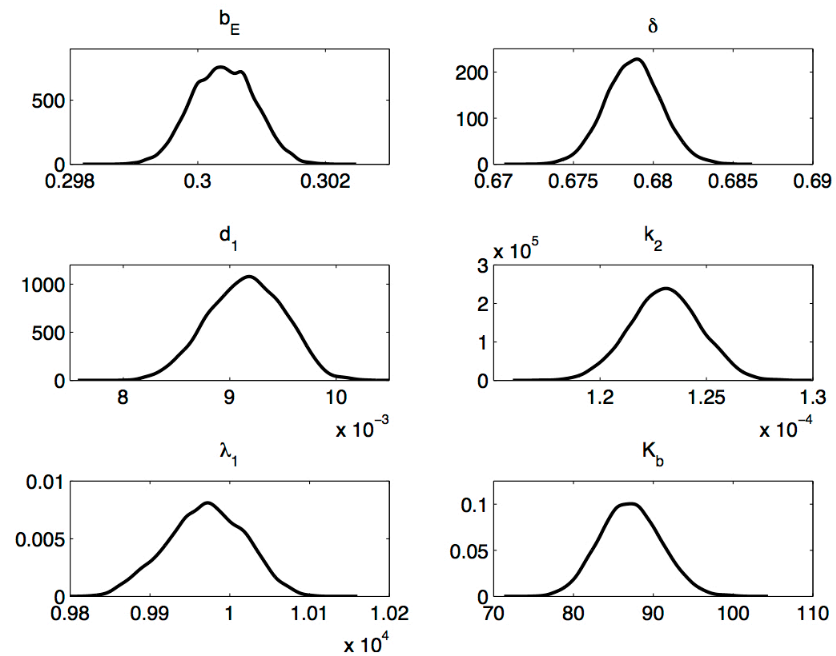
Uncertainty Propagation

Setting:

- We assume that we have determined distributions for parameters
  - e.g., Bayesian inference, prior experiments, expert opinion

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon)k_1 V T_1$$
$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon)k_2 V T_2$$
$$\dot{T}_1^* = (1-\varepsilon)k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$
$$\dot{T}_2^* = (1-f\varepsilon)k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$
$$\dot{V} = N_T \delta(T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2]V$$
$$\dot{E} = \lambda_E + \frac{b_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_b}E - \frac{d_E(T_1^* + T_2^*)}{T_1^* + T_2^* + K_d}E - \delta_E E$$



Goal: Construct statistics for quantities of interest

- e.g., Expected viral load in HIV patient with appropriate uncertainty intervals
- Note: Often involves moderate to high-dimensional integration

$$\mathbb{E}[V(t)] = \int_{\mathbb{R}^6} V(t,q)\rho(q)dq$$

Questions:

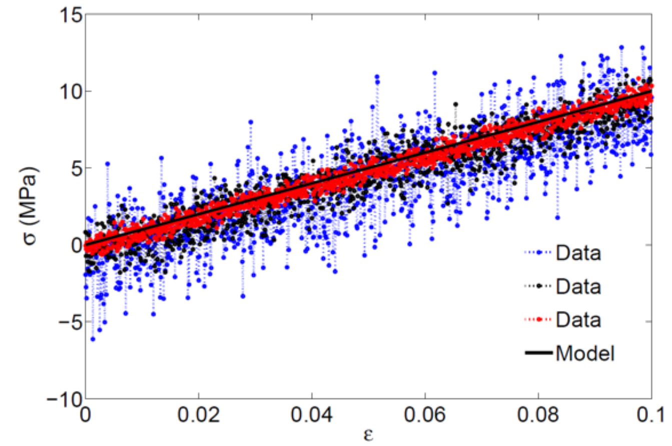
- How do we effectively propagate input uncertainties?
- Efficient quadrature techniques

Uncertainty Propagation Techniques

Techniques and Issues:

- Analytic expressions for linearly parameterized problems
- Perturbation methods for nonlinearly parameterized problems
- Direct sampling methods
  - Often require surrogate models
- Computation of moments using stochastic spectral methods
  - Stochastic Galerkin – aka polynomial chaos
  - Discrete projection
  - Stochastic collocation

Forward Uncertainty Propagation: Linear Models



Linear Models: Analytic mean and variance relations

Example: Linear stress-strain relation

$$\Upsilon_i = Ee_i + E_2 e_i^3 + \varepsilon_i \ , \ i = 1, \ldots, n$$

Model Statistics:

Let $\overline{E}, \overline{E}_2$ and $\mathrm{var}(E), \mathrm{var}(E_2)$ denote parameter means and variance. Then

$$\mathbb{E}[Ee_i + E_2 e_i^3] = \overline{E}e_i + \overline{E}_2 e_i^3$$

$$\mathrm{var}[Ee_i + E_2 e_i^3] = e_i^2 \mathrm{var}(E) + e_i^6 \mathrm{var}(E_2) + 2e_i^4 \mathrm{cov}(E, E_2)$$

Response Statistics: Assume measurement errors uncorrelated from model response.

$$\mathbb{E}[\Upsilon_i] = \overline{E}e_i + \overline{E}_2 e_i^3$$

$$\mathrm{var}[\Upsilon_i] = e_i^2 \mathrm{var}(E) + e_i^6 \mathrm{var}(E_2) + 2e_i^4 \mathrm{cov}(E, E_2) + \mathrm{var}(\varepsilon_i)$$

