Markov Chain Monte Carlo (MCMC) for model and parameter identification

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Multidisciplinary Course: Monte Carlo Simulation Methods for the Quantitative Analysis of Stochastic and Uncertain Systems
Problem statement: statistical inference

On the basis of the experimental data \( x \), estimate the (unknown) parameters \( \theta \) of the (known) model

\[
\hat{\theta}
\]
**SYSTEM MODEL (hypothesis)**

Component failure time

**Exponential distribution**

\[ f(t) = \lambda e^{-\lambda t} = \theta e^{-\theta t} \]

**EXPERIMENTAL DATA (from real components)**

\[ \mathbf{x} = \{ x_1, x_2, \ldots, x_N \} = \mathbf{t} = \{ t_1, t_2, \ldots, t_N \} = \{ 1.71 \text{h}, 48.8 \text{h}, \ldots, 0.39 \text{h} \} \]

\( (N = 100 \text{ failure times from } N = 100 \text{ ‘identical’ components}) \)

**MODEL PARAMETER \( \theta \)? (\( = \text{FAILURE RATE } \lambda \)?)
• Only the (random) data are used to estimate the parameter

(e.g.) MAXIMUM LIKELIHOOD ESTIMATION

\[ x = \{x_1, x_2, \ldots, x_N\} = t = \{t_1, t_2, \ldots, t_N\} \quad (N = 100 \text{ failure times}) \]

\[ \hat{\theta} = \hat{\lambda} = \left[ \frac{\text{failures}}{\text{time}} \right] = \frac{\text{Number of collected failures}}{\text{Total observed time}} = \frac{N}{\sum_{i=1}^{N} t_i} = \frac{100}{3.05 \cdot 10^3 \text{ h}} = 3.28 \cdot 10^{-2} \text{ h}^{-1} \]

(NB: also confidence intervals can be computed, reflecting the variability in the random data)
Statistical inference: the Bayesian approach

- In addition to the (random) data, it uses the analyst’s degree of belief (state of knowledge) about the true value of the parameter.

- The analyst’s state of knowledge about the parameter before obtaining the data is represented by a (prior) probability distribution (Bayesian interpretation of probability).

\[ p(\theta) = p(\lambda) \]

Combination to obtain the “posterior” distribution:

\[ p(\theta | x) = p(\lambda | t) \]

\[ x = t = \{t_1, t_2, \ldots, t_N\} \]

\(N = 100\) failure times
Bayesian statistical inference: definitions

\[ p(\theta \text{ and } x) = p(\theta | x)p(x) = p(x | \theta)p(\theta) \]

Definition of ‘and’

\[ p(\theta | x) = \frac{p(x | \theta)p(\theta)}{p(x)} = \frac{p(x | \theta)p(\theta)}{\int p(x | \theta)p(\theta)d\theta} \]

Bayes theorem

\[ p(\theta | x) = \pi(\theta | x) \]

Posterior distribution of the parameters given the data
(objective of the analysis)

\[ p(x | \theta) = L(\theta | x) \]

Likelihood of the parameters given dataset
(dependent on the functional form of the chosen model)

\[ p(\theta) \]

Prior distribution of the parameters
(dependent on the a priori knowledge on the values of the parameters)

\[ p(x) \]

Probability of the experimental dataset
(“normalization” factor: requires the evaluation of a complex integral)
Bayesian statistical inference – Example: component with constant failure rate

Exponential model for the failure times

\[ f(t) = \lambda e^{-\lambda t} \Rightarrow \text{“Exponential likelihood”} \]

\[ L(\theta | x) = L(\lambda | t) = (\lambda \exp[-\lambda t_1]) \cdot (\lambda \exp[-\lambda t_2]) \cdot \ldots \cdot (\lambda \exp[-\lambda t_N]) = \lambda^N \exp[-\lambda \sum_{i=1}^{N} t_i] \]

**Expert “prior” knowledge**

\[ p(\theta) = p(\lambda) \]

\[ x = t = \{ t_1, t_2, \ldots, t_N \} \]

