Introduction to Bayesian Inference and Uncertainty Propagation

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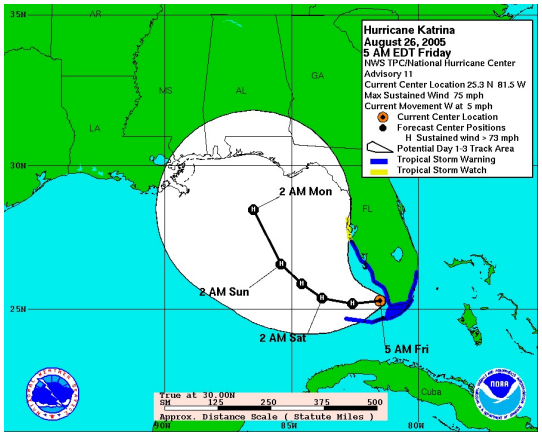
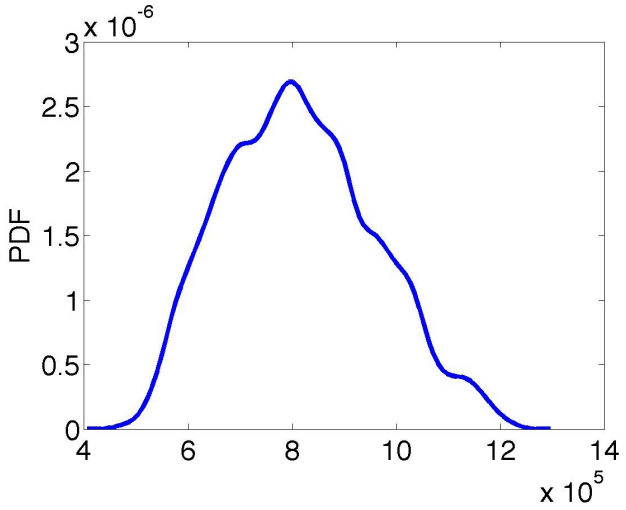
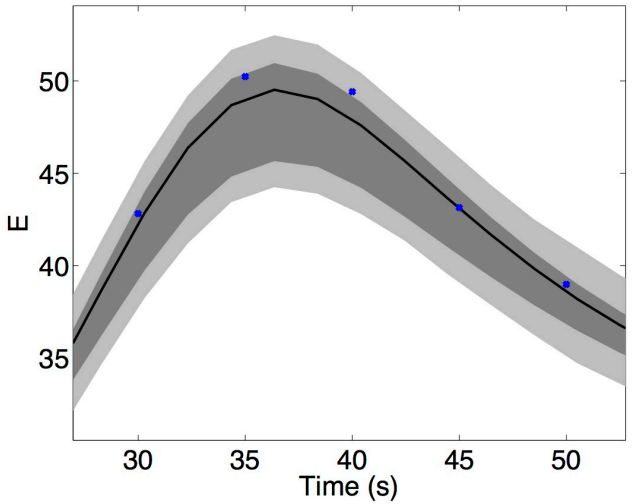






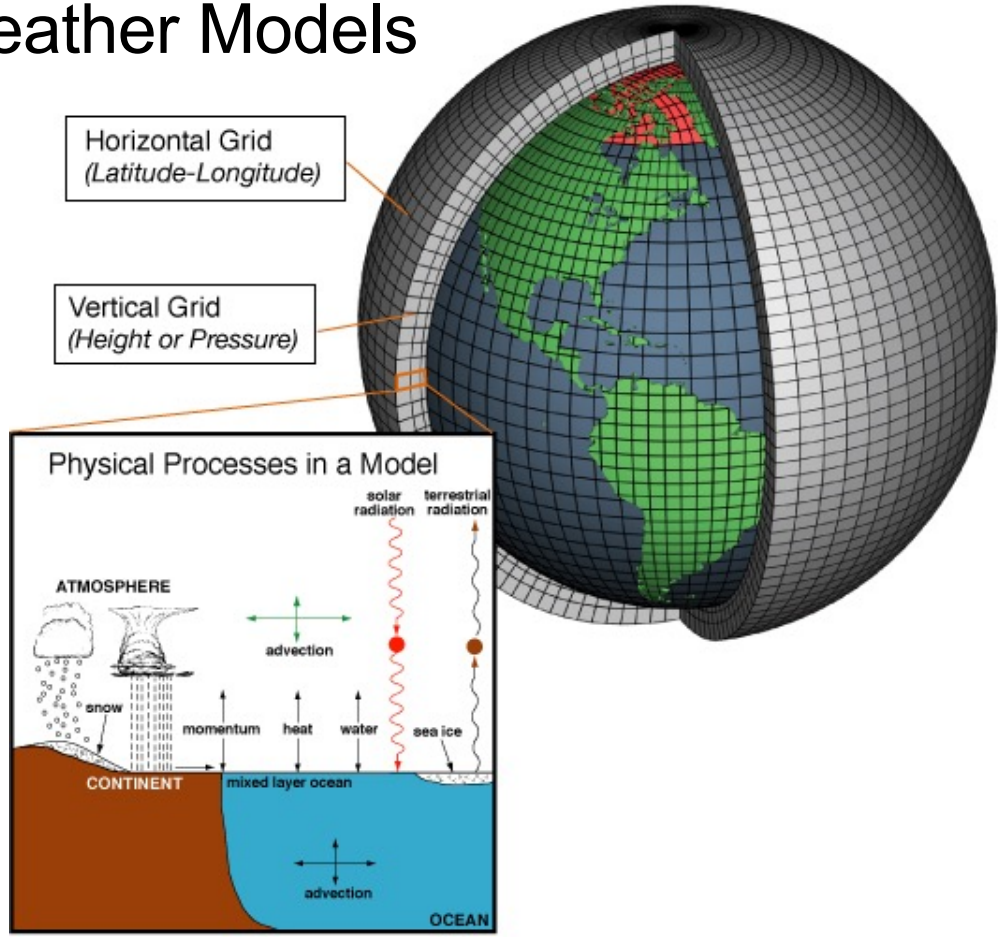
Essentially, all models are wrong, but some are useful, George E.P. Box, Industrial Statistician.

Support: DOE Consortium for Advanced Simulation of LWR (CASL)
NNSA Consortium for Nonproliferation Enabling Capabilities (CNEC)
National Science Foundation (NSF)
Air Force Office of Scientific Research (AFOSR)

Example 1: Weather Models

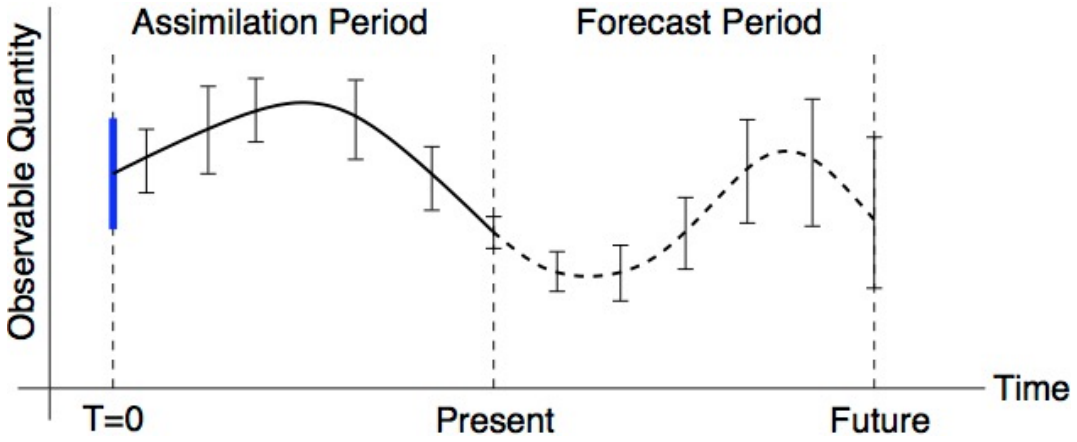
Challenges:

- Coupling between temperature, pressure gradients, precipitation, aerosol, 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:

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

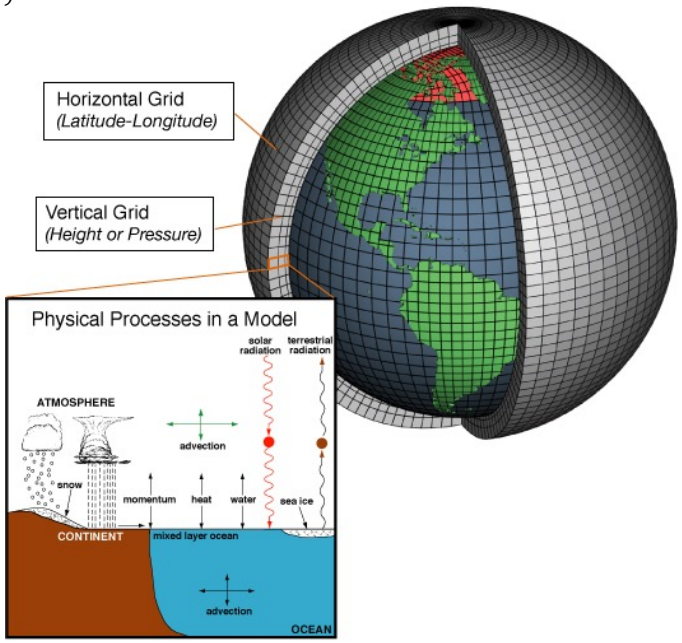
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

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

$$p = \rho RT$$

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.,

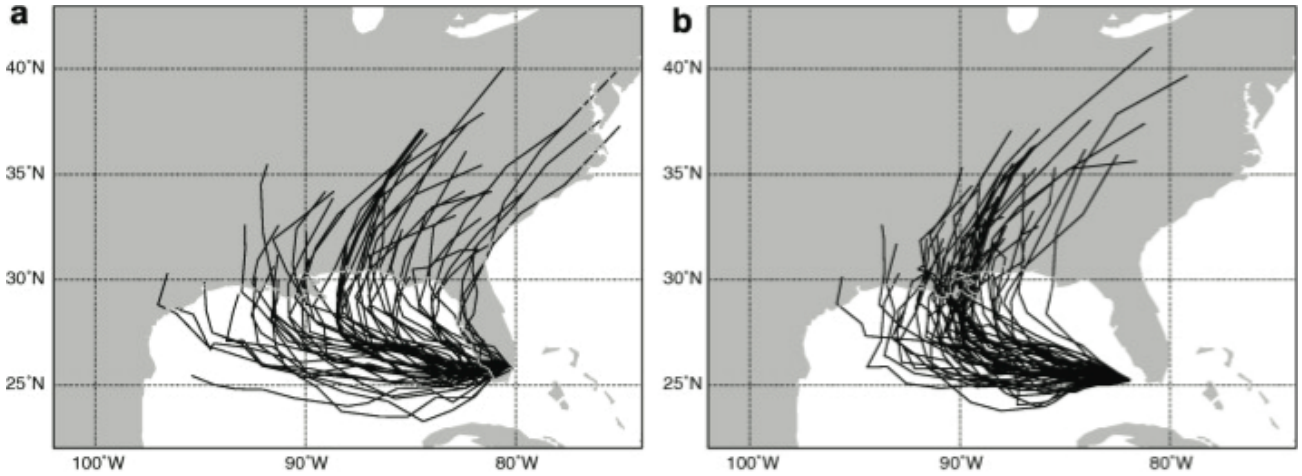
$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

where

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

Ensemble Predictions

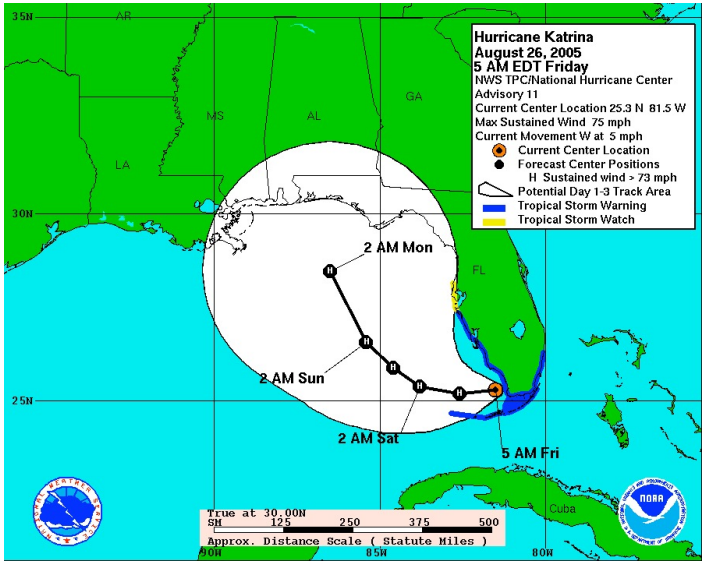
Ensemble Predictions:



