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An Overview of Sensitivity Analysis and Uncertainty Quantification Methods

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NNSA National Nuclear Security Administration

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Outline

- Motivation
- Background
  - Sensitivity Analysis & Uncertainty Quantification (UQ)
- Intro to Sensitivity Analysis and UQ
  - Cantilever Beam Sensitivity Analysis
  - UQ Example #1: probabilistic uncertainty
  - UQ Example #2: lack of knowledge uncertainty
- Summary

Goals for this Briefing

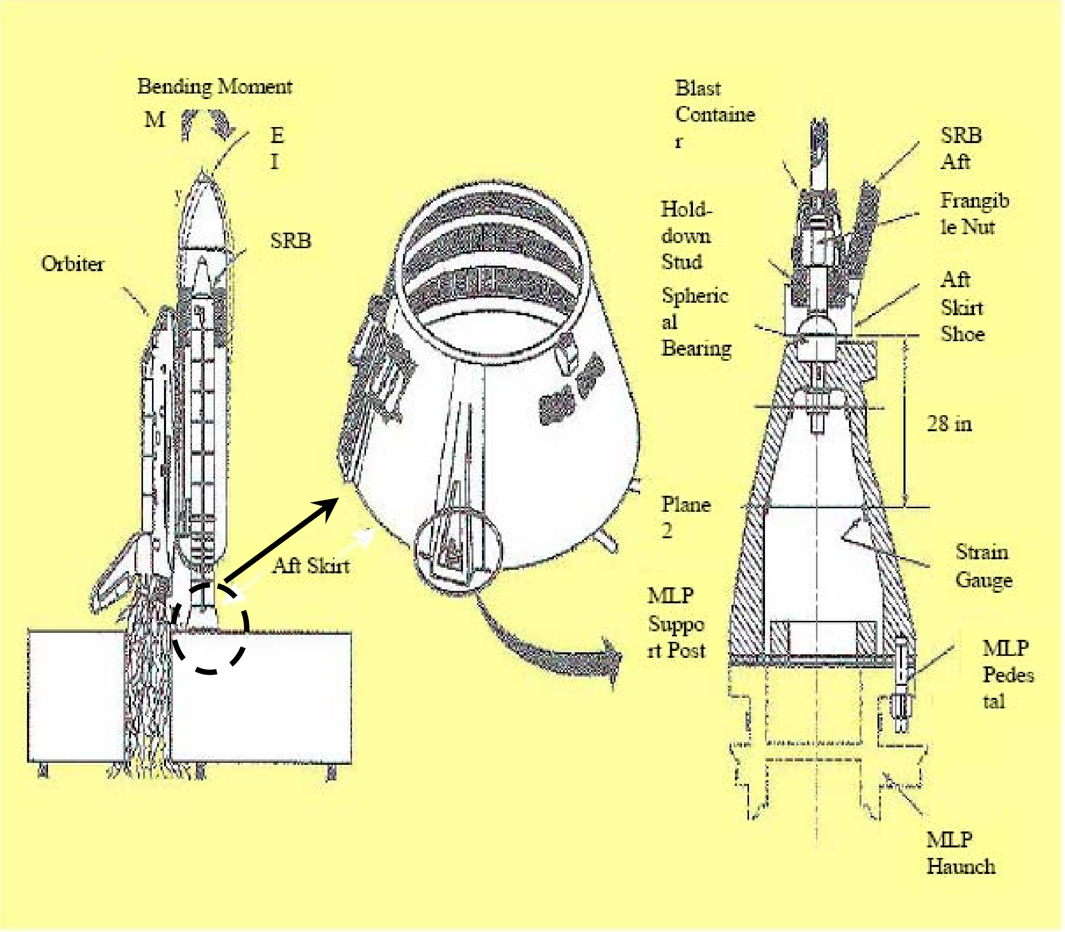
- Understand the connection between verification & validation (V&V), sensitivity analysis (SA), and uncertainty quantification (UQ).
  - And the basic SA and UQ methods & software tools.

- Understand the difference between aleatory (probabilistic) uncertainty and epistemic (lack of knowledge) uncertainty.
  - And how this impacts what you can and cannot learn from a UQ study.

- Know where to go for more info:
  - SNL staff resources
  - Key documents

Example of Analysis w/o UQ: Space Shuttle Solid Rocket Booster Skirt

- Deterministic analysis indicates stress within allowable limit
- Skirt sometimes yields at launch
- Probabilistic analysis reveals high probability of plastic deformation due to scatter in loads and material strength



Take home messages:

1. The best deterministic analysis can yield only limited insight.
2. Neglecting or overlooking uncertainty invites problems. (NASA: O-rings, foam debris,...)

Sensitivity Analysis & UQ Terminology & Issues

- Sensitivity Analysis (SA):
  - How do my code outputs vary due to changes in my code inputs?
  - Need both “local sensitivity” and “global sensitivity” information.
  - Local sensitivity: code output gradient data for a specific set of code input parameter values
  - Global sensitivity: the general trends of the code outputs over the full range of code input parameter values (linear, quadratic, etc.)
- Uncertainty Quantification (UQ):
  - What are the probability distributions on my code outputs, given the probability distributions on my code inputs? (aleatoric UQ)
    - Estimate Probability[f > f*], i.e., the probability that the system will fail
  - What are the possible/plausible code outputs? (epistemic UQ)
- Quantification of margins and uncertainties (QMU):
  - How “close” are my code output predictions (incl. UQ) to the system’s required performance level?

