Applications of Uncertainty Quantification and Sensitivity Analysis in Smart Materials and Adaptive Structures

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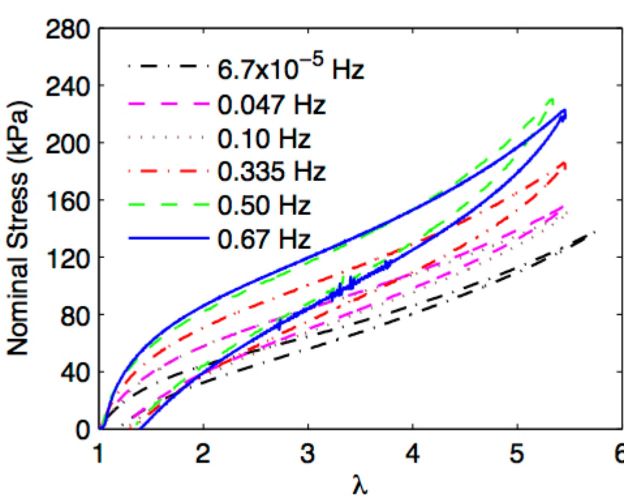
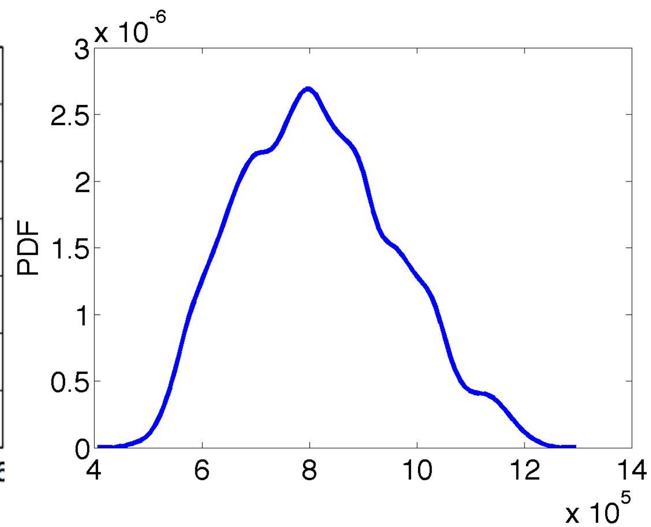
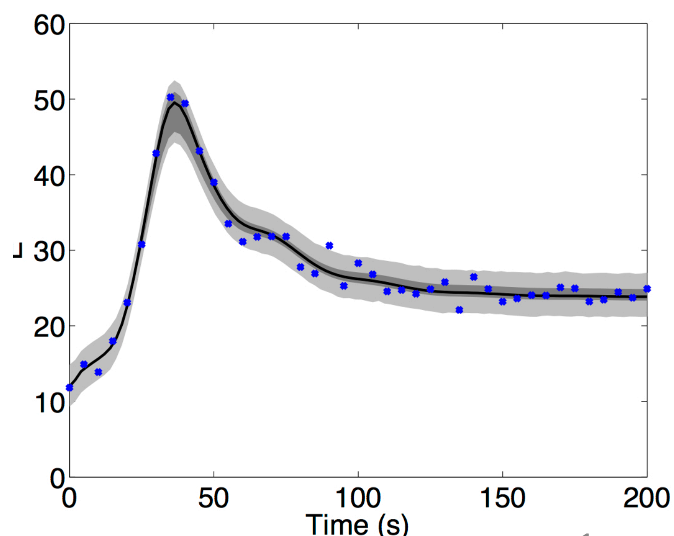






Course Structure

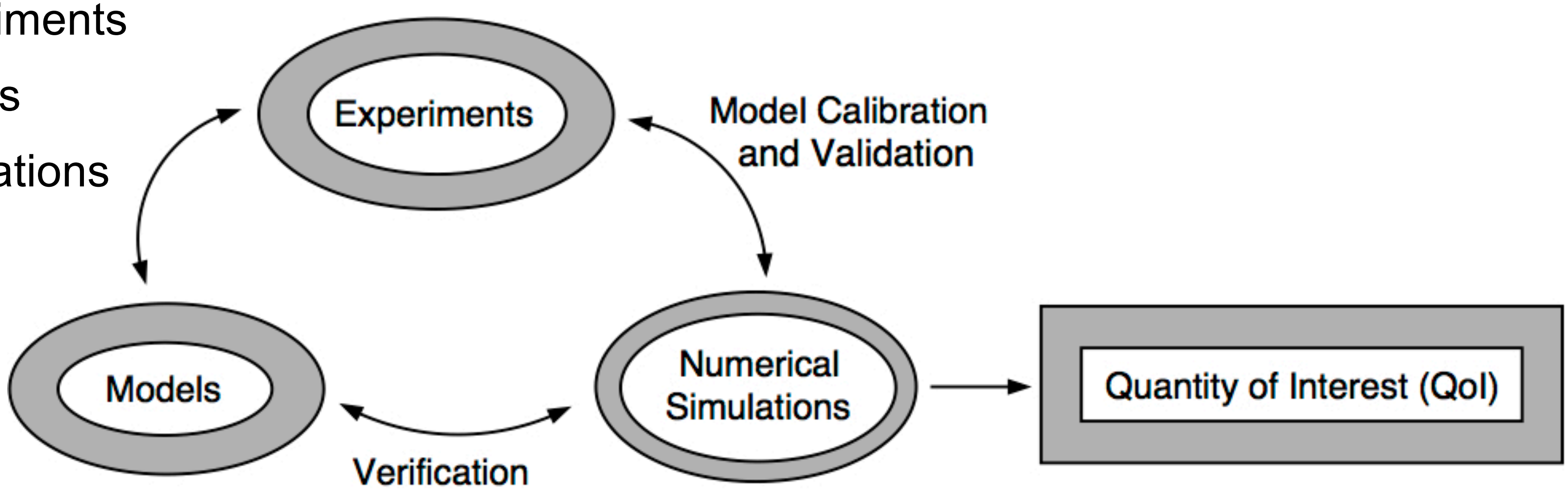
Overview: 10:00-4:00

1. Introduction: Motivating examples
2. Overview of terminology and inverse problems
3. Bayesian inference
4. Forward uncertainty propagation
5. Global sensitivity analysis and active subspaces
6. Surrogate model construction

1. Introduction: Predictive Science

Components: All involve uncertainty

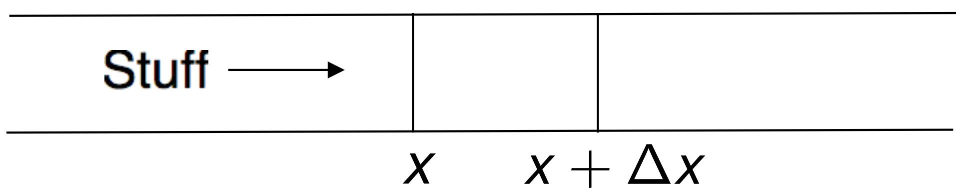
- Experiments
- Models
- Simulations



- *Experimental results are believed by everyone, except for the person who ran the experiment*, source anonymous, quoted by Max Gunzburger, Florida State University.
- *Essentially, all models are wrong, but some are useful,* George E.P. Box, Industrial Statistician.
- *Computational results are believed by no one, except the person who wrote the code*, source anonymous, quoted by Max Gunzburger, Florida State University.
- *I have always done uncertainty quantification. The difference now is that it is capitalized.* Bill Browning, Applied Mathematics Incorporated.

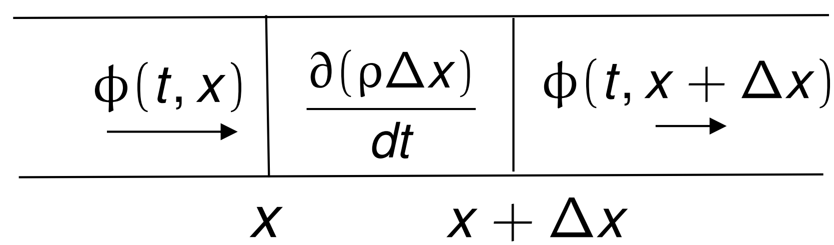
Modeling Strategy

General Strategy: Conservation of stuff



$$\boxed{\frac{dStuff}{dt} = \text{Stuff in - Stuff out + Stuff created - Stuff destroyed}}$$

Continuity Equation:



$$\frac{\partial(\rho\Delta x)}{\partial t} = \phi(t,x) - \phi(t,x+\Delta x)$$

$$\Rightarrow \lim_{\Delta x \to 0} \frac{\partial \rho}{\partial t} = \lim_{\Delta x \to 0} \frac{\phi(t,x) - \phi(t,x+\Delta x)}{\Delta x}$$

$$\boxed{\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = 0}$$

Density: $\rho(t,x)$ - Stuff per unit length or volume

Rate of Flow: $\phi(t,x)$ - Stuff per second

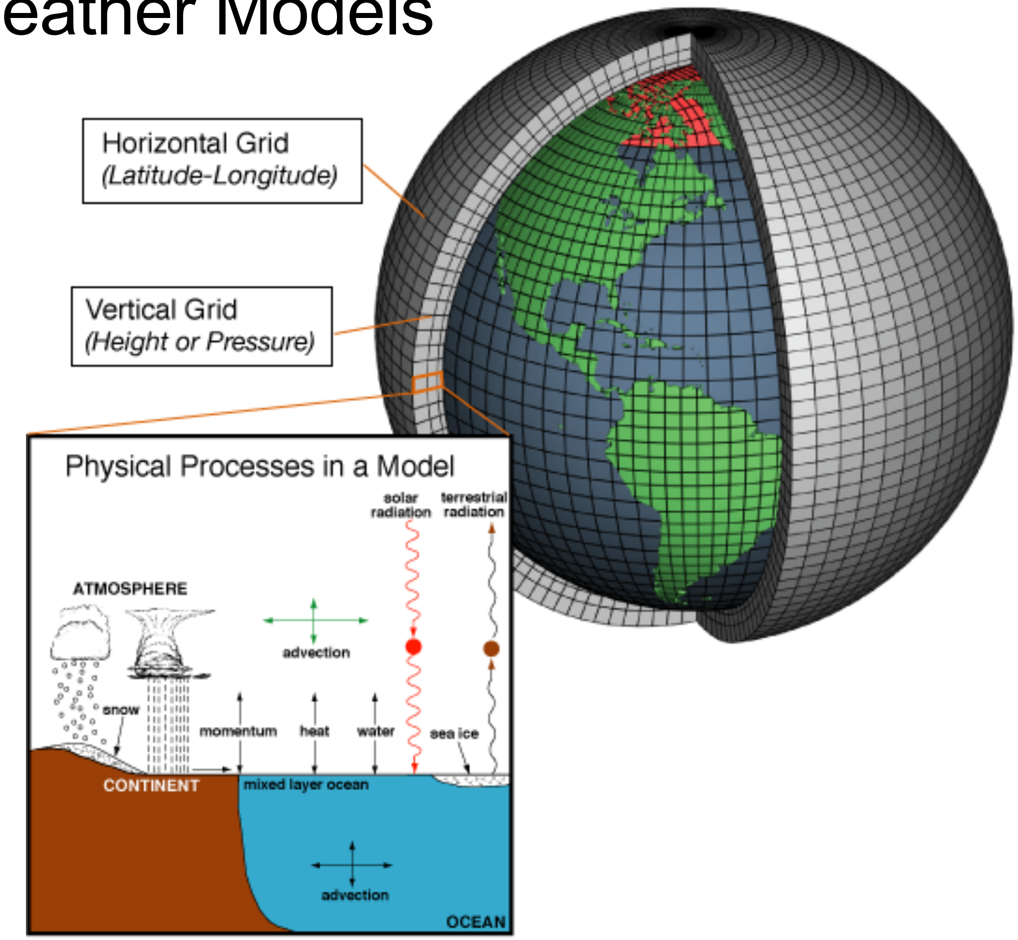
More Generally:

$$\boxed{\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}}$$

Example 1: Weather Models

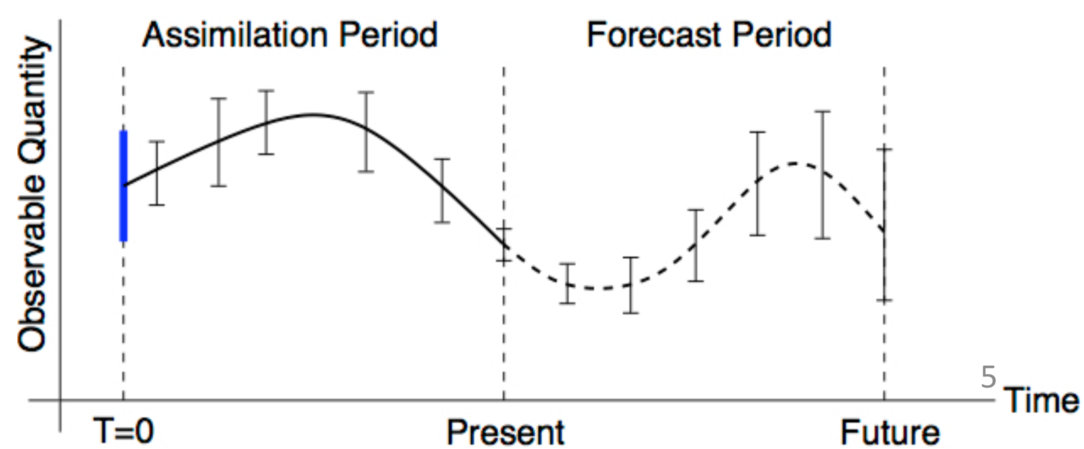
Challenges:

- Coupling between temperature, pressure gradients, precipitation, aerosol species, etc.;
- Models and inputs contain uncertainties;
- Numerical grids necessarily larger than many phenomena; e.g., clouds
- Sensors positions may be uncertain; e.g., weather balloons, ocean buoys.



Goal:

- Assimilate data to quantify uncertain initial conditions and parameters;
- Make predictions with quantified uncertainties.



Equations of Atmospheric Physics

Conservation Relations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}$$

Mass $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

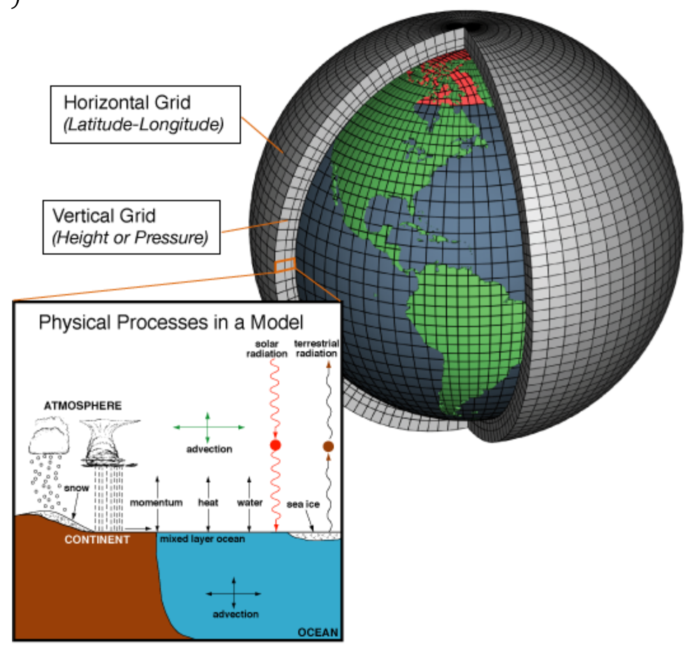
Momentum $$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy $$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water $$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho)\ ,\ j = 1, 2, 3,$$

Aerosol $$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho)\ ,\ j = 1, \cdots, J,$$



Constitutive Closure Relations: e.g.,

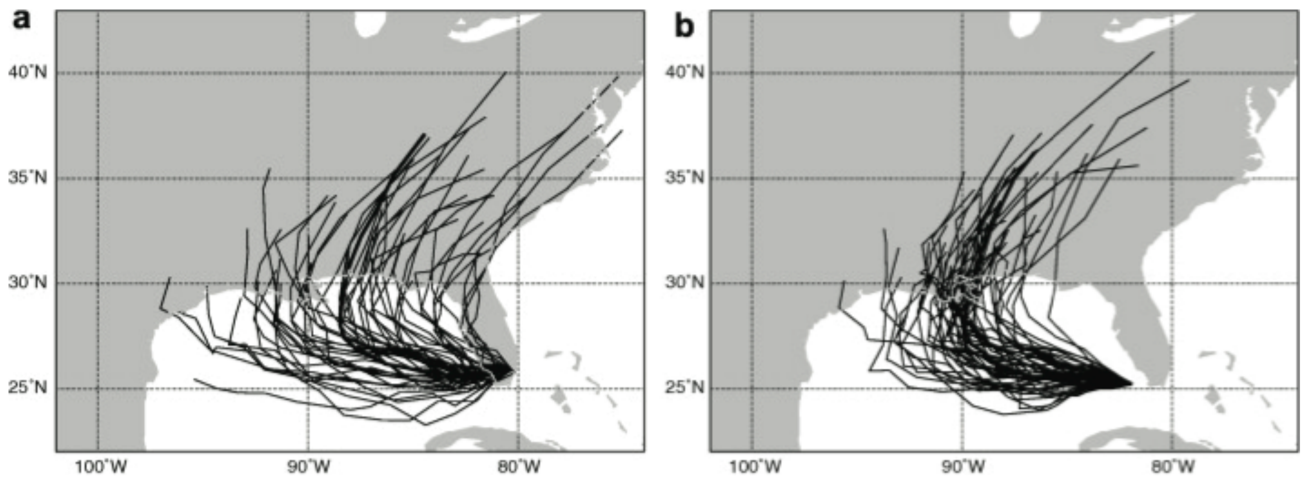
$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

where

$$S_1 = \bar{\rho}(m_2 - m_2^*)^2 \left[\underline{1.2 \times 10^{-4}} + \left(\underline{1.569 \times 10^{-12}} \frac{n_r}{d_0 (m_2 - m_2^*)} \right) \right]^{-1}$$

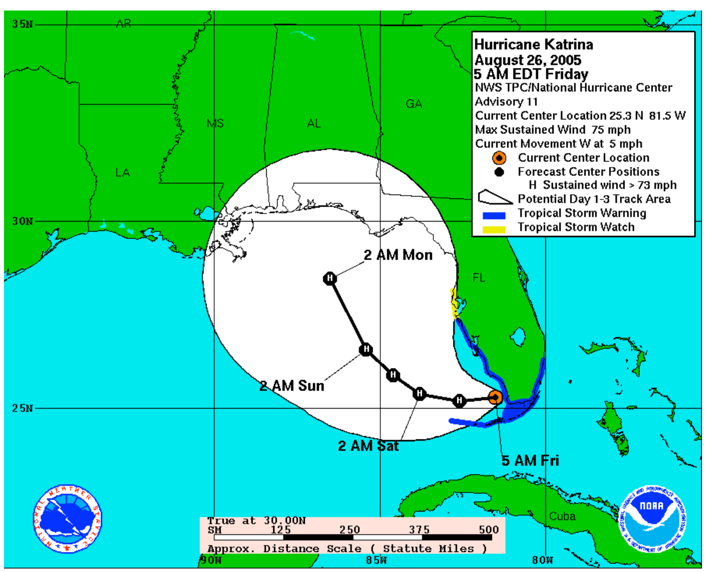
Ensemble Predictions

Ensemble Predictions:



00 UTC on August 26, 2005 12 UTC on August 26, 2005

Cone of Uncertainty:



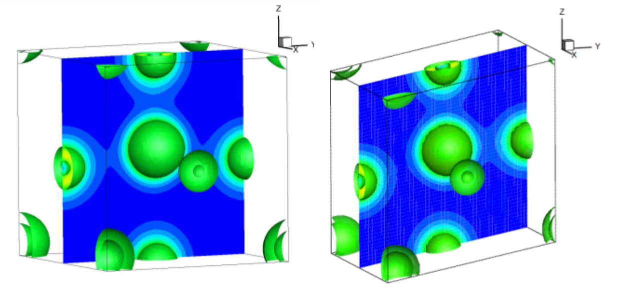
General Questions:

- What is expected rainfall at Eglin AFB on July 22?
- What are average high and low temperatures?
- Note: Quantities are statistical in nature.

Example 2: Quantum-Informed Continuum Models

Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
- Polydomain structure – Lead titanate



DFT Electronic Structure Simulation

$$u(P_i, \varepsilon_{ij}, P_{i,j}) = u_M(\varepsilon_{ij}) + u_L(P_i) + u_C(P_i, \varepsilon_{ij}) + u_G(P_{i,j})$$

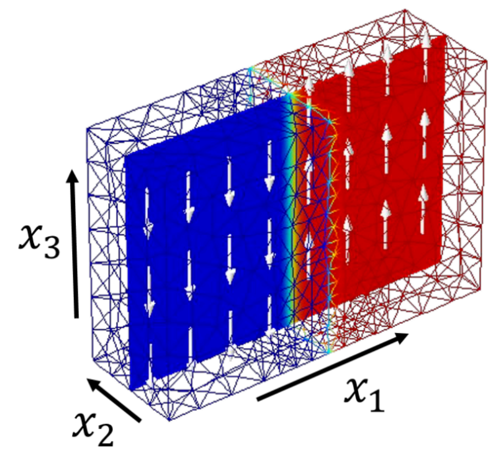
where

$$u_L(P_3) = \alpha_1 P_3^2 + \alpha_{11} P_3^4 + \alpha_{111} P_3^6$$

$$u_C(P_3, \varepsilon_{ii}) = -q_{11}\varepsilon_{11} P_3^2 - q_{12}\left(\varepsilon_{11} P_3^2 + \varepsilon_{22} P_3^2\right)$$

$$u_G(P_{3,1}) = \frac{1}{2} g_{44} P_{3,1}^2$$

180^o Domain Wall



Domain Wall Energy: $E_{180}(q_{180}) = \int_{-\infty}^{\infty} (u - u_0)\, dx_1$

Question: Can parameters be uniquely determined by DFT simulations?

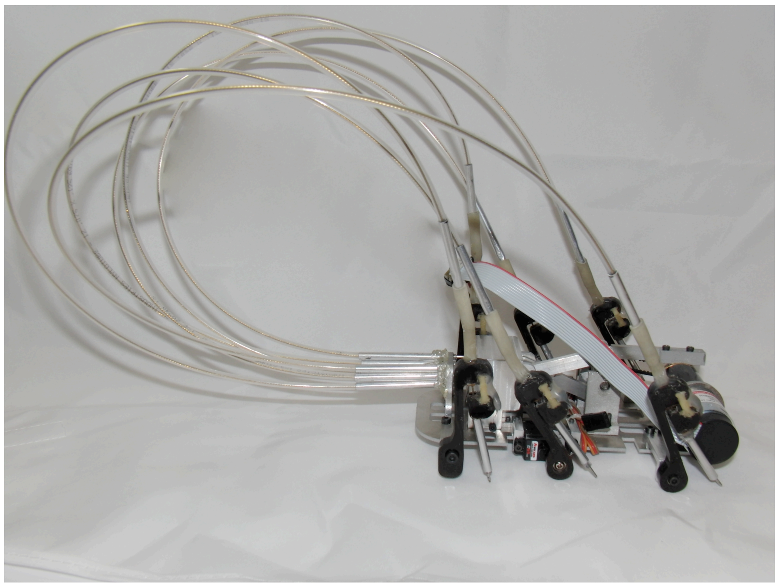
Broad Objective:

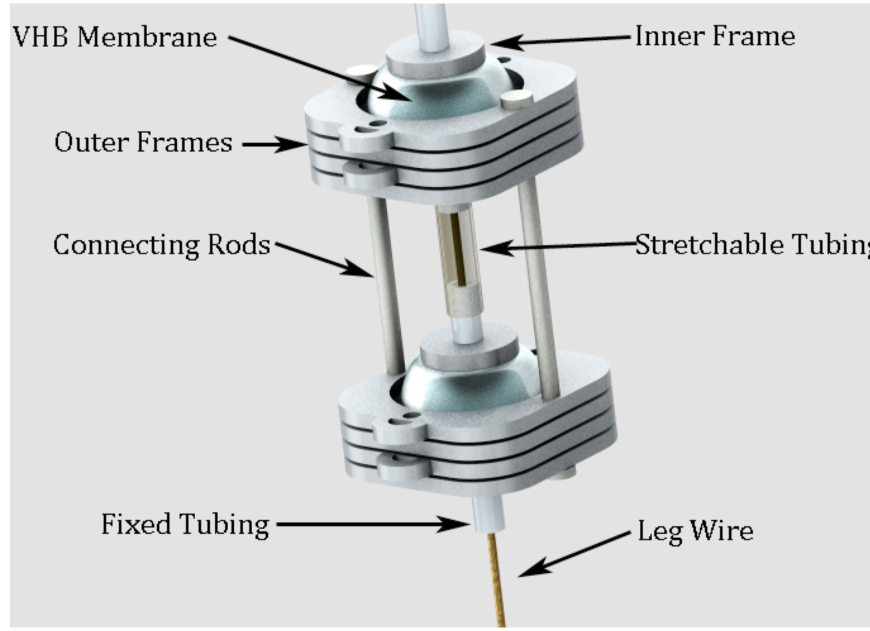
- Use UQ/SA to help bridge scales from quantum to system

Example 3: Viscoelastic Material Models

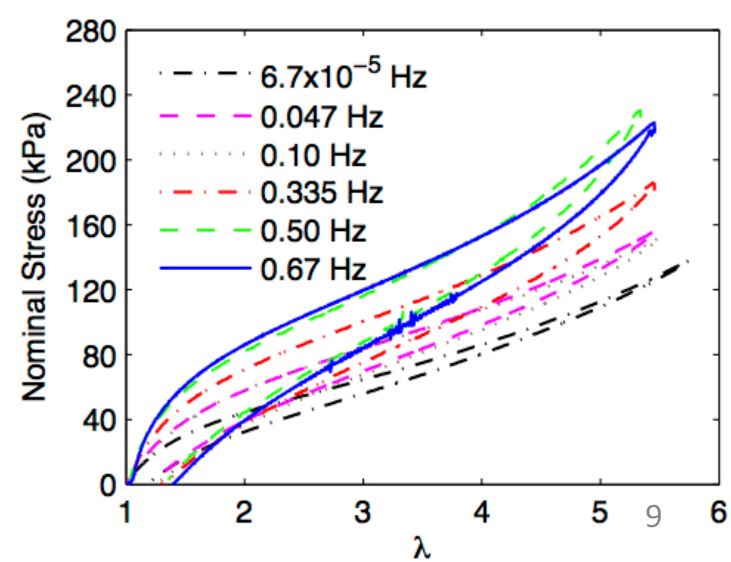
Application: Adaptive materials for legged robotics

- Figure: Billy Oates





Material Behavior: Significant rate dependence



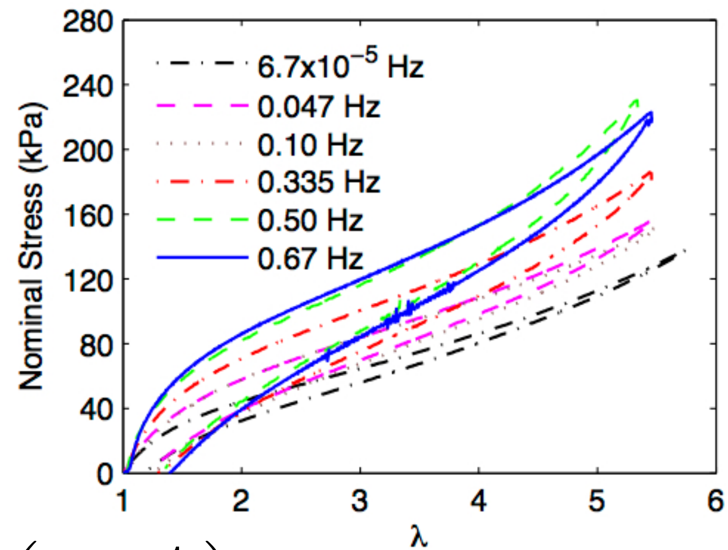
Example: Viscoelastic Material Models

Material Behavior: Significant rate dependence

Finite-Deformation Model: Nonlinear, non-affine

$$\psi(q) = \psi_\infty(G_e, G_c, \lambda_{\max}) + \Upsilon(\eta, \beta, \gamma)$$

- Dissipative energy function Υ
- Conserved hyperelastic energy function



$$\psi_\infty^N = \frac{1}{6}\underline{G_c} I_1 - \underline{G_c\lambda_{\max}^2}\ln(3\underline{\lambda_{\max}^2} - I_1) + \underline{G_e}\sum_j\left(\lambda_j + \frac{1}{\lambda_j}\right)$$

Parameters:

$$q = [G_e, G_c, \lambda_{\max}, \eta, \beta, \gamma]$$

G_c: Crosslink network modulus

G_e: Plateau modulus

$\lambda_{\max}$: Max stretch effective affine tube

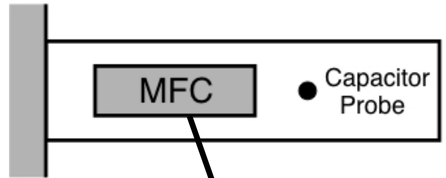
$[\eta, \beta, \gamma]$: Viscoelastic parameters

Uncertainty Quantification Goals:

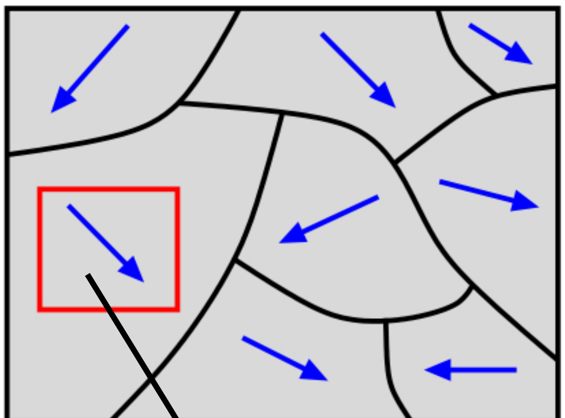
- Quantify measurement errors.
- Quantify uncertainty in parameters.
- Use statistics to quantify accuracy of considered models.

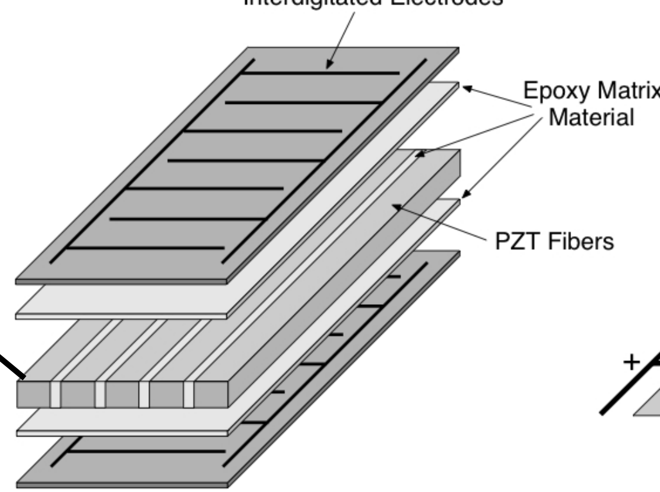
Example 4: Multiscale Model Development

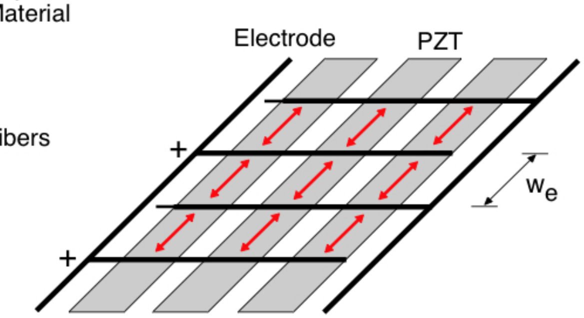
Example: PZT-Based Macro-Fiber Composites

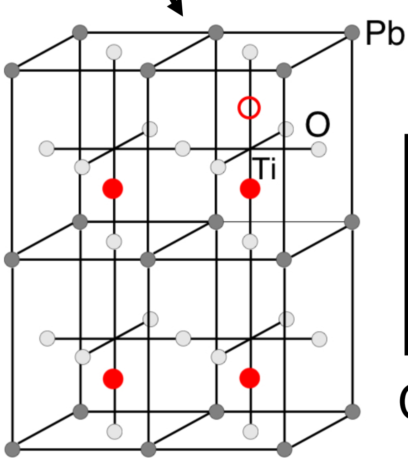


$$\rho \ddot{u} = \nabla \cdot \sigma + F$$
$$\nabla \cdot D = 0\,,\;\; D = \varepsilon_0 E + P$$
$$\nabla \times E = 0\,,\;\; E = -\nabla \varphi$$









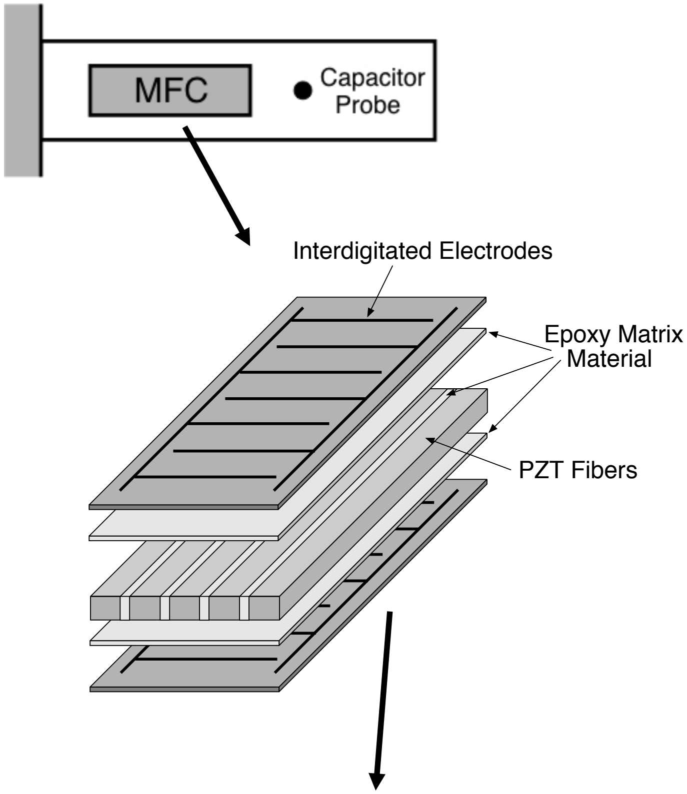
$$P^\alpha = d_\alpha \sigma + \chi_\alpha^\sigma E + P_R^\alpha$$
$$\varepsilon^\alpha = s_\alpha^E \sigma + d_\alpha E + \varepsilon_R^\alpha$$

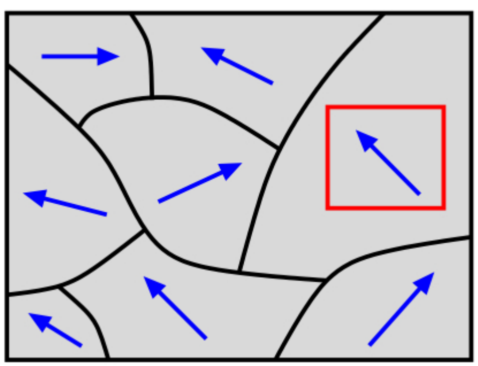
Continuum Energy Relations

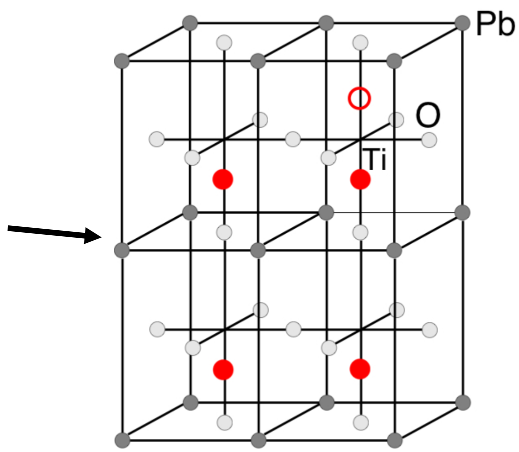
$$P = d(E,\sigma)\sigma + \chi^\sigma E + P_{irr}(E,\sigma)$$
$$\varepsilon = s^E \sigma + d(E,\sigma)E + \varepsilon_{irr}(E,\sigma)$$

Homogenized Energy Model (HEM)

Example: PZT-Based MFC and Robobee







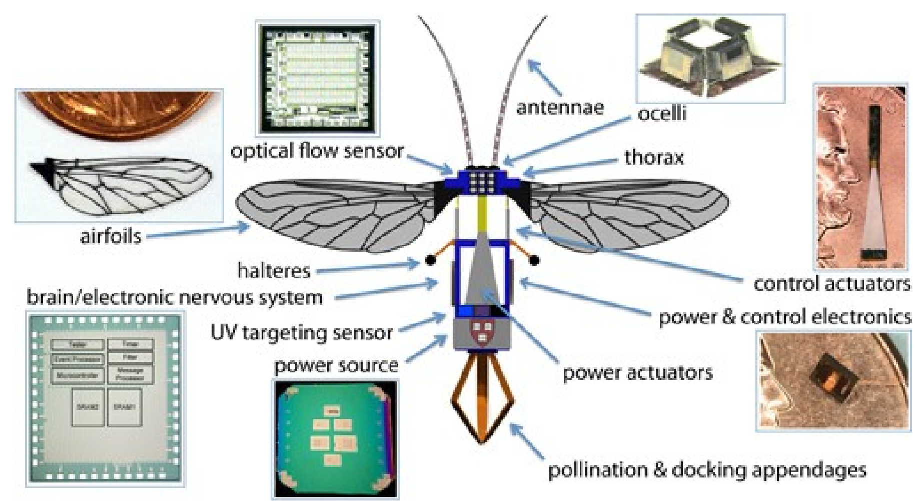
Beam Model: 20 parameters -- quantify uncertainties

$$\rho \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0$$

$$M = -c^E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} - [k_1 e(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)] \chi_{MFC}(x)$$

Homogenized Energy Model (HEM)

2nd Example: Robobee Drive Mechanism



2. Challenge: Terminology and Notation

Terminology:

- Inputs: Parameters, initial conditions, boundary conditions, exogenous forces; e.g., parameters in HIV models, initial conditions in weather models.

