

Introduction to Markov chain Monte Carlo

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Introduction

- Let π be a discrete or continuous distribution.

Goal: Sample from π or estimate $\pi(f)$, where

$$\pi(f) = \sum_x f(x)\pi(x), \quad \text{or} \quad \pi(f) = \int f(x)\pi(dx).$$

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- **Difficulty:** At times it is impossible to apply classical Monte Carlo methods, since π is often of the form

$$\pi(x) = \frac{e^{-\beta H(x)}}{Z},$$

where Z is a normalization constant that cannot be computed.

- **Idea of Markov chain Monte Carlo (MCMC):**
Construct a Markov chain that converges to π , which only depends on the ratio

$$\frac{\pi(y)}{\pi(x)}.$$

Thus there is no need to know Z .

Motivation from Bayesian statistics

- Suppose that we have a statistical model on the parameter θ , and we observe data $\mathbf{x} = (x_i)_{i=1}^n$ generated from this model.

Likelihood function of \mathbf{x} given θ : $L(\theta|\mathbf{x})$.

Prior distribution of θ : $f(\theta)$.

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- By Bayes theorem, the **posterior distribution** of θ given \mathbf{x} is

$$\pi(\theta|\mathbf{x}) = \frac{L(\theta|\mathbf{x})f(\theta)}{\int L(\theta|\mathbf{x})f(\theta) d\theta},$$

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- To conduct Bayesian inference, we need to sample from $\pi(\theta|\mathbf{x})$ or estimate $\pi(f)$ (e.g. the posterior mean). MCMC is thus very useful in the Bayesian statistics community.

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The Metropolis-Hastings algorithm

- Two ingredients:
 - (i). **Target distribution:** π
 - (ii). **Proposal chain** with transition matrix $Q = (Q(x, y))_{x, y}$.

The Metropolis-Hastings algorithm

Algorithm 1: The Metropolis-Hastings algorithm

Input: Proposal chain Q , target distribution π

- 1 Given X_n , generate $Y_n \sim Q(X_n, \cdot)$
- 2 Take

$$X_{n+1} = \begin{cases} Y_n, & \text{with probability } \alpha(X_n, Y_n), \\ X_n, & \text{with probability } 1 - \alpha(X_n, Y_n), \end{cases}$$

where

$$\alpha(x, y) := \min \left\{ \frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}, 1 \right\}$$

is known as the acceptance probability.

The Metropolis-Hastings algorithm

Definition

The Metropolis-Hastings algorithm, with proposal chain Q and target distribution π , is a Markov chain $X = (X_n)_{n \geq 1}$ with transition matrix

$$P(x, y) = \begin{cases} \alpha(x, y)Q(x, y), & \text{for } x \neq y, \\ 1 - \sum_{y; y \neq x} P(x, y), & \text{for } x = y. \end{cases}$$

The Metropolis-Hastings (MH) algorithm

Theorem

Given target distribution π and proposal chain Q , the Metropolis-Hastings chain is

- **reversible**, that is, for all x, y ,

$$\pi(x)P(x, y) = \pi(y)P(y, x).$$

- (Ergodic theorem of MH) If P is irreducible, then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n f(X_i) = \pi(f).$$

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- Different choices of Q give rise to different MH algorithms

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- **Symmetric MH:** We take a symmetric proposal chain with $Q(x, y) = Q(y, x)$, and so the acceptance probability is

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- **Random walk MH:** We take a random walk proposal chain with $Q(x, y) = Q(y - x)$. E.g., $Q(x, \cdot)$ is the probability density function of $N(x, \sigma^2)$.

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- **Random walk MH:** We take a random walk proposal chain with $Q(x, y) = Q(y - x)$. E.g., $Q(x, \cdot)$ is the probability density function of $N(x, \sigma^2)$.
- **Independence sampler:** Here we take $Q(x, y) = q(y)$, where $q(y)$ is a probability distribution. In words, $Q(x, y)$ does not depend on x .

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Example 1: logistic regression

- We observe $(x_i, y_i)_{i=1}^n$ according to the model

$$Y_i \sim \text{Bernoulli}(p(x_i)), \quad p(x) = \frac{e^{\alpha + \beta x}}{1 + e^{\alpha + \beta x}}.$$

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- The likelihood function is

$$L(\alpha, \beta | \mathbf{x}, \mathbf{y}) \propto \prod_{i=1}^n \left(\frac{e^{\alpha + \beta x_i}}{1 + e^{\alpha + \beta x_i}} \right)^{y_i} \left(\frac{1}{1 + e^{\alpha + \beta x_i}} \right)^{1 - y_i},$$

and prior distribution

$$\pi_{\alpha}(\alpha | \hat{b}) \pi_{\beta}(\beta) = \frac{1}{\hat{b}} e^{\alpha} e^{-e^{\alpha} / \hat{b}},$$

i.e. exponential prior on $\log \alpha$ and a flat prior on β . \hat{b} is chosen such that $\mathbb{E}(\alpha) = \hat{\alpha}$, where $\hat{\alpha}$ is the MLE of α .

