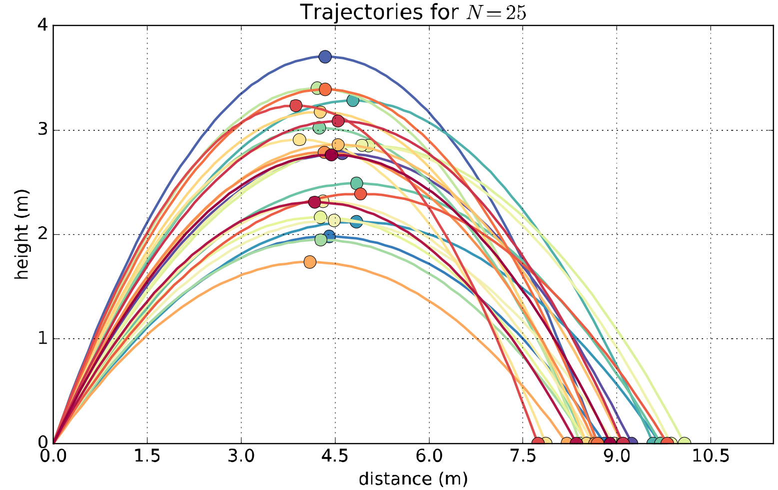
Propagation of Uncertainty

- Sampling methods – Latin Hypercube Sampling (LHS)
  - Exact same as for sensitivity analysis
  - Difference – uncertainty context
  - Based on characterization of parameter uncertainty
- MOST other methods can be formulated as
  1. Construct a surrogate model with as few realizations as possible
  2. Sample the surrogate model with many, many more samples
  3. Compute desired quantities
     - Discussed in Advanced topics

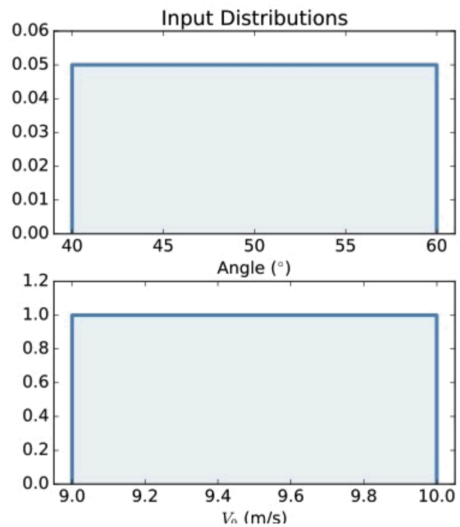
Example: Ballistic Trajectory

Neglect gravity and assume other parameters are uncertain. What can we figure out about the output?



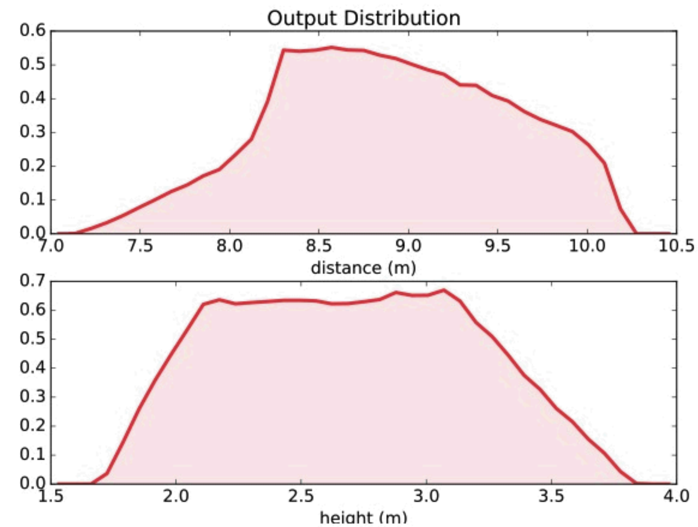


Uniform input parameter PDF's



UQ Process: Sample many times (model or surrogate)

Sample 10^5 times



Non-uniform output PDF

Types of Uncertainty – Definitions

- Epistemic (Reducible uncertainty)
  - Lack of knowledge about the appropriate value to use
  - Reduced through increased understanding or more data.
- Aleatoric (Irreducible uncertainty)
  - Cannot be reduced by further data
  - Variability (due to part-to-part, test-to-test variation, etc.)

