

*Exceptional service in the national interest*



# ESP700 Pre-Lecture 3: Crash Course on Probability & Decision Theory, and Dakota

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

3 April, 2014



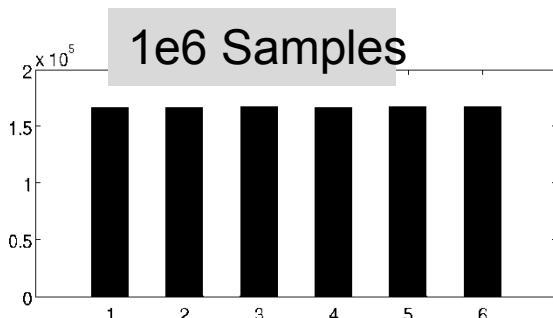
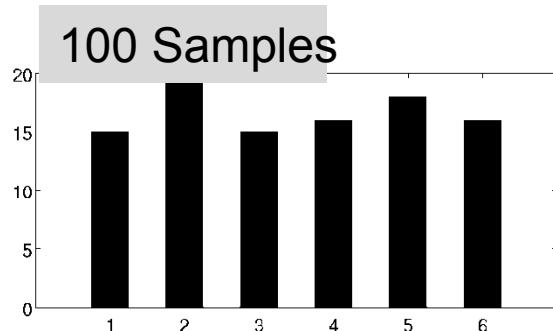
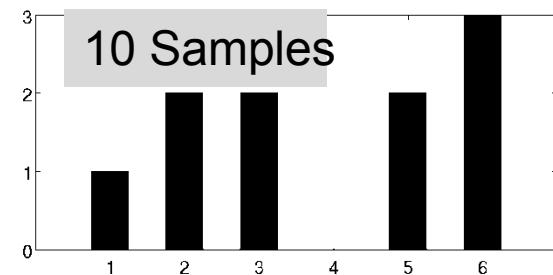
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXX

- 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**

# Statistics question: Is the Die fair?

- Observe data, find correlations  
→ Hypothesize causation
- Statistics issues:
  - Inputs & Responses/ QoI:
    - Shooter, face number before throw
    - Number of tumbles, face after throw
  - Quantity & Quality of data
- Not a focus of this course

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

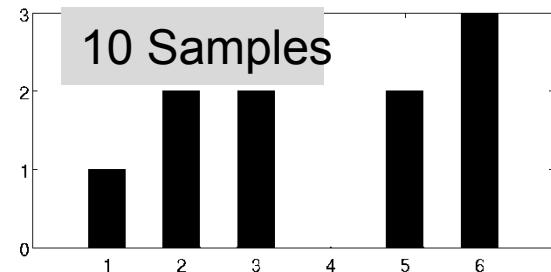


# Probability Question: What is the next roll?

- 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

# Known unknowns, unknown unknowns?

- 10 rolls of a die
  - What is the statistical model?

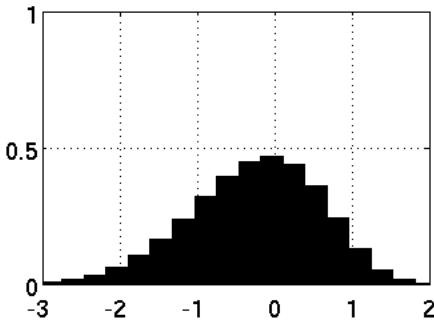
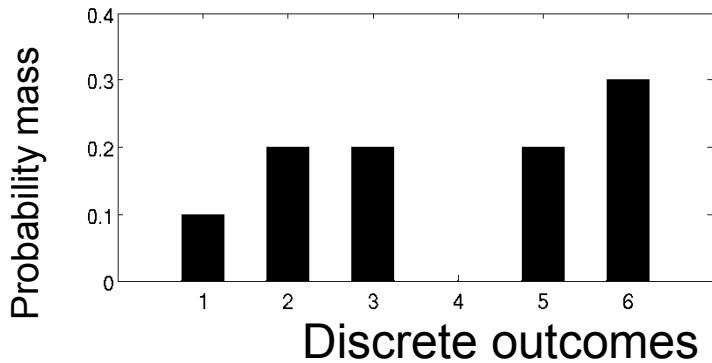


- Probability: what is the probability model?
$$P(\text{face} = 4) = 0?$$
- Inherent weakness of models
  - They include only what you put in
  - “Garbage in, garbage out”
  - “Models are wrong, some are useful”

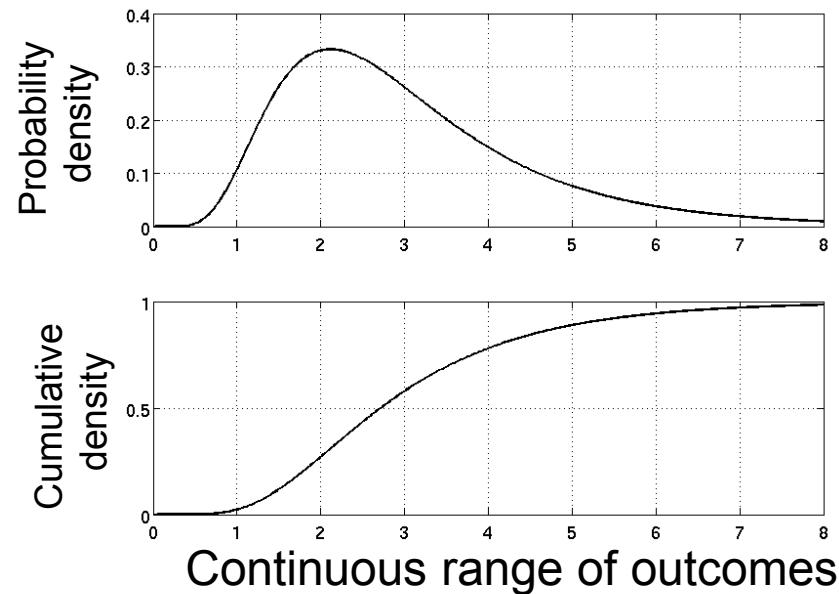
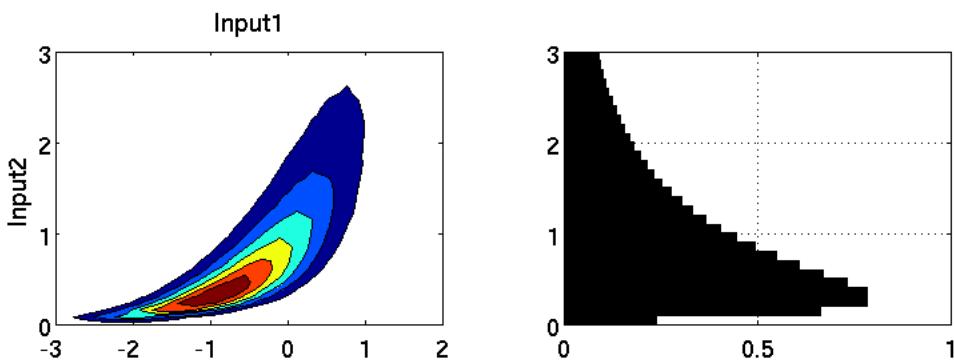
# A bit of jargon

- (Real valued) Random Variable
  - A function that associates *outcomes* with *probabilities* of their occurrence
- Discrete:
  - Coin flip – *outcome* is heads,  $P(\text{heads}) = 1/2$
- Continuous:
  - Failure – *outcome* is that material will fail if subjected to impact at 1km/s, prob =  $1/2$
- Random variable  $\longleftrightarrow$  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 datapoints

- Sample Mean  $\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$  Estimates from data can have error
- Sample Variance  $s_x^2 = \frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2$  Cannot calculate variance from 1 datapoint
- Variance of the mean  $\text{var}(\bar{x}) = \frac{s_x^2}{N}$

- 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

# Uncertainty, Probability, Decisions

- What is uncertainty? Lack of information
  - Dice example
- Mathematically describe the amount of available info
- Probability distributions are ONE way to model information and uncertainty
  - It's JUST A MODEL
- Decision theory: formal way to choose actions when the outcomes are uncertain, using probability theory

# Decision Theory

Decision = select a action

Enumerate actions

1. Actions have costs

Estimate costs & benefits

2. Actions impact the possible outcomes

Use Models

3. Outcomes have benefits

4. Value = benefit – cost

Possibility that value < desired  
→ risk

Pick the action to maximize the predicted value,  
based on which outcomes you expect to happen

Engineering question:  
Can you make money from this?

