Bayesian Theory and Computation

Lecture 3: Monte Carlo Methods

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Background

- We saw previously that in certain situations, the posterior distribution has a closed form (e.g., when the prior is conjugate), and the integrals are tractable.
- For many other problems, however, finding the posterior distribution and obtaining the expectation are far from trivial.
- Remember that even for the case of simple normal distribution with two parameters, the posterior didn't have a closed form unless we were willing to use noninformative priors or tie the variance of the mean to the variance of the data.
- In the following few lectures, we focus on problems where the posterior distribution is not analytically tractable.
- For this, we need to learn about Monte Carlo methods and Markov chain stochastic processes.

Monte Carlo Method

- Suppose we are interested in estimating $I(h) = \int_a^b h(x)dx$
- If we can draw iid samples, $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ uniformly from (a, b), we can approximate the integral as

$$\hat{I}_n = (b-a)\frac{1}{n}\sum_{i=1}^{n} h(x^{(i)})$$

- Note that we can think about the integral as

$$(b-a)\int_a^b h(x) \cdot \frac{1}{b-a} dx$$

where $\frac{1}{b-a}$ is the density of Uniform(a, b)

Monte Carlo Method

- In general, we are interested in integrals of the form $\int_{\mathcal{X}} h(x)f(x)dx$, where $f(x)$ is a probability density function
- Analogous to the above argument, we can approximate this integral (or expectation) by drawing iid samples $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ from the density $f(x)$ and then

$$\hat{I} = \frac{1}{n}\sum_{i=1}^{n} h(x^{(i)})$$

- Based on the law of large numbers, we know that

$$\lim_{n\to\infty} \hat{I}_n \xrightarrow{p} I$$

- And based on the central limit theorem

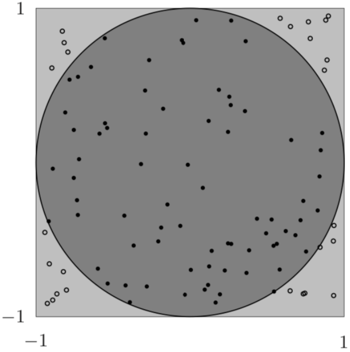
$$\sqrt{n}(\hat{I}_n - I) \to \mathcal{N}(0, \sigma^2), \quad \sigma^2 = \mathbb{V}\mathrm{ar}(h(X))$$

Example: estimating π

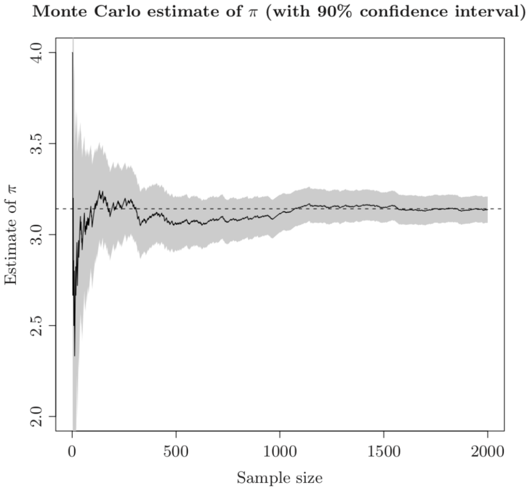
- Let $h(x) = \mathbf{1}_{B(0,1)}(x)$, then $\pi = 4\int_{[-1,1]^2} h(x) \cdot \frac{1}{4}\, dx$
- Monte Carlo estimate of π

$$\hat{I}_n = \frac{4}{n}\sum_{i=1}^{n} \mathbf{1}_{B(0,1)}(x^{(i)})$$

$$x^{(i)} \sim \text{Uniform}([-1,1]^2)$$



Example: estimating π



Monte Carlo vs Quadrature

- Convergence rate for Monte Carlo: $\mathcal{O}(n^{-1/2})$

  $$p\left(|\hat{I}_n - I| \leq \frac{\sigma}{\sqrt{n\delta}}\right) \geq 1 - \delta, \quad \forall \delta$$

  often slower than quadrature methods ($\mathcal{O}(n^{-2})$ or better)
- However, the convergence rate of Monte Carlo does not depend on dimensionality
- On the other hand, quadrature methods are difficult to extend to multidimensional problems, because of the curse of dimensionality. The actual convergence rate becomes $\mathcal{O}(n^{-k/d})$, for any order k method in dimension d
- This makes Monte Carlo strategy very attractive for high dimensional problems