- Outputs or Responses: Quantities that we experimentally or numerically measure; e.g., viral load, outlet temperature in reactor.

- Quantities of Interest (QoI): Statistical quantity that we want to compute; e.g., average CRUD buildup, expected profit for a given design.

Input Notation: Can vary even within disciplines!

- Math Control Community: $q = [q_1, \ldots, q_p]$
- Math Reduced-Order Community: $p = [p_1, \ldots, p_q]$
- Statistics: $\theta = [\theta_1, \ldots, \theta_d]$
- Nuclear Engineering: $\alpha = [\alpha_1, \ldots, \alpha_k]$
- Active subspace community: $x = [x_1, \ldots, x_p]$

Note: Same variability in notation for outputs and quantities of interest

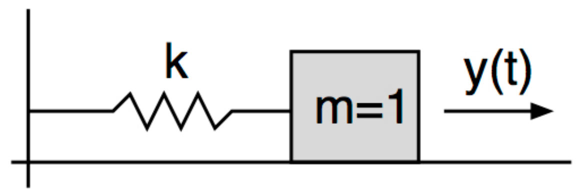
First Challenge: Terminology and Notation

Terminology:

- Linearly parameterized problems: e.g., portfolio model $y = c_1 q_1 + c_2 q_2$
  - Rare in applications except constitutive relations and image processing
- Nonlinearly parameterized problems: typical case
  - Differs from linear or nonlinear in state; e.g., spring model

$$\frac{d^2 y(t)}{dt^2} + ky(t) = 0$$

$$y(0) = y_0 \ , \ \frac{dy}{dt}(0) = 0$$



Notation: $\dot{y} \equiv \dfrac{dy}{dt} \ , \ \ddot{y} \equiv \dfrac{d^2 y}{dt^2}$

Inputs: $q = [k, y_0]$

Response: Displacement $y(t) = y_0 \cos(\sqrt{k} \cdot t)$

$$\Rightarrow \quad \begin{aligned} &\ddot{y}(t) + ky(t) = 0 \\ &y(0) = y_0 \ , \ \frac{dy}{dt}(0) = 0 \end{aligned}$$

Note:

- Linear state dependence
- Nonlinear parameter dependence

Uncertainty Quantification

I have always done uncertainty quantification. The difference now is that it is capitalized. Bill Browning, Applied Mathematics Incorporated.

Note: The field of "Uncertainty Quantification" has grown rapidly over the last 20 years. How is "Capital UQ" different from what statisticians do extremely well every day?

- E.g., When I proposed a course on "Uncertainty Quantification" in Mathematics, I had to carefully justify its existence to Statistics.
- Statistics students are now starting to take the course.

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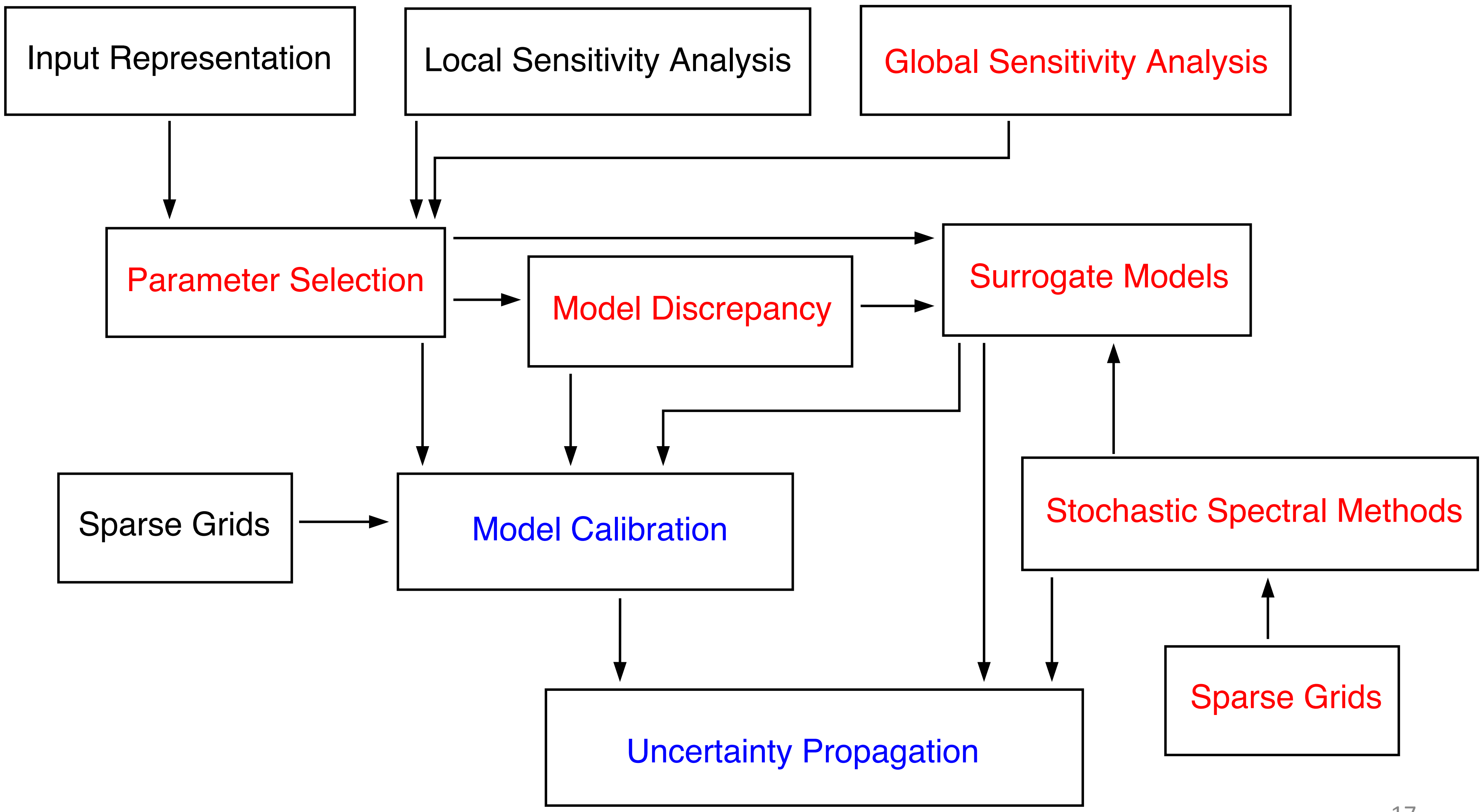
My Definition of “Capital UQ”: The synergy between statistics, applied mathematics and domain sciences required to quantify uncertainties in inputs and QoI when models are too computationally complex to permit sole reliance on sampling-based methods.”

- Involves orthogonal polynomial techniques, sparse grids, high-D (infinite-D) approximation theory, randomized linear algebra … and a lot of statistics!

No one trusts a model except the man who wrote it; everyone trusts an observation except the man who made it, Harlow Shapely.

Steps in Uncertainty Quantification

Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



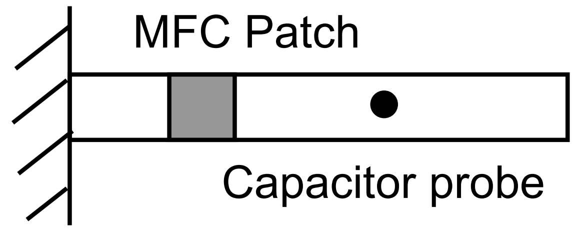
Deterministic Model Calibration

Example: MFC

$$\rho \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0$$

$$M = \quad -c^E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t}$$
$$- \left[k_1 e(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)\right] \chi_{MFC}(x)$$

Homogenized Energy Model (HEM)

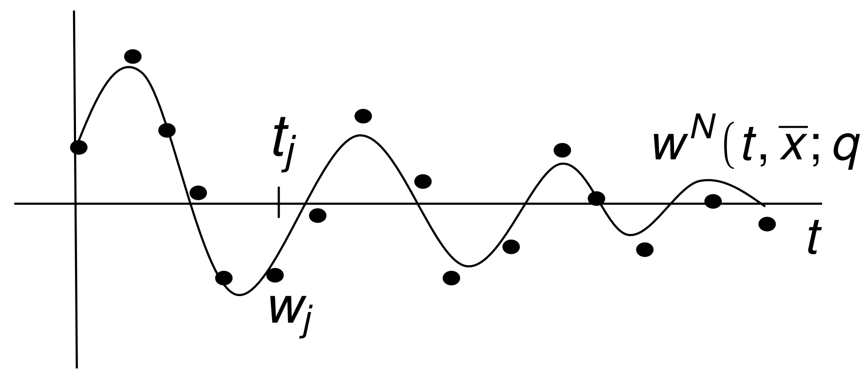


Macro-Fiber Composite

Note: 20 parameters

Point Estimates: Ordinary least squares

$$q^0 = \arg\min_q \frac{1}{2} \sum_{j=1}^{N} \left[w_j - w^N(t_j, \overline{x}, q)\right]^2$$

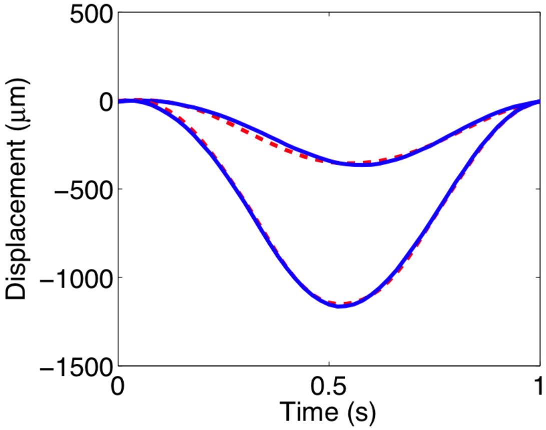


Deterministic Model Calibration

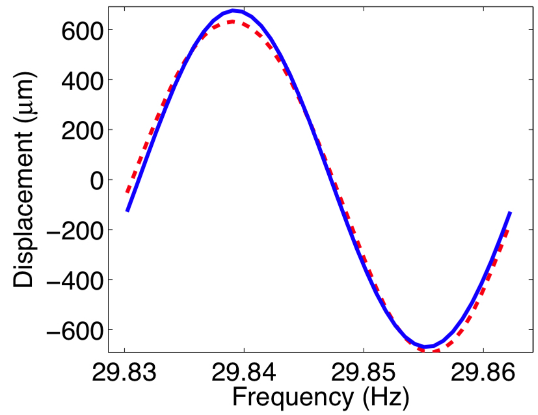
Representative Parameter Values:

d_+ (m/V)	σ_I (V/m)	τ_{180} (s)
478.10×10^{-12}	6.47×10^{6}	2.80×10^{-3}

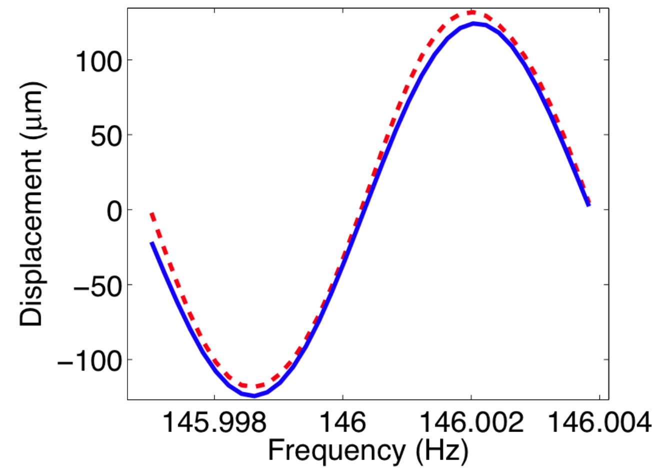
1 Hz Input
(400, 800 VDC)



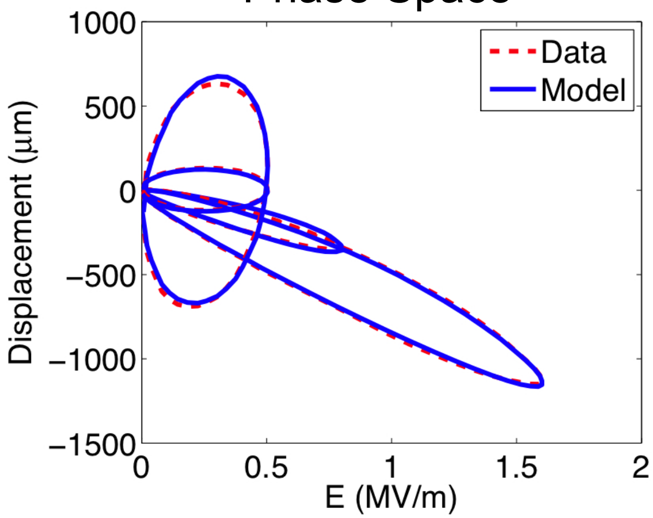
30 Hz Input



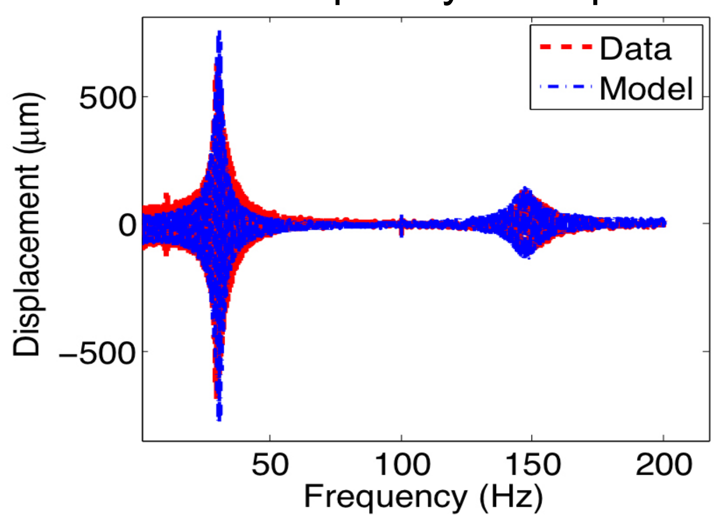
146 Hz Input



Phase Space



Frequency Sweep



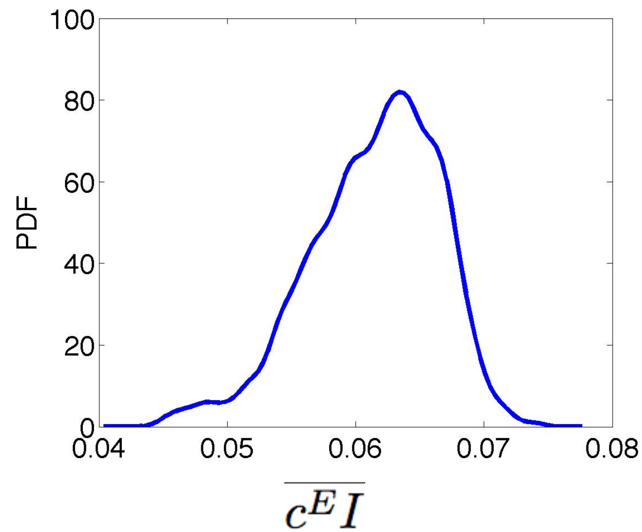
Note: Point estimates but no quantification of uncertainty in:

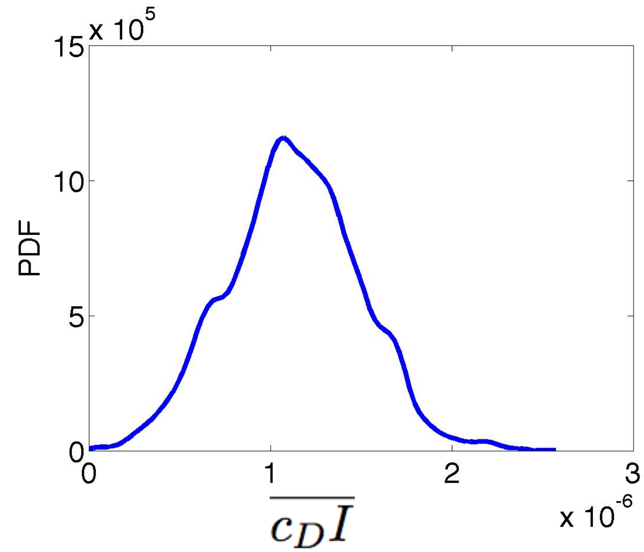
- Model
- Parameters
- Data

Objectives for Uncertainty Quantification

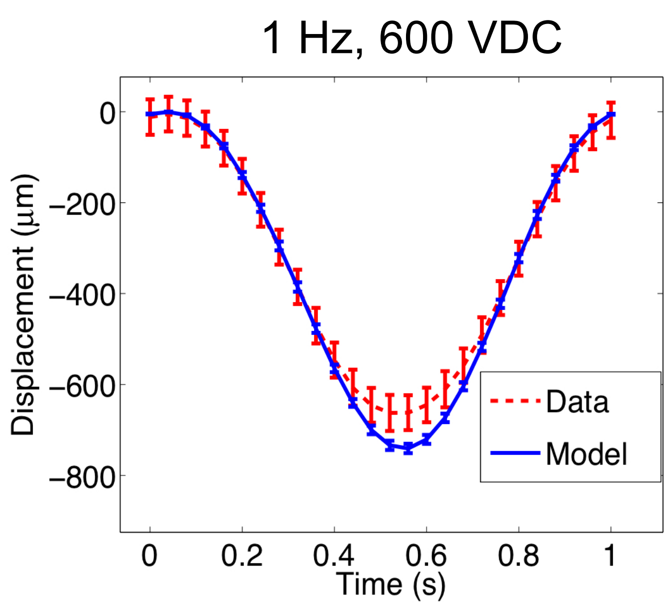
Goal: Replace point estimates with distributions or credible intervals

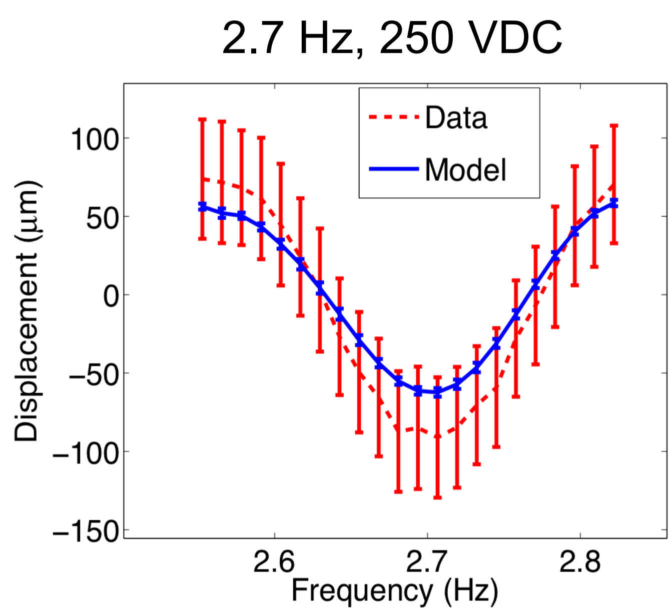
E.g., Parameter Densities





E.g., Response Intervals





Objectives for Uncertainty Quantification

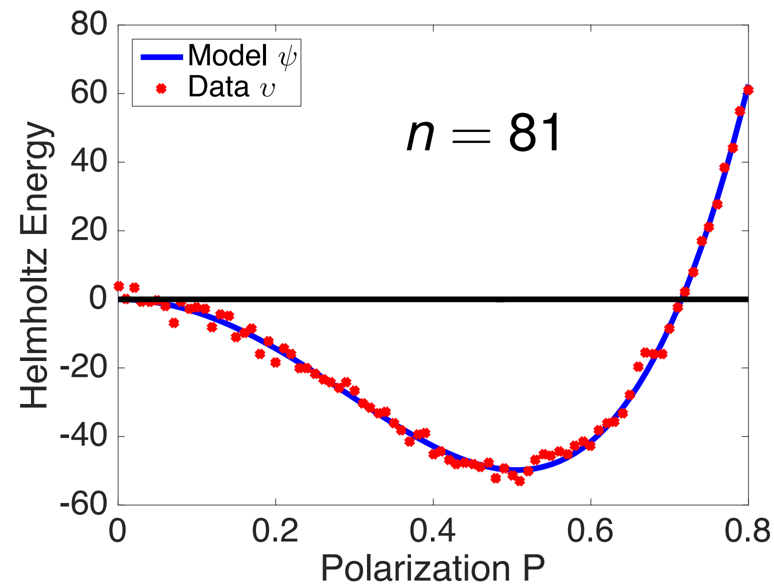
Example: Helmholtz energy $\psi(P, q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$

Statistical Model: Describes observation process

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \quad , \; i = 1, \ldots, n$$

Common Assumption: $\varepsilon_i \sim N(0, \sigma^2)$

UQ Goals: Quantify parameter and response uncertainties

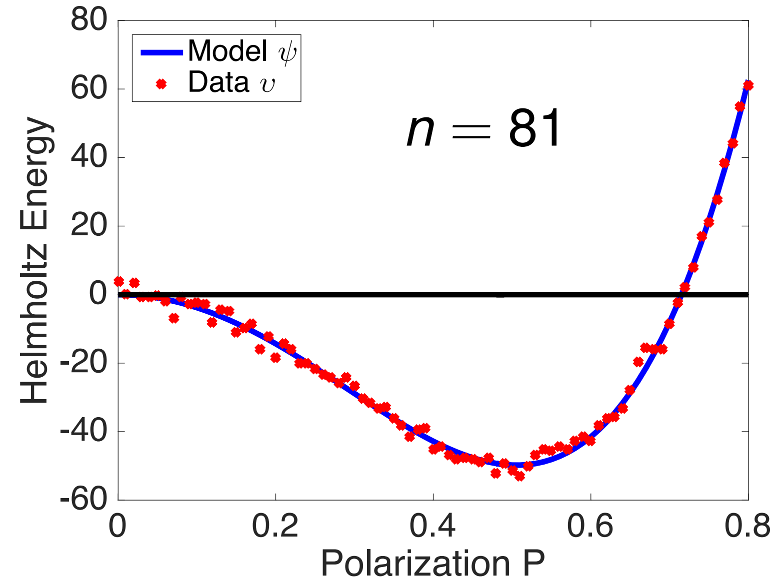


Strategy 1: Perform Experiments or High-Fidelity Simulations

Example: Helmholtz energy $\psi(P,q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$

Statistical Model: Describes observation process

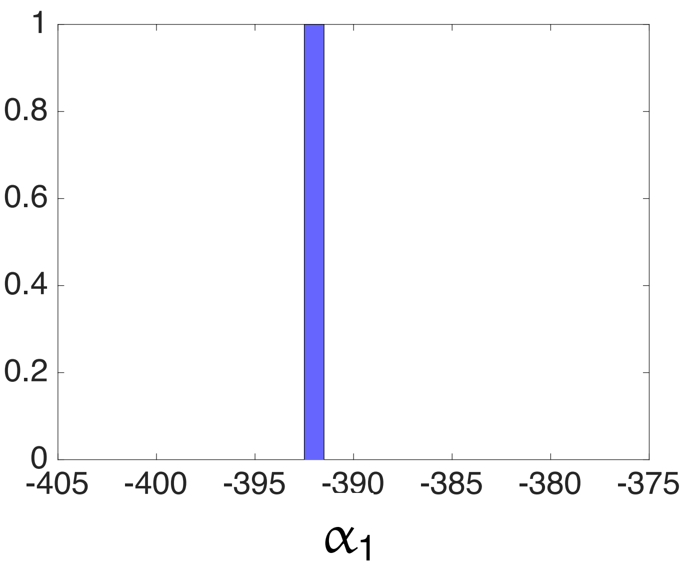
$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \quad , \; i = 1, \ldots, n$$

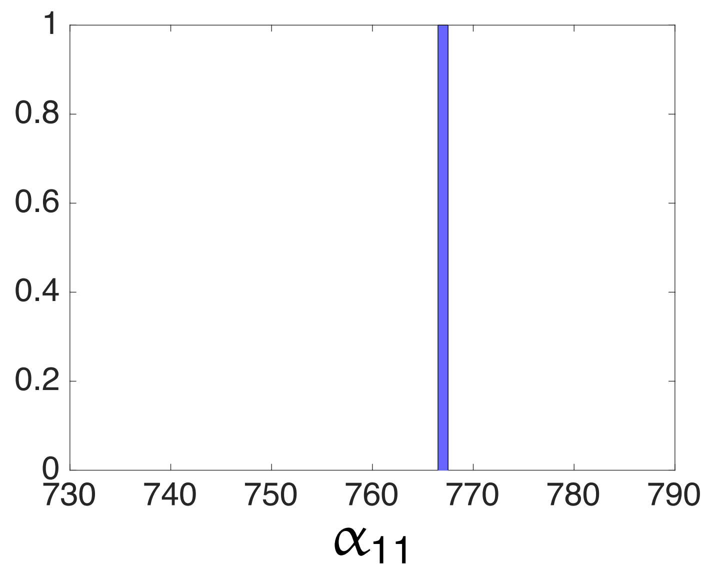


Common Assumption: $\varepsilon_i \sim N(0, \sigma^2)$

UQ Goals: Quantify parameter and response uncertainties

Strategy 1: Perform experiments; e.g., 1





Strategy 1: Perform Experiments or High-Fidelity Simulations

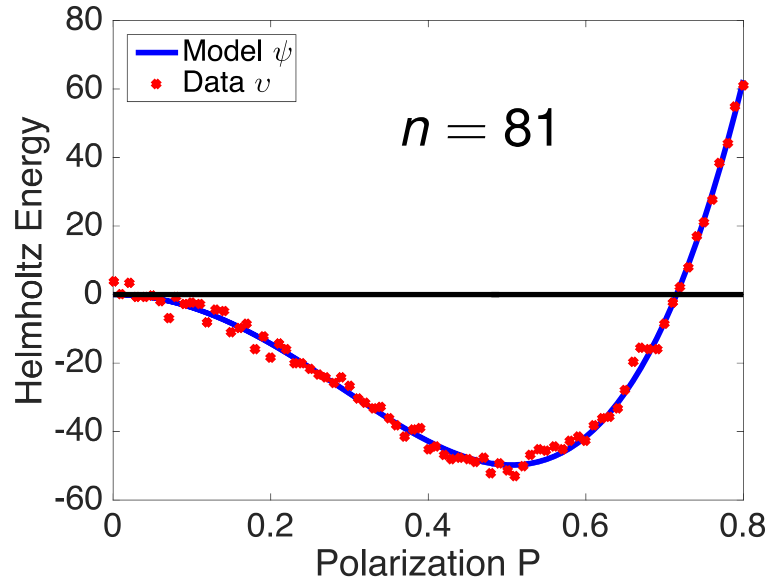
Example: Helmholtz energy $\psi(P,q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$

Statistical Model: Describes observation process

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \quad , \; i = 1, \ldots, n$$

Common Assumption: $\varepsilon_i \sim N(0, \sigma^2)$

UQ Goals: Quantify parameter and response uncertainties



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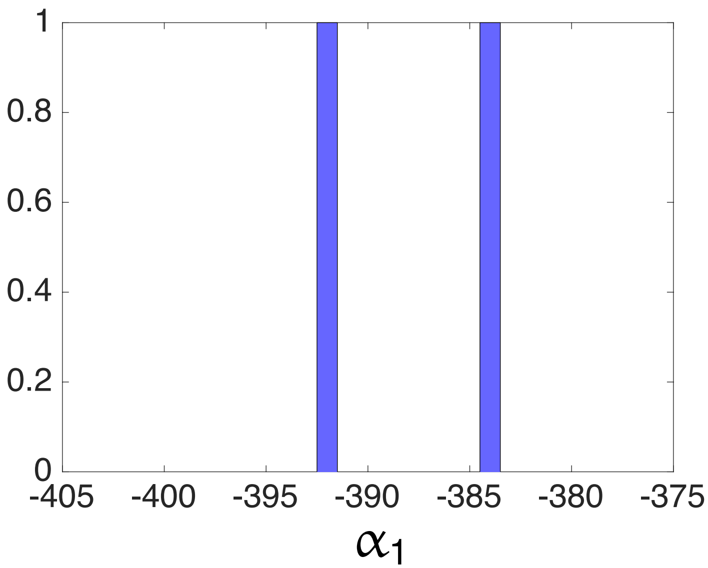

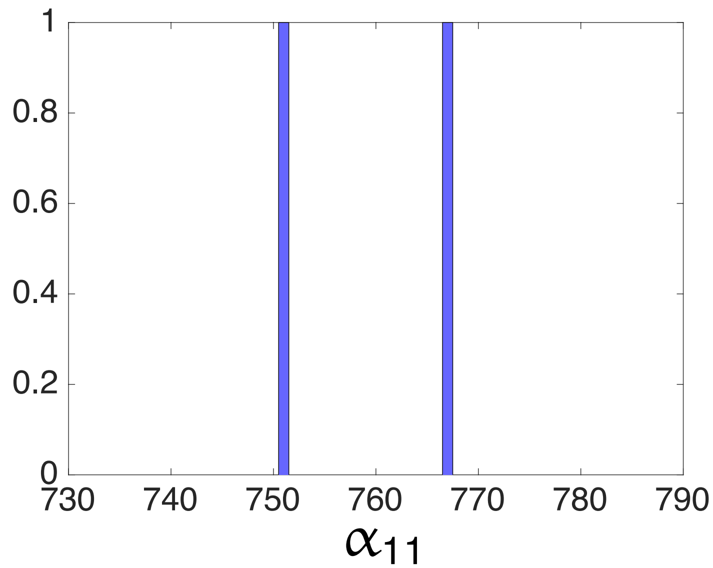

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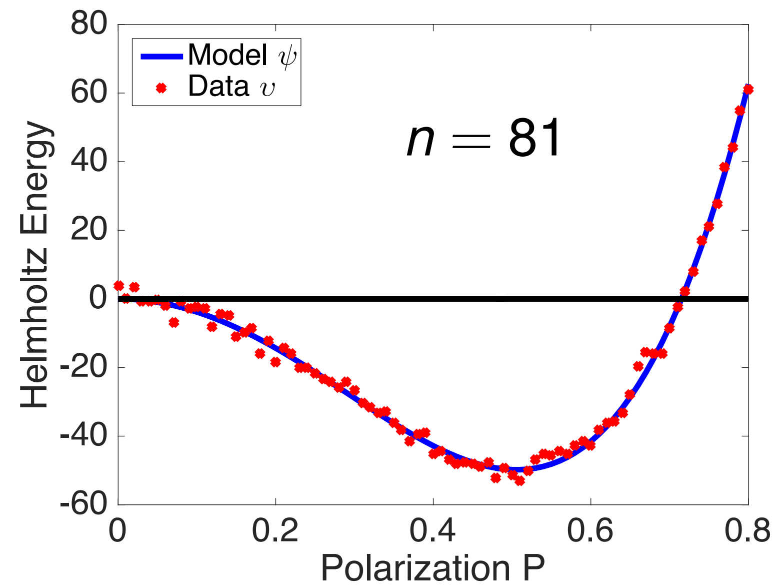

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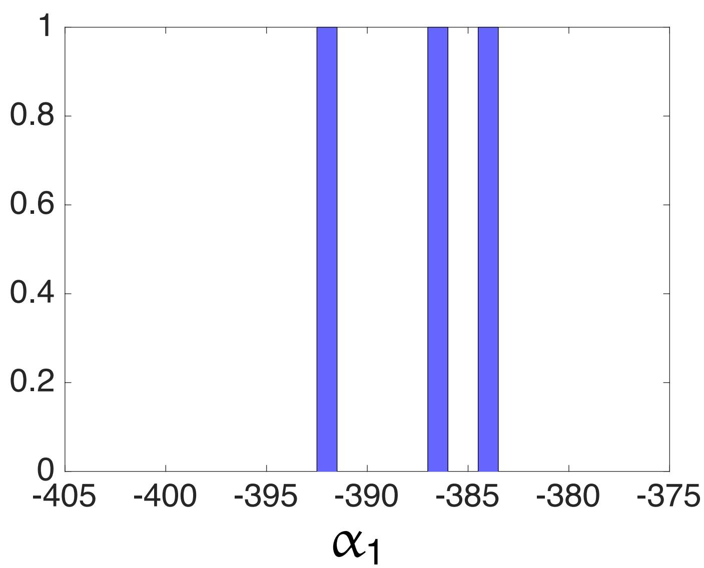