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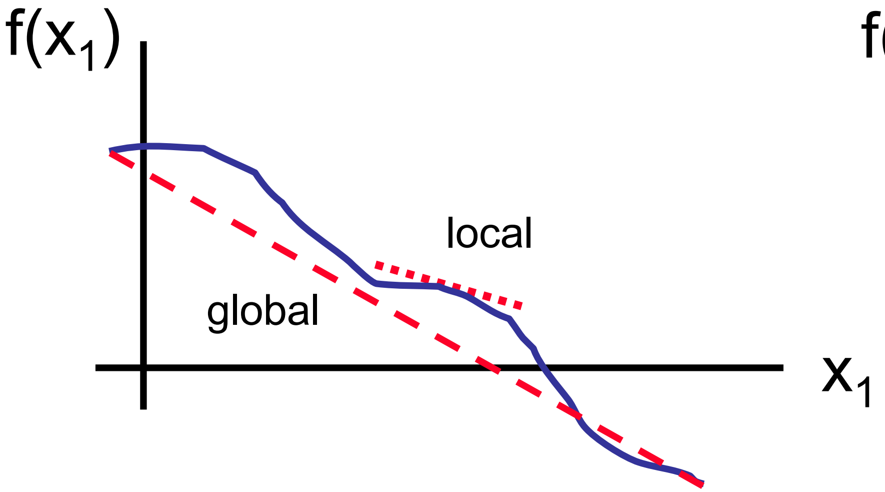
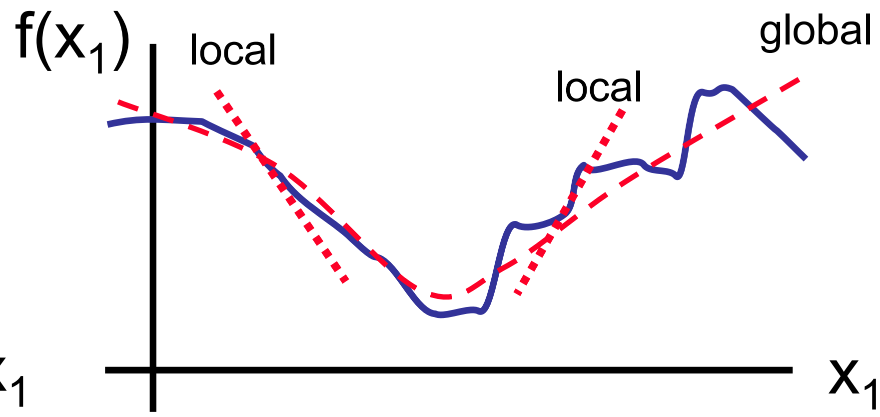
Examples of Sensitivity Analysis
Local vs. Global Sensitivity





- Sensitivity analysis examines variations in $f(x_1)$ due to perturbations in x_1
  - Local sensitivities are typically partial derivatives.
    - Given a specific x_1, what is the slope at that point?
  - Global sensitivities are typically found via least squares.
    - What is the trend of the function over all values of x_1?

Getting Started with Sensitivity Studies and UQ Studies

- **Make a list of the relevant parameters:**
  - Experimental conditions and parameters
  - Physics parameters
  - Code algorithm parameters

- **The next step is to identify what is known about each parameter:**
  - Bounds?, Discrete or continuous?, Probabilistic?

- **Initial sensitivity analysis studies can identify:**
  - High impact parameters
  - Where to focus resources ($, people, simulations, tests, etc.)

- ***Goal: Out of the O(10-100) parameters going into a simulation code, identify the most important parameters & their interactions.***

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Sensitivity Analysis Methods

- An abridged list of sensitivity analysis methods:
  - Simple 1-parameter and multi-parameter studies*
  - Importance factors*
  - Scaled sensitivity coefficients
  - Design of experiments and data analysis*
  - Random sampling and correlation analysis*
  - Variance based decomposition*
  - Many others....

Workhorse methods

** SA capability in SNL's DAKOTA software toolkit*

- Software tools:
  - DAKOTA
  - Minitab statistics package (SNL site license)
  - JMP statistics package (~80 licenses around SNL)
  - Mathematica
  - Matlab with Statistics Toolbox
  - Others (Origin, etc.)

Sensitivity Analysis Example

- Let's use a simple cantilever beam example to illustrate some of these sensitivity analysis concepts.
  - Sensitivity analysis with gradients
  - Sensitivity analysis with DAKOTA's sampling methods and correlation analysis

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Example: Cantilever Beam Deterministic Analysis

Goal:
We want to understand how deflection varies with respect to the length, width, height, load, and elastic modulus.

- **L = Length = 1 m**
- **W = Width = 1 cm, H = Height = 2 cm**
- **I = Area Moment of Inertia = (1/12)WH^3**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa, Yield Stress = 255 MPa (from a handbook)**

Beam theory: (assumes: elastic, isotropic, neglects beam mass, etc.)