Most parameters in engineering models have both aleatoric / epistemic components of uncertainty

Importance

- Epistemic vs. aleatoric distinction is subtle
- **What is the model attempting to predict?**
  - Ex: modeling a validation experiment
  1. Response of a specific unit to a specific event?
  2. Possible responses from a population of units, and population of events *consistent* with a scenario?
- **What do we expect to match?**
  - Only aleatoric uncertainties should match

Ballistic Trajectory Example

- Angle is determined by launcher and base
  - Launch tube creates shot-to-shot variability
  - Base is not always on level ground
- What is aleatoric vs. epistemic?
- What are we attempting to predict?

To estimate WHERE the shot will hit, we don't need to decompose into aleatoric and epistemic nature of uncertainty.

The distinction provides additional insight into the *quality* of the predictions → this is important for decisions

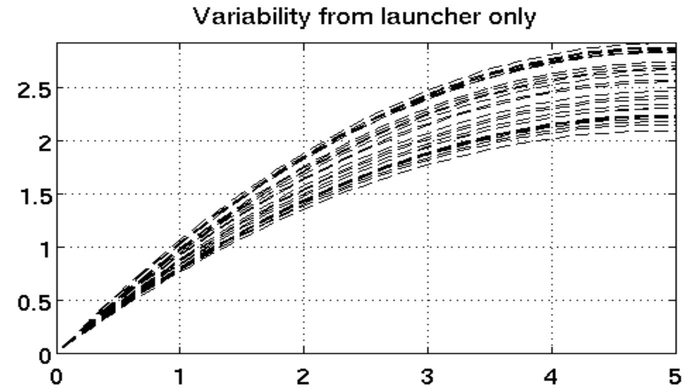
Example: Ballistic Trajectory

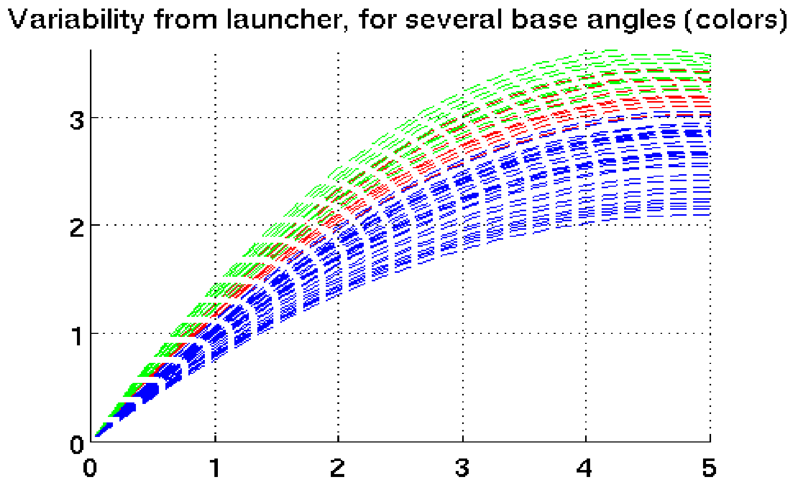
Base is fixed but unmeasured, velocity is known

Scenarios:

1. Predict range for next shot
2. Predict ranges for next dozen shots
3. Observe shots, validate model – Is our understanding of physics & uncertainty consistent w/ observed data?

Q: What is aleatoric vs. epistemic? Is the separation useful? How to use this information?