00 UTC on August 26, 2005

12 UTC on August 26, 2005

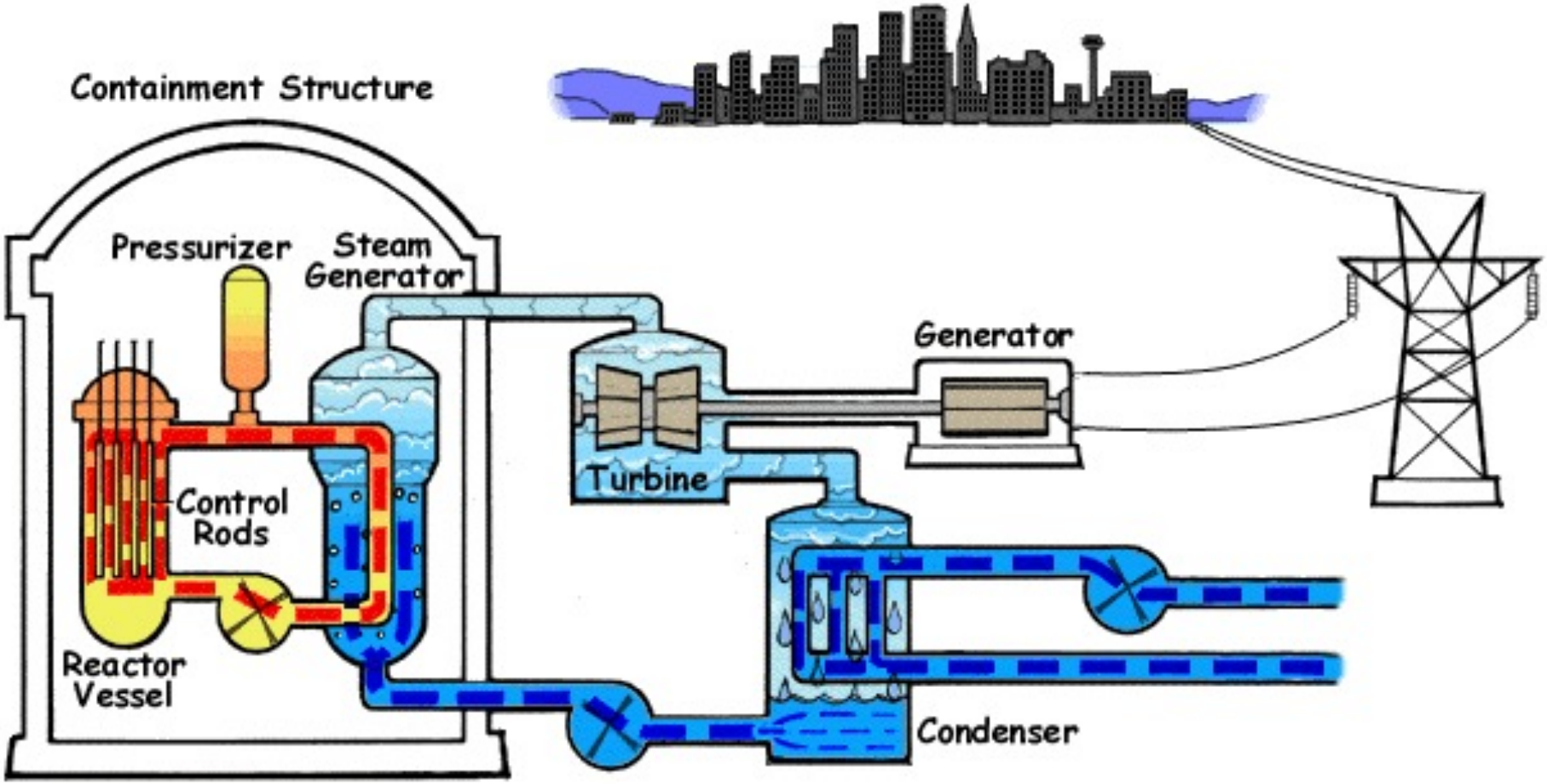
Cone of Uncertainty:



General Questions:

- What is expected rainfall in Research Triangle on July 12?
- What are average high and low temperatures?
- What is predicted average snow fall?
- Note: Quantities are statistical in nature.

Example 2: Pressurized Water Reactors (PWR)



Models:

- Involve neutron transport, thermal-hydraulics, chemistry, fuels
- Inherently multi-scale, multi-physics -- Must be incorporated in surrogate models

Objective: Develop Virtual Environment for Reactor Applications (VERA)

Example: Pressurized Water Reactors (PWR)

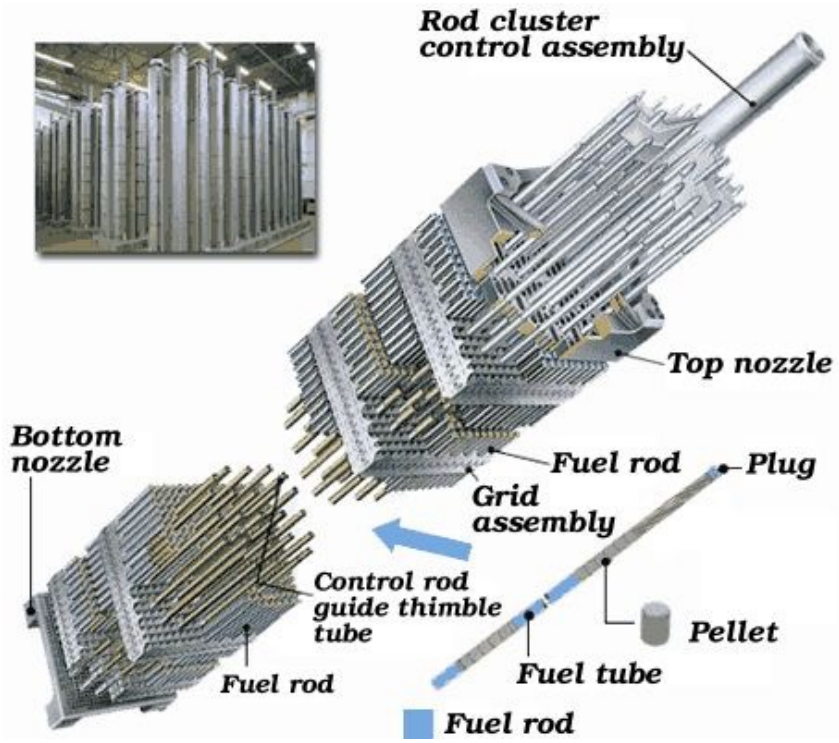
Challenges:

• Models linear in the state but function of 7 independent variables:

$$r = x, y, z; E; \Omega = \theta, \phi; t$$

• Very large number of inputs or parameters; e.g., 100,000. Parameter selection critical.

• Codes can take hours to days to run.



Example: Shearon Harris outside Raleigh

UQ Questions:

• What is peak operating temperature?

• What is expected level of CRUD buildup?

• What is associated risk?

• What is expected profit for new design?

Example 3: HIV Model for Characterization and Control Regimes

HIV Model:

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

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

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

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

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

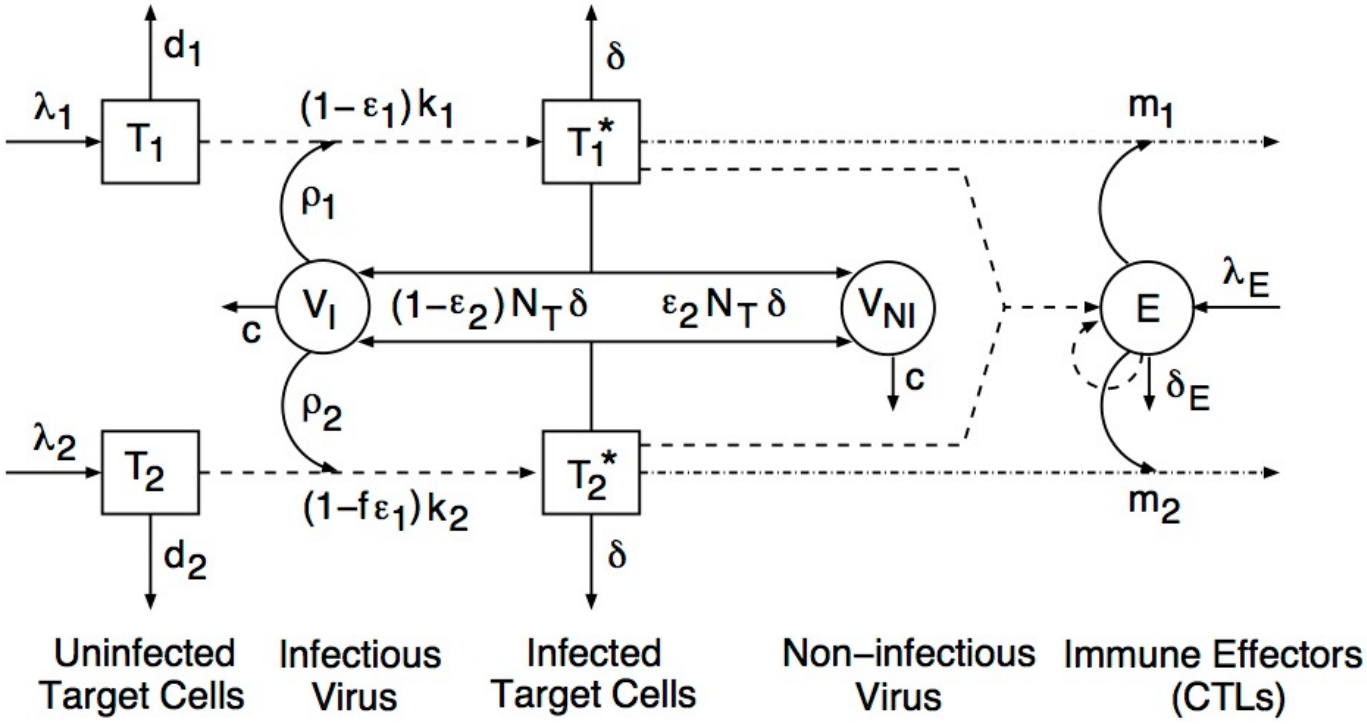
$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E$$

Notes: 21 parameters

[Adams, Banks et al., 2005, 2007]

Notation: $\dot{E} \equiv \frac{dE}{dt}$

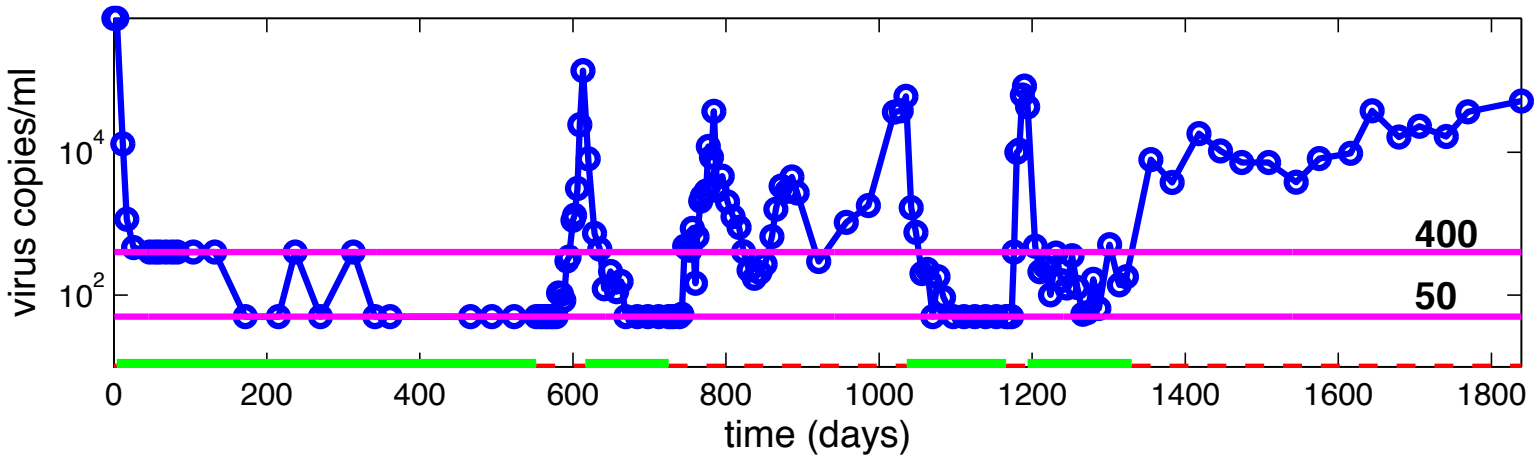
Compartments:



Example: HIV Model for Characterization and Treatment Regimes

HIV Model: Several sources of uncertainty including viral measurement techniques

Example: Upper and lower limits to assay sensitivity



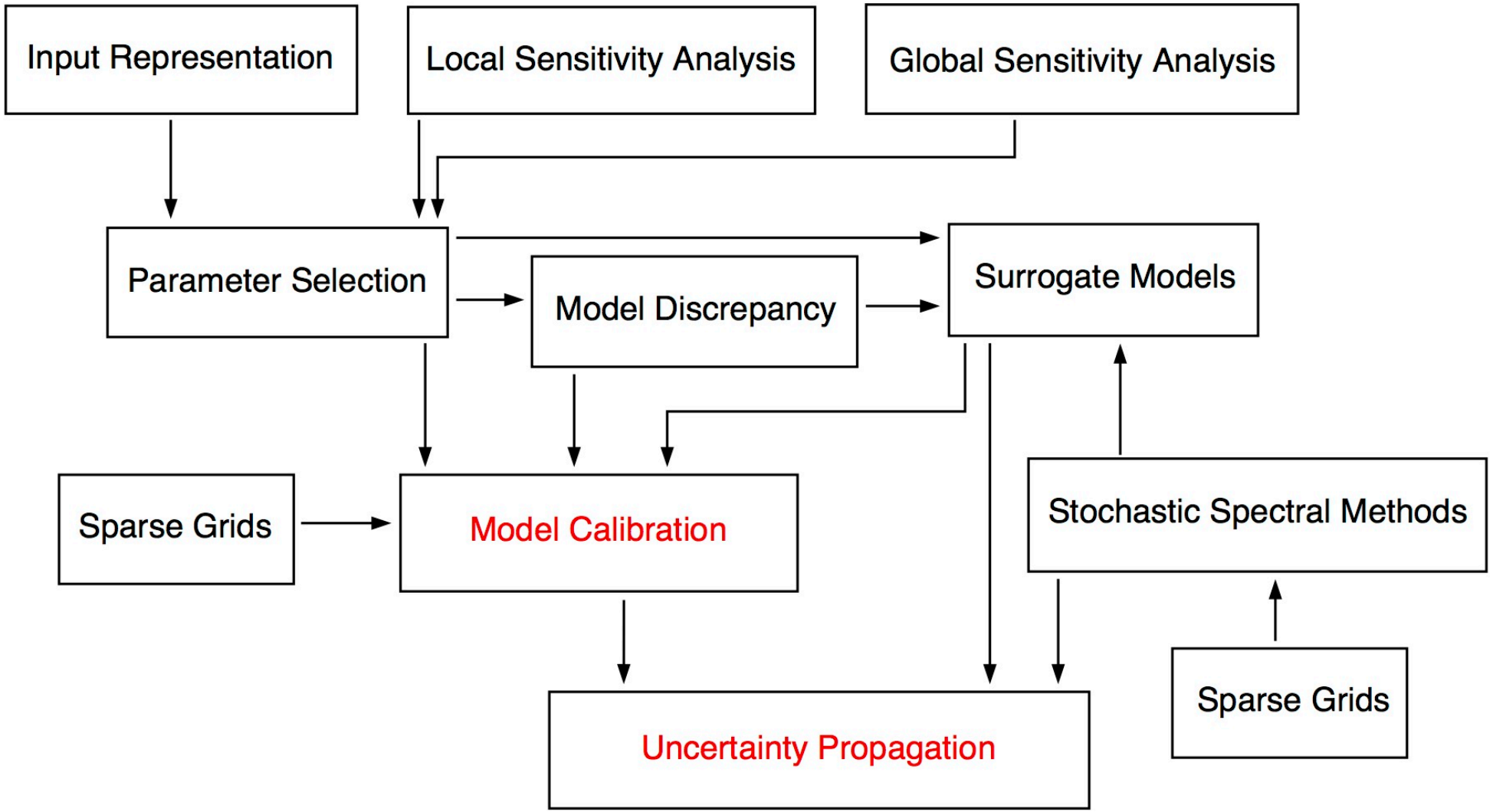
UQ Questions:

- What are the uncertainties in parameters that cannot be directly measured?
- What is optimal treatment regime that is "safe" for patient?
- What is expected viral load? Issue: very often requires high-dimensional integration!
- e.g., $\mathbb{E}[V(t)] = \int_{\mathbb{R}^{21}} V(t,q)\rho(q)dq$

Experimental results are believed by everyone, except for the person who ran the experiment, source anonymous, quoted by Max Gunzburger, Florida State University.

