

CPSC 535

Trans-dimensional MCMC

AD

March 2007

- Bayesian Model Selection

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- Metropolis-Hastings on a General State-Space

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- Metropolis-Hastings on a General State-Space
- Trans-dimensional Markov chain Monte Carlo.

- Most Bayesian models discussed until now: prior $p(\theta)$ and likelihood $p(y|\theta)$. Using MCMC, we sample from

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- We discuss several examples where the model under study is fully specified.
- In practice, we might have a collection of candidate models. This class of problems include cases where “the number of unknowns is something you don’t know” (Green, 1995).

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 - The likelihood is $p(y | k, \theta_k)$.
- You can think of it as a “standard” Bayesian model of parameter $(k, \theta_k) \in \cup_{i \in \mathcal{K}} (\{i\} \times \Theta_i)$.

- The Bayes' rule gives the posterior

$$p(k, \theta_k | y) = \frac{p(k) p(\theta_k | k) p(y | k, \theta_k)}{\sum_{i \in \mathcal{K}} \int_{\Theta_i} p(i) p(\theta_i | i) p(y | i, \theta_i) d\theta_i}$$

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- From this posterior, we can compute

$$p(k | y) \text{ and } \frac{p(y | k)}{p(y | j)} = \frac{p(k | y) p(j)}{p(j | y) p(k)}$$

or performing Bayesian model averaging

$$p(y' | y) = \sum_{i \in \mathcal{K}} \int_{\Theta_i} p(y' | i, \theta_i) p(i, \theta_i | y) d\theta_i$$

Example: Autoregression

- The model $k \in \mathcal{K} = \{1, \dots, k_{\max}\}$ is given by an AR of order k

$$Y_n = \sum_{i=1}^k a_i Y_{n-i} + \sigma V_n \text{ where } V_n \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$$

and we have $\theta_k = (a_{1:k}, \sigma^2) \in \mathbb{R}^k \times \mathbb{R}^+$.

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- We need to defined a prior $p(k, \theta_k) = p(k) p(\theta_k | k)$, say

$$\begin{aligned} p(k) &= k_{\max}^{-1} \text{ for } k \in \mathcal{K}, \\ p(\theta_k | k) &= \mathcal{N}(a_{1:k}; 0, \sigma^2 \delta^2 I_k) \mathcal{IG}\left(\sigma^2; \frac{\nu_0}{2}, \frac{\gamma_0}{2}\right). \end{aligned}$$

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- One should be careful, the parameters denoted similarly can have a different “meaning” so that computing say $p(\sigma^2 | y)$ does not mean much.
- Some authors favour a more precise notation $\theta_k = (a_{k,1:k}, \sigma_k^2)$ but this can be cumbersome.

Example: Finite Mixture of Gaussians

- The model $k \in \mathcal{K} = \{1, \dots, k_{\max}\}$ is given by a mixture of k Gaussians

$$Y_n \sim \sum_{i=1}^k \pi_i \mathcal{N}(\mu_i, \sigma_i^2).$$

and we have $\theta_k = (\pi_{1:k}, \mu_{1:k}, \sigma_{1:k}^2) \in S_k \times \mathbb{R}^k \times (\mathbb{R}^+)^k$.

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$$p(k) = \frac{1}{k_{\max}},$$

$$p(\theta_k | k) = \mathcal{D}(\pi_{1:k}; 1, \dots, 1) \prod_{i=1}^k \mathcal{N}(\mu_i; \alpha, \beta) \mathcal{IG}(\sigma_i^2; \frac{\nu_0}{2}, \frac{\gamma_0}{2}).$$

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Problem Statement

- As stated before, Bayesian model selection problems corresponds to the case where the parameter space is simply $\cup_{k \in \mathcal{K}} (\{k\} \times \Theta_k)$.
- Can we define MCMC algorithms - i.e. Markov chain kernels with fixed invariant distribution $\pi(k, \theta_k) = \pi(k) \pi_k(\theta_k)$ - ?
- We are going to present a generalization of MH after revisiting first the MH algorithm.

