Reversible Jump Markov Chain Monte Carlo

Extending Metropolis-Hastings to Varying Dimensional Spaces

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Motivation: Sampling Across Model Spaces

- Many scientific problems require comparing models of different complexity (i.e. different paramter spaces)
- Traditional MCMC methods aren't able to compare different models of different complexity due to the time reversibility constraint.
- Solution: Reversible Jump Markov Chain Monte Carlo (RJMCMC)

Metropolis-Hastings: Problem Setup

Core Challenge

- Goal: Sample from target distribution $\pi(x)$
- Direct sampling often impossible
- Requires clever proposal mechanisms

Key Components

- Target distribution: $\pi(x)$
- Candidate/Proposal distribution: $q(x, x') = q(x'|x)$ (for notation)
- Acceptance probability: α

Acceptance Probability Derivation

$$\alpha = \underbrace{\frac{\pi(x')}{\pi(x_t)}}_{\text{Target Distribution Ratio}} \underbrace{\frac{q(x_t, x')}{q(x', x_t)}}_{\text{Proposal Density Correction}}$$

First Ratio

- Compares likelihood of proposed state
- Drives exploration of high-probability regions

Second Ratio

- Corrects for asymmetric proposals
- Ensures detailed balance

Detailed Balance Condition

Theorem (Detailed Balance)

A Markov chain satisfies the detailed balance condition if:

$$\pi(x)p(x,x') = \pi(x')p(x',x)$$

where $p(x,x')$ is the transition density. The above can be rewritten as:

- Guarantees long-run convergence to target distribution

Fix any sets $A, A' \subseteq \mathbb{R}^k$.

$$\int_A \int_{A'} \pi(x)p\left(x,x'\right) dx' dx = \int_A \int_{A'} \pi\left(x'\right) p\left(x',x\right) dx dx'$$

RJMCMC: Example

Suppose we want to sample from the following mixture model: $(\mathrm{m}, \theta_{\mathrm{m}})$ where m is the model choice indicator.
Consider a mixture model: $Y_i = \sum_{m=1}^{M} w_m \pi_m(\cdot|\theta_m)$

- Different models might have different dimensions, hence the use of RJMCMC

Mathematical Formulation

Consider a case where we only need to take on trans-dimensional jump

Consider moving from a n-dimensional state x to a n'-dimentional state x':

- Add auxilliarry random vectors u and u' with densities g and g' and dimensions r and r' so that $n + r = n' + r'$
- The new proposed state of the chain is given by a smooth, continuous function $(x', u') = h(x, u)$ [1]

The transition density is now just:

$$q(x, x') = g(u)$$

[1] Note that the proposals are no longer generated directly from a candidate density, by rather there is an immediate step to generate $h(x, u)$

Detailed Balance Condition

Recall the 'old' detailed balance was:

Fix any sets $A, A' \subseteq \mathbb{R}^k$.

$$\int_A \int_{A'} \pi(x) p\left(x, x'\right) dx' dx = \int_A \int_{A'} \pi\left(x'\right) p\left(x', x\right) dx' dx$$

However, since we have that $q(x, x') = g(u)$ [2], the detailed balance in this case can be rewritten as:

$$\int_A \int_{A'} \pi(x) g(u) \alpha(x, x') du dx = \int_{A'} \int_A \pi(x) g(u') \alpha(x', x) dx' du'$$

[2] Can be though of as the randomization of x via u

The Acceptance Probability

The detailed balance condition holds if:

$$\pi(x)g(u)\alpha\left(x,x'\right)=\pi\left(x'\right)g'\left(u'\right)\alpha\left(x',x\right)\left|\frac{\partial\left(x',u'\right)}{\partial(x,u)}\right|$$

Thus, a valid choice for α is

$$\alpha\left(x,x'\right)=\min\left\{1,\frac{\pi\left(x'\right)g'\left(u'\right)}{\pi(x)g(u)}\left|\frac{\partial\left(x',u'\right)}{\partial(x,u)}\right|\right\}$$

In General

From the *Handbook of Markov Chain Monte Carlo*

Step 1. Initialize m and θ_m at iteration $t = 1$.

Step 2. For iteration $t \geq 1$ perform

- *Within-model move*: with a fixed model m, update the parameters θ_m according to any MCMC updating scheme.
- *Between-models move*: simultaneously update model indicator m and the parameters θ_m according to the general reversible proposal/acceptance mechanism

Step 3. Increment iteration $t = t + 1$. If $t < N$, go to Step 2.

Example

We will do an example where $(\mathrm{m}, \theta_{\mathrm{m}})$ where m is the model choice indicator. Consider a mixture model: $Y_i = \sum_{m=1}^{M} w_m \pi_m(\cdot|\theta_m)$
For $k = 1$:

$$Y_i \sim Poisson(\lambda)$$

For $k = 2$:

$$Y_i \sim Neg - Binomial(\lambda, \kappa)$$

References

- Green, Peter J., and David I. Hastie. "Reversible jump MCMC." Genetics 155.3 (2009): 1391-1403.
- Brooks, Steve, et al., eds. Handbook of markov chain monte carlo. CRC press, 2011.