Steps in Uncertainty Quantification

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



Model Calibration and Uncertainty Propagation

Sources of Uncertainty:

- Model
- Parameters
- Sensor measurements
- Initial conditions

Strategy:

- Quantify uncertainty in parameters
- Propagate uncertainty through model

Example: HIV model

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

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

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

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

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

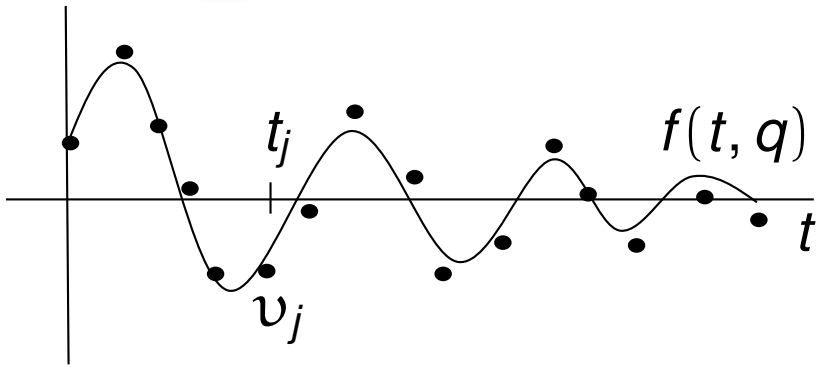
$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E$$

Parameters: Reduced set

$$q = [b_E, \delta, d_1, k_2, \lambda_1, K_b]$$

Point Estimates: Ordinary least squares

$$q^0 = \arg\min_q \frac{1}{2} \sum_{j=1}^{N} [\upsilon_j - f(t_j, q)]^2$$



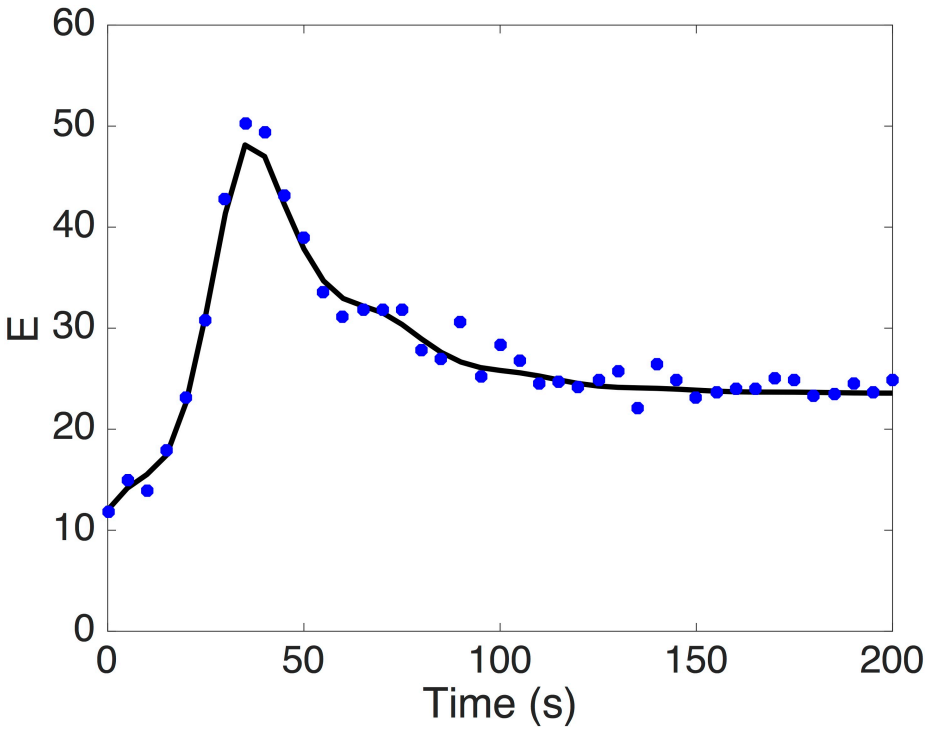
Note: Scaling critical since parameter values vary by 8 orders of magnitude.

Model Calibration and Predictions

Optimization Results:

b_E	δ	d_1	k_2	λ_1	K_b
0.30	0.68	9.1×10^{-3}	1.22×10^{-4}	9.95×10^{3}	88.5

Data and Prediction of Immune Effector Response E:



Note: Point estimates but no quantification of uncertainty in:

- Model
- Parameters
- Data

Goals:

- Replace point estimates with distributions.
- Construct credible and prediction intervals.
- Natural in a Bayesian framework

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.
- Parameter Estimation:
  - Relies on estimators derived from different data sets and a specific sampling distribution.
  - Parameters may be unknown but are fixed and deterministic.

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

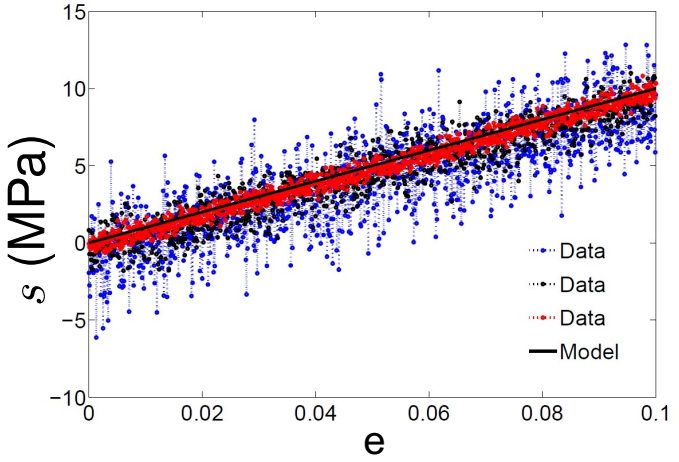
- Parameter Estimation: Parameters are considered to be random variables having associated densities.

Bayesian Inference: Motivation

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

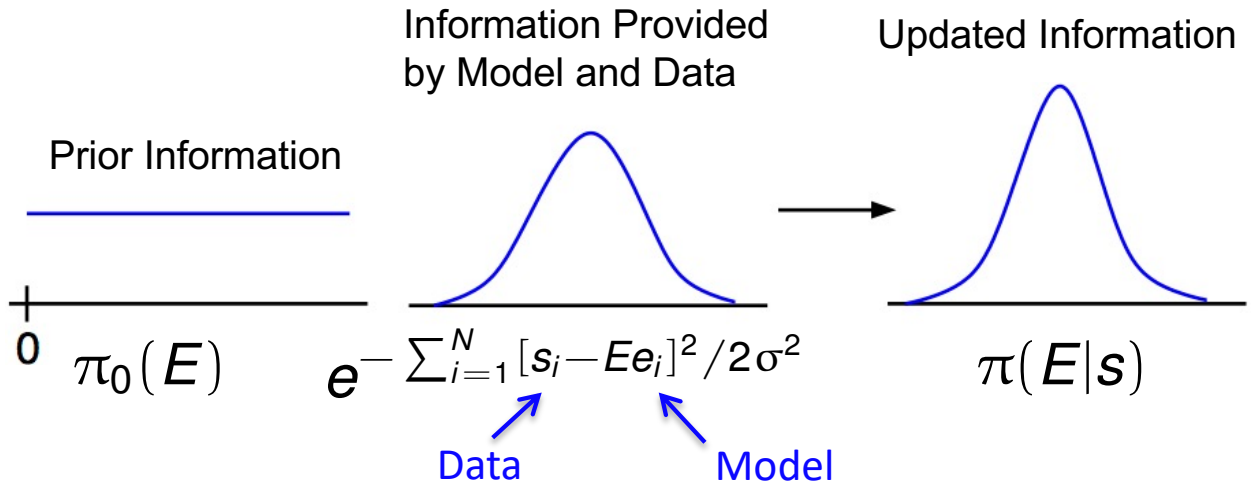
$$s_i = Ee_i + \varepsilon_i \ , \ i = 1, \ldots, N$$

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



Parameter: Stiffness E

Strategy: Use model fit to data to update prior information

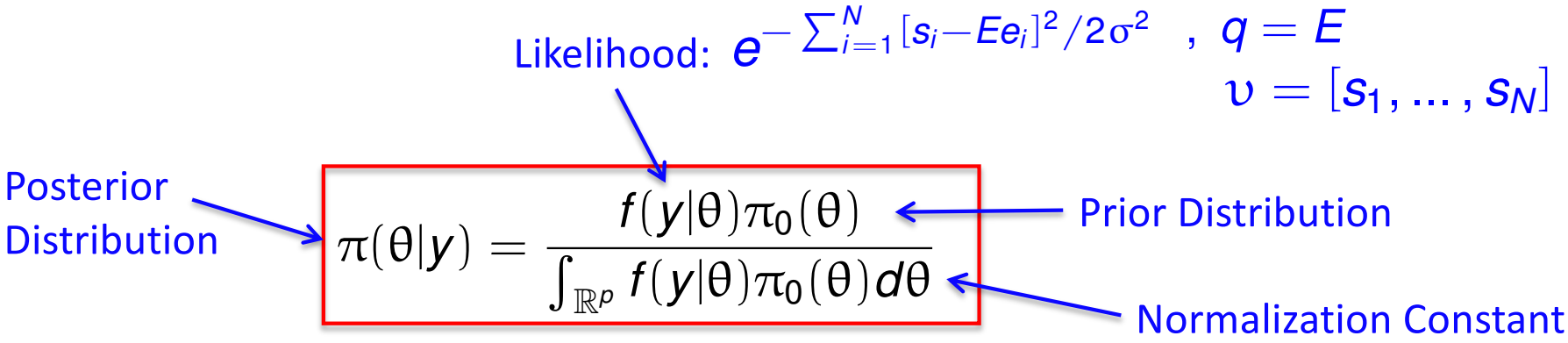


Non-normalized Bayes' Relation:

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

Bayesian Inference

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



- 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., Many applications: p = 10-50!
- 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.

Parameter Estimation Problem

Observation Model:

$$y_i = f_i(\theta) + \varepsilon_i \ , \ i = 1, \ldots, n$$

Assumption: Assume that measurement errors are iid and $\varepsilon_i \sim N(0, \sigma^2)$

Likelihood:

$$f(y|\theta) = L(\theta, \sigma|y) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_\theta/2\sigma^2}$$

where

$$SS_\theta = \sum_{j=1}^{n} [y_j - f_i(\theta)]^2$$

is the sum of squares error.

Parameter Estimation: Example

Example: Consider the spring model

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

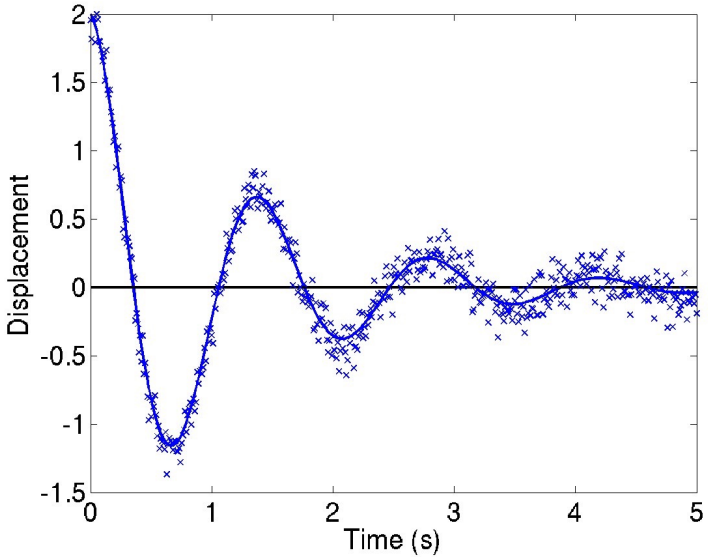
$$z(0) = 2\,,\ \dot{z}(0) = -C$$

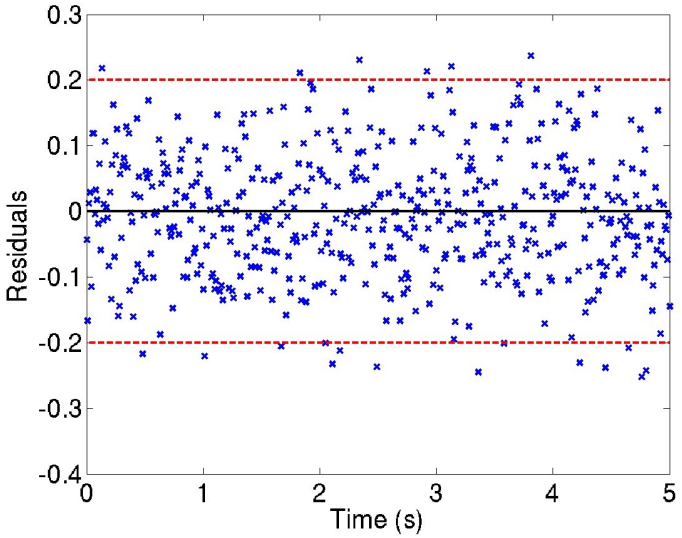
which has the solution

$$z(t) = 2e^{-Ct/2}\cos(\sqrt{K - C^2/4}\cdot t)$$

Note: Take $K = 20.5$, $C^0 = 1.5$

Take K to be known and $\theta = C$. Assume that $\varepsilon_i \sim N(0, \sigma_0^2)$ where $\sigma_0 = 0.1$





Parameter Estimation: Example

Example: The sensitivity matrix is

$$\mathcal{X}(\theta) = \left[\frac{\partial y}{\partial C}(t_1, \theta), \cdots, \frac{\partial y}{\partial C}(t_n, \theta)\right]^T$$

where

$$\frac{\partial y}{\partial C} = e^{-Ct/2}\left[\frac{Ct}{\sqrt{4K - C^2}}\sin\left(\sqrt{K - C^2/4}\cdot t\right) - t\cos\left(\sqrt{K - C^2/4}\cdot t\right)\right]$$

Here

$$V = \sigma_c^2 = \sigma_0^2\left[\mathcal{X}^T(\theta)\mathcal{X}(\theta)\right]^{-1} = 3.35 \times 10^{-4}$$

so that

$$\widehat{C} \sim N\left(C_0, \sigma_c^2\right)\ ,\ \sigma_c = 0.0183$$

Note: In 10,000 simulations, 9455 of confidence intervals contained true parameter value.