\( (N = 100 \text{ failure times}) \)
Bayesian statistical inference: Markov Chain Monte Carlo (MCMC) simulation approach

It generates samples according to any desired probability distribution

Randomly chosen value $\theta^0$

MCMC rules + Data, $x$

$\{\theta^1, \theta^2, ..., \theta^j, ..., \theta^{N_s}\}$

If $N_s$ is large enough, then $\{\theta^1, \theta^2, ..., \theta^j, ..., \theta^{N_s}\} \sim \pi(\theta \mid x)$ independently on the initial point $\theta^0$
MCMC simulation: the Metropolis-Hastings algorithm (1)

- Randomly choose an initial value $\theta^0 = \{\theta_1^0, \theta_2^0, \ldots, \theta_i^0, \ldots, \theta_n^0\}$ for the Markov chain
- For $j = 0, 1, \ldots, N_s$ (chain length)

1. Sample a proposal value $\theta' = \{\theta_1', \theta_2', \ldots, \theta_i', \ldots, \theta_n'\}$ from a proposal distribution $K(\theta' | \theta^j)$

Example for variable $\theta_i$, $i = 1, 2, \ldots, n$
MCMC simulation: the Metropolis-Hastings algorithm (2)

2. Calculate the acceptance probability $\alpha$ for proposal value $\theta'$

$$\alpha = \min \left\{ 1, \frac{\pi(\theta' \mid x)K(\theta^j \mid \theta')}{\pi(\theta^j \mid x)K(\theta' \mid \theta^j)} \right\}$$

Since $\pi(\theta \mid x) = \frac{L(\theta \mid x)p(\theta)}{p(x)}$

$$\alpha = \min \left\{ 1, \frac{L(\theta' \mid x)p(\theta')K(\theta^j \mid \theta')}{L(\theta^j \mid x)p(\theta^j)K(\theta' \mid \theta^j)} \right\}$$

NO NEED FOR NORMALIZATION FACTOR CALCULATION

3. Accept/reject proposal value $\theta'$
   - Draw a uniform random number $r \sim U[0, 1)$
   - If $r \leq \alpha$, then accept the proposal value $\theta'$, i.e. set $\theta^{j+1} = \theta'$
     else reject the proposal value $\theta'$, i.e. set $\theta^{j+1} = \theta^j$

- End For ($j = 0, 1, \ldots, N_s$)
Application:
 component with constant failure rate
Application: component with constant failure rate

**Exponential distribution**

\[ f(t) = \lambda e^{-\lambda t} \]

Failure rate \( \lambda \) = constant

Experimental dataset:

\[ x = \{x_1, x_2, \ldots, x_N\} = t = \{t_1, t_2, \ldots, t_N\} \quad (N = 100 \text{ failure times}) \]

Likelihood function (given by the chosen model)

\[ L(\theta | x) = L(\lambda | t) = (\lambda \exp[-\lambda t_1]) \cdot (\lambda \exp[-\lambda t_2]) \cdots (\lambda \exp[-\lambda t_N]) = \lambda^N \exp\left[ -\lambda \sum_{i=1}^{N} t_i \right] \]

Prior distribution

\[ p(\theta) = p(\lambda) = U[0, \lambda_{\text{max}}] = 1/\lambda_{\text{max}} \quad ("\text{uninformative}") \]

Proposal distribution

\[ K(\lambda' | \lambda) = N(\lambda, \sigma); K(\lambda | \lambda') = N(\lambda', \sigma) \quad ("\text{symmetric}") \]

\[ \alpha = \min\left\{ 1, \frac{L(\lambda' | t)p(\lambda')K(\lambda | \lambda')}{L(\lambda | t)p(\lambda)K(\lambda' | \lambda)} \right\} = \min\left\{ 1, \frac{L(\lambda' | t)}{L(\lambda | t)} \right\} = \min\left\{ 1, \frac{(\lambda')^N \exp\left[ -\lambda' \sum_{i=1}^{N} t_i \right]}{(\lambda)^N \exp\left[ -\lambda \sum_{i=1}^{N} t_i \right]} \right\} \]
GOOD AGREEMENT WITH "TRUE" VALUE, $\lambda = 0.01$
The reversible-jump MCMC algorithm
Problem statement