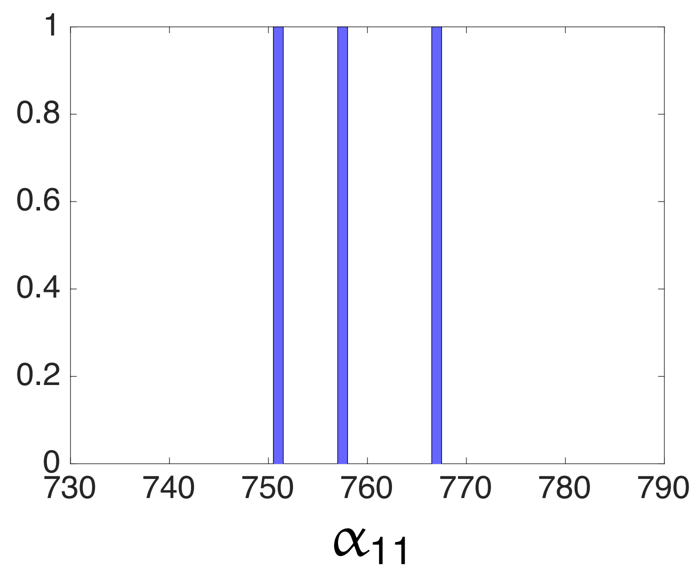

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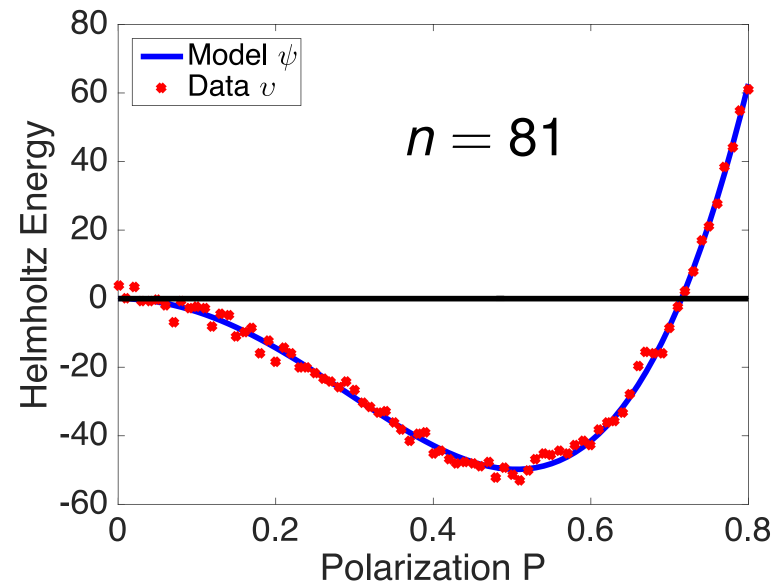
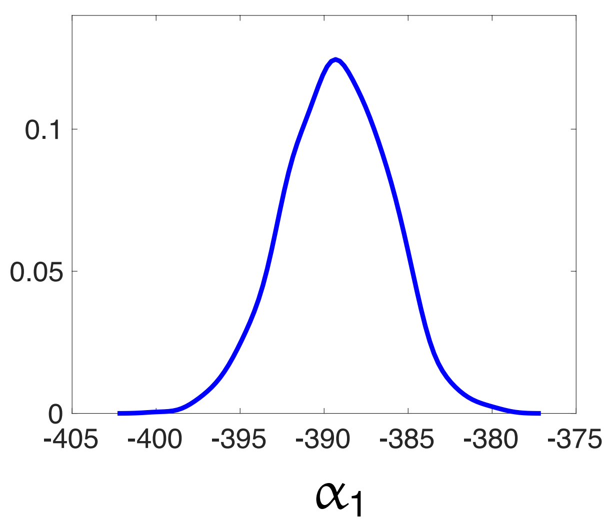
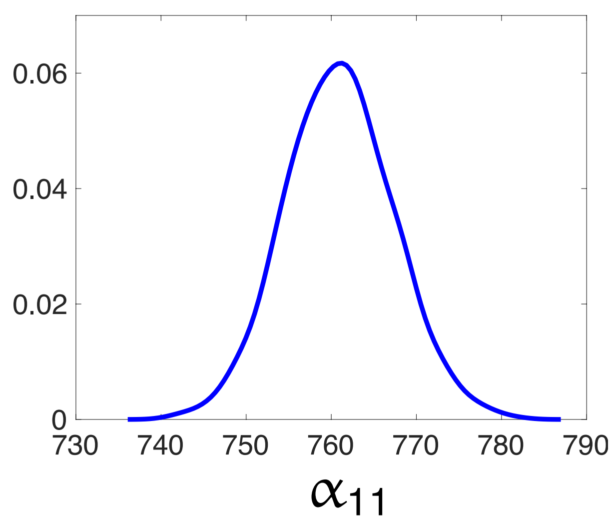
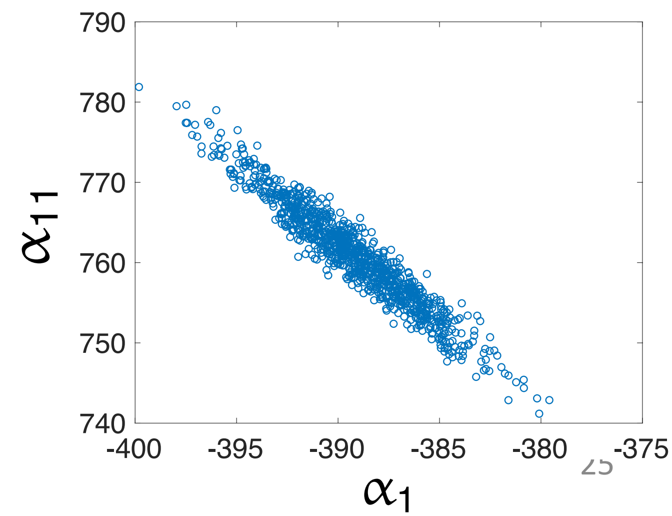


Strategy 1: Perform many experiments; e.g., 1000







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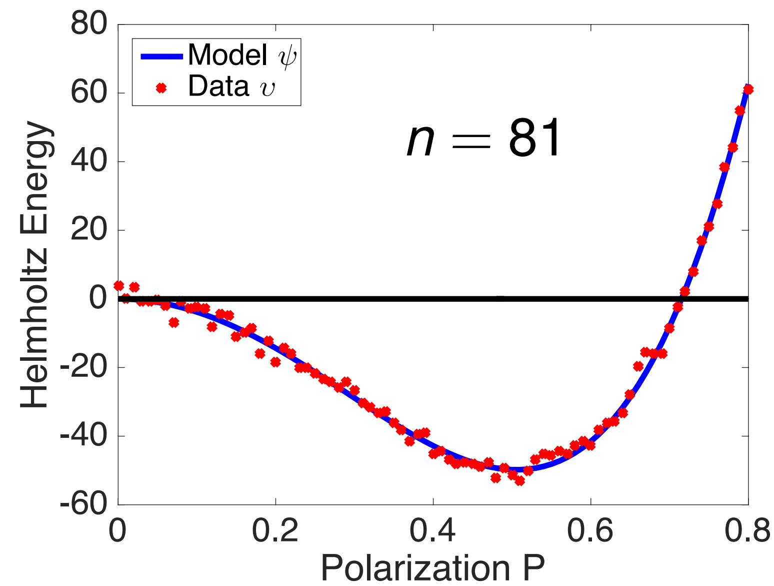

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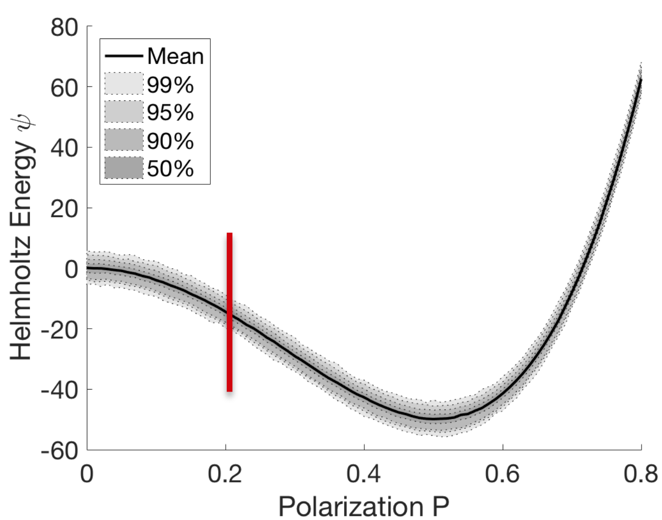

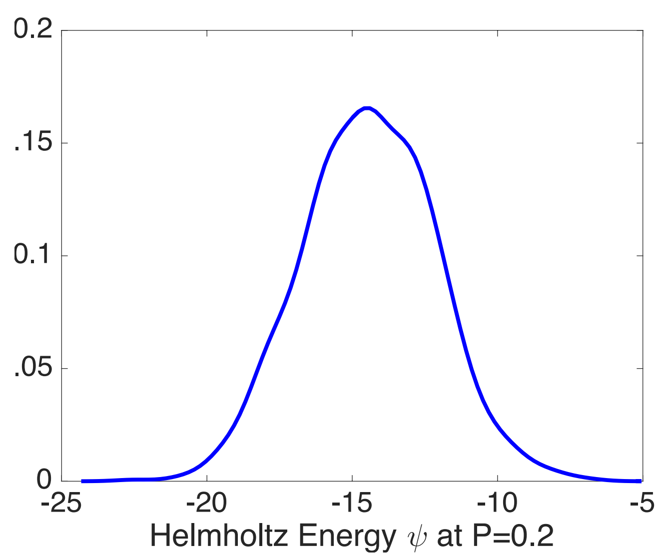

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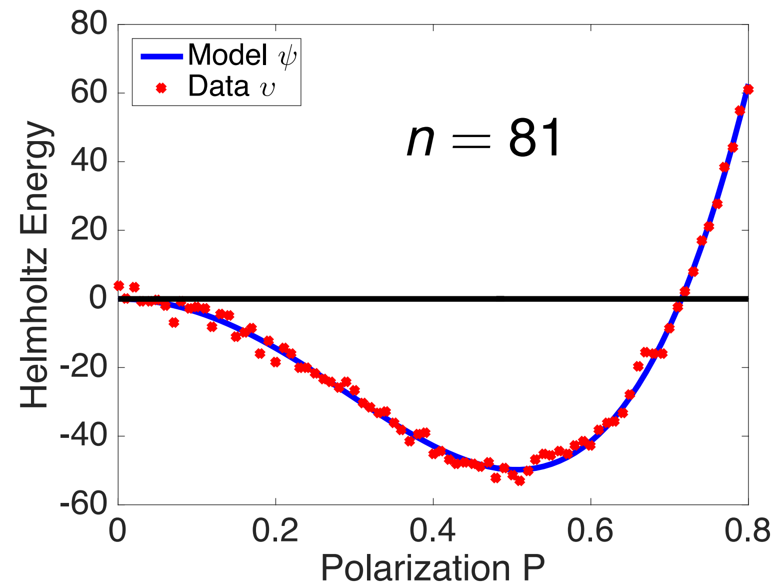

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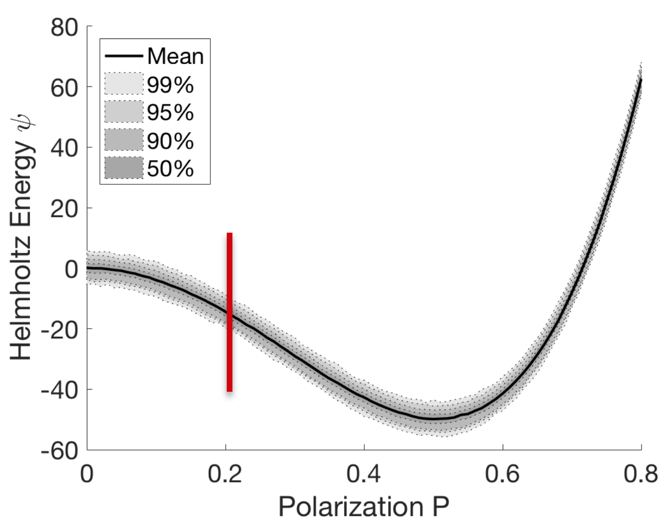

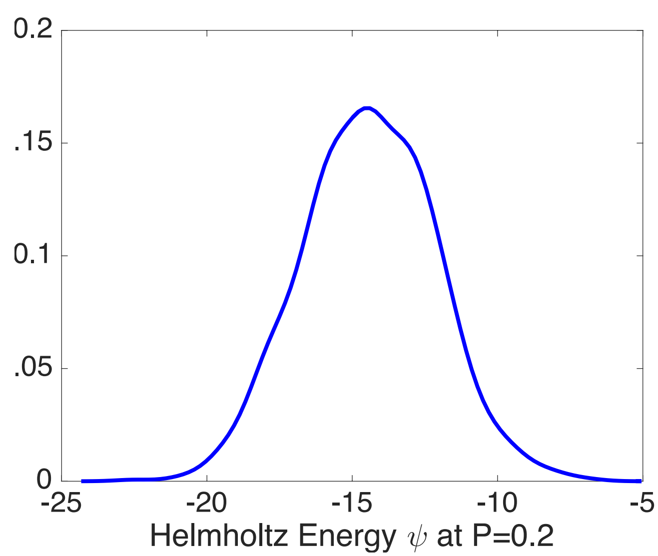

Problem: Often cannot perform required number of experiments or high-fidelity simulations.

Solution: Statistical inference

3. Statistical Inference

Goal: The goal in statistical inference is to make conclusions about a phenomenon based on observed data.

Frequentist: Observations made in the past are analyzed with a specified model. Result is regarded as confidence about state of real world.

- Probabilities defined as frequencies with which an event occurs if experiment is repeated several times.
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  - o Parameters may be unknown but are fixed and deterministic.

Bayesian: Interpretation of probability is subjective and can be updated with new data.

- Parameter Estimation: Parameters are considered to be random variables having associated densities.

Linear Regression

Statistical Model:

$$\Upsilon = Xq_0 + \varepsilon$$

Assumptions:

(i) $\mathbb{E}(\varepsilon_i) = 0$

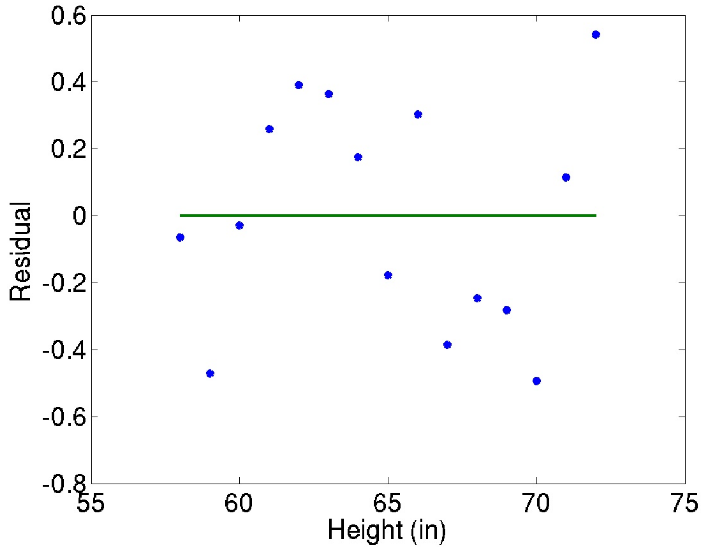
(ii) ε_i iid (independent and identically distributed)

$$\Rightarrow \quad \mathrm{var}(\varepsilon_i) = \sigma_0^2$$

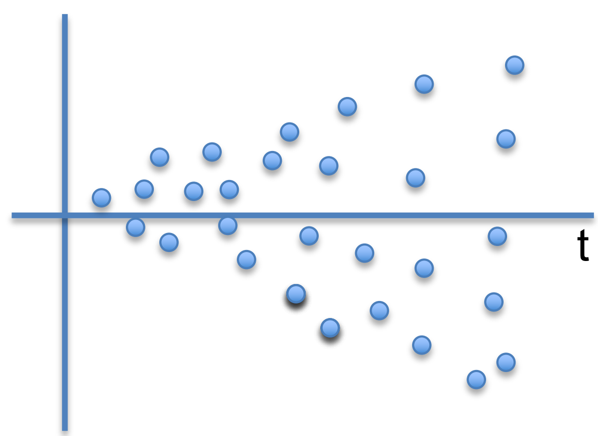
$$\mathbb{E}[(\varepsilon_i - \mathbb{E}(\varepsilon_i))(\varepsilon_j - \mathbb{E}(\varepsilon_j))] = \mathrm{cov}(\varepsilon_i, \varepsilon_j) = 0 \text{ for } i \neq j$$

Examples:

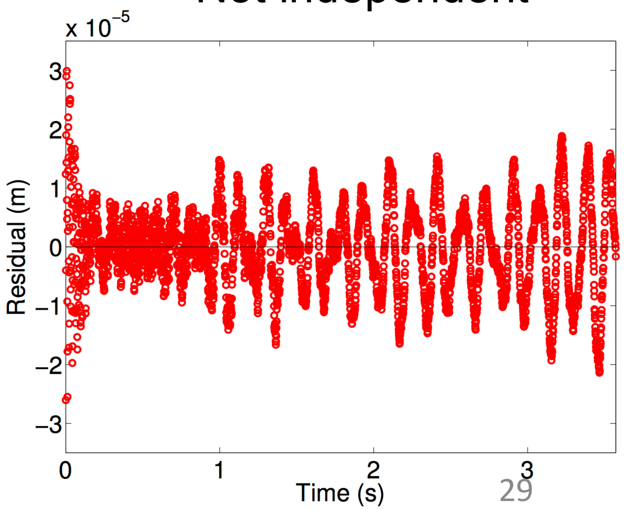
iid errors



Not identically distributed



Not independent



Polarization Example

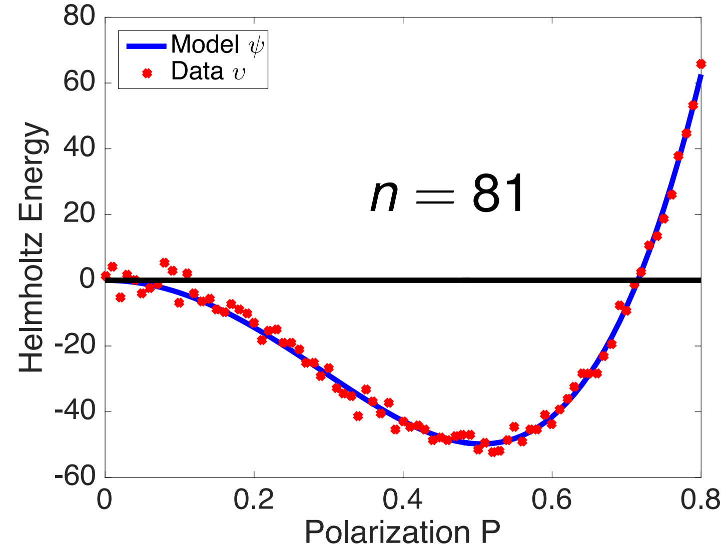
Statistical Model: For i = 1, …, n

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$

$$= \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i$$

$$\Rightarrow \begin{bmatrix} \upsilon_i \end{bmatrix} = \begin{bmatrix} P_i^2 & P_i^4 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_{11} \end{bmatrix} + \begin{bmatrix} \varepsilon_i \end{bmatrix}$$

$$\Rightarrow \upsilon = Xq + \varepsilon$$



Statistical Quantities:

$$q = (X^T X)^{-1} X^T \upsilon$$

Polarization Example

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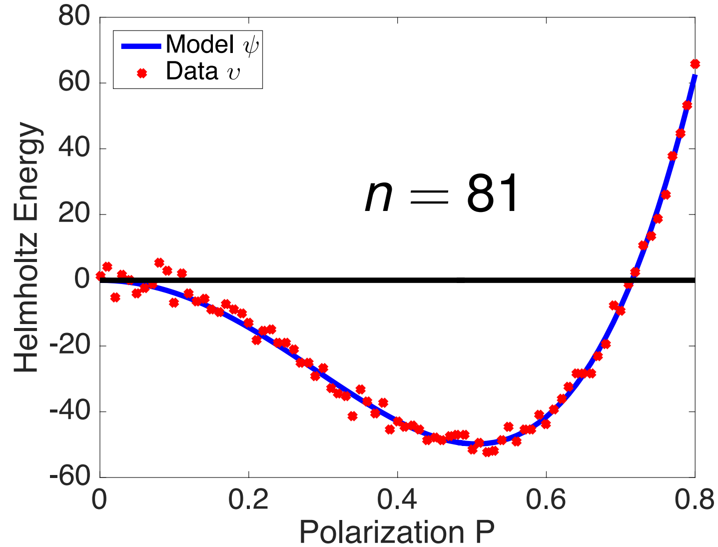


Statistical Quantities:

$$q = (X^T X)^{-1} X^T \upsilon$$

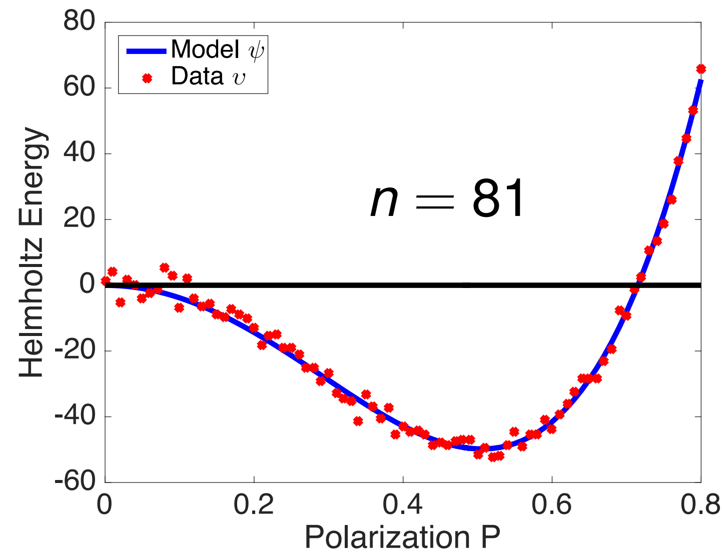
Note: $\mathbb{E}(q) = \mathbb{E}[(X^T X)^{-1} X^T \upsilon]$

$$= (X^T X)^{-1} X^T \mathbb{E}(\upsilon)$$

$$= q_0$$

$$\upsilon = Xq_0 + \varepsilon$$

Polarization Example



Statistical Model: For i = 1, …, n

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$$\upsilon = Xq_0 + \varepsilon$$

And: Let $A = (X^T X)^{-1} X^T$

$$\begin{aligned} V(q) &= \mathbb{E}[(q - q_0)(q - q_0)^T] \\ &= \mathbb{E}[(q_0 + A\varepsilon - q_0)(q_0 + A\varepsilon - q_0)^T] \ \text{ since } q = A\Upsilon = A(Xq_0 + \varepsilon) \\ &= A\mathbb{E}(\varepsilon\varepsilon^T)A^T \\ &= \sigma^2 (X^T X)^{-1} \end{aligned}$$

Polarization Example

Statistical Model: For i = 1, …, n

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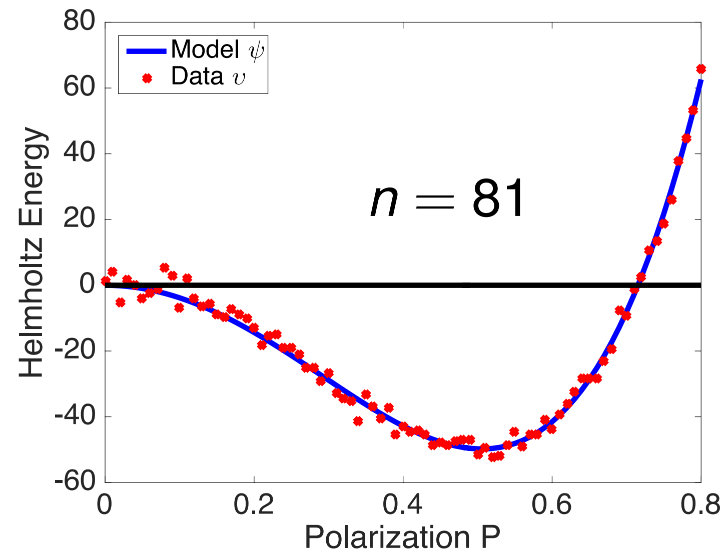


Statistical Quantities:

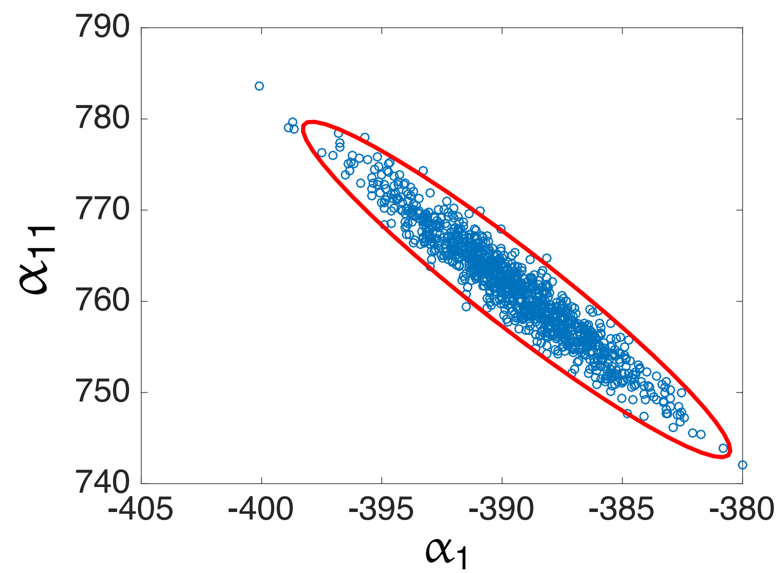
$$q = (X^T X)^{-1} X^T \upsilon$$

$$V = \underline{\sigma^2} (X^T X)^{-1} = \begin{bmatrix} 8.8 & -17.4 \\ -17.4 & 37.6 \end{bmatrix}$$

var(α_1)

cov(α_1, α_{11})

var(α_{11})



Note: Covariance matrix incorporates “geometry”

Goal: Employ Bayesian inference for UQ

Statistical Inference

Goal: The goal in statistical inference is to make conclusions about a phenomenon based on observed data.

Frequentist: Observations made in the past are analyzed with a specified model. Result is regarded as confidence about state of real world.

- Probabilities defined as frequencies with which an event occurs if experiment is repeated several times.
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Bayesian: Interpretation of probability is subjective and can be updated with new data.

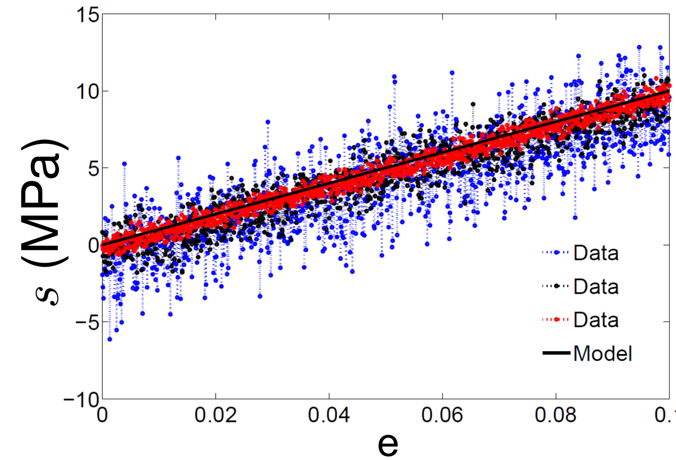
- Parameter Estimation: Parameters are considered to be random variables having associated densities.

Bayesian Inference: Simpler Model

Example: Displacement-force relation (Hooke's Law)

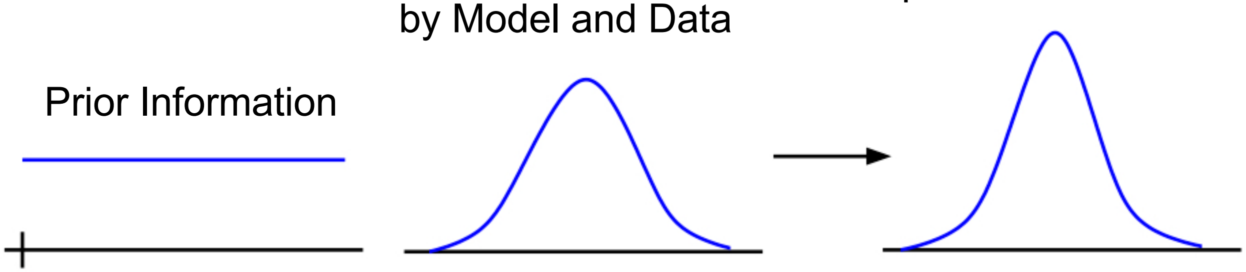
$$s_i = Ee_i + \varepsilon_i \ , \ i = 1, \ldots, N$$

$$\varepsilon_i \sim N(0, \sigma^2)$$



Parameter: Stiffness E

Strategy: Use model fit to data to update prior information



$$\pi_0(E) \qquad e^{-\sum_{i=1}^N [s_i - Ee_i]^2/2\sigma^2} \qquad \pi(E|s)$$

Data Model

Non-normalized Bayes' Relation:

$$\pi(E|s) = e^{-\sum_{i=1}^N [s_i - Ee_i]^2/2\sigma^2} \pi_0(E)$$

Bayesian Inference

Bayes' Relation: Specifies posterior in terms of likelihood and prior

Likelihood: $e^{-\sum_{i=1}^{N}[s_i - Ee_i]^2/2\sigma^2}$, $q = E$

$\upsilon = [s_1, \ldots, s_N]$

Posterior Distribution

$$\boxed{\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}}$$

Prior Distribution

Normalization Constant

- Prior Distribution: Quantifies prior knowledge of parameter values
- Likelihood: Probability of observing a data given set of parameter values.
- Posterior Distribution: Conditional distribution of parameters given observed data.

Problem: Can require high-dimensional integration

- e.g., MFC Model: p = 20!
- Solution: Sampling-based Markov Chain Monte Carlo (MCMC) algorithms.
- Metropolis algorithms first used by nuclear physicists during Manhattan Project in 1940's to understand particle movement underlying first atomic bomb.

Bayesian Inference: Motivation

Bayes' Relation for Sets:

$$\boxed{P(B_i|A) = \frac{P(B_i \cap A)}{P(A)} = \frac{P(A|B_i)P(B_i)}{\sum_i P(A|B_i)P(B_i)}}$$

Bayes' Relation for Functions: Specifies posterior in terms of likelihood, prior, and normalization constant.

Likelihood

Posterior Distribution

Prior Distribution

$$\boxed{\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}}$$

Normalization factor

Note:

- Prior Distribution: Quantifies prior knowledge of parameter values.
- Likelihood: Probability of observing a data if we have a certain set of parameter values.
- Posterior Distribution: Conditional probability distribution of unknown parameters given observed data (Updated distribution based on how model fits new data).

Bayesian Model Calibration

Bayesian Model Calibration:

- Parameters assumed to be random variables

$$\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}$$

Example: Coin Flip

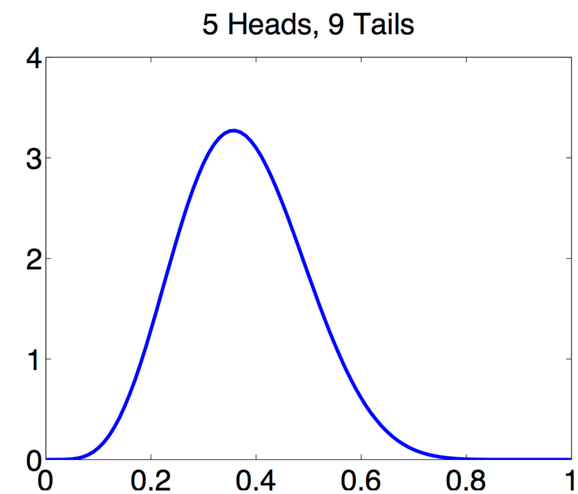
$$\Upsilon_i(\omega) = \begin{cases} 0 & , \quad \omega = T \\ 1 & , \quad \omega = H \end{cases}$$

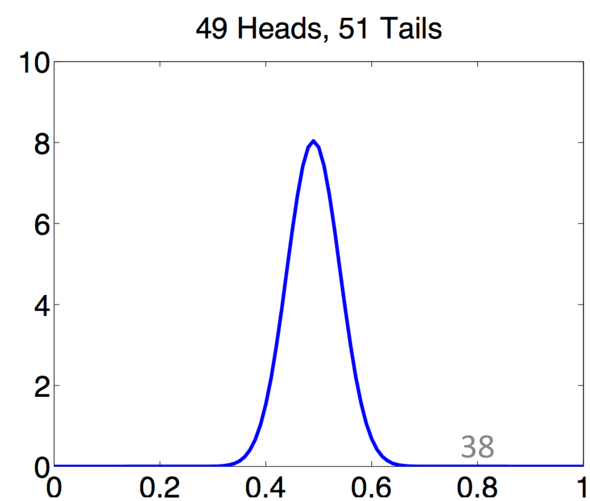
Likelihood:

$$\begin{aligned} \pi(\upsilon|q) &= \prod_{i=1}^{N} q^{\upsilon_i}(1-q)^{1-\upsilon_i} \\ &= q^{N_1}(1-q)^{N_0} \end{aligned}$$

Posterior with Noninformative Prior: $\pi_0(q) = 1$

$$\pi(q|\upsilon) = \frac{q^{N_1}(1-q)^{N_0}}{\int_0^1 q^{N_1}(1-q)^{N_0}dq} = \frac{(N+1)!}{N_0!N_1!}q^{N_1}(1-q)^{N_0}$$





Bayesian Model Calibration

Bayesian Model Calibration:

• Parameters considered to be random variables with associated densities.