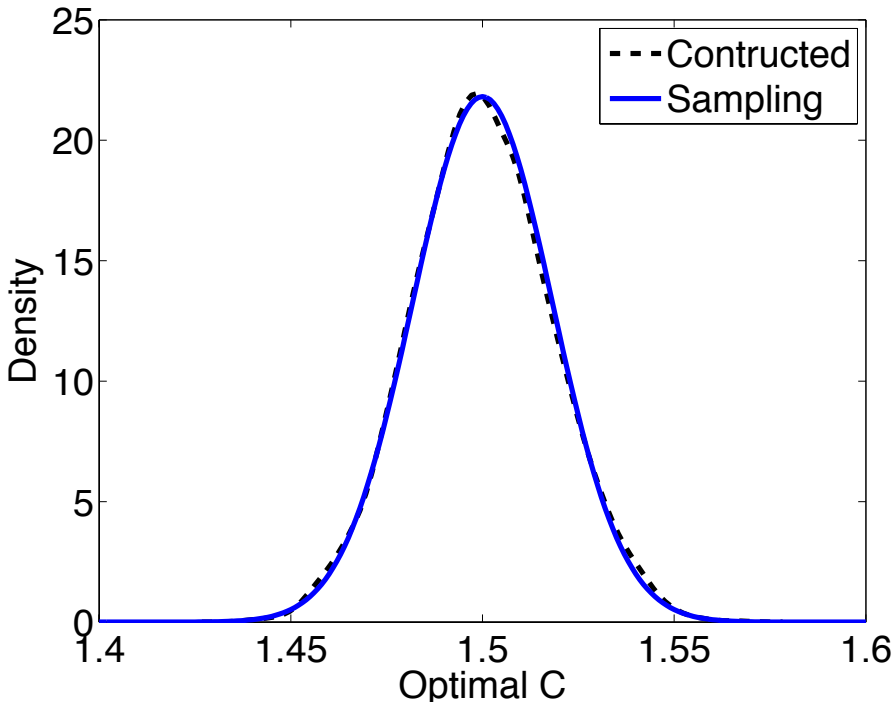


Figure: Sampling distribution compared with that constructed using 10,000 estimated values of C.

Parameter Estimation: Example

Bayesian Inference: Employ the flat prior

$$\pi_0(\theta) = \chi_{[0,\infty)}(\theta)$$

Posterior Distribution:

$$\pi(\theta|y) = \frac{e^{-SS_\theta/2\sigma_0^2}}{\int_0^\infty e^{-SS_\zeta/2\sigma_0^2} d\zeta} = \frac{1}{\int_0^\infty e^{-(SS_\zeta - SS_\theta)/2\sigma_0^2} d\zeta}$$

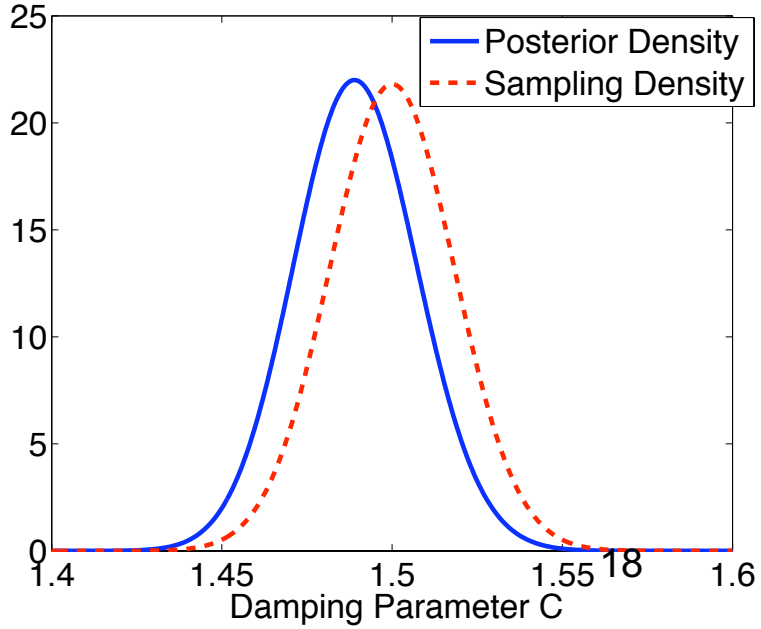
Issue: $e^{-SS_{\theta\,MAP}} \approx 3 \times 10^{-113}$

Midpoint formula:

$$\pi(\theta|y) \approx \frac{1}{\sum_{i=1}^{k} e^{-(SS_{\zeta_i} - SS_\theta)/2\sigma_0^2} w_i}$$

Note:

- Slow even for one parameter.
- Strategy: create Markov chain using random sampling so that created chain has the posterior distribution as its limiting (stationary) distribution.



Markov Chain Monte Carlo Methods

General Strategy:

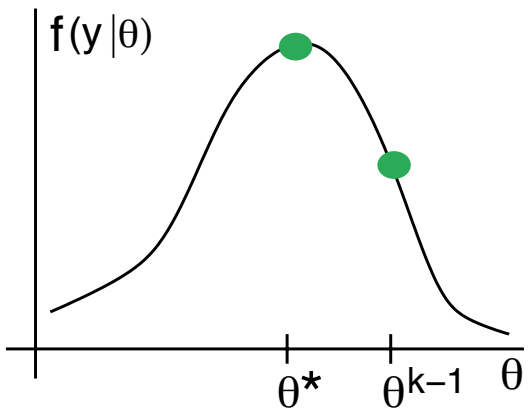
- Current value: $X_{k-1} = \theta^{k-1}$
- Propose candidate $\theta^* \sim J(\theta^*|\theta^{k-1})$ from proposal (jumping) distribution
- With probability $\alpha(\theta^*, \theta^{k-1})$, accept θ^*; i.e., $X_k = \theta^*$
- Otherwise, stay where you are: $X_k = \theta^{k-1}$

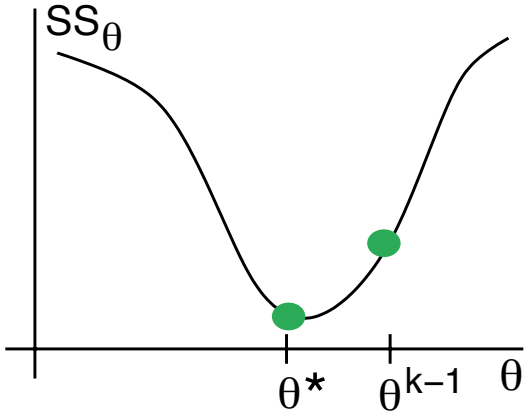
Intuition: Recall that

$$\pi(\theta|y) = \frac{f(y|\theta)\pi_0(\theta)}{\int_{\mathbb{R}^p} f(y|\theta)\pi_0(\theta)d\theta}$$

where

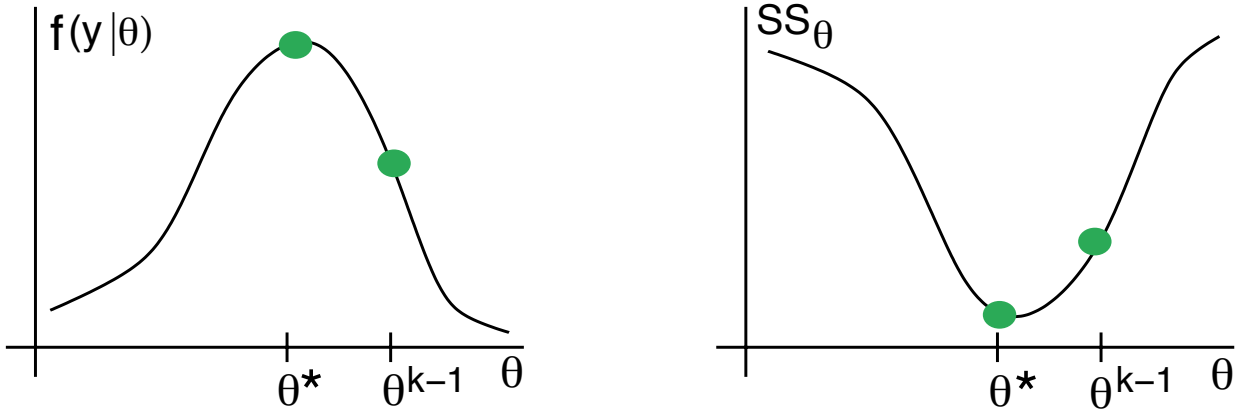
$$f(y|\theta) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\sum_{i=1}^{n}[y_i - f_i(\theta)]^2/2\sigma^2} = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_\theta/2\sigma^2}$$





Markov Chain Monte Carlo Methods

Intuition:

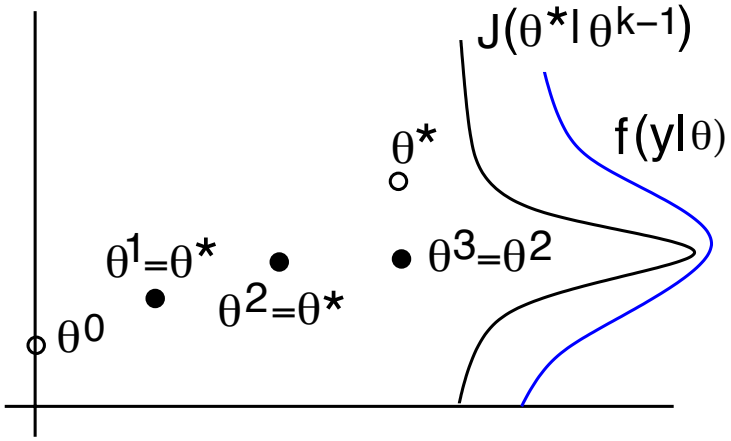


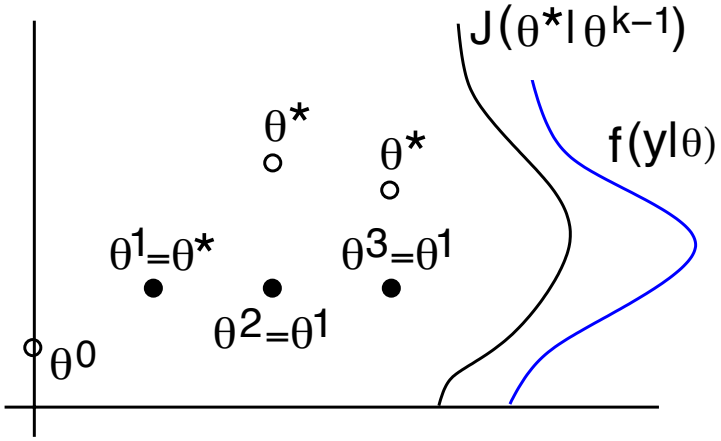
- Consider $r(\theta^*|\theta^{k-1}) = \frac{\pi(\theta^*|y)}{\pi(\theta^{k-1}|y)} = \frac{f(y|\theta^*)\pi_0(\theta^*)}{f(y|\theta^{k-1})\pi_0(\theta^{k-1})}$
  - If $r < 1 \Rightarrow \ f(y|\theta^*) < f(y|\theta^{k-1})$, accept with probability $\alpha = r$
  - If $r > 1$, accept with probability $\alpha = 1$

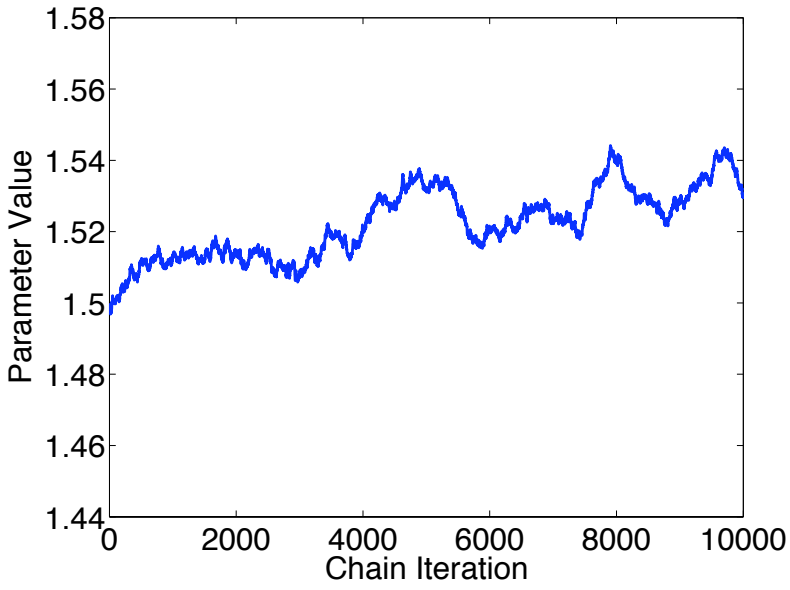
Note: Narrower proposal distribution yields higher probability of acceptance.