Presence of changepoints in model parameter $\theta$

Assumption: step changes in model parameter $\theta$
Objectives of the Bayesian inference

- Location(s) $s_i$, $i = 1, 2, \ldots, k$, of the changepoints
  \[ \pi(s_i \mid x), i = 1, 2, \ldots, k \]

- Values $\theta_i$, $i = 0, 1, \ldots, k$, of the parameter(s) before and after the transitions
  \[ \pi(\theta_i \mid x), i = 0, 1, \ldots, k \]

- **Number $k$ of changepoints**
  \[ \pi(k \mid x) \]

\[ \text{THE NUMBER OF CHANEGPOINTS IS NOT KNOWN} \Rightarrow \text{IT IS AN UNCERTAIN VARIABLE!} \]
Reversible-jump MCMC: prior distributions

Prior distribution $p(k)$ for the number of changepoints $k$:

$$p(k) = \frac{e^{-\lambda} \lambda^k}{k!} \quad \text{(Truncated) Poisson distribution}$$

Given $k$, prior distribution for step positions $s_1, s_2, \ldots, s_k$:

Even numbered order statistics from $(2k + 1)$ points uniform in $[s_0, s_{k+1}]$

Given the step positions $s_1, s_2, \ldots, s_k$, prior distributions for parameters $\theta_0, \theta_1, \ldots, \theta_k$:

$$p(\theta_i) = \frac{\beta^\alpha}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta \theta} \quad \text{Gamma distribution}$$
Four possible random moves to explore the uncertain parameter space:

1. The parameter value $\theta$ is varied at a random location $s_i$

2. A randomly chosen step location $s_i$ is moved

3. A new step location is created at random in the interval $[s_0, s_{k+1}]$ (*birth move*)

4. A randomly chosen location $s_i$ is eliminated (*death move*)
Reversible-jump MCMC - Random move 1: variation of the parameter value

\[ \theta_i = \text{“old” value} \]
\[ \theta_i' = \text{proposed value} \]

Selected at random

Proposed value:
\[
\log\left( \frac{\theta_i'}{\theta_i} \right) \approx U[-0.5, 0.5] \rightarrow \theta_i' = \theta_i \cdot e^U
\]

Acceptance probability:
\[
\alpha_n = \min\left\{ 1, l \cdot \left( \frac{\theta_i'}{\theta_i} \right)^\alpha e^{-\beta(\theta_i' - \theta_i)} \right\}
\]

where
\[
l = \frac{L(\theta_i' | x)}{L(\theta_i | x)} = \text{likelihood ratio (dependent on the problem)}
\]
Reversible-jump MCMC - Random move 2: variation of a step location

Selected at random

Proposed value: \( s_i' \approx U[s_{i-1}, s_{i+1}] \)

Acceptance probability: \( \alpha_x = \min \left\{ 1, l \cdot \frac{(s_{i+1} - s_i')(s_{i'} - s_{i-1})}{(s_{i+1} - s_i)(s_i - s_{i-1})} \right\} \)

where \( l = \frac{L(s_i' | x)}{L(s_i | x)} = \) likelihood ratio (dependent on the problem)
Reversible-jump MCMC - Random move 3: “birth” of a new location

Proposed values:
\[ S^* \approx U\left[ S_0, S_{k+1} \right] \] (and identify the interval where it lies)

\[
\begin{align*}
\left( S^* - S_i \right) \theta_i' + \left( S_{i+1} - S^* \right) \theta_{i+1}' &= \left( S_{i+1} - S_i \right) \theta_i \quad \text{(perturbation of } \theta_i) \\
\frac{\theta_{i+1}'}{\theta_i} &= \frac{1-r}{r}, \quad r \approx U[0,1] \quad \text{(imposed)}
\end{align*}
\]

Acceptance probability, \( \alpha_b \): very complex structure! \( \rightarrow \) see (Green, 1995)
Reversible-jump MCMC - Random move 4: “death” of a new location