Exact Simulation

- Monte Carlo methods require sampling a set of points chosen randomly from a probability distribution
- For simple distribution $f(x)$ whose inverse cumulative distribution functions (CDF) exists, we can sampling x from f as follows

$$x = F^{-1}(u), \quad u \sim \mathrm{Uniform}(0,1)$$

where F^{-1} is the inverse CDF of f

- Proof.

$$p(a \leq x \leq b) = p(F(a) \leq u \leq F(b)) = F(b) - F(a)$$

Examples

- Exponential distribution: $f(x) = \theta\exp(-\theta x)$. The CDF is

$$F(a) = \int_0^a \theta\exp(-\theta x) = 1 - \exp(-\theta a)$$

therefore, $x = F^{-1}(u) = -\frac{1}{\theta}\log(1-u) \sim f(x)$. Since $1-u$ also follows the uniform distribution, we often use $x = -\frac{1}{\theta}\log(u)$ instead

- Normal distribution: $f(x) = \frac{1}{\sqrt{2\pi}}\exp(-\dfrac{x^2}{2})$. Box-Muller Transform

$$X = \sqrt{-2\log U_1}\cos 2\pi U_2$$
$$Y = \sqrt{-2\log U_1}\sin 2\pi U_2$$

where $U_1 \sim \text{Uniform}(0,1), \quad U_2 \sim \text{Uniform}(0,1)$

Intuition for Box-Muller Transform

- Assume $Z = (X, Y)$ follows the standard bivariate normal distribution. Consider the following transform

$$X = R\cos\Theta, \quad Y = R\sin\Theta$$

- From symmetry, clearly Θ follows the uniform distribution on the interval $(0, 2\pi)$ and is independent of R
- What distribution does R follow? Let's take a look at its CDF

$$\begin{aligned} p(R \le r) &= p(X^2 + Y^2 \le r^2) \\ &= \frac{1}{2\pi}\int_0^r t\exp(-\frac{t^2}{2})dt \int_0^{2\pi} d\theta = 1 - \exp(-\frac{r^2}{2}) \end{aligned}$$

Therefore, using the inverse CDF rule, $R = \sqrt{-2\log U_1}$

Rejection Sampling

- If it is difficult or computationally intensive to sample directly from $f(x)$ (as described above), we need to use other strategies
- Although it is difficult to sample from $f(x)$, suppose that we can evaluate the density at any given point up to a constant $f(x) = f^*(x)/Z$, where Z could be unknown (remember that this make Bayesian inference convenient since we usually know the posterior distribution only up to a constant)
- Furthermore, assume that we can easily sample from another distribution with the density $g(x) = g^*(x)/Q$, where Q is also a constant

Rejection Sampling

- Now we choose the constants c such that $cg^*(x)$ becomes the envelope (blanket) function for $f^*(x)$:

$$cg^*(x) \geq f^*(x), \quad \forall x$$

- Then, we can use a strategy known as *rejection sampling* in order to sample from $f(x)$ indirectly
- The rejection sampling method works as follows
    1. draw a sample x from $g(x)$
    2. generate $u \sim \text{Uniform}(0, 1)$
    3. if $u \leq \frac{f^*(x)}{cg^*(x)}$ we accept x as the new sample, otherwise, reject x (discard it)
    4. return to step 1

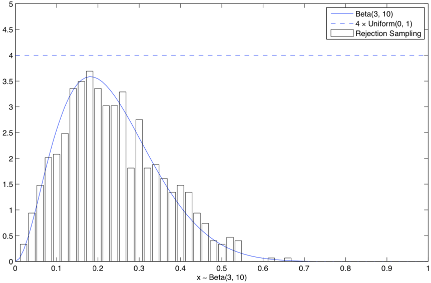
Rejection Sampling

Rejection sampling generates samples from the target density, no approximation involved

$$\begin{aligned}
p(X^R \leq y) &= p(X^g \leq y | U \leq \frac{f^*(X^g)}{cg^*(X^g)}) \\
&= p(X^g \leq y, U \leq \frac{f^*(X^g)}{cg^*(X^g)}) / p(U \leq \frac{f^*(X^g)}{cg^*(X^g)}) \\
&= \frac{\int_{-\infty}^{y} \int_0^{\frac{f^*(z)}{cg^*(z)}} du g(z) dz}{\int_{-\infty}^{\infty} \int_0^{\frac{f^*(z)}{cg^*(z)}} du g(z) dz} \\
&= \int_{-\infty}^{y} f(z) dz
\end{aligned}$$

