Monte Carlo Methods

Edward Ionides

2016-03-23

Contents

Produced in R version 3.4.3.

Objectives

1. To review some basic ideas in Monte Carlo computation and simulating random variables.
2. To provide a basic introduction to the Monte Carlo approach, and the generation of simulated random variables, for those who haven't seen it before.

Our context: Monte Carlo methods for POMP models.

Let's consider a general POMP model. As before, let $y^*_{1:N}$ be the data, and let the model consist of a latent process $X_{0:N}$ and an observable process $Y_{1:N}$. Then the likelihood function is

$$\begin{aligned}
\mathcal{L}(\theta) &= f_{Y_{1:N}}(y^*_{1:N}\,;\theta) && (1)\\
&= \int_{x_0}\cdots\int_{x_N} f_{X_0}(x_0\,;\theta)\prod_{n=1}^{N} f_{Y_n|X_n}(y^*_n\,|\,x_n\,;\theta)\, f_{X_n|X_{n-1}}(x_n|x_{n-1}\,;\theta)\, dx_0\dots dx_N. && (2)
\end{aligned}$$

i.e., computation of the likelihood requires integrating (or summing, for a discrete model) over all possible values of the unobserved latent process at each time point. This is very hard to do, in general.

Let's review, and/or learn, some *Monte Carlo* approaches for evaluating this and other difficult integrals. An excellent technical reference on Monte Carlo techniques is @robert04.

The fundamental theorem of Monte Carlo integration

- The basic insight of Monte Carlo methods is that we can get a numerical approximation to a challenging integral,
$$H = \int h(x)\, f(x)\, dx,$$

if we can simulate (i.e., generate random draws) from the distribution with probability density function f.

- This insight is known as the *fundamental theorem of Monte Carlo integration.*

Theorem. Let $f(x)$ be the probability distribution function for a random variable X, and let $X_{1:J} = \{X_j, j = 1, \dots, J\}$ be an independent and identically distributed sample of size J from f. Let H_J be the sample average of $h(X_1) \dots, h(X_J)$,

$$H_J = \frac{1}{J} \sum_{j=1}^{J} h(X_j).$$

Then H_J converges to H as $J \to \infty$ with probability 1. Less formally, we write

$$H_J \approx \int h(x)\, f(x)\, dx.$$

Proof. This is the strong law of large numbers, together with the identity that

$$\mathbb{E}[h(X)] = \int h(x)\, f(x)\, dx.$$

- We can estimate the error in this approximation, because the empirical variance

$$V_J = \frac{1}{J-1} \sum_{j=1}^{J} \big[h(X_j) - H_J\big]^2$$

approximates the true variance, $\mathrm{Var}[h(X)] = \mathbb{E}\big[\big(h(X) - \mathbb{E}[h(X)]\big)^2\big]$.

- The standard error on the approximation $H_J \approx \mathbb{E}[h(X)]$ is therefore

$$\sqrt{\frac{V_J}{J}}.$$

- From the central limit theorem, the error is approximately normally distributed:

$$H_J - \mathbb{E}[h(X)] \;\sim\; \text{normal}\left(0, \frac{V_J}{J}\right).$$

- The fundamental theorem of Monte Carlo inspires us to give further thought on how to simulate from a desired density function f, which may itself be a challenging problem.
- We will review simulation, but first let's consider a useful generalization of the fundamental theorem.

Importance sampling

- Sometimes it is difficult to sample directly from the distribution of X.
- In this case, we can often make use of *importance sampling*, in which we generate random samples from another distribution (easier to simulate) and make the appropriate correction.

- Specifically, suppose we wish to compute $\mathbb{E}[h(X)]$, where $X \sim f$, but it is difficult or impossible to draw random samples from f.
- Suppose g is a probability distribution from which it's relatively easy to draw samples and let $Y_{1:J}$ be i.i.d. random variables drawn from g.
- Notice that
$$\mathbb{E}[h(X)] = \int h(x)\, f(x)\, \mathrm{d}x = \int h(x)\, \frac{f(x)}{g(x)}\, g(x)\, dx.$$
- So, we can generalize the Monte Carlo integration theorem to give the **Monte Carlo importance sampling theorem**,
$$\mathbb{E}[h(X)] \approx \frac{1}{J} \sum_{j=1}^{J} h(Y_j)\, \frac{f(Y_j)}{g(Y_j)}.$$
- We call $w_j = f(Y_j)/g(Y_j)$ the **importance weights**, and then we can write
$$\mathbb{E}[h(X)] \approx \frac{1}{J} \sum_{j=1}^{J} w_j\, h(Y_j).$$
- Since $\mathbb{E}[w_j] = \mathbb{E}[f(Y)/g(Y)] = 1$, we can modify this formula to give a **self-normalized importance sampling** estimate,
$$\mathbb{E}[h(X)] \approx \frac{\sum w_j\, h(Y_j)}{\sum w_j}.$$
- The self-normalized estimate requires computation of w_j only up to a constant of proportionality.
- The Monte Carlo variance associated with this estimate is
$$\frac{\sum w_j\, (h(Y_j) - \overline{h})^2}{\sum w_j}.$$
- Obtaining accurate estimates requires some thought to the importance distribution g. Specifically, if the tails of g are lighter than those of f, the Monte Carlo variance will be inflated and the estimates can be unusable.

Simulation techniques for general distributions

- Simulation refers to the generation of random variables.
- The general problem of simulation is: given a probability distribution f, find a procedure that generates random draws from f.
- This is a very important problem in scientific computing and much thought and effort has gone into producing reliable simulators for many basic random variables.
- There are two basic ways of solving this problem:
  1. The transformation method,
  2. The rejection method.