- How would you find out?
- Do these theories actually help?
  - Design of Experiments
  - Statistics
  - Probability
  - Sensitivity analysis
  - Uncertainty quantification
  - Decision theory

# Die Game

- Pay \$, guess the face number & win!
- Have Sandia's \$\$\$\$ to spend
- Based on available knowledge:
  - Should you play?
  - Which number to pick?
  - How much to bet?
- What is the expected value? Risk?

# Layers of Decisions

- Gather more info to improve the decision?
  - **This is ALSO a decision problem**
- Examples:
  - Consider additional actions
  - Characterize the die ( **improve models** )
  - Understand the payout ( **understand models** )
  - See if model predictions match gameplay ( **validate** )
- Is the added benefit worth the additional cost??

**If you don't know how the top decision is made,  
you will not make the best sub-decisions**

# Questions?

- **Probability Theory** – Introduction to Probability (Bertsekas)
- **Decision Theory** – Making Hard Decisions (Robert T. Clemen)

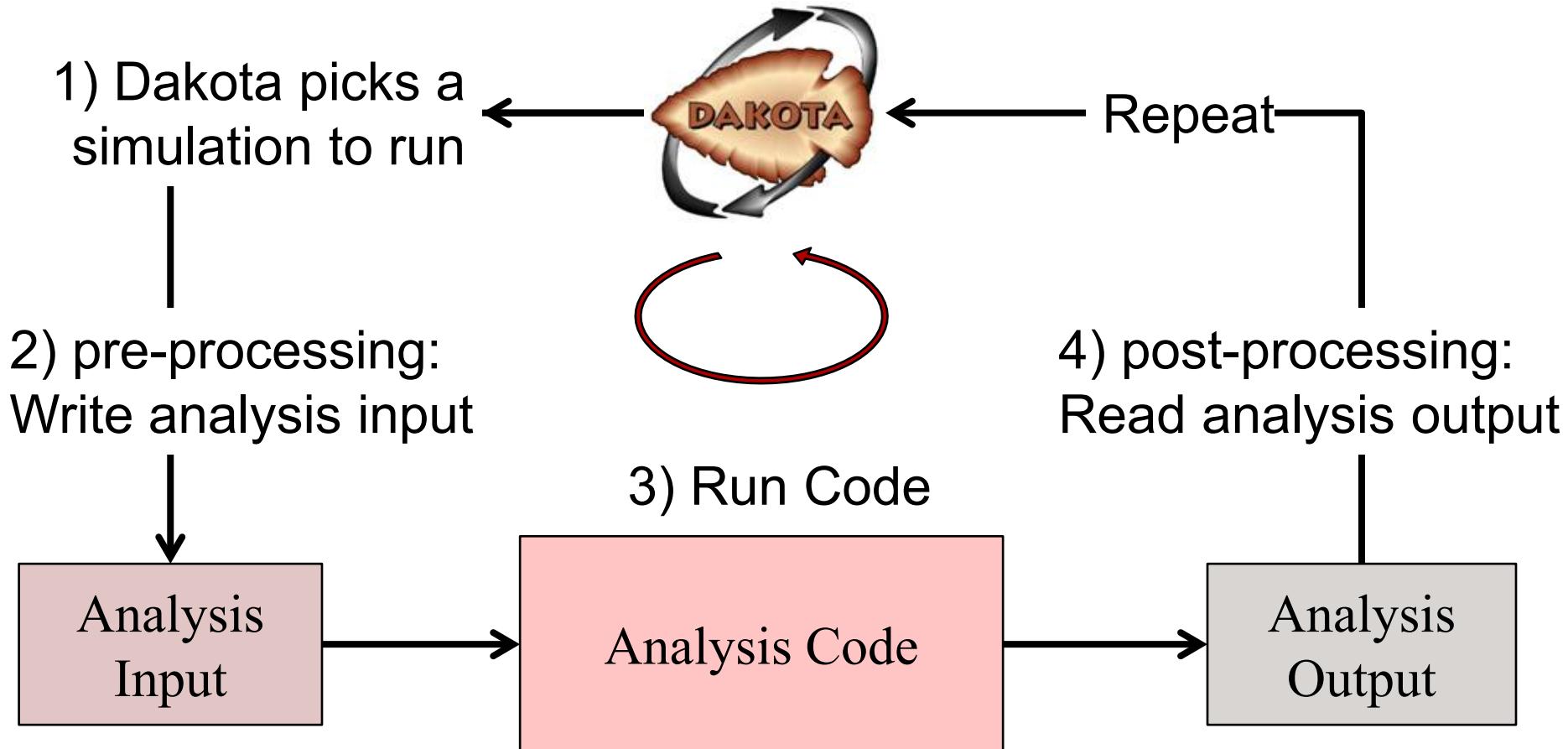
# What is Dakota?

- **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.
- No scripts

## Automation

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

HOW LONG CAN YOU WORK ON MAKING A ROUTINE TASK MORE  
EFFICIENT BEFORE YOU'RE SPENDING MORE TIME THAN YOU SAVE?  
(ACROSS FIVE YEARS)

		HOW OFTEN YOU DO THE TASK					
		50/DAY	5/DAY	DAILY	WEEKLY	MONTHLY	YEARLY
HOW MUCH TIME YOU SHAVE OFF	1 SECOND	1 DAY	2 HOURS	30 MINUTES	4 MINUTES	1 MINUTE	5 SECONDS
	5 SECONDS	5 DAYS	12 HOURS	2 HOURS	21 MINUTES	5 MINUTES	25 SECONDS
	30 SECONDS	4 WEEKS	3 DAYS	12 HOURS	2 HOURS	30 MINUTES	2 MINUTES
	1 MINUTE	8 WEEKS	6 DAYS	1 DAY	4 HOURS	1 HOUR	5 MINUTES
	5 MINUTES	9 MONTHS	4 WEEKS	6 DAYS	21 HOURS	5 HOURS	25 MINUTES
	30 MINUTES		6 MONTHS	5 WEEKS	5 DAYS	1 DAY	2 HOURS
	1 HOUR		10 MONTHS	2 MONTHS	10 DAYS	2 DAYS	5 HOURS
	6 HOURS				2 MONTHS	2 WEEKS	1 DAY
	1 DAY					8 WEEKS	5 DAYS

Good news – Dakota team can help

# Tools in ESP700

- See Dakota in action
  - Demonstrate capabilities/ methods
  - Simple workflow
- Learn about available resources
- What you won't see
  - Dakota tutorial
  - Scripting details
  - Complicated data analysis
- Today's examples also use Matlab
- Similar tools:
  - JMP
  - Minitab
  - R
  - Octave
  - Excel
  - Etc...