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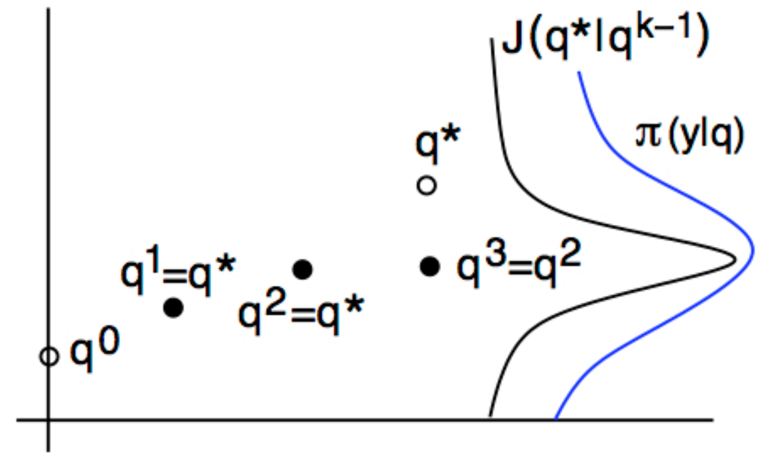
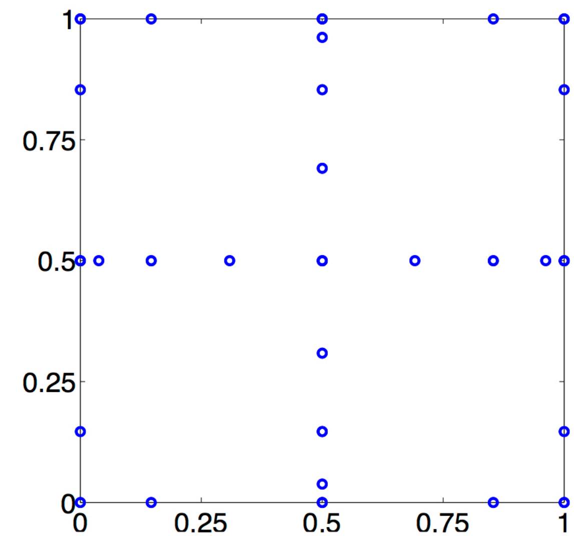


Problem:

• Often requires high dimensional integration;

  ○ p = 20 for MFC example



Strategies:

• Sampling methods

• Sparse grid quadrature techniques

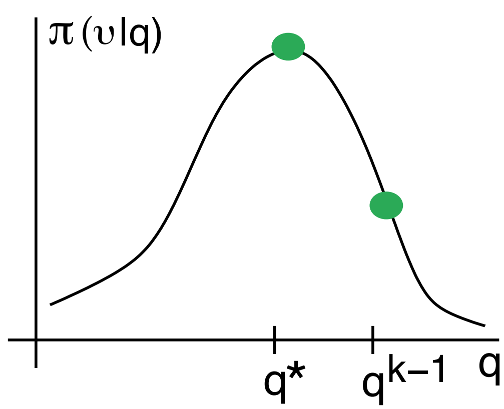
Markov Chain Monte Carlo Methods

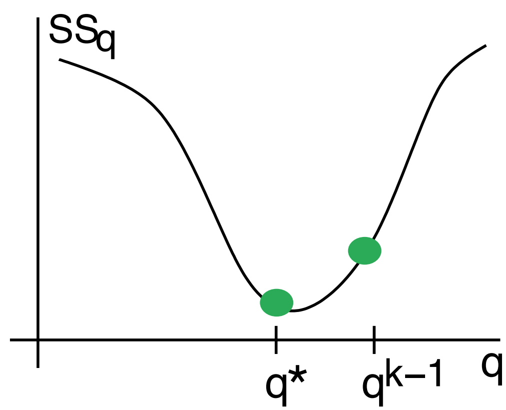
Strategy:

- Sample values from proposal distribution $J(q^*|q^{k-1})$ that reflects geometry of posterior distribution
- Compute $r(q^*|q^{k-1}) = \frac{\pi(\upsilon|q^*)\pi_0(q^*)}{\pi(\upsilon|q^{k-1})\pi_0(q^{k-1})}$
  - $*$ If $r \geqslant 1$, accept with probability $\alpha = 1$
  - $*$ If $r < 1$, accept with probability $\alpha = r$

Intuition: Consider flat prior $\pi_0(q) = 1$ and Gaussian observation model

$$\pi(\upsilon|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2} \qquad SS_q = \sum_{i=1}^{N} [\upsilon_i - f(t_i, q)]^2$$





Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006] – MATLAB, Python, R

1. Determine $q^0 = \arg\min_q \sum_{i=1}^{N} [\upsilon_i - \psi(P_i, q)]^2]$

Example: Helmholtz energy

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$
$$= \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i$$

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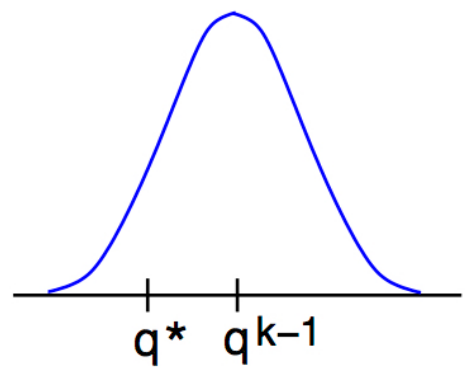
   (a) Construct candidate $q^* \sim N(q^{k-1}, \underline{V})$



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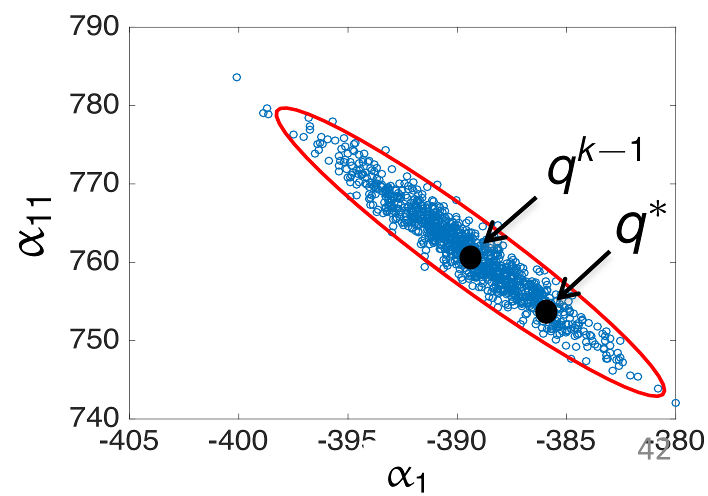
Recall: Covariance V incorporates geometry



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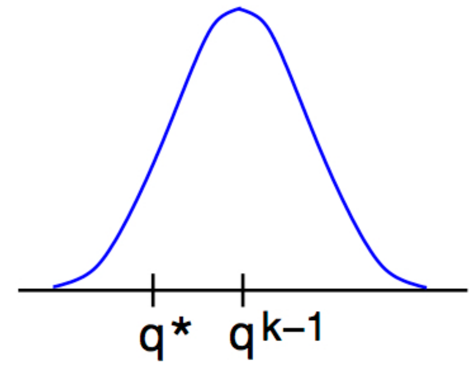

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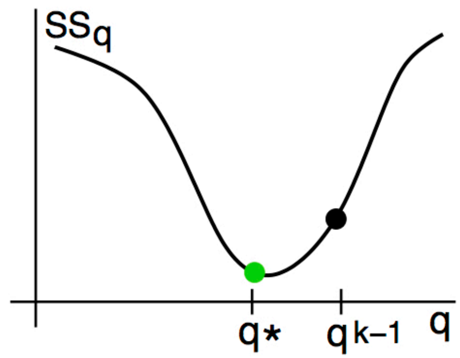
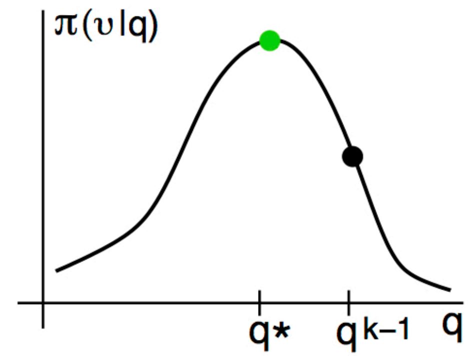
   (a) Construct candidate $q^* \sim N(q^{k-1}, V)$
   (b) Compute likelihood

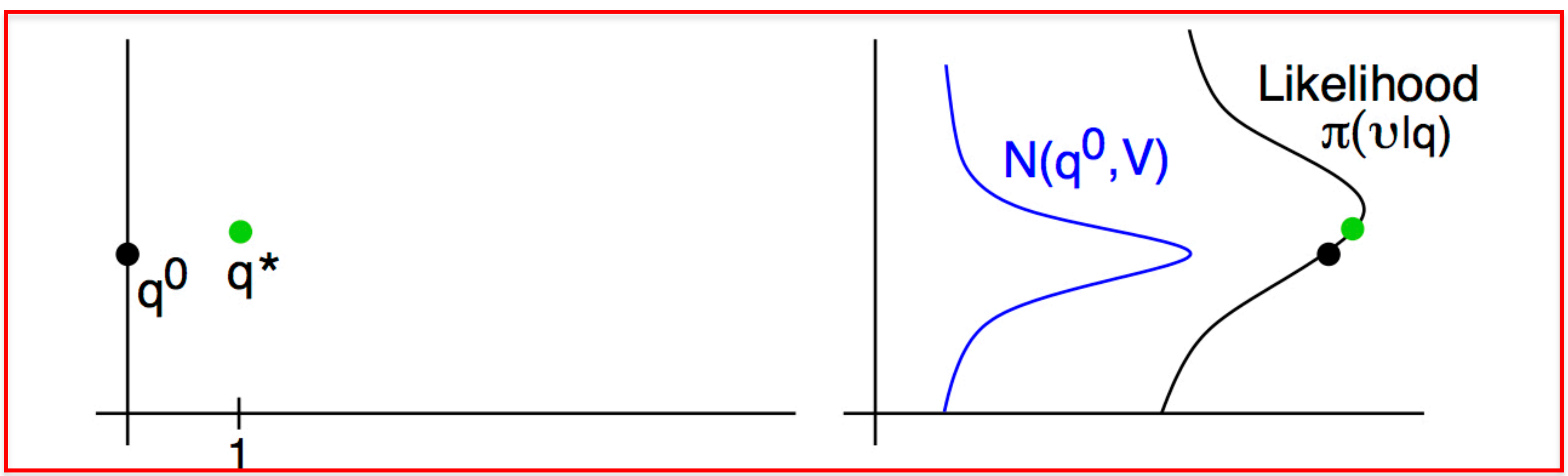
$$SS_{q^*} = \sum_{i=1}^{N} \upsilon_i - \psi(P_i, q^*)]^2$$

$$\pi(\upsilon|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}$$



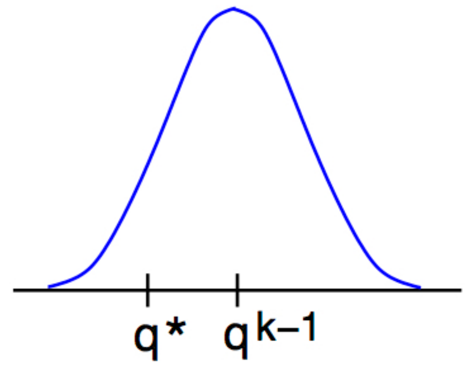


   (c) Accept q^* with probability dictated by likelihood



Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006] – MATLAB, Python, R



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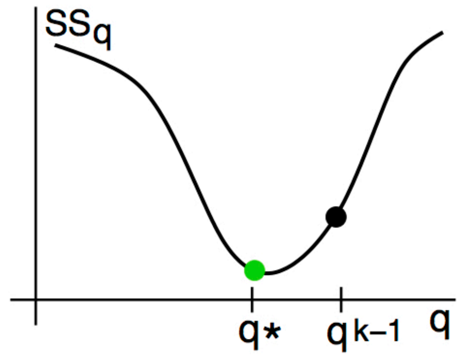

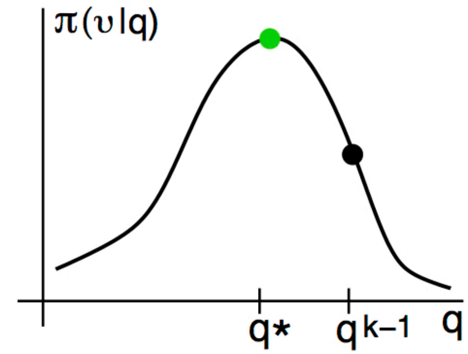

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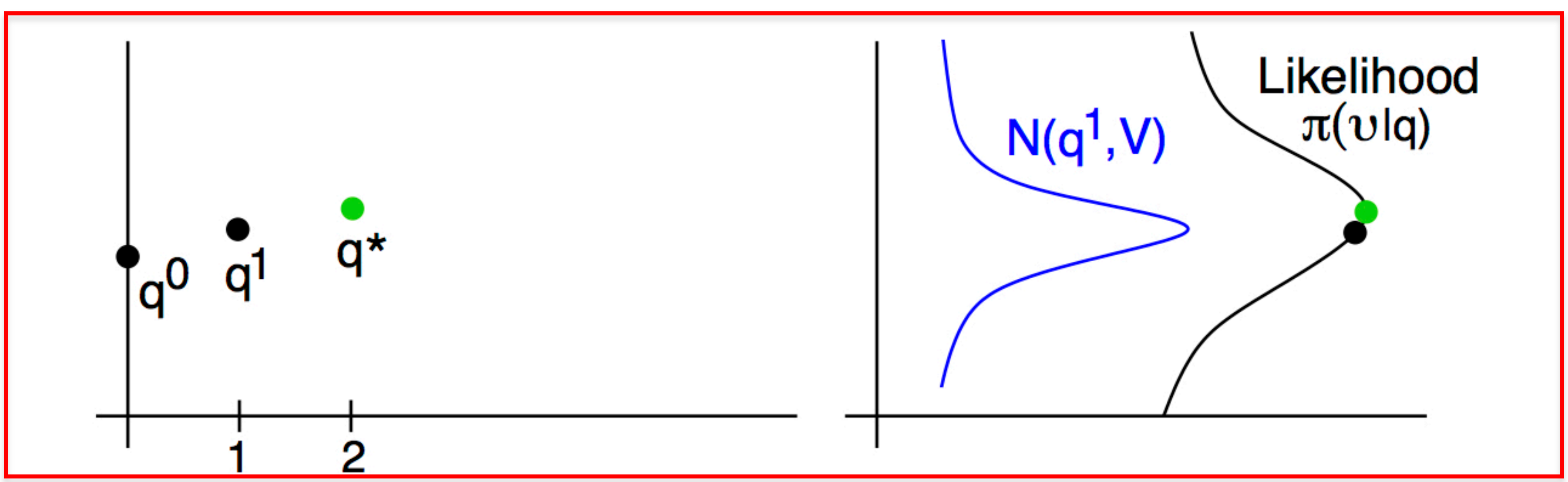

Delayed Rejection Adaptive Metropolis (DRAM)

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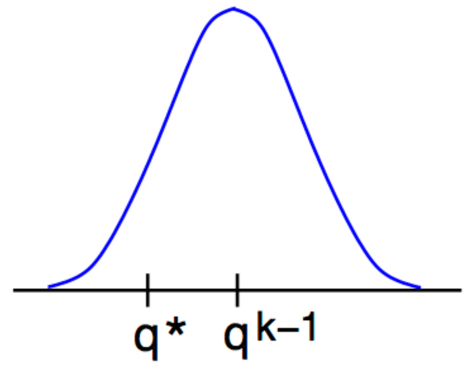

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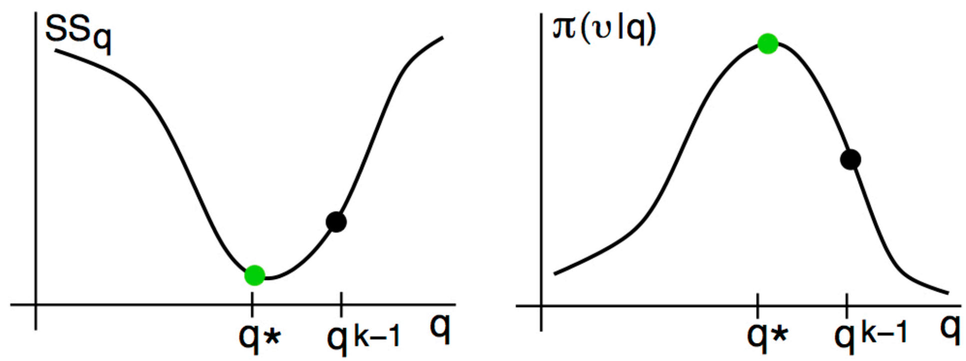

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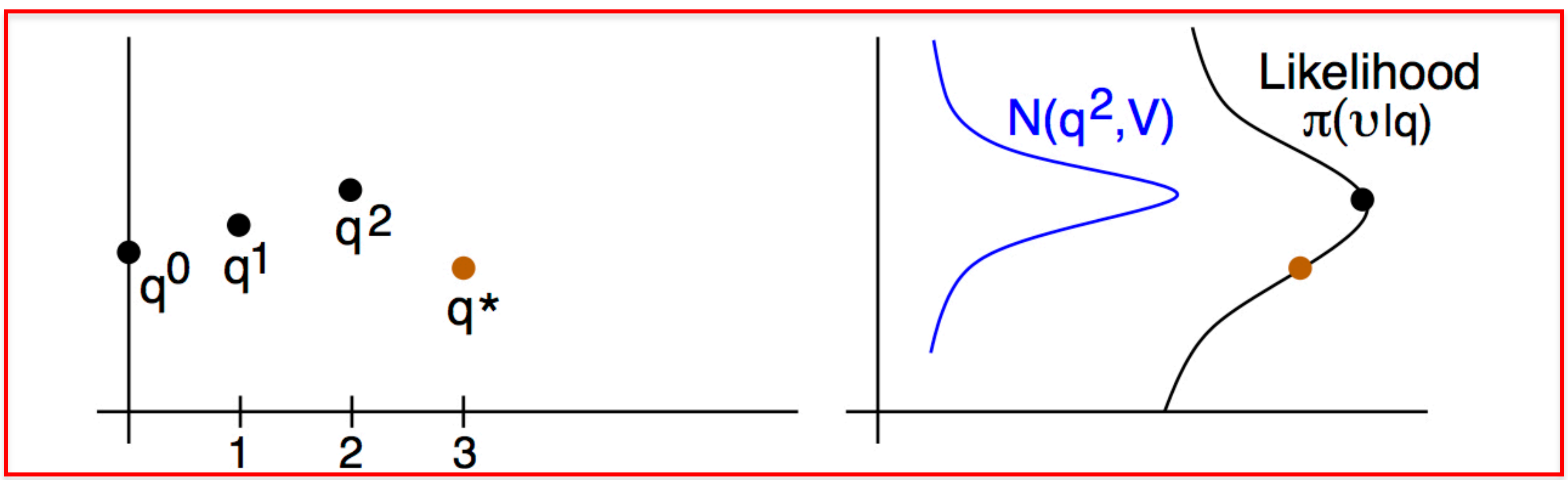
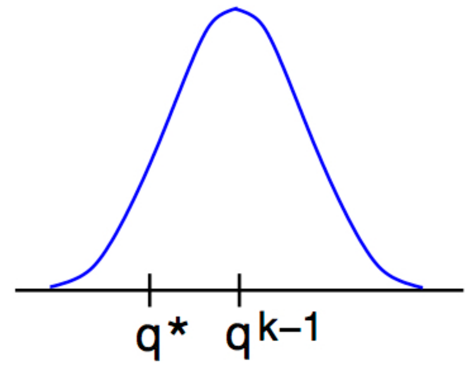


Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006] – MATLAB, Python, R



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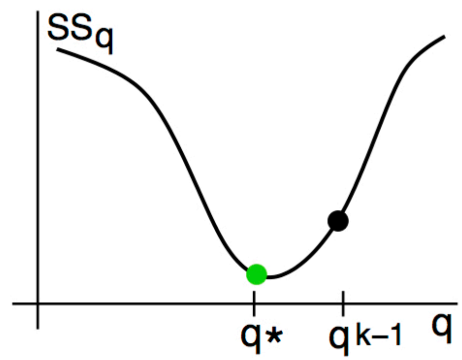

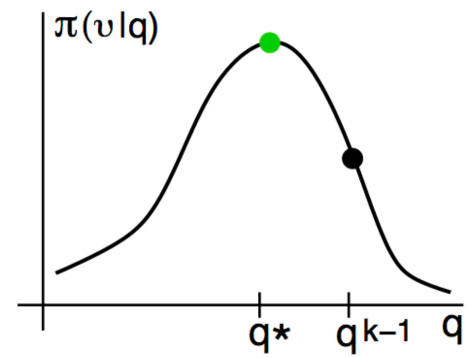

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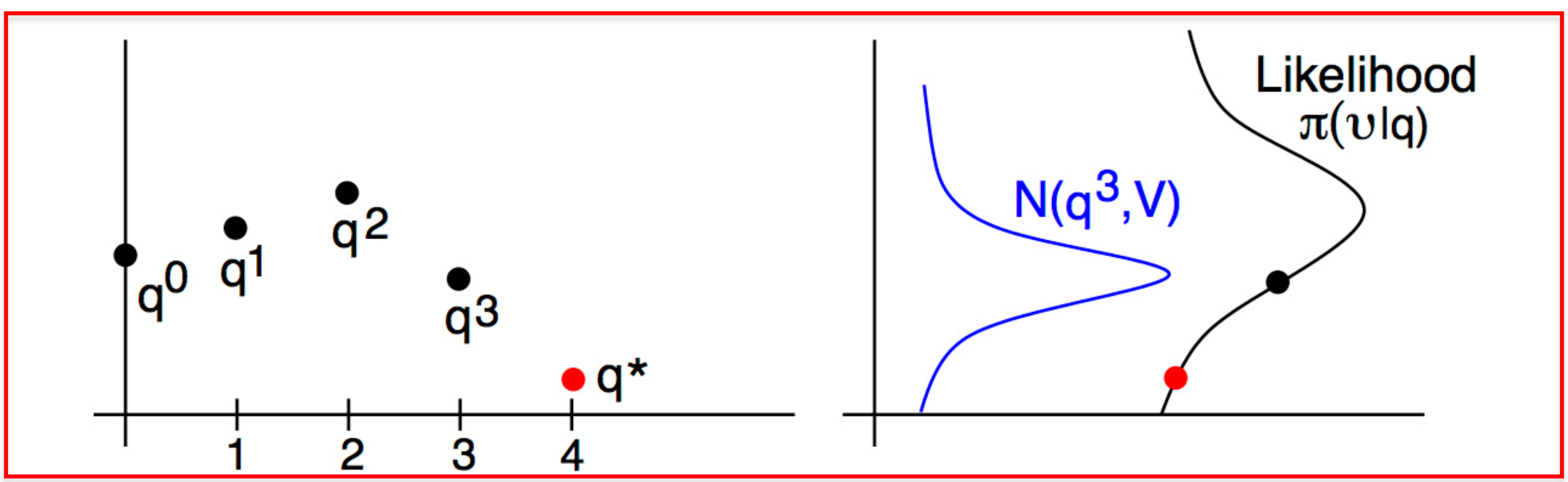

Delayed Rejection Adaptive Metropolis (DRAM)

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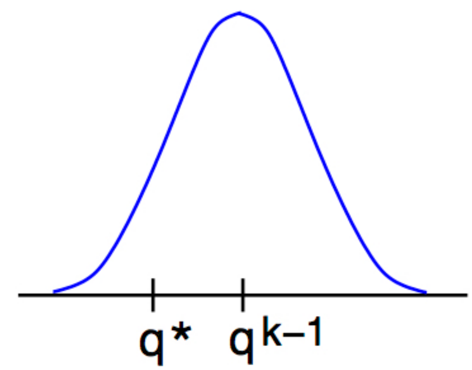

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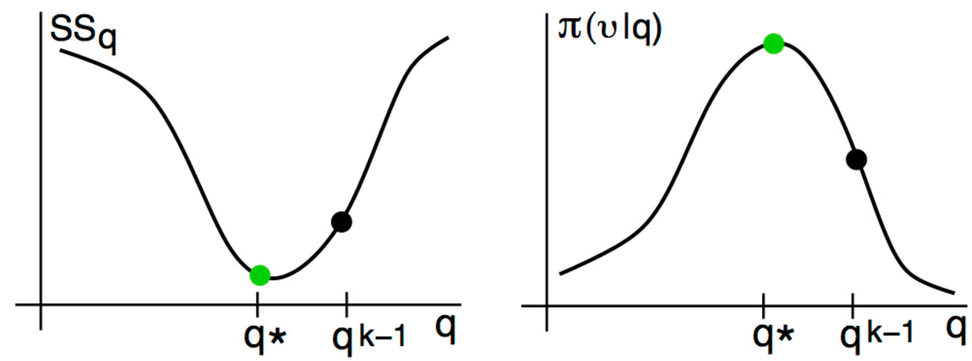

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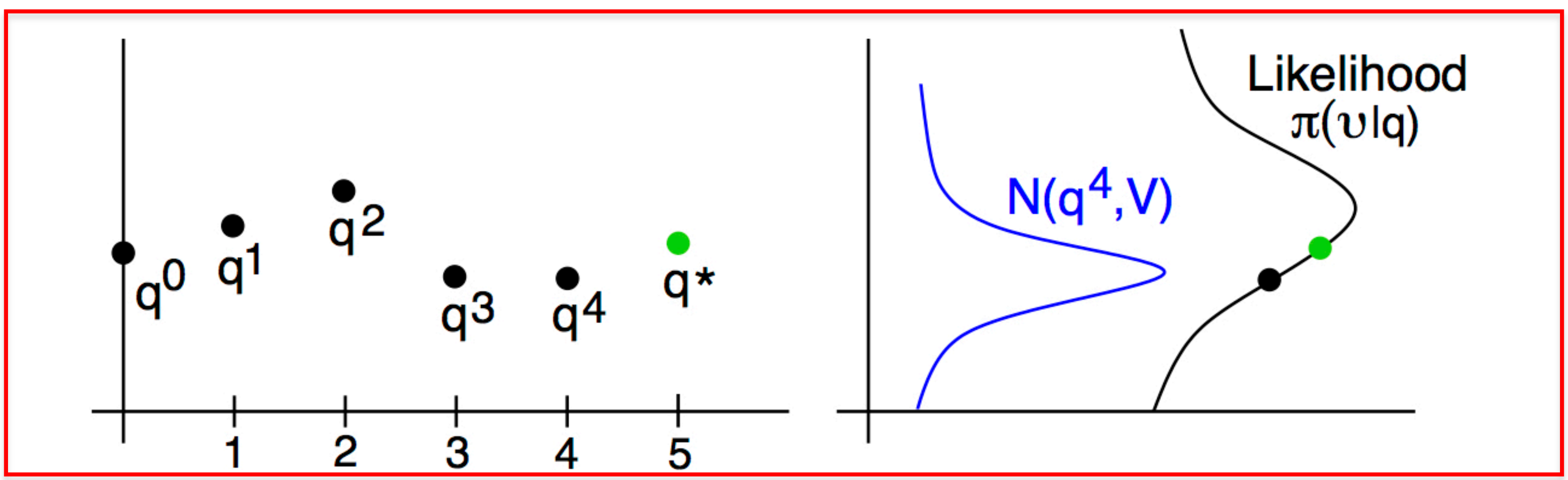

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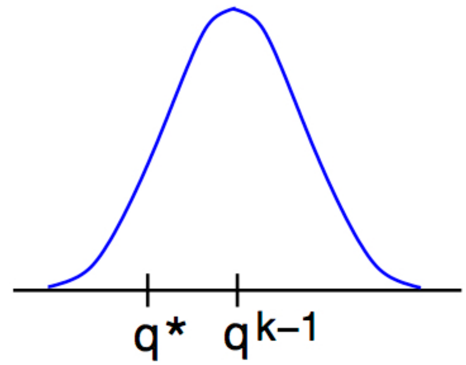

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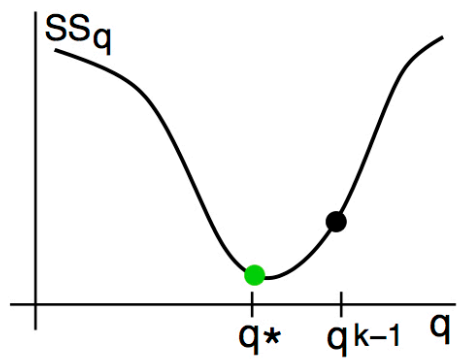

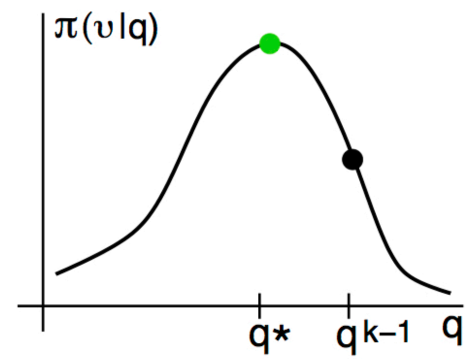

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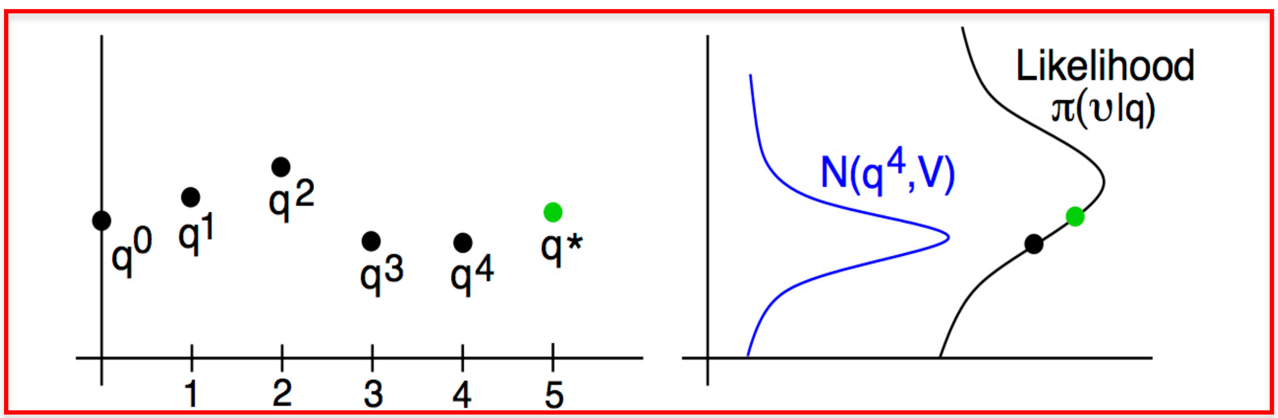


Note:

- Delayed Rejection: Shrink proposal: γV
- Adaptive Metropolis: Update proposal as samples are accepted

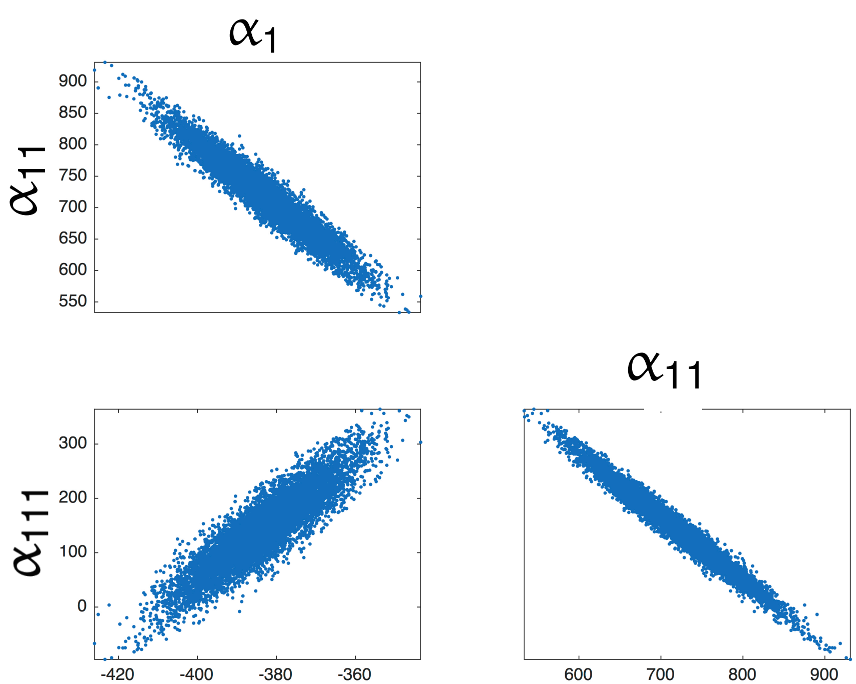
Delayed Rejection Adaptive Metropolis (DRAM)

Example: Helmholtz energy with 3 parameters

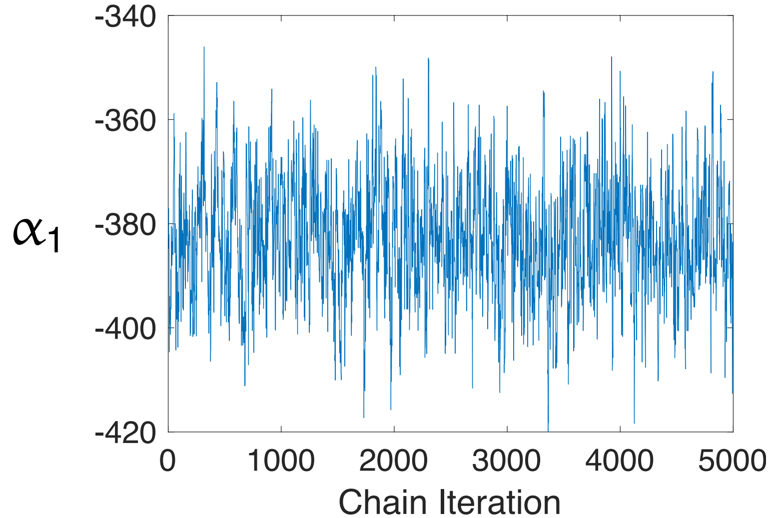
$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Note: Similar results for α_{11} and α_{111}

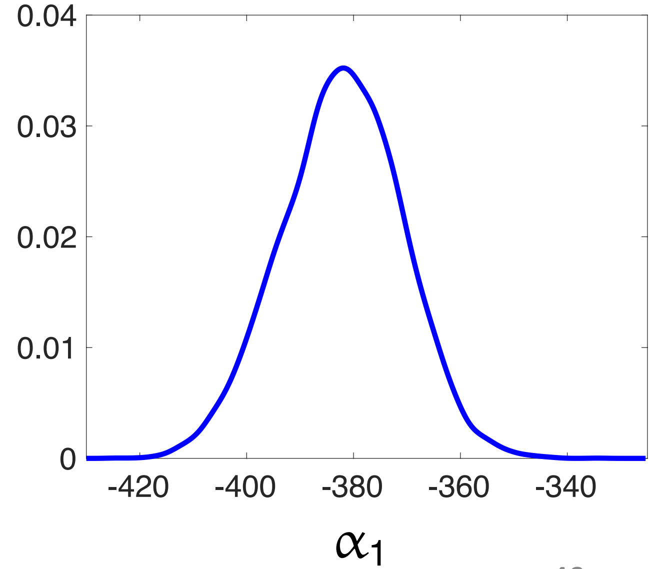
Pairwise Plots: Quantify correlation



Chain for α_1 with 5000 samples



Marginal density for α_1



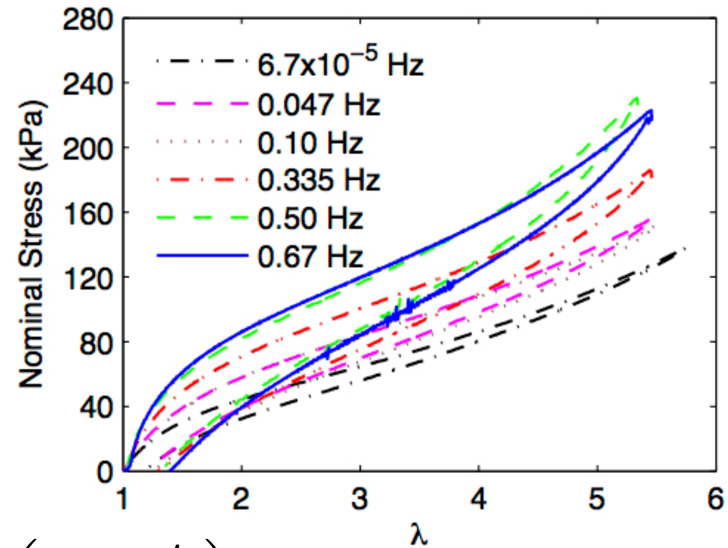
Example: Viscoelastic Material Models

Material Behavior: Significant rate dependence

Finite-Deformation Model: Nonlinear, non-affine

$$\psi(q) = \psi_\infty(G_e, G_c, \lambda_{\max}) + \Upsilon(\eta, \beta, \gamma)$$

- Dissipative energy function Υ
- Conserved hyperelastic energy function



$$\psi_\infty^N = \frac{1}{6}\underline{G_c} I_1 - \underline{G_c \lambda_{\max}^2} \ln(3\underline{\lambda_{\max}^2} - I_1) + \underline{G_e} \sum_j \left(\lambda_j + \frac{1}{\lambda_j}\right)$$

Parameters:

$$q = [G_e, G_c, \lambda_{\max}, \eta, \beta, \gamma]$$

G_c: Crosslink network modulus

G_e: Plateau modulus

$\lambda_{\max}$: Max stretch effective affine tube

$\boxed{[\eta, \beta, \gamma]\text{: Viscoelastic parameters}}$

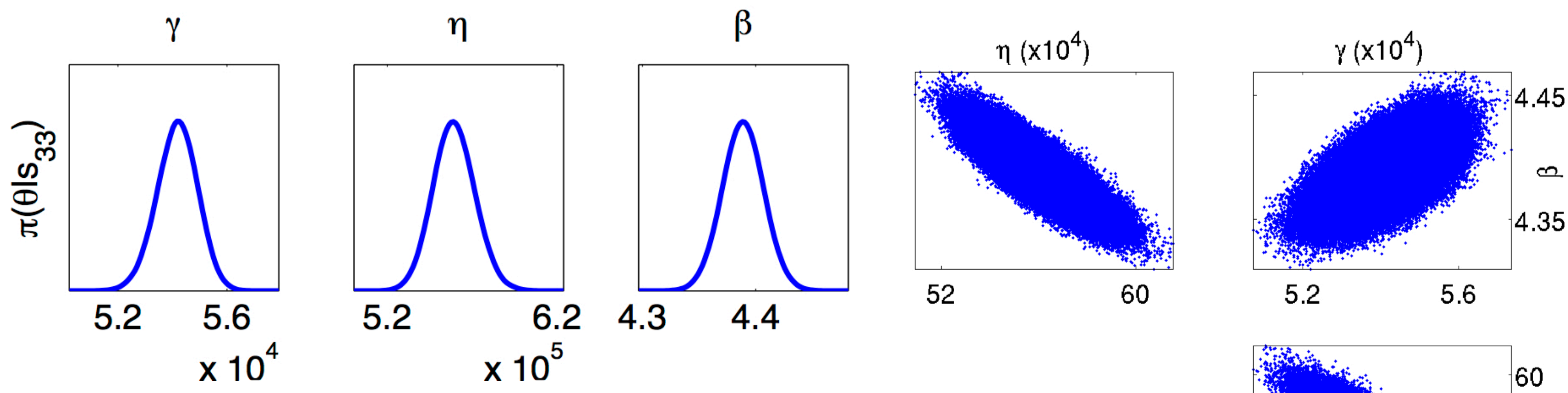
UQ Goals:

- Quantify uncertainty in parameters.
- Use UQ for model selection
  - E.g., linear versus nonlinear.
- Quantify models' predictive capabilities for range of stretch rates.