The transformation method

- This method works for discrete or continuous scalar random variables.
- Let f be the probability distribution function we seek to draw from (known as the **target distribution**) and F be the corresponding cumulative distribution function, i.e., $F(x) = \int_{-\infty}^{x} f(v)\,dv$.
- Let $F^{-1}(u) = \inf\{x : F(x) \geq u\}$ be the inverse of F.
- A basic fact is that, if $X \sim f$, then $F(X) \sim \text{uniform}(0, 1)$. Proof: If $f(X) > 0$, then

$$\begin{aligned} \mathbb{P}[F(X) \leq u] &= \mathbb{P}[X < F^{-1}(u)] && (3) \\ &= F\big(F^{-1}(u)\big) = u. && (4) \end{aligned}$$

- This suggests that, if we can compute F^{-1}, we use the following algorithm to generate $X \sim f$:

1. draw $U \sim \text{uniform}(0, 1)$.
2. let $X = F^{-1}(U)$.

The rejection method

- The transformation method is very efficient in that we are guaranteed to obtain a valid X from the density f for every $U \sim \text{uniform}(0, 1)$ we generate.
- Sometimes, however, we cannot compute the inverse of the cumulative distribution function, as required by the transformation method.
- Under such circumstances, the rejection method offers a less efficient, but more flexible, alternative.
- We'll see how and why this method works.

The rejection method for uniform random variables on arbitrary sets

- Let a random variable X take values in $\mathbb{R}^{\dim(X)}$.
- Suppose that X is **uniformly distributed** over a region $D \subset \mathbb{R}^{\dim(X)}$. This means that, for any $A \subset D$,

$$\mathbb{P}[X \in A] = \frac{\text{area}(A)}{\text{area}(D)}.$$

  We write

$$X \sim \text{uniform}(D).$$

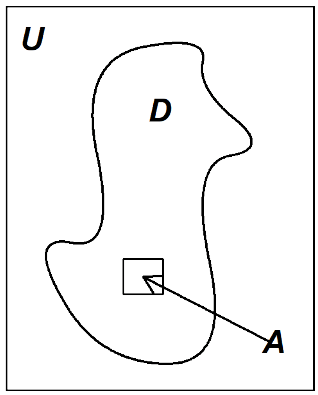
- Let's suppose that we wish to simulate $X \sim \text{uniform}(D)$.
- Suppose that we don't know how to directly simulate a random draw from D, but we know D is a subset of some nicer region $U \subset \mathbb{R}^{\dim(X)}$.
- If we know how to generate $Y \sim \text{uniform}(U)$, then we can simply do so until $Y \in D$, at which point we take $X = Y$.

- Since for any $A \subset D$,

$$\begin{aligned}
\mathbb{P}[X \in A] &= \mathbb{P}[Y \in A | Y \in D] && (5)\\
&= \frac{\text{area}(A)}{\text{area}(U)} \Big/ \frac{\text{area}(D)}{\text{area}(U)} && (6)\\
&= \frac{\text{area}(A)}{\text{area}(D)}, && (7)
\end{aligned}$$

  it follows that $Y \sim \text{uniform}(D)$.

- Consider an analogy to throwing darts. If the darts are thrown in such a way as to be equally likely to land anywhere in U, then those that do land in D are equally likely to land anywhere in D.



The rejection method for dominated densities

- A useful little fact allows us to extend the rejection method from uniform distributions to arbitrary densities.
- @robert04 refer to this fact the *fundamental theorem of simulation.*

- Let h be an arbitary positive, integrable function.
- Define

$$D = \{(x, u) : 0 \leq u \leq h(x)\},$$

  i.e., D is the graph of h.

- Consider the random pair $(X, U) \sim \text{uniform}(D)$.
- What is the marginal distribution of X?

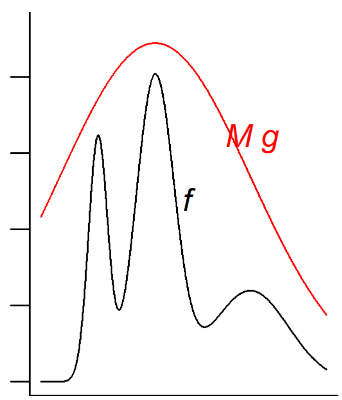
$$\int_0^{h(x)} \mathrm{d}u = h(x)$$

- So h is the probability distribution function for X!

- To carry out the rejection method, simulating from g to obtain a sample from f, we take our region D to be the **graph** of Mg, i.e.,
$$D = \{(x, y) : 0 \leq y \leq Mg(x),$$
where M is a constant chosen so that $Mg(x) \leq f(x)$ for all x.
- We propose points (X, Y) by drawing them uniformly from the area under the graph of $M\,g$.
- We **accept** the point (X, Y) if it lies under the graph of f.
- Then, the X-component of the (X, Y) pair is distributed according to f.

- This suggests the following rejection method for simulating an arbitrary random variable.
- Let f be the target distribution and g be another distribution function (from which it is easy to simulate) (see Figure below).
- Let M be such that $M\,g(x) {\geq} f(x)$ for all x.
- The following procedure simulates $X \sim f$.

1. draw $Y \sim g$ and $U \sim \text{uniform}(0, M\,g(Y))$.
2. if $U {\leq} f(Y)$, then let $X = Y$ else repeat step 1.



Acknowledgement: These notes derive from notes by Aaron King.