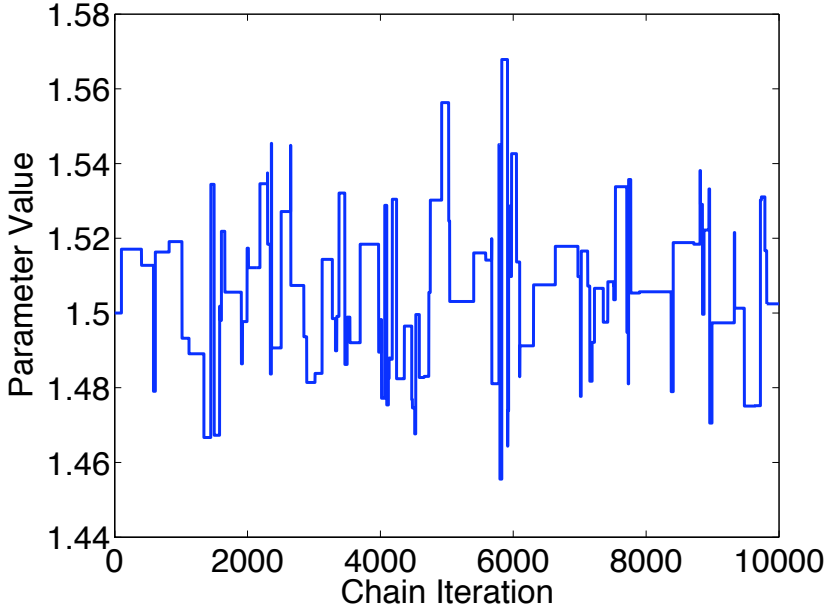
Markov Chain Monte Carlo Methods

Note: Narrower proposal distribution yields higher probability of acceptance.









Proposal Distribution

Proposal Distribution: Two basic approaches

- Choose a fixed proposal function
  - o Independent Metropolis
- Random walk (local Metropolis)

$$\theta^* = \theta^{k-1} + Rz$$

o Two (of several) choices: $Z \sim N(0, 1)$

(i) $R = cI \Rightarrow \theta^* \sim N(\theta^{k-1}, cI)$

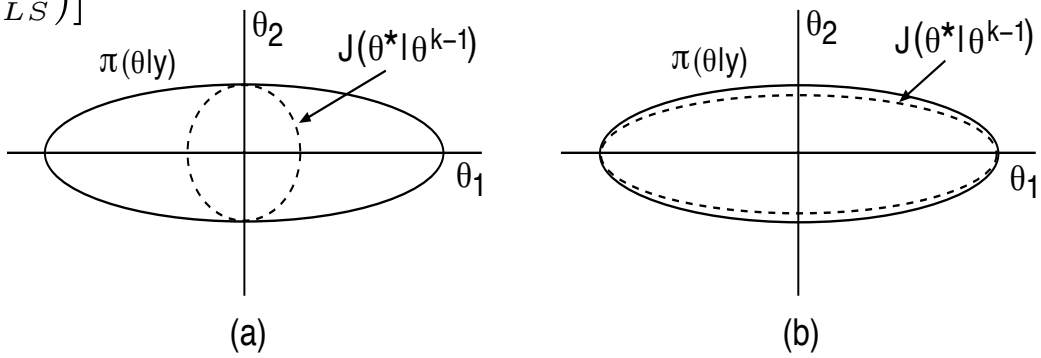
(ii) $R = \text{chol}(V) \Rightarrow \theta^* \sim N(\theta^{k-1}, V)$

where

Sensitivity Matrix

$$V = \sigma^2_{OLS} \left[\mathcal{X}^T(\theta_{OLS})\mathcal{X}(\theta_{OLS})\right]^{-1}$$

$$\sigma^2_{OLS} = \frac{1}{n-p}\sum_{i=1}^{n}\left[y_i - f_i(\theta_{OLS})\right]^2$$



Metropolis Algorithm

Metropolis Algorithm: [Metropolis and Ulam, 1949]

1. Initialization: Choose an initial parameter value θ^0 that satisfies $\pi(\theta^0|y) > 0$.
2. For $k = 1, \cdots, M$

   (a) For $z \sim N(0, 1)$, construct the candidate

   $$\theta^* = \theta^{k-1} + Rz$$

   where R is the Cholesky decomposition of V or D. This ensures that

   $$\theta^* \sim N(\theta^{k-1}, V) \text{ or } \theta^* \sim N(\theta^{k-1}, D).$$

   (b) Compute the ratio

   $$r(\theta^*|\theta^{k-1}) = \frac{\pi(\theta^*|y)}{\pi(\theta^{k-1}|y)} = \frac{\pi(y|\theta^*)\pi_0(\theta^*)}{\pi(y|\theta^{k-1})\pi_0(\theta^{k-1})}.$$

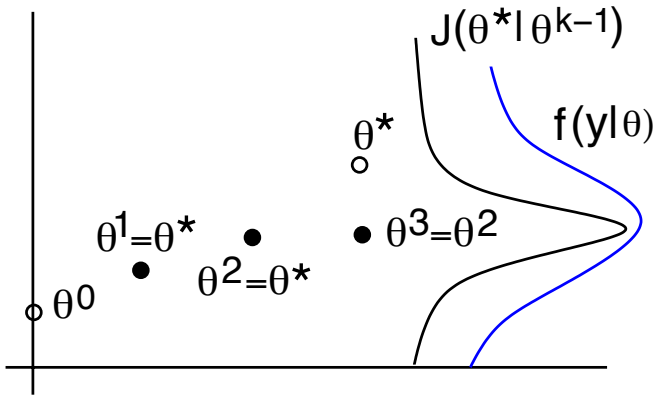
   (c) Set

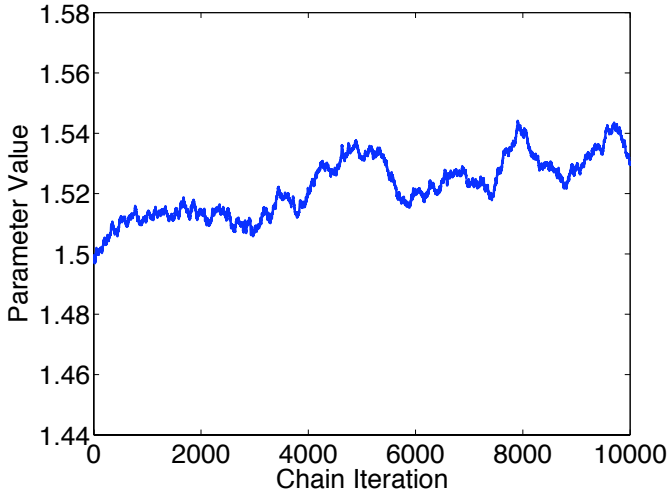
   $$\theta^k = \begin{cases} \theta^* & , \text{ with probability } \alpha = \min(1, r) \\ \theta^{k-1} & , \text{ else.} \end{cases}$$

   That is, we accept θ^* with probability 1 if $r \geqslant 1$ and we accept it with probability r if $r < 1$.

Random Walk Metropolis Algorithm for Parameter Estimation

1. Set number of chain elements M and design parameters n_s, σ_s
2. Determine $\theta^0 = \arg\min_\theta \sum_{i=1}^{N} [y_i - f_i(\theta)]^2$
3. Set $SS_{\theta^0} = \sum_{i=1}^{N} [y_i - f_i(\theta^0)]^2$
4. Compute initial variance estimate: $s_0^2 = \frac{SS_{\theta^0}}{n-p}$
5. Construct covariance estimate $V = s_0^2 [\mathcal{X}^T(\theta^0)\mathcal{X}(\theta^0)]^{-1}$ and $R = \text{chol}(V)$
6. For $k = 1, \cdots, M$
   - (a) Sample $z_k \sim N(0, 1)$
   - (b) Construct candidate $\theta^* = \theta^{k-1} + Rz_k$
   - (c) Sample $u_\alpha \sim \mathcal{U}(0, 1)$
   - (d) Compute $SS_{\theta^*} = \sum_{i=1}^{N} [y_i - f_i(\theta^*)]^2$
   - (e) Compute
     $$\alpha(\theta^* | \theta^{k-1}) = \min\left(1, e^{-[SS_{\theta^*} - SS_{\theta^{k-1}}]/2s_{k-1}^2}\right)$$
   - (f) If $u_\alpha < \alpha$,
     Set $\theta^k = \theta^*$, $SS_{\theta^k} = SS_{\theta^*}$
     else
     Set $\theta^k = \theta^{k-1}$, $SS_{\theta^k} = SS_{\theta^{k-1}}$
     endif
   - (g) Update $s_k \sim \text{Inv-gamma}(a_{val}, b_{val})$ where
     $$a_{val} = 0.5(n_s + n) \ , \ b_{val} = 0.5(n_s \sigma_s^2 + SS_{\theta^k})$$





Random Walk Metropolis

Example: We revisit the spring model

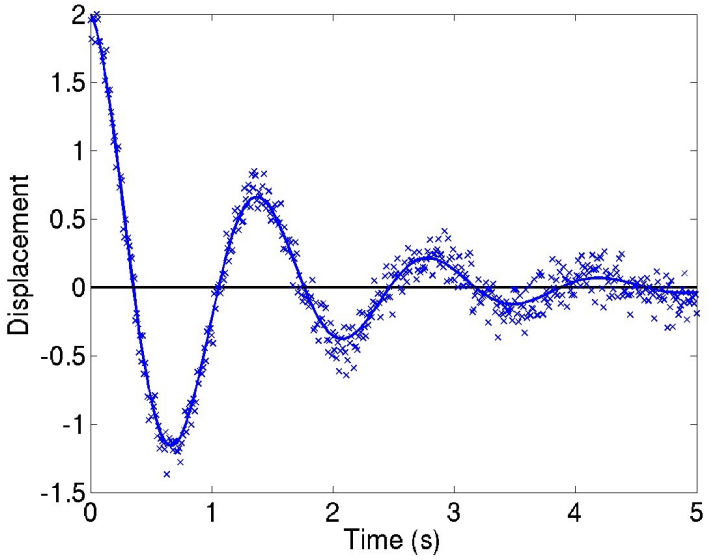
$$\ddot{z} + C\dot{z} + Kz = 0$$

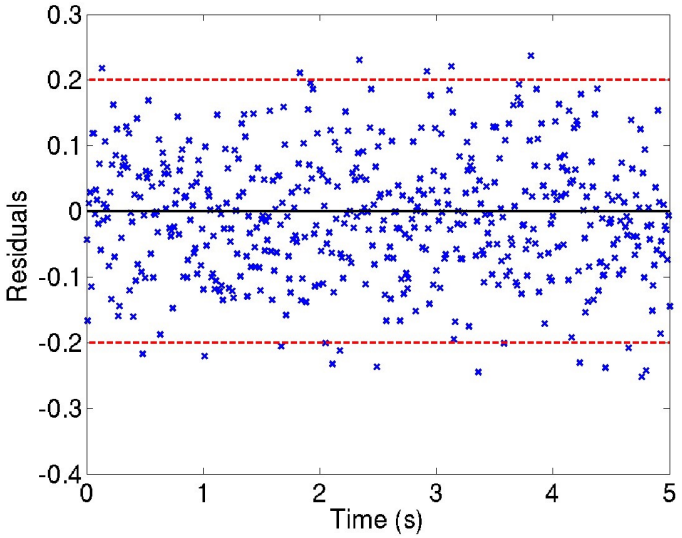
$$z(0) = 2\,,\ \dot{z}(0) = -C$$

which has the solution

$$z(t) = 2e^{-Ct/2}\cos(\sqrt{K - C^2/4}\cdot t)$$

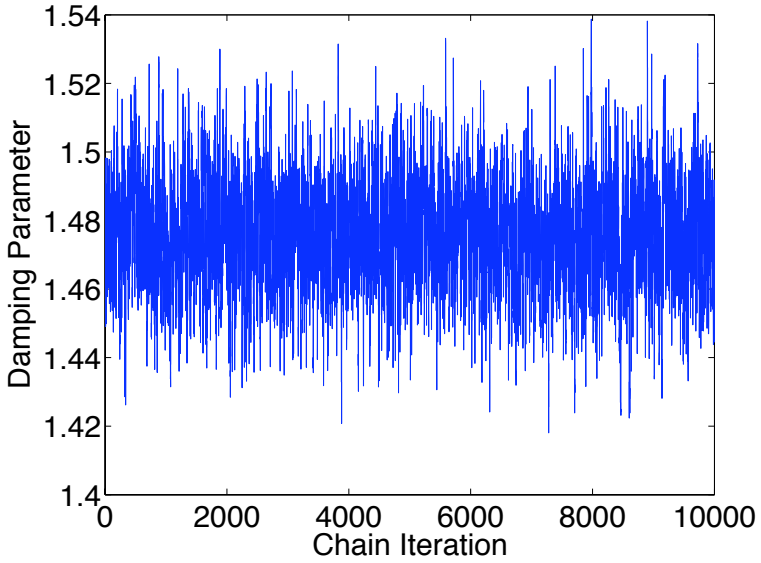
We assume that $\varepsilon_i \sim N(0, \sigma_0^2)$ where $\sigma_0 = 0.1$.

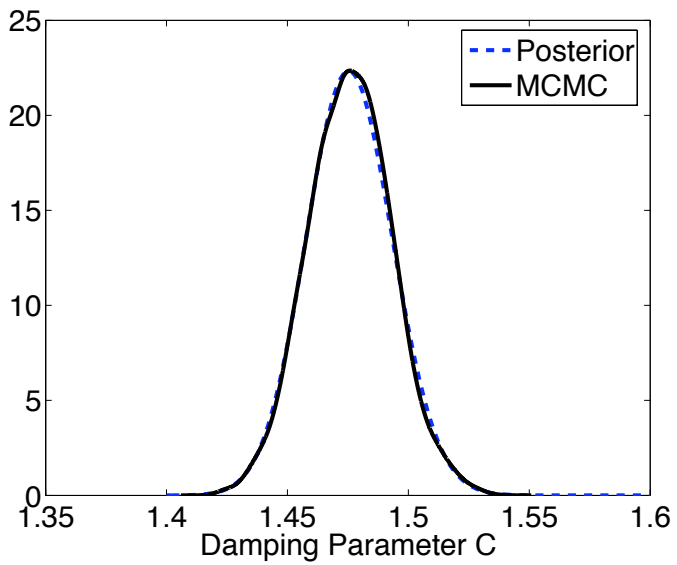




Random Walk Metropolis

Case i: Take K =20.5 and $\theta = [C, \sigma^2]$





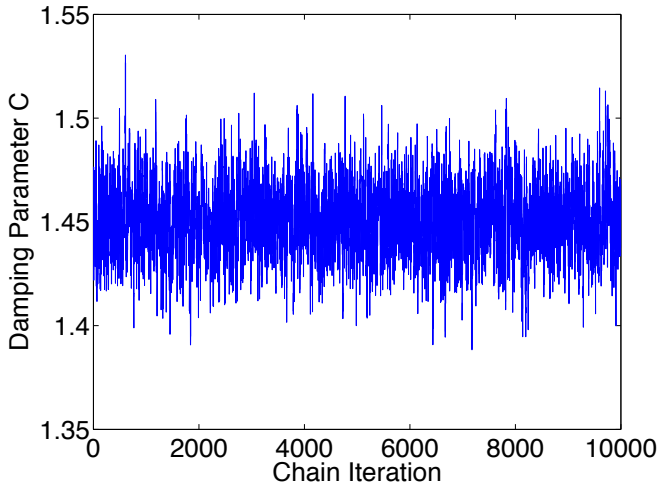
Note: Kernel density estimator (KDE) used to construct density.