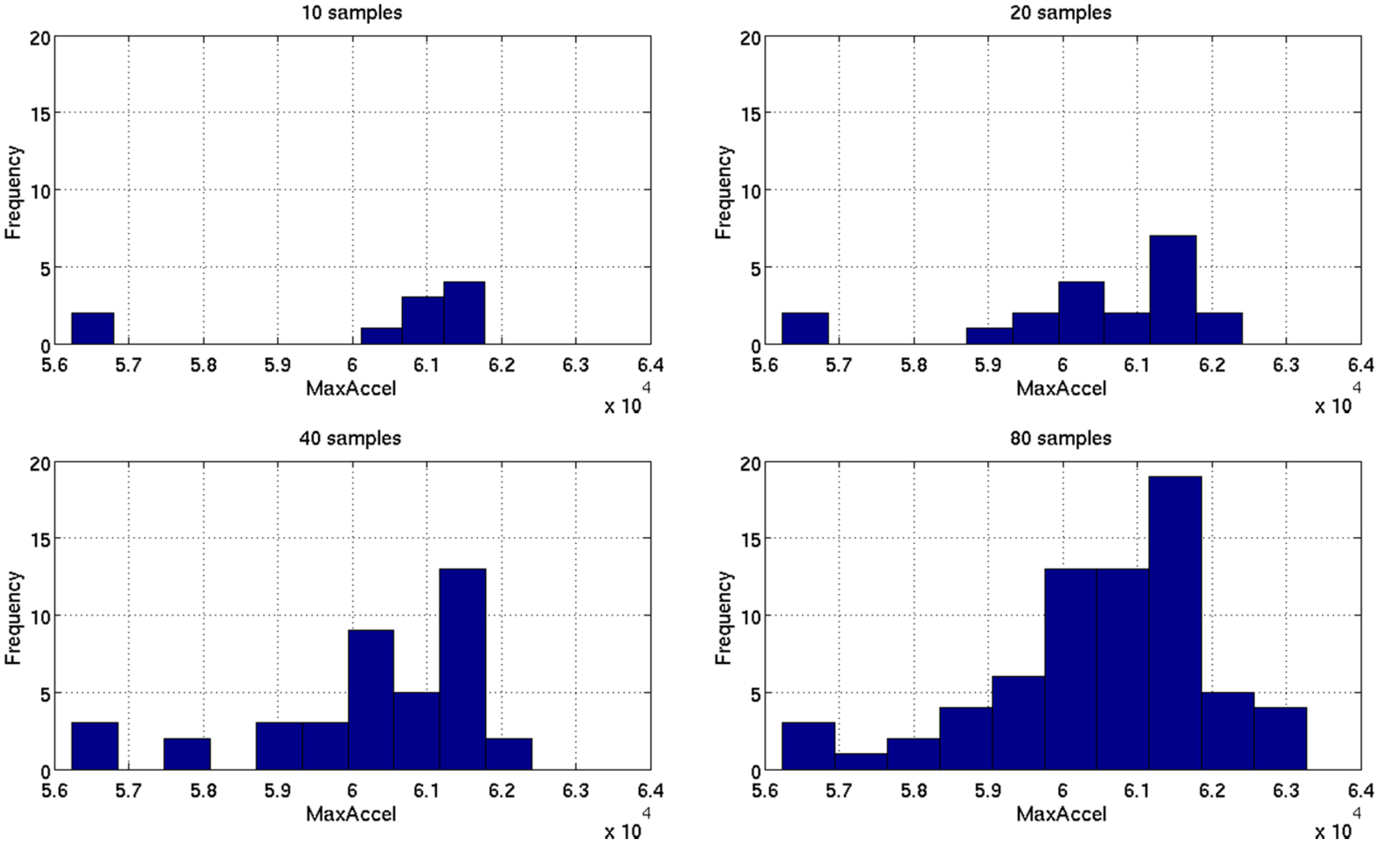


Example: 3leg Characterization

- Experimental data – 20 tests on different joints
- Iwan Model: Calibrate 4 model parameters to each
  - Result – 20 “best estimates”
  - Represents variability of joint behaviors
  - Aleatoric uncertainty
- Generalize this small set of data to a 4D joint pdf
  - Make assumptions → find a pdf that is (mostly) consistent with data
  - Example – Multivariate Gaussian, Karhunen-Loeve Expansions
- Also have epistemic uncertainty with the parameters
  - Related to assumptions
  - Related to imperfect calibration
  - Related to model form uncertainty, experimental uncertainty
  - Advanced topic – we will ignore this for now…