- We say that a measure $\gamma(dx)$ admits a density with respect to a measure $\lambda(dx)$ if for any (measurable) set $A \in B(\mathcal{X})$

$$\lambda(A) = 0 \Rightarrow \gamma(A) = 0$$

and we call

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- In 99% of the applications in statistics $\lambda(dx)$ is the Lebesgue measure dx and we write

$$\frac{\gamma(dx)}{\lambda(dx)} = \frac{\gamma(dx)}{dx} = \gamma(x).$$

- The standard MH algorithm where $\mathcal{X} \subset \mathbb{R}^d$ corresponds to

$$K(x, dx') = \alpha(x, x') q(x, dx') + \left(1 - \int \alpha(x, z) q(x, dz)\right) \delta_x(dx')$$

where

$$\alpha(x, x') = \min \left\{ 1, \frac{\pi(x') q(x', x)}{\pi(x) q(x, x')} \right\}$$

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- You should think of

$$\frac{\pi(x') q(x', x)}{\pi(x) q(x, x')}$$

not as just a “number”!

- The acceptance ratio corresponds to a ratio of probability measures -importance weight- defined on the same spaces

$$\frac{\pi(dx') q(x', dx)}{\pi(dx) q(x, dx')} = \frac{\pi(x') dx' q(x', x) dx}{\pi(x) dx q(x, x') dx'} = \frac{\pi(x') q(x', x)}{\pi(x) q(x, x')}.$$

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- You can only compared points defined on the same joint space. If you have $x = (x_1, x_2)$ and $\pi_1(dx_1) = \pi_1(x_1) dx_1$, $\pi_2(dx_1, dx_2) = \pi_2(x_1, x_2) dx_1 dx_2$, you can compute numerically

$$\frac{\pi_2(x_1, x_2)}{\pi_1(x_1)}$$

but it means *nothing* as the measures π_1 and π_2 are not defined on the same space. You CANNOT compare a surface to a volume!

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- To construct this move, you can use $u \in \mathbb{R}^r$ and $u' \in \mathbb{R}^{r'}$ and a *one-to-one differentiable* mapping $h: \mathbb{R}^d \times \mathbb{R}^r \rightarrow \mathbb{R}^{d'} \times \mathbb{R}^{r'}$

$$(x', u') = h(x, u) \text{ where } u \sim g$$

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- We need $d + r = d' + r'$ and typically, if $d < d'$, then $r' = 0$ and $r = d' - d$, that is in most case the variable u' is not introduced.

- We can rewrite formally

$$\pi(dx) q(x, (dx', du')) = \pi(x) g(u) dx du$$

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$$\pi(dx') q(x', (dx, du)) = \pi(x') g'(u') dx' du'.$$

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- An acceptance ratio ensuring π -reversibility of this trans-dimensional move is given by

$$\frac{\pi(dx') q(x', (dx, du))}{\pi(dx) q(x, (dx', du'))} = \frac{\pi(x') g'(u')}{\pi(x) g(u)} \left| \frac{\partial(x', u')}{\partial(x, u)} \right|.$$

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- In this respect, the RJMCMC is an extension of standard MH as you need to introduce auxiliary variables u and u' .

- Assume we have a distribution defined on $\{1\} \times \mathbb{R} \cup \{2\} \times \mathbb{R} \times \mathbb{R}$. We want to propose some moves to go from $(1, \theta)$ to $(2, \theta_1, \theta_2)$.

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i.e. we do not need to introduce a variable u' . Its inverse is given by

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- The acceptance probability for this “birth” move is given by

$$\begin{aligned} & \min \left(1, \frac{\pi(2, \theta_1, \theta_2)}{\pi(1, \theta)} \frac{1}{g(u)} \left| \frac{\partial(\theta_1, \theta_2)}{\partial(\theta, u)} \right| \right) \\ &= \min \left(1, \frac{\pi(2, \theta_1, \theta_2)}{\pi(1, \theta_1) g(\theta_2)} \right). \end{aligned}$$

- The acceptance probability for the associated “death move” is

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- Once the birth move is defined then the death move follows automatically. In the death move, we do not simulate from g but its expression still appear in the acceptance probability.