# Questions?

- Dakota resources:
  - [dakota.sandia.gov](http://dakota.sandia.gov)
  - Dakota Product Manager for 1500: Ken Hu
  - 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

3 April, 2014



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-XXXX

## 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?**

# 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

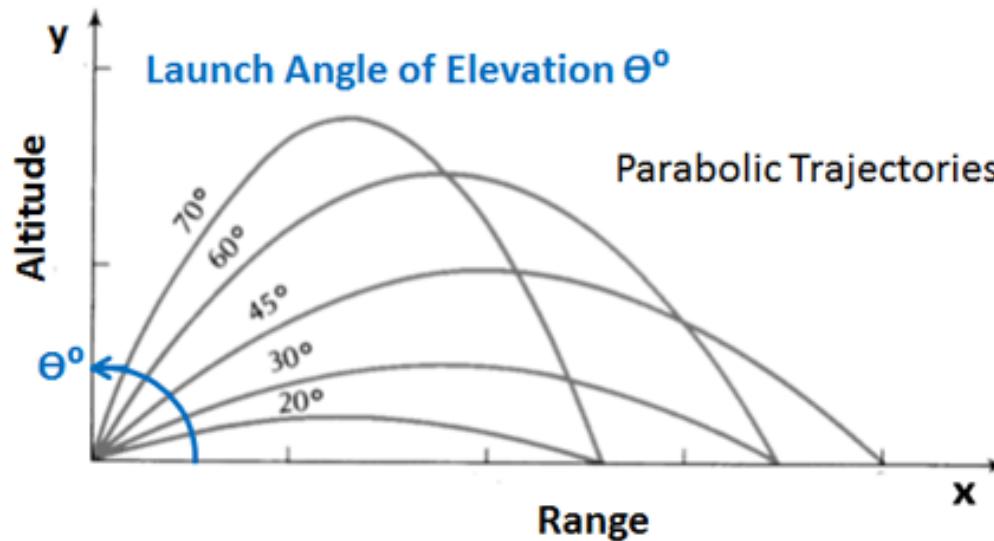
- Introduce topics at a high level
- Describe the basic methods
- Promote Dakota usage
- Demonstrate methods and tools
  - Simple example – compute ballistic trajectory
  - Case study – 3 leg structural dynamics problem
- **Leave with a basic knowledge of methods, tools, context – there is much more**

# 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

Range  $R$  vs Launch Angle  $\Theta$  for a Given Initial Velocity  $V_0$

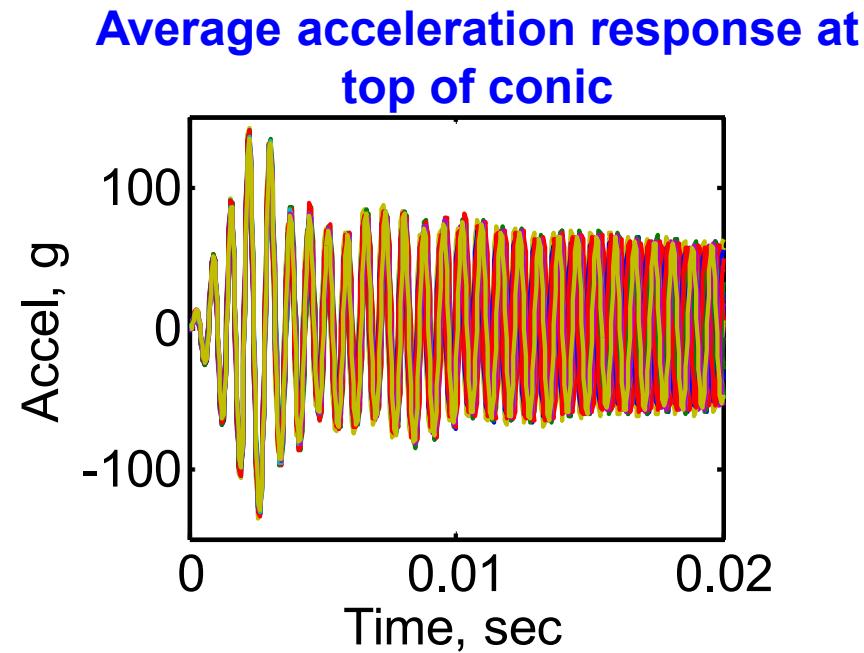
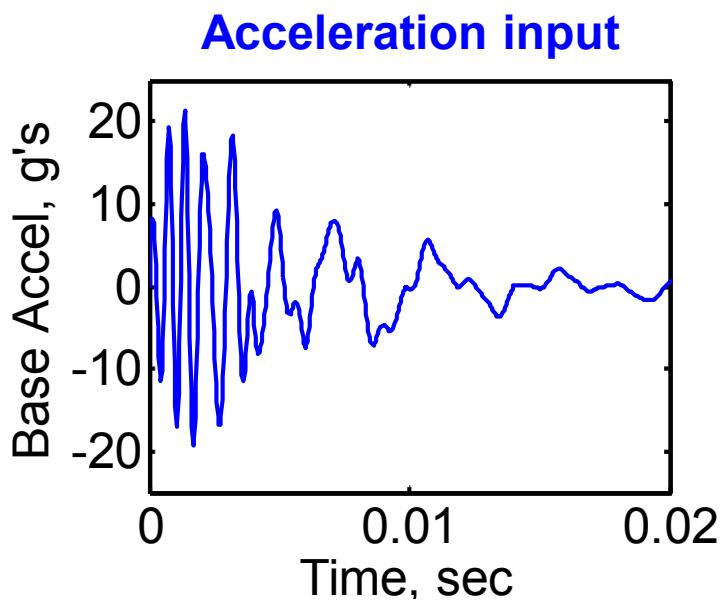


- Inputs
  - Angle,  $\theta$
  - Initial Velocity,  $V_0$
  - Gravity
- Quantities of Interest
  - Max Height,  $H$
  - Range,  $R$

