Parameter Selection, Model Calibration, and Uncertainty Propagation for Physical Models

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Experimental Setup

Heat Model

\[
\frac{d^2 T_s}{dx^2} = \frac{2(a + b)}{ab} \frac{h}{k} \left[ T_s(x) - T_{amb} \right]
\]

\[
\frac{dT_s}{dx}(0) = \frac{\Phi}{k}, \quad \frac{dT_s}{dx}(L) = \frac{h}{k} \left[ T_{amb} - T_s(L) \right]
\]
Heat Model Example

Experimental Setup and Data:

Steady State Model:

\[
\frac{d^2 T_s}{dx^2} = \frac{2(a + b)}{ab} \frac{h}{k} [T_s(x) - T_{amb}]
\]

\[
\frac{dT_s}{dx}(0) = \frac{\Phi}{k}
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\[
\frac{dT_s}{dx}(L) = \frac{h}{k} [T_{amb} - T_s(L)]
\]

Objectives: Employ Bayesian analysis for

- Model calibration
- Uncertainty propagation
- Experimental design

Note: Parameter set \( q = [h, k, \Phi] \) is not identifiable
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 Model Calibration

Bayes’ Theorem:

\[ P(A|B) = \frac{P(B|A)P(A)}{P(B)} \]

Example: Coin Flip

\[ \gamma_i(\omega) = \begin{cases} 0 & , \quad \omega = T \\ 1 & , \quad \omega = H \end{cases} \]

Likelihood:

\[ \pi(v|q) = \prod_{i=1}^{N} q^{v_i} (1 - q)^{1-v_i} = q \sum v_i (1 - q)^{N - \sum v_i} = q^{N_1} (1 - q)^{N_0} \]

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

\[ \pi(q|v) = \frac{q^{N_1} (1 - q)^{N_0}}{\int_0^1 q^{N_1} (1 - q)^{N_0} dq} = \frac{(N + 1)!}{N_0!N_1!} q^{N_1} (1 - q)^{N_0} \]
Bayesian Model Calibration:

- Parameters considered to be random variables with associated densities.

\[ \pi(q|v) = \frac{\pi(v|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(v|q)\pi_0(q) dq} \]

Problem:
- Often requires high dimensional integration;
  - e.g., \( p = 18 \) for MFC model
  - \( p = \) thousands to millions for some models

Strategies:
- Sampling methods
- Sparse grid quadrature techniques
Markov Chain Techniques

Markov Chain: Sequence of events where current state depends only on last value.

Baseball: States are $S = \{\text{win}, \text{lose}\}$. Initial state is $p^0 = [0.8, 0.2]$.

- Assume that team which won last game has 70% chance of winning next game and 30% chance of losing next game.
- Assume losing team wins 40% and loses 60% of next games.

![Transition Diagram]

- Percentage of teams who win/lose next game given by
  \[
p^1 = [0.8, 0.2] \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix} = [0.64, 0.36]
  \]

- Question: does the following limit exist?
  \[
p^n = [0.8, 0.2] \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix}^n
  \]
Markov Chain Techniques

**Baseball Example:** Solve constrained relation

\[ \pi = \pi P , \quad \sum \pi_i = 1 \]

\[ \Rightarrow [\pi_{\text{win}}, \pi_{\text{lose}}] \begin{bmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{bmatrix} = [\pi_{\text{win}}, \pi_{\text{lose}}] , \quad \pi_{\text{win}} + \pi_{\text{lose}} = 1 \]

to obtain

\[ \pi = [0.5714, 0.4286] \]
Markov Chain Techniques

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**Alternative:** Iterate to compute solution

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**Notes:**

- Forms basis for Markov Chain Monte Carlo (MCMC) techniques
- Goal: construct chains whose stationary distribution is the posterior density
Markov Chain Monte Carlo Methods

**Strategy:** Markov chain simulation used when it is impossible, or computationally prohibitive, to sample \( q \) directly from

\[
\pi(q|v) = \frac{\pi(v|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(v|q)\pi_0(q) dq}
\]

- Create a Markov process whose stationary distribution is \( \pi(q|v) \).

**Note:**

- In Markov chain theory, we are given a Markov chain \( P \), and we construct its equilibrium distribution.
- In MCMC theory, we are “given” a distribution and we want to construct a Markov chain that is reversible with respect to it.
Model Calibration Problem

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

![Graph showing displacement over time](image1)

**Likelihood:**

\[
\pi(v|q) = L(q, \sigma|v) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}
\]

where

\[
SS_q = \sum_{i=1}^{n} [v_i - f_i(q)]^2
\]

is the sum of squares error.
Markov Chain Monte Carlo Methods

General Strategy:

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

Intuition: Recall that

\[
\pi(q|\nu) = \frac{\pi(\nu|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\nu|q)\pi_0(q) dq}
\]

where

\[
\pi(\nu|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\sum_{i=1}^{n} [\nu_i - f_i(q)]^2 / 2\sigma^2} = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q / 2\sigma^2}
\]
Markov Chain Monte Carlo Methods

Intuition:

\[ \pi(v|q) \]

\[ q^* \quad q^{k-1} \quad q \]

\[ \text{SS}_q \]

\[ q^* \quad q^{k-1} \quad q \]

- Consider \( r(q^*|q^{k-1}) = \frac{\pi(q^*|v)}{\pi(v|q^{k-1})} = \frac{\pi(v|q^*)\pi_0(q^*)}{\pi(v|q^{k-1})\pi_0(q^{k-1})} \)
  - If \( r < 1 \) \( \Leftrightarrow \) \( \pi(v|q^*) < \pi(v|q^{k-1}) \), 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**: Significantly affects mixing

- Too wide: Too many points rejected and chain stays still for long periods;
- Too narrow: Acceptance ratio is high but algorithm is slow to explore parameter space
- Ideally, it should have similar “shape” to posterior distribution.

Problem:

- Anisotropic posterior, isotropic proposal;
- Efficiency nonuniform for different parameters

Result:

- Recovers efficiency of univariate case
Proposal Distribution

Proposal Distribution: Two basic approaches

- Choose a fixed proposal function
  - Independent Metropolis
- Random walk (local Metropolis)
  \[ q^* = q^{k-1} + Rz \]
  - Two (of several) choices: \( z \sim N(0, 1) \)
    1. \( R = cI \Rightarrow q^* \sim N(q^{k-1}, cI) \)
    2. \( R = \text{chol}(V) \Rightarrow q^* \sim N(q^{k-1}, V) \)

where

\[
V = \sigma_{OLS}^2 \left[ \mathcal{X}^T(q_{OLS}) \mathcal{X}(q_{OLS}) \right]^{-1}
\]

\[
\sigma_{OLS}^2 = \frac{1}{n-p} \sum_{i=1}^{n} \left[ v_i - f_i(q_{OLS}) \right]^2
\]

\[
\mathcal{X}_{ik}(q_{OLS}) = \frac{\partial f_i(q_{OLS})}{\partial q_k}
\]