Reversible Jump Markov Chain Monte Carlo

Based on Chapter 3 in Handbook of Markov Chain Monte Carlo

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Talk by Nir Levin, July 2015

Y. Fan, S. A. Sisson RJMCMC

Outline

Introduction

- Motivation
- Model
- The M.H Algorithm
- M.H to Reversible Jump
- Some Use Cases

2 Implementation

- General Approach
- Marginalization
- Centering & Order Methods
- Generic Samplers
- ③ Simulation
 - Model Formulation
 - Results

Motivation

Model The M.H Algorithm M.H to Reversible Jump Some Use Cases

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Motivation Model The M.H Algorithm M.H to Reversible Jump Some Use Cases

Start With The End

$$y = \sum_{i=1}^n x_i b_i + \varepsilon$$

- n ≤ m where m is the number of possible inputs, x_i's are the inputs, y is the output (what we measure), ε is the measurment noise.
- We wish to estimate {n, b₁,.., b_n} using Bayesian modeling, given k independent measurments.
- Next, we define relevant distributions for the model.

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- Next, we define relevant distributions for the model.

Motivation Model The M.H Algorithm M.H to Reversible Jump Some Use Cases

Starting With The End (Cont'd)

• The likelihood is given by,

$$L(y|n,b) = \left(\frac{1}{\sqrt{2\pi\sigma_0^2}}\right)^k \cdot \exp\left\{-\frac{\left\|y - X^T b\right\|^2}{2\sigma_0^2}\right\}$$

• The prior over b is given by,

$$p(b|n) = \left(\frac{1}{\sqrt{2\pi\sigma_p^2}}\right)^n \cdot \exp\left\{-\frac{\|b-\mu\|^2}{2\sigma_p^2}\right\}$$

• The prior over *n* is given by,

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Motivation Model The M.H Algorithm M.H to Reversible Jump Some Use Cases

Understanding the Problem

- Bayesian modeling context for observed data.
- Countable collection Models *M* = {*M*₁, *M*₂, ..} indexed by k ∈ *K*.
- Each model *M_k* has an *n_k*-dimensional vector of unknown parameters, θ_k ∈ ℝ^{n_k}. *n_k* can be different for different k ∈ *X*.

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Understanding the Problem (Cont'd)

• The joint posterior of $(k, \theta_k | x)$ is given by,

$$\pi(k,\theta_k|x) = \frac{L(x|k,\theta_k) p(\theta_k|k) p(k)}{\sum_{k' \in \mathscr{K}} \int_{\mathbb{R}^{n_{k'}}} L(x|k',\theta'_{k'}) p(\theta'_{k'}|k') p(k')}$$

- L(x|k, θ_k) is the likelihood distribution, ρ(θ_k|k) is the prior of θ_k under model M_k and ρ(k) is the prior for model M_k.
- Reversible Jump sets the posterior distribution as the target of MCMC sampler over the state space Θ = ∪_{k∈𝔅} ({k} × ℝ^{n_k}).

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Motivation Model **The M.H Algorithm** M.H to Reversible Jump Some Use Cases

Reminder

- Propose some transition distribution $q(\theta, \theta') \equiv q(\theta'|\theta)$ and target distribution π .
- Starting with some initial state θ_0 , the algorithm proceeds as follows:
 - **()** Given the current state heta, generate $heta' \sim q(heta, \cdot)$.

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 $eta:=egin{cases} heta' & ext{w.p.} \ lpha(heta, heta') \ heta & ext{otherwise} \end{cases}$

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

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Motivation Model **The M.H Algorithm** M.H to Reversible Jump Some Use Cases



- The motivation behind M.H algorithm is satisfying the detailed balance condition, so that π is the stationary distribution.
- Following the same concept we can suggest MCMC for multi-models as well, let's call it Reversible Jump MCMC.

Motivation Model The M.H Algorithm M.H to Reversible Jump Some Use Cases

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Motivation Model The M.H Algorithm **M.H to Reversible Jump** Some Use Cases

Basically the Same

- Initialize the state for some (k, θ_k) .
- Proceed as follows:
 - Generate a new state $\left(\, k', \, heta_{k'}' \,
 ight)$ by,
 - [] Within-model move: fixed k, update $ilde{ heta}_k$.
 - Between-models move: generate $(k', \theta'_{k'})$ using $(k, \tilde{\theta}_k)$ and a mapping function.