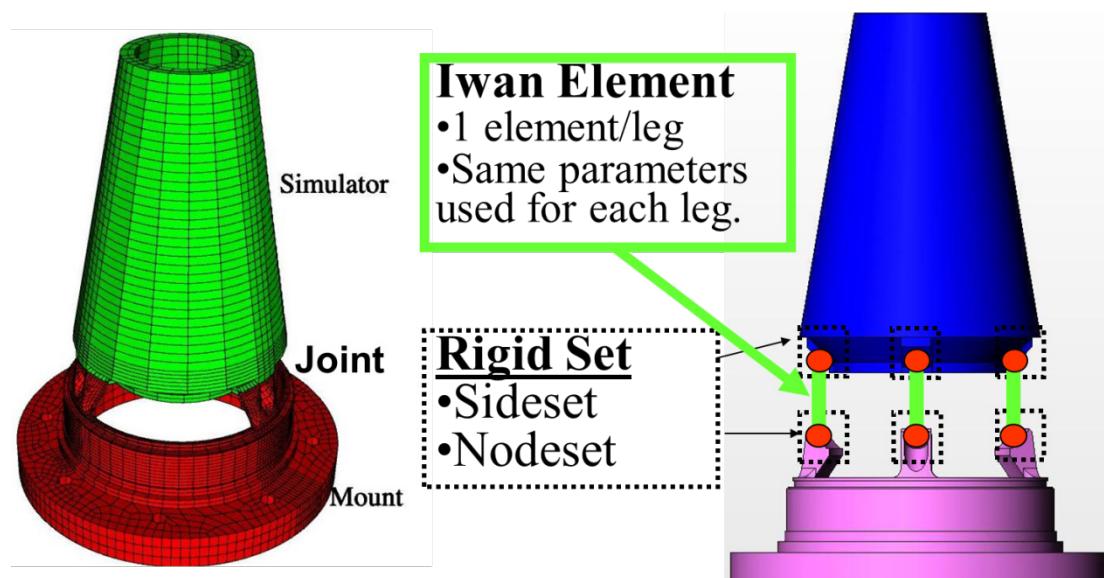
# Case Study: 3leg model



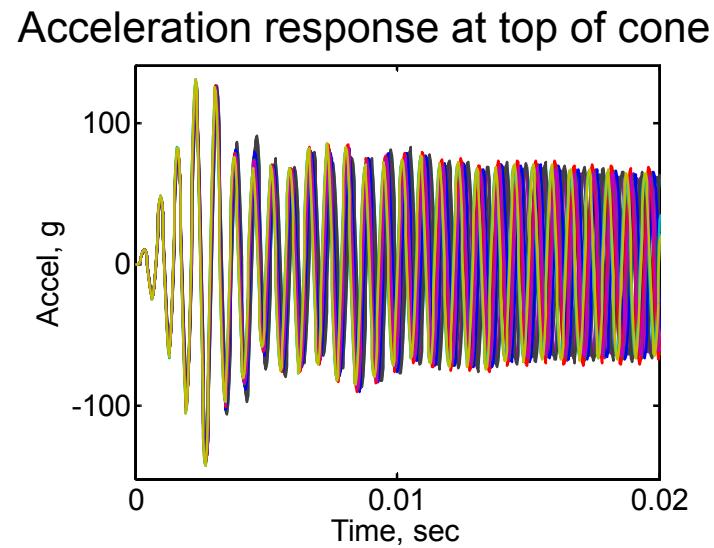
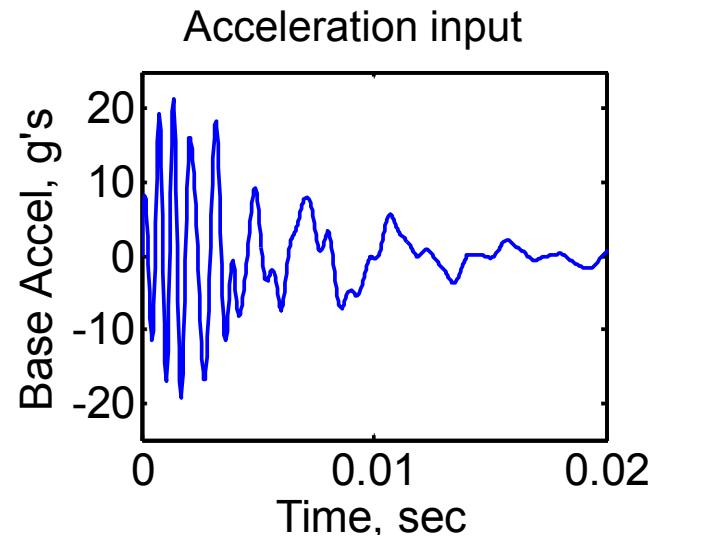
- Hardware consists of 3 top conic sections and 3 bottom sections
- 9 total combinations of top/bottoms



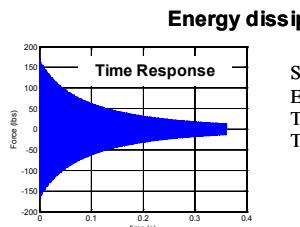
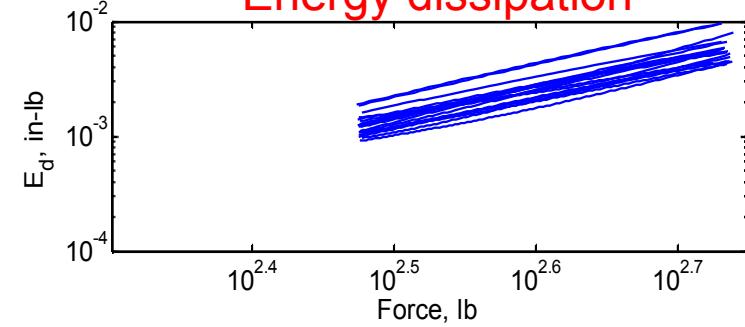
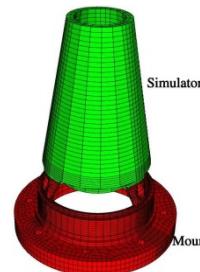
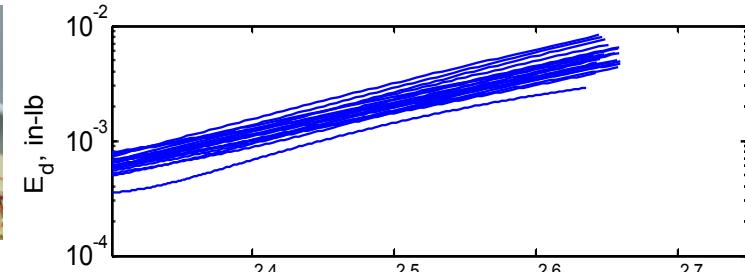
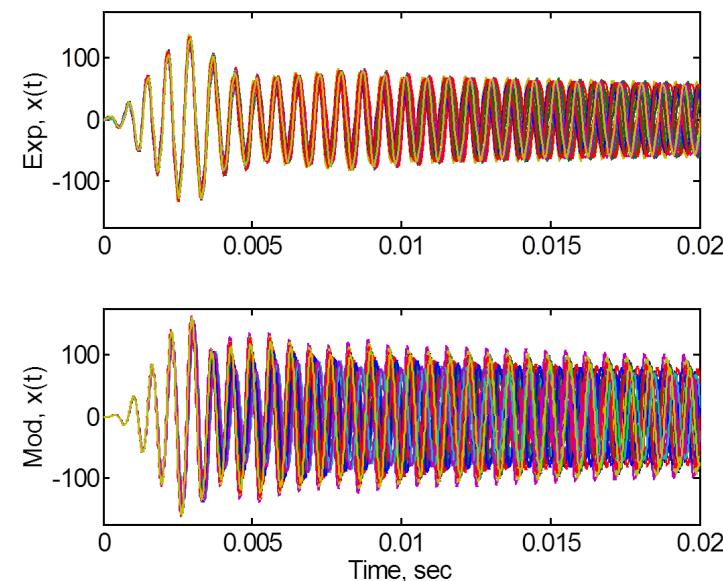
# Case Study: 3leg model



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



# Quantities of interest

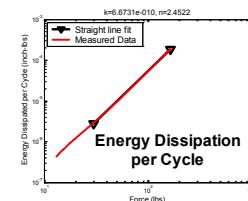
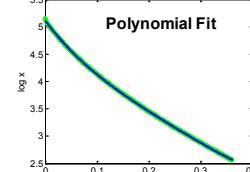


Simple free decay:  $x(t) = e^{-\zeta\omega_n t} \cos(\omega_n t)$

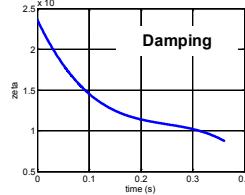
Envelope of the peaks:  $x(t) = e^{-\zeta\omega_n t}$

