Computational statistics

Chapter 4: Classical simulation of probability distributions

Thierry Denœux
Université de technologie de Compiègne

Fall 2021

Overview

1. Introduction
2. Exact simulation
   - Generating from Standard Parametric Families
   - Probability integral transform
   - Rejection Sampling
3. Sampling Importance Resampling

Purpose of this chapter

- This chapter addresses the simulation of random draws $X_1, \ldots, X_n$ from a target distribution f.
- The most frequent use of such draws is to estimate the expectation of a function of a random variable, say $\mathbb{E}\{h(X)\}$. For instance: $\mathbb{E}\{X^k\}$, $\mathbb{P}(X \in A) = \mathbb{E}\{I(X \in A)\}$, etc.
- Example of applications:
  - E-step in the EM algorithm ("Monte-carlo EM")
  - Calculation of some likelihood functions ("simulated likelihood")
  - In Bayesian analyses, approximation of posterior moments, posterior probabilities, credible intervals, etc.
  - Estimation of risk, power of tests, etc.
  - etc.

Monte Carlo integration

- Let f denote the density of X, and μ denote the expectation of $h(X)$ with respect to f.
- When an i.i.d. random sample $X_1, \ldots, X_n$ is obtained from f, we can approximate μ by a sample average:

$$\widehat{\mu} = \frac{1}{n}\sum_{i=1}^{n} h(X_i) \rightarrow \int h(x)f(x)dx = \mu$$

as $n \rightarrow \infty$, by the strong law of large numbers.

Error estimation

- Further, let $\sigma^2 = \mathbb{E}\{(h(X) - \mu)^2\}$ be the variance of $h(X)$, assuming that this quantity exists.
- The Monte Carlo approach can be used to estimate σ^2 by

$$\widehat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^{n} [h(X_i) - \widehat{\mu}]^2 \tag{1}$$

- The Monte Carlo or simulation standard error (sse) of $\widehat{\mu}$ is $\sigma/\sqrt{n}$. It can be estimated by $\widehat{\sigma}/\sqrt{n}$.
- When σ^2 exists, the central limit theorem implies that $\widehat{\mu}$ has an approximate normal distribution for large n, so we get the following approximate confidence bounds for μ with confidence level $1 - \alpha$:

$$\widehat{\mu} \pm u_{1-\alpha/2} \frac{\widehat{\sigma}}{\sqrt{n}}$$

Non standard distributions

- Problem: how to generate draws from a target distribution f?
- When the target distribution comes from a standard parametric family, abundant software exists to easily generate random deviates.
- We focus on what should be done when the target density is not one easily sampled using the software.
- For example, nearly all Bayesian posterior distributions are not members of standard parametric families. Posteriors obtained when using conjugate priors in exponential families are exceptions.

Difficulties

- There can be additional difficulties beyond the absence of an obvious method to sample f. In many cases – especially in Bayesian analyses – the target density may be known only up to a multiplicative proportionality constant. In such cases, f cannot be sampled and can only be evaluated up to that constant. Fortunately, there are a variety of simulation approaches that still work in this setting.
- Finally, it may be possible to evaluate f, but computationally expensive. If each computation of $f(x)$ requires an optimization, an integration, or other time-consuming computations, we may seek simulation strategies that avoid direct evaluation of f as much as possible.
- Simulation methods can be categorized by whether they are exact or approximate.

Overview

1. Introduction
2. Exact simulation
   - Generating from Standard Parametric Families
   - Probability integral transform
   - Rejection Sampling
3. Sampling Importance Resampling

Overview

1 Introduction

2 Exact simulation
- Generating from Standard Parametric Families
- Probability integral transform
- Rejection Sampling

3 Sampling Importance Resampling

Standard uniform distribution

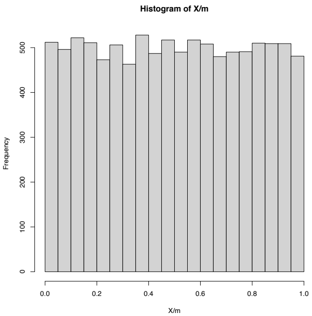
- At some level, all of code for simulation relies on the generation of Pseudorandom number generators (PRNGs), which are algorithms that can automatically create long runs of numbers that are statistically indistinguishable from independent standard uniform variates.
- The series of values generated by such algorithms is generally determined by a fixed number called a seed X_0. One of the most common PRNG is the linear congruential generator, which uses the recurrence

$$X_{n+1} = (aX_n + b) \bmod m$$

to generate numbers, where $0 < a < m$, $0 \leq b < m$ and $m > 0$ are large integers, and mod is the remainder of the integer division. The maximum number of numbers the formula can produce is the modulus, m.

