Metropolis-Hastings Algorithm

MCMC Seminar

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Historical Notes

- 1970 paper generalized the original Metropolis algorithm to allow for non-symmetric proposal moves.
- From 1966 to 1971, Hastings was an Associate Professor in the Department of Mathematics at the University of Toronto.*

  When I returned to the University of Toronto, after my time at Bell Labs, I focused on Monte Carlo methods and at first on methods of sampling from probability distributions with no particular area of application in mind. [University of Toronto Chemistry professor] John Valleau and his associates consulted me concerning their work. They were using Metropolis's method to estimate the mean energy of a system of particles in a defined potential field. With 6 coordinates per particle, a system of just 100 particles involved a dimension of 600. When I learned how easy it was to generate samples from high dimensional distributions using Markov chains, I realised how important this was for Statistics, and I devoted all my time to this method and its variants which resulted in the 1970 paper.

- Wrote only 3 papers and a mentored a single graduate student.

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*`http://probability.ca/hastings/`

Detailed Balance

Given states i and j, the condition of detailed balance requires that "at equilibrium" the net traffic between the two states be equal:

$$\pi_i q_{ij} \alpha_{ij} = \pi_j q_{ji} \alpha_{ji} \tag{1}$$

where,

- π_i is the probability of state i
- q_{ij} is the probability of proposing a MC move from state i to state j (sometimes written as $q(j|i)$ or $q(i \to j)$).
- α_{ij} is the probability of accepting such a move.

The equation above implies:

$$\frac{\alpha_{ij}}{\alpha_{ji}} = \frac{\pi_j q_{ji}}{\pi_i q_{ij}} = r_H \tag{2}$$

Metropolis

Proposals are symmetric:

$$q_{ij} = q_{ji}.$$

Thus,

$$\frac{\alpha_{ij}}{\alpha_{ji}} = \frac{\pi_j}{\pi_i} \tag{3}$$

There are many different ways in which can specify a form for α_{ij} so that it satisfies the equation above.

Metropolis and company suggested:

$$\alpha_{ij} = \begin{cases} \frac{\pi_j}{\pi_i} & \text{if } \frac{\pi_j}{\pi_i} < 1 \\ 1 & \text{otherwise} \end{cases} \tag{4}$$

Let us check if this indeed satisfies eqn. 5.

Metropolis

Suppose $\pi_j/\pi_i < 1$. Then, $\alpha_{ij} = \pi_j/\pi_i$ from eqn. 6.

Since, $\pi_i/\pi_j > 1$, $\alpha_{ji} = 1$, again, according to eqn. 6.

Hence,

$$\frac{\alpha_{ij}}{\alpha_{ji}} = \frac{\pi_j/\pi_i}{1} \tag{5}$$

Checks out!

Metropolis

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Since, $\pi_i/\pi_j > 1$, $\alpha_{ji} = 1$, again, according to eqn. 6.

Hence,

$$\frac{\alpha_{ij}}{\alpha_{ji}} = \frac{\pi_j/\pi_i}{1} \tag{5}$$

Checks out!

Hastings suggested what seems like a not so big change. He suggested, for $q_{ij} \neq q_{ji}$:

$$\alpha_{ij} = \begin{cases} \frac{\pi_j q_{ji}}{\pi_i q_{ij}} & \text{if } \frac{\pi_j q_{ji}}{\pi_i q_{ij}} < 1 \\ 1 & \text{otherwise} \end{cases} \tag{6}$$

We can see that it satisfies eqn. 2, as required.

Example of Asymmetric Proposal

Suppose we want to sample a *wide and asymmetric* probability distribution like a log-normal distribution:

$$\pi(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}}\, e^{-\frac{(\ln x-\mu)^2}{2\sigma^2}}, \quad x > 0 \tag{7}$$

Suppose, we set $\mu = 2.0$, and $\sigma = 0.75$.

logN.pdf