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- Clearly if we have $g(\theta_2|\theta_1) = \pi(\theta_2|2, \theta_1)$ then the expressions simplify

$$\begin{aligned} \min \left(1, \frac{\pi(2, \theta_1, \theta_2)}{\pi(1, \theta_1) g(\theta_2|\theta_1)} \right) &= \min \left(1, \frac{\pi(2, \theta_1)}{\pi(1, \theta_1)} \right), \\ \min \left(1, \frac{\pi(1, \theta) g(u|\theta)}{\pi(2, \theta, u)} \right) &= \min \left(1, \frac{\pi(1, \theta)}{\pi(2, \theta)} \right). \end{aligned}$$

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- We can propose $u \sim g \in \mathbb{R}$ and set

$$(\theta_1, \theta_2) = h(\theta, u) = (\theta - u, \theta + u).$$

Its inverse is given by

$$(\theta, u) = h^{-1}(\theta_1, \theta_2) = \left(\frac{\theta_1 + \theta_2}{2}, \frac{\theta_2 - \theta_1}{2} \right).$$

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- The acceptance probability for this “split” move is given by

$$\begin{aligned} & \min \left(1, \frac{\pi(2, \theta_1, \theta_2)}{\pi(1, \theta)} \frac{1}{g(u)} \left| \frac{\partial(\theta_1, \theta_2)}{\partial(\theta, u)} \right| \right) \\ &= \min \left(1, \frac{\pi(2, \theta_1, \theta_2)}{\pi\left(1, \frac{\theta_1 + \theta_2}{2}\right)} \frac{2}{g\left(\frac{\theta_2 - \theta_1}{2}\right)} \right). \end{aligned}$$

- The acceptance probability for the associated “merge move” is

$$\begin{aligned} & \min \left(1, \frac{\pi(1, \theta)}{\pi(2, \theta_1, \theta_2)} g(u) \left| \frac{\partial(\theta, u)}{\partial(\theta_1, \theta_2)} \right| \right) \\ = & \min \left(1, \frac{\pi(1, \theta)}{\pi(2, \theta - u, \theta + u)} \frac{g(u)}{2} \right) \end{aligned}$$

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- Once the split move is defined then the merge move follows automatically. In the merge move, we do not simulate from g but its expression still appear in the acceptance probability.

- In practice, the algorithm is based on a combination of moves to move from $x = (k, \theta_k)$ to $x' = (k', \theta_{k'})$ indexed by $i \in \mathcal{M}$ and in this case we just need to have

$$\begin{aligned} & \int_{(x, x') \in A \times B} \pi(dx) \alpha_i(x, x') q_i(x, dx') \\ &= \int_{(x, x') \in A \times B} \pi(dx') \alpha_i(x', x) q_i(x', dx) \end{aligned}$$

to ensure that the kernel $P(x, B)$ defined for $x \notin B$

$$P(x, B) = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} \int_B \alpha_i(x, x') q_i(x, dx')$$

is π -reversible.

- In practice, the algorithm is based on a combination of moves to move from $x = (k, \theta_k)$ to $x' = (k', \theta_{k'})$ indexed by $i \in \mathcal{M}$ and in this case we just need to have

$$\begin{aligned} & \int_{(x,x') \in A \times B} \pi(dx) \alpha_i(x, x') q_i(x, dx') \\ &= \int_{(x,x') \in A \times B} \pi(dx') \alpha_i(x', x) q_i(x', dx) \end{aligned}$$

to ensure that the kernel $P(x, B)$ defined for $x \notin B$

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- In practice, we would like to have

$$P(x, B) = \sum_{i \in \mathcal{M}} j_i(x) \int_B \alpha_i(x, x') q_i(x, dx')$$

where $j_i(x)$ is the probability of selecting the move i once we are in x and $\sum_{i \in \mathcal{M}} j_i(x) = 1$.

- In this case reversibility is ensured if

$$\begin{aligned} & \int_{(x,x') \in A \times B} \pi(dx) j_i(x) \alpha_i(x, x') q_i(x, dx') \\ &= \int_{(x,x') \in A \times B} \pi(dx') j_i(x') \alpha_i(x', x) q_i(x', dx) \end{aligned}$$

which is satisfied if

$$\alpha_i(x, x') = \min \left(1, \frac{\pi(x') j_i(x') g'_i(u')}{\pi(x) j_i(x) g_i(u)} \left| \frac{\partial(x', u')}{\partial(x, u)} \right| \right).$$

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- In practice, we will only have a limited number of moves possible from each point x .

Reversible Jump MCMC Algorithm

- For each point $x = (k, \theta_k)$, we define a collection of potential moves selected randomly with probability $j_i(x)$ where $i \in \mathcal{M}$

Reversible Jump MCMC Algorithm

- For each point $x = (k, \theta_k)$, we define a collection of potential moves selected randomly with probability $j_i(x)$ where $i \in \mathcal{M}$
- To move from $x = (k, \theta_k)$ to $x' = (k', \theta_{k'})$, we build one (or several) deterministic differentiable and invertible mapping(s)

$$(\theta_{k'}, u_{k',k}) = T_{k,k'}(\theta_k, u_{k,k'})$$

where $u_{k,k'} \sim g_{k,k'}$ and $u_{k',k} \sim g_{k',k}$ and we accept the move with proba

$$\min \left(1, \frac{\pi(k', \theta_{k'}) j_i(k', \theta_{k'}) g_{k',k}(u_{k',k})}{\pi(k, \theta_k) j_i(k, \theta_k) g_{k,k'}(u_{k,k'})} \left| \frac{\partial T_{k,k'}(\theta_k, u_{k,k'})}{\partial (\theta_k, u_{k,k'})} \right| \right).$$

Example: Autoregression

- The model $k \in \mathcal{K} = \{1, \dots, k_{\max}\}$ is given by an AR of order k

$$Y_n = \sum_{i=1}^k a_i Y_{n-i} + \sigma V_n \text{ where } V_n \sim \mathcal{N}(0, 1)$$

and we have $\theta_k = (a_{k,1:k}, \sigma_k^2) \in \mathbb{R}^k \times \mathbb{R}^+$ where

$$\begin{aligned} p(k) &= k_{\max}^{-1} \text{ for } k \in \mathcal{K}, \\ p(\theta_k | k) &= \mathcal{N}(a_{k,1:k}; 0, \sigma_k^2 \delta^2 I_k) \mathcal{IG}\left(\sigma^2; \frac{\nu_0}{2}, \frac{\gamma_0}{2}\right). \end{aligned}$$

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- Note that this is not very clever as $p(k | y_{1:T})$ is known up to a normalizing constant!

- We propose the following moves. If we have $(k, a_{1:k}, \sigma_k^2)$ then with probability b_k we propose a birth move if $k \leq k_{\max}$, with proba u_k we propose an update move and with proba $d_k = 1 - b_k - u_k$ we propose a death move.

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- We have $d_1 = 0$ and $b_{k_{\max}} = 0$.
- The *update move* can simply be done in a Gibbs step as

$$p(\theta_k | y_{1:T}, k) = \mathcal{N}(a_{k,1:k}; m_k, \sigma^2 \Sigma_k) \mathcal{IG}\left(\sigma^2; \frac{\nu_k}{2}, \frac{\gamma_k}{2}\right)$$

- *Birth move*: We propose to move from k to $k + 1$

$$(a_{k+1,1:k}, a_{k+1,k+1}, \sigma_{k+1}^2) = (a_{k,1:k}, u, \sigma_k^2) \text{ where } u \sim g_{k,k+1}$$

and the acceptance probability is

$$\min \left(1, \frac{p(a_{k,1:k}, u, \sigma_k^2, k+1 | y_{1:T}) d_{k+1}}{p(a_{k,1:k}, \sigma_k^2, k | y_{1:T}) b_k g_{k,k+1}(u)} \right).$$