- **Deflection = (PL^3)/(3EI), stress = My/I (y = distance from neutral axis)**
- **Deflection ~ 7.2 cm for P = 100 N**
- **Yield Load = 170 N, Deflection at Yield Load ~ 12.3 cm**

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Example: Cantilever Beam Sensitivity Analysis with Gradients

- L = Length = 1 m
- Width = 1 cm, Height = 2 cm
- P = load = 100 N
- Material = Aluminum 6061-T6:
- E = Elastic Modulus = 69 GPa
- Deflection = PL^3/(3EI)

Sensitivity Analysis of deflection (δ)vs. P, L, and E

Scaled Sensitivity Coefficients

$\mu_x*(\partial\delta/\partial x)$

$\mu_P*(\partial\delta/\partial P) = 0.0724$

$\mu_L*(\partial\delta/\partial L) = 0.217$

$\mu_E*(\partial\delta/\partial E) = -0.0724$

Notes:

1. Gradients typically computed via finite difference estimates (4-7 code runs).
2. Be wary of extrapolating trends.
3. No interaction data from this approach, but still useful.
4. *For a follow-on UQ study, maybe I'd freeze P and E at nominal values, and focus resources to study uncertainty in L.*

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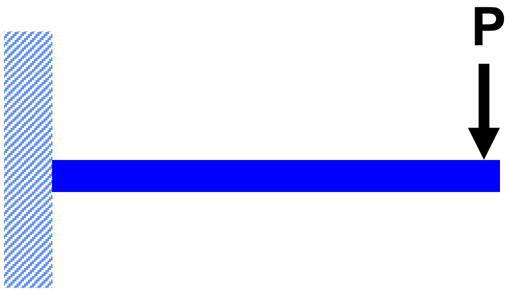
Example: Cantilever Beam Sensitivity Analysis with DAKOTA



- **L = Length = 1 m**
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- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa**
- **Deflection = PL^3/(3EI)**

Sensitivity Analysis of deflection (δ)vs. P, L, and E via random sampling over +/- 5% bounds around nominal values.

Correlation Analysis Method

1. Use DAKOTA to generate 20 random samples of L, P, E within +/-5% bounds.
2. Compute deflection for each random sample.
3. Look at partial correlation results generated by DAKOTA software.
4. Result: "L" most important parameter, but all have about equal impact.

Partial Correlation Table

	Load	Length	Modulus	Deflection
Load	.	-0.1177	-0.0753	0.2624
Length	-0.1177	.	0.2146	0.3251
Modulus	-0.0753	0.2146	.	-0.3088
Deflection	0.2624	0.3251	-0.3088	.

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Moving from Sensitivity Analysis to UQ Studies

- **The remaining parameters of interest will probably have some uncertainty associated with them, e.g.:**
  - **Lower and upper bounds (not necessarily uniform probabilities!!!)**
  - **Probabilistic data (vague or well-substantiated)**
- ***UQ is the process of propagating this uncertainty through a simulation model, and assessing the resulting uncertainty on the simulation output data.***
  - **Recall, typically we want to compute something like Probability(f > f*)**
- **Issues:**
  - **There are many methods to propagate uncertainty – all requiring multiple code runs (actual time/expense are problem dependent)**
  - **Special methods needed for UQ with epistemic parameters**

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Uncertainty Quantification Methods

- **An abridged list of UQ methods:**
  - **Exact analytic methods**
  - **(Structural) reliability methods*** — Workhorse methods
  - **Monte Carlo-type sampling methods*** — Workhorse methods
  - **Polynomial chaos methods*** — Research methods
  - **Dempster-Shafer evidence theory*** — Research methods
  - **Bayesian methods**
  - **Many others....**

**** UQ capability in SNL's DAKOTA software toolkit***

- **Reliability methods are simple and cheap, but can have limited accuracy and applicability.**
- **Sampling methods are simple and can be expensive, but are more generally applicable.**
  - **<u>Latin hypercube sampling</u> is my method of choice,**
  - **Sampling methods can be used when there is a mix of aleatory and epistemic uncertain parameters**

Uncertainty Quantification Example #1

- **Let's return to the simple cantilever beam example to illustrate some of these UQ concepts.**
  - <u>**Aleatory**</u> **(probabilistic) uncertainty**

Example: Cantilever Beam Deterministic Analysis

Goal:
We want to understand how deflection varies with respect to the length, width, height, load, and elastic modulus.

- **L = Length = 1 m**
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- **<u>Deflection ~ 7.2 cm for P = 100 N</u>**
- **<u>Yield Load = 170 N, Deflection at Yield Load ~ 12.3 cm</u>**

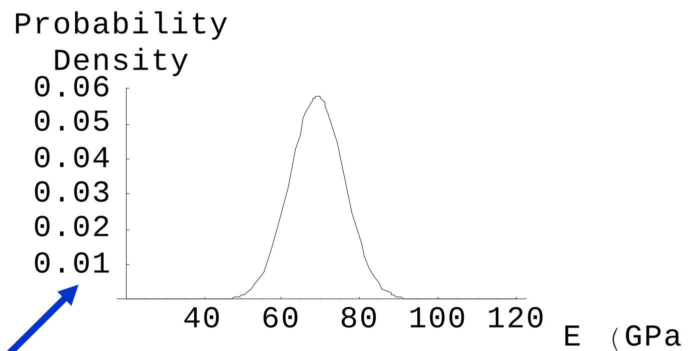
Example: Cantilever Beam UQ Analytical Approach

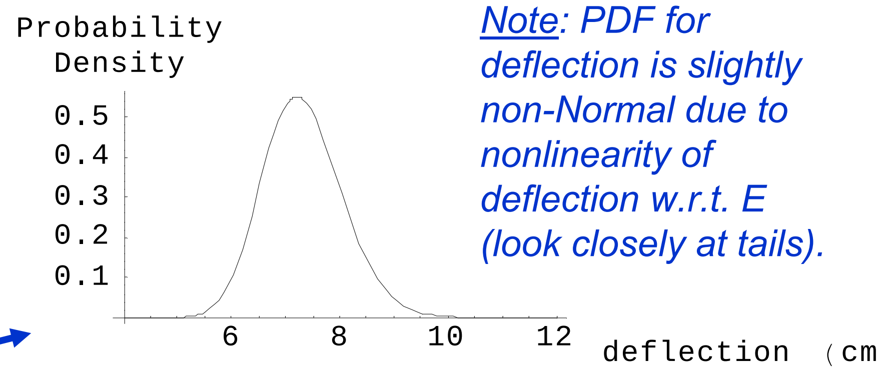
- **Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus**
  - **Mean = μ = 69 GPa**
  - **Std Deviation = σ = 6.9 GPa**

