Computational Statistics

Lecture 8: Accept-Reject Methods

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Content of Lecture

Principles of Monte Carlo integration

The generic problem of Monte Carlo Integration (MCI) consists in evaluating the following integral:

$$E_f[h(X)] = \int_{S_x} h(x)f(x)dx, \qquad (*)$$

where S_x denotes the set where the random variable X takes its value, which is usually equal to the support of the density f. The principle of MCI method for approximating Integral (*) is to generate a sample $(X_1.X_2, ..., X_n)$ from the density f and propose as an approximation for $E_f[h(X)]$ the empirical average $\overline{h_n}$ as follows:

$$\overline{h_n} = \frac{1}{n}\sum_{j=1}^{n} h(x_j). \qquad (**)$$

By the Strong Law of Large Numbers, $\overline{h_n}$ converges indeed to $E_f[h(X)]$.

Monte Carlo Integration – continue

When $h(X)$ has a finite expectation under f, the convergence takes place at a speed $O(\sqrt{n})$ and the asymptotic variance of the approximation (**) is

$$var(\overline{h_n}) = \frac{1}{n}\int_{\mathcal{X}} (h(x) - E_f[h(X)])^2 f(x)dx,$$

which can be estimated from the sample $(X_1.X_2, ..., X_n)$ through

$$v_n = \frac{1}{n^2}\sum_{j=1}^{n}[h(x) - \overline{h_n}]^2.$$

Due to the CLT, for large n,

$$\frac{\overline{h_n} - E_f[h(X)]}{\sqrt{v_n}} \rightsquigarrow \mathcal{N}(0,1).$$

MCI application

MCI of $h(x) = \left(\cos(50x) + \sin(20x)\right)^2$ over the interval $[0,1]$ may be achieved with a sample $(U_1, ..., U_n)$ of 10^4 i.i.d $\mathcal{U}(0,1)$ random variables. We approximate $\int h(x)dx$ with $\sum h(U_i)/n$.

Example R session:

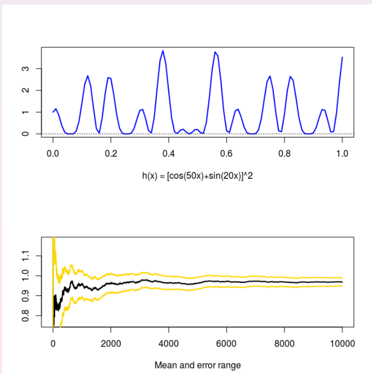
```
> h = function(x){
+         ( cos(50*x) + sin(20*x) )^2 }
> integrate(h,0,1)
0.9652009 with |error| < 1.9e-10
> n = 10^4
> x = runif(n)
> hx = h(x)
> estint=cumsum(hx)/(1:n)
> estint[n]
[1] 0.9681744
> esterr=sqrt(cumsum(
+          (hx-estint)^2) / (1:n)^2 )
> esterr[n]
[1] 0.01044141
```


MCI application – continue

The upper panel in the figure below shows the function $h(x)$ over the domain $[0,1]$. The lower panel shows the running means with bounds of $2\times$ the estimated standard error depending on the sample size $n = 10^4$.

Example R session:

```
> par(mfrow=c(2,1))
> curve(h,0,1,xlab="h(x) =
+ [cos(50x)+sin(20x)]^2",ylab="",
+ lwd=2,col="blue")
> abline(h=0,lty=3)
> plot(estint,
+  xlab="Mean and error range",
+  type="l",lwd=2,,ylab="",
+  ylim=mean(hx)+
+        20*c(-esterr[n],esterr[n]))
> lines(estint-2*esterr,col="gold",
+                            lwd=2)
> lines(estint+2*esterr,col="gold",
+                            lwd=2)
```



Simple MC integration in action

Examples

1. To approximate the integral $\int_0^1 x^4 dx$ in the interval $[0,1]$ one may use the following R code:

```
> U = runif(10^5)
> mean(U^4)
[1] 0.2008846
```

The exact answer naturally is $[x^5/5]_0^1 = 1/5 - 0 = 0.2$

2. To approximate the integral $\int_2^5 \sin(x)dx$ one may use the following R code:

```
> U = runif(10^5, min=2, max = 5)
> mean(sin(U)) * (5-2)
[1] -0.6984924
```

The exact answer is $[-cos(x)]_2^5$, with

```
> cos(2) - cos(5)
[1] -0.699809
```

multiple Monte Carlo integration

Let U_1, U_2, ...,U_n and V_1, V_2, ...,V_n be two sets of independent uniform distributed random variables on the interval $[0,1]$, and suppose $g(x,y)$ is now an integrable function of two variables x and y, then the CLT states that

$$\left(\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\left(g(U_i,V_i)\right)\right)(b-a)(d-c) \;=\; \int_a^b\int_c^d g(x,y)dxdy$$

with probability 1.
So we can approximate the integral $\int_a^b\int_c^d g(x,y)dxdy$ by generating two sets of independent uniform numbers, computing $g(U_i,V_i)$ for each one, and taking the sampled average multiplied by the respective integration intervals.

Example of MMC integration

Example

To approximate the integral $\int_3^{10}\int_1^7 \sin(x-y)dxdy$ one may use the following R code:

```
> U = runif(10^5,min=1,max=7)
> V = runif(10^5,min=3,max=10)
> mean(sin(U-V)) * (7-1) * (10-3)
[1] 0.07989664
```


Importance Sampling Principle

If the density of a random variable is $f(x)$ then

$$E\left[\frac{f(x)}{g(x)}\right] \;=\; \int_{-\infty}^{+\infty}\left(\frac{f(x)}{g(x)}\right)g(x)dx \;=\; \int_{-\infty}^{+\infty} f(x)dx$$

Hence we can approximate the last integral by taking the average of a sample X_i of ratios $f(X_i)/g(X_i)$.

Example

If we are interested in tail probabilities like $P(Z>4.5)=\int_{4.5}^{\infty} f(z)dz$ if $Z\sim\mathcal{N}(0,1)$, which is very small (3.4e-06), we may enhance the MCI approach by using a smart instrumental density $g(x)$ like the exponential distribution truncated at 4.5:

