

Forward Uncertainty Propagation: Perturbation Methods

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

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

Then

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

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

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

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

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

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

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

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

Compare:

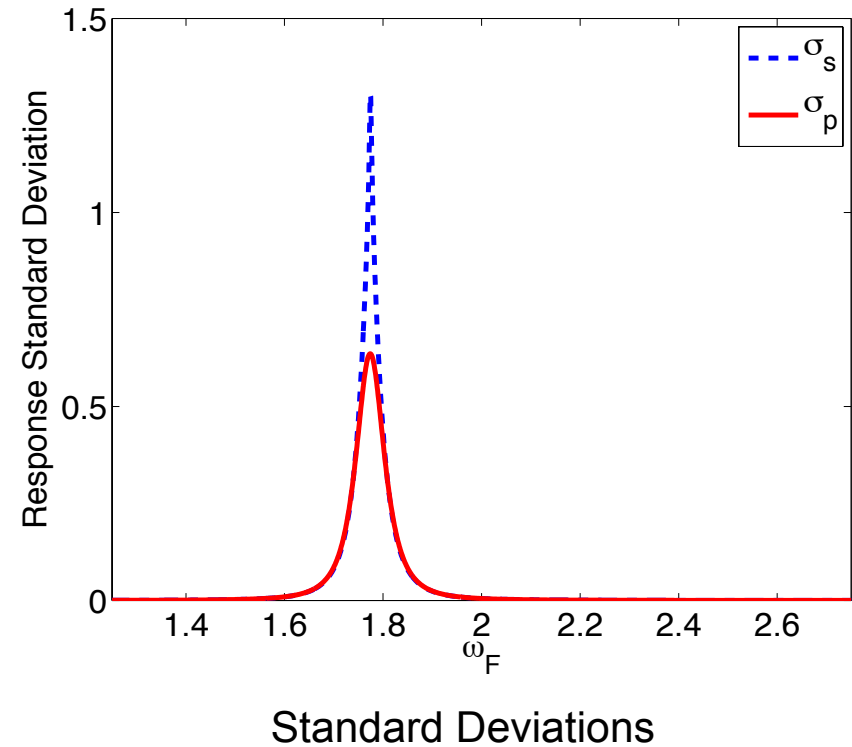
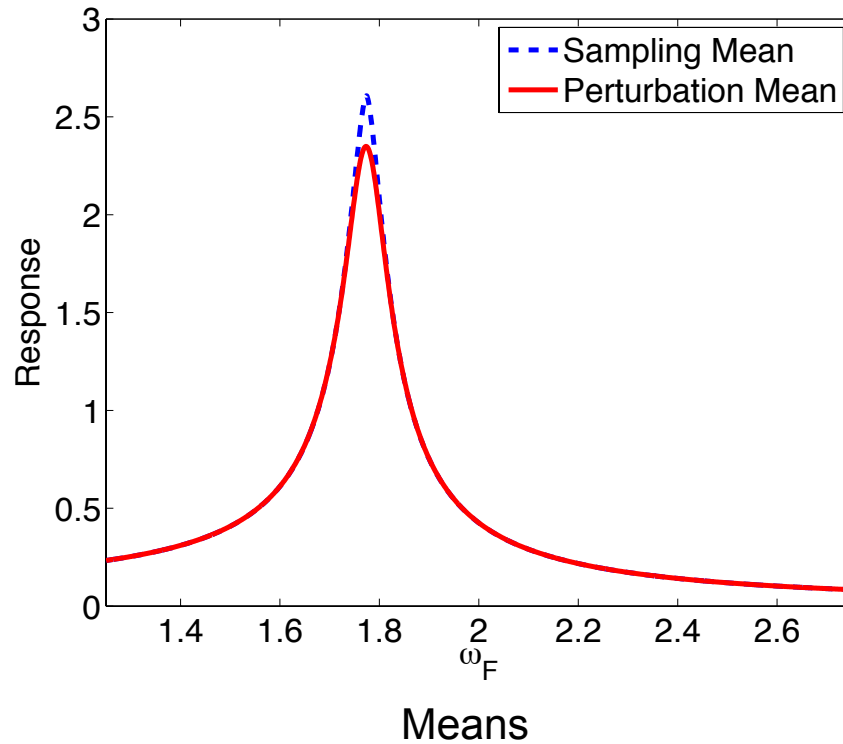
- Perturbation result
- Sample $M = 10,000$ and construct sample mean and variance

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

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

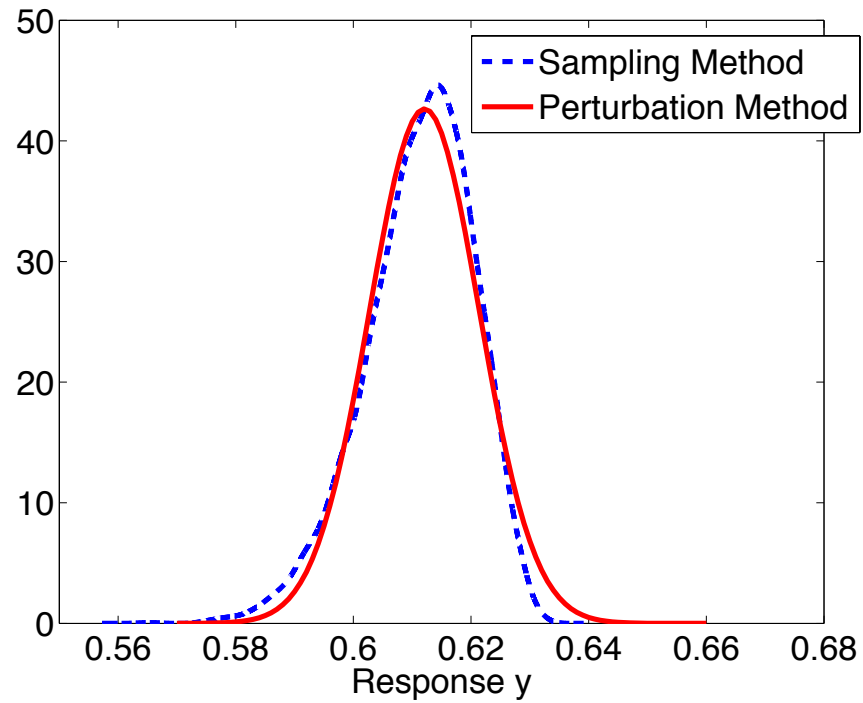
Perturbation and Sampling for Forward Propagation

Results:

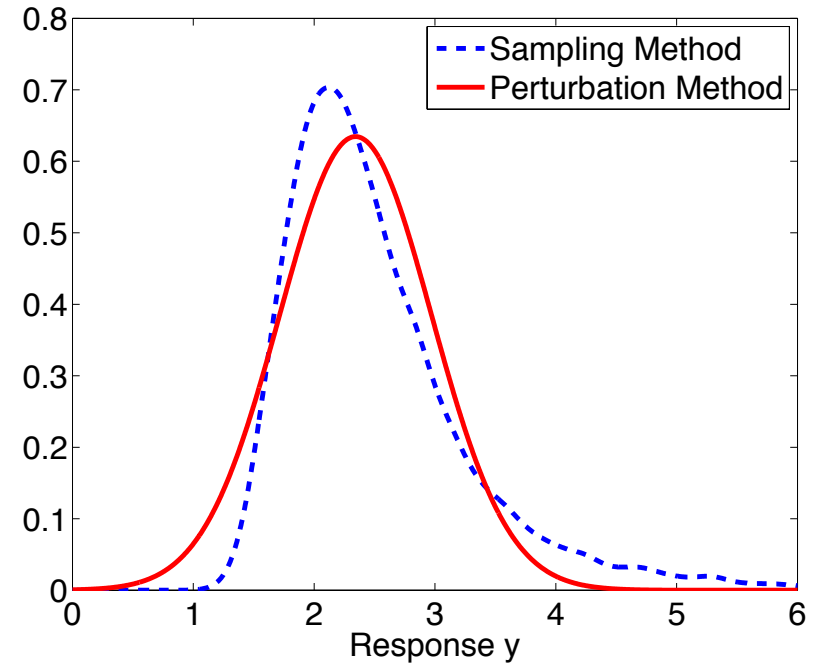


Perturbation and Sampling for Forward Propagation

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



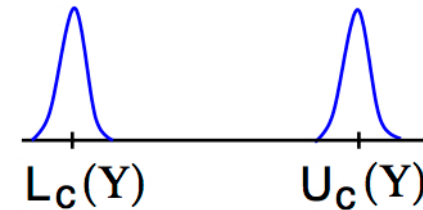
1.60 Hz



1.77 Hz

Review of Confidence and Credible Intervals for Parameters

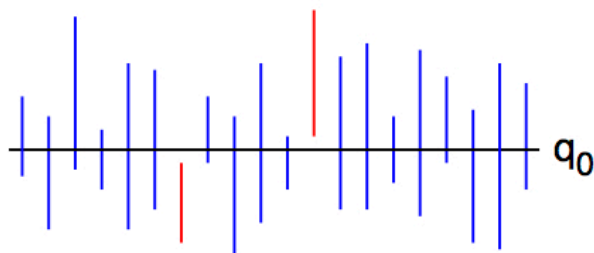
Data: $\Upsilon = [\Upsilon_1, \dots, \Upsilon_n]$ of iid random observations



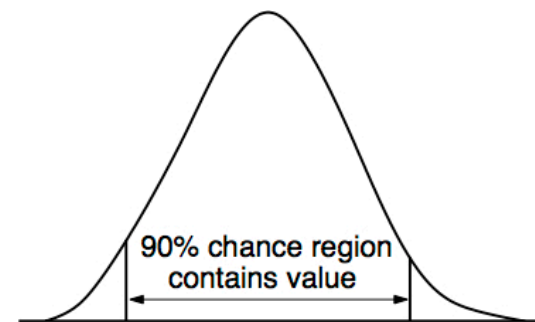
Confidence Interval (Frequentist): A $100 \times (1 - \alpha)\%$ confidence interval for a fixed, unknown parameter q_0 is a random interval $[L_c(\Upsilon), U_c(\Upsilon)]$, having probability at least $1 - \alpha$ of covering q_0 under the joint distribution of Υ .

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:

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

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

Example: Linear regression

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

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

Two Cases:

- (i) New prediction Y_{x_0}
- (ii) Mean response $\mu_{x_0} = \mathbb{E}(Y_{x_0})$

Case (ii) First: Consider the unbiased estimator

$$\hat{Y}_{x_0} = x_0^T \hat{q}$$

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

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

Estimator:

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

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

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

Confidence and Prediction Intervals for Responses

Using Property 7.10 and 7.11, it follows that

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

Confidence Interval:

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

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

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

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

Prediction Intervals for Responses

Prediction Interval:

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

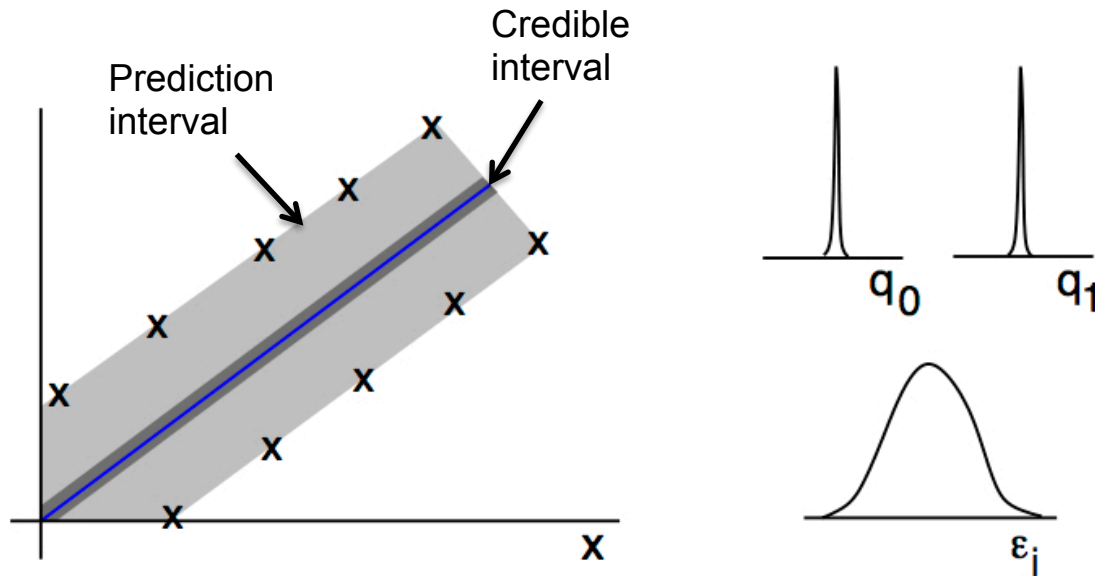
Data: $\Upsilon = [\Upsilon_1, \dots, \Upsilon_n]$ of iid random observations