Example: 3leg

- 20 sets of best estimates for 4 parameters
  - Assume Gaussian distributions w/ correlations
- Propagate w/ incremental LHS: 10, 20, 40, 80 samples



Samples	Mean	Std Dev
10	60297	2131.5
20	60488	1700.4
40	60365	1558.6
80	60589	1496.3

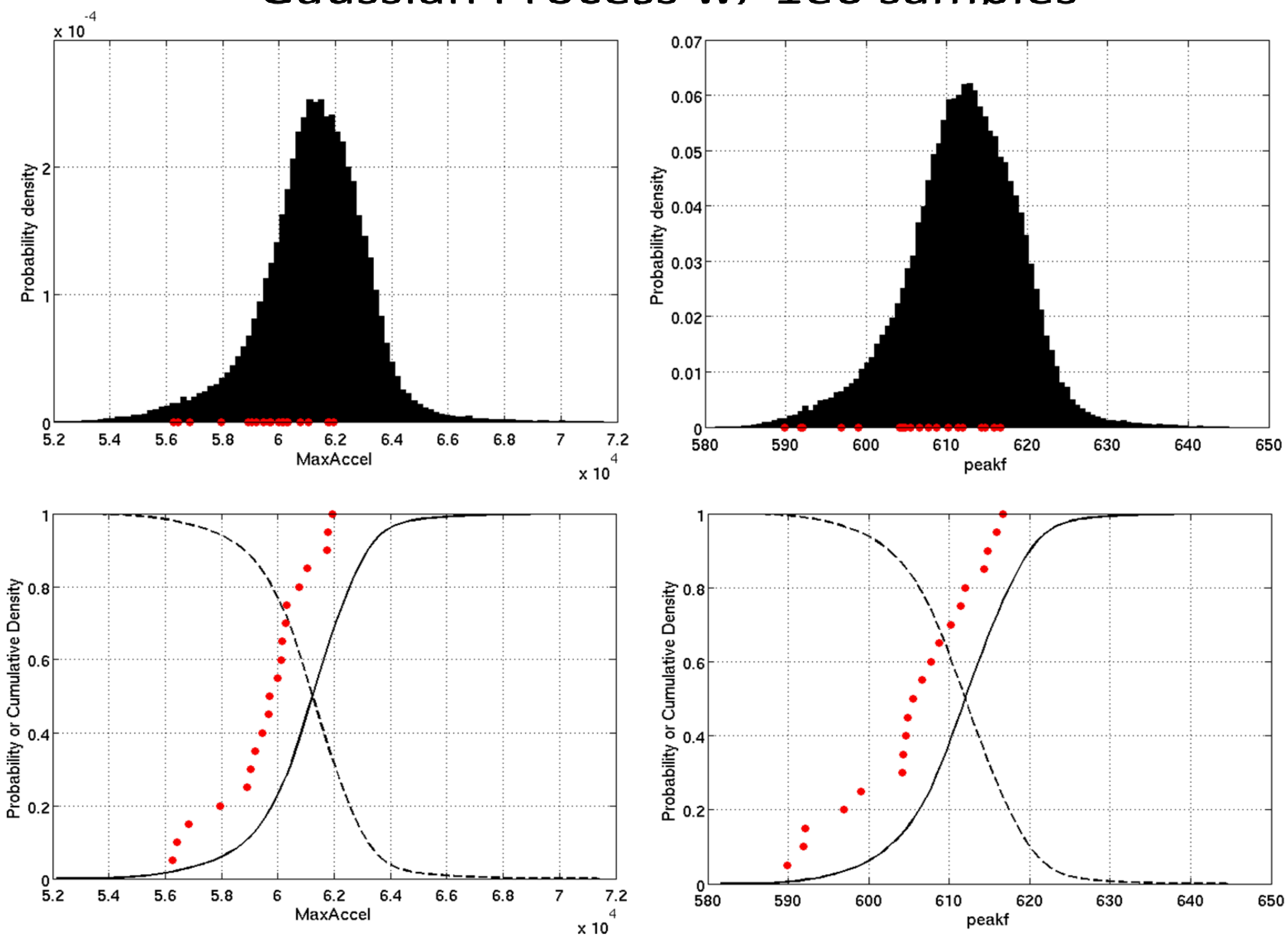
Higher moments need more samples to converge