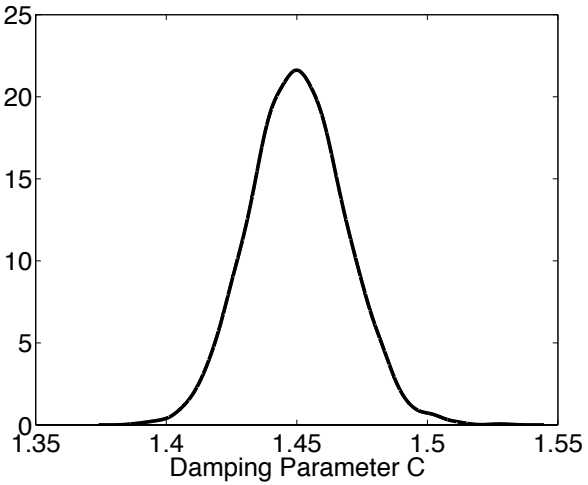
Posted MATLAB Code: spring_mcmc_C.m

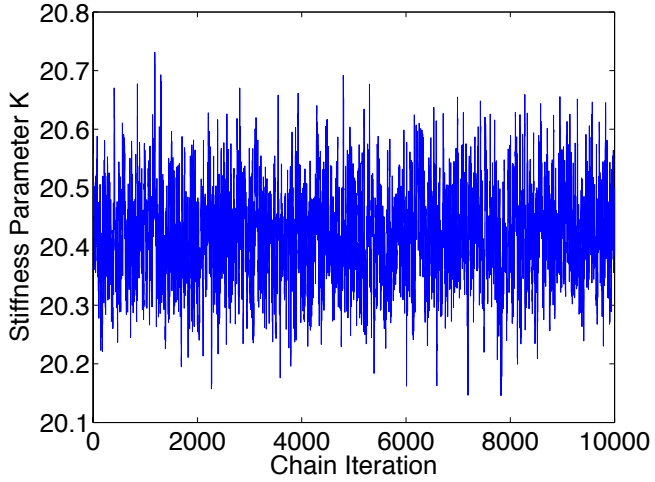
Random Walk Metropolis

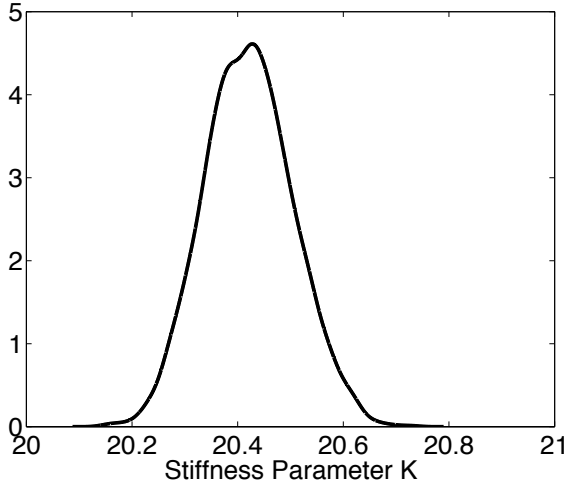
Case ii: Take $\theta = [C, K, \sigma^2]$ with $J(\theta^*|\theta^{k-1}) = N(\theta^{k-1}, V)$ and

$$V = \begin{bmatrix} 0.000345 & 0.000268 \\ 0.000268 & 0.007071 \end{bmatrix}$$









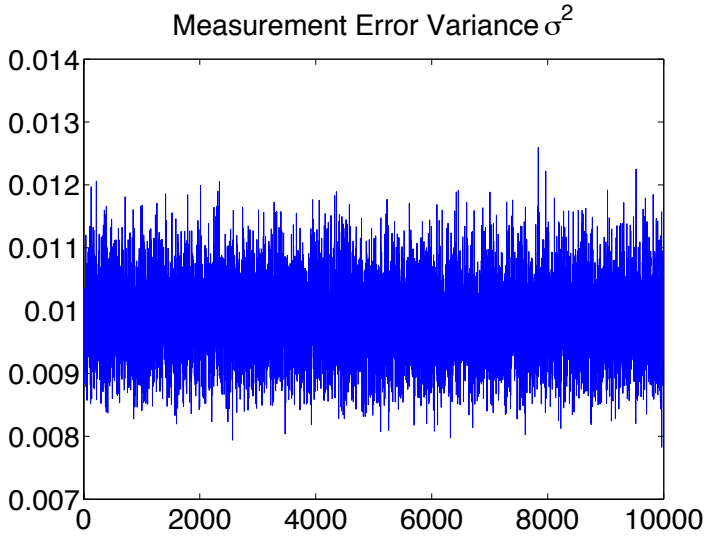
Note:

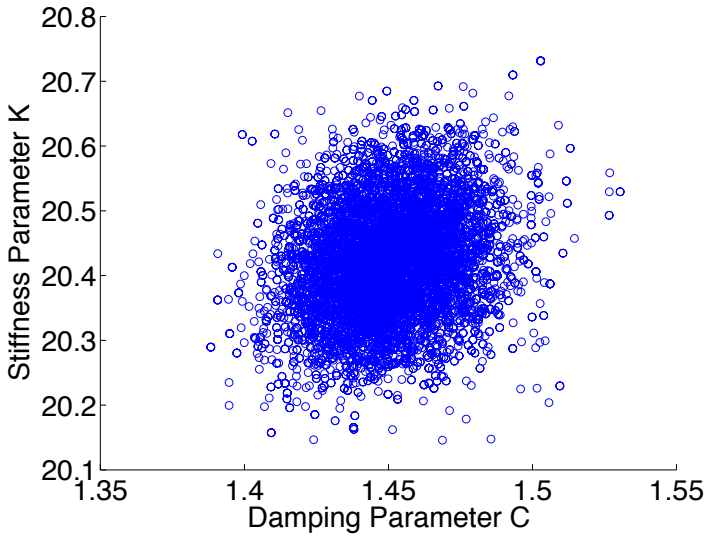
$$2\sigma_C \approx 0.04$$
$$\Rightarrow \sigma_C^2 \approx 0.4 \times 10^{-3}$$

$$2\sigma_K \approx 0.18$$
$$\Rightarrow \sigma_K^2 \approx 0.0081$$

Random Walk Metropolis

Case ii: Measurement error variance and joint samples





Posted MATLAB Code: spring_mcmc_C_K_sigma.m

Delayed Rejection Adaptive Metropolis (DRAM)

Example: HIV model

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

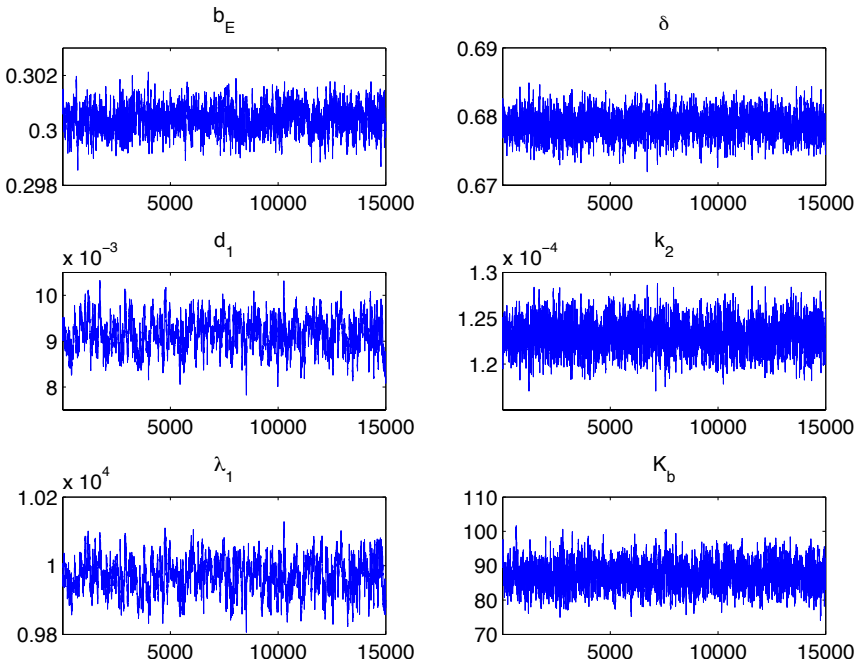
$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

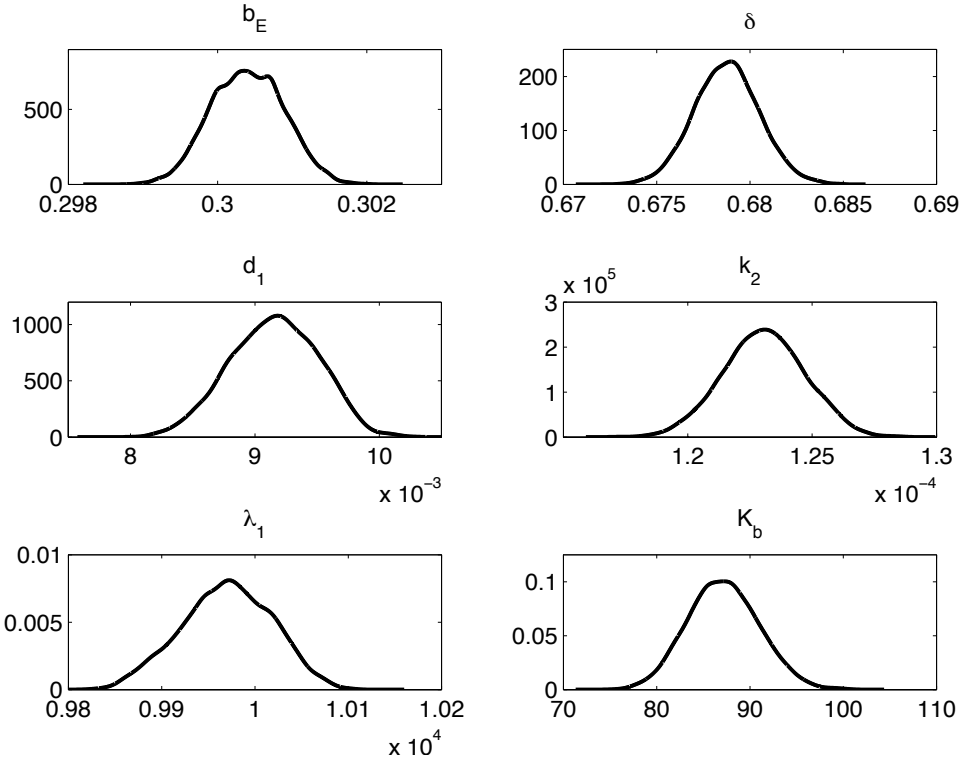
$$\dot{T}_1^* = (1-\varepsilon) k_1 V T_1 - \delta T_1^* - m_1 E T_1^*$$

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

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

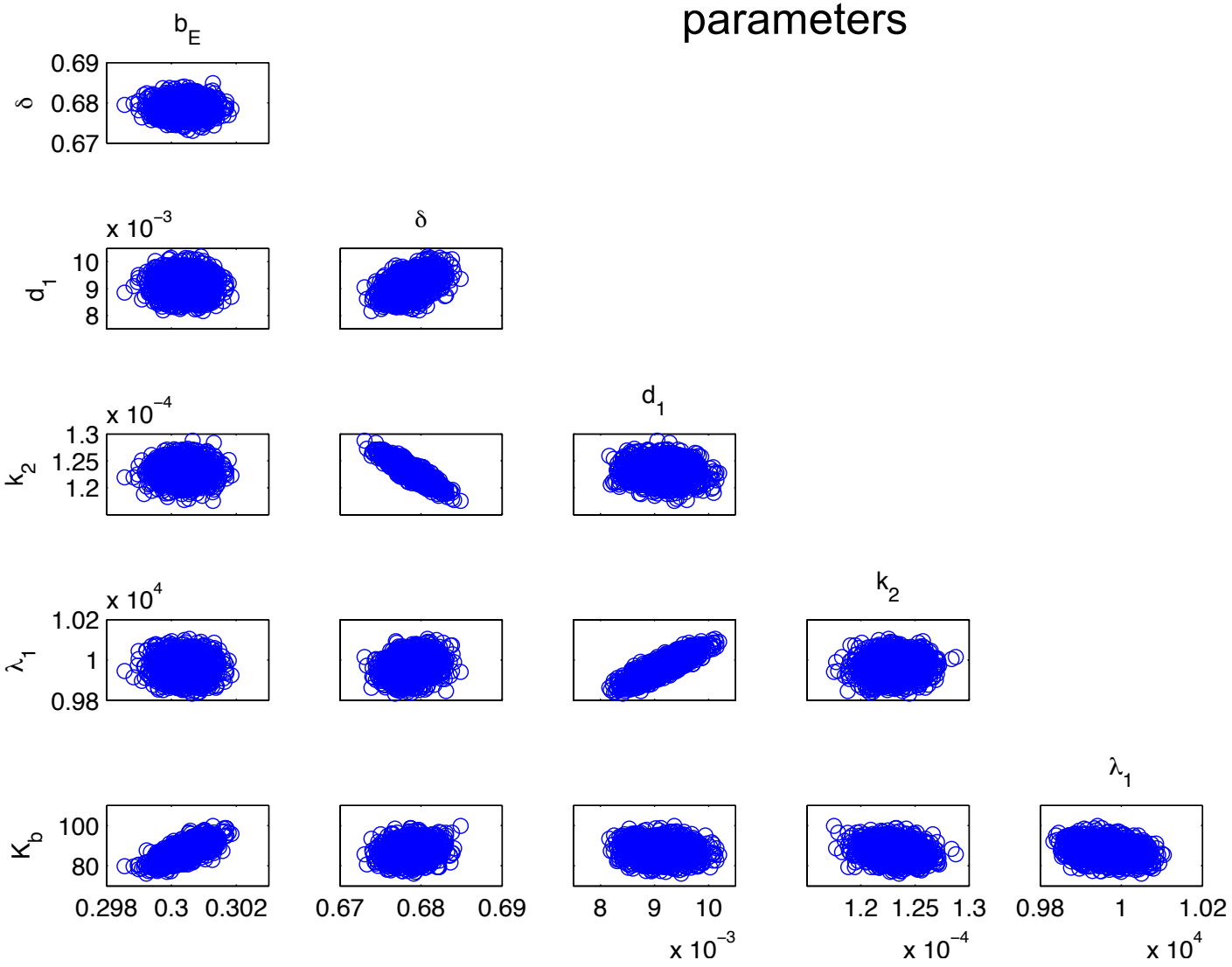
$$\dot{E} = \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta_E E.$$





