Metropolis-Hastings

MCMC algorithm

- Goal: generate samples from a target distribution π on state space $\mathbb{X}$.
- Idea: construct a Markov chain $\{X^{(t)}\}_{t\geq 1}$ with invariant distribution π.
- After an initial burn-in period, the samples $X^{(t)}$ can be treated as approximate samples from π.
- Metropolis-Hastings is a general MCMC algorithm that uses a proposal distribution to suggest new states and an acceptance-rejection mechanism to ensure the correct invariant distribution.

Metropolis-Hastings Algorithm

- Target distribution on $\mathbb{X} = \mathbb{R}^d$ of density $\pi(x)$.
- Proposal distribution: for any $x, x' \in \mathbb{X}$, we have $q(x'|x) \geq 0$ and $\int_{\mathbb{X}} q(x'|x)\, dx' = 1$.
- Starting with $X^{(1)}$, for $t = 2, 3, \ldots$

Algorithm

1. Sample $X^\star \sim q(\cdot|X^{(t-1)})$.
2. Compute $\alpha(X^\star|X^{(t-1)}) = \min\left(1, \frac{\pi(X^\star)q(X^{(t-1)}|X^\star)}{\pi(X^{(t-1)})q(X^\star|X^{(t-1)})}\right)$.
3. Sample $U \sim \mathcal{U}_{[0,1]}$. If $U \leq \alpha(X^\star|X^{(t-1)})$, set $X^{(t)} = X^\star$, otherwise set $X^{(t)} = X^{(t-1)}$.

Role of Acceptance Probability

- The acceptance probability $\alpha(X^\star|X^{(t-1)})$ is crucial for ensuring that the Markov chain has the desired stationary distribution π.
- It corrects for the discrepancy between the proposal distribution q and the target distribution π.
- If the proposed state $X^\star$ has a higher density than the current state $X^{(t-1)}$, then it favors acceptance but doesn't guarantee it.[1]
- This mechanism helps to avoid getting stuck in local modes.
- Reverse proposal ratio: how easy is it to propose reverse move compared to forward move? If proposal mechanism makes it easy to reach certain states, we need to be more selective accepting such moves, otherwise the chain will be biased towards such easy-to-propose-to regions rather than high probability regions.

[1] In case the proposal is symmetric e.g RWM it will always be accepted.

Transition Kernel

Kernel for Metropolis–Hastings algorithm

$K(x, y) = \alpha(y \mid x)q(y \mid x) + (1 - a(x))\delta_x(y)$ where a is the average acceptance probability from the current state. That is, $a(x) = \int q(x^* \mid x)\alpha(x^* \mid x)\, dx^*$

Proof:

$$\begin{aligned} K(x, y) &= \int q(x^* \mid x)\Big\{\alpha(x^* \mid x)\delta_{x^*}(y) + (1 - \alpha(x^* \mid x))\delta_x(y)\Big\}\, dx^* \\ &= q(y \mid x)\alpha(y \mid x) + \left\{\int q(x^* \mid x)(1 - \alpha(x^* \mid x))\, dx^*\right\}\delta_x(y) \\ &= q(y \mid x)\alpha(y \mid x) + \left\{1 - \int q(x^* \mid x)\alpha(x^* \mid x)\, dx^*\right\}\delta_x(y) \\ &= q(y \mid x)\alpha(y \mid x) + \{1 - a(x)\}\delta_x(y). \end{aligned}$$

if we accept we move to x^* so $y = x^*$ and $\delta_{x^*}(y) = 1$. If we reject we stay at x so $y = x$ and $\delta_x(y) = 1$.

Reversibility

Proposition

The Metropolis–Hastings kernel K is π-reversible (i.e., $\pi(x)K(x,y) = \pi(y)K(y,x)$) and thus admits π as invariant distribution.

Proof: If $x = y$, then obviously $\pi(x)K(x,y) = \pi(y)K(y,x)$. For any $x \neq y$

$$\begin{align}
\pi(x)K(x,y) &= \pi(x)q(y \mid x)\alpha(y \mid x) \tag{1}\\
&= \pi(x)q(y \mid x)\left(1 \wedge \frac{\pi(y)q(x \mid y)}{\pi(x)q(y \mid x)}\right) \tag{2}\\
&= \pi(x)q(y \mid x) \wedge \pi(y)q(x \mid y) \tag{3}\\
&= \pi(y)q(x \mid y)\left(\frac{\pi(x)q(y \mid x)}{\pi(y)q(x \mid y)} \wedge 1\right) = \pi(y)K(y,x). \tag{4}
\end{align}$$

1: kernel definition, 2: acceptance probability definition, 3: symmetry of min operation, 4: algebraic rearrangement.

Metropolis-Hastings Algorithm

Convergence: We also need irreducibility and aperiodicity to ensure convergence to π.

RWM: If q is symmetric, i.e., $q(x'|x) = q(x|x')$, then the acceptance probability simplifies to $\alpha(x'|x) = \min\left(1, \frac{\pi(x')}{\pi(x)}\right)$. This is also known as Random Walk Metropolis.

Independent MH: If q does not depend on the current state, i.e., $q(x'|x) = q(x')$, then the algorithm reduces to the Independent Metropolis-Hastings algorithm.