Interpret UQ: present and assess results

- Sampling → histogram
  - With many LHS samples, normalized histogram → pdf
  - CDF – cumulative distribution function, "integrated pdf"
  - CCDF – complementary CDF
  - Many other ways to present information
- Statistics: mean, median, variance, percentiles
- Layers of information!
  - Inputs → Model → Quantity of interest
  - UQ → uncertainty / information quantification on QoI
  - Quality of UQ – convergence, data analysis on uncertainty

Example: 3leg w/ surrogate

- Construct surrogate models from LHS
  - Gaussian Process w/ 1e6 samples



Salinas propagated best estimates

Surrogate propagated Gaussians

Same information as pdf
Different look

Do we trust the surrogate?

Surrogate Models

- Difference: mathematical form and expense
  - Polynomials / PCEs
  - Collocation / Interpolation
  - Gaussian process / kriging
  - MARS/"Earth"
  - Radial basis functions
  - Neural Network
- Train from "data" = full model evaluations
  - **No physics, just fitting to data**
- Diagnostic metrics: R^2, mean absolute error, sum-squared error, cross-validation metrics
- Often the surrogate is less accurate at bounds or endpoints: use caution

- Challenge: Build a sufficiently-accurate surrogate with as few model evaluations as possible
  - What are the best model evaluation points? LHS? Grid? Sparse-Grid?
- Potentially very high dimension