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- Goal: sample from the posterior of (α, β) using the MH algorithm

Example 1: logistic regression

- **Choosing a good \mathbf{Q} to accelerate convergence:** Let $\hat{\alpha}$ and $\hat{\beta}$ be the MLE of α and β respectively, and $\widehat{\sigma}_{\hat{\beta}}^2$ be the variance of $\hat{\beta}$.

Example 1: logistic regression

- **Choosing a good Q to accelerate convergence:** Let $\hat{\alpha}$ and $\hat{\beta}$ be the MLE of α and β respectively, and $\widehat{\sigma}_{\hat{\beta}}^2$ be the variance of $\hat{\beta}$.
- We take an independent MH with proposal chain

$$f(\alpha, \beta) = \pi_{\alpha}(\alpha|\hat{b})\phi(\beta),$$

where $\phi(\beta)$ is the pdf of normal distribution with mean $\hat{\beta}$ and variance $\widehat{\sigma}_{\hat{\beta}}^2$.

Example 1: logistic regression

Algorithm 2: Independent MH on logistic regression

- 1 Given (α_n, β_n) , generate $(\alpha', \beta') \sim f(\alpha, \beta)$, that is, generate $\log \alpha'$ following exponential distribution with parameter \hat{b} , and $\beta' \sim N(\hat{\beta}, \widehat{\sigma_{\hat{\beta}}^2})$.
- 2 Accept (α', β') with probability

$$\min \left\{ \frac{L(\alpha', \beta' | \mathbf{x}, \mathbf{y}) \phi(\beta_n)}{L(\alpha_n, \beta_n | \mathbf{x}, \mathbf{y}) \phi(\beta')}, 1 \right\}$$

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Example 2: graph colouring

- Let $G = (V, E)$ be an undirected graph without self-loop on the vertex set V and edge set E . We want to colour each vertex with one of the q colours such that a vertex's colour differs from that of all its neighbours.

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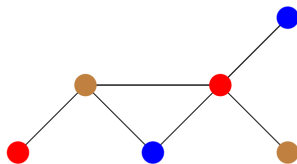


Photo courtesy of Olivier Leveque (EPFL)

Example 2: graph colouring

- Let S be the set of possible colour configurations on G , and $x = (x_v, v \in V) \in S$ is a particular colour configuration. A **proper q -colouring** of G is any configuration x such that for all $v, w \in V$, if $(v, w) \in E$, then $x_v \neq x_w$.

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- **Goal:** Sample uniformly among the proper q -colourings of G . In other words, we would like to sample from

$$\pi(x) = \frac{\mathbf{1}_{\{x \text{ is a proper } q\text{-colouring}\}}}{Z}, \quad x \in S,$$

where Z is the number of proper q -colourings of G .

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- Computing Z is non-trivial. Using Metropolis-Hastings, we can still sample π without computing Z .

Example 2: graph colouring

Algorithm 3: MH on graph colouring

- 1 Given a proper q -colouring x
 - 2 Select a vertex $v \in V$ uniformly at random
 - 3 Select a colour $c \in \{1, 2, \dots, q\}$ uniformly at random
 - 4 If c is an allowed colour at v , then recolour v , i.e. set $x_v = c$;
do nothing otherwise
 - 5 Repeat step 2 - 4
-

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Example 3: Ising model

- Let $G = (V, E)$ be an undirected graph without self-loop on the vertex set $V = \{1, 2, \dots, N\}$ and edge set E . Variables $\sigma_v \in \{-1, 1\}$ are attached to the vertices $v \in V$. These variables are called spins. The state space is made up of spin assignments $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_N) \in \{-1, 1\}^N$.

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- We would like to sample from the **Gibbs** distribution:

$$\pi(\sigma) = \frac{1}{Z} \exp \left(\sum_{(v,w) \in E} \beta J_{vw} \sigma_v \sigma_w \right),$$

where $\beta > 0$ is the inverse temperature, $J_{vw} \in \mathbb{R}$ is the interaction strength and Z is the normalization constant

$$Z = \sum_{\sigma \in \{-1, 1\}^N} \exp \left(\sum_{(v,w) \in E} \beta J_{vw} \sigma_v \sigma_w \right).$$

Example 3: Ising model

Algorithm 4: MH on Ising model

- 1 Given an initial spin assignment σ
- 2 Select a vertex $v \in V$ uniformly at random
- 3 Consider the spin assignment $\sigma^{(v)}$ where the initial spin σ_v is flipped, i.e. $\sigma_v^{(v)} = -\sigma_v$.
- 4 Accept $\sigma^{(v)}$ with probability

$$\min \left\{ \frac{\pi(\sigma^{(v)})}{\pi(\sigma)}, 1 \right\} = \min \left\{ e^{-\beta 2\sigma_v \sum_w J_{vw}\sigma_w}, 1 \right\}$$

; do nothing otherwise.