Viscoelastic Model

Reduced Parameter Set:

$$q = [\gamma, \eta, \beta] \quad , \text{ Fixed hyperelastic parameters}$$



Note: Fastest stretch rate (0.67 Hz)

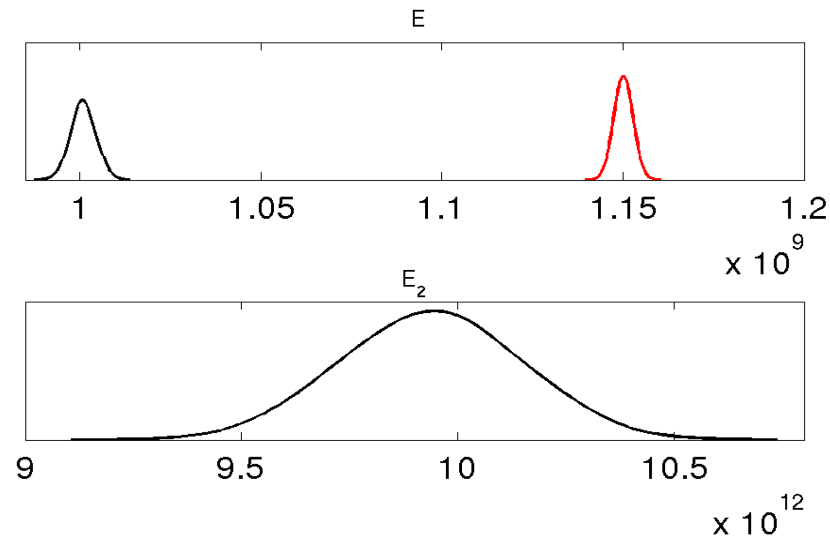
Question: How do we quantify uncertainty in response (stress)?

Solution: Propagate parameter and measurement uncertainties through model … in a few slides!

Bayesian Inference: Exercise

Example: Stress-strain relation

$$\sigma = Ee + E_2 e^3$$



Notes:

- Nonlinear dependence on strain
- Linear dependence on parameters E, E_2

Website: http://www.eng.fsu.edu/~woates/template/research.html

Exercise:

1. Using the small synthetic data set, use DRAM to estimate the parameters using the default code assuming the stress depends both linearly and nonlinear on strain (equation above).
2. Repeat but neglect the nonlinear term in the model; i.e., $\sigma = Ee$. How does this change the uncertainty on the estimated modulus *E*?

Bayesian Inference: Exercise

Example: Spring relation (parameter identifiability example)

Consider the following idealized model:

$$\sigma = E_1 e + E_2 e$$

This model can be easily created by changing the file:
elastic_model_Bayesian.m

Exercise:

1. Assess question on parameter uniqueness and issues arising with the initial guesses for the two parameters E_1 and E_2.
2. What are the posterior densities for the two parameters E_1 and E_2? What if the bounds on the parameter space is changed; will the posterior densities change?
3. Review the pairwise correlation between these two parameters.

Bayesian Inference: Exercise

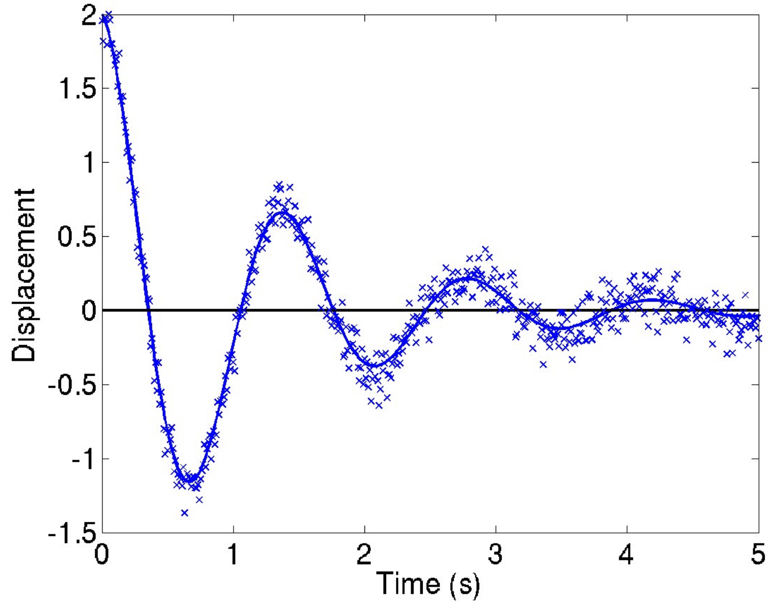
Example: Consider the spring model

$$\ddot{z} + C\dot{z} + Kz = 0$$

$$z(0) = 2 \; , \; \dot{z}(0) = -C$$

and synthetic data generated with errors

$\varepsilon \overset{iid}{\sim} N(0, \sigma^2)$ where $\sigma = 0.1$.



Website: https://rsmith.math.ncsu.edu /UQ_TIA/

Exercise:

Download the code spring_mcmc_C_K_sigma.m from Chapter 8 of the website, which is a basic Metropolis algorithm for inferring C, K and the measurements. Run the code and familiarize yourself with the algorithm.

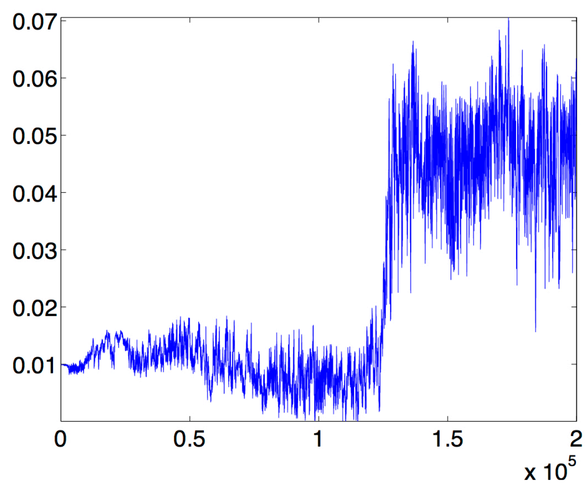
Bayesian Inference: Advantages and Disadvantages

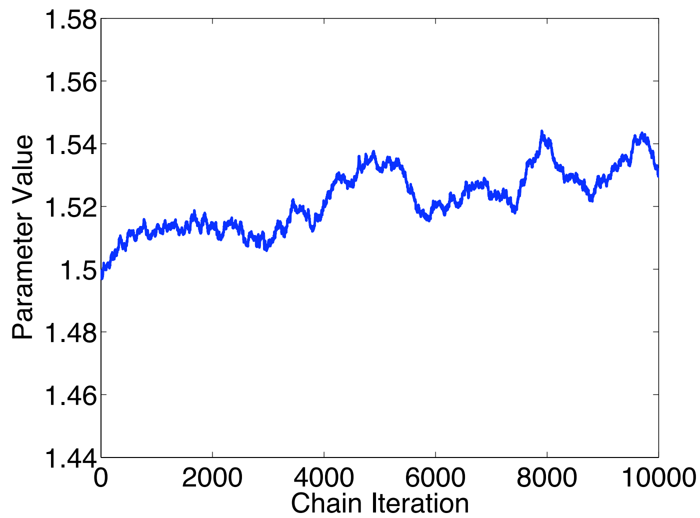
Advantages:

- Advantageous over frequentist inference when data is limited.
- Directly provides parameter densities, which can subsequently be propagated to construct response uncertainties.
- Can be used to infer non-identifiable parameters if priors are tight.
- Provides natural framework for experimental design.

Disadvantages:

- More computationally intense than frequentist inference.
- Can be difficult to confirm that chains have burned-in or converged.





Delayed Rejection Adaptive Metropolis (DRAM)

Websites:

- https://rsmith.math.ncsu.edu/UQ_TIA/CHAPTER8/index_chapter8.html
- http://helios.fmi.fi/~lainema/mcmc/

Delayed Rejection Adaptive Metropolis (DRAM)

We fit the Monod model

$$y = \theta_1 \frac{1}{\theta_2 + 1} + \epsilon \quad , \quad \epsilon \sim N(0, I\sigma^2)$$

to observations

x (mg / L COD): 28 55 83 110 138 225 375

y (1 / h): 0.053 0.060 0.112 0.105 0.099 0.122 0.125

First clear some variables from possible previous runs.

```
clear data model options
```

Next, create a data structure for the observations and control variables. Typically one could make a structure data that contains fields xdata and ydata.

```
data.xdata = [28    55    83    110   138   225   375]';   % x (mg / L COD)
data.ydata = [0.053 0.060 0.112 0.105 0.099 0.122 0.125]'; % y (1 / h)
```

Construct model

```
modelfun = @(x,theta) theta(1)*x./(theta(2)+x);
ssfun = @(theta,data) sum((data.ydata-modelfun(data.xdata,theta)).^2);
model.ssfun = ssfun;
model.sigma2 = 0.01^2;
```

Delayed Rejection Adaptive Metropolis (DRAM)

Input parameters

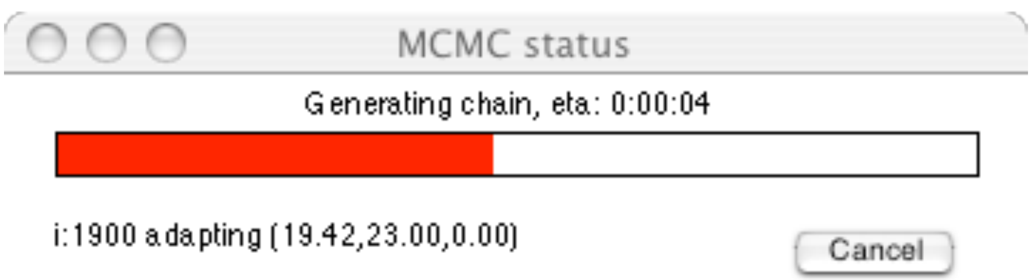
```
params = {
    {'theta1', tmin(1), 0}
    {'theta2', tmin(2), 0} };
```

and set options

```
options.nsimu = 4000;
options.updatesigma = 1;
options.qcov = tcov;
```

Run code

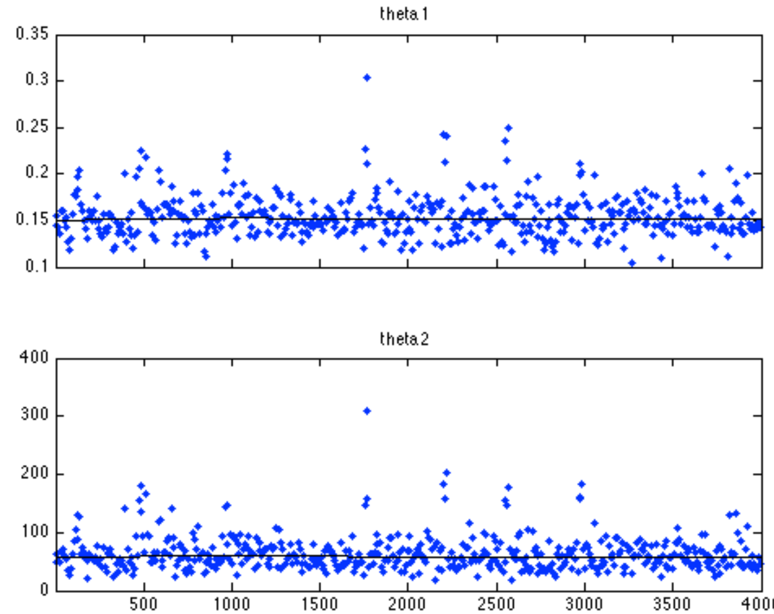
```
[res,chain,s2chain] = mcmcrun(model,data,params,options);
```

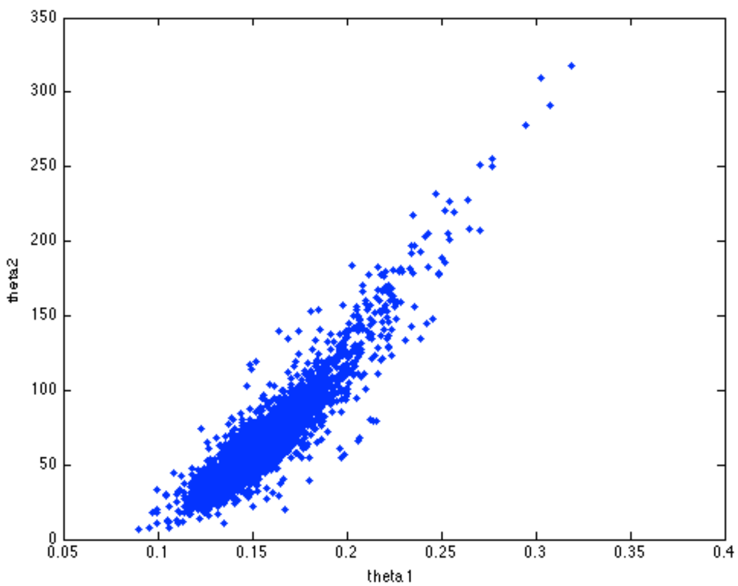


Delayed Rejection Adaptive Metropolis (DRAM)

Plot results

```
figure(2); clf
mcmcplot(chain,[],res,'chainpanel');
figure(3); clf
mcmcplot(chain,[],res,'pairs');
```





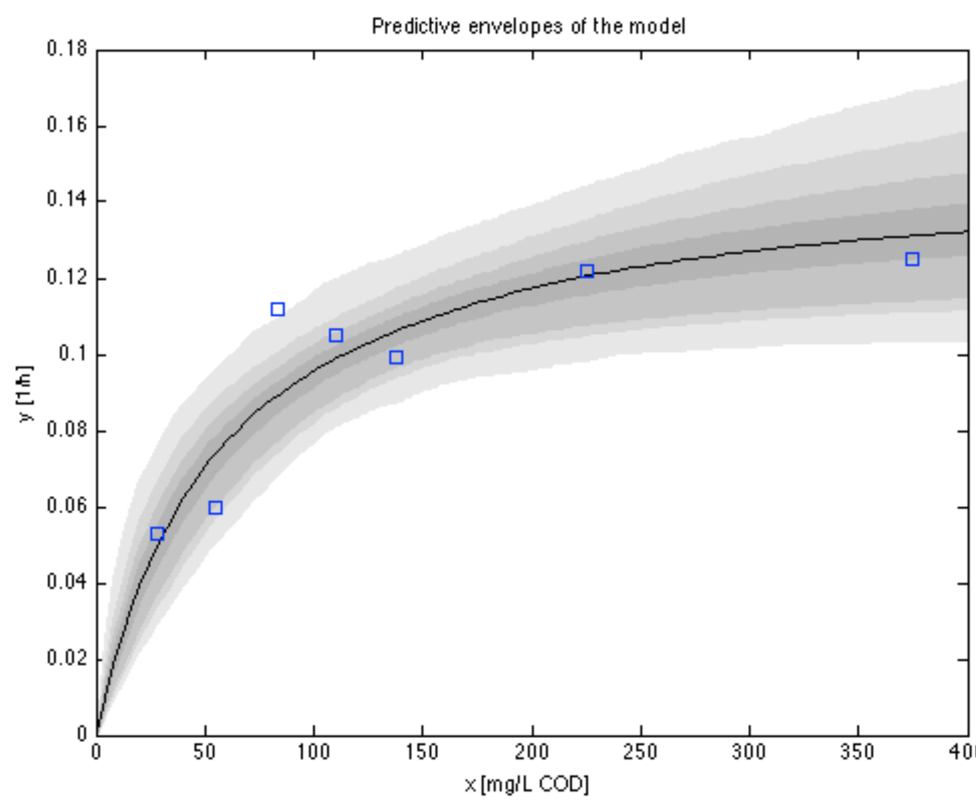
Examples:

- Several available in MCMC_EXAMPLES
- ODE solver illustrated in algae example

Delayed Rejection Adaptive Metropolis (DRAM)

Construct credible and prediction intervals

```
figure(5); clf
out = mcmcpred(res,chain,[],x,modelfun);
mcmcpredplot(out);
hold on
plot(data.xdata,data.ydata,'s');  % add data points to the plot
xlabel('x [mg/L COD]');
ylabel('y [1/h]');
hold off
title('Predictive envelopes of the model')
```



Bayesian Inference: Exercise

Example: Helmholtz energy with 3 parameters

$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Exercise:

1. Download the code Helmholtz_DRAM.m, and associated functions and data Helmholtz.txt, from the website

https://rsmith.math.ncsu.edu/AFRL_SHORT_COURSE19/

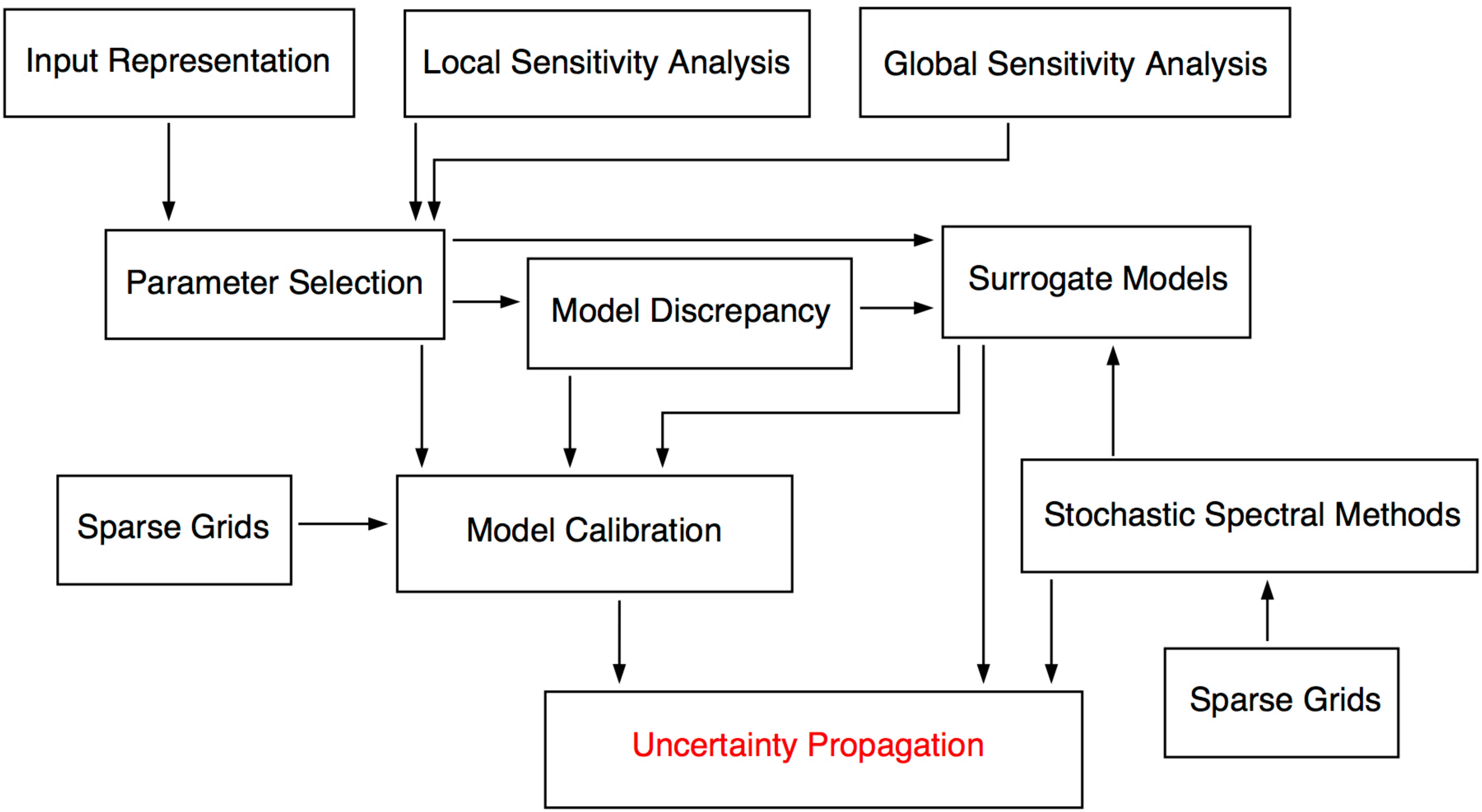
Also download and unzip MCMC_Stat.zip, which contains the DRAM software. You will need to set your paths. Run the code and generate the chains, marginal distributions and pairwise plots. The final plot are credible and prediction intervals, which we will discuss later.

2. Now modify the code to infer just the first two parameters. You may need to additionally modify your initial values.

3. Run the Jupyter notebooks example Landau_Energy.ipynb

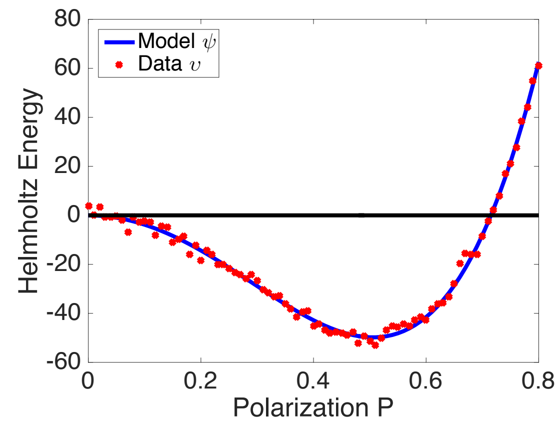
Steps in Uncertainty Quantification

Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



4. Forward Uncertainty Propagation: Linear Models

Note: Analytic mean and variance relations



Example: Helmholtz energy

$$\Upsilon_i = \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i \ , \ \text{var}[\varepsilon_i] = \sigma^2$$

Model Statistics:

Let $\overline{\alpha}_1, \overline{\alpha}_{11}$ and $\text{var}(\alpha_1), \text{var}(\alpha_{11})$ denote parameter means and variance. Then

$$\mathbb{E}[\alpha_1 P_i^2 + \alpha_{11} P_i^4] = \overline{\alpha}_1 P_i^2 + \overline{\alpha}_{11} P_i^4$$

$$\text{var}[\alpha_1 P_i^2 + \alpha_{11} P_i^4] = P_i^4 \text{var}[\alpha_1] + P_i^8 \text{var}[\alpha_{11}] + 2 P_i^6 \text{cov}[\alpha_1, \alpha_{11}]$$

Response Statistics: Assume measurement errors uncorrelated from model response.

$$\mathbb{E}[\Upsilon] = \overline{\alpha}_1 P_i^2 + \overline{\alpha}_{11} P_i^4$$

$$\text{var}[\Upsilon] = P_i^4 \text{var}[\alpha_1] + P_i^8 \text{var}[\alpha_{11}] + 2 P_i^6 \text{cov}[\alpha_1, \alpha_{11}] + \sigma^2$$

Problem: Models almost always nonlinearly parameterized

Forward Uncertainty Propagation: Sampling Methods

Strategy 1: Randomly sample from parameter and measurement error distributions and propagate through model to quantify response uncertainty.

Advantages:

- Applicable to nonlinear models.
- Parameters can be correlated and non-Gaussian.
- Straight-forward to apply and convergence rate is independent of number of parameters.
- Can directly incorporate both parameter and measurement uncertainties.

Disadvantages:

- Very slow convergence rate: $\mathcal{O}(1/\sqrt{M})$ where M is the number of samples.
- 100-fold more evaluations required to gain additional place of accuracy.
- This motivates numerical analysis techniques.

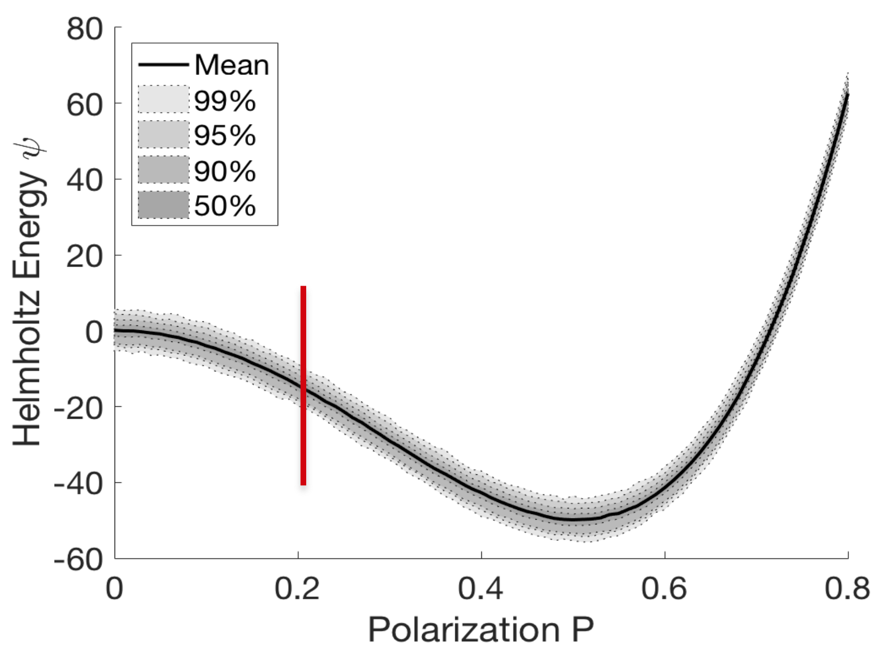
Strategy 2: Employ numerical surrogate representations to analytically propagate uncertainties.

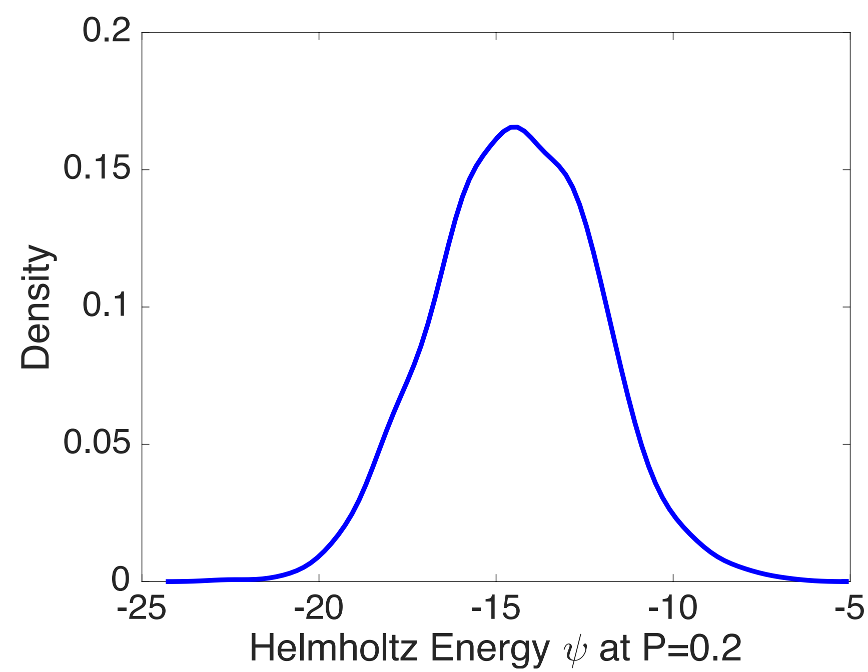
Confidence, Credible and Prediction Intervals

Note:

- We now know how to compute the mean response for the QoI.
- How do we compute appropriate intervals?

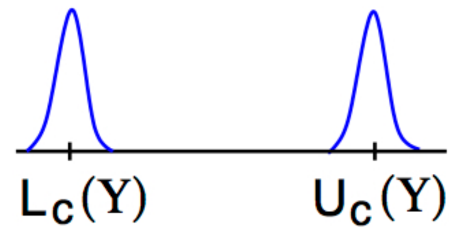
Example: Helmholtz energy $\psi(P,q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$





Confidence, Credible and Prediction Intervals

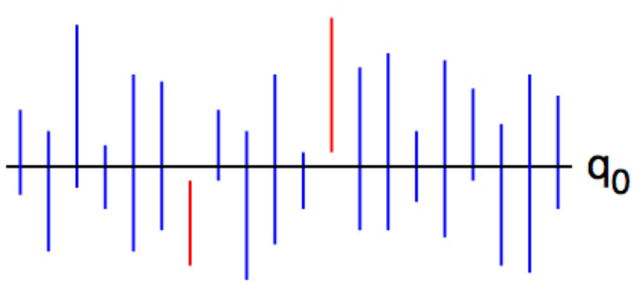
Data: $\Upsilon = [\Upsilon_1, \cdots, \Upsilon_n]$ of iid random observations



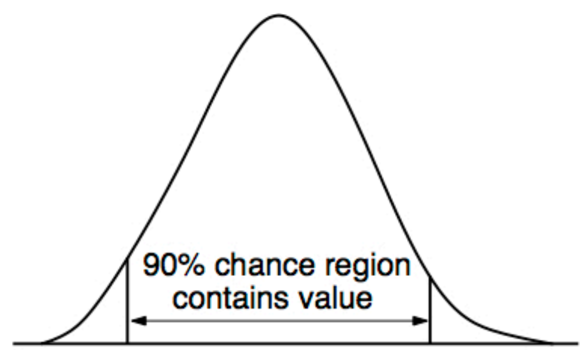
Confidence Interval (Frequentist): A $100 \times (1-\alpha)$% confidence interval for a fixed, unknown parameter q_0 is a random interval $[L_c(\Upsilon), U_c(\Upsilon)]$, having probability at least $1-\alpha$ of covering q_0 under the joint distribution of Υ.

Credible Interval (Bayesian): A $100 \times (1-\alpha)$ % credible interval is that having probability at least $1-\alpha$ of containing q.

Strategy: Sample out of parameter density $\rho_Q(q)$



90% Confidence Intervals



90% Credible Interval

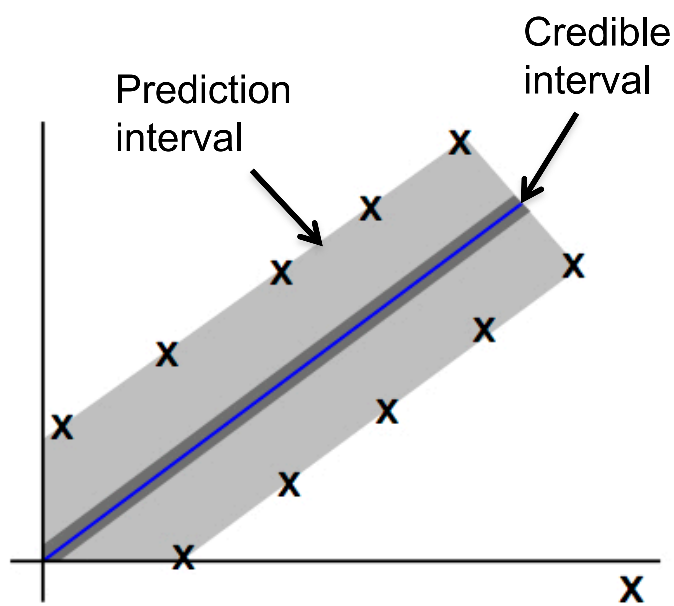
Confidence, Credible and Prediction Intervals

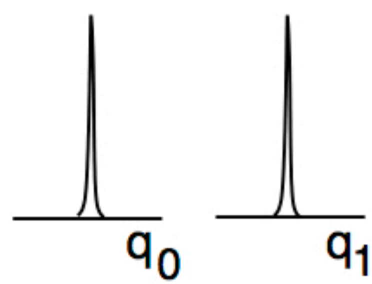
Data: $\Upsilon = [\Upsilon_1, \cdots, \Upsilon_n]$ of iid random observations

Prediction Interval: A $100 \times (1-\alpha)$% prediction interval for a future observable Υ_{n+1} is a random interval $[L_c(\Upsilon), U_c(\Upsilon)]$ having probability at least $1-\alpha$ of of containing Υ_{n+1} under the joint distribution of $(\Upsilon, \Upsilon_{n+1})$.