Example in R

```
m<-2^32
a<-1664525
b<-1013904223
N<-10000
X<-rep(2^20,N)
for(i in 2:N) X[i]<-(a*X[i-1]+b)%%m
hist(X/m)
```



Familiar distributions

Methods to draw from some standard parametric distributions. The methods may be special case of a general method, or may be specific to the particular parametric family (ex: Student, Chi-square, etc.)

Distribution	Method
Uniform	See [195, 227, 383, 538, 539, 557]. For $X \sim \text{Unif}(a, b)$; draw $U \sim \text{Unif}(0, 1)$; then let $X = a + (b - a)U$.
Normal(μ, σ^2) and Lognormal(μ, σ^2)	Draw $U_1, U_2 \sim$ i.i.d. Unif(0, 1); then $X_1 = \mu + \sigma\sqrt{-2\log U_1}\cos\{2\pi U_2\}$ and $X_2 = \mu + \sigma\sqrt{-2\log U_1}\sin\{2\pi U_2\}$ are independent $N(\mu, \sigma^2)$. If $X \sim N(\mu, \sigma^2)$ then $\exp\{X\} \sim \text{Lognormal}(\mu, \sigma^2)$.
Multivariate $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$	Generate standard multivariate normal vector, $\mathbf{Y}$, coordinatewise; then $\mathbf{X} = \boldsymbol{\Sigma}^{-1/2}\mathbf{Y} + \boldsymbol{\mu}$.
Cauchy(α, β)	Draw $U \sim \text{Unif}(0, 1)$; then $X = \alpha + \beta\tan\{\pi(U - \frac{1}{2})\}$.
Exponential(λ)	Draw $U \sim \text{Unif}(0, 1)$; then $X = -(\log U)/\lambda$.
Poisson(λ)	Draw $U_1, U_2, \ldots \sim$ i.i.d. Unif(0, 1); then $X = j - 1$, where j is the lowest index for which $\prod_{i=1}^{j} U_i < e^{-\lambda}$.
Gamma(r, λ)	See Example 6.1, references, or for integer r, $X = -(1/\lambda)\sum_{i=1}^{r}\log U_i$ for $U_1, \ldots, U_r \sim$ i.i.d. Unif(0, 1).
Chi-square (df $= k$)	Draw $Y_1, \ldots, Y_k \sim$ i.i.d. $N(0, 1)$, then $X = \sum_{i=1}^{k} Y_i^2$; or draw $X \sim \text{Gamma}(k/2, \frac{1}{2})$.
Student's t (df $= k$) and $F_{k,m}$ distribution	Draw $Y \sim N(0, 1)$, $Z \sim \chi^2_k$, $W \sim \chi^2_m$ independently, then $X = Y/\sqrt{Z/k}$ has the t distribution and $F = (Z/k)/(W/m)$ has the F distribution.
Beta(a, b)	Draw $Y \sim \text{Gamma}(a, 1)$ and $Z \sim \text{Gamma}(b, 1)$ independently; then $X = Y/(Y + Z)$.
Bernoulli(p) and Binomial(n, p)	Draw $U \sim \text{Unif}(0, 1)$; then $X = 1_{\{U<p\}}$ is Bernoulli(p). The sum of n independent Bernoulli(p) draws has a Binomial(n, p) distribution.
Negative Binomial(r, p)	Draw $U_1, \ldots, U_r \sim$ i.i.d. Unif(0, 1); then $X = \sum_{i=1}^{r}\lfloor(\log U_i)/\log\{1-p\}\rfloor$, and $\lfloor\cdot\rfloor$ means greatest integer.
Multinomial$(1, (p_1, \ldots, p_k))$	Partition [0, 1] into k segments so the ith segment has length p_i. Draw $U \sim \text{Unif}(0, 1)$; then let X equal the index of the segment into which U falls. Tally such draws for Multinomial$(n, (p_1, \ldots, p_k))$.
Dirichlet$(\alpha_1, \ldots, \alpha_k)$	Draw independent $Y_i \sim \text{Gamma}(\alpha_i, 1)$ for $i = 1, \ldots, k$; then $\mathbf{X}^T = \left(Y_1/\sum_{i=1}^{k} Y_i, \ldots, Y_k/\sum_{i=1}^{k} Y_i\right)$.