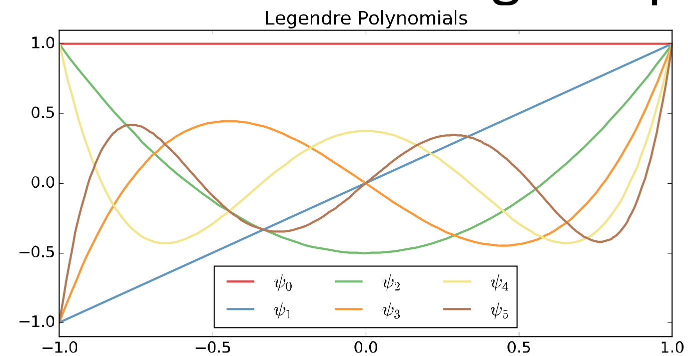
Quick Look at Surrogates: PCE

- PCE – Polynomial Chaos Expansion

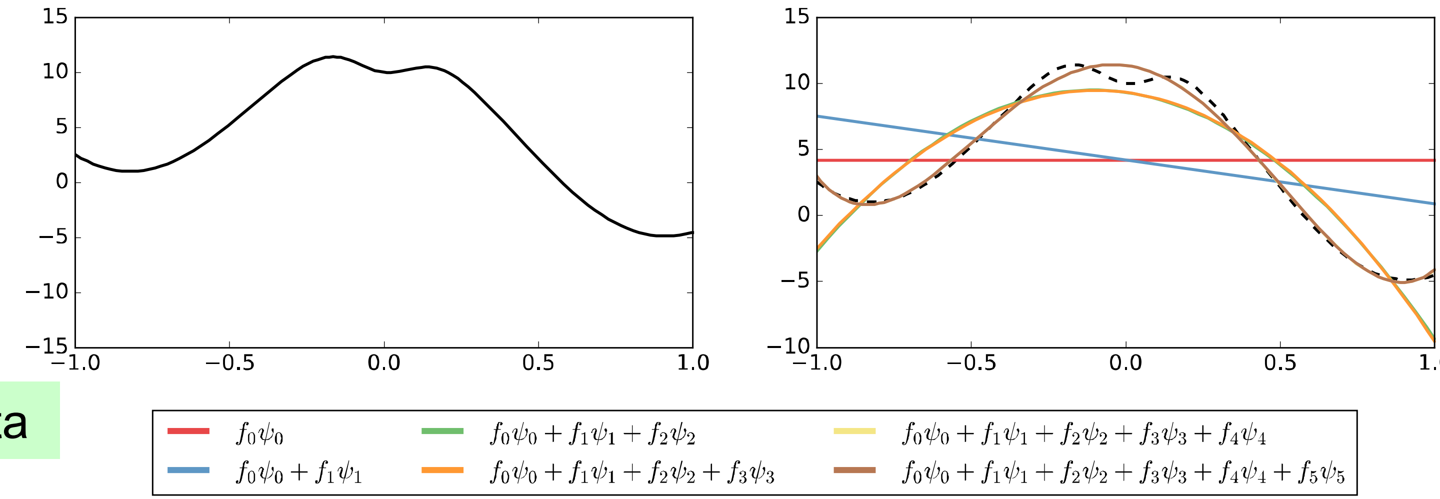
Nothing to do with dynamical chaos

  - Generalized Fourier method on orthogonal polynomials

$$\text{model},\ F \approx \sum_{k=0}^{P} f_k \Psi_k$$



Estimate coefficients with
- Regression
- Integration
- Advanced Techniques

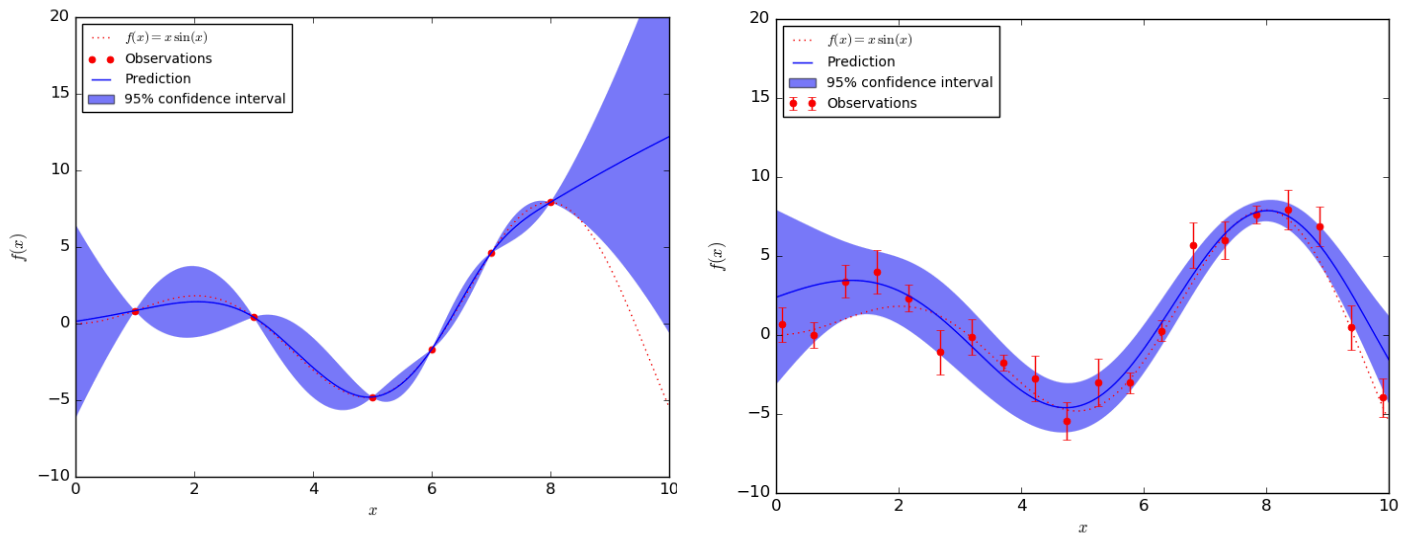


Built in to Dakota

Quick Look at Surrogates: GP

- Gaussian Processes (aka Kriging)
  - Model the function as a multivariate Gaussian distribution with a set covariance function with a noise model
  - Use optimization to find “best” parameters
  - Also provides confidence

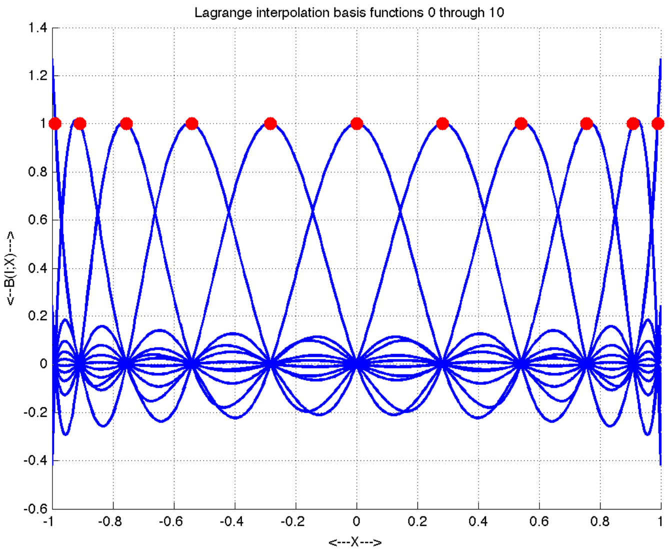