Example: Consider linear model

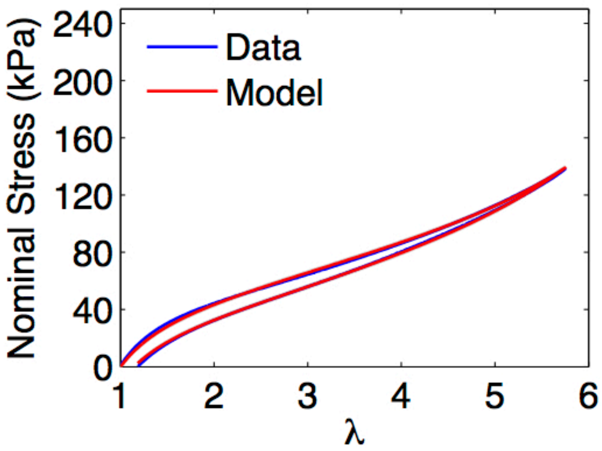
$$\Upsilon_i = q_0 + q_1 x_i + \varepsilon_i \ , \ i = 1, \cdots, n$$



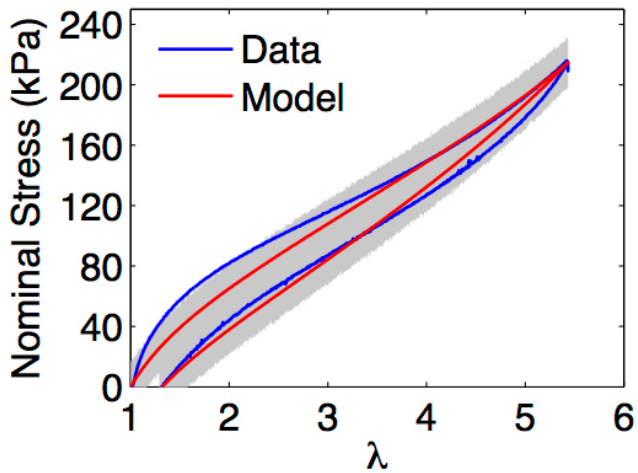


Prediction Intervals for the Viscoelastic Model

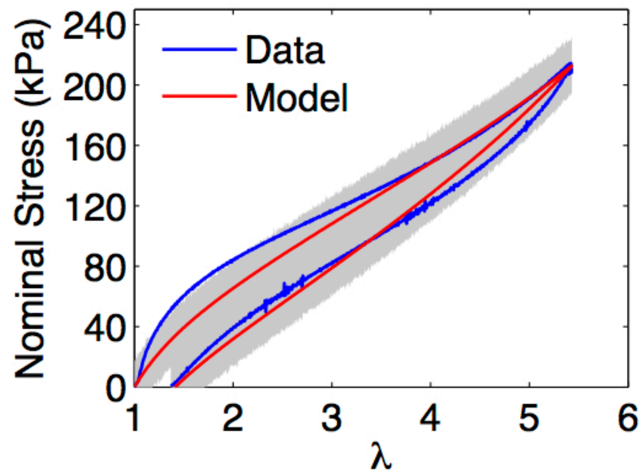
Linear Non-Affine Model: Not accurate for predicting higher stretch rates



$$\frac{d\lambda}{dt} = 6.7 \times 10^{-5} \text{ Hz}$$



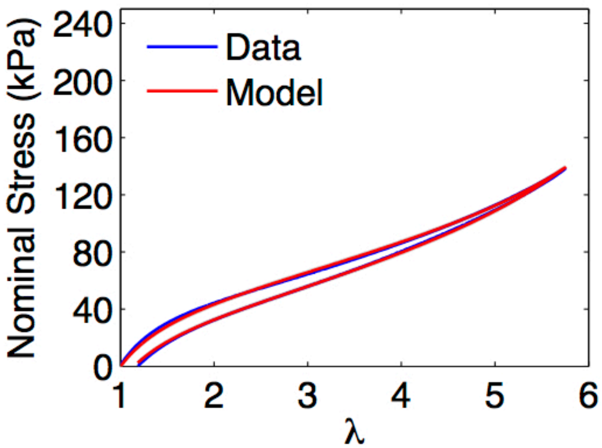
$$\frac{d\lambda}{dt} = 0.335 \text{ Hz}$$

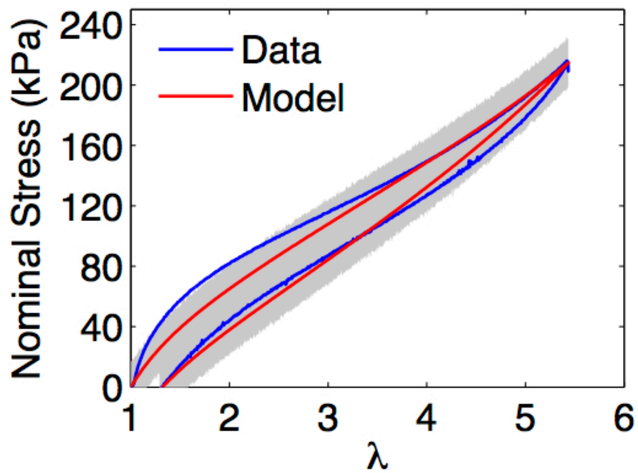


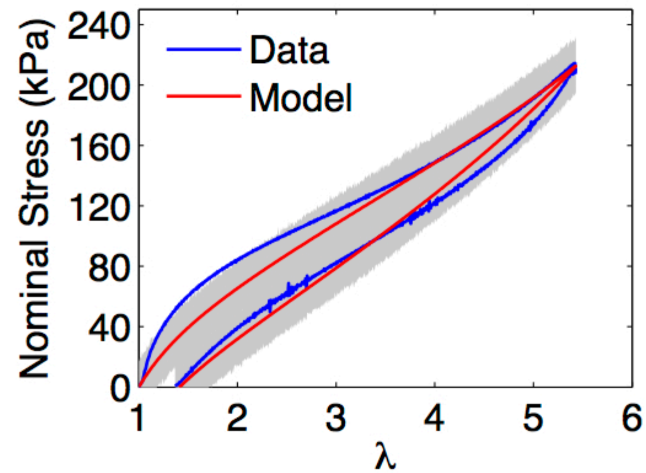
$$\frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

Prediction Intervals for the Viscoelastic Model

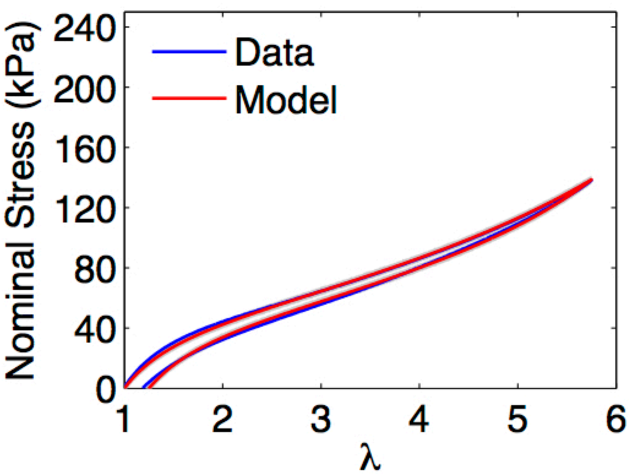
Linear Non-Affine Model:







Nonlinear Non-Affine Model: Significantly more accurate over range of stretch rates!



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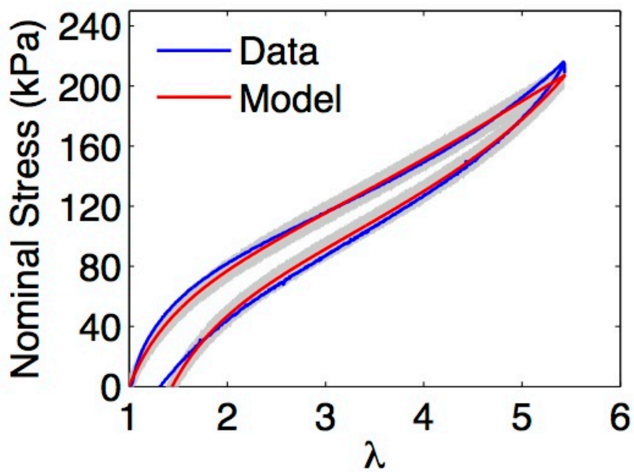

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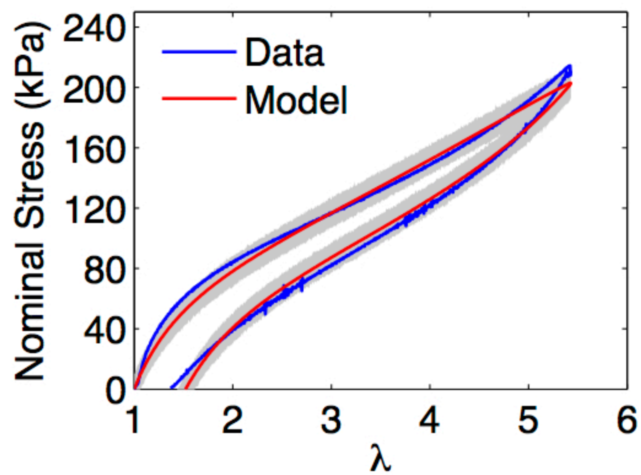
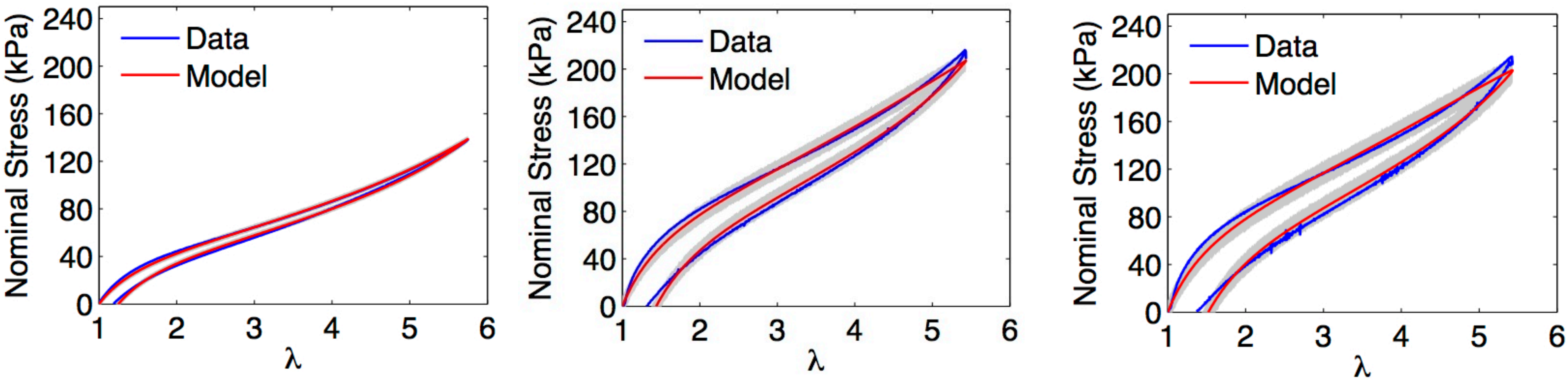


$$\frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

Bayesian Inference: Exercise

Nonlinear Non-Affine Model: Significantly more accurate over range of stretch rates!



$$\frac{d\lambda}{dt} = 6.7 \times 10^{-5} \text{ Hz} \qquad \frac{d\lambda}{dt} = 0.335 \text{ Hz} \qquad \frac{d\lambda}{dt} = 0.67 \text{ Hz}$$

Exercise:

Run the Jupyter notebooks examples:

- Viscoelasticity.ipynb
- Landau_energy.ipynb

Prediction Intervals: Exercise

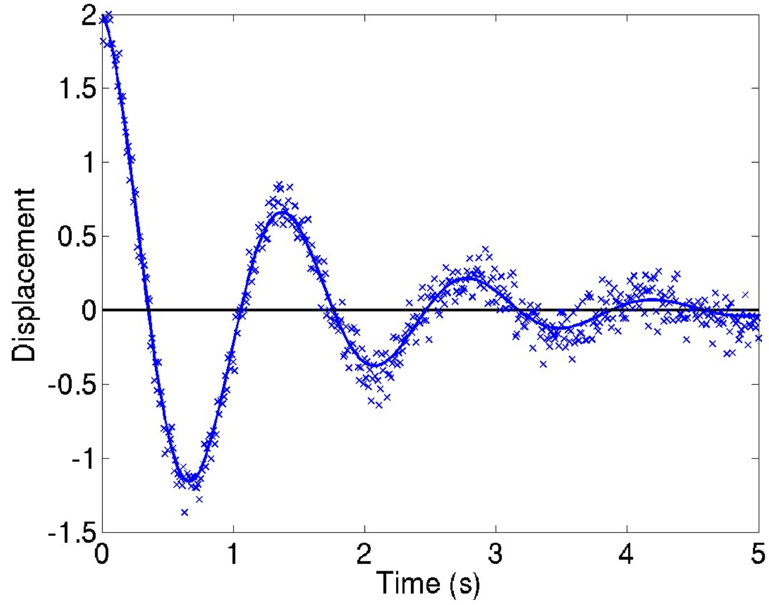
Example: Consider the spring model

$$\ddot{z} + \underline{C}\dot{z} + \underline{K}z = 0$$

$$z(0) = 2\ ,\ \ \dot{z}(0) = -\underline{C}$$

and synthetic data generated with errors

$$\varepsilon \overset{iid}{\sim} N(0, \sigma^2) \text{ where } \sigma = 0.1.$$



Exercise:

1. Use the code spring_mcmc_C_K_sigma.m, which you downloaded from Chapter 8 of the website https://rsmith.math.ncsu.edu /UQ_TIA/ to compute the uncertainty in the displacement z(2) by sampling out of the densities for K, C and the measurement error.

2. Now download the code spring_dram.m and functions from the website https://rsmith.math.ncsu.edu/AFRL_SHORT_COURSE19/ and run it to construct 95% prediction intervals for the spring model.

What UQ Can and Cannot Do (Not Comprehensive)

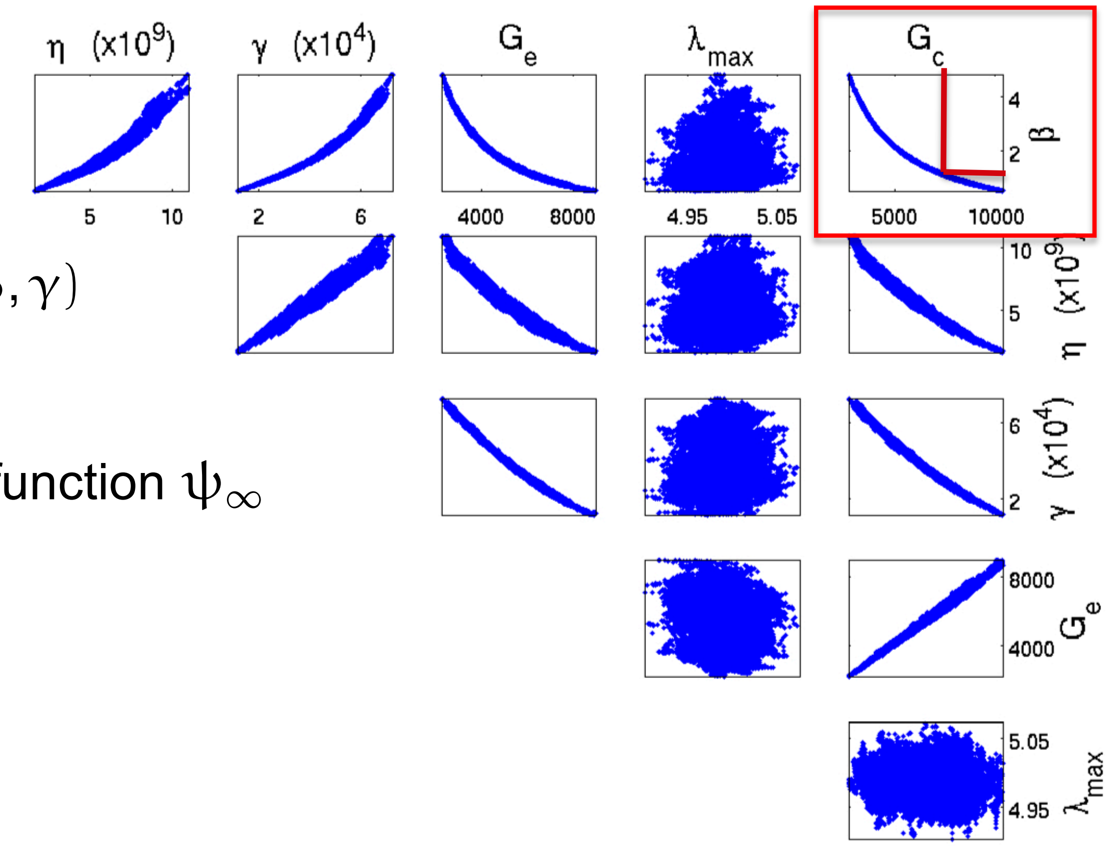
Can Do:

- Quantify uncertainty in model parameters or inputs based on experimental data or high-fidelity model simulations.
- Quantify correlation between model inputs.
- Quantify uncertainties in statistical quantities-of-interest. This is critical when specifying model predictions with quantified uncertainty

Cannot Do:

- Accommodate or replace missing physics in models.
  - However, when combined with validation, it can indicate missing physics.
  - Research topic: quantifying model discrepancy
- Guarantee optimal parameter values. However, it can be more robust than gradient-based optimization.
- Rank parameter sensitivity. This is addressed next!

Uncertainty Quantification Challenges



E.g., Viscoelastic model

$$\psi(q) = \psi_\infty(G_e, G_c, \lambda_{\max}) + \Upsilon(\eta, \beta, \gamma)$$

- Dissipative energy function Υ
- Conserved hyperelastic energy function ψ_∞

Parameters:

$$q = [G_e, \underline{G_c}, \lambda_{\max}, \eta, \underline{\beta}, \gamma]$$

Challenge 1:

• How do we isolate set of parameters that are identifiable in the sense that they can be uniquely inferred from data?

Challenge 2:

• How do we do uncertainty propagation for computationally intensive models? E.g., we have computational budget of 5000 but UQ requires 120,000 evaluations.

Parameter Selection Techniques

First Issue: Parameters often *not identifiable* in the sense that they are not uniquely determined by the data.

Example 1: Spring model

$$\underline{m}\frac{dy}{dt^2} + \underline{k}y = 0$$

$$y(0) = y_0 \ , \ \frac{dy}{dt}(0) = 0$$

Solution: $y(t,q) = y_0 \cos\left(\sqrt{\underline{k/m}} \cdot t\right)$

Note: q = [k,m] not jointly identifiable

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Solution: $y(t,q) = y_0 \cos\left(\sqrt{k/m} \cdot t\right)$

Note: q = [k,m] not jointly identifiable

Example 2: Polydomain structure – Lead Titanate

$$u(P_i, \varepsilon_{ij}, P_{i,j}) = u_M(\varepsilon_{ij}) + u_L(P_i) + u_C(P_i, \varepsilon_{ij}) + u_G(P_{i,j})$$

where

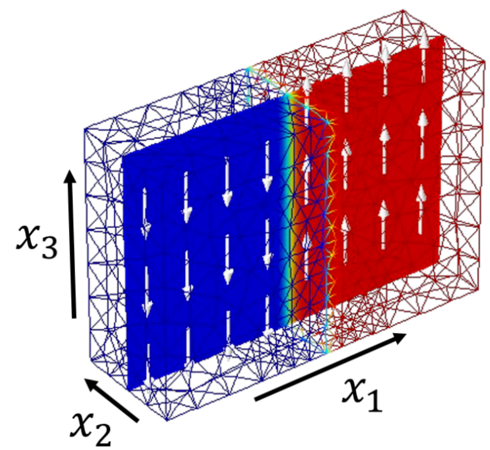
$$u_L(P_3) = \alpha_1 P_3^2 + \alpha_{11} P_3^4 + \alpha_{111} P_3^6$$

$$u_C(P_3, \varepsilon_{ii}) = -q_{11}\varepsilon_{11}P_3^2 - q_{12}\left(\varepsilon_{11}P_3^2 + \varepsilon_{22}P_3^2\right)$$

$$u_G(P_{3,1}) = \frac{1}{2} g_{44} P_{3,1}^2$$

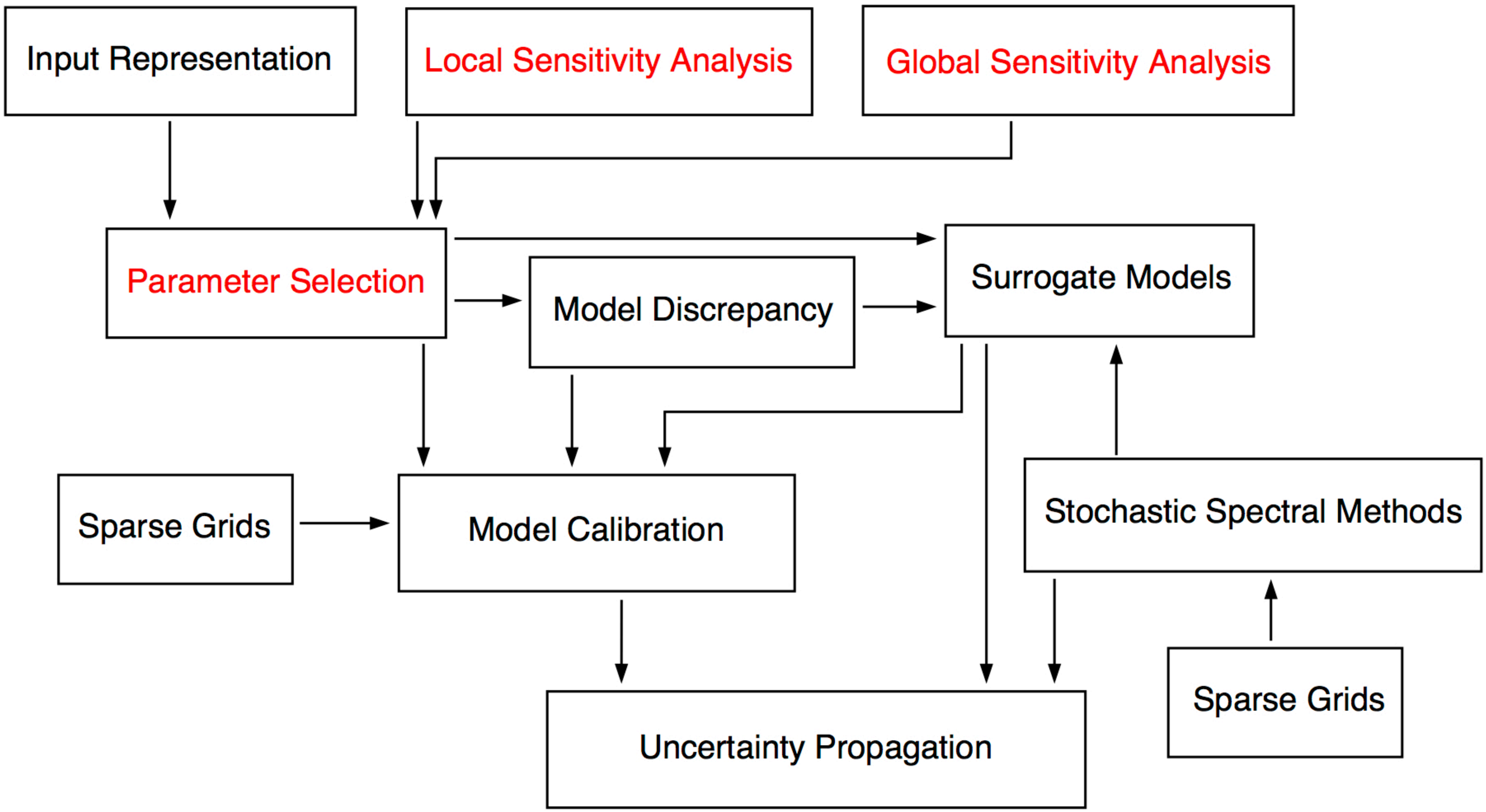
Domain Wall Energy: $E_{180}(q_{180}) = \int_{-\infty}^{\infty} (u - u_0)\, dx_1$

180^o Domain Wall



Question: Can parameters be uniquely determined by DFT simulations?

Steps in Uncertainty Quantification



Parameter Selection: Required for models with unidentifiable or noninfluential inputs

- e.g., Nuclear neutron transport codes can have 100,000 inputs

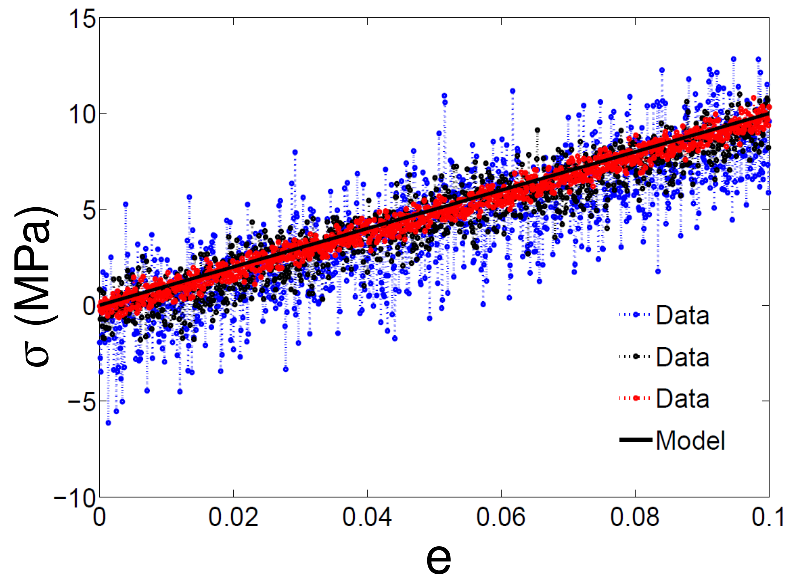
Sensitivity Analysis: Motivation

Example: Linear constitutive relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100$, $c = 0.1$

$$e = 0.001 \ , \ \frac{de}{dt} = 0.1$$



Question: To which parameter E or c is stress most sensitive?

Local Sensitivity Analysis:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\boxed{\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1}$$

Conclusion: Model most sensitive to damping parameter c

Limitations:

- Does not accommodate potential uncertainty in parameters.
- Does not accommodate potential correlation between parameters.
- Sensitive to units and magnitudes of parameters.

Global Sensitivity Analysis

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100,\ c = 0.1$

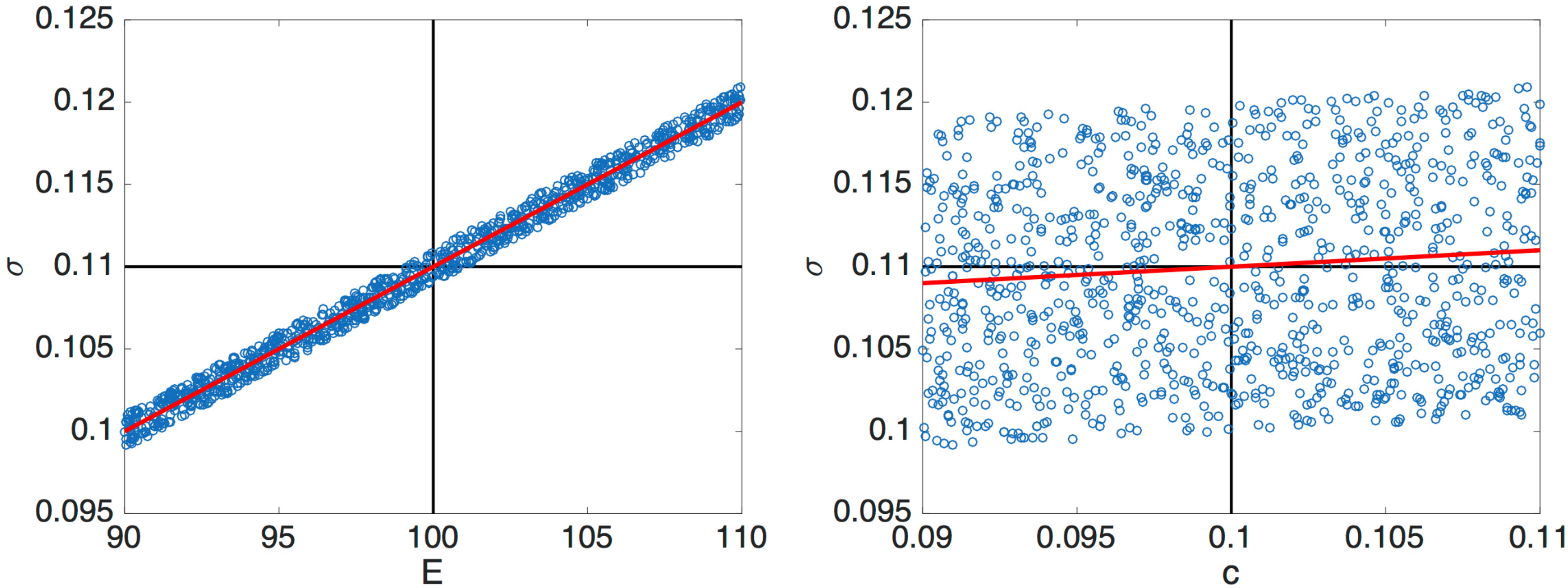
Uncertainty: 10% of nominal values

$$E \sim \mathcal{U}(90, 110)\ ,\ c \sim \mathcal{U}(0.09, 0.11)$$

Local Sensitivities:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1$$



Global Sensitivity: E is more influential

Global Sensitivity Analysis

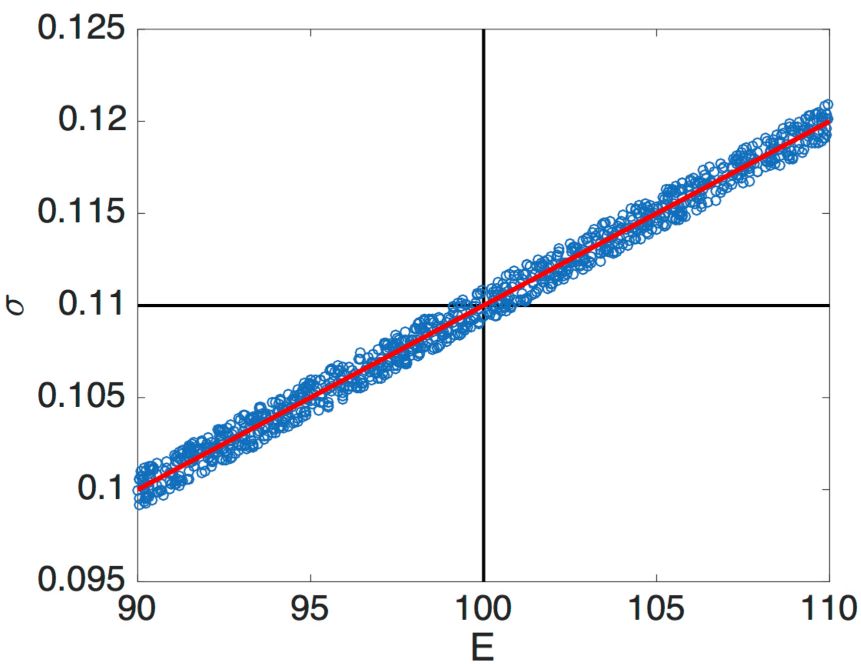
Example: Linear elastic constitute relation

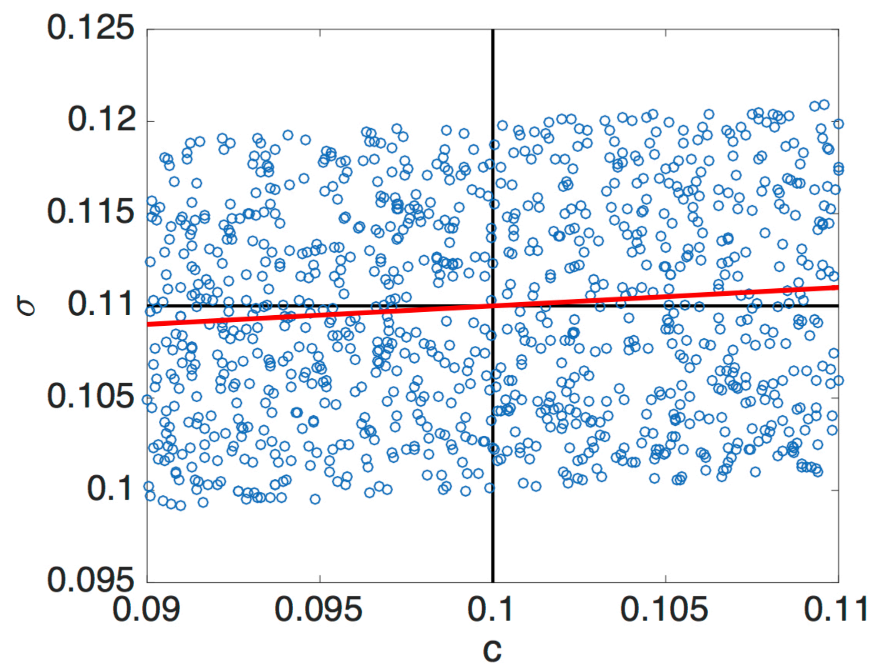
$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100, \; c = 0.1$

Uncertainty: 10% of nominal values

$$E \sim \mathcal{U}(90, 110) \;, \; c \sim \mathcal{U}(0.09, 0.11)$$





Statistical Motivation: Consider variability of expected values $D_i = \text{var}[\mathbb{E}(Y|q_i)]$

Variance-Based Methods

Sobol Representation: For now, take $Q_i \sim \mathcal{U}(0,1)$ and $\Gamma = [0,1]^p$

Take

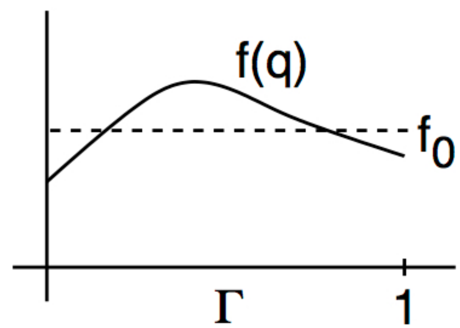
$$f(q) = f_0 + \sum_{i=1}^{p} f_i(q_i) + \sum_{1 \leqslant i < j \leqslant p} f_{ij}(q_i, q_j)$$