Delayed Rejection Adaptive Metropolis (DRAM)

Example: HIV model

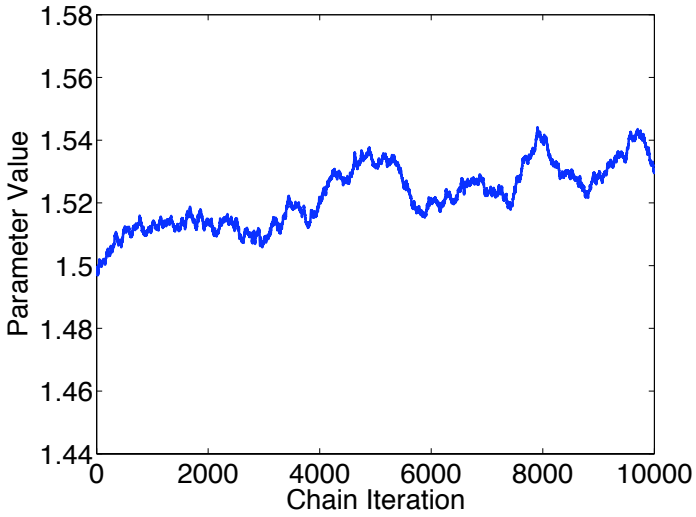


Note: Correlated versus nonidentifable parameters

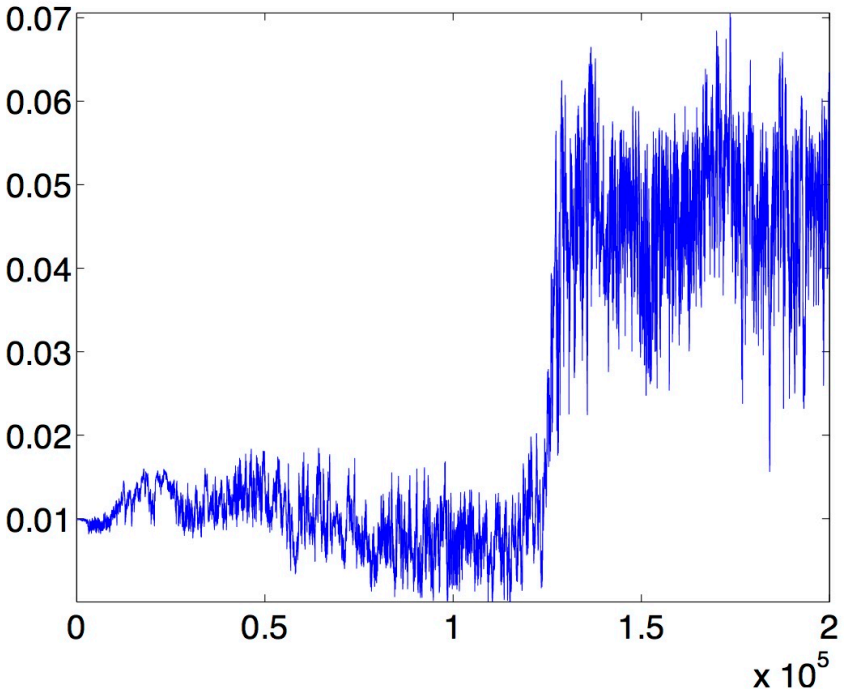
Chain Convergence (Burn-In)

Techniques:

- Visually check chains
- Statistical tests
- Often abused in the literature



Chain not converged



Chain for nonidentifiable parameter

Effects of Parameter Non-identifiability

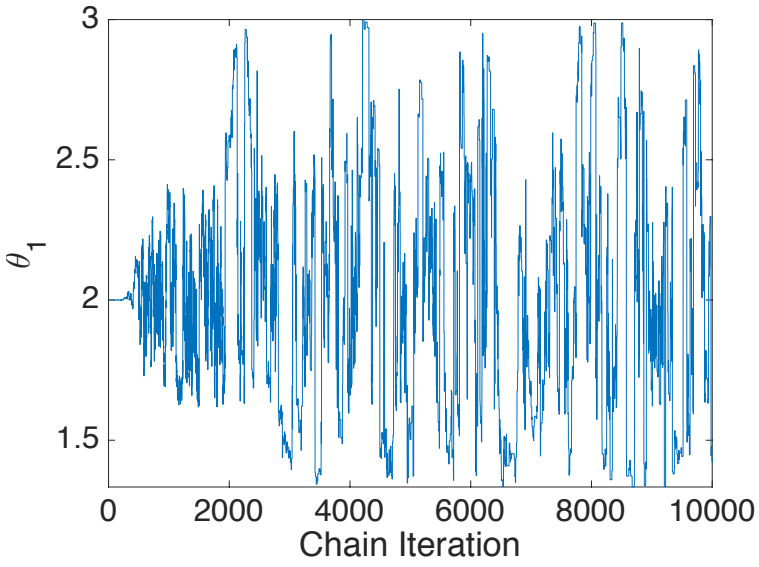
Example:

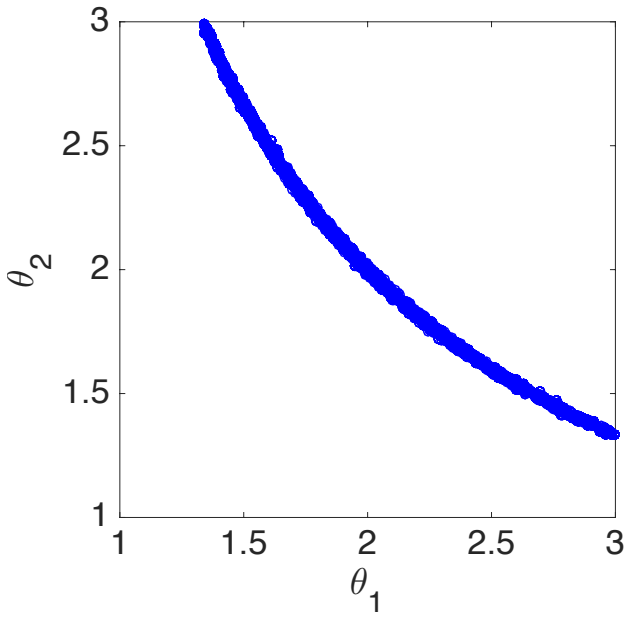
$$y_i = \theta_1 \theta_2 t_i + \varepsilon_i \ , \ i = 1, \ldots, n$$

Parameter values: $\theta_1 = \theta_2 = 2$

Times: $t_i \in [0, 1]$

Prior: $\mathcal{U}^2(4/3, 3)$





Note: Non-identifiable on manifold $h(\theta_{sub}) = 4 - \theta_1 \theta_2$

Uncertainty Propagation

Setting:

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

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

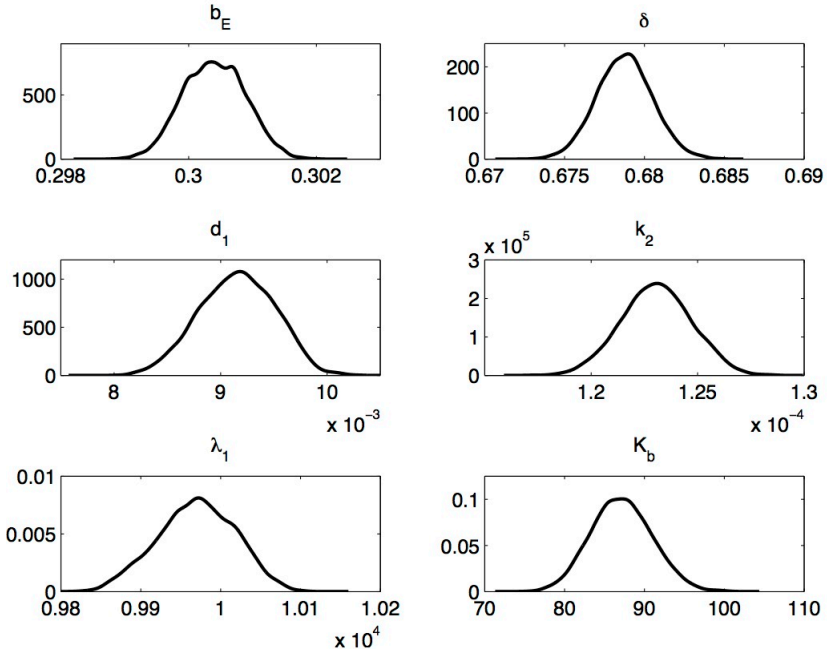
$$\dot{T}_2 = \lambda_2 - d_2 T_2 - (1-f\varepsilon) k_2 V T_2$$

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

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

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

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



Goal: Construct statistics for QoI

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

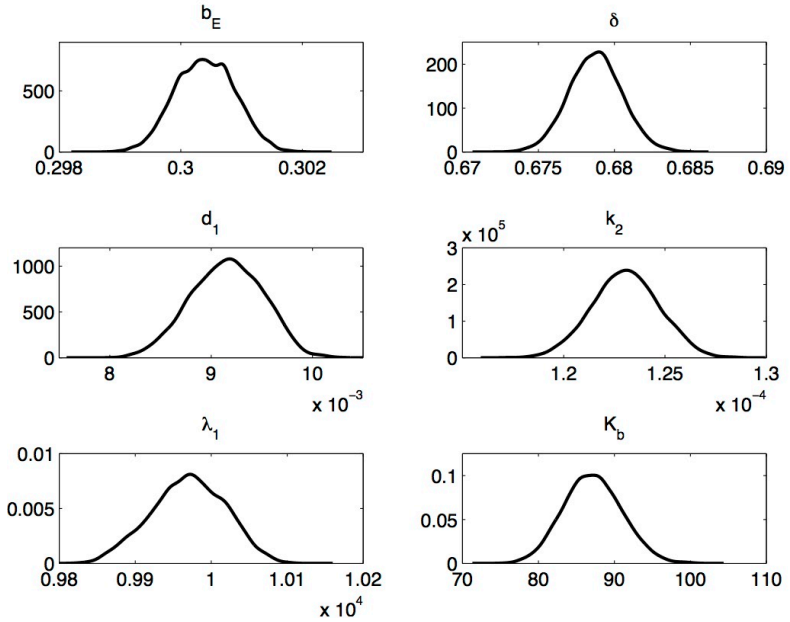
$$\mathbb{E}[V(t)] = \int_{\mathbb{R}^6} V(t,q)\rho(q)dq$$

Issues:

- How do we efficiently propagate input uncertainties through models? Surrogate models.
- How do we approximately integrate in moderate to high dimensions; e.g., p = 50-100?

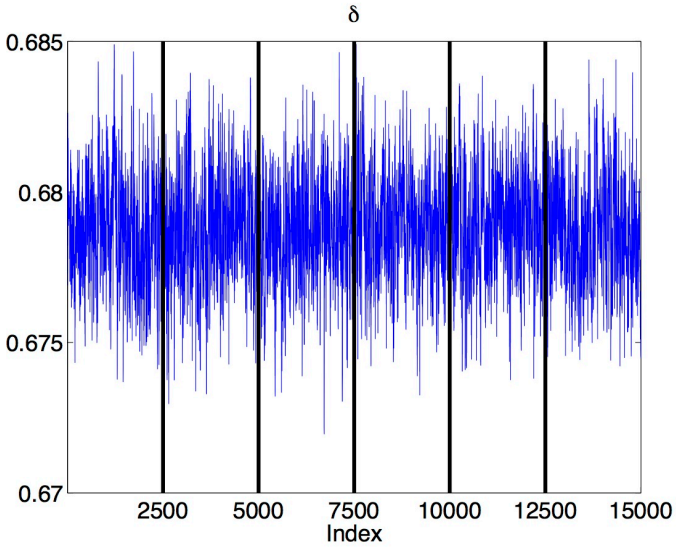
Propagation of Uncertainty in Models – HIV Example

Parameter Densities:

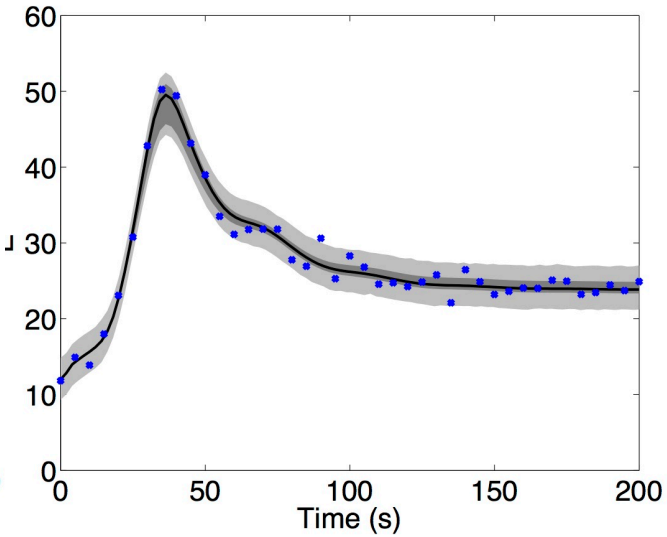


Techniques:

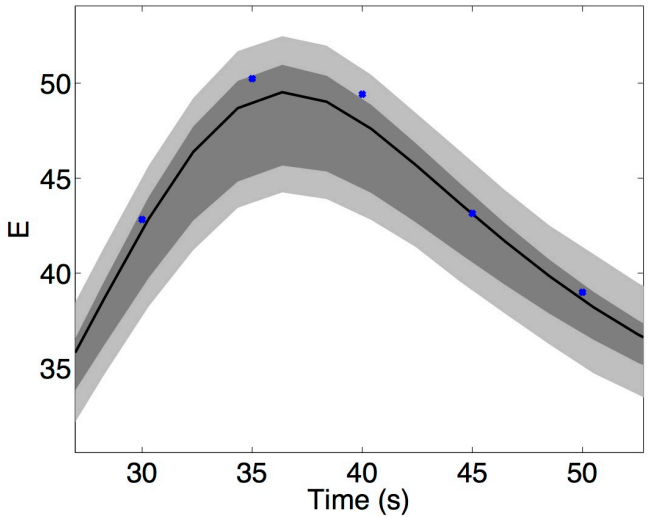
- Sample from parameter densities to construct prediction intervals for QoI.
- Slow convergence rate $O(1/\sqrt{M})$
- 100-fold more evaluations required to gain additional place of accuracy.
- Significant numerical analysis used to efficiently propagate densities.