Built in to Dakota



Source: Scikit_Learn Documentation: http://scikit-learn.org/stable/modules/gaussian_process.html

Quick Look at Surrogates: Collocation

- Collocation is essentially advanced interpolation
- Can be adaptive both locally and globally to minimize sample evaluations
- Similar to PCEs except *exact* interpolation

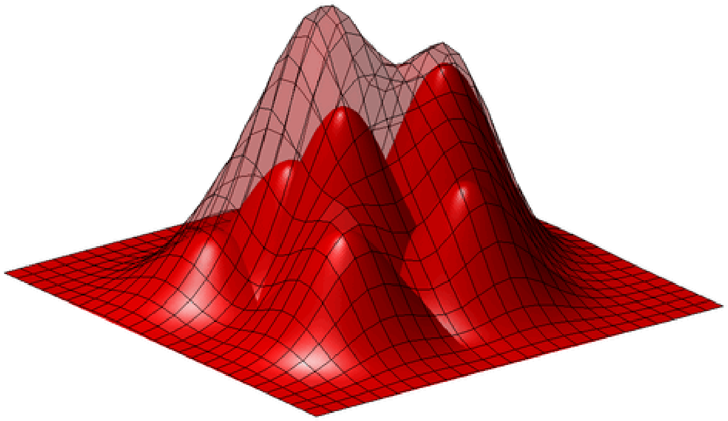


Built in to Dakota

Source: https://people.sc.fsu.edu/~jburkardt/m_src/lagrange_basis_display/lagrange_basis_display.html

Quick Look at Surrogates: RBF

- Radial Basis Functions are an *interpolation* technique
- Interpolate function as a linear combination of functions that only depend on radial distance
- Developed for geosciences
- Can handle high dimensional problems