Analogy: Taylor or Fourier series

With appropriate assumptions,

$$f_0 = \int_\Gamma f(q)dq$$

$$f_i(q_i) = \int_{\Gamma^{p-1}} f(q)dq_{\sim i} - f_0$$



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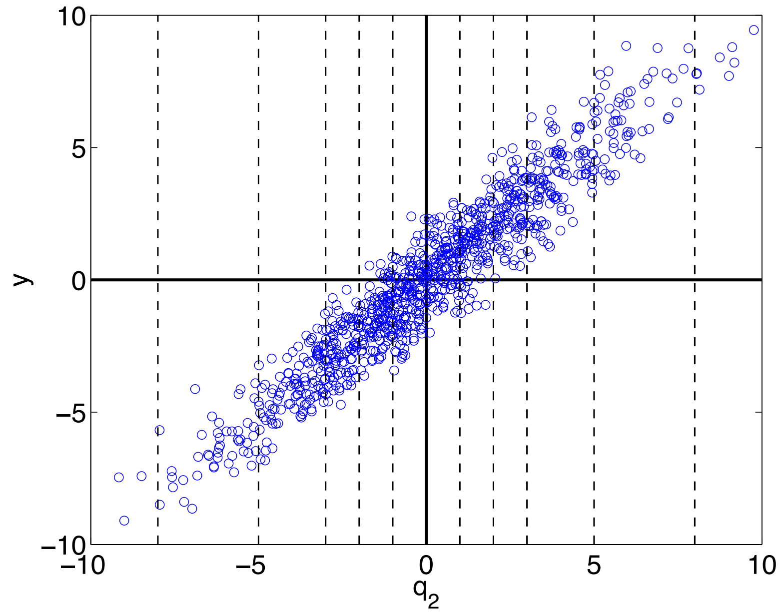
Analogy: Taylor or Fourier series

Assumption: Mutually independent parameters



With appropriate assumptions,

$$f_0 = \int_\Gamma f(q)dq$$

$$f_i(q_i) = \int_{\Gamma^{p-1}} f(q)dq_{\sim i} - f_0$$

Variances:

$$D_i = \int_0^1 f_i^2(q_i)dq_i$$

$$D = \text{var}(Y)$$

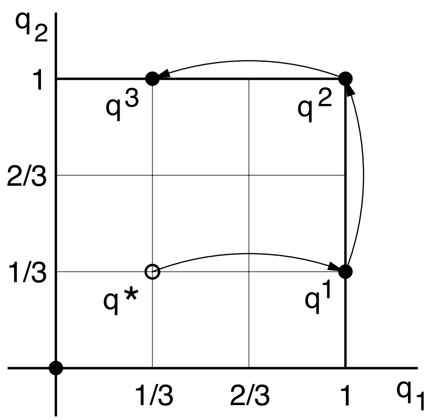
Sobol Indices: $S_i = \frac{D_i}{D}$

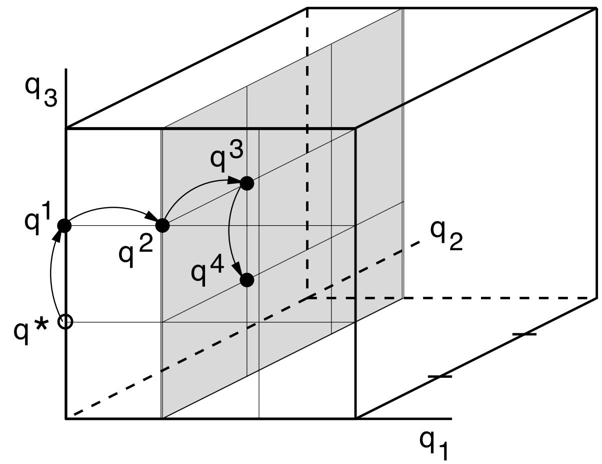
Statistical Interpretation:

$$D_i = \text{var}[\mathbb{E}(Y|q_i)] \Rightarrow S_i = \frac{\text{var}[\mathbb{E}(Y|q_i)]}{\text{var}(Y)}$$

Global Sensitivity Analysis: Morris Screening

Example: Consider independent uniformly distributed parameters on $\Gamma = [0,1]^p$





Elementary Effect:

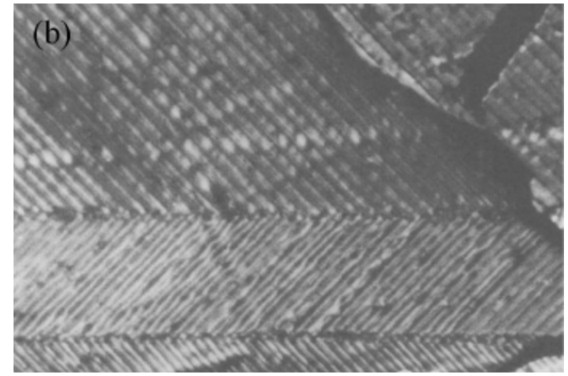
$$d_i^j = \frac{f(q^j + \Delta e_i) - f(q^j)}{\Delta} \quad , i^{th} \text{ parameter }, \; j^{th} \text{ sample}$$

Global Sensitivity Measures: r samples

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r} |d_i^j(q)|$$

$$\sigma_i^2 = \frac{1}{r-1}\sum_{j=1}^{r}\left(d_i^j(q) - \mu_i\right)^2 \quad , \quad \mu_i = \frac{1}{r}\sum_{j=1}^{r} d_i^j(q)$$

Parameter Subset Selection: Materials



Example: Polydomain structure – Lead Titanate

$$u(P_i, \varepsilon_{ij}, P_{i,j}) = u_M(\varepsilon_{ij}) + u_L(P_i) + u_C(P_i, \varepsilon_{ij}) + u_G(P_{i,j})$$

where

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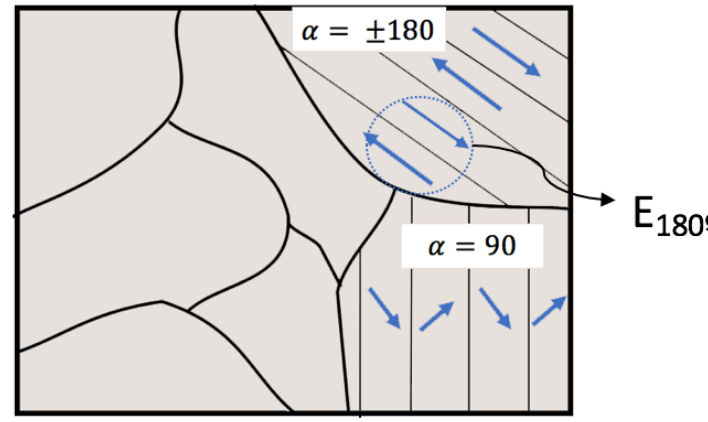
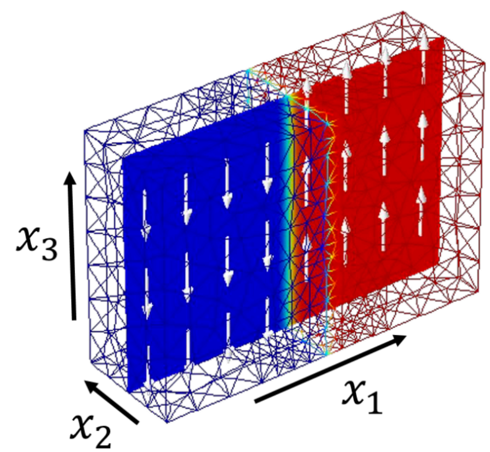


Domain Wall Energy:

$$E_{180}(q_{180}) = \int_{-\infty}^{\infty} (u - u_0)\, dx_1$$

$$q_{180} = [\alpha_1, \alpha_{11}, \alpha_{111}, q_{11}, q_{12}, g_{44}]$$

180^o Domain Wall



Result: Linear-algebra based techniques

- Only $\alpha_{11}, q_{11}, g_{44}$ influential and can be inferred
- Prior distributions for $\alpha_1, \alpha_{111}, q_{12}$ not informed by data

Global Sensitivity Analysis

Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

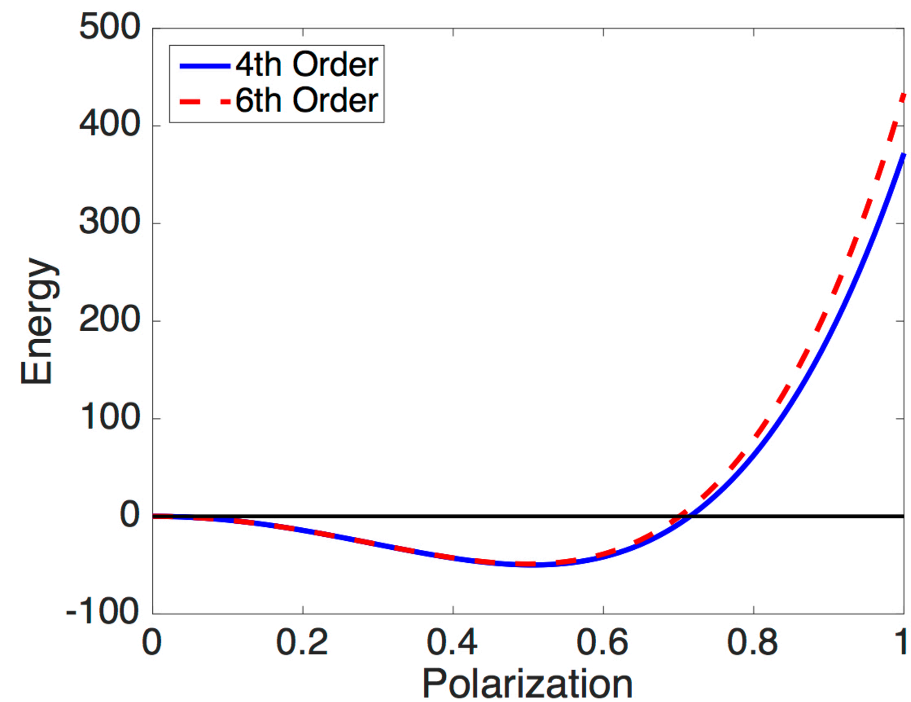
$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03



Conclusion: α_{111} insignificant and can be fixed

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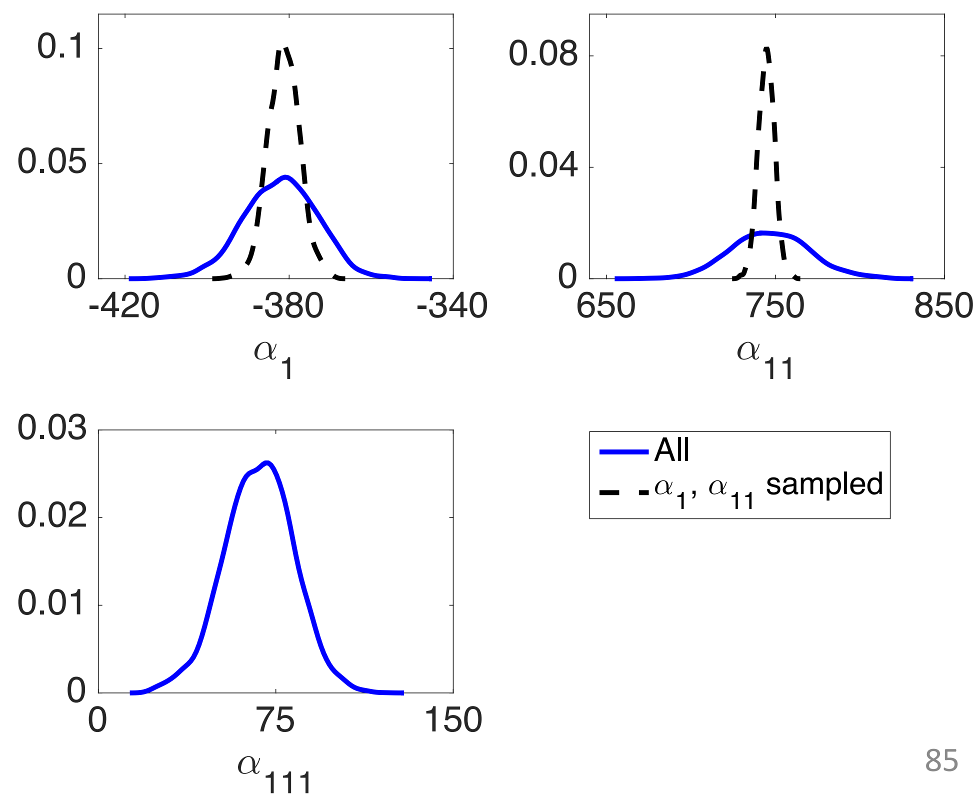
Conclusion:

α_{111} insignificant and can be fixed

Problem: We obtain different distributions when we perform Bayesian inference with fixed non-influential parameters



Global Sensitivity Analysis

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Question: Do we use 4th or 6th-order Landau energy?

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Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

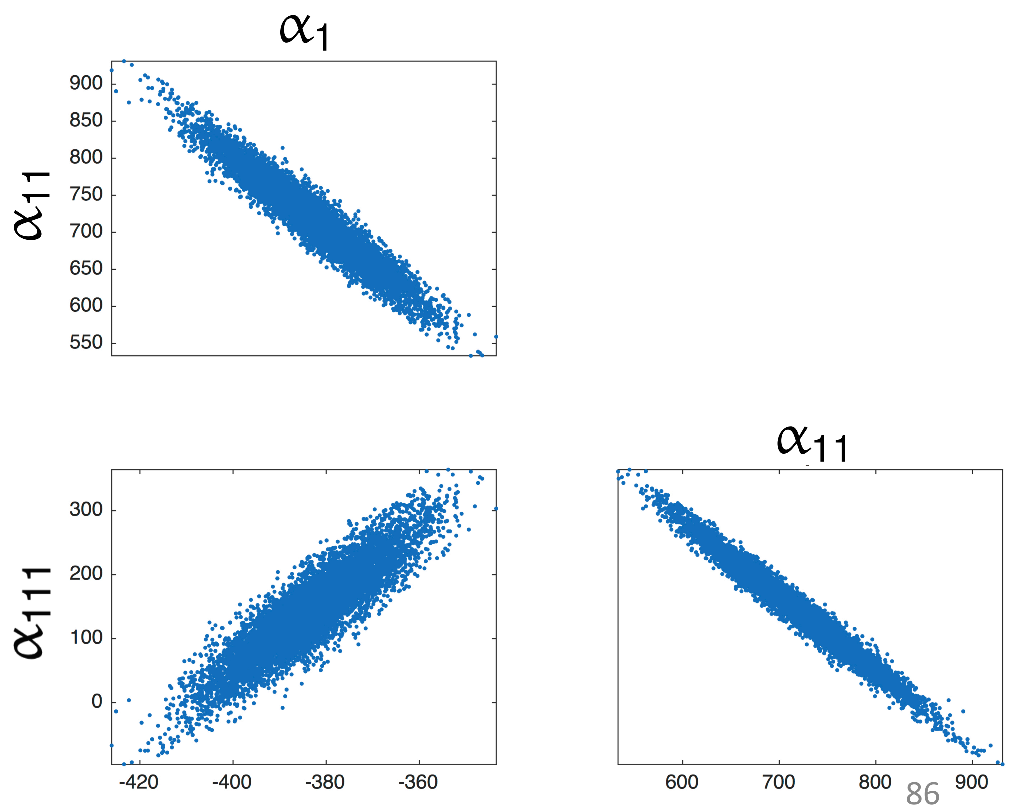
Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_k	0.62	0.39	0.01
T_k	0.66	0.38	0.06
μ_k^*	0.17	0.07	0.03

Note: Must accommodate correlation

Problem:

- Parameters correlated
- Cannot fix α_{111}



One Solution: Parameter Subset Selection

Consider

$$\psi(P_i, q) \approx \psi(P_i, q^*) + \nabla_q \psi(P_i, q^*) \Delta q$$

where

$$\nabla_q \psi(P_i, q^*) = \left[\frac{\partial \psi}{\partial \alpha_1}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{11}}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{111}}(P_i, q^*) \right]$$

Functional: Since $\upsilon_i \approx \psi(P_i, q^*)$

$$\begin{aligned} J(q) &= \frac{1}{n} \sum_{i=1}^{n} [\upsilon_i - \psi(P_i, q)]]^2 \\ &\approx \frac{1}{n} \sum_{i=1}^{n} [\nabla_q \psi(P_i, q^*) \cdot \Delta q]^2 \\ &= \frac{1}{n} (\chi \Delta q)^T (\chi \Delta q) \end{aligned}$$

Sensitivity Matrix:

$$\chi(q^*) = \begin{bmatrix} \frac{\partial \psi}{\partial \alpha_1}(P_1, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_1, q^*) \\ \vdots & \dots & \vdots \\ \frac{\partial \psi}{\partial \alpha_1}(P_n, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_n, q^*) \end{bmatrix}$$

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

One Solution: Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

Note: $\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable

Note: Estimator for covariance matrix

$$V = s^2 \left[\chi^T \chi\right]^{-1} = \begin{bmatrix} \mathrm{var}(q_1) & \mathrm{cov}(q_1, q_2) & \cdots & \mathrm{cov}(q_1, q_n) \\ \mathrm{cov}(q_2, q_1) & \mathrm{var}(q_2) & \mathrm{cov}(q_2, q_3) & \\ \vdots & & & \vdots \\ \mathrm{cov}(q_n, q_1) & \cdots & \cdots & \mathrm{var}(q_n) \end{bmatrix}$$

One Solution: Parameter Subset Selection

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$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

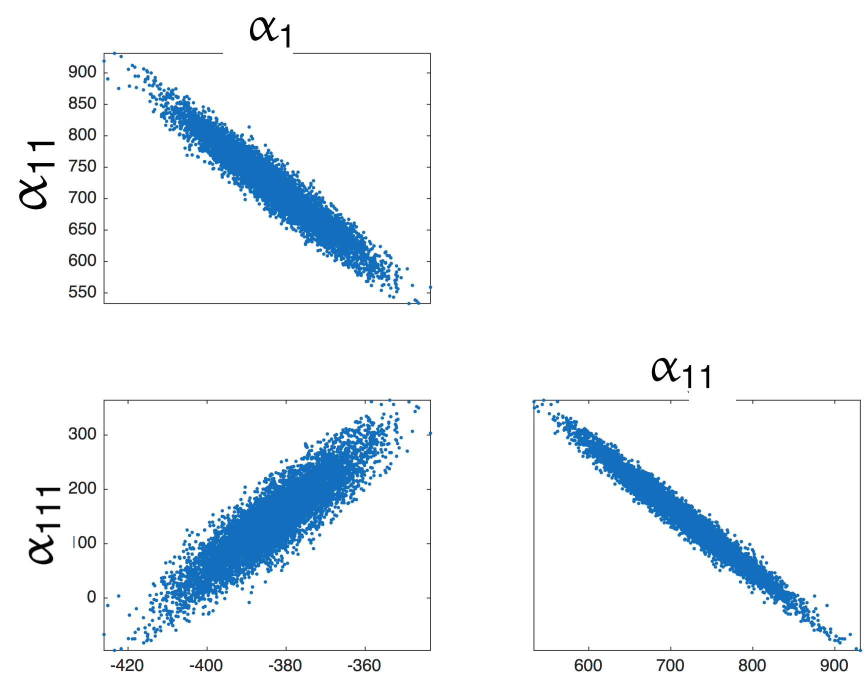
Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

$\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable



Example:

$$\psi(P, q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Result: rank($\chi^T \chi$) = 3 so all parameters identifiable

Case Study: Spring Model

Example: Spring model

$$m\frac{d^2z}{dt^2} + kz = 0$$

$$z(0) = 1\ ,\ \frac{dz}{dt}(0) = 0$$

Responses: For q = [k,m], consider

$$y = f(q) = \cos\left(\sqrt{\frac{k}{m}} \cdot \frac{\pi}{2}\right)$$

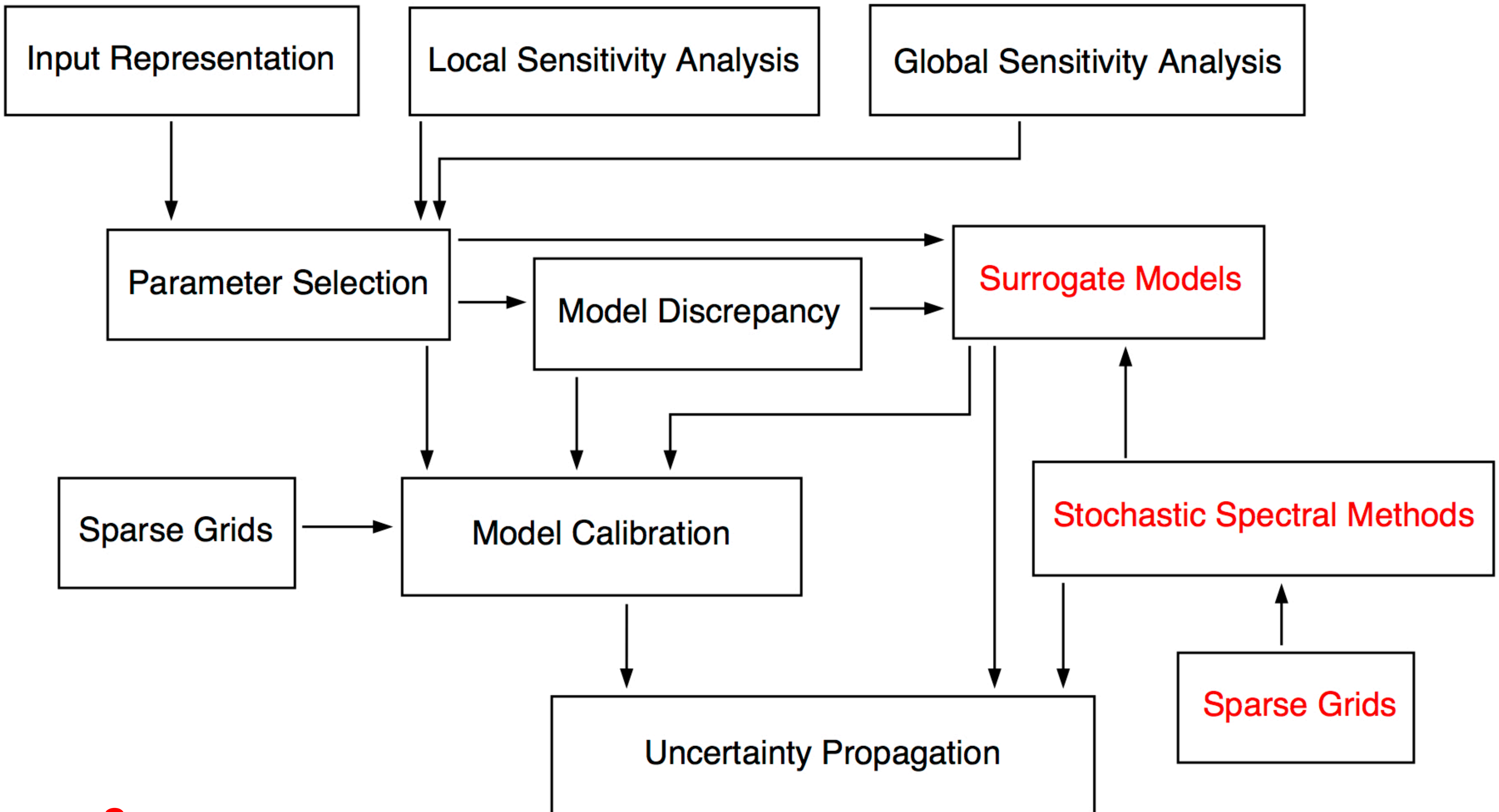
$$y = \int_0^{\pi/2} \cos\left(\sqrt{\frac{k}{m}}t\right) dt = \sqrt{\frac{m}{k}}$$

Exercise: Download MATLAB software from the website

https://rsmith.math.ncsu.edu/AFRL_SHORT_COURSE19/

and run the codes spring_morris.m and spring_Saltelli.m. What do you conclude about the parameter sensitivity?

Steps in Uncertainty Quantification

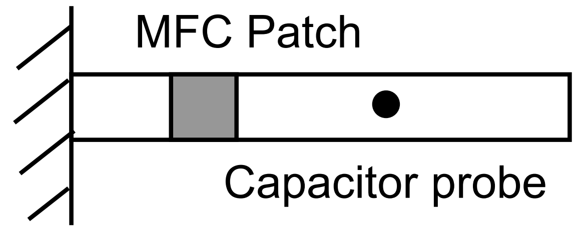


Challenge 2:

- How do we do uncertainty quantification for computationally expensive models?
- Example:
  - We have a computational budget of 5000 model evaluations.
  - Bayesian inference and uncertainty propagation require 120,000 evaluations.

Uncertainty Quantification Challenges

Example: MFC model – Fourth-order PDE

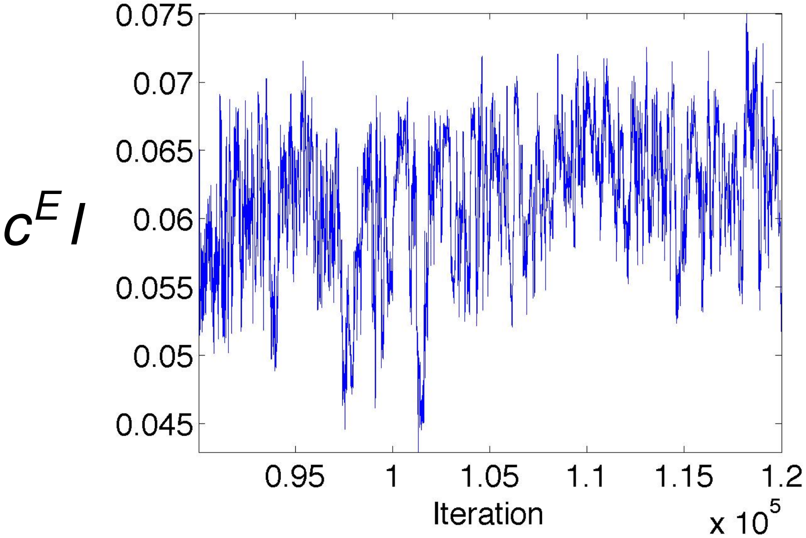


$$\rho \frac{\partial^2 w}{\partial t^2} + \gamma \frac{\partial w}{\partial t} - \frac{\partial^2 M}{\partial x^2} = 0$$

$$M = -c^E I \frac{\partial^2 w}{\partial x^2} - c_D I \frac{\partial^3 w}{\partial x^2 \partial t} - [k_1 e(E, \sigma_0) E + k_2 \varepsilon_{irr}(E, \sigma_0)] \chi_{MFC}(x)$$

Macro-Fiber Composite

Bayesian Inference: 20 parameters -- Took 6 days!



Problem:

1.2×10^5 PDE solutions

Solution: Highly efficient surrogate models

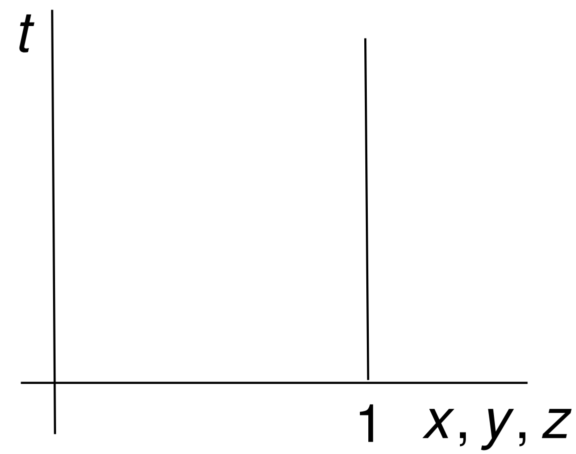
Surrogate Models: Motivation

Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

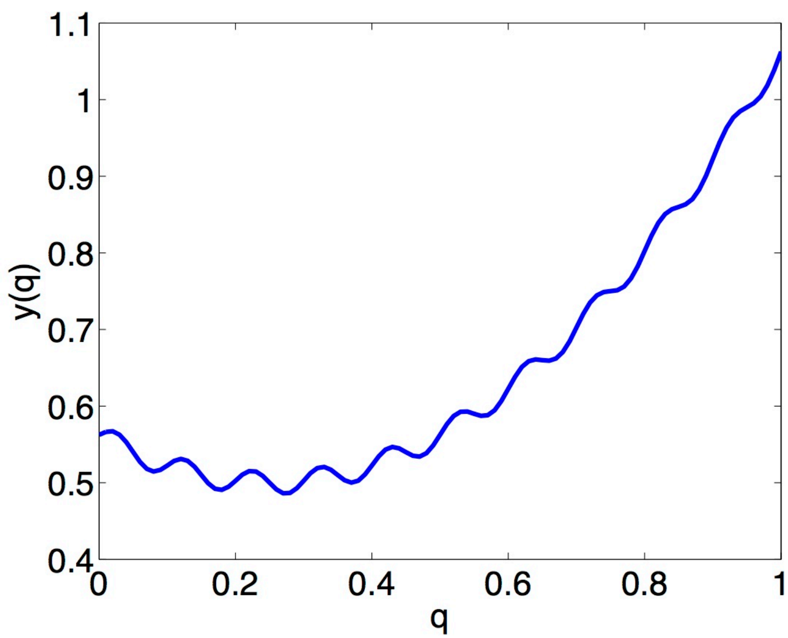
Boundary Conditions

Initial Conditions



with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\, dxdydzdt$$



Notes:

- Requires approximation of PDE in 3-D
- What would be a simple surrogate?

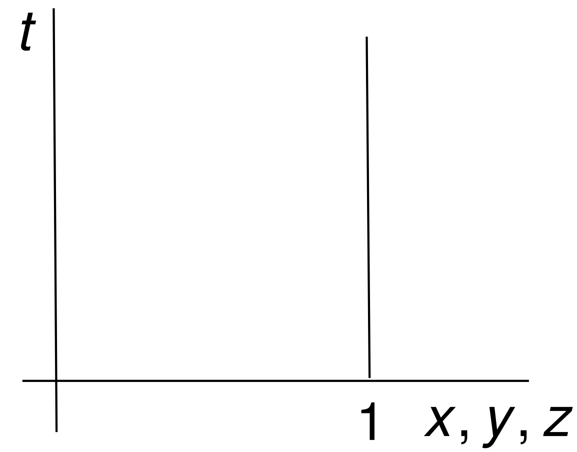
Surrogate Models

Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions



with the response

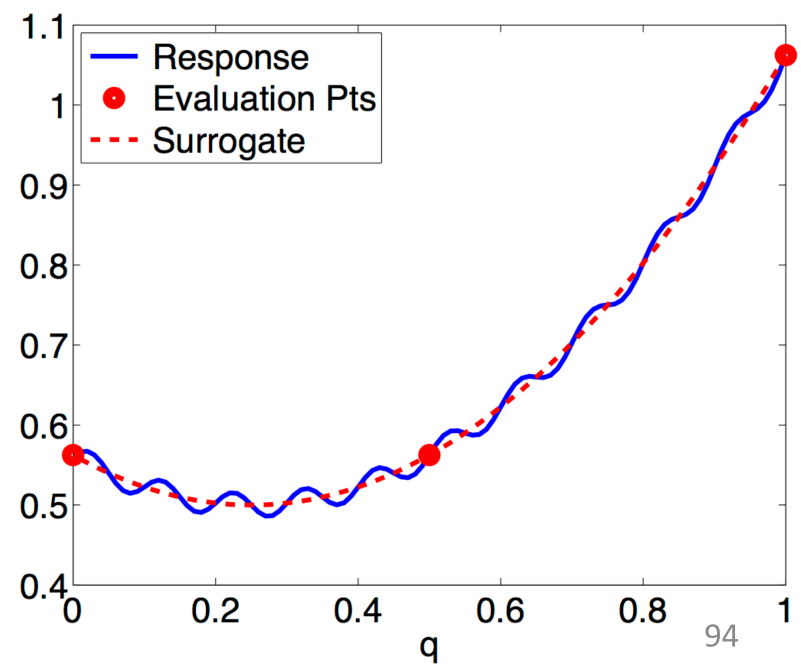
$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\,dxdydzdt$$

Surrogate: Quadratic

$$y_s(q) = (q - 0.25)^2 + 0.5$$

Question: How do you construct a polynomial surrogate?

- Regression
- Interpolation



Surrogate Models

Recall: Consider the model

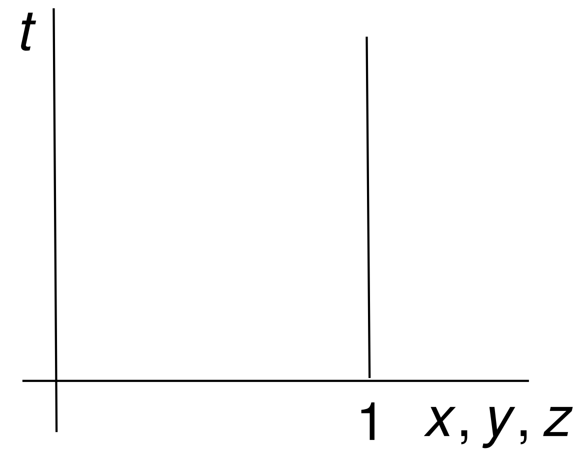
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

Boundary Conditions

Initial Conditions

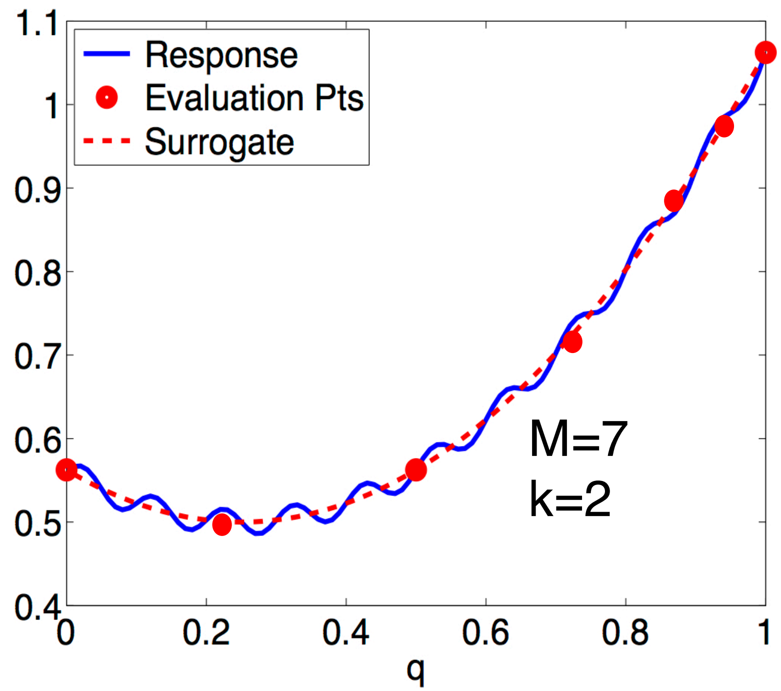
with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\,dxdydzdt$$



Surrogate: Quadratic

$$y_s(q) = (q - 0.25)^2 + 0.5$$



Question: How do you construct a polynomial surrogate?