- **Deflection = PL^3/(3EI)**
- **E is Normal[μ, σ]**

- **Exact PDF of E**
- **Exact PDF of deflection**

Probability Density Functions (aka PDFs)

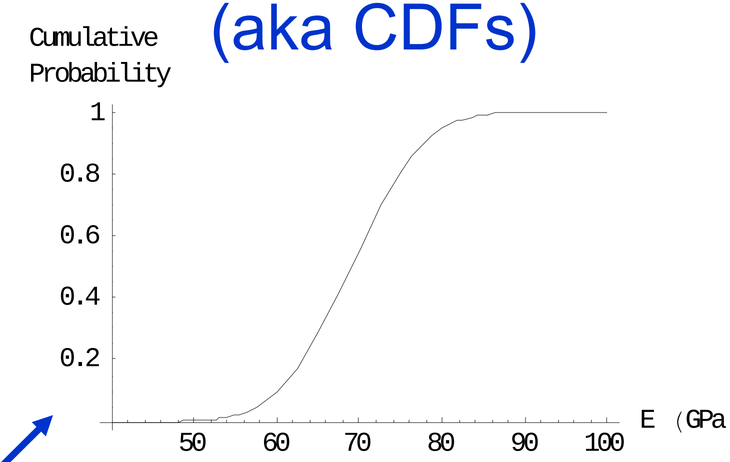


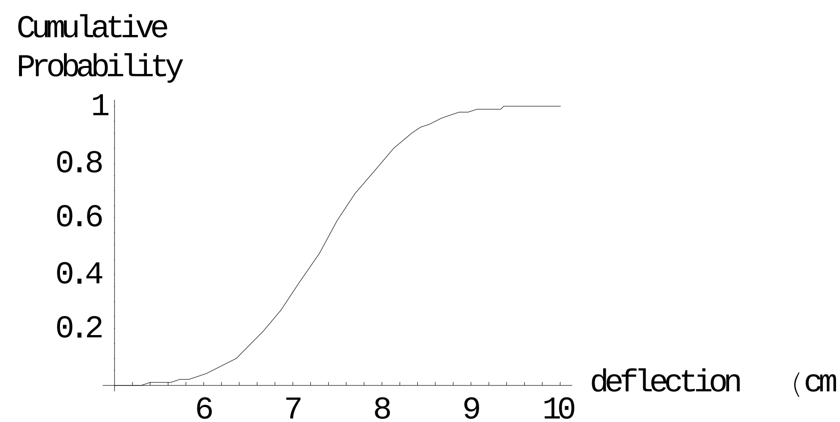


<u>Note</u>: PDF for deflection is slightly non-Normal due to nonlinearity of deflection w.r.t. E (look closely at tails).

Example: Cantilever Beam UQ Analytical Approach

Cumulative Distribution Functions (aka CDFs)





- **Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus**
  - **Mean = μ = 69 GPa**
  - **Std Deviation = σ = 6.9 GPa**

- **Deflection = PL^3/(3EI)**
- **E is Normal[μ, σ]**

- **Exact CDF of E**
- **Exact CDF of deflection**

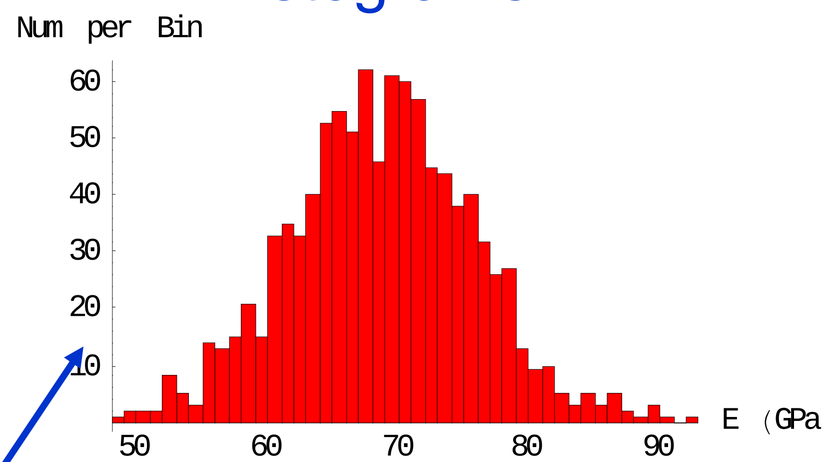
Example: Cantilever Beam UQ
Monte Carlo Sampling – Single Parameter