Overview

1. Introduction
2. Exact simulation
   - Generating from Standard Parametric Families
   - Probability integral transform
   - Rejection Sampling
3. Sampling Importance Resampling

Principle

- The methods for the Cauchy and exponential distributions in the previous table are justified by the inverse cumulative distribution function or probability integral transform approach, based on the following proposition:

Proposition

For any continuous univariate distribution function F, if $U \sim Unif(0,1)$, then $X = F^{-1}(U)$ has a cumulative distribution function equal to F.

Proof: $\mathbb{P}(X \leq x) = \mathbb{P}(F^{-1}(U) \leq x) = \mathbb{P}(U \leq F(x)) = F(x)$.

- If F^{-1} is available for the target density, then this strategy is probably the simplest option.

Approximation

- If F^{-1} is not available but F is either available or easily approximated, then a crude approach can be built upon linear interpolation.
- Using a grid of $x_1, \dots, x_m$ spanning the region of support of f, calculate or approximate $u_i = F(x_i)$ at each grid point. Then, draw $U \sim \text{Unif}(0,1)$ and linearly interpolate between the two nearest grid points for which $u_i \leq U \leq u_j$ according to

$$X = \frac{u_j - U}{u_j - u_i} x_i + \frac{U - u_i}{u_j - u_i} x_j.$$

Discussion

- This approach is not exact, but its the degree of approximation is deterministic and can be reduced to any desired level by increasing m sufficiently.
- Compared to the alternatives, this simulation method is not appealing because
  - It requires a complete approximation to F regardless of the desired sample size
  - It does not generalize to multiple dimensions
  - It is less efficient than other approaches.

Overview

1 Introduction

2 Exact simulation
- Generating from Standard Parametric Families
- Probability integral transform
- Rejection Sampling

3 Sampling Importance Resampling

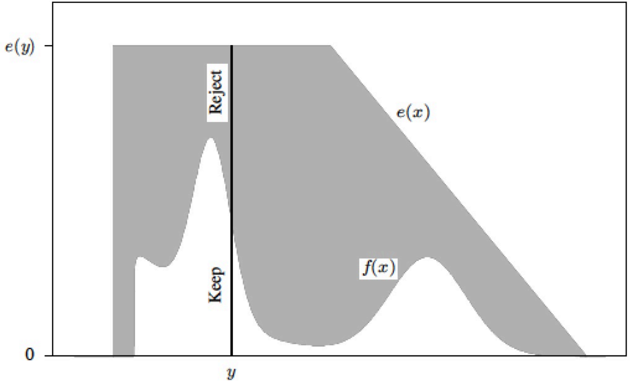
Basic idea

- If $f(x)$ can be calculated, at least up to a proportionality constant, then we can use rejection sampling to obtain a random draw from exactly the target distribution.
- This strategy relies on sampling candidates from an easier distribution and then correcting the sampling probability through random rejection of some candidates.

Algorithm

- Let g denote another density from which we know how to sample and for which we can easily calculate $g(x)$. Let $e(\cdot)$ denote an envelope, having the property $e(x) = g(x)/\alpha \geq f(x)$ for all x for which $f(x) > 0$, for a given constant $\alpha \leq 1$.
- Rejection sampling proceeds as follows:
  1. Sample $Y \sim g$.
  2. Sample $U \sim \text{Unif}(0, 1)$.
  3. Reject Y if $U > f(Y)/e(Y)$. In this case, do not record the value of Y as an element in the target random sample. Instead, return to step 1.
  4. Otherwise, keep the value of Y. Set $X = Y$, and consider X to be an element of the target random sample. Return to step 1 until you have accumulated a sample of the desired size.

