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: $L(\theta|\mathbf{x})$.
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- By Bayes theorem, the **posterior distribution** of θ given $\mathbf{x}$ is
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  where the integral is often impossible to calculate.
- 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.

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*

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

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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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- **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.

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

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

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 $\beta^{'} \sim N(\hat{\beta}, \widehat{\sigma^2_{\hat{\beta}}})$.

2 Accept $(\alpha^{'}, \beta^{'})$ with probability

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

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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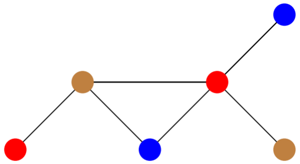

Example 2: graph colouring

- 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

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

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

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

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

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- 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

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

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.

Simulated annealing

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

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- **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 $T(t) \to 0$ as $t \to \infty$, and we expect the Markov chain get "frozen" at the set of global minima U_{min}:

$$\pi_\infty(x) := \lim_{t\to\infty} \pi_{T(t)}(x) = \begin{cases} \dfrac{1}{|U_{min}|}, & \text{for } x \in U_{min}, \\ 0, & \text{for } x \notin U_{min}. \end{cases}$$

$$U_{min} := \{x;\ U(x) \leq U(y) \text{ for all } y\}.$$

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

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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.

Other MCMC algorithms

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

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Thank you! Question(s)?