Built in to Dakota

Source: http://www.it.uu.se/research/project/rbf

Assess UQ results

- UQ → what we know about QoI's
  - Based on model, inputs, parameters
- Also need to consider the process!
  1. Characterization of parameter uncertainty
  2. Limited LHS sampling
  3. Constructing surrogates
- What to do? How to assess the effect?
  1. Verify data analysis, document assumptions
  2. Incremental LHS → check convergence of statistics
  3. Surrogate diagnostics, cross-validation, multiple surrogates

Notes on Uncertainty Quantification

- More samples → more information
- Sampling, especially LHS, gives more samples in high probability areas
  - Very good for mean, standard deviation – “bulk properties”
  - **NOT good for tails, “extreme events”**
- Same for characterization of parameter uncertainty
- Surrogate models – accurate where training data exists

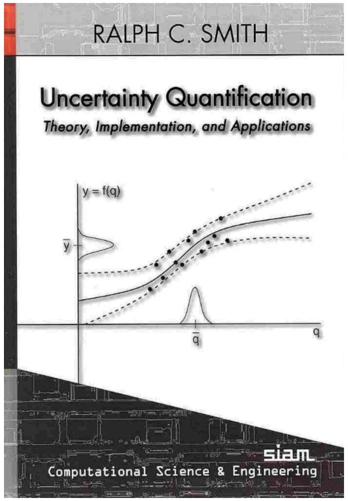
- For tails: Advanced methods – reliability

Uncertainty Quantification Conclusion

- How to do UQ? Method, # samples, surrogates?
- **Recall goal: understand QoI information**
  - **Why?: QMU? PLoAS? Design study? Validation?**
- Principles
  - Fidelity of UQ should be determined by intended use
  - Always have option to do more UQ – iterate w/ application
  - Balance sources of uncertainty ("the uncertainty budget")
    - Uncertain parameters, mesh, code, model form, UQ methods, surrogate
    - Don't need high fidelity UQ when mesh is poor quality

Questions?

- No “standard” texts
- Recent book:

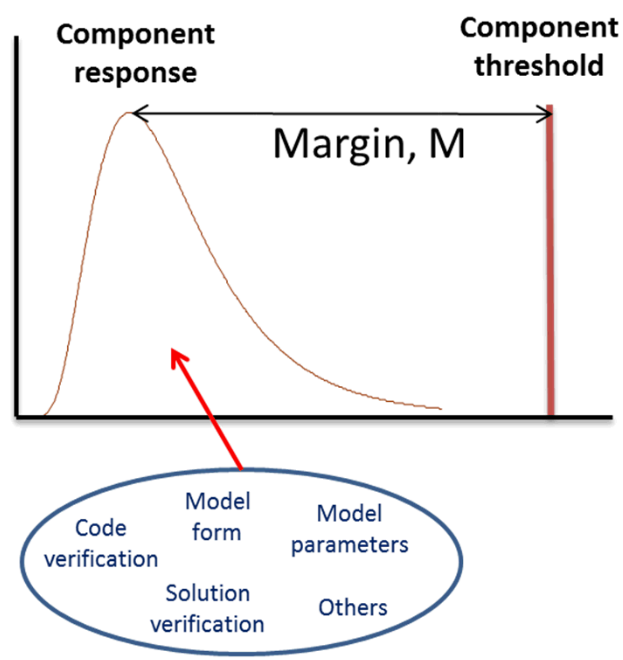


- Dakota Users and Theory Manuals have many references
- Course: *Verification, Validation and Uncertainty Quantification- Hands on Lab* – April at AWE

Big Picture

- Discussed sensitivity analysis, uncertainty quantification for model parameters
  - SA → prioritization of resources
  - UQ → pdf of QoI
- Demonstrate how each is used for an engineering project
  - 3leg example
- Understand cost and benefit
  - Uncertainty budget concept
  - Driven by the decision to be made, not math/ computer time

QMU Example



Contact

Uncertainty Quantification

Justin Winokur, Dept. 1544
(505) 844-0630
jgwinok@sandia.gov