MSA101/MVE187 2020 Lecture 5.1
More on basic simulation methods

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Review: Rejection sampling; example

- Sometimes we cannot easily simulate from a density $f(x)$, (the "target density") but we *can* simulate from an "instrumental" density $g(x)$ that approximates $f(x)$.
- If we can find a constant M such that $f(x)/g(x) \leq M$ for all x (and if f and g have the same support), we can use *rejection sampling* to sample from f:
  - Sample X using $g(x)$.
  - Draw u uniformly on $[0, 1]$.
  - If $u \cdot M \cdot g(x) \leq f(x)$ accept x as a sample, otherwise reject x and start again.
- Toy example in R: Simulate from the Beta$(2.3, 5.2)$ distribution using a Uniform$(0, 1)$ as the instrumental density.

Importance sampling

- Monte Carlo integration computes

$$\mathrm{E}_f(h(x)) = \int h(x)f(x)\,dx$$

where $f(x)$ is a probability density function, by simulating $x_1, \ldots, x_m$ according to f and taking the average of $h(x_1), \ldots, h(x_m)$. The result has accuracy $\sqrt{Var_f(h(X))/m}$.

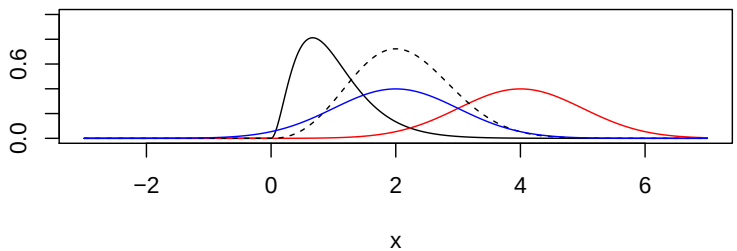
- Instead, we may re-write the integral as

$$\int \left[\frac{h(x)f(x)}{g(x)}\right] g(x)\,dx$$

and simulate x_i according to g, taking the averages of $h(x_1)f(x_1)/g(x_1), \ldots, h(x_m)f(x_m)/g(x_m)$.

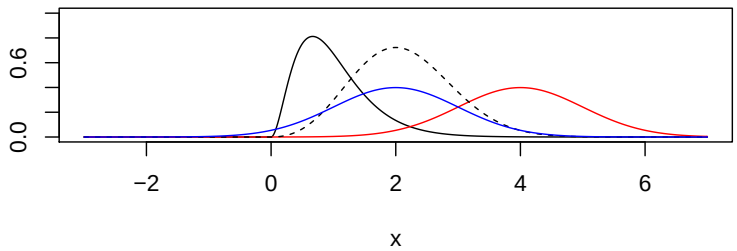
- A good idea if $Var_g(h(X)f(X)/g(X))$ is much smaller than $Var_f(h(X))$.
- Note: This is not really a "sampling" method, but a method to do Monte Carlo integration more accurately.

Importance sampling: Example



- In figure above, the black curve is $h(x)$ and the red curve is the density $f(x)$. The dotted curve is a scaled version of their product.
- Simulating points according to the red curve to compute the integral under the dotted curve will not be efficient.
- Better to simulate using the blue curve, which approximates the dotted curve, and then adjust using the quotient of the densities, as shown in the previous overhead.

Sampling Importance Resampling (SIR)



- In the figure above, assume you want to sample from a density proportional to the dotted curve: $\pi(x) \propto_x v(x)$.
- An *approximate* procedure starts with generating a sample

$$x_1, x_2, \ldots, x_N$$

  according to the density given by the blue curve $g(x)$.
- Then one *resamples* from this sample (with replacement) using probability weights

$$w_i = \frac{v(x_i)/g(x_i)}{\sum_{j=1}^{N} v(x_j)/g(x_j)}.$$

MSA101/MVE187 2020 Lecture 5.2
Review of Markov chains

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Where are we??

- We want to make probabilistic predictions using the posterior predictive.
- For all but the simplest models, we do this by generating a sample from the posterior for the model parameters, and then using the sample in Monte Carlo integration to make predictions.
- Often simple methods such as rejection sampling cannot easily be used to generate a sample.
- A very general and useful method is then *Markov chain Monte Carlo* (MCMC).
- To study it we first need to review(?) a bit about Markov chains.

Review of Markov chains

- Definition: A (discrete time, time-homogeneous) Markov chain with kernel K is a sequence of random variables $X^{(0)}, X^{(1)}, X^{(2)}, \ldots$ satisfying, for all t,

$$\pi(X^{(t)} \mid X^{(0)}, X^{(1)}, \ldots, X^{(t-1)}) = \pi(X^{(t)} \mid X^{(t-1)}) = K(X^{(t-1)}, X^{(t)})$$

- Example: In the case of a state space with n possible values, a distribution is represented by a vector of length n summing to 1, and the *transition probabilities* are given in an $(n \times n)$ matrix K.
- A *stationary distribution* f is one satisfying

$$f(y) = \int K(x, y) f(x)\, dx.$$

In the discrete case, a simpler notation for this is to say a stationary distribution is a vector v so that $vK = v$, i.e., a left eigenvector for K.