“Reverse” the “birth” move:

Proposed values: \((s_i - s_{i-1})\theta_{i-1} + (s_{i+1} - s_i)\theta_i = (s_{i+1} - s_{i-1})\theta'_{i-1}\)

Acceptance probability, \(\alpha_d\): very complex structure! \(\rightarrow\) see (Green, 1995)
Reversible-jump MCMC: sequential steps of the algorithm (1)

1. Select prior values of the Markov chain

\[ p(k) = \frac{e^{-\lambda} \lambda^k}{k!} \]

\( \Rightarrow \) Prior value for \( k \) (number of changepoints)

Prior positions of the changepoints: \( s_1, s_2, \ldots, s_k \)

\[ p(\theta_i) = \frac{\beta^\alpha}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta \theta} \]

\( \Rightarrow \) Prior values of the parameter: \( \theta_0, \theta_1, \ldots, \theta_k \)

2. Calculate the probabilities for each possible move

\( \eta_k + \chi_k + b_k + d_k = 1 \) \quad \text{Normalization}

\( \chi_0 = b_{k_{\text{max}}} = d_0 = 0 \) \quad \text{“Physical” considerations}

\( \eta_k = \chi_k \quad \text{if} \ k \neq 0 \)

\[ b_k = c \min \left\{ 1, \frac{p(k+1)}{p(k)} \right\}, d_k = c \min \left\{ 1, \frac{p(k-1)}{p(k)} \right\} \]

Suggested by (Green, 1995) to obtain “good” chains (i.e., fast convergence and exploration of the parameter space)

\[ b_k + d_k \leq 0.9 \]
3. Sample a uniform random number \( r \) in \([0, 1)\) and select one of the possible moves according to the probabilities computed in step 2.

\[
\begin{array}{cccc}
\eta_k & \chi_k & b_k & d_k \\
\end{array}
\]

4. Generate proposal values according to the selected move
   - If move 1: variation of parameter value \((\theta'_i)\)
   - If move 2: variation of step location \((s'_i)\)
   - If move 3: “birth” of a new location \((s^*, \theta'_i \text{ and } \theta'_{i+1})\)
   - If move 4: “death” of a location \((s_i \text{ removed and } \theta'_i \text{ proposed})\)

5. Calculate the acceptance probability for the move(s) proposed in step 4. (i.e., \( a_\eta, a_\chi, a_b \) or \( a_d \))
5. Sample a uniform random number $u$ in $[0, 1)$ and accept/reject the proposed move(s) according to the acceptance probabilities computed in step 4.

\[ \begin{array}{c}
\alpha_b \\
0 \quad \quad \quad 1 - \alpha_b \\
\end{array} \]

6. Update the values of the uncertain parameters in the chain:
   - New number $k$ of changepoints,
   - New locations $s_i, \ i = 1, 2, \ldots, k,$ of the changepoints,
   - New values $\theta_i, \ i = 0, 1, \ldots, k,$ of the parameter in each interval

7. Return to step 2. above (i.e., update the values of the probabilities for each possible move $\eta_k, \chi_k, b_k, d_k$ and so on ...)

8. Stop the algorithm when the number of iterations (i.e., the number of samples in the chain) reaches a predefined (large) value
Reversible-jump MCMC: example (1)

- Iteration 0 (i.e., sample the prior values)

\[ p(k) = \frac{e^{-\lambda} \lambda^k}{k!}, \lambda = 1, k_{\max} = 3 \quad \Rightarrow k^0 = 2 \text{ (prior number of changepoints)} \]

\[ [s_{\min}, s_{\max}] = [0,100] \rightarrow \{61,35,10,43,87\} \rightarrow \{10,35,43,61,87\} \]

(uniform random sampling of \(2k^0+1\) values)

\[ p(\theta_i) = \frac{\beta^\alpha}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta \theta}, \alpha = 3, \beta = 2 \quad \Rightarrow \{\theta_1^0, \theta_2^0, \theta_3^0\} = \begin{cases} 4.04, \text{if } s \in [s_{\min}, s_1^0] \\ 1.51, \text{if } s \in [s_1^0, s_2^0] \\ 5.75, \text{if } s \in [s_2^0, s_{\max}] \end{cases} \]

<table>
<thead>
<tr>
<th>(k^0)</th>
<th>(s_1^0)</th>
<th>(s_2^0)</th>
<th>(\theta_1^0)</th>
<th>(\theta_2^0)</th>
<th>(\theta_3^0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 0</td>
<td>2</td>
<td>35</td>
<td>61</td>
<td>4.04</td>
<td>1.51</td>
</tr>
</tbody>
</table>
Reversible-jump MCMC: example (2)

- Iteration 1:

- Calculate the probabilities for each possible move given $k = 2$

$$\eta_k + \chi_k + b_k + d_k = 1$$

$$b_k = c \min \left\{ 1, \frac{p(k+1)}{p(k)} \right\}, d_k = c \min \left\{ 1, \frac{p(k-1)}{p(k)} \right\}$$

$$b_k + d_k \leq 0.9$$

$$\eta_k = \chi_k$$

- Sample one of the possible moves

$$\eta_2 = 0.0500$$

$$\chi_2 = 0.0500$$

$$b_2 = 0.2250$$

$$d_2 = 0.6750$$

$$r = 0.085$$

VARIATION OF A STEP LOCATION
Reversible-jump MCMC: example (3)

- Select randomly one of the changepoints \( \rightarrow s^0_1 = 35 \)

- Sample a new proposal value \( s'_1 \) from a uniform distribution:
  \[
  U[s^0_{\text{min}}, s^0_2] = U[0, 61] \rightarrow s'_1 = 51
  \]

- Accept/reject the candidate according to \( \alpha_x \) \( \rightarrow \) e.g., accept: \( s^1_1 = s'_1 \)

\[
\begin{array}{ccccccc}
  k^l & s^1_1 & s^1_2 & \theta^1_1 & \theta^1_2 & \theta^1_3 \\
  \text{Sample 1} & 2 & 51 & 61 & 4.04 & 1.51 & 5.75
\end{array}
\]
Reversible-jump MCMC: example (4)

- Iteration 2:

- Calculate the probabilities for each possible move: since \( k \) still = 2 the probabilities are the same as before!

\[
\begin{align*}
\eta_k &= \eta_2 = 0.0500 \\
\chi_k &= \chi_2 = 0.0500 \\
b_k &= b_2 = 0.2250 \\
d_k &= d_2 = 0.6750
\end{align*}
\]

- Sample one of the possible moves

\[ r = 0.65 \]

"DEATH" OF A LOCATION
Reversible-jump MCMC: example (5)

- Select randomly one of the changepoints \( \rightarrow s_2^1 = 61 \)

- Proposed value: 
  \[
  (s_2^1 - s_1^1)\theta_2^1 + (s_{\text{max}} - s_2^1)\theta_3^1 = (s_{\text{max}} - s_1^1)\theta_2^2 \rightarrow \theta_2^2 = 4.88
  \]

- Accept/reject the candidate according to \( \alpha_d \rightarrow \) e.g., accept: \( \theta_2^2 = \theta_2^{'2} \)

<table>
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<th>Sample 2</th>
<th>( k^2 )</th>
<th>( s_1^2 )</th>
<th>( s_2^2 )</th>
<th>( \theta_1^2 )</th>
<th>( \theta_2^2 )</th>
<th>( \theta_3^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>51</td>
<td>/</td>
<td>4.04</td>
<td>4.88</td>
<td>/</td>
</tr>
</tbody>
</table>
### Reversible-jump MCMC: example (6)