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 containing Υ_{n+1} under the joint distribution of $(\Upsilon, \Upsilon_{n+1})$.

Credible and Prediction Intervals

Example: Consider linear model

$$Y_i = q_0 + q_1 x_i + \varepsilon_i, \quad i = 1, \dots, n$$



Bayesian Intervals:

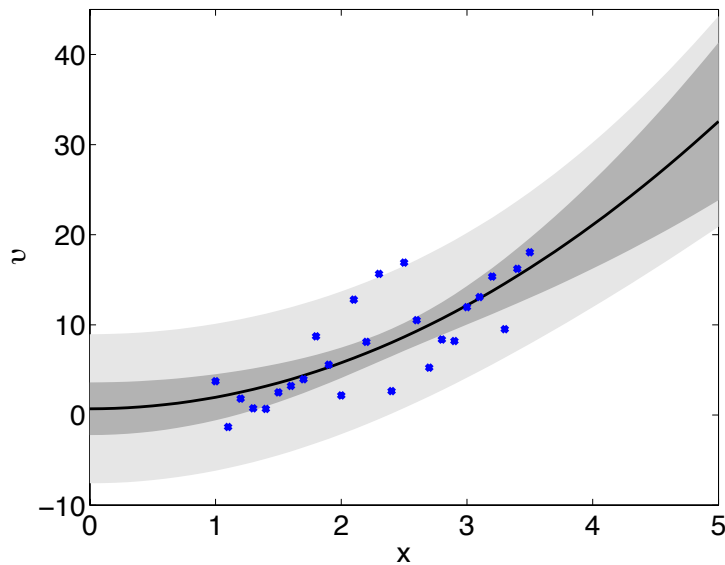
- Credible Intervals: Sample from joint parameter density $\rho_Q(q)$ and propagate through model.
- Prediction Intervals: Sample from $\rho_Q(q)$ and $\rho_\varepsilon(\varepsilon)$ and propagate through model.