Take the logarithm:  $\log(x) = -\zeta\omega_n t$

Take the derivative:  $\frac{d(\log(x))}{dt} = -\zeta\omega_n$



$$E_d = c \frac{\xi F^2}{m^2 f_n^2}$$



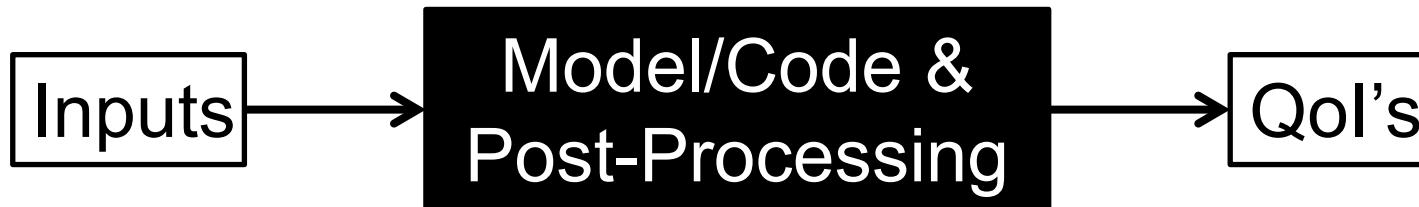
Slope  
Peak Force  
Max Acceleration

# 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

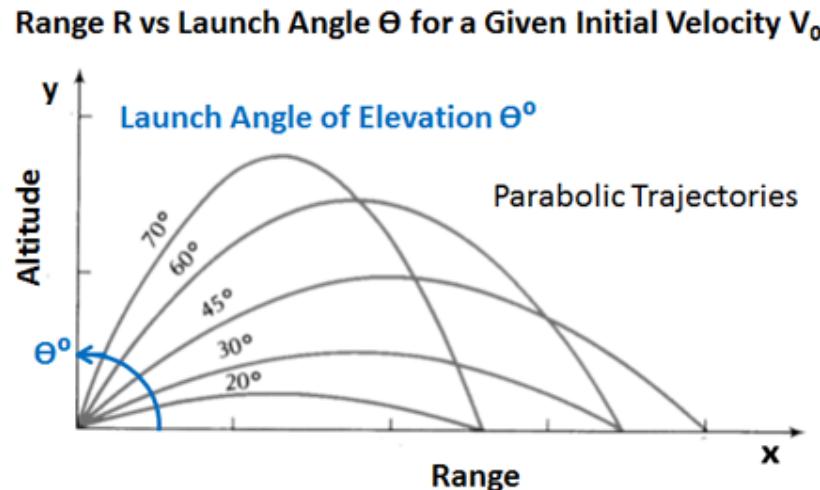
- Think of models / code as a black box
  - Inputs go in, QoI's come out



- 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

- How do changes to inputs affect the response?
  - How “sensitive” is the response to each input?
  - Direction and magnitude
- 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”
    - $V_0 \uparrow$  → Height  $\uparrow$  & Range  $\uparrow$
    - Gravity  $\uparrow$  → Height  $\downarrow$  & Range  $\downarrow$
    - $\theta \uparrow$  → Height  $\uparrow$  & Range ??
    - $V_0 \uparrow, \theta \downarrow$  → 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: Finite differences
- Must pick nominal point and step sizes
- Example: Ballistic Trajectory
  - Nominal  $\theta = 45^\circ, V_0 = 10 \text{ m/s}, g = 10 \text{ m/s}^2$
  - Step size = +10%
  - Results:

$$\text{Range} \quad \left. \frac{\partial R}{\partial \theta}, \frac{\partial R}{\partial V_0}, \frac{\partial R}{\partial g} \right|_{nom} = [-0.00 \ 0.21 \ -0.09]$$

$$\text{Height} \quad \left. \frac{\partial H}{\partial \theta}, \frac{\partial H}{\partial V_0}, \frac{\partial H}{\partial g} \right|_{nom} = [0.04 \ 0.21 \ -0.09]$$

# Lessons

- Sensitivities:  $V_0 > g > \theta$ 
  - On Earth: how much does gravity vary?
  - **Most sensitive  $\neq$  most significant**
  - Must consider the possible range of values
- Compare sensitivity of height and range
  - Depends on the QoI
- Repeat at:  $\theta = 1^\circ, V_0 = 10 \text{ m/s}, g = 10 \text{ m/s}^2$ 
  - Sensitivities:  $\theta > V_0 > g$
  - Nominal value matters

Cheap – bare minimum of model evaluations

Limited – Estimate of main effects, no interactions

# Case Study: 3leg

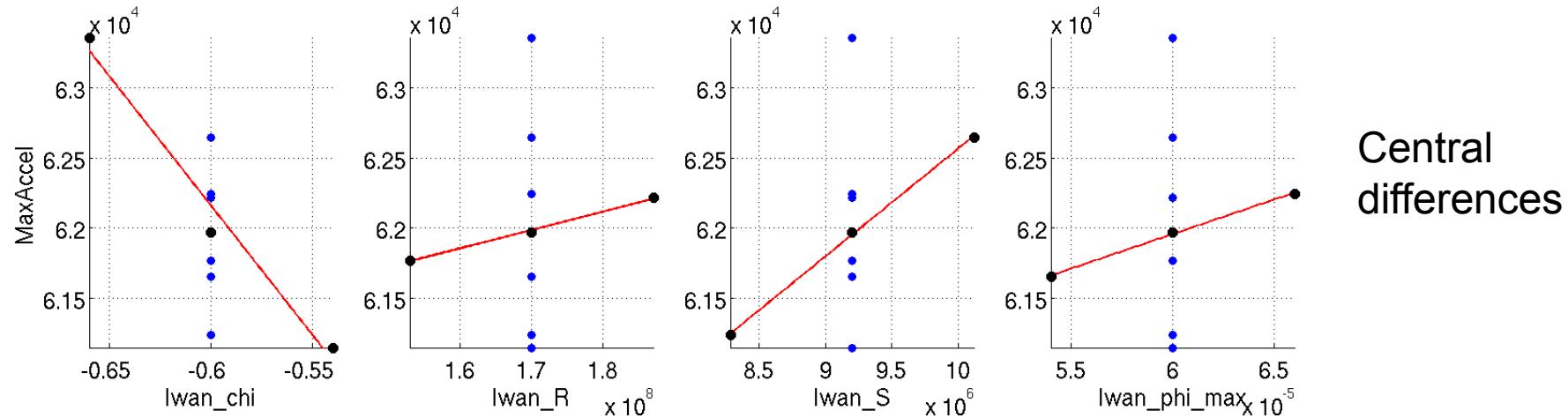
- Local sensitivity
  - Pick nominal values for 4 Iwan parameters
  - Pick range & step size = 10%
  - QoI's are most sensitive to  $\text{Phi}_{\text{max}}$
- Absolute change in response over whole range
  - $\text{chi}$  and  $\text{S}$  are most significant

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

**'chi' >> 'S' >> 'phi\_max'  $\approx$  'R'**

# “Projection” Plots

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



- 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
4. Analysis: plotting + correlation coefficients

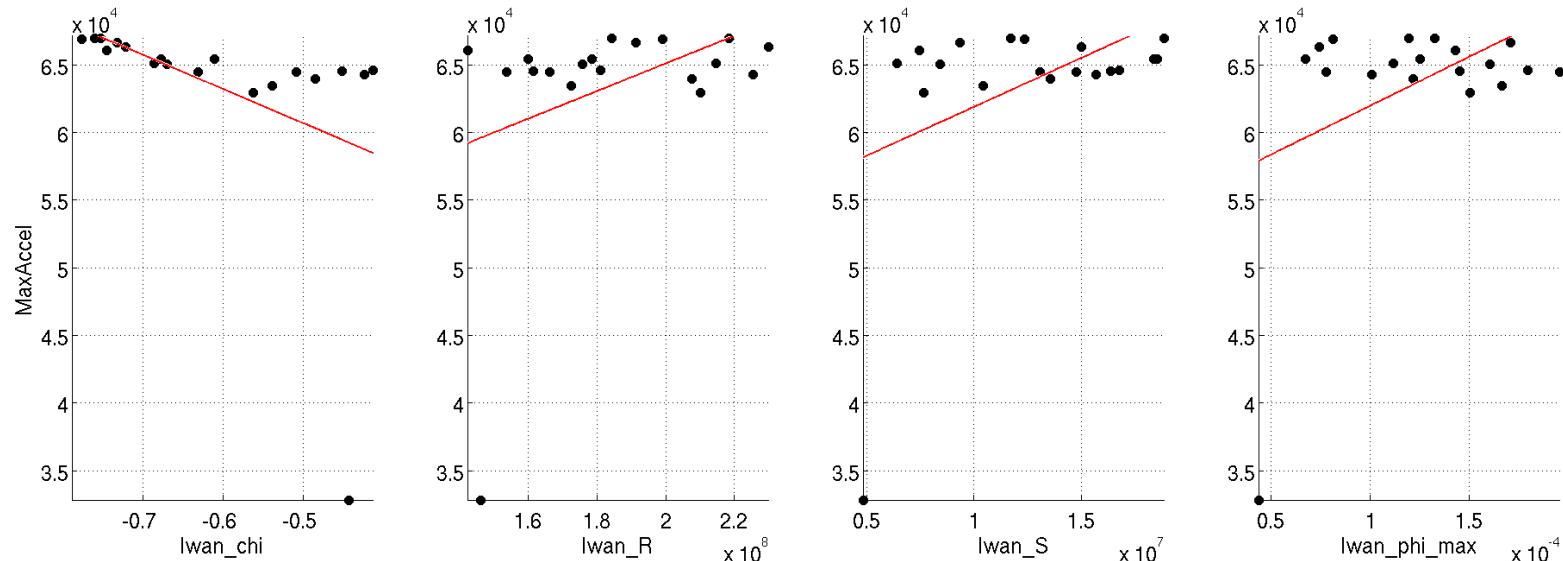
## Matlab demo – Latin Hypercube Sampling