<table>
<thead>
<tr>
<th></th>
<th>$k$</th>
<th>$s_1$</th>
<th>$s_2$</th>
<th>$s_3$</th>
<th>$\theta_1$</th>
<th>$\theta_2$</th>
<th>$\theta_3$</th>
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</tr>
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<td>Sample 1</td>
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<td></td>
<td>4.04</td>
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<tr>
<td>Sample $u$</td>
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<td>$s_1^u$</td>
<td>$s_2^u$</td>
<td>$s_3^u$</td>
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<td>$\theta_2^u$</td>
<td>$\theta_3^u$</td>
<td>$\theta_4^u$</td>
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<tr>
<td>Sample $u+1$</td>
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<td>$s_3^{u+1}$</td>
<td>$\theta_1^{u+1}$</td>
<td>$\theta_2^{u+1}$</td>
<td>$\theta_3^{u+1}$</td>
<td>$\theta_4^{u+1}$</td>
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<tr>
<td>Sample $Ns$</td>
<td>1</td>
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<td></td>
<td></td>
<td>$\theta_1^{Ns}$</td>
<td>$\theta_2^{Ns}$</td>
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</table>

**Posterior distribution of the number of changepoints**

![Graph showing the posterior distribution of the number of changepoints](image)
Reversible-jump MCMC: example (7)

<table>
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<tr>
<th></th>
<th>$k$</th>
<th>$s_1$</th>
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<th>$\theta_2$</th>
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<td>$\theta_4^{u+1}$</td>
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<td>$s_1^{Ns}$</td>
<td></td>
<td></td>
<td>$\theta_1^{Ns}$</td>
<td>$\theta_2^{Ns}$</td>
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</tr>
</tbody>
</table>

$$
\pi(s \mid x, k = 2) \\
\pi(s \mid x, k = 1) \\
\pi(s \mid x, k = 3)
$$

$$
\pi(s \mid x) = \sum_k \pi(s \mid x, k) \pi(k \mid x)
$$
Application 1: Component degradation due to reparations or aging
Application 1: inhomogeneous Poisson process

Synthetic dataset

λ₁ = 1  λ₂ = 2  λ₃ = 4

Experimental dataset:

\[ x = \{x₁, x₂, \ldots, xₙ\} \]
\[ t = \{t₁, t₂, \ldots, tₙ\} \] (N = 240 failure times)

Likelihood function

\[ L(\theta | x) = L(\lambda | t) = \prod_{i=1}^{N} \lambda(t_i) \exp \left[ -\int_{s_0=0}^{s_{k+1}=T} \lambda(t) \, dt \right] \]
Application 1 – Results: posterior distributions

Number of changepoints $k$

Changepoint locations $s_i$

Failure rates, $\lambda_i$

$\lambda_1 = 1$

$\lambda_2 = 2$

$\lambda_3 = 4$

$s_1 = 84$

$s_2 = 120$
Application 2: 
Deterioration due to fatigue
Application: crack growth due to fatigue

Synthetic dataset

Paris-Erdogan law:

\[
\frac{dZ_t}{dt} = a_0 Z_t^b X_t
\]

\(a_0, b = \text{constant}\)

\(Z_t = \text{crack size}\)

\(X_t = \text{multiplicative noise } \sim \exp[N(\mu, \sigma)]\)

Experimental dataset:

\(x = \{x_1, x_2, \ldots, x_N\}\)

\(Z = \{Z_1, Z_2, \ldots, Z_N\} \ (N = 90 \text{ observations})\)

Likelihood function

Setting \(Y_t(X_t) = \log\left(\frac{1}{a_0} \frac{dZ_t}{dt} Z_t^{-b}\right) = \log(X_t) \approx N(\mu, \sigma)\) then

\[
L(Y_t(Z_t) | \mu, \sigma) \propto \frac{1}{\sigma^N} \exp\left[-\sum_{i=1}^{N} \frac{(Y_i - \mu)^2}{2\sigma^2}\right]
\]
Application 2 – Results: posterior distributions

- Number of changepoints $k$
  - $k = 2$

- Changepoint locations $s_i$
  - $s_1 = 20$
  - $s_2 = 60$

- Parameter $a_i = \exp(\mu_i)$
  - $a_1 = 1.2$
  - $a_2 = 1.6$

- Standard deviation, $\sigma_i$
  - $\sigma_1 = 0.9$
  - $\sigma_2 = 0.4$