Uncertainty Propagation in Models

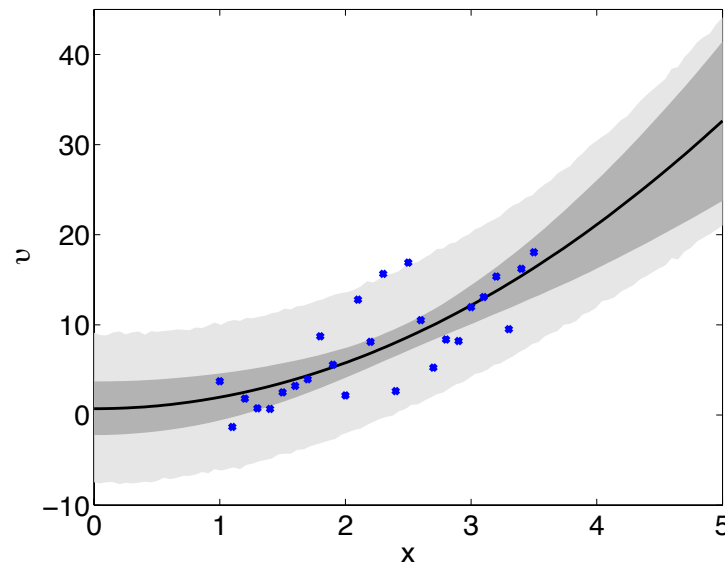
Example: Linear model

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

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

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

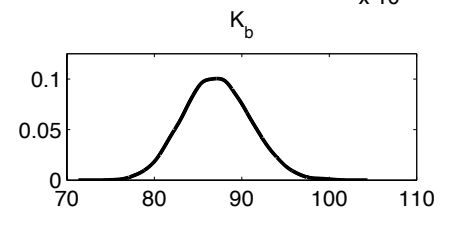
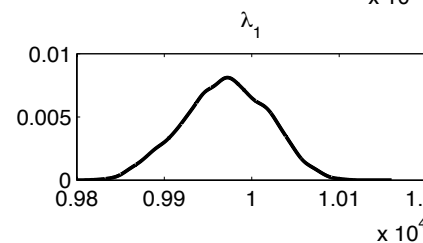
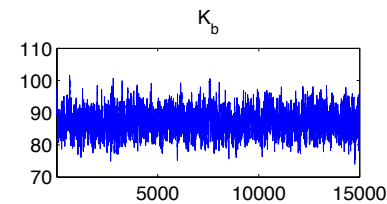
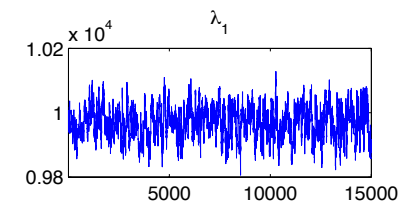
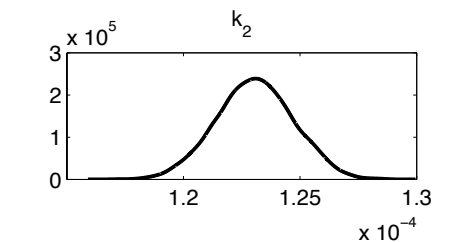
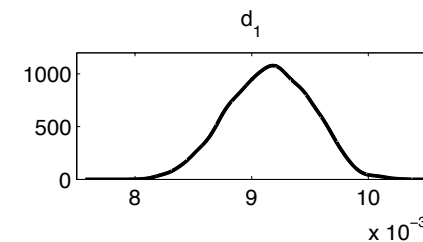
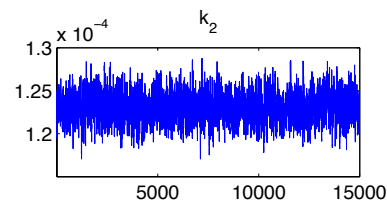
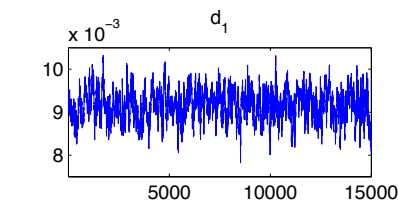
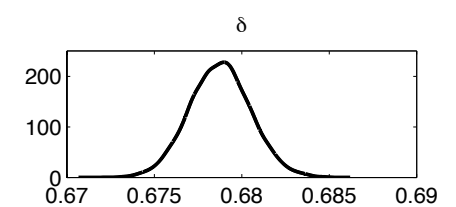
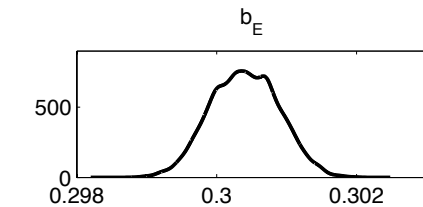
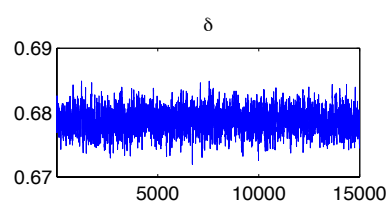
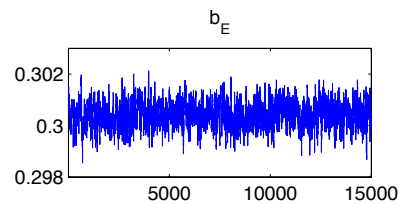
$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1 - f\varepsilon) k_2 V T_2$$

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

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

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

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



Uncertainty Propagation in Models

Example: HIV model