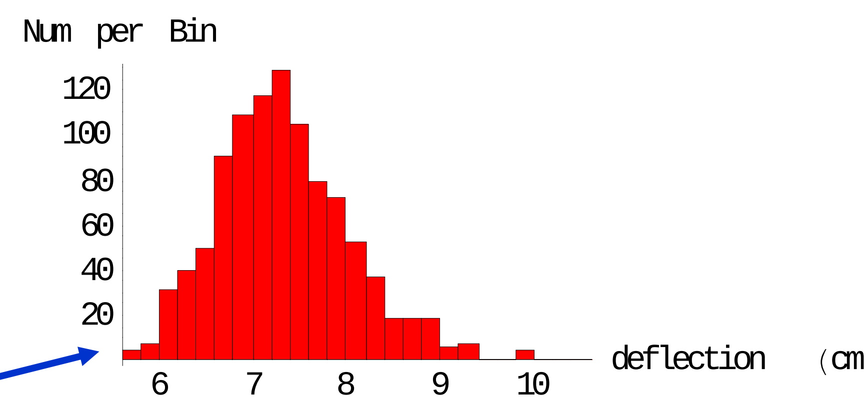
- Length = 1 m
- Width = 1 cm, Height = 2 cm
- P = load = 100 N
- Material = Aluminum 6061-T6:
- E = Elastic Modulus
  - Mean = μ = 69 GPa
  - Std Deviation = σ = 6.9 GPa

- Deflection = PL^3/(3EI)
- E is Normal[μ, σ]

- <u>1000 random samples of E</u>
- <u>1000 computed deflections</u>

Histograms





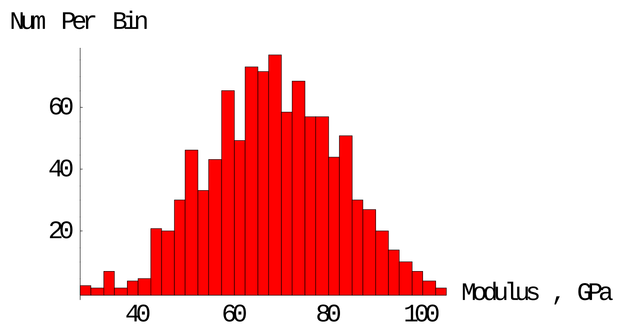
Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters

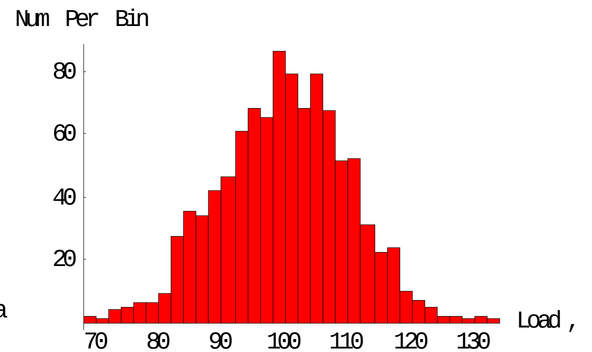
- **<u>Now make several parameters uncertain:</u>**

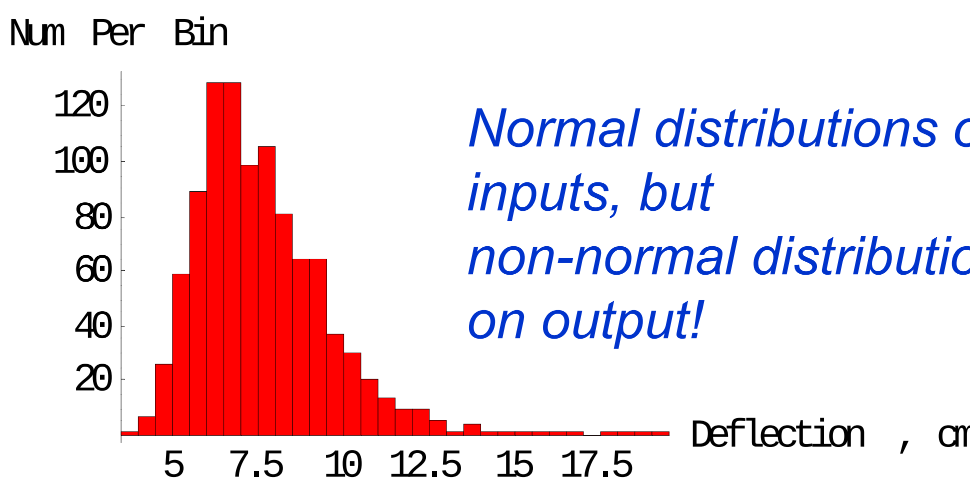
- **Deflection = PL^3/(3EI)**
- **E is Normal[69,13.8] GPa**
- **P is Normal[100,5] N**
- **L is Normal[1.0m, 1cm]**

- **1000 random samples of E, P, and L (top – for E & P)**
- **1000 computed deflections (bottom)**