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- *Death move*: We propose to move from k to $k - 1$

$$(a_{k-1,1:k-1}, u, \sigma_{k-1}^2) = (a_{k,1:k-1}, a_{k,k}, \sigma_k^2)$$

and the acceptance probability is

$$\min \left(1, \frac{p(a_{k,1:k-1}, \sigma_k^2, k-1 | y_{1:T}) b_{k-1} g_{k-1,k}(a_{k,k})}{p(a_{k,1:k}, \sigma_k^2, k | y_{1:T}) d_k} \right).$$

- The performance are obviously very dependent on the selection of the proposal distribution. We select whenever possible the full conditional distribution, i.e. we have

$$u = a_{k+1,k+1} \sim p(a_{k+1,k+1} | y_{1:T}, a_{k,1:k}, \sigma_k^2, k+1) \text{ and}$$

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- In such cases, it is actually possible to reject a candidate before sampling it!

- We simulate 200 data with $k = 5$ and use 10,000 iterations of RJMCMC.

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- Histograms of $(\theta_k^{(i)})$ for which $k^{(i)} = k_0$ yields estimates of $p(\theta_{k_0} | y, k_0)$.
- The algorithm provides us with an estimate of $p(k | y)$ which matches analytical expressions.

Example: Finite Mixture of Gaussians

- The model $k \in \mathcal{K} = \{1, \dots, k_{\max}\}$ is given by a mixture of k Gaussians

$$Y_n \sim \sum_{i=1}^k \pi_i \mathcal{N}(\mu_i, \sigma_i^2).$$

and we have $\theta_k = (\pi_{1:k}, \mu_{1:k}, \sigma_{1:k}^2) \in \mathcal{S}_k \times \mathbb{R}^k \times (\mathbb{R}^+)^k$.

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- We need to defined a prior $p(k, \theta_k) = p(k) p(\theta_k | k)$, say

$$p(k) = k_{\max}^{-1} \text{ for } k \in \mathcal{K}$$

$$p(\theta_k | k) = \mathcal{D}(\pi_{k,1:k}; 1, \dots, 1) \prod_{i=1}^k \mathcal{N}(\mu_{k,i}; \alpha, \beta) \mathcal{IG}\left(\sigma_{k,i}^2; \frac{\nu_0}{2}, \frac{\gamma_0}{2}\right).$$

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- Given T data, we are interested in $\pi(k, \theta_k | y_{1:T})$.

- When k is fixed, we will use Gibbs steps to sample from $\pi(\theta_k, z_{1:T} | y_{1:T}, k)$ where $z_{1:T}$ are the discrete latent variables such that $\Pr(z_n = i | k, \theta_k) = \pi_{k,i}$.

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- To allow to move in the model space, we define a birth and death move.
- The birth and death moves use as a target $\pi(\theta_k | y_{1:T}, k)$ and not $\pi(\theta_k, z_{1:T} | y_{1:T}, k) \Rightarrow$ Reduced dimensionality, easier to design moves.

- We propose a naive move to go from $k \rightarrow k + 1$ where $j \sim \mathcal{U}_{\{1, \dots, k+1\}}$

$$\begin{aligned}\mu_{k+1, -j} &= \mu_{k, 1:k}, \quad \sigma_{k+1, -j}^2 = \sigma_{k, 1:k}^2, \\ \pi_{k+1, -j} &= (1 - \pi_{k+1, j}) \pi_{k, -j},\end{aligned}$$

where $(\pi_{k+1, j}, \mu_{k+1, j}, \sigma_{k+1, j}^2) \sim g_{k, k+1}$ (prior distribution in practice).

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- The Jacobian of the transformation is $(1 - \pi_{k+1, j})^{k-1}$ (only $k - 1$ “true” variables for $\pi_{k, -j}$)

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- The Jacobian of the transformation is $(1 - \pi_{k+1,j})^{k-1}$ (only $k - 1$ “true” variables for $\pi_{k,-j}$)
- Now one has to be careful when considering the reverse death move. Assume the death move going from $k + 1 \rightarrow k$ by removing the component j .

- The acceptance probability of the birth move is given by $\min(1, A)$ where

$$A = \frac{\pi(k+1, \pi_{k+1,1:k+1}, \mu_{k+1,1:k+1}, \sigma_{k+1,1:k+1}^2 | y_{1:T})}{\pi(k, \pi_{k,1:k}, \mu_{k,1:k}, \sigma_{k,1:k}^2 | y_{1:T})} \times \frac{(d_{k+1,k} / (k+1)) (1 - \pi_{k+1,j})^{k-1}}{(b_{k,k+1} / (k+1)) g_{k,k+1}(\pi_{k+1,j}, \mu_{k+1,j}, \sigma_j^2)}.$$

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- This move will work properly if the prior is not too diffuse. Otherwise the acceptance probability will be small.
- We have $(k+1)$ birth moves to move from $k \rightarrow k+1$ and $k+1$ associated death moves.

- To move from $k \rightarrow k + 1$, one can also select a split move of the component $j \sim \mathcal{U}_{\{1, \dots, k\}}$

$$\begin{aligned} \pi_{k+1,j} &= u_1 \pi_{k,j}, \quad \pi_{k+1,j+1} = (1 - u_1) \pi_{k,j}, \\ \mu_{k+1,j} &= u_2 \mu_{k,j}, \quad \mu_{k+1,j+1} = \frac{\pi_{k,j} - \pi_{k+1,j} u_2}{\pi_{k,j} - \pi_{k+1,j}} \mu_{k,j}, \\ \sigma_{k+1,j}^2 &= u_3 \sigma_{k,j}^2, \quad \sigma_{k+1,j+1}^2 = \frac{\pi_{k,j} - \pi_{k+1,j} u_3}{\pi_{k,j} - \pi_{k+1,j}} \sigma_{k,j}^2 \end{aligned}$$

with $u_1, u_2, u_3 \sim \mathcal{U}(0, 1)$.

- The associated merge move is

$$\pi_{k,j} = \pi_{k+1,j} + \pi_{k+1,j+1},$$

$$\pi_{k,j}\mu_{k,j} = \pi_{k+1,j}\mu_{k+1,j} + \pi_{k+1,j+1}\mu_{k+1,j+1},$$

$$\pi_{k,j}\sigma_{k,j}^2 = \pi_{k+1,j}\sigma_{k+1,j}^2 + \pi_{k+1,j+1}\sigma_{k+1,j+1}^2.$$

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- The Jacobian of the transformation of the split is given by

$$\left| \frac{\partial (\pi_{k+1,1:k+1}, \mu_{k+1,1:k+1}, \sigma_{k+1,1:k+1}^2)}{\partial (\pi_{k,1:k}, \mu_{k,1:k}, \sigma_{k,1:k}^2, u_1, u_2, u_3)} \right| = \frac{\pi_{k,j}^3}{(1-u_1)^2} |\mu_{k,j}| \sigma_{k,j}^2.$$

- It follows that the acceptance probability of the split move with $j \sim \mathcal{U}_{\{1, \dots, k\}}$ is $\min(1, A)$ where

$$A = \frac{\pi(k+1, \pi_{k+1,1:k+1}, \mu_{k+1,1:k+1}, \sigma_{k+1,1:k+1}^2 \mid y_{1:T})}{\pi(k, \pi_{k,1:k}, \mu_{k,1:k}, \sigma_{k,1:k}^2 \mid y_{1:T})} \times \frac{(m_{k+1,k}/k)}{(s_{k,k+1}/k)} \times \frac{\pi_{k,j}^3}{(1-u_1)^2} \mid \mu_{k,j} \mid \sigma_{k,j}^2.$$

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- You should think of the split move as a mixture of k split moves and you have k associated merge moves.

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- We run the algorithm for over 1,000,000 iterations.
- We set additional constraints on the mean $\mu_{k,1} < \mu_{k,2} < \dots < \mu_{k,k}$.
- The cumulative averages stabilize very quickly.

