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
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nu) = 0 \]

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

Energy
\[ \rho c_v \frac{\partial T}{\partial t} + p \nabla \cdot \nu = -\nabla \cdot F + \nabla \cdot (k \nabla T) + \rho \dot{q}(T, p, \rho) \]

\[ p = \rho RT \]

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

Aerosol
\[ \frac{\partial \chi_j}{\partial t} = -\nu \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho), \quad j = 1, \ldots, J, \]

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:

Cone of Uncertainty:

00 UTC on August 26, 2005

12 UTC on August 26, 2005

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)
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:

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

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

\[ \mathbb{E}[V(t)] = \int_{\mathbb{R}^{21}} V(t, q) \rho(q) dq \]

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!

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

\[
\begin{align*}
\dot{T}_1 &= \lambda_1 - d_1 T_1 - (1 - \varepsilon) k_1 VT_1 \\
\dot{T}_2 &= \lambda_2 - d_2 T_2 - (1 - f\varepsilon) k_2 VT_2 \\
\dot{T}_1^* &= (1 - \varepsilon) k_1 VT_1 - \delta T_1^* - m_1 ET_1^* \\
\dot{T}_2^* &= (1 - f\varepsilon) k_2 VT_2 - \delta T_2^* - m_2 ET_2^* \\
\dot{V} &= N_T \delta (T_1^* + T_2^*) - cV - [(1 - \varepsilon) \rho_1 k_1 T_1 + (1 - f\varepsilon) \rho_2 k_2 T_2]V \\
\dot{E} &= \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta E E
\end{align*}
\]

Parameters: Reduced set

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

Point Estimates: Ordinary least squares

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

Note: Scaling critical since parameter values vary by 8 orders of magnitude.
Model Calibration and Predictions

Optimization Results:

<table>
<thead>
<tr>
<th>( b_E )</th>
<th>( \delta )</th>
<th>( d_1 )</th>
<th>( k_2 )</th>
<th>( \lambda_1 )</th>
<th>( K_b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.30</td>
<td>0.68</td>
<td>( 9.1 \times 10^{-3} )</td>
<td>( 1.22 \times 10^{-4} )</td>
<td>( 9.95 \times 10^3 )</td>
<td>88.5</td>
</tr>
</tbody>
</table>

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)

\[ s_i = E e_i + \varepsilon_i, \; i = 1, \ldots, N \]

\[ \varepsilon_i \sim N(0, \sigma^2) \]

**Parameter:** Stiffness \( E \)

**Strategy:** Use model fit to data to update prior information

**Non-normalized Bayes’ Relation:**

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

**Bayes’ Relation:** Specifies posterior in terms of likelihood and prior

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

- **Likelihood:** \(e^{-\sum_{i=1}^{N}(s_i-Ee_i)^2/2\sigma^2}\), \(q = E\)
- **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:

\[ y_i = f_i(\theta) + \varepsilon_i, \quad i = 1, \ldots, n \]

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

Likelihood:

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

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

\[ \ddot{z} + C\dot{z} + Kz = 0 \]

\[ z(0) = 2, \quad \dot{z}(0) = -C \]

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

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

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

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

so that

\[
\hat{C} \sim N \left( C_0, \sigma_c^2 \right), \quad \sigma_c = 0.0183
\]

**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.
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 $\theta^*$; 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:

Note: Narrower proposal distribution yields higher probability of acceptance.

- 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
  - Independent Metropolis
  - Random walk (local Metropolis)
    \[ \theta^* = \theta^{k-1} + Rz \]
  - Two (of several) choices: \( Z \sim N(0, 1) \)
    1. \( R = cl \Rightarrow \theta^* \sim N(\theta^{k-1}, cl) \)
    2. \( R = \text{chol}(V) \Rightarrow \theta^* \sim N(\theta^{k-1}, V) \)

where

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

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

**Metropolis Algorithm:** [Metropolis and Ulam, 1949]

1. Initialization: Choose an initial parameter value \( \theta^0 \) 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 \( \theta^* \) with probability 1 if \( r \geq 1 \) 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 $n_s, \sigma_s$.