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Use acceptance/rejection scheme to determine next state.

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Examples Time

Finite Mixture Models

Model is in the form

$$f(x|\theta_k) = \sum_{j=1}^k \omega_j f_j(x|\phi_j)$$

where $\theta_k = (\phi_1, ..., \phi_k)$, $\sum_{j=1}^k \omega_j = 1$, and the number of mixture models, k, is also unknown.

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Examples Time (Cont'd)

Variable Selection

Model is in the form

$$Y = X_{\gamma}\beta_{\gamma} + \varepsilon$$

where γ is a binary vector indexing the subset of X to be included, β are the regression coefficients and ε is noise.

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Examples Time (Cont'd)

Autoregressive Process

Model is in the form

$$X_t = \sum_{ au=1}^k a_ au X_{t- au} + arepsilon_t$$

where a_{τ} are the coefficients, \mathcal{E}_t is white noise and the order, k, is also unknown.

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In Practice - "Dimension Matching"

- Say we wish to perform transition to a model with higher dimension, $\mathcal{M}_k : (k, \theta_k) \to \mathcal{M}_{k'} : (k', \theta'_{k'})$.
 - Generate a RV *u* of length $d_{k\to k'} = n_{k'} n_k$ from a known distribution $q_{d_{k\to k'}}(u)$.
 - Output Description ($heta_{k'} = g_{k o k'}(heta_k, u)$).

Accept new state w.p.

$$\alpha \left[(k, \theta_k), (k', \theta'_{k'}) \right] = \min \{1, A\}$$
$$A = \frac{\pi \left(k', \theta'_{k'} \right) q(k' \to k)}{\pi (k, \theta_k) q(k \to k') q_{d_{k \to k'}}(u)} \left| \frac{\partial g_{k \to k'}(\theta_k, u)}{\partial (\theta_k, u)} \right.$$

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② Use a deterministic one-to-one mapping $m{ heta}'_{k'}=g_{k
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Some Notes

- The term $q(k \to k')$ denotes probability distribution over transition $\mathcal{M}_k \to \mathcal{M}_{k'}$.
- In this setup the transition from higher to lower dimension is deterministic.
- More generally, we can simply impose

$$n_k + d_{k \to k'} = n_{k'} + d_{k' \to k}$$

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Image: A matrix

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Example Time

• Two models,

$$\mathscr{M}_1: (k=1, heta_1 \in \mathbb{R})\,, \quad \mathscr{M}_2: ig(k=2, heta_2 \in \mathbb{R}^2ig)$$

• Transition $\mathcal{M}_1 \to \mathcal{M}_2$ (stochastic)

$$\theta_2^{(1)} = \theta_1 + u, \quad \theta_2^{(2)} = \theta_1 - u$$

• Transition $\mathscr{M}_2 \to \mathscr{M}_1$ (deterministic)

$$\boldsymbol{\theta}_1 = \frac{1}{2} \left(\boldsymbol{\theta}_2^{(1)} + \boldsymbol{\theta}_2^{(2)} \right)$$

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A B > A B > A

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Making Life Easier

- In some Bayesian models, integrating over all (or parts of) θ_k is possible.
- Usually arises when assuming some structures such as conjugate priors.
- Results in smaller state space, thus often easier to implement.

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Revisit Variable Selection

$$Y = X_{\gamma}\beta_{\gamma} + \varepsilon$$

- Under some prior assumptions, β can be integrated out of the posterior.
- A Gibbs Sampler (for example) is available directly on γ .