Problem: Models are almost always nonlinearly parameterized

Forward Uncertainty Propagation: Perturbation Methods

Strategy: Consider $Q = [Q_1, \ldots, Q_p]$ with joint pdf $\rho_Q(q)$. Take

$$\begin{aligned} Q = & \quad \bar{q} + \delta Q \\ = & \quad [\bar{q}_1 + \delta Q_1, \ldots, \bar{q}_p + \delta q_p] \end{aligned}$$

Then

$$\begin{aligned} f(Q) = & \quad f(\bar{q}) + \sum_{i=1}^{p} \frac{\partial f}{\partial Q_i}\bigg|_{\bar{q}} \delta Q_I + H.O.T \\ \approx & \quad \bar{y} + \sum_{i=1}^{p} s_i \delta Q_i \end{aligned}$$

and

$$\mathbb{E}(Q_i) = \bar{q}_i$$

$$\text{var}(Q_i) = \int_{\mathbb{R}^p} (q_i - \bar{q}_i)^2 \rho_Q(q) dq = \int_{\mathbb{R}^p} (\delta q_i)^2 \rho_Q(q) dq$$

$$\text{cov}(Q_i, Q_j) = \int_{\mathbb{R}^p} (q_i - \bar{q}_i)(q_j - \bar{q}_j) \rho_Q(q) dq = \int_{\mathbb{R}^p} \delta q_i \delta q_j \rho_Q(q) dq$$

Forward Uncertainty Propagation: Perturbation Methods

It follows that

$$\mathbb{E}[f(Q)] = \bar{y} \int_{\mathbb{R}^p} \rho_Q(q)dq + \sum_{i=1}^{p} s_i \int_{\mathbb{R}^p} (q_i - \bar{q}_i)\rho_Q(q)dq = \bar{y}$$

and

$$\begin{aligned}
\mathrm{var}[f(Q)] &= \mathbb{E}[(f(Q) - \bar{y})^2] \\
&= \int_{\mathbb{R}^p} \left(\sum_{i=1}^{p} s_i \delta q_i \right)^2 \rho_Q(q)dq \\
&= \sum_{i=1}^{p} s_i^2 \int_{\mathbb{R}^p} (\delta q_i)^2 \rho_Q(q)dq + \sum_{i=1}^{p} \sum_{\substack{j=1 \\ j \neq i}}^{p} s_i s_j \int_{\mathbb{R}^p} (\delta q_i)(\delta q_j)\rho_Q(q)dq \\
&= \sum_{i=1}^{p} s_i^2 \mathrm{var}(Q_i) + \sum_{i=1}^{p} \sum_{\substack{j=1 \\ j \neq i}}^{p} s_i s_j \mathrm{cov}(Q_i, Q_j) \\
&= S^T V S
\end{aligned}$$

Notes:

- S and V are the local sensitivity vector and covariance matrix.
- This is often termed the “sandwich relation”.
- Suppose $Q_i \sim N(\bar{q}_i, \sigma_i^2)$ are mutually independent. Then $F(Q) \sim N(\bar{y}, S^T V S)$.

Forward Uncertainty Propagation: Sampling Methods

Strategy: 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.
- No additional cost for DRAM if interpolating.

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.

Perturbation and Sampling for Forward Propagation

Example: Consider

$$m\frac{d^2z}{dt^2} + c\frac{dz}{dt} = kz = f_0\cos(\omega_F t)$$

$$z(0) = z_0 \; , \; \frac{dz}{dt}(0) = z_1$$

with Q = [m,c,k]. This has the amplitude

$$z_0(Q) = \frac{f_0}{\sqrt{m^2(\omega_0^2 - \omega_F^2)^2 + c^2\omega_F^2}} \quad , \; \omega_0 = \sqrt{k/m}$$

Consider the response

$$y = f(\omega_F, Q) = \frac{z_0(Q)}{f_0} = \frac{1}{\sqrt{(k - m\omega_F^2)^2 + (c\omega_F^2)}}$$

Take $q = [m, c, k] \sim N(\bar{q}, V)$ where

$$\bar{q} = [2.7, 0.24, 8.5] \quad , \quad V = \begin{bmatrix} 0.002^2 & 0 & 0 \\ 0 & 0.065^2 & 0 \\ 0 & 0 & .001^2 \end{bmatrix}$$

Perturbation and Sampling for Forward Propagation

Notes:

- Natural frequency $\bar{\omega}_0 = 1.7743 \text{ Hz}$
- Analytic sensitivity relations

$$s^T = \left[\frac{\partial f}{\partial m}, \frac{\partial f}{\partial c}, \frac{\partial f}{dk} \right]$$

Compare:

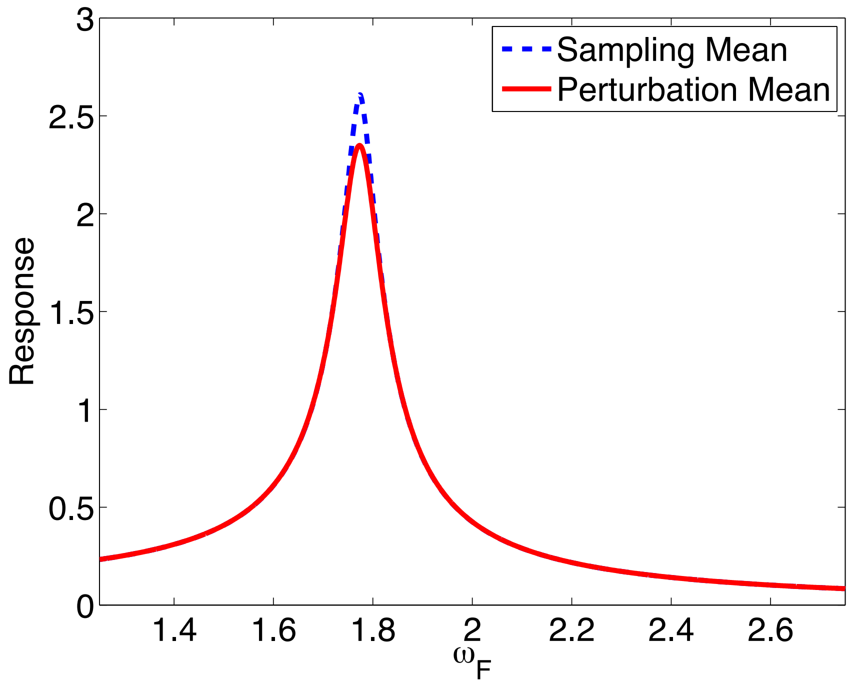
- Perturbation result
- Sample M = 10,000 and construct sample mean and variance

$$\bar{y}_s(\omega_F) = \frac{1}{M} \sum_{m=1}^{M} f(\omega_F, q^m)$$

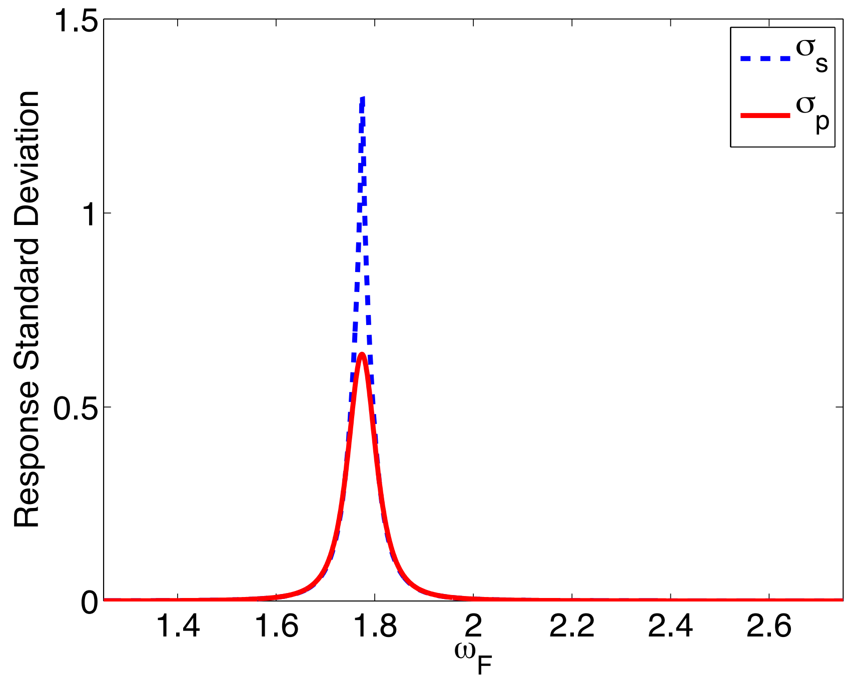
$$\omega_s^2(\omega_F) = \frac{1}{M-1} \sum_{m=1}^{M} \left[f(\omega_F, q^m) - \bar{y}_s(\omega_F) \right]^2$$

Perturbation and Sampling for Forward Propagation

Results:



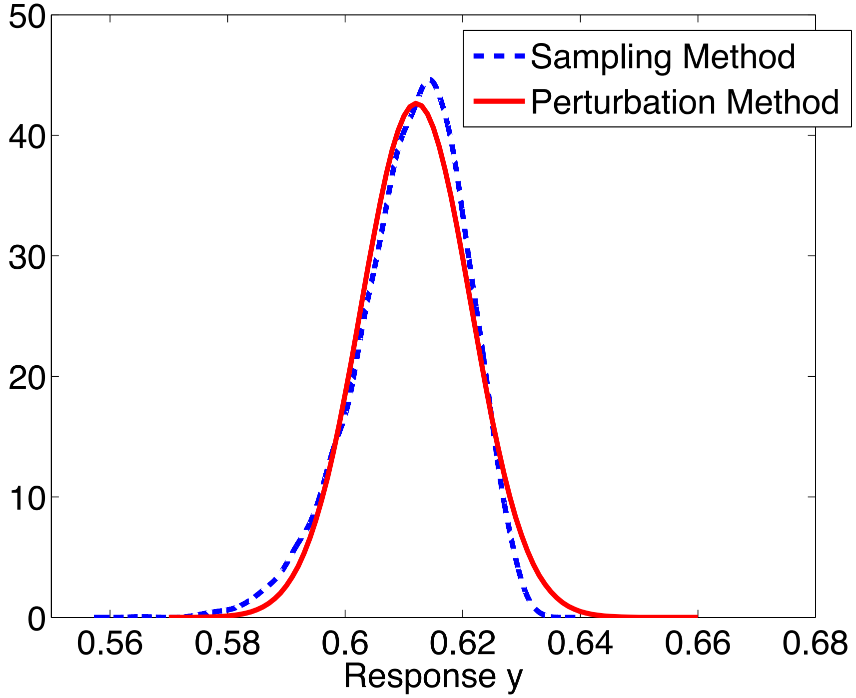
Means



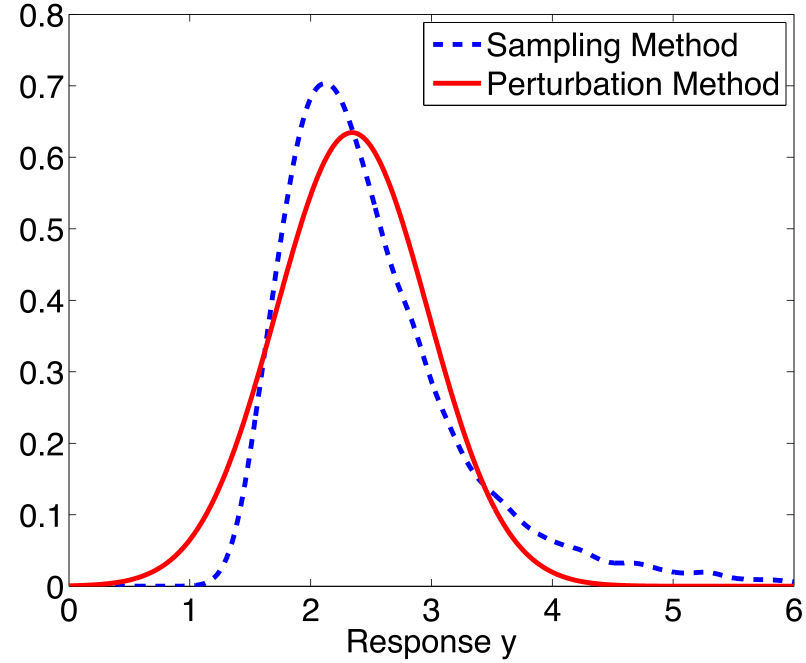
Standard Deviations

Perturbation and Sampling for Forward Propagation

Results: Recall the natural frequency $\bar{\omega}_0 = 1.7743 \text{ Hz}$



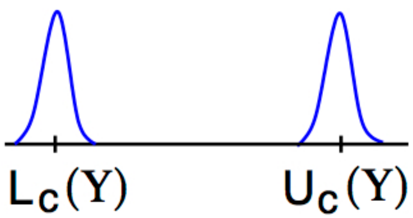
1.60 Hz



1.77 Hz

Review of Confidence and Credible Intervals for Parameters

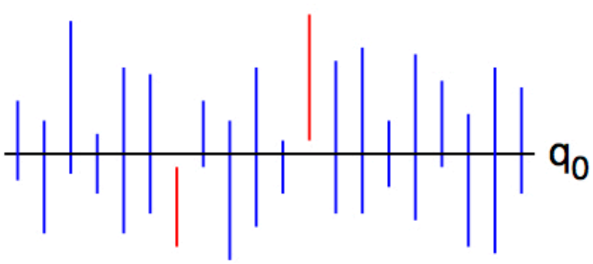
Data: $\Upsilon = [\Upsilon_1, \cdots, \Upsilon_n]$ of iid random observations



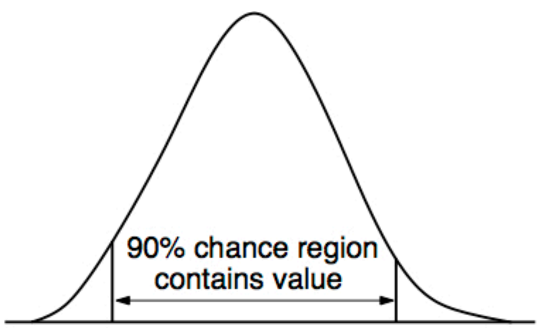
Confidence Interval (Frequentist): A $100 \times (1-\alpha)$% confidence interval for a fixed, unknown parameter q_0 is a random interval $[L_c(\Upsilon), U_c(\Upsilon)]$, having probability at least $1-\alpha$ of covering q_0 under the joint distribution of Υ.

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 and Prediction Intervals for Responses

Linear Model:

$$\Upsilon = Xq_0 + \varepsilon \quad , \quad \varepsilon_i \sim N(0, \sigma_0^2)$$

Consider x_0 in domain but not among data used to estimate q and σ.

Example: Linear regression

$$\Upsilon_i = q_1 + \sum_{j=2}^{p} x_{ij} q_j + \varepsilon_i \ , \ i = 1, \cdots, n$$

$$x_0 = [1, x_{02}, \cdots, x_{0p}]^T$$

Two Cases:

(i) New prediction Υ_{x_0}

(ii) Mean response $\mu_{x_0} = \mathbb{E}(\Upsilon_{x_0})$

Case (ii) First: Consider the unbiased estimator

$$\widehat{\Upsilon}_{x_0} = x_0^T \hat{q}$$

Confidence and Prediction Intervals for Responses

From the properties

$$\text{var}\left(\sum_{i=1}^{n} a_i X_i\right) = \sum_{i=1}^{n} a_i^2 \text{var}(X_i)$$

$$\text{var}(\hat{q}) = \sigma_0^2 (X^T X)^{-1}$$

it follows that

$$\text{var}(\widehat{\Upsilon}_{x_0}) = \sigma_0^2 \left[x_0^T (X^T X)^{-1} x_0\right]$$

Estimator:

$$\widehat{\sigma}^2(\widehat{\Upsilon}_{x_0}) = \widehat{\sigma}^2 \left[x_0^T (X^T X)^{-1} x_0\right]$$

Note: $\varepsilon_i \sim N(0, \sigma_0^2)$ implies that

$$\frac{\widehat{\Upsilon}_{x_0} - \mu_{x_0}}{\sigma_0 \sqrt{x_0^T (X^T X)^{-1} x_0}} \sim N(0,1)$$