Histograms

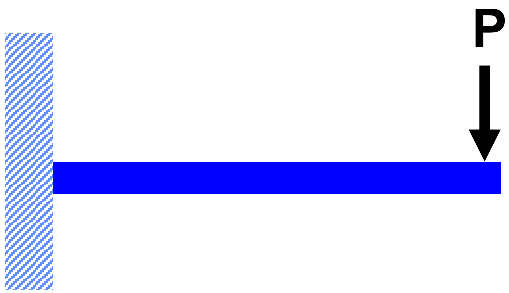




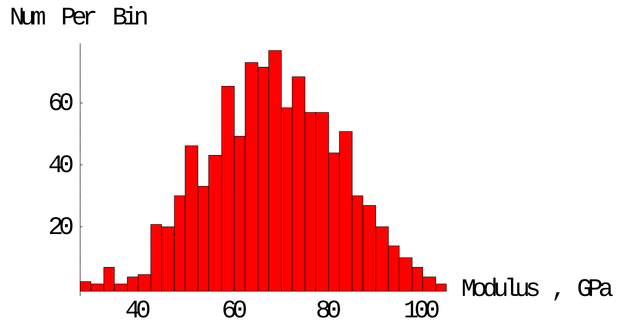


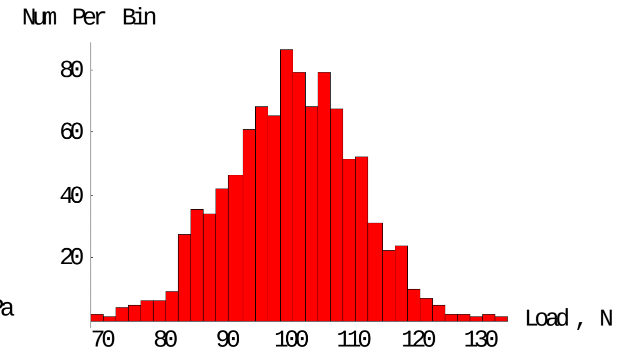
Normal distributions on inputs, but non-normal distribution on output!

Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters



Histograms





- **<u>Now make several parameters uncertain:</u>**

- **Deflection = PL^3/(3EI)**
- **E is Normal[69,13.8] GPa**
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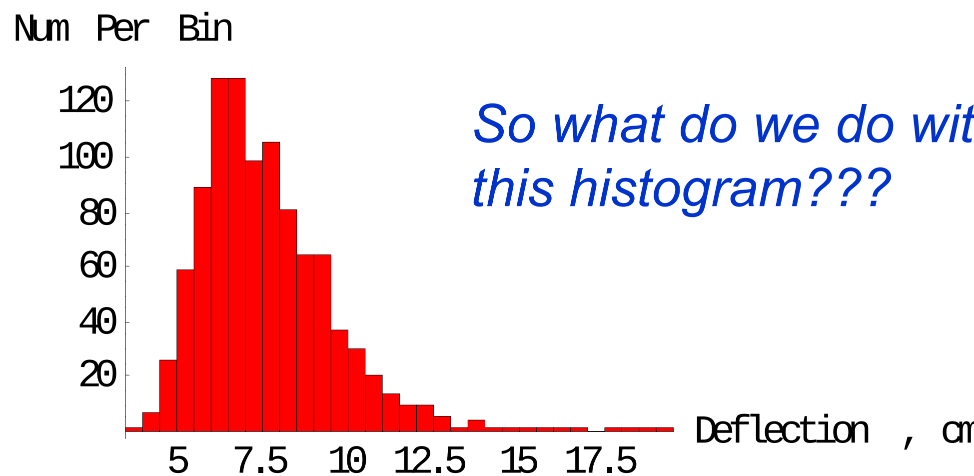
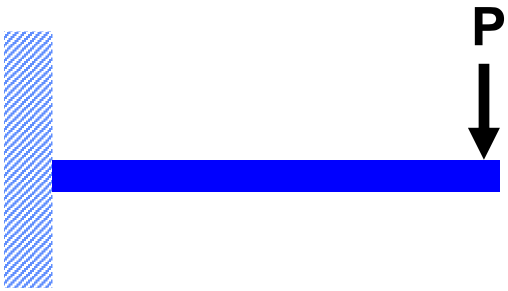
- **1000 random samples of E, P, and L (top – for E & P)**
- **1000 computed deflections (bottom)**



So what do we do with this histogram???

Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters

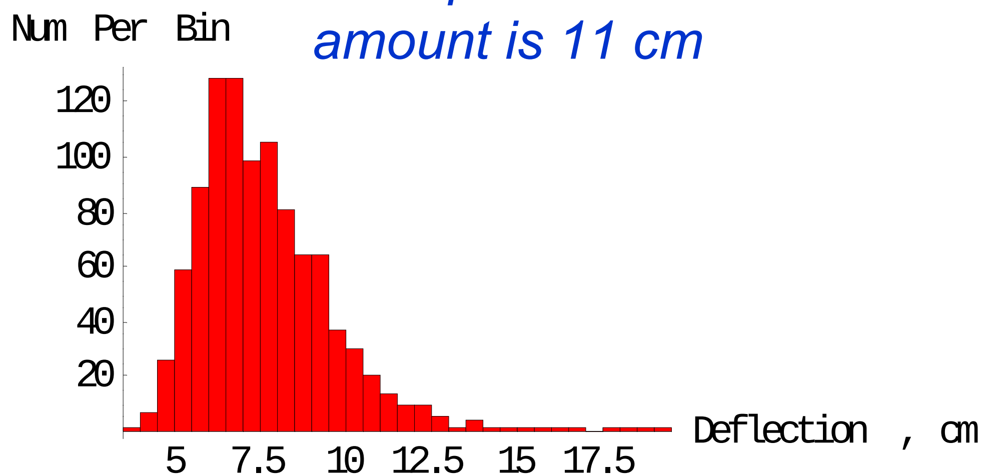


- **<u>Now make several parameters uncertain:</u>**

- **Deflection = PL^3/(3EI)**
- **E is Normal[69,13.8] GPa**
- **P is Normal[100,5] N**
- **L is Normal[1.0m, 1cm]**

- **1000 random samples of E, P, and L**
- **1000 computed deflections**
- ***<u>DAKOTA computes these simple statistics</u>***

Example: "Critical" deflection amount is 11 cm



Estimate failure probability as # of samples with deflection > 11 cm , e.g.
P_{fail} ~ 52/1000 = 0.052
(plus, can also estimate P_{fail} uncertainty)

What if few or no points exceed limit?