- Interpolation
- Regression

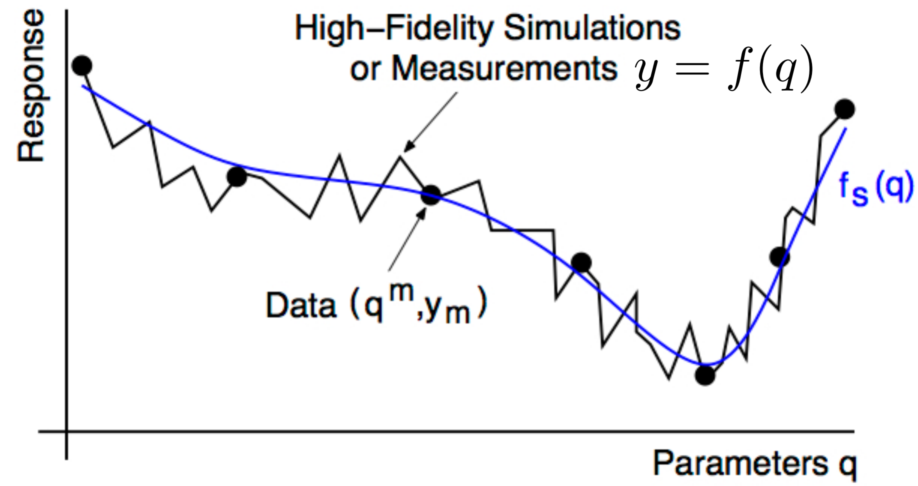
Data-Fit Models

Notes:

• Often termed response surface models, emulators, meta-models.

• Constructed via interpolation or regression.

• Data can consist of high-fidelity simulations or experiments.



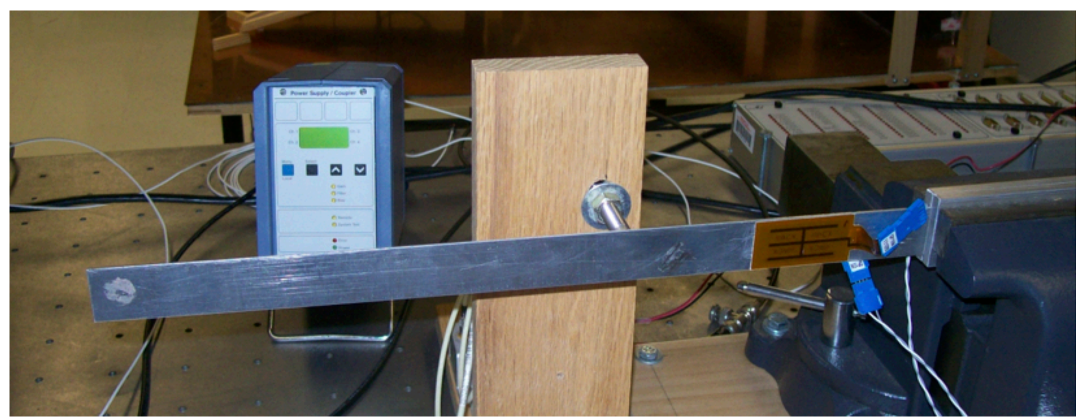
Example: Steady-state Euler-Bernouilli beam model with PZT patch

$$YI\frac{d^4 w}{dx^4}(x) = k_p V \chi_{pzt}(x)$$

Data: Displacement observations

Parameter: YI

Simulations: Nikolas Bravo



Data-Fit Models

Example: Steady-state Euler-Bernouilli beam model with PZT patch

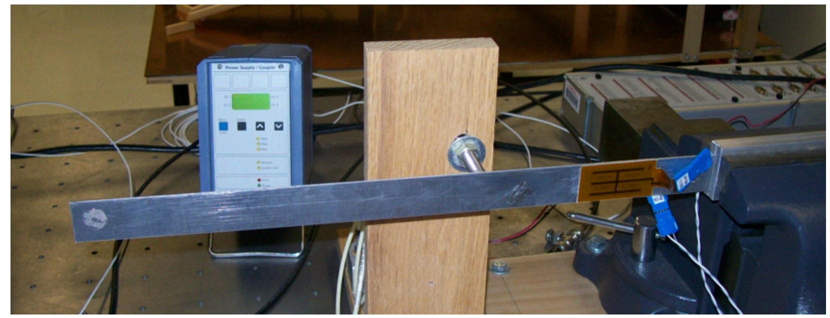
$$YI\frac{d^4w}{dx^4}(x) = k_p V \chi_{pzt}(x)$$

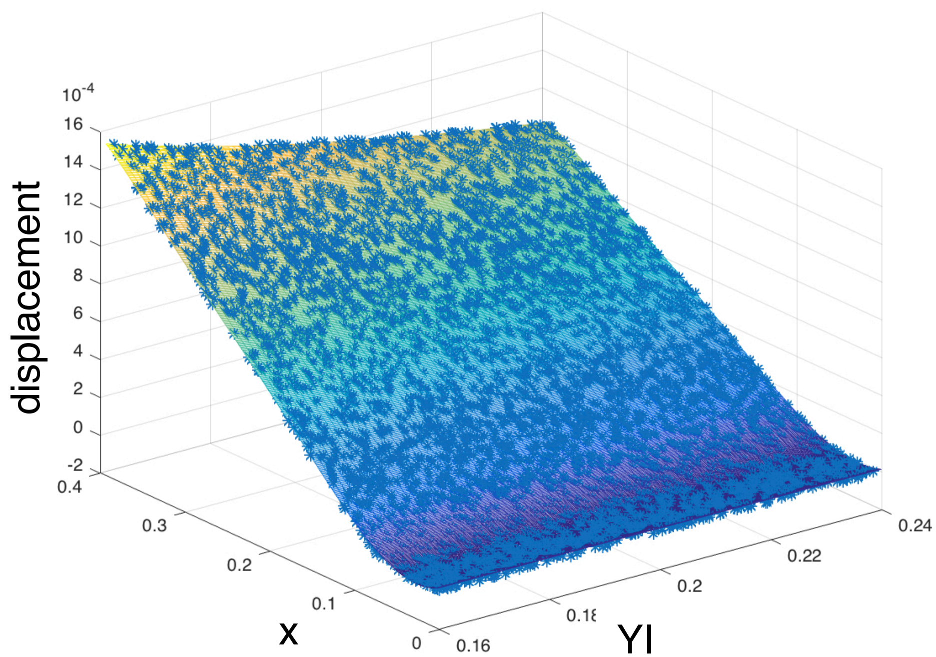
Data: Displacement observations

Parameter: YI

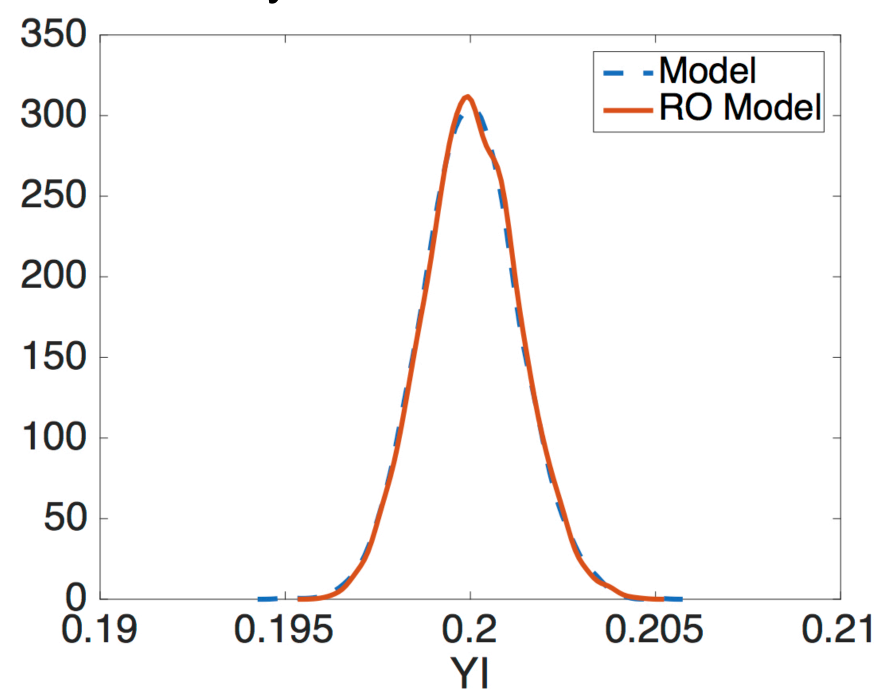
Training points: 5000

Polynomial surrogate: 6th order





Bayesian Inference



Data-Fit Models

Notes:

- Often termed response surface models, surrogates, emulators, meta-models.
- Rely on interpolation or regression.
- Data can consist of high-fidelity simulations or experiments.
- Common techniques: polynomial models, kriging (Gaussian process regression), orthogonal polynomials.

Strategy: Consider high fidelity model

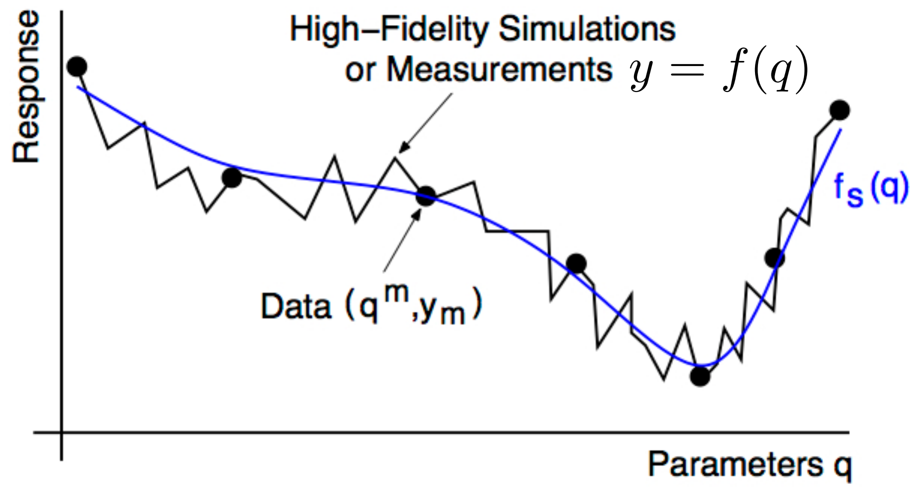
$$y = f(q)$$

with M model evaluations

$$y_m = f(q^m)\ ,\ \ m = 1, \ldots, M$$

Statistical Model: $f_s(q)$: Surrogate for $f(q)$

$$y_m = f_s(q^m) + \varepsilon_m\ ,\ \ m = 1, \ldots, M$$



Surrogate:

$$y^K(Q) = f_s(Q) = \sum_{k=0}^{K} \alpha_k \Psi_k(Q)$$

Note: $\Psi_k(Q)$ orthogonal with respect to inner product associated with pdf

e.g., $Q \sim N(0,1)$: Hermite polynomials

$Q \sim U(-1,1)$: Legendre polynomials

Orthogonal Polynomial Representations

Representation:

$$y^K(Q) = \sum_{k=0}^{K} \alpha_k \Psi_k(Q)$$

Note: $\Psi_0(Q) = 1$ implies that

$$\begin{aligned} \mathbb{E}[\Psi_0(Q)] &= 1 \\ \mathbb{E}[\Psi_i(Q)\Psi_j(Q)] &= \int_\Gamma \Psi_i(q)\Psi_j(q)\rho(q)dq \\ &= \delta_{ij}\gamma_i \end{aligned}$$

where $\gamma_i = \mathbb{E}[\Psi_i^2(Q)]$

Properties:

(i) $\mathbb{E}[y^K(Q)] = \alpha_0$

(ii) $\mathrm{var}[y^K(Q)] = \sum_{k=1}^{K} \alpha_k^2 \gamma_k$

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

Issue: How does one compute α_k , $k = 0, \ldots, K$?

- Stochastic Galerkin techniques (Polynomial Chaos Expansion – PCE)
- Nonintrusive PCE (Discrete projection)
- Stochastic collocation
- Regression-based methods with sparsity control (Lasso)

Note: Methods nonintrusive and treat code as blackbox.

Orthogonal Polynomial Representations

Nonintrusive PCE: Take weighted inner product of $y(q) = \sum_{k=0}^{\infty} \alpha_k \Psi_k(q)$ to obtain

$$\alpha_k = \frac{1}{\gamma_k} \int_{\Gamma} y(q) \Psi_k(q) \rho(q) dq$$

Quadrature:

$$\alpha_k \approx \frac{1}{\gamma_k} \sum_{r=1}^{R} y(q^r) \Psi_k(q^r) w^r$$

Note:

(i) Low-dimensional: Tensored 1-D quadrature rules – e.g., Gaussian

(ii) Moderate-dimensional: Sparse grid (Smolyak) techniques

(iii) High-dimensional: Monte Carlo or quasi-Monte Carlo (QMC) techniques

Regression-Based Methods with Sparsity Control (Lasso): Solve

$$\min_{\alpha \in \mathbb{R}^{K+1}} \|\Lambda \alpha - d\|^2 \quad \text{subject to} \quad \sum_{k=0}^{K} |\alpha_k| \leqslant \tau$$

Note: Sample points $\{q^m\}_{m=1}^{M}$

$\Lambda \in \mathbb{R}^{M \times (K+1)}$ where $\Lambda_{jk} = \Psi_k(q^j)$

$d = [y(q^1) \text{ , ... , } y(q^m)]$

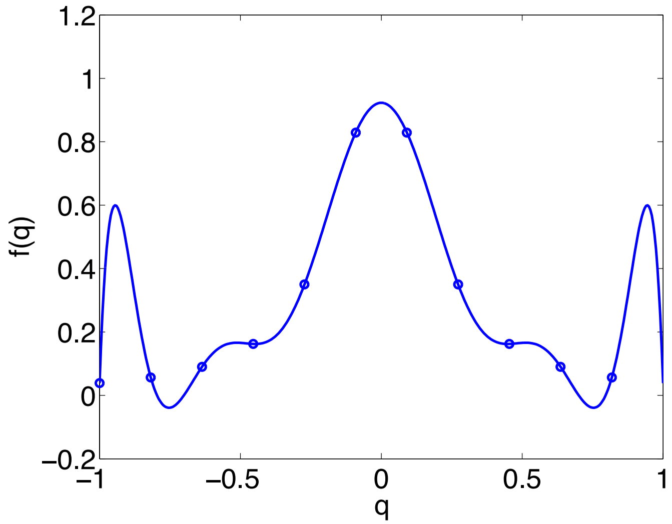
e.g., SPGL1

- MATLAB Solver for large-scale sparse reconstruction

Surrogate Models – Grid Choice

Example: Consider the Runge function $f(q) = \frac{1}{1+25q^2}$ with points

$$q^j = -1 + (j-1)\frac{2}{M} \ , \ j = 1, \ldots, M$$



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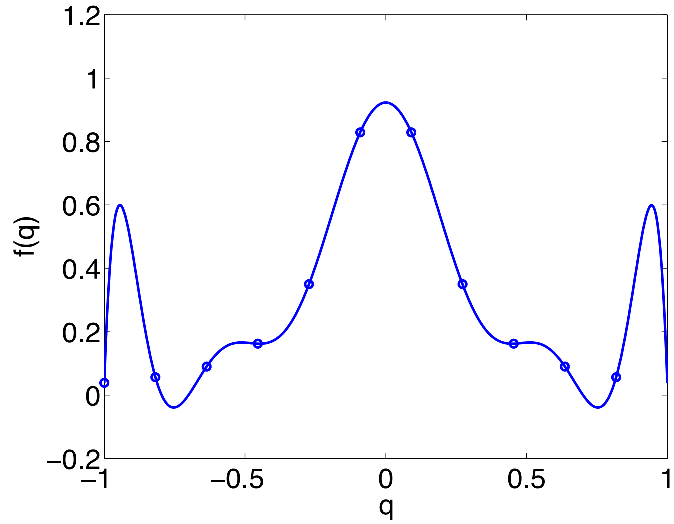

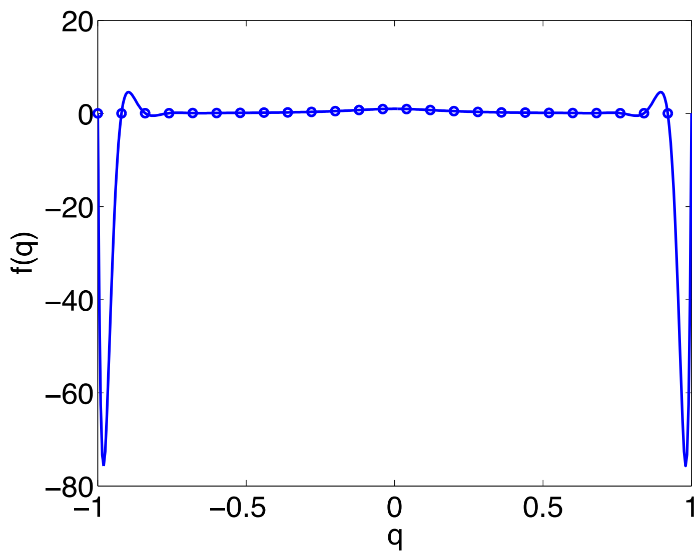

Surrogate Models – Grid Choice

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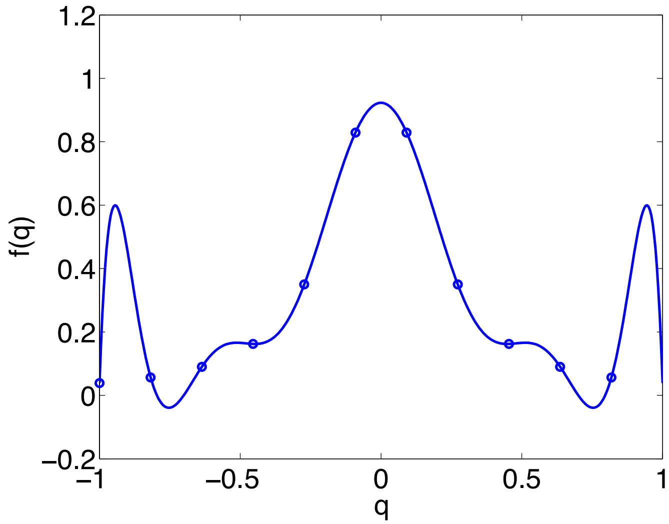
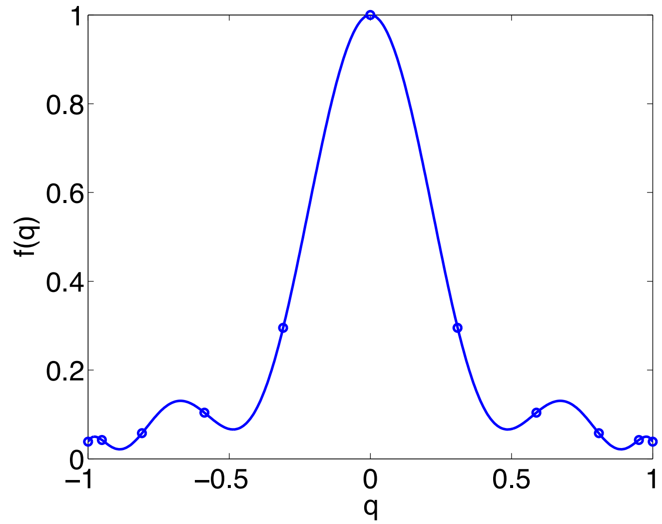
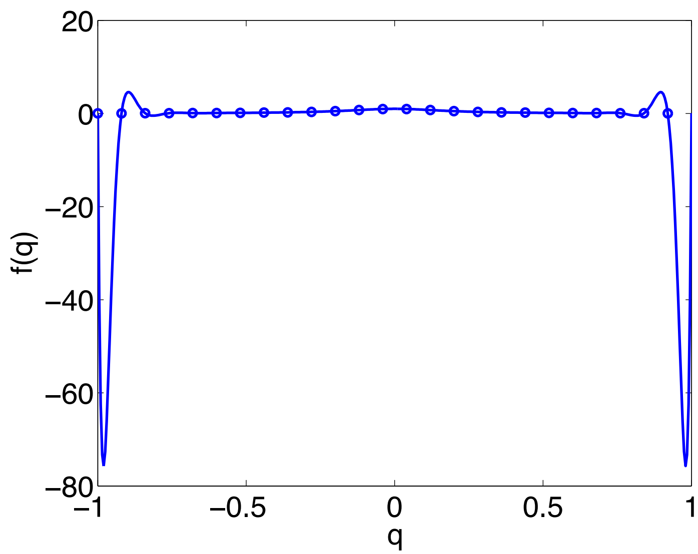
$$q^j = -1 + (j-1)\frac{2}{M}\ ,\ j = 1, \ldots, M \qquad\qquad q^j = -\cos\frac{\pi(j-1)}{M-1}\ ,\ j = 1, \ldots, M$$







Surrogate Models – Grid Choice

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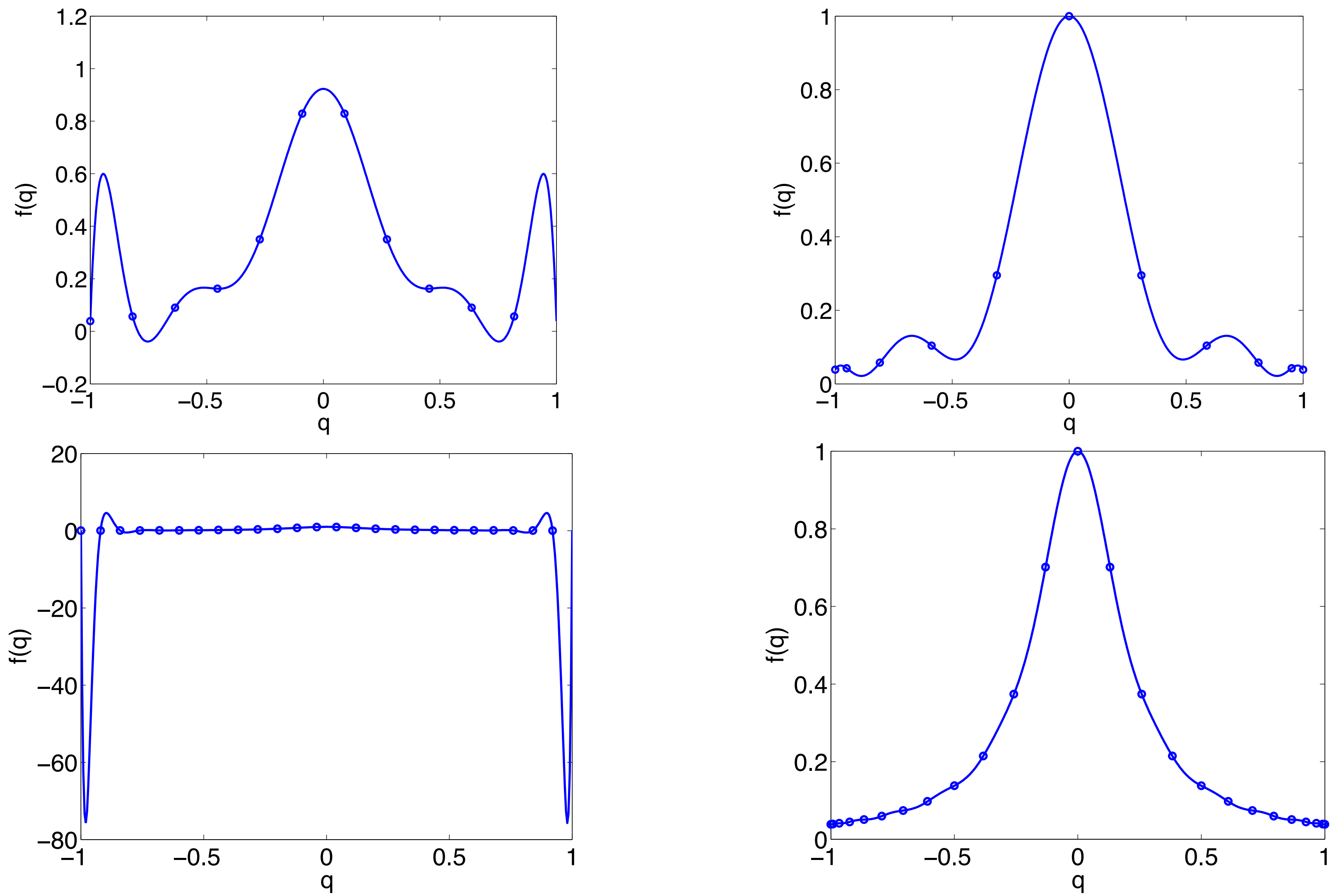
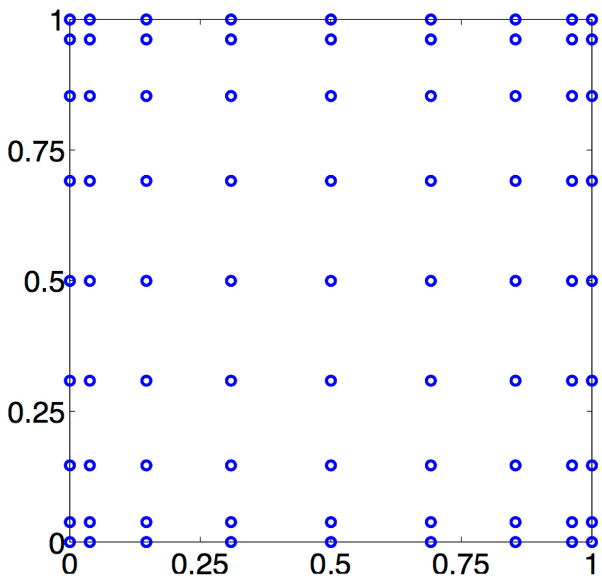
$$q^j = -1 + (j-1)\frac{2}{M}\ ,\ j = 1, \ldots, M \qquad q^j = -\cos\frac{\pi(j-1)}{M-1}\ ,\ j = 1, \ldots, M$$

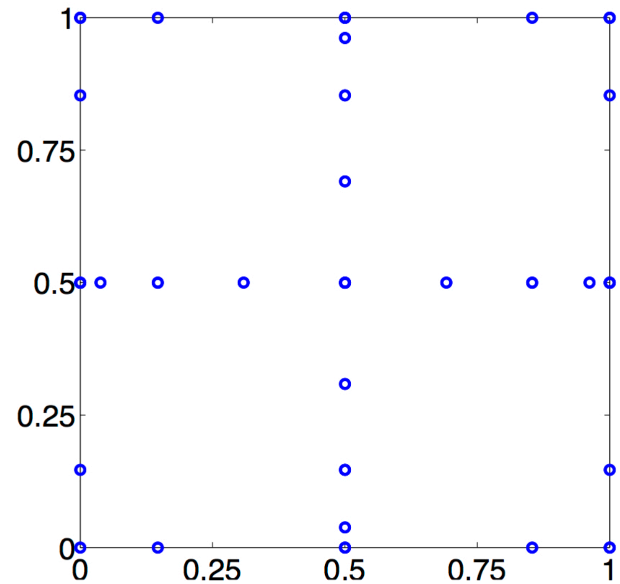


Sparse Grid Techniques

Tensored Grids: Exponential growth



Sparse Grids: Same accuracy



p	R_ℓ	Sparse Grid $\mathcal{R}$	Tensored Grid $R = (R_\ell)^p$
2	9	29	81
5	9	241	59,049
10	9	1581	$> 3 \times 10^9$
50	9	171,901	$> 5 \times 10^{47}$
100	9	1,353,801	$> 2 \times 10^{95}$

Surrogate Models

Question: How do we keep from fitting noise?

- Akaike Information Criterion (AIC)

$$AIC = 2k - 2\log[\pi(y|q)]$$

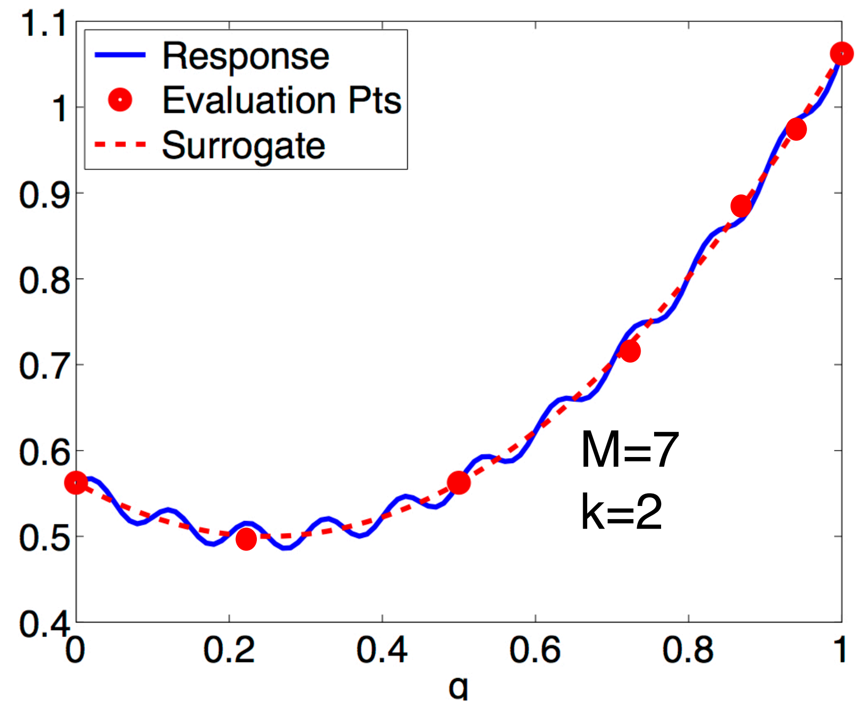
- Bayesian Information Criterion (AIC)

$$BIC = k\log(M) - 2\log[\pi(y|q)]$$

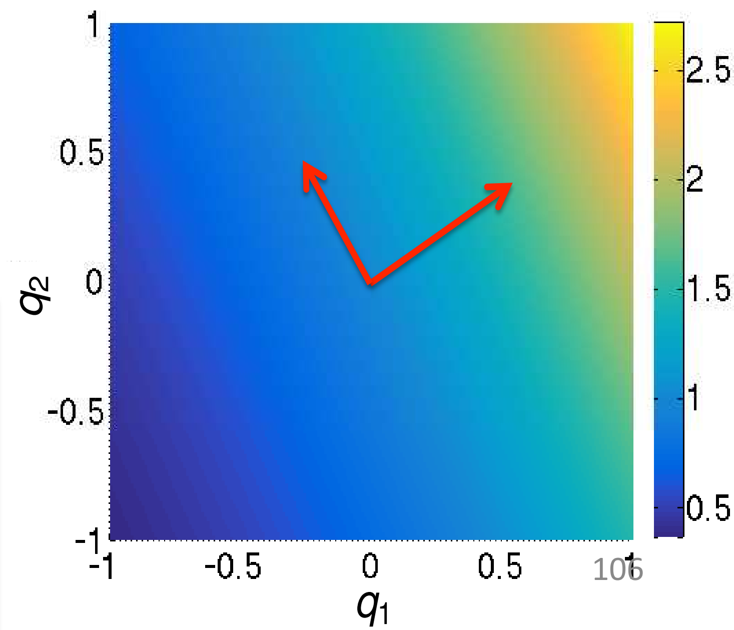
Likelihood:

$$\pi(y|q) = \frac{1}{(2\pi\sigma^2)^{M/2}} e^{-SS_q/2\sigma^2}$$ Maximize

$$SS_q = \sum_{m=1}^{M} [y_m - y_s(q^m)]^2$$ Minimize



Example: $y = \exp(0.7q_1 + 0.3q_2)$



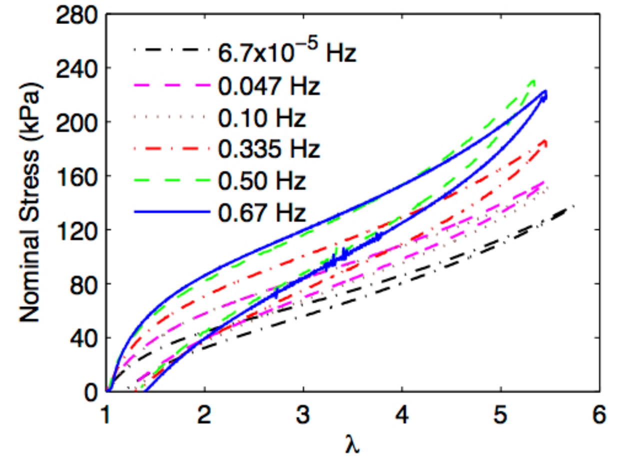
Exercise:

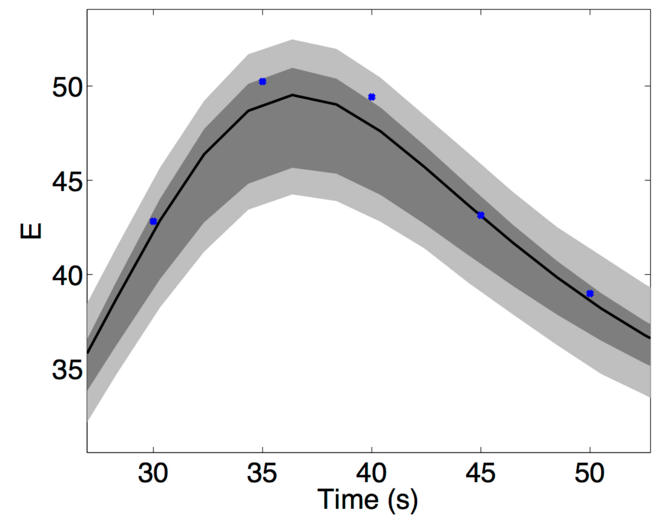
- Construct a polynomial surrogate using the code response_surface.m.
- What order seems appropriate?

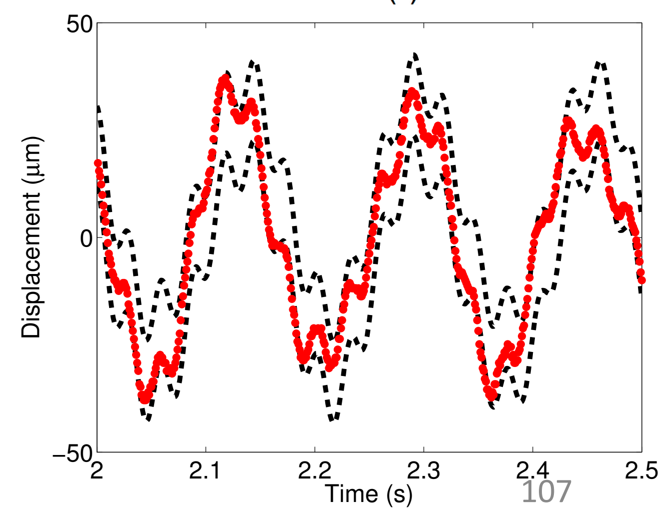
Concluding Remarks

Notes:

- UQ requires a synergy between engineering, statistics, and applied mathematics.
- Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.
- Goal is to predict model responses with quantified and reduced uncertainties.
- Parameter selection is critical to isolate identifiable and influential parameters.
- Surrogate models critical for computationally intensive simulation codes.
- Codes and packages: Sandia Dakota, R, MATLAB, Python, nanoHUB.
- Algorithms are new and evolving.
- *Prediction is very difficult, especially if it's about the future*, Niels Bohr.







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Papers:

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