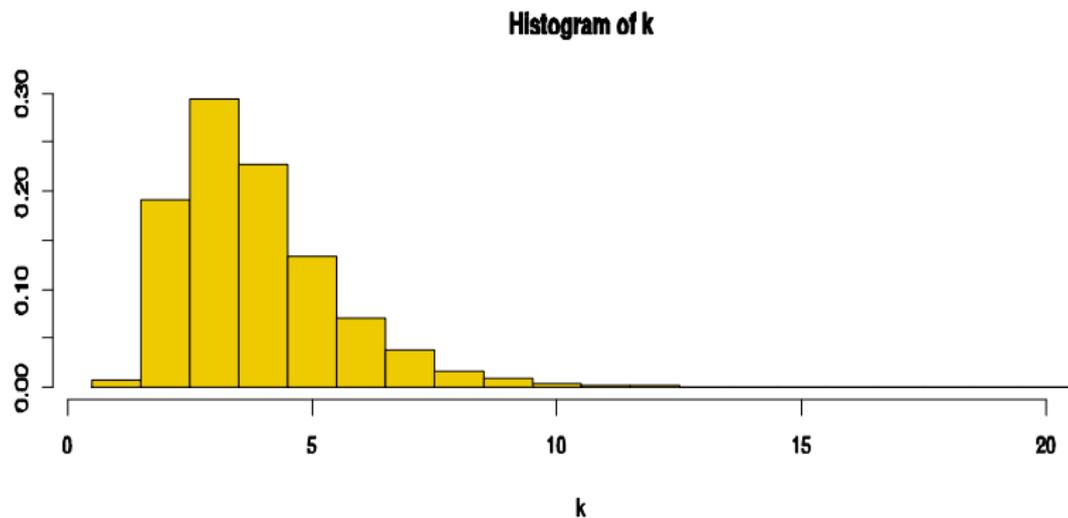


Figure: Estimation of the marginal posterior distribution $p(k|y_{1:T})$

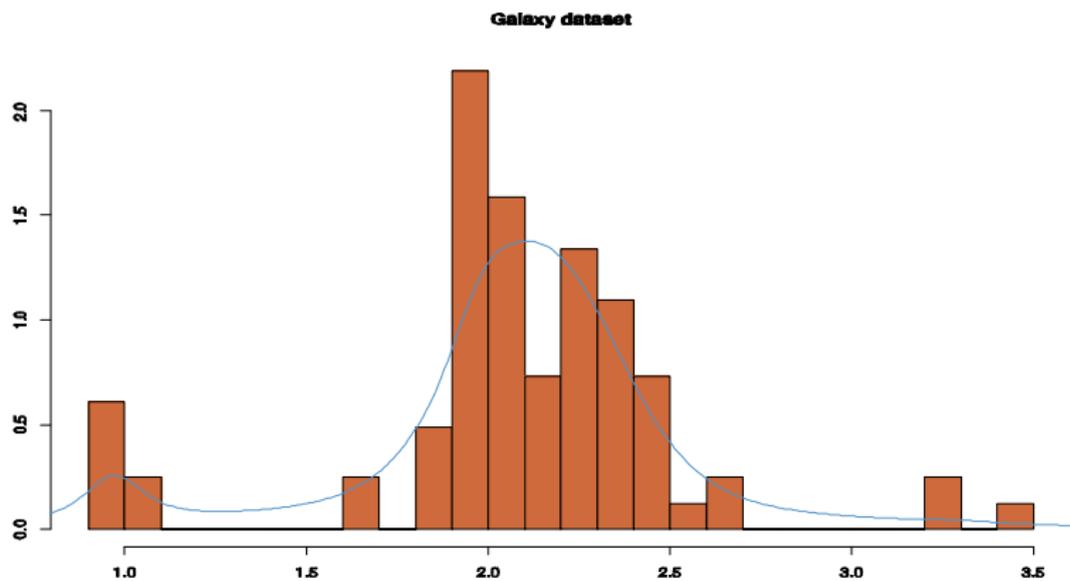


Figure: Estimation of $\mathbb{E}[f(y|k, \theta_k) | y_{1:T}]$

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- Designing efficient trans-dimensional MCMC algorithms is still a research problem.