- **Concept** – local sensitivity at many nominal values
  - Average the sensitivities “globally” over parameter space
  - Need a lot of samples

No connotations of probability

# Qualitative LHS Analysis

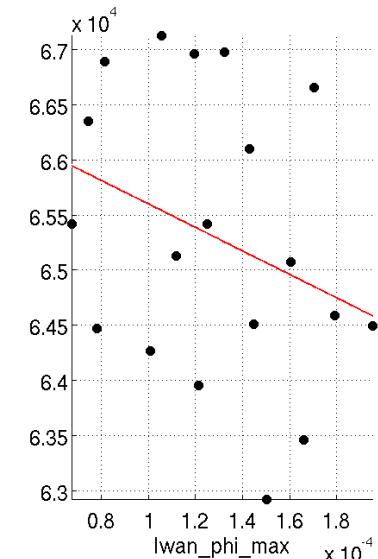
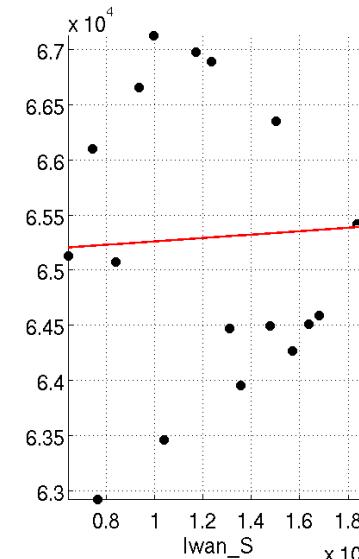
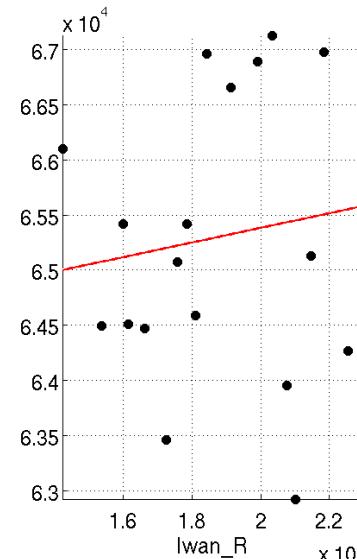
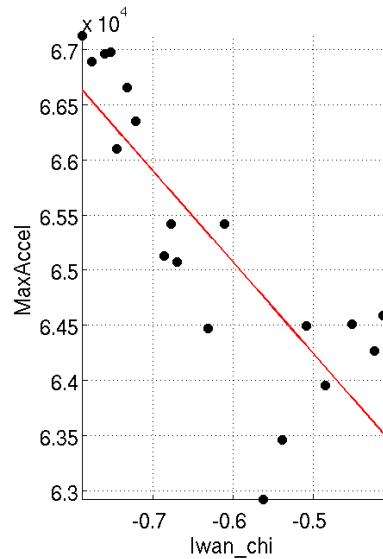
- Projection, scatterplot see nonlinear trends
- Compare vertical spread vs. trendline
  - Qualitative indicator of significance



**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  $\propto$  simple correlation
- Linear assumptions!
- Compare simple vs. partial
  - Difference indicates significance of interactions between inputs

## Show Dakota Output –

most data analysis software will compute these also

# 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
- Rank correlations:  
simple and partial correlations performed on “rank” of data

**Correlation coefficients have range [-1 , 1]**

0, no relationship

1, strong positive relationship

-1, strong negative relationship

# List Sensitivity Methods

- Expert Opinion
  - Local methods
    - **Finite differences**
    - Design of Computer Experiments
  - Global methods
    - Morris one at a time
    - Sampling
      - Monte Carlo, Quasi-Monte Carlo
      - **Latin Hypercube Sampling (LHS)**
- Partial derivatives  
ANOVA
- Correlation coefficients  
Variance Based Decomposition  
Sobol indices

# 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:**  $10^*N \rightarrow$  get trends, mean, variance
- **Use incremental studies –  $N, 2N, 4N, 8N, 16N \dots$** 
  - Can predict computational cost
  - When benefit stops increasing, stop analysis

# 3leg Sampling

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

Simple Correlation Matrix MaxAccel				Partial Correlation Matrix MaxAccel			
# samples	10	20	40	# samples	10	20	40
chi	-0.33	-0.43	-0.46	chi	-0.68	-0.56	-0.59
R	-0.14	0.25	0.17	R	-0.59	0.18	0.15
S	0.62	0.52	0.49	S	0.78	0.64	0.61
phi_max	0.39	0.45	0.39	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

# Time Permitting

- Sensitivity Analysis workflow
  - Automation of Salinas runs
  - Post-processing in Matlab
  - Dakota study
- Advanced Methods
  - Morris one at a time
  - Variance based decomposition w/ Sobol indices

# 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*



# ESP700 Lecture 3: Methods and Tools for Uncertainty Quantification

Org 1544: V&V/UQ and Credibility Processes

Sandia National Laboratories

3 April, 2014



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

## 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 Very confusing!  
We'll return to this later
  - Provide more insight into the information we have
- Quantitative methods
  - parameters require mathematical description

# Mathematical Description of Uncertainty

- None – deterministic

Increasing cost, complexity,  
information content

- 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

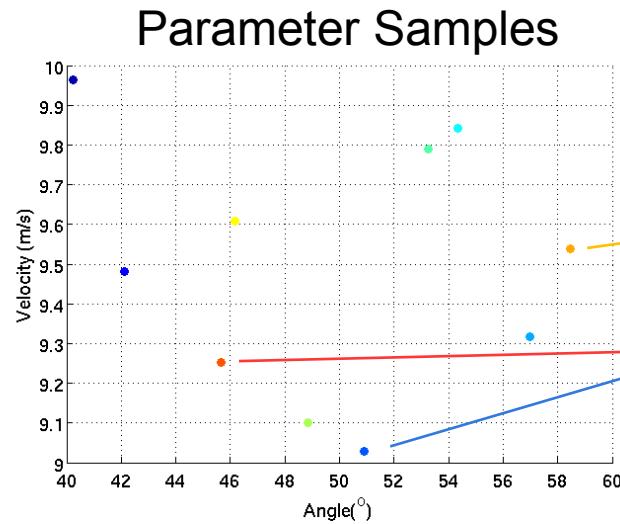
# Propagation of Uncertainty

- 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
  - Construct a surrogate model
  - Sample the surrogate model
  - Discussed in Advanced topics