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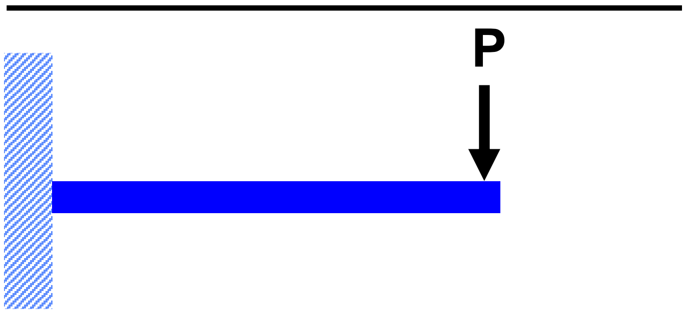
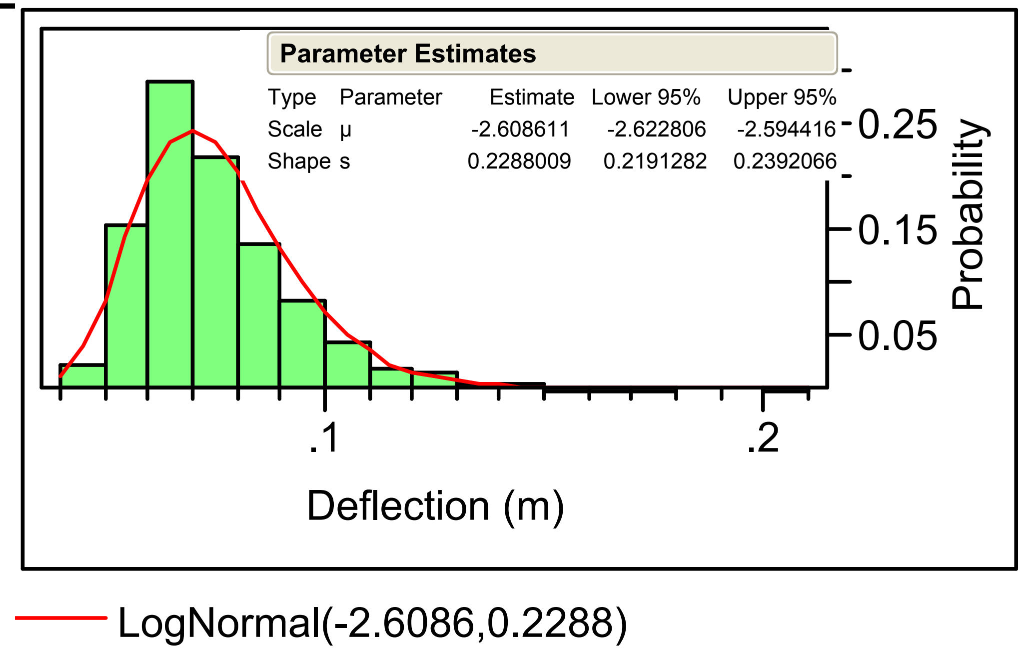
Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters





- **<u>Now make several parameters uncertain:</u>**

- **Deflection = PL^3/(3EI)**
- **E is Normal[69,13.8] GPa**
- **P is Normal[100,5] N**
- **L is Normal[1.0m, 1cm]**

- **1000 random samples of E, P, and L**
- **1000 computed deflections**
- ***<u>Use JMP, Minitab, or other statistics software</u>***

Fit a probability distribution function to the histogram & estimate P_{fail} values:
Prob(δ > 11 cm) ~ 0.04
Prob(δ > 21.8 cm) ~ $1.0e^{-6}$
(note: there is uncertainty on the lognormal parameters!)

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Uncertainty Quantification Example #2

- What happens in the UQ study if some or all of the parameters have <u>epistemic</u> (lack of knowledge) uncertainty?

- This is an active research area:
  - Bayesian methods
  - Dempster-Shafer methods
  - Interval methods, etc.

- Approach used in WIPP and Nuclear Reg. Comm. studies:
  - "2^{nd} order sampling" methods
  - Epistemic parameters define "possible" scenarios.
  - Aleatoric parameters give probability estimates <u>within each scenario</u>.
  - Result: yields a collection of failure probability estimates, but user cannot know which scenario is most likely.

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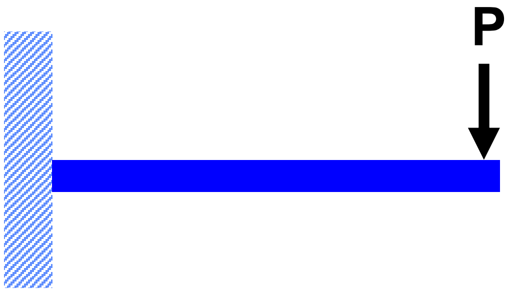
Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters



- **Now make two parameters have <u>epistemic</u> uncertainty:**

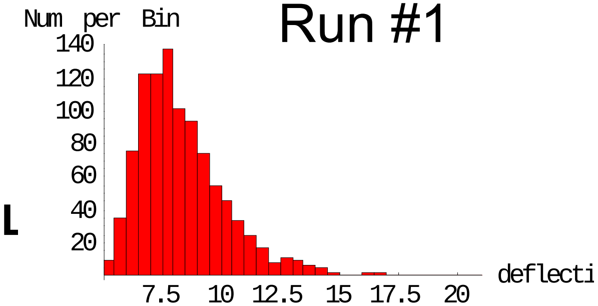
- **Deflection = PL^3/(3EI)**
- **<u>E is Normal[69, 13.8] GPa</u>**
- **<u>L is in [0.97, 1.03] m</u>**
- **<u>P is in [85, 115] N</u>**