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Helpful Heuristics - Centering Methods

- A class of methods to achieve scaling based on "local" between-models moves. Assumes g_{k→k} is given.
- Based on equal likelihood values under current and proposed models.
- Say we wish to move $\mathcal{M}_k \to \mathcal{M}_{k'}$. The RV "centering point" $c_{k \to k'}(\theta_k) = g_{k \to k'}(\theta_k, u)$, is *u* such that,

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$$L(x|k,\theta_k) = L(x|k',c_{k\to k'}(\theta_k))$$

General Approach Marginalization Centering & Order Methods Generic Samplers

Helpful Heuristics - Centering Methods

- A class of methods to achieve scaling based on "local" between-models moves. Assumes g_{k→k} is given.
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Example Time

Revisit Autoregressive Process

Remeber the model,

$$X_t = \sum_{\tau=1}^k a_\tau X_{t-\tau} + \varepsilon_t$$

• Say \mathcal{M}_k is a model of order k, and $\mathcal{M}_{k'}$ is a model order k+1. We wish to move $\mathcal{M}_k \to \mathcal{M}_{k'}$.

• In this case, we have $c_{k
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Helpful Heuristics - Order Methods

- Assume we have the "centering" constraint on u. We wish to determine a suitable $q_{k \rightarrow k'}(u)$.
- If u is a scalar, choose q_{k→k'} such that α[(k,θ_k),(k', c_{k→k'}(θ_k))] is exactly one. Intuition: Proposals close to the "centering point" will also have large acceptance probability.
- If *u* is *n*-length vector, choose $q_{k\to k'}$ such that $\nabla^n \alpha [(k, \theta_k), (k', c_{k\to k'}(\theta_k))] = 0.$ *Intuition*: Accepatance probability becomes flatter around $c_{k\to k'}(\theta_k).$

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- M.H to Reversible Jump
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 - Model Formulation
 - Results

General Approach Marginalization Centering & Order Methods Generic Samplers

- In centering & order methods, we assume we know g_{k→k'}. But how one should choose it?
- Moreover, it's not necessarily easy to compute $q_{k\to k'}$ from $g_{k\to k'}$ using the above heuristics.
- New stradegy move towards a more generic proposal machanism.
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General Approach Marginalization Centering & Order Methods Generic Samplers

Example Time

Green's Proposal

- Suppose that for each $k \in \mathcal{K}$, first and second moments of θ_k are available (denote by μ_k and $B_k B_k^T$ respectively).
- Suppose we wish to move from (k, θ_k) to model $\mathscr{M}_{k'}$.
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Example Time (Cont'd)

Green's Proposal

$$\theta_{k'}^{'} = \begin{cases} \mu_{k'} + B_{k'} \left[RB_{k}^{-1}(\theta_{k} - \mu_{k}) \right]_{1}^{n_{k'}} & \text{if } n_{k'} < n_{k} \\ \mu_{k'} + B_{k'}RB_{k}^{-1}(\theta_{k} - \mu_{k}) & \text{if } n_{k'} = n_{k} \\ \mu_{k'} + B_{k'}R \begin{pmatrix} B_{k}^{-1}(\theta_{k} - \mu_{k}) \\ u \end{pmatrix} & \text{if } n_{k'} > n_{k} \end{cases}$$

where $[\cdot]_1^m$ denotes the first *m* components, *R* fixed orthogonal matrix of order max $\{n_k, n_{k'}\}$, and $u \sim q_{n_{k'}-n_k}(u)$.
Model Formulation Results

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③ Simulation

• Model Formulation

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Model Formulation Results

Setting Up The Model

• Model is given by,

$$y = \sum_{i=1}^{n} x_i b_i + \varepsilon$$

- n ≤ m where m is the number of predictors, x_i's are the inputs, y is the output (what we measure), ε is the measurment noise.
- We wish to estimate {n, b₁,.., b_n} using Bayesian modeling, given k independent measurments.
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Model Formulation Results

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$$L(y|n,b) = \left(\frac{1}{\sqrt{2\pi\sigma_0^2}}\right)^k \cdot \exp\left\{-\frac{\left\|y - X^T b\right\|^2}{2\sigma_0^2}\right\}$$

• The prior over b is given by,

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Y. Fan, S. A. Sisson RJMCMC

Introduction Simulation

Model Formulation

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Model Formulation Results

What Model Is It From?

A simulation for n = 3:



Model Formulation Results

What Model Is It From?

A simulation for n = 7:



Model Formulation Results

Examining a Model - PDF

A simulation for n = 2. Real coefficients are $\{4.99, 5.12\}$. "Clutter" - State Space Samples.



Model Formulation Results

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Model Formulation Results

Examining a Model - Clutter

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