Ergodic Markov chains

- A Markov chain is *irreducible* if for any pairs of states x and y there is an n so that the probability that the chain moves from x to y in n steps is nonzero.
- If a chain starts at x the (random) number of steps T before it revisits x is called the return time. A state is called positive recurrent if the expectation of T is finite.
- The *period* of a state x is the greatest common divisor of the numbers m so that $\Pr(T = m) > 0$. In an irreducible chain all states have the same period. If this period is 1 the chain is called *aperiodic*.
- A Markov chain is called *ergodic* if it is irreducible, aperiodic, and all states have a finite expected return time.

Fundamental limit theorem for ergodic Markov chains

- If $X_0, X_1, X_2, \ldots$ is an ergodic Markov chain then there exists a *unique* positive stationary distribution which is the *limiting distribution* for the chain.
- In other words, if we run an ergodic Markov chain long enough, its values will eventually be an approximate sample from the limiting distribution, which can be identified as the unique distribution that is stationary for the chain.

How to use this for MCMC

- The MCMC algorithm constructs a Markov chain which has a stationary distribution equal to the target density we would like to generate a sample from. (We look at how in Lecture 5.3).
- To use MCMC one needs to check that the constructed Markov chain is ergodic, but this is usually simple.
- Running the Markov chain will then eventually create values which are an approximate sample from the target distribution. But is this good enough?

The Ergodic theorem

- This theorem says that, when $X^{(0)}, \ldots, X^{(t)}, \ldots$, is sampled from an ergodic Markov chain with stationary distribution f, we have that

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} h(X^{(t)}) = E_f[h(X)]$$

- When the sample is instead a random sample from f, this is the law of large numbers; we then also have the extension to the Central Limit Theorem, telling us how fast the convergence is.
- In the ergodic case, we still have convergence, but we don't know as easily how fast it is.

MSA101/MVE187 2020 Lecture 5.3 Introduction to Markov chain Monte Carlo (MCMC)

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MCMC simulation: General idea

- We have a "target density" $f(x)$ and we would like to generate a sample (or approximate sample) from this density.
- We use the *Metropolis-Hastings algorithm* to construct a Markov chain $x_0, x_1, \ldots$ which has the target density as a stationary distribution.
- After checking that the chain is ergodic, we know that if we simulate long enough, the chain will provide an approximate sample which can be used for Bayesian inference and predictions with Monte Carlo integration.

The Metropolis-Hastings algorithm

Given a probability density f that we want to simulate from. Construct a *proposal function* $q(y \mid x)$ which for every x gives a probability density for a proposed new value y. The algorithm starts with a choice of an initial value $x^{(0)}$ for x, and then simulates $x^{(t+1)}$ given $x^{(t)}$ for $t \geq 0$. Specifically, given $x^{(t)}$,

- Simulate a new value y according to $q(y \mid x^{(t)})$.
- Compute the acceptance probability

$$\rho(x^{(t)}, y) = \min\left(\frac{f(y)q(x^{(t)} \mid y)}{f(x^{(t)})q(y \mid x^{(t)})}, 1\right).$$

- Set

$$x^{(t+1)} = \begin{cases} y & \text{with probability } \rho(x^{(t)}, y) \\ x^{(t)} & \text{with probability } 1 - \rho(x^{(t)}, y) \end{cases}$$

Proving that the Metropolis-Hastings algorithm works

- The missing ingredient is to prove that the Metropolis-Hastings (MH) algorithm has the target density as a stationary distribution.
- We do this by showing
  - The MH chain satisfies the *detailed balance condition* relative to the target density.
  - If a chain satisfies the detailed balance condition relative to a density f then f is a stationary distribution.

The detailed balance condition

- A Markov chain satisfies the *detailed balance condition* relative to a density f if, for all x, y,

$$f(x)K(x,y) = f(y)K(y,x)$$

  where $K(x,y)$ is the kernel of the Markov chain. The chain is then called a *time reversible* Markov chain.
- If a chain satisfies detailed balance relative to f, then f must be a stationary distribution.
- Prove by integrating over x!

The chain defined by Metropolis-Hastings satisfies the detailed balance condition relative to $f(x)$

- Assume first that $\rho(x, y) < 1$ (with $x \neq y$). Then

$$\begin{aligned} f(x)K(x,y) &= f(x)q(y \mid x)\rho(x,y) = f(x)q(y \mid x)\frac{f(y)q(x \mid y)}{f(x)q(y \mid x)} \\ &= f(y)q(x \mid y) = f(y)q(x \mid y)\rho(y,x) = f(y)K(y,x) \end{aligned}$$

  The next to last step is because $\rho(y, x) = 1$ when $\rho(x, y) < 1$.
- If we start with $\rho(x, y) = 1$ the situation is clearly symmetrical, and we get the same result.

Note that...

- ...the Metropolis-Hastings algorithm *only* requires knowledge of the target density $f(x)$ up to a constant not involving x, as the density only appears in the quotient $f(y)/f(x)$ in the algoritm.
- ...the Metropolis-Hastings algorith *only* requires knowledge of the proposal density up to a constant, for the same reason.
- ...similarly, smart versions of the Metropolis-Hastings algorithm uses proposal flunctions so that many factors in the acceptance probability

$$\frac{f(y)q(x \mid y)}{f(x)q(y \mid x)}$$

cancel each other.