Metropolis–Hastings MCMC in general spaces

Jeffrey W. Miller

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This instructional note shows why the Metropolis–Hastings algorithm for Markov chain Monte Carlo (MCMC) works in general spaces, provided that the target distribution and the proposal distributions have densities (that is, Radon–Nikodym derivatives) with respect to a common sigma-finite measure.

Let $(\mathcal{X}, \mathcal{A}, \mu)$ be a sigma-finite measure space. Let P be a probability measure on $(\mathcal{X}, \mathcal{A})$ with density p with respect to μ. For $x \in \mathcal{X}$, let Q_x be a probability measure on $(\mathcal{X}, \mathcal{A})$ with density q_x with respect to μ. (Note: P will serve as the target distribution, and the Q_x's as the proposal distributions.) It is assumed that $(x, y) \mapsto q_x(y)$ is measurable. For $x, y \in \mathcal{X}$, define

$$\alpha(x, y) = \min\Big\{1, \frac{p(y)q_y(x)}{p(x)q_x(y)}\Big\}$$

if $p(x)q_x(y) > 0$, and $\alpha(x, y) = 0$ otherwise.

Theorem. *Let $X \sim P$, let $Y' \sim Q_X$, let $Z \sim \mathrm{Bernoulli}(\alpha(X, Y'))$, and let*

$$Y = \begin{cases} Y' & \text{if } Z = 1 \\ X & \text{if } Z = 0. \end{cases}$$

Then $(X, Y) \overset{D}{=} (Y, X)$, that is, (X, Y) has the same distribution as (Y, X), and in particular, $Y \sim P$.

This shows that the Metropolis–Hastings algorithm "works" in the sense that it induces a Markov chain $(X_1, X_2, \dots)$ that is reversible and has stationary distribution P. (Note, however, that irreducibility and aperiodicity must still be verified.) For, if $X_n \sim P$, and X_{n+1} is sampled using the Metropolis–Hastings algorithm, then with (X, Y) as in the statement of the theorem,

$$(X_n, X_{n+1}) \overset{D}{=} (X, Y) \overset{D}{=} (Y, X) \overset{D}{=} (X_{n+1}, X_n).$$

Proof. For any $x, y \in \mathcal{X}$, we have

$$\alpha(x, y)p(x)q_x(y) = \min\{p(x)q_x(y), p(y)q_y(x)\} = \alpha(y, x)p(y)q_y(x) \tag{1}$$

by checking each of the following three cases: $p(x)q_x(y)$ and $p(y)q_y(x)$ are (i) both positive, (ii) both zero, or (iii) one is positive and one is zero. Therefore, for any $A, B \in \mathcal{A}$,

$$\begin{aligned}
&\int\int \mathbb{1}(x \in A, y \in B)\alpha(x,y)p(x)q_x(y)\mu(dx)\mu(dy) \qquad (2)\\
&\overset{(a)}{=} \int\int \mathbb{1}(x \in A, y \in B)\alpha(y,x)p(y)q_y(x)\mu(dx)\mu(dy)\\
&\overset{(b)}{=} \int\int \mathbb{1}(y \in A, x \in B)\alpha(x,y)p(x)q_x(y)\mu(dy)\mu(dx)\\
&\overset{(c)}{=} \int\int \mathbb{1}(x \in B, y \in A)\alpha(x,y)p(x)q_x(y)\mu(dx)\mu(dy)
\end{aligned}$$

where (a) follows by Equation 1, (b) by swapping the symbols x and y, and (c) by the Fubini–Tonelli theorem. Next, we have

$$\begin{aligned}
&\mathbb{P}(X \in A, Y \in B, Z = 1)\\
&\overset{(a)}{=} \mathbb{P}(X \in A, Y' \in B, Z = 1)\\
&= \mathbb{E}\big(\mathbb{1}(X \in A, Y' \in B, Z = 1)\big)\\
&= \mathbb{E}\Big(\mathbb{E}\big(\mathbb{1}(X \in A, Y' \in B, Z = 1)|X, Y'\big)\Big)\\
&= \mathbb{E}\Big(\mathbb{1}(X \in A, Y' \in B)\mathbb{E}\big(\mathbb{1}(Z = 1)|X, Y'\big)\Big)\\
&= \mathbb{E}\Big(\mathbb{1}(X \in A, Y' \in B)\mathbb{P}(Z = 1|X, Y')\Big)\\
&= \mathbb{E}\Big(\mathbb{1}(X \in A, Y' \in B)\alpha(X, Y')\Big)\\
&= \int\int \mathbb{1}(x \in A, y \in B)\alpha(x,y)p(x)q_x(y)\mu(dx)\mu(dy)
\end{aligned}$$

where (a) follows since $Y = Y'$ when $Z = 1$. Along with Equation 2, this implies

$$\mathbb{P}(X \in A, Y \in B, Z = 1) = \mathbb{P}(X \in B, Y \in A, Z = 1).$$

Since $X = Y$ when $Z = 0$,

$$\mathbb{P}(X \in A, Y \in B, Z = 0) = \mathbb{P}(X \in B, Y \in A, Z = 0).$$

Therefore,

$$\begin{aligned}
\mathbb{P}(X \in A, Y \in B) &= \mathbb{P}(X \in A, Y \in B, Z = 0) + \mathbb{P}(X \in A, Y \in B, Z = 1)\\
&= \mathbb{P}(X \in B, Y \in A, Z = 0) + \mathbb{P}(X \in B, Y \in A, Z = 1)\\
&= \mathbb{P}(X \in B, Y \in A),
\end{aligned}$$

and since $A, B \in \mathcal{A}$ are arbitrary, this implies $(X, Y) \overset{D}{=} (Y, X)$. $\square$