- 5 Repeat step 2 - 4
-

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MH as L^1 minimizer

Theorem (Billera and Diaconis '01, Choi and Huang '19)

Given a target distribution π and proposal chain Q on a finite state space, let P be the transition matrix of MH. Then

$$d_\pi(Q, P) = \inf_{K \in R(\pi)} d_\pi(Q, K),$$

where $R(\pi)$ is the set of reversible transition matrix with respect to π , and

$$d_\pi(Q, K) = \sum_x \sum_{y \neq x} \pi(x) |Q(x, y) - K(x, y)|.$$

In words, P minimizes the distance d_π between Q and $R(\pi)$.

The scaling limit of MH is the Langevin diffusion

- Suppose that $U : \mathbb{R}^d \rightarrow \mathbb{R}$, and U is continuously differentiable with Lipschitz continuous gradient.

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- Suppose that $U : \mathbb{R}^d \rightarrow \mathbb{R}$, and U is continuously differentiable with Lipschitz continuous gradient.
- Target distribution: Gibbs distribution with density

$$\pi(\mathbf{x}) = \frac{e^{-U(\mathbf{x})/T}}{\int e^{-U(\mathbf{x})/T} dx}$$

Proposal chain: Gaussian proposal with $Q_\epsilon(\mathbf{x}, \mathbf{y})$ being the pdf of $N(\mathbf{x}, \epsilon I)$.

The scaling limit of MH is the Langevin diffusion

Theorem (Gelfand and Mitter '91)

Given target distribution π and proposal chain Q_ϵ , let $(X_n^\epsilon)_{n \geq 0}$ be the MH chain. Then

$$X_{\lfloor t/\epsilon \rfloor}^\epsilon \Rightarrow X_t,$$

where $(X_t)_{t \geq 0}$ is a rescaled version of the Langevin diffusion described by the SDE

$$dX_t = -\nabla U(X_t)/2T dt + dW_t,$$

where $(W_t)_{t \geq 0}$ is the standard d -dimensional Brownian motion. In words, the scaled MH chain converges weakly in the Skorokhod topology to a rescaled Langevin diffusion.

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Simulated annealing

- **Goal:** Find the global minimizers of a target function U .

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- **Idea of simulated annealing:** Construct a **non-homogeneous** Metropolis-Hastings Markov chain that converges to π_∞ , which is supported on the set of global minima of U .

Simulated annealing

- **Goal:** Find the global minimizers of a target function U .
- **Idea of simulated annealing:** Construct a **non-homogeneous** Metropolis-Hastings Markov chain that converges to π_∞ , which is supported on the set of global minima of U .
- **Target distribution:** Gibbs distribution $\pi_{T(t)}$ with temperature $T(t)$ that depends on time t

$$\pi_{T(t)}(x) = \frac{e^{-U(x)/T(t)}}{Z_{T(t)}},$$

$$Z_{T(t)} = \sum_x e^{-U(x)/T(t)}.$$

Proposal chain Q : symmetric

Simulated annealing

- The temperature cools down $T(t) \rightarrow 0$ as $t \rightarrow \infty$, and we expect the Markov chain get “frozen” at the set of global minima U_{min} :

$$\pi_{\infty}(x) := \lim_{t \rightarrow \infty} \pi_{T(t)}(x) = \begin{cases} \frac{1}{|U_{min}|}, & \text{for } x \in U_{min}, \\ 0, & \text{for } x \notin U_{min}. \end{cases}$$
$$U_{min} := \{x; U(x) \leq U(y) \text{ for all } y\}.$$

Simulated annealing

Algorithm 5: Simulated annealing

Input: Symmetric proposal chain Q , target distribution $\pi_{T(t)}$, temperature schedule $T(t)$

- 1 Given X_t , generate $Y_t \sim Q(X_t, \cdot)$
- 2 Take

$$X_{t+1} = \begin{cases} Y_t, & \text{with probability } \alpha_t(X_t, Y_t), \\ X_t, & \text{with probability } 1 - \alpha_t(X_t, Y_t), \end{cases}$$

where

$$\alpha_t(x, y) := \min \left\{ \frac{\pi_{T(t)}(y)Q(y, x)}{\pi_{T(t)}(x)Q(x, y)}, 1 \right\} = \min \left\{ e^{\frac{U(x) - U(y)}{T(t)}}, 1 \right\}$$

is the acceptance probability.

Optimal cooling schedule

- The temperature schedule $T(t)$ cannot be too slow: it may take too long for the Markov chain to converge

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Theorem (Hajek '88, Holley and Stroock '88)

The Markov chain generated by simulated annealing converges to π_∞ if and only if for any $\epsilon > 0$,

$$T(t) = \frac{c + \epsilon}{\ln(t + 1)},$$

where c is known as the optimal hill-climbing constant that depends on the target function U and proposal chain Q .

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Other MCMC algorithms

- Glauber dynamics/heat bath algorithm/Gibbs sampler
- Perfect simulation/Coupling from the past
- Hamiltonian Monte Carlo
- Metropolis adjusted Langevin algorithm (MALA)

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Thank you! Question(s)?