2. Determine $\theta^0 = \arg \min_\theta \sum_{i=1}^{N} [y_i - f_i(\theta)]^2$.

3. Set $\text{SS}_{\theta^0} = \sum_{i=1}^{N} [y_i - f_i(\theta^0)]^2$.

4. Compute initial variance estimate: $s_0^2 = \frac{\text{SS}_{\theta^0}}{n - p}$.

5. Construct covariance estimate $V = s_0^2 [\chi^T(\theta^0)\chi(\theta^0)]^{-1}$ 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 $u_\alpha \sim U(0, 1)$
   - (d) Compute $\text{SS}_{\theta^*} = \sum_{i=1}^{N} [y_i - f_i(\theta^*)]^2$
   - (e) Compute
     \[
     \alpha(\theta^*|\theta^{k-1}) = \min \left( 1, e^{-[\text{SS}_{\theta^*} - \text{SS}_{\theta^{k-1}}]/2s_k^2} \right)
     \]
   - (f) If $u_\alpha < \alpha$, Set $\theta^k = \theta^*$, $\text{SS}_{\theta^k} = \text{SS}_{\theta^*}$
     else Set $\theta^k = \theta^{k-1}$, $\text{SS}_{\theta^k} = \text{SS}_{\theta^{k-1}}$
     endif
   - (g) Update $s_k \sim \text{Inv-gamma}(a_{val}, b_{val})$ where $a_{val} = 0.5(n_s + n)$, $b_{val} = 0.5(n_s\sigma_s^2 + \text{SS}_{\theta^k})$
Random Walk Metropolis

**Example:** We revisit the spring model

\[ \ddot{z} + C \dot{z} + Kz = 0 \]

\[ z(0) = 2, \quad \dot{z}(0) = -C \]

which has the solution

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

We assume that \( \epsilon_i \sim N(0, \sigma_0^2) \) where \( \sigma_0 = 0.1 \).
Random Walk Metropolis

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

![Graph of Chain Iteration vs Damping Parameter](image)

**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 \( J(\theta^*|\theta^{k-1}) = \mathcal{N}(\theta^{k-1}, V) \) 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

![Graphs showing measurement error variance and joint samples](image)

**Posted MATLAB Code:** spring_mcmc_C_K_sigma.m
Delayed Rejection Adaptive Metropolis (DRAM)

**Example:** HIV model

\[
\begin{align*}
\dot{T}_1 &= \lambda_1 - d_1 T_1 - (1 - \epsilon) k_1 V T_1 \\
\dot{T}_2 &= \lambda_2 - d_2 T_2 - (1 - f \epsilon) k_2 V T_2 \\
\dot{T}_1^- &= (1 - \epsilon) k_1 V T_1 - \delta T_1^- - m_1 E T_1^- \\
\dot{T}_2^- &= (1 - f \epsilon) k_2 V T_2 - \delta T_2^- - m_2 E T_2^- \\
\dot{V} &= N_T \delta (T_1^- + T_2^-) - c V - [(1 - \epsilon) \rho_1 k_1 T_1 + (1 - f \epsilon) \rho_2 k_2 T_2] V \\
\dot{E} &= \lambda_E + \frac{b_E (T_1^- + T_2^-)}{T_1^- + T_2^- + K_b} E - \frac{d_E (T_1^- + T_2^-)}{T_1^- + T_2^- + K_d} E - \delta_E E.
\end{align*}
\]
 Delayed Rejection Adaptive Metropolis (DRAM)

**Example:** HIV model

**Note:** Correlated versus nonidentifiable 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

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

\[
\begin{align*}
\dot{T}_1 &= \lambda_1 - d_1 T_1 - (1 - \varepsilon) k_1 VT_1 \\
\dot{T}_2 &= \lambda_2 - d_2 T_2 - (1 - f\varepsilon) k_2 VT_2 \\
\dot{T}_1^* &= (1 - \varepsilon) k_1 VT_1 - \delta T_1^* - m_1 ET_1^* \\
\dot{T}_2^* &= (1 - f\varepsilon) k_2 VT_2 - \delta T_2^* - m_2 ET_2^* \\
\dot{V} &= N_T \delta(T_1^* + T_2^*) - cV - [(1 - \varepsilon) \rho_1 k_1 T_1 + (1 - f\varepsilon) \rho_2 k_2 T_2] V \\
\dot{E} &= \lambda_E + \frac{b_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_b} E - \frac{d_E (T_1^* + T_2^*)}{T_1^* + T_2^* + K_d} E - \delta E E
\end{align*}
\]

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:

- \( b_E \)
- \( \delta \)
- \( d_1 \)
- \( k_2 \)
- \( \lambda_1 \)
- \( K_b \)

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

\[ \begin{align*}
\Delta\left(0.0035\right) &= 2\sigma \\
\Delta(0.06) &= 2\sigma \\
\Delta(0.03) &= 2\sigma
\end{align*} \]

**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://mjilaine.github.io/mcmcstat/
Delayed Rejection Adaptive Metropolis (DRAM)

We fit the Monod model

\[ y = \frac{\theta_1 t}{\theta_2 + t} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, I\sigma^2) \]

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.

```matlab
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`.

```matlab
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

```matlab
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

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

and set options

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

Run code

```matlab
[res,chain,s2chain] = mcmcrun(model,data,params,options);
```
Delayed Rejection Adaptive Metropolis (DRAM)

Plot results

```matlab
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

```matlab
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')
```