- **1000 random samples of E for <u>each</u> instance of P and L**

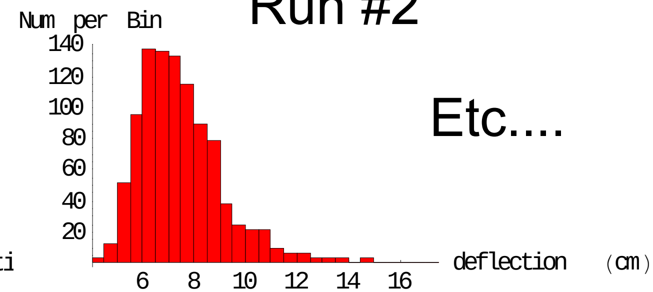
- **<u>Report range of failure probability estimates to decision maker, including the worst-case failure probability.</u>**

<u>Approach</u>:
1. Randomly choose a Load and a Length from their respective intervals.
2. Perform Monte Carlo (or Latin hypercube) sampling over the Elastic Modulus PDF
3. Compute probability deflection > 11 cm
4. Return to step 1 and repeat until computational budget limit reached.

Run #1



Run #2



Etc....

Run #1: P_{fail} ~ 0.043

Run #2: P_{fail} ~ 0.055

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What are the Issues for Real World Sensitivity Analysis and UQ Studies?

- Constrained resources - time, test/simulation budget.
- Combo of aleatory, epistemic, and mixed aleatory/epistemic uncertain parameters.

- What to do:
  - Get a knowledgeable engineer-stats person involved early.
  - If you can do more than one test/simulation, you probably can get some statistical data.
  - Rules of thumb for # of test/simulations needed:
    - Sensitivity analysis: ~[n+1, n^2/2] (where n=# of uncertain parameters)
    - UQ for mean response: ~[n+1, n^2/2]
    - UQ for low-probability events: ~10*(1/desired probability level) (see note)

- Note: There are special stats/math methods to do SA & UQ when you can't afford a large # of tests or simulations!

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Conclusion Slides

- Summary
- Points of contact

Summary: UQ Applications in Sandia Mission Areas

- **Sandia's engineering practices are evolving to include UQ concepts to enable risk-informed design.**
- **Risk-informed design leverages past work on analysis of low-probability and high-consequence systems:**
  - **Waste Isolation Pilot Plant (WIPP)**
  - **Nuclear Regulatory Commission (NRC) studies on reactor safety**
- **Programmatic front:**
  - **Partner statisticians with engineers on projects.**
  - **Educate engineers on basic statistical methods and relevant topics, e.g., V&V, sensitivity analysis, UQ, QMU.**
- **Technical front:**
  - **Employ UQ methods that accommodate both probabilistic (aleatoric) and lack of knowledge (epistemic) uncertainty.**
  - **Employ existing software tools: both in-house (DAKOTA) and commercial.**
  - **Perform UQ within the time/simulation run budget of the study.**
  - **Produce "best estimate + quantified uncertainty" for our customers.**

Closing Remarks

- **Sensitivity analysis and UQ are key components of ASC verification & validation studies:**
  - **Also, SA and UQ have much utility outside of ASC applications**
  - **Must discriminate between epistemic (lack of knowledge) uncertainty and aleatory (probabilistic) uncertainty.**
  - ***Just assuming that every uncertain parameter has a normal or uniform probability distribution is not good engineering practice.***

- **Sandia has software tools (DAKOTA, JMP, Minitab, etc.) for SA and UQ studies.**
  - **Training in these software tools is available -- by SNL staff, online "webinars", multi-day courses, etc.**
  - **In my experience, the most productive SA/UQ studies involve a collaboration between engineering experts and SA/UQ experts**

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Points of Contact

- There is a growing cadre of SNL managers and staff with V&V/UQ/QMU knowledge.

- SNL/NM:
  - Tony Giunta, Channy Wong, Hal Morgan (1500), Jim Stewart (1400), David Womble (1400), Marty Pilch (1200), Kathleen Diegert (12300), Janet Sjulin (12300), Sheryl Hingorani (2900), Bob Paulsen (2100), et al.

- SNL/CA:
  - Mike Hardwick and Heidi Ammerlahn (8900)
  - Artie Ortega (8200)
  - et al.

My apologies to those I've inadvertently left off this list!

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V&V/UQ/QMU Reading List

- **Ideas underlying quantification of margins and uncertainties (QMU): a white paper. SAND2006-5001**
  - Tim Trucano, Martin Pilch, Jon Helton Unclassified Unlimited Release
- **V&V 10 - 2006 Guide for Verification and Validation in Computational Solid Mechanics**
  - ASME Publication ($42)
  - http://catalog.asme.org/Codes/PrintBook/VV_10_2006_Guide_Verification.cfm
- **SNL Integrated Stockpile Evaluation Program website:**
  - http://ise.sandia.gov/
- ***Probability, Reliability, and Statistical Methods in Engineering Design***
  - Achintya Haldar and Sankaran Mahadevan

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Extensive Reference List

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Extra Vugraphs

Common UQ Pitfall:
(Cannot have PDF on results if no PDFs on inputs!)

The "Model"

$Y = A^B$ Indisputable

$A = [0,2]$ Only Bounds Are Known

$B = [1,3]$ Only Bounds Are Known

How do you interpret the results?

(a) Y as a probability distribution? $\boxed{\text{(b) Y bounded by (0,8)?}}$