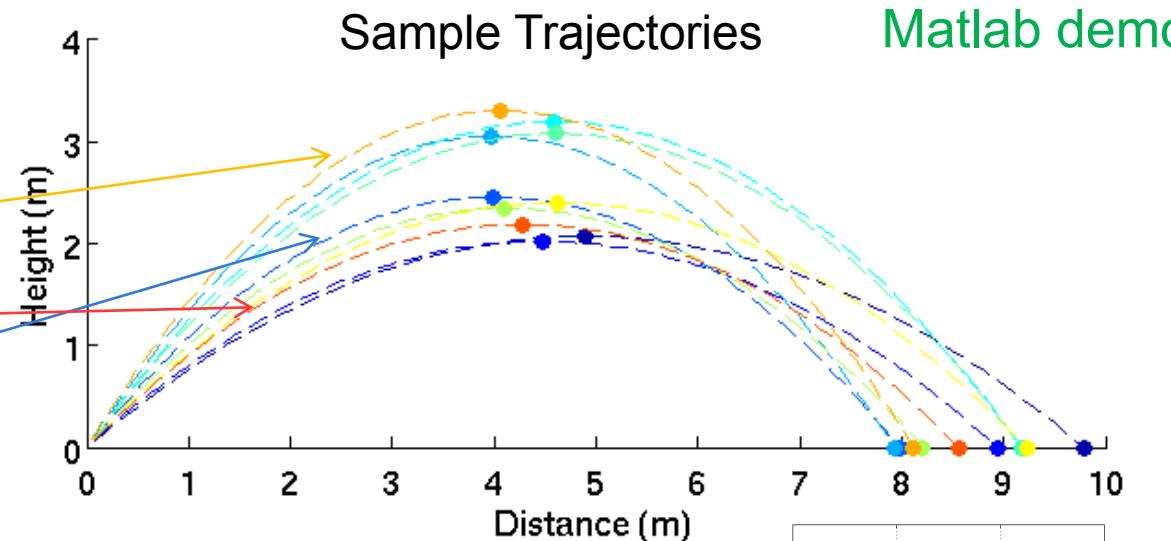
# Example: Ballistic Trajectory

- If we assume  $\theta, V_0$  are uncertain  $\rightarrow$  pdf's
- Then what do we know about QoI: Range?

SA  $\rightarrow$  neglect gravity

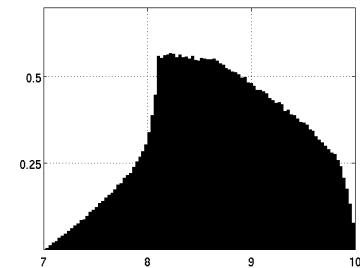


Uniform  
parameter pdf's



Matlab demo

**UQ result:** Normalized histogram of predicted QoI:Range based on (a LOT of) parameter sampling



Non-uniform QoI 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?

## Matlab demo

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

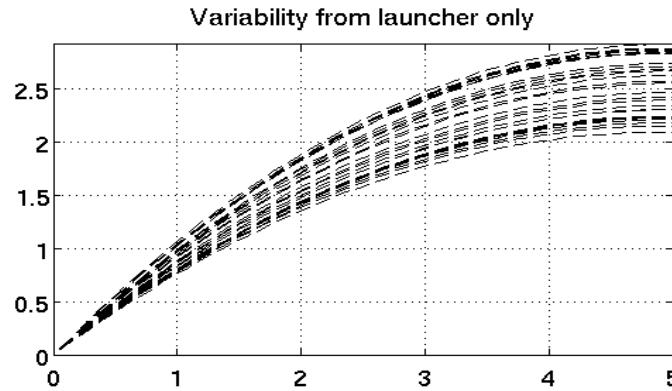
# Example: Ballistic Trajectory

Base is fixed but unmeasured, velocity is known

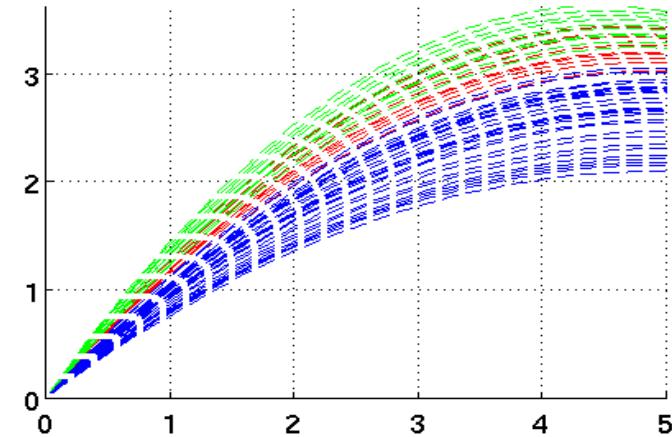
Scenarios:

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?



Variability from launcher, for several base angles (colors)

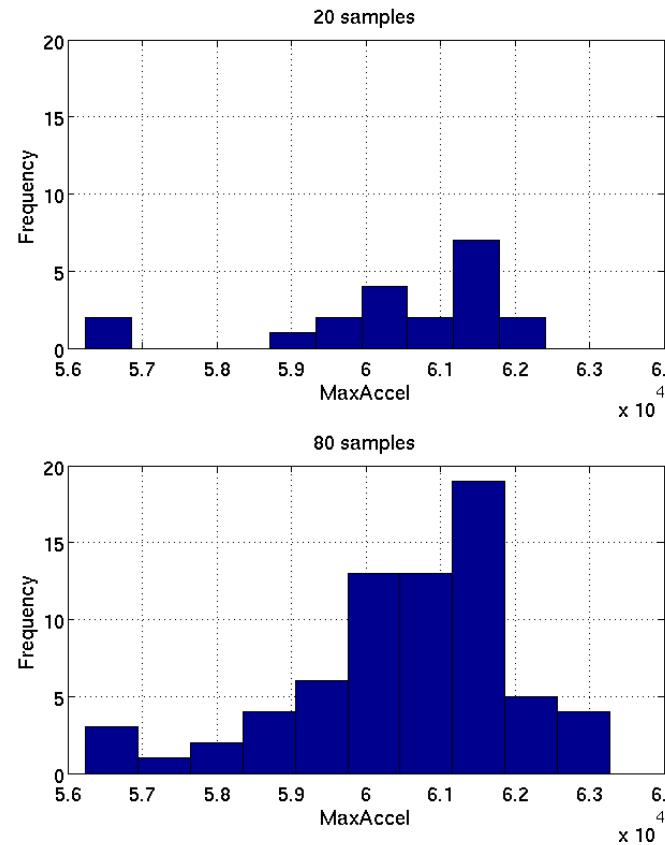
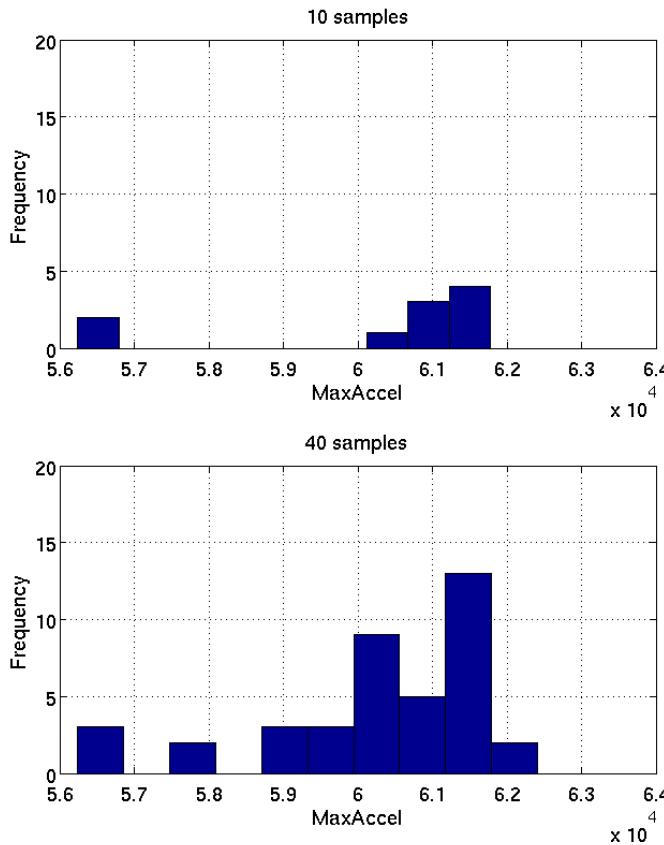