Samples from Chain



Data, Credible Intervals and Prediction Intervals



Non-Gaussian Credible and Prediction Intervals

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.

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.

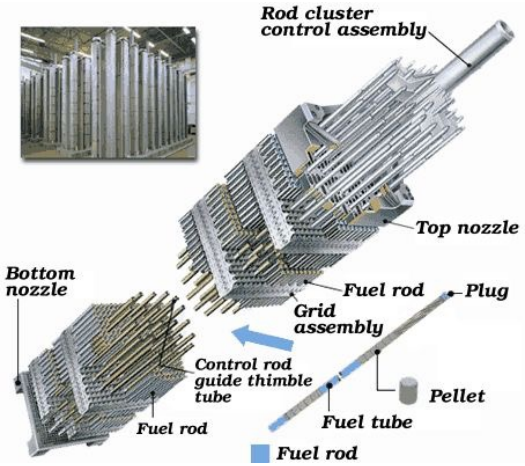
Use of Prediction Intervals: Nuclear Power Plant Design

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

e.g., Dittus—Boelter Relation

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

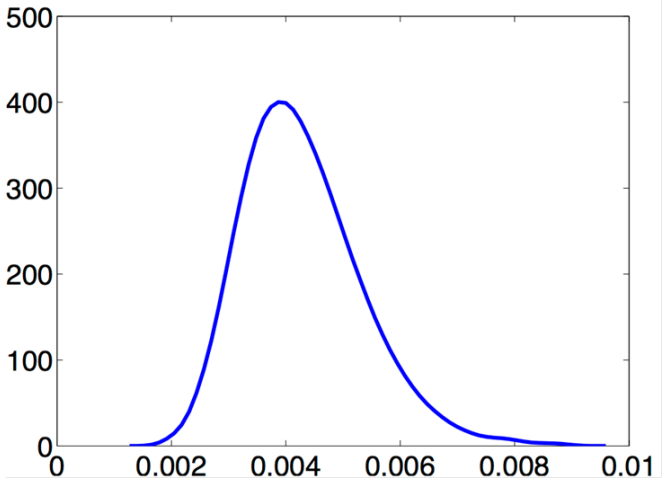
Nu: Nusselt number
Re: Reynolds number
Pr: Prandtl number



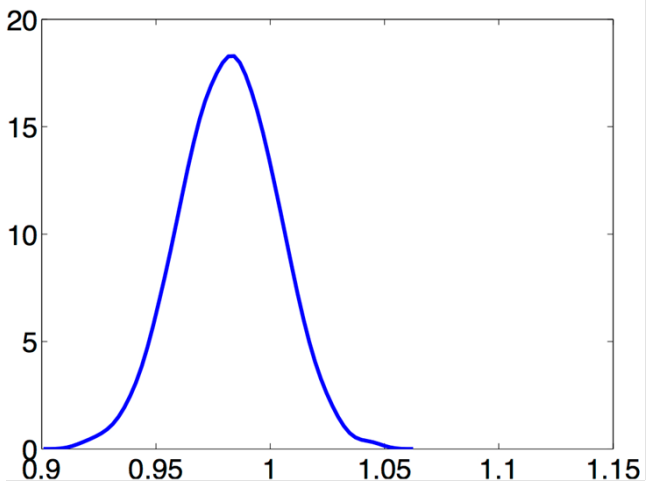
Industry Standard: Employ conservative, uniform, bounds

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

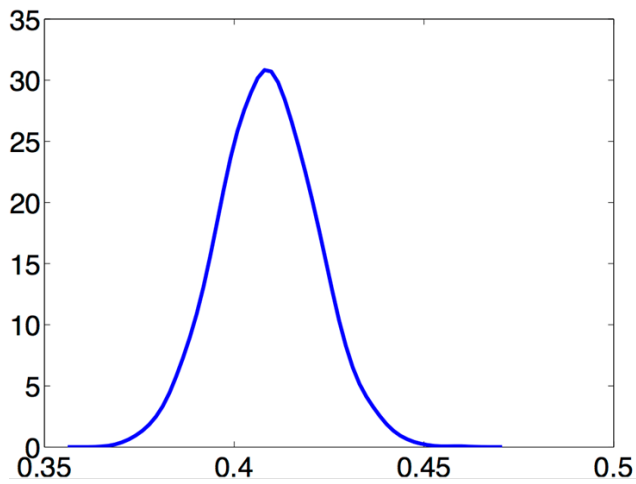
Bayesian Analysis: Employ conservative bounds as priors



$2\sigma \approx 0.0035$



$2\sigma \approx 0.06$

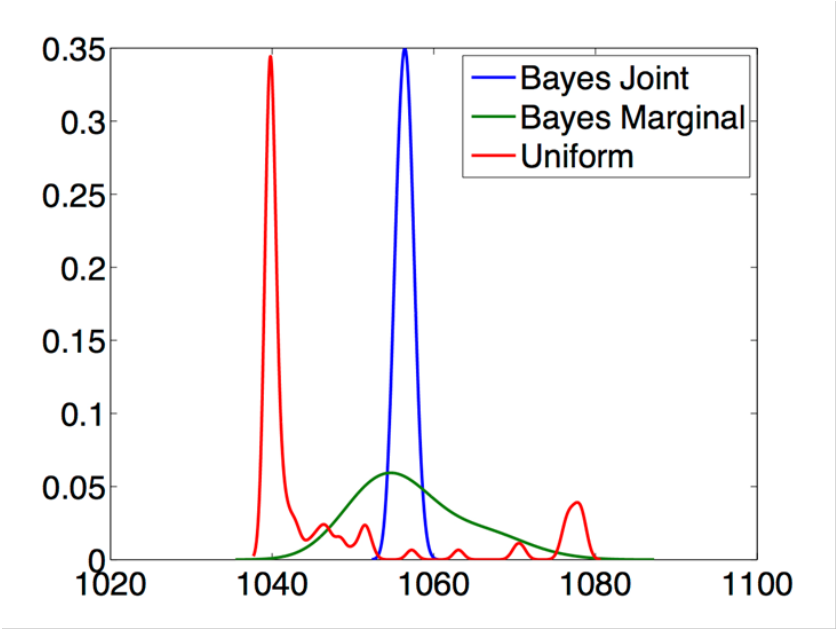


$2\sigma \approx 0.03$

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 physical relations
- Nuclear regulatory commission takes years to change requirements and codes

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

Delayed Rejection Adaptive Metropolis (DRAM)

Websites

- https://rsmith.math.ncsu.edu/UQ_TIA/CHAPTER8/index_chapter8.html
- https://mjlaine.github.io/mcmcstat/

Delayed Rejection Adaptive Metropolis (DRAM)

We fit the Monod model

$$y = \theta_1 \frac{t}{\theta_2 + t} + \varepsilon \ , \ \varepsilon \sim \mathcal{N}(0, I\sigma^2)$$

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

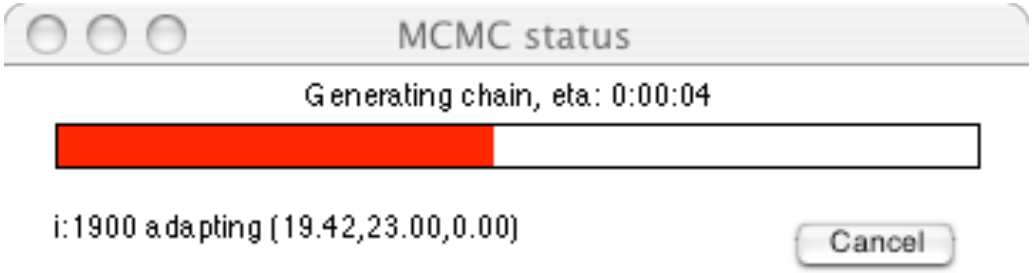
```
params = {
    {'theta1', tmin(1), 0}
    {'theta2', tmin(2), 0} };
```

and set options

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

Run code

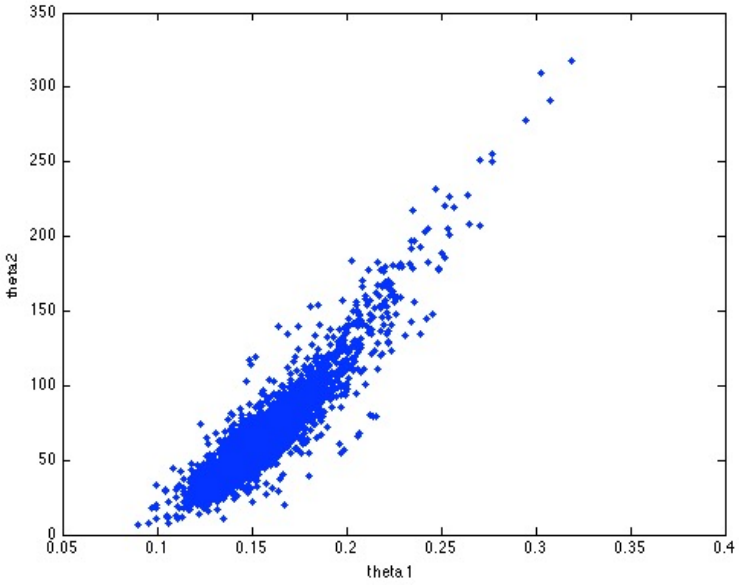
```
[res,chain,s2chain] = mcmcrun(model,data,params,options);
```

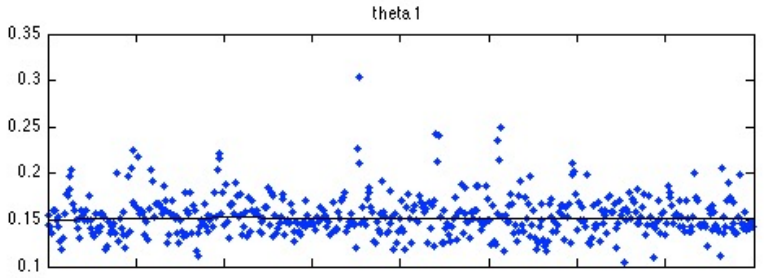


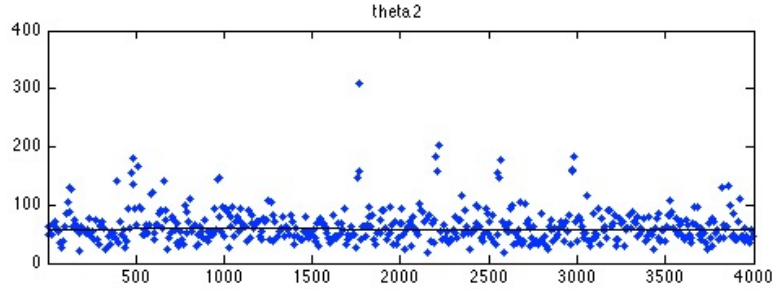
Delayed Rejection Adaptive Metropolis (DRAM)

Plot results

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



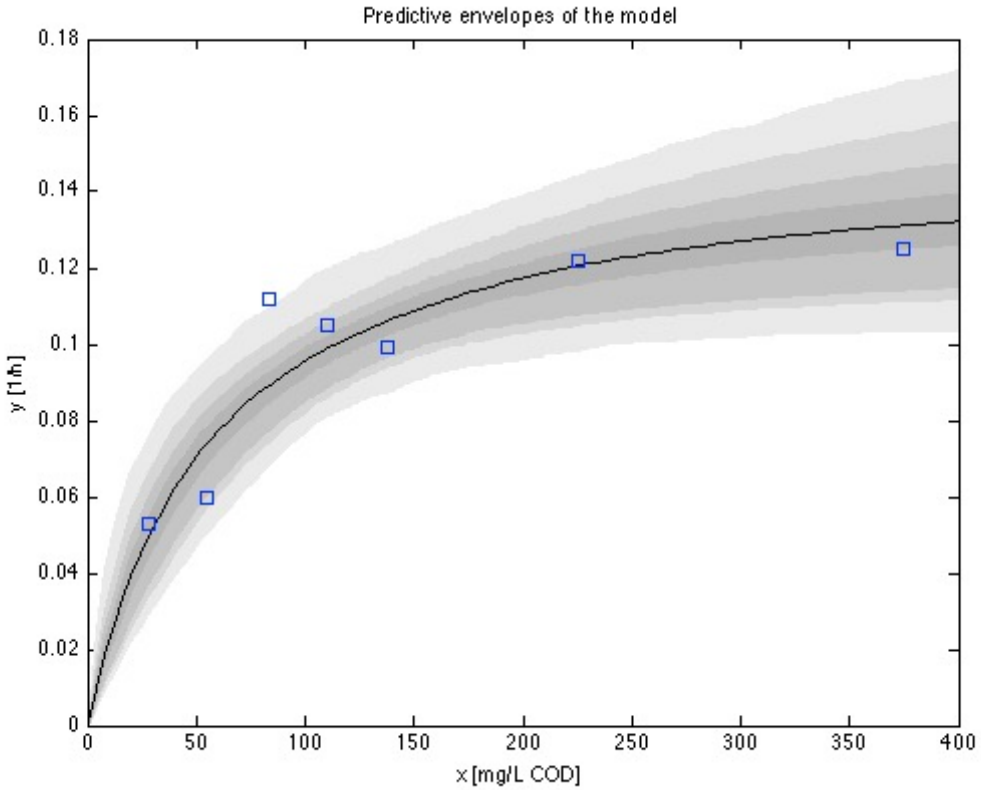




Examples:

- 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')
```