Confidence and Prediction Intervals for Responses

Using Property 7.10 and 7.11, if follows that

$$T = \frac{\widehat{\Upsilon}_{x_0} - \mu_{x_0}}{\widehat{\sigma}\sqrt{x_0^T (X^T X)^{-1} x_0}} \sim t(n-p)$$

Confidence Interval:

$$\left[\widehat{\Upsilon}_{x_0} \pm t_{n-p,1-\alpha/2} \cdot \widehat{\sigma}\sqrt{x_0^T (X^T X)^{-1} x_0}\right]$$

Prediction Interval: Assume that estimators $\hat{q}$ and $\hat{\sigma}^2$ have been computed using previous data so independent from Υ_{x_0}. Then $\Upsilon_{x_0} - \widehat{\Upsilon}_{x_0}$ is normally distributed with

$$\mathbb{E}(\Upsilon_{x_0} - \widehat{\Upsilon}_{x_0}) = x_0^T q_0 - x_0^T \mathbb{E}(\hat{q}) = 0$$

$$\begin{aligned} \mathrm{var}(\Upsilon_{x_0} - \widehat{\Upsilon}_{x_0}) &= \mathrm{var}(\Upsilon_{x_0}) + \mathrm{var}(\widehat{\Upsilon}_{x_0}) \\ &= \sigma_0^2 + \sigma_0^2 x_0^T (X^T X)^{-1} x_0 \\ &= \sigma_0^2 \left[1 + x_0^T (X^T X)^{-1} x_0\right] \end{aligned}$$

Prediction Intervals for Responses

Prediction Interval:

$$\left[\Upsilon_{x_0} \pm t_{n-p,1-\alpha/2} \cdot \widehat{\sigma}\sqrt{1 + x_0^T(X^TX)^{-1}x_0}\right]$$

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

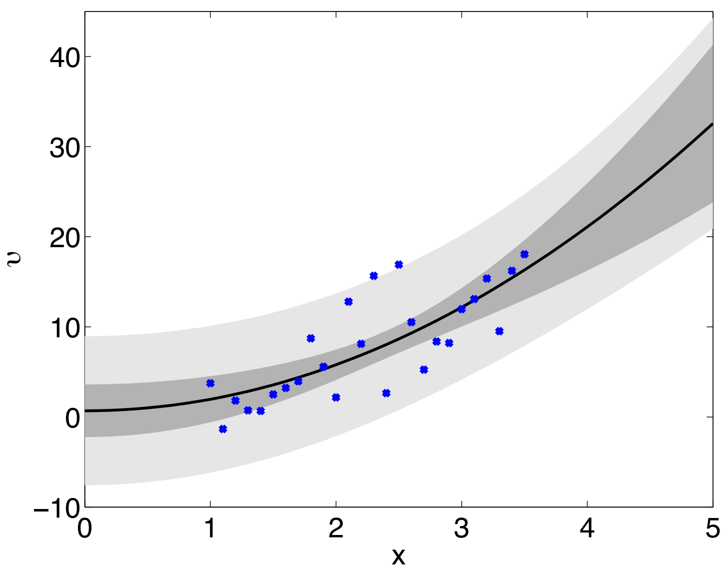
Prediction Interval: A $100 \times (1-\alpha)$% prediction interval for a future observable Υ_{n+1} is a random interval $[L_c(\Upsilon), U_c(\Upsilon)]$ having probability at least $1-\alpha$ of of containing Υ_{n+1} under the joint distribution of $(\Upsilon, \Upsilon_{n+1})$.

Uncertainty Propagation in Models

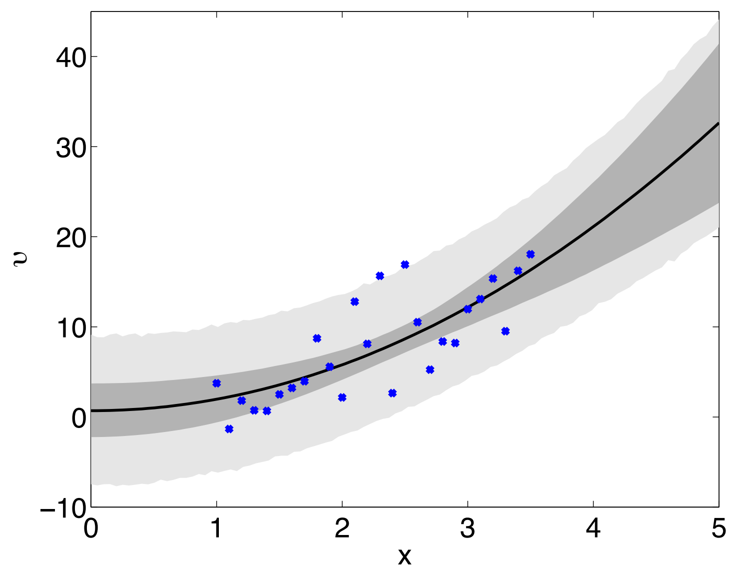
Example: Linear model

$$\Upsilon_i = q_1 + q_2 x_i^2 + \varepsilon_i$$

with $q_0 = [0.6, 1.2]$ and $\sigma_0 = 3$.



Frequentist Confidence and Prediction Intervals



Bayesian Credible and Prediction Intervals

Note: Confidence and credible intervals grow for extrapolatory predictions.