Rejection sampling



The shaded region above f and below e indicates the waste. The draw $Y = y$ is very likely to be rejected when $e(y)$ is far larger than $f(y)$. Envelopes that exceed f everywhere by at most a slim margin produce fewer wasted (i.e., rejected) draws and correspond to α values near 1.

Property

Proposition

The draws kept using this algorithm constitute an i.i.d. sample from the target density f; there is no approximation involved.

Proof

$$
\begin{aligned}
P[X \leq y] =& P\left[Y \leq y \mid U \leq \frac{f(Y)}{e(Y)}\right] && \text{(2a)}\\
&= P\left[Y \leq y \text{ and } U \leq \frac{f(Y)}{e(Y)}\right] \Big/ P\left[U \leq \frac{f(Y)}{e(Y)}\right] && \text{(2b)}\\
&= \int_{-\infty}^{y} \int_{0}^{f(z)/e(z)} du \, g(z) \, dz \Big/ \int_{-\infty}^{+\infty} \int_{0}^{f(z)/e(z)} du \, g(z) \, dz \\
&= \int_{-\infty}^{y} \frac{f(z)}{e(z)} g(z) \, dz \Big/ \int_{-\infty}^{+\infty} \frac{f(z)}{e(z)} g(z) \, dz && \text{(2c)}\\
&= \frac{\int_{-\infty}^{y} \alpha f(z) \, dz}{\alpha} = \int_{-\infty}^{y} f(z) \, dz. && \text{(2d)}
\end{aligned}
$$

Efficiency of the algorithm

- We have shown that

$$P\left[U \leq \frac{f(Y)}{e(Y)}\right] = \alpha.$$

Consequently, α can be interpreted as the expected proportion of candidates that are accepted.

- Hence α is a measure of the efficiency of the algorithm.
- We may continue the rejection sampling procedure until it yields exactly the desired number of sampled points, but this requires a random total number of iterations that will depend on the proportion of rejections.

Case where f is known up to a proportionality constant

- Suppose now that the target distribution f is only known up to a proportionality constant c. That is, suppose we are only able to compute easily $q(x) = f(x)/c$, where c is unknown.
- Such densities arise, for example, in Bayesian inference when f is a posterior distribution known to equal the product of the prior and the likelihood scaled by some normalizing constant.
- Fortunately, rejection sampling can be applied in such cases. We find an envelope e such that $e(x) \geq q(x)$ for all x for which $q(x) > 0$.
- A draw $Y = y$ is rejected when $U > q(y)/e(y)$. The sampling probability remains correct because the unknown constant c cancels out in the numerator and denominator of (2c) when f is replaced by q. The proportion of kept draws is α/c.

Good rejection sampling envelopes

Good rejection sampling envelopes have three properties:

1. They are easily constructed to exceed the target everywhere
2. They are easy to sample
3. They generate few rejected draws.

Sampling from a Bayesian posterior

- Suppose we want to sample from

$$f(\theta \mid x) \propto f(x \mid \theta) f(\theta) = L(\theta \mid x) f(\theta)$$

- Let $q(\theta \mid x) = L(\theta \mid x) f(\theta)$. We have

$$q(\theta \mid x) \leq L(\widehat{\theta} \mid x) f(\theta) = e(\theta)$$

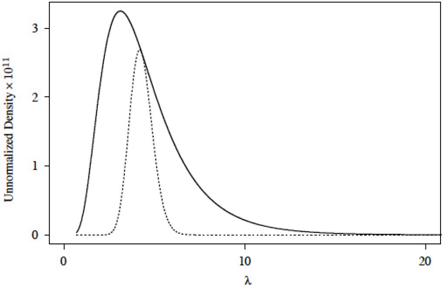
  where $\widehat{\theta}$ is the MLE of θ.