# Example: 3leg Characterization

- 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



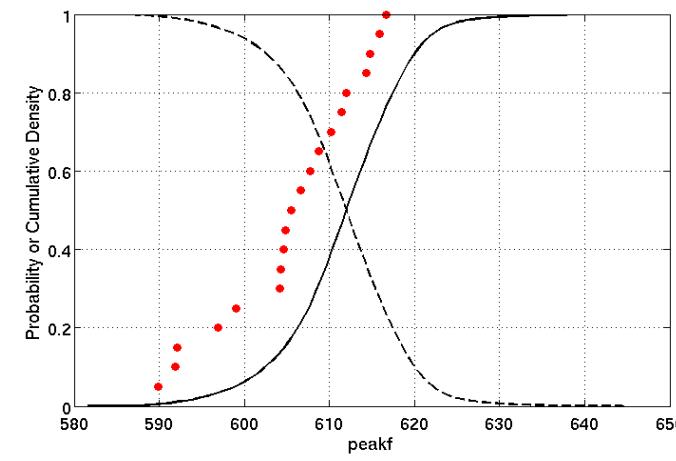
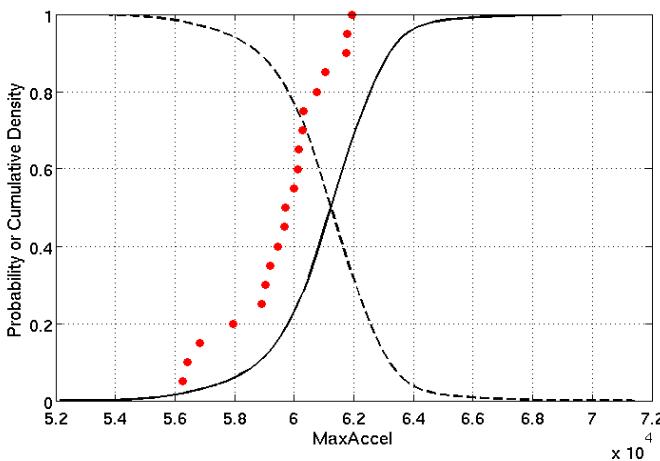
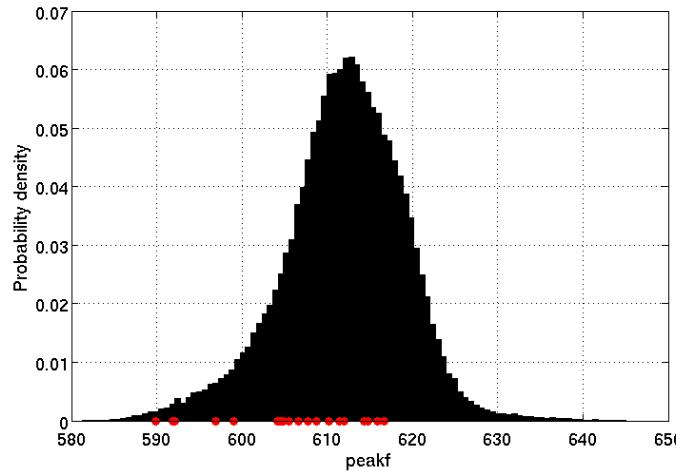
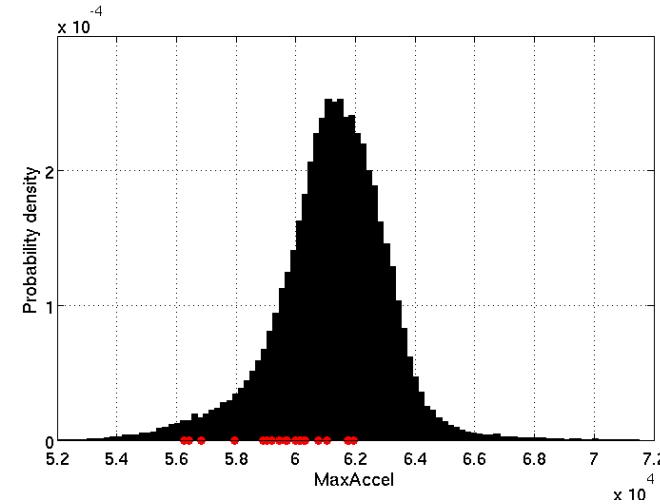
Samples	Mean	Std Dev
10	60297	2131.5
20	60488	1700.4
40	60365	1558.6
80	60589	1496.3

Higher moments  
need more samples  
to converge

- 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

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



Salinas propagated  
best estimates  
Surrogate propagated  
Gaussians

Same information as pdf  
Different look

- Difference: mathematical form
  - Polynomials
  - Polynomial chaos expansions
  - Gaussian process
  - MARS
  - 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

# 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

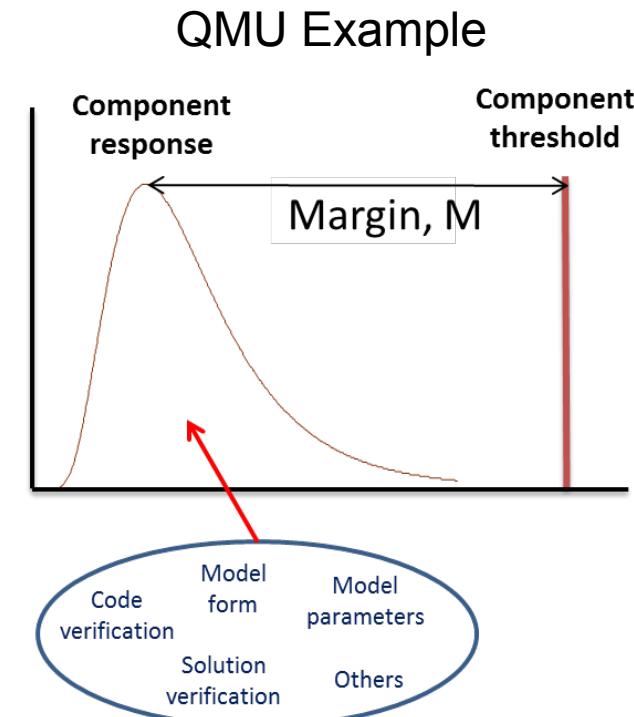
- How to do UQ? Method, # samples, surrogates?
- **Recall goal: understand QoI information**
  - Why?: QMU? PLoAS? Design study? Validation?
- Principles
  - Fidelity of UQ should be determined by intended use
  - Always have option to do more UQ – iterate w/ application
  - Balance sources of uncertainty (“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:
  - [http://www4.ncsu.edu/~rsmith/UQ\\_TIA/](http://www4.ncsu.edu/~rsmith/UQ_TIA/)
- Dakota Users and Theory Manuals have many references

# 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



# Contact

## V&V/UQ Applications and Credibility



Angel Urbina, Dept. 1544  
(505) 844-4988  
[aurbina@sandia.gov](mailto:aurbina@sandia.gov)

## Uncertainty Quantification



Ken Hu, Dept. 1544  
(505) 284-2894  
[khu@sandia.gov](mailto:khu@sandia.gov)