Example

- Assume that it is difficult to sample from the Beta(3, 10) distribution (this is not the case of course)
- We use the Uniform$(0, 1)$ distribution with $g(x) = 1$, $\forall x \in [0, 1]$, which has the envelop proporty: $4g(x) > f(x)$, $\forall x \in [0, 1]$. The following graph shows the result after 3000 iterations



Advanced Rejection Sampling

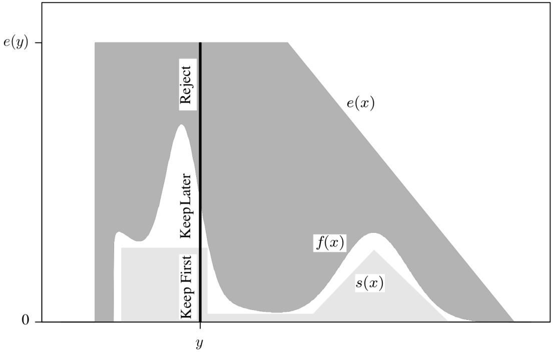
Rejection sampling becomes challenging as the dimension of x increases. A good rejection sampling algorithm must have three properties

- It should be easy to construct envelops that exceed the target everywhere
- The envelop distributions should be easy to sample
- It should have a low rejection rate

Squeezed Rejection Sampling

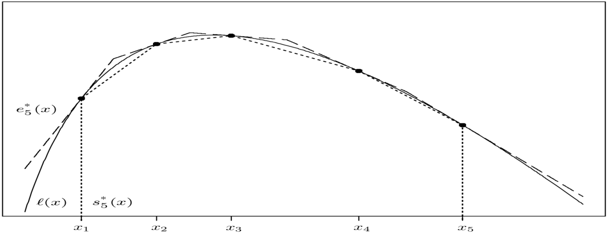
- When evaluating f^* is computationally expensive, we can improve the simulation speed of rejection sampling via *squeezed rejection sampling*
- Squeezed rejection sampling reduces the evaluation of f via a nonnegative squeezing function s that does not exceed f^* anywhere on the support of f: $s(x) \leq f^*(x), \forall x$
- The algorithm proceeds as follows:
  1. draw a sample x from $g(x)$
  2. generate $u \sim \text{Uniform}(0, 1)$
  3. if $u \leq \frac{s(x)}{cg^*(x)}$, we accept x as the new sample, return to step 1
  4. otherwise, determine whether $u \leq \frac{f^*(x)}{cg^*(x)}$. If this inequality holds, we accept x as the new sample, otherwise, we reject it.
  5. return to step 1

Squeezed Rejection Sampling



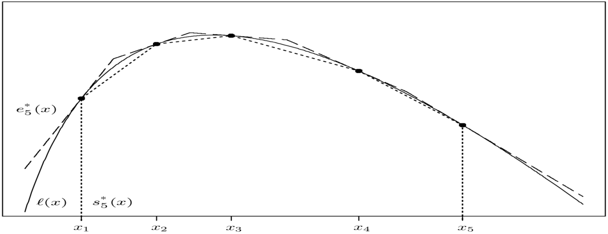
Remark: The proportion of iterations in which evaluation of f is avoided is $\int s(x)dx / \int e(x)dx$

Adaptive Rejection Sampling



- For a continuous, differentiable, log-concave density on a connected region of support, we can adapt the envelope construction (Gilks and Wild, 1992)
- Let $T = \{x_1, \ldots, x_k\}$ be the set of k starting points.
- We first sample x^* from the piecewise linear upper envelop $e(x)$, formed by the tangents to the log-likelihood ℓ at each point in T_k.

Adaptive Rejection Sampling



- To sample from the upper envelop, we need to transform from log space by exponentiating and using properties of the exponential distribution
- We then either accept or reject x^* as in squeeze rejection sampling, with $s(x)$ being the piecewise linear lower bound formed from the chords between adjacent points in T
- Add x^* to T whenever the squeezing test fails.

Markov Chain Monte Carlo

- For more complex distributions, we can use a Markov chain process to generate samples (which would not be independent anymore) and approximate the target distribution.
- This method is known as Markov chain Monte Carlo (MCMC) technique.
- However, we first need to discuss Markov chains and stochastic processes in general.

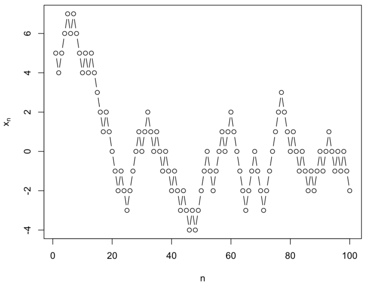
Stochastic Processes & Random Walks

- Stochastic processes is a family of random variables, usually indexed by a set of numbers (time). A discrete time stochastic process is simply a sequence of random variables, $X_0, X_1, \ldots, X_n$ defined on the same probability space
- One of the simplest stochastic processes (and one of the most useful) is the simple random walk
- Consider a simple random walk on a graph $G = (\Omega, E)$. The stochastic process starts from an initial position $X_0 = x_0 \in \Omega$, and proceeds following a simple rule:

$$p(X_{n+1}|X_n = x_n) \sim \text{Discrete}(\mathcal{N}(x_n)),\ \forall n \geq 0$$

  where $\mathcal{N}(x_n)$ denotes the neighborhood of x_n

Random Walk: One Dimension

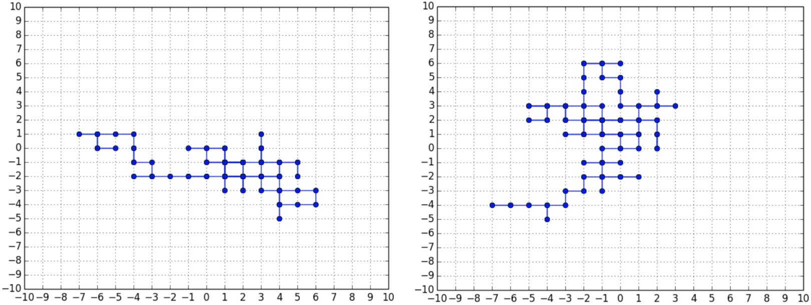


- Consider a sequence of iid random variables $\{Z_i\}$ such that $p(Z_i = 1) = p$, $p(Z_i = -1) = 1 - p$. A one dimension random work process can be defined as $X_0 = a,\ X_n = a + Z_1 + \cdots + Z_n$.
- The distribution of X_n

$$p(X_n = a + k) = \binom{n}{(n+k)/2} p^{(n+k)/2} (1 - p)^{(n-k)/2}$$

Random Walk: Two Dimension

Two random walks on a 20 × 20 grid graph



- The above simple random walk is a special case of another well-known stochastic process called *Markov chains*
- A Markov chain represents the stochastic movement of some particle in the state space over time. The particle initially starts from state i with probability $\pi_i^{(0)}$, and after that moves from the current state i at time t to the next state j with probability $p_{ij}(t)$
- A Markov chain has three main elements:
    1. A state space $\mathcal{S}$
    2. An initial distribution $\pi^{(0)}$ over $\mathcal{S}$
    3. Transition probabilities $p_{ij}(t)$ which are non-negative numbers representing the probability of going from state i to j, and $\sum_j p_{ij}(t) = 1$.
- When $p_{ij}(t)$ does not depend on time t, we say the Markov chain is time-homegenous

Markov Property

- Chain rule (in probability)

$$p(X_n = x_n, \dots, X_0 = x_0) = \prod_{i=1}^{n} p(X_i = x_i | X_{<i} = x_{<i})$$

- **Markov property**

$$p(X_{i+1} = x_{i+1} | X_i = x_i, \dots, X_0 = x_0) = p(X_{i+1} = x_{i+1} | X_i = x_i)$$

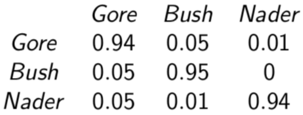
- Joint probability with Markov property

$$p(X_n = x_n, \dots, X_0 = x_0) = \prod_{i=1}^{n} p(X_i = x_i | X_{i-1} = x_{i-1})$$

fully determined by the transition probabilities

Example

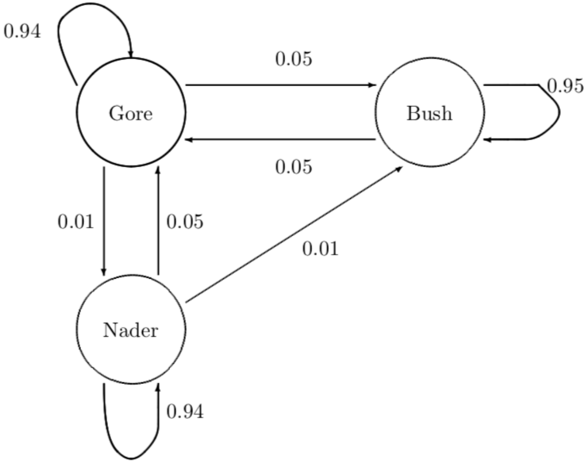
- Consider the 2000 US presidential election with three candidates: Gore, Bush and Nader (just an illustrative example and does not reflect the reality of that election)
- We assume that the initial distribution of votes (i.e., probability of winning) was $\pi = (0.49, 0.45, 0.06)$ for Gore, Bush and Nader respectively
- Further, we assume the following transition probability matrix



	Gore	*Bush*	*Nader*
Gore	0.94	0.05	0.01
Bush	0.05	0.95	0
Nader	0.05	0.01	0.94

Example

A probabilistic graph presentation of the Markov chain



Stationary Distribution

- If we represent the transition probability a square matrix P such that $P_{ij} = p_{ij}$, we can obtain the distribution of states in step n, $\pi^{(n)}$, as follows

$$\pi^{(n)} = \pi^{(n-1)} P = \ldots = \pi^{(0)} P^n$$

- For the above example, we have

$$\begin{aligned}
\pi^{(0)} &= (0.4900, 0.4500, 0.0600) \\
\pi^{(10)} &= (0.4656, 0.4655, 0.0689) \\
\pi^{(100)} &= (0.4545, 0.4697, 0.0758) \\
\pi^{(200)} &= (0.4545, 0.4697, 0.0758)
\end{aligned}$$

Stationary Distribution

- As we can see last, after several iterations, the above Markov chain converges to a distribution, $(0.4545, 0.4697, 0.0758)$
- In this example, the chain would have reached this distribution regardless of what initial distribution $\pi^{(0)}$ we chose. Therefore, $\pi = (0.4545, 0.4697, 0.0758)$ is the stationary distribution for the above Markov chain
- **Stationary distribution**. A distribution of Markov chain states is called to be stationary if it remains the same in the next time step, i.e.,

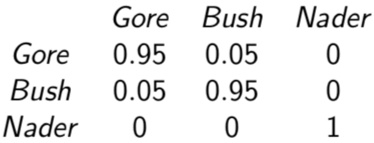
$$\pi = \pi P$$

Stationary Distribution

- How can we find out whether such distribution exists?
- Even if such distribution exists, is it unique or not?
- Also, how do we know whether the chain would converge to this distribution?
- To find out the answer, we briefly discuss some properties of Markov chains

Irreducibility

- Irreducible: A Markov chain is irreducible if the chain can move from any state to another state.
- Examples
  - The simple random walk is irreducible
  - The following chain, however, is reducible since Nader does not communicate with the other two states (Gore and Bush)



	Gore	*Bush*	*Nader*
Gore	0.95	0.05	0
Bush	0.05	0.95	0
Nader	0	0	1

Aperiodicity

- Period: the period of a state i is the greatest common divisor of the times at which it is possible to move from i to i.
- For example, all the states in the following Markov chain have period 3.

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

- Aperiodic: a Markov chain is said to be aperiodic if the period of each state is 1, otherwise the chain is periodic.

Recurrent vs. Transient

- **Recurrent** states: a state i is called recurrent if with probability 1, the chain would ever return to state i given that it started in state i.

	Gore	*Bush*	*Nader*
Gore	0.94	0.05	0.01
Bush	0.05	0.95	0
Nader	0.05	0.01	0.94

- **Positive recurrent**: a recurrent state j is called positive recurrent if the expected amount of time to return to state j given that the chain started in state j is finite
- For a positive recurrent Markov chain, the stationary distribution exists and is unique

Reversibility

- **Reversibility**: a Markov chain is said to be reversible with respect to a probability distribution π if $\pi_i p_{ij} = \pi_j p_{ji}$
- In fact, if a Markov chain is reversible with respect to π, then π is also a stationary distribution

$$\begin{aligned}\sum_i \pi_i p_{ij} &= \sum_i \pi_j p_{ji} \\ &= \pi_j \sum_i p_{ji} \\ &= \pi_j\end{aligned}$$

  since $\sum_i p_{ji} = 1$ for all transition probability matrices
- This is also known as *detailed balance condition*.

Discrete Time, General Space Markov Chains

- We can define a Markov chain on a general state space $\mathcal{X}$ with initial distribution $\pi^{(0)}$ and transition probabilities $p(x, A)$ defined as the probability of jumping to the subset A from point $x \in \mathcal{X}$
- Similarly, with Markov property, we have the joint probability

$$p(X_0 \in A_0, \ldots, X_n \in A_n) = \int_{A_0} \pi^{(0)}(dx_0) \ldots \int_{A_n} p(x_{n-1}, dx_n)$$

- Example. Consider a Markov chain with the real line as its state space. The initial distribution is $\mathcal{N}(0, 1)$, and the transition probability is $p(x, \cdot) = \mathcal{N}(x, 1)$. This is just a Brownian motion (observed at discrete time)

ϕ-irreducibility and ϕ-aperiodicity

- Unlike the discrete space, we now need to talk about the property of Markov chains with a continuous non-zero measure ϕ, on $\mathcal{X}$, and use sets A instead of points
- A chain is ϕ-irreducible if for all $A \subseteq \mathcal{X}$ with $\phi(A) > 0$ and for all $x \in \mathcal{X}$, there exists a positive integer n such that

$$p^n(x, A) = p(X_n \in A | X_0 = x) > 0$$

- Similarly, we need to modify our definition of period

Stationary Distribution

- A distribution π is a stationary distribution if

$$\pi(A) = \int_{\mathcal{X}} \pi(dx)p(x, A), \quad \forall A \subseteq \mathcal{X}$$

- As for the discrete case, a continuous space Markov chain is reversible with respect to π if

$$\pi(dx)p(x, dy) = \pi(dy)p(y, dx)$$

- Similarly, if the chain is reversible with respect to π, then π is a stationary distribution
- Example. Consider a Markov chain on the real line with initial distribution $\mathcal{N}(1, 1)$ and transition probability $p(x, \cdot) = \mathcal{N}(\frac{x}{2}, \frac{3}{4})$. It is easy to show that the chain converges to $\mathcal{N}(0, 1)$ (Exercise)

Ergodicity

- Ergodic: a Markov chain is ergodic if it is both irreducible and aperiodic, with stationary distribution π
- **Ergodic Theorem**. For an ergodic Markov chain on the state space $\mathcal{X}$ having stationary distribution π, we have: (i) for all measurable $A \subseteq \mathcal{X}$ and π-a.e. $x \in \mathcal{X}$,

$$\lim_{t\to\infty} p^t(x, A) = \pi(A)$$

(ii) $\forall f$ with $\mathbb{E}_\pi |f(x)| < \infty$,

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} f(X_t) = \int_{\mathcal{X}} f(x)\pi(x)dx, \quad \text{a.s.}$$

In particular, π is the unique stationary probability density function for the chain

References

- P. J. Davis and P. Rabinowitz. Methods of Numerical Integration. Academic, New York, 1984.
- W. R. Gilks and P. Wild. Adaptive rejection sampling for Gibbs sampling. Applied Statistics, 41:337–348, 1992.