- The rejection sampling algorithm becomes:
  1. Sample $\theta_i \sim f(\theta)$ (the prior)
  2. Sample $U_i \sim \mathrm{Unif}(0, 1)$
  3. Keep θ_i if

$$U_i < \frac{q(\theta_i \mid x)}{e(\theta)} = \frac{L(\theta_i \mid x)}{L(\widehat{\theta} \mid x)}$$

Example

- Suppose 10 independent observations $(8, 3, 4, 3, 1, 7, 2, 6, 2, 7)$ are collected from the model $X_i|\lambda \sim \mathcal{P}(\lambda)$. A lognormal prior distribution for λ is assumed: $\log \lambda \sim \mathcal{N}(\log 4, 0.52)$. We have $\widehat{\lambda} = \overline{x} = 4.3$.
- Unnormalized target $q(\lambda \mid x)$ (dotted) and envelope $e(\lambda)$ (solid):

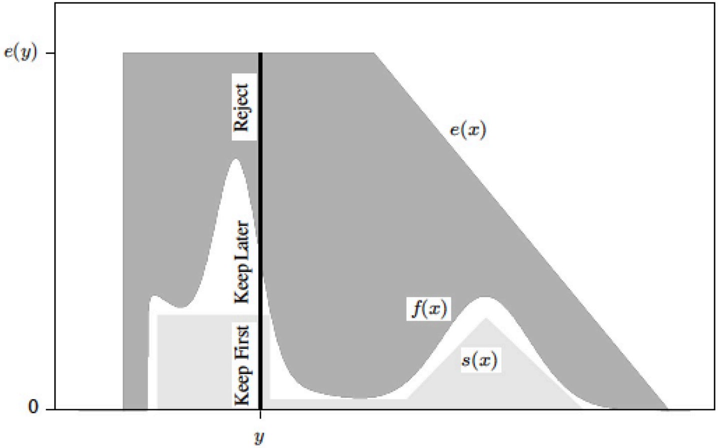


- Although not efficient – only about 30% of candidate draws are kept – this approach is easy and exact.

Squeezed rejection sampling

- When evaluating f is computationally expensive, we can use a nonnegative squeezing function s such that $s(x) \leq f(x)$ for all x such that $f(x) > 0$.
- The algorithm becomes
  1. Sample $Y \sim g$.
  2. Sample $U \sim \text{Unif}(0, 1)$.
  3. If $U \leq s(Y)/e(Y)$, keep Y and set $X = Y$.
  4. Else if $U \leq f(Y)/e(Y)$, keep Y and set $X = Y$.
  5. Otherwise, reject Y and return to step 1.

Squeezed rejection sampling



Overview

1. Introduction
2. Exact simulation
   - Generating from Standard Parametric Families
   - Probability integral transform
   - Rejection Sampling
3. Sampling Importance Resampling

Need for approximations

- Although the methods described above have the appealing feature that they are exact, there are many cases when an approximate method is easier or perhaps the only feasible choice.
- Approximation is not a critical flaw as long as the degree of approximation can be controlled by user-specified parameters in the algorithms.
- Many approximate simulation methods are based to some extent on the Sampling Importance Resampling (SIR) principle.

Basic idea

- The SIR algorithm simulates realizations approximately from some target distribution.
- SIR is based upon the notion of importance sampling.
- Briefly, importance sampling proceeds by drawing a sample from an importance sampling function, g. Informally, we will call g an envelope.
- Each point in the sample is weighted to correct the sampling probabilities so that the weighted sample can be related to a target density f.

SIR algorithm

- Let X denotes a random variable or vector with density $f(x)$, and let g denote the density corresponding to an envelope for the target density f, such that the support of g includes the entire support of f $(\forall x, g(x) = 0 \Rightarrow f(x) = 0)$.
- SIR algorithm:
  1. Sample candidates $Y_1, \ldots, Y_m$ i.i.d. from g.
  2. Calculate the standardized importance weights, $w(Y_1), \ldots, w(Y_m)$, with
  $$w(Y_i) = \frac{f(Y_i)/g(Y_i)}{\sum_{j=1}^m f(Y_j)/g(Y_j)} \quad (3)$$
  3. Resample $X_1, \ldots, X_n$ from $Y_1, \ldots, Y_m$ with replacement with probabilities $w(Y_1), \ldots, w(Y_m)$.
- Remark: when $f = cq$ for some unknown proportionality constant c, the unknown c cancels in the numerator and denominator of (3).