Uncertainty Propagation in Models

Example: HIV model

$$\dot{T}_1 = \lambda_1 - d_1 T_1 - (1-\varepsilon) k_1 V T_1$$

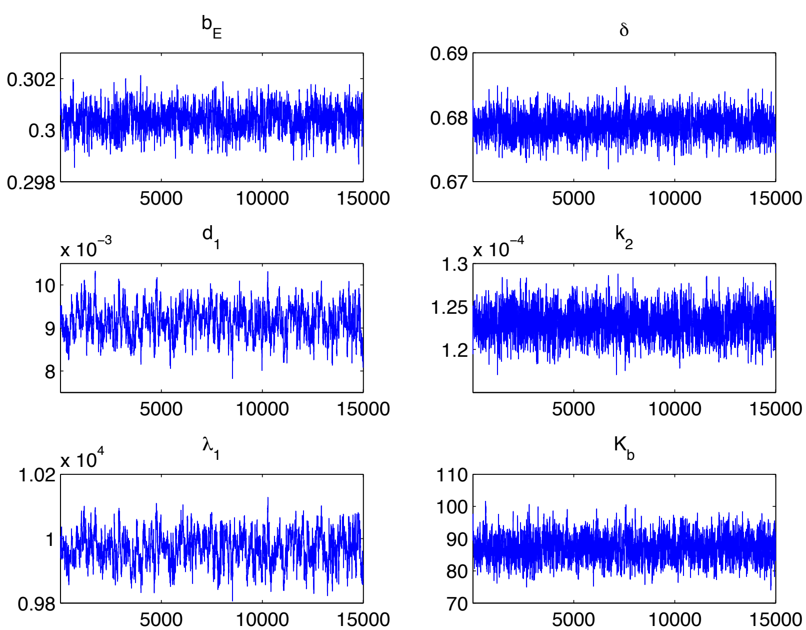
$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

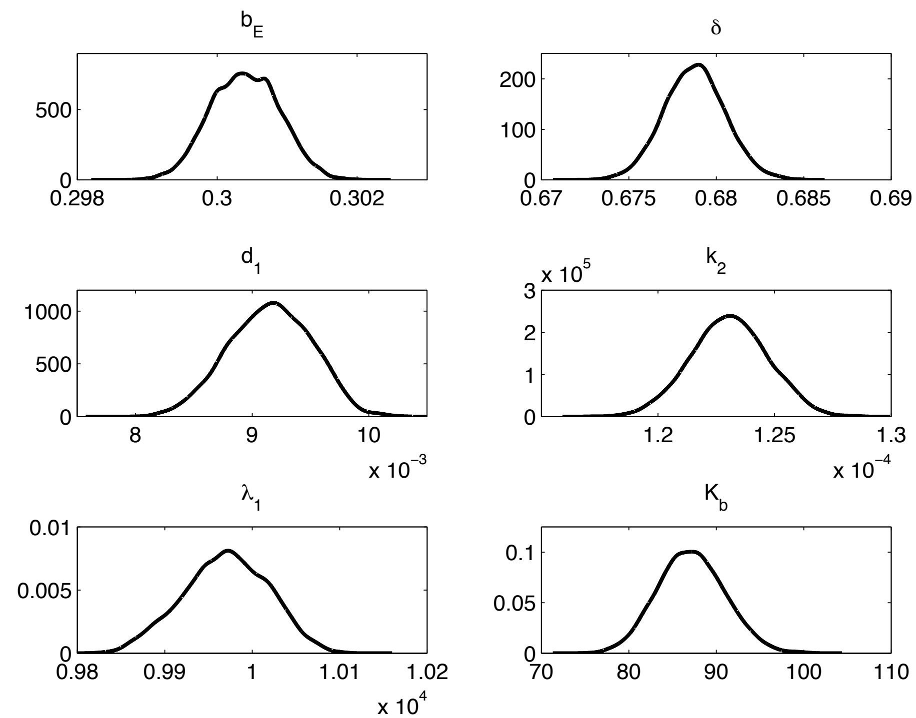
$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

$$\dot{T}_2^* = (1-f\varepsilon) k_2 V T_2 - \delta T_2^* - m_2 E T_2^*$$

$$\dot{V} = N_T \delta (T_1^* + T_2^*) - cV - [(1-\varepsilon)\rho_1 k_1 T_1 + (1-f\varepsilon)\rho_2 k_2 T_2] V$$

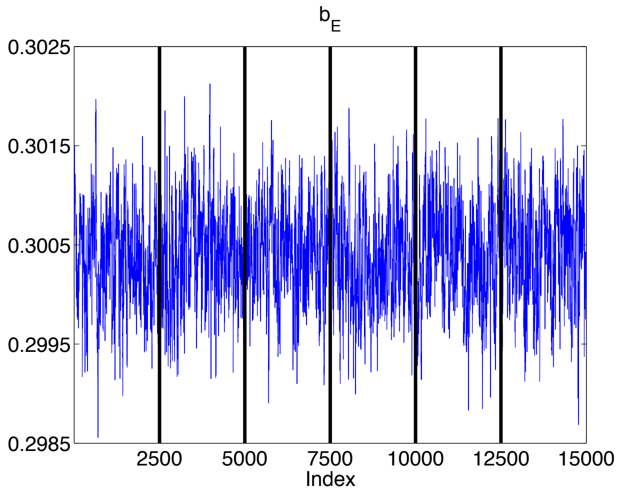
$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E.$$

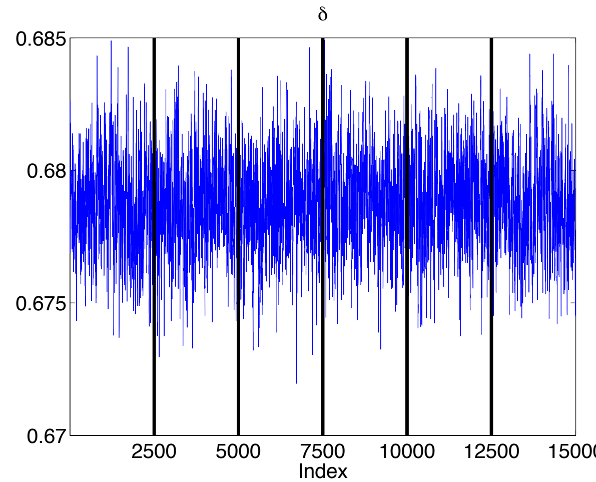


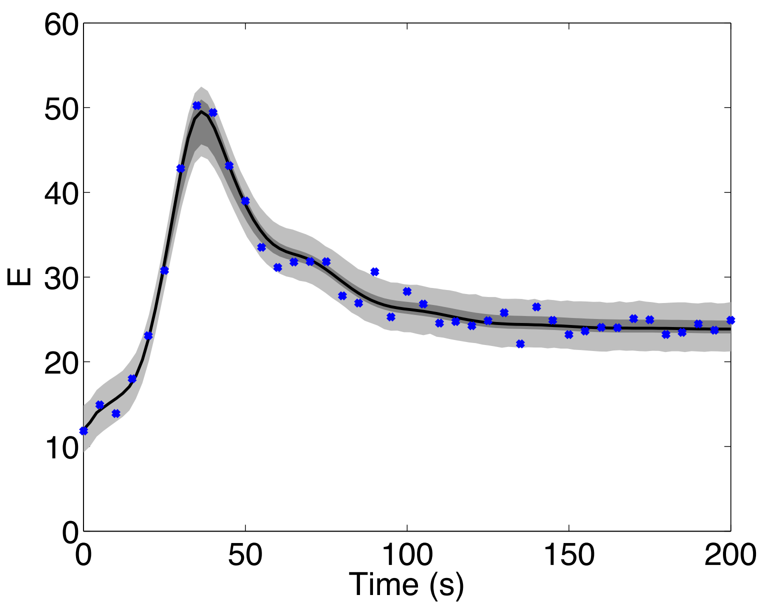


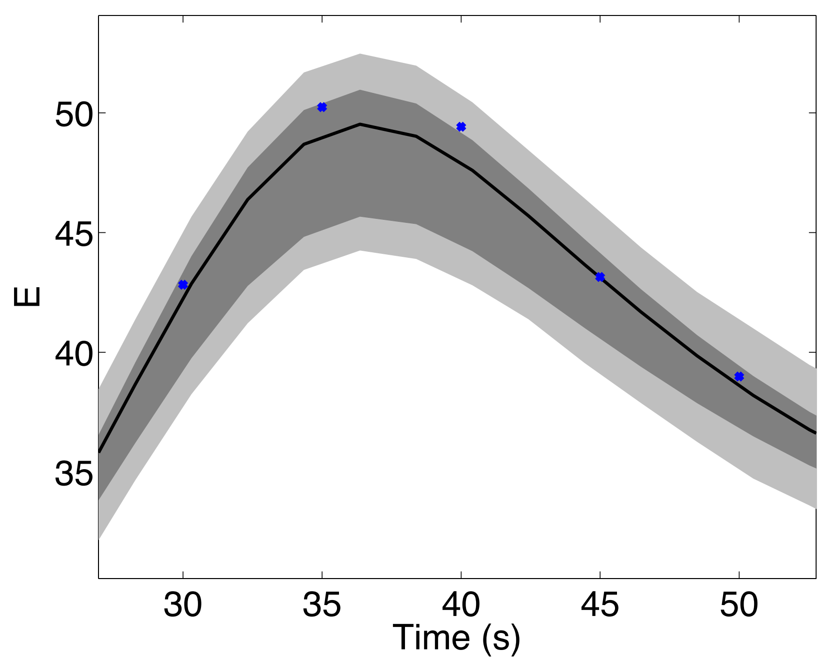
Uncertainty Propagation in Models

Example: HIV model









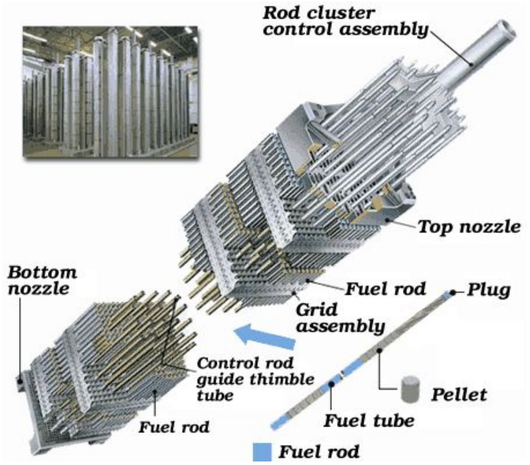
Use of Prediction Intervals: Nuclear Power Plant Design

Subchannel Code (COBRA-TF): numerous closure relations, ~70 parameters

e.g., Dittus—Boelter Relation

$$Nu = 0.023 Re^{0.8} Pr^{0.4}$$

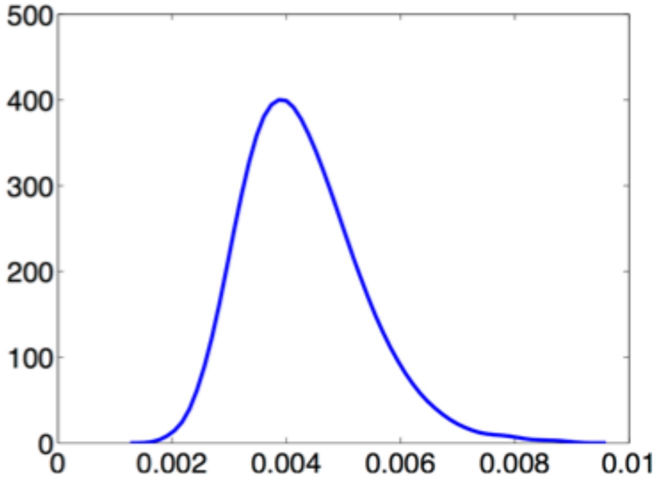
Nu: Nusselt number
Re: Reynolds number
Pr: Prandtl number



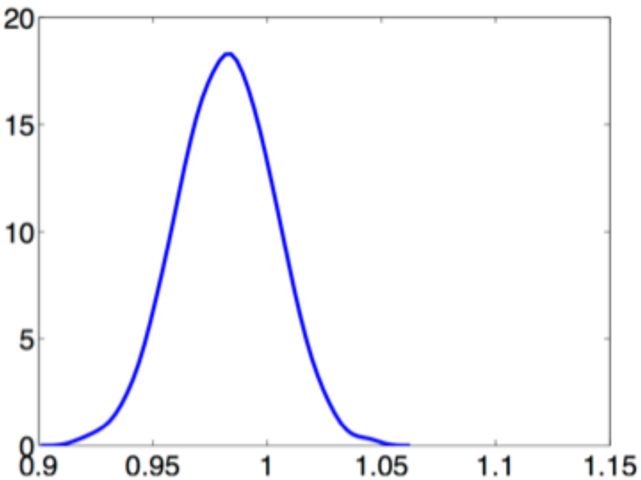
Industry Standard: Employ conservative, uniform, bounds

i.e., [0, 0.046], [0, 1.6], [0,0.8]

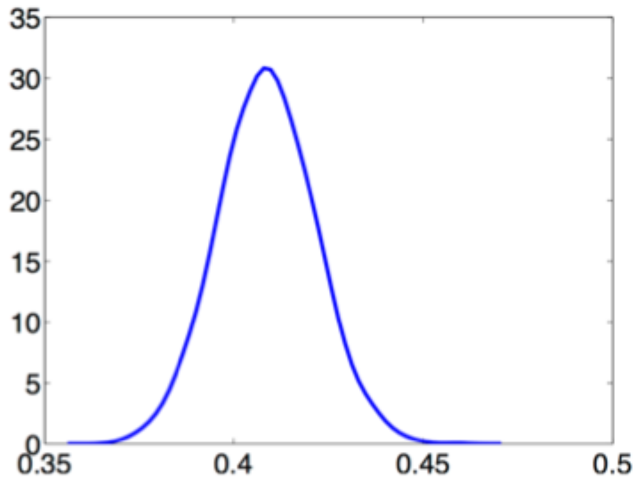
Bayesian Analysis: Employ conservative bounds as priors



$2\sigma \approx 0.0035$



$2\sigma \approx 0.06$

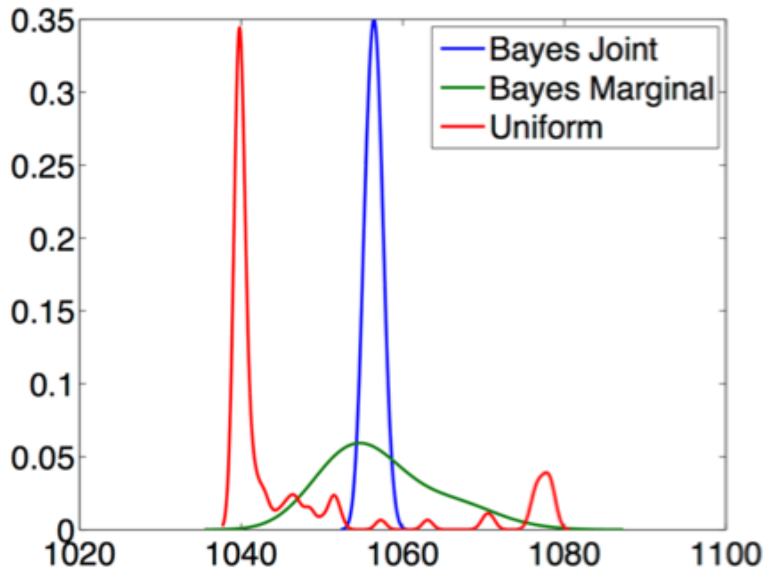


$2\sigma \approx 0.03$

Note: Substantial reduction in parameter uncertainty

Use of Prediction Intervals: Nuclear Power Plant Design

Strategy: Propagate parameter uncertainties through COBRA-TF to determine uncertainty in maximum fuel temperature



Notes:

- Temperature uncertainty reduced from 40 degrees to 5 degrees
- Can run plant 20 degrees hotter, which significantly improves efficiency

Ramification: Savings of 10 billion dollars per year for US power plants

Issues:

- We considered only one of many closure relations
- Nuclear regulatory commission takes years to change requirements and codes

Good News: We are now working with Westinghouse to reduce uncertainties.