Property

Proposition

A random variable X drawn with the SIR algorithm has distribution that converges to f as $m \to \infty$.

Sketch of proof

- Let X be a r.v. drawn with the SIR algorithm. Define $w^*(y) = f(y)/g(y)$, let $Y_1, \ldots, Y_m$ i.i.d. from g and consider an event A.

$$\mathbb{P}(X \in A \mid Y_1, \ldots, Y_m) = \sum_{\{i | Y_i \in A\}} w(Y_i)$$
$$= \sum_{i=1}^{m} I(Y_i \in A) w^*(Y_i) \Big/ \sum_{i=1}^{m} w^*(Y_i)$$

- From the strong law of large numbers,

$$\frac{1}{m}\sum_{i=1}^{m} I(Y_i \in A) w^*(Y_i) \to \mathbb{E}\left\{I(Y \in A) w^*(Y)\right\} = \int_A w^*(y) g(y) dy$$

and

$$\frac{1}{m}\sum_{i=1}^{m} w^*(Y_i) \to \mathbb{E}\left\{w^*(Y)\right\} = \int w^*(y) g(y) dy = 1$$

Sketch of proof (continued)

- Consequently,

$$\mathbb{P}(X \in A \mid Y_1, \ldots, Y_m) \to \int_A w^*(y)g(y)dy = \int_A f(y)dy$$

- Finally, we have

$$\mathbb{P}(X \in A) = \mathbb{E}\left\{\mathbb{P}(X \in A \mid Y_1, \ldots, Y_m)\right\} \to \int_A f(y)dy$$

(by Lebesgue's dominated convergence theorem)

Sample sizes

- When conducting SIR, it is important to consider the relative sizes of the initial sample and the resample. These sample sizes are m and n, respectively.
- In principle, we require $n/m \to 0$ for distributional convergence of the sample. In the context of asymptotic analysis of Monte Carlo estimates based on SIR, where $n \to \infty$, this condition means that $m \to \infty$ even faster than $n \to \infty$.
- For fixed n, distributional convergence of the sample occurs as $m \to \infty$, therefore in practice one wants to initiate SIR with the largest possible m. However, one faces the competing desire to choose n as large as possible to increase the inferential precision.
- Rule of thumb: ensure $n/m \leq 1/10$ so long as the resulting resample does not contain too many replicates of any initial draw.

Envelope

- The SIR algorithm can be sensitive to the choice of g.
- First, the support of g must include the entire support.
- Further, g should have heavier tails than f, or more generally g should be chosen to ensure that $f(x)/g(x)$ never grows too large.
- If $g(x)$ is nearly zero anywhere where $f(x)$ is positive, then a draw from this region will happen only extremely rarely, but when it does it will receive a huge weight. When this problem arises, one or a few standardized importance weights are enormous compared to the other weights, and the secondary sample consists nearly entirely of replicated values of one or a few initial draws.
- When the distribution of weights is found to be highly skewed, it is probably wiser to switch to a different envelope or a different sampling strategy altogether.

Application to Bayesian inference

- Suppose that we seek a sample from the posterior distribution from a Bayesian analysis.
- Let $f(\theta)$ denote the prior, and $L(\theta \mid x)$ the likelihood, so the posterior is $f(\theta \mid x) = c \cdot f(\theta)L(\theta \mid x)$ for some constant c that may be difficult to determine.
- If the prior does not seriously restrict the parameter region favored by the data via the likelihood function, then the prior can serve as a useful importance sampling function.
- Sample $\theta_1, \ldots, \theta_m$ i.i.d. from $f(\theta)$. Since the target density is the posterior, the i-th unstandardized weight equals $c \cdot L(\theta_i \mid x)$. Thus the SIR algorithm has a very simple form: Sample from the prior, weight by the likelihood, and resample.
- Remark: we do not need to know $\widehat{\theta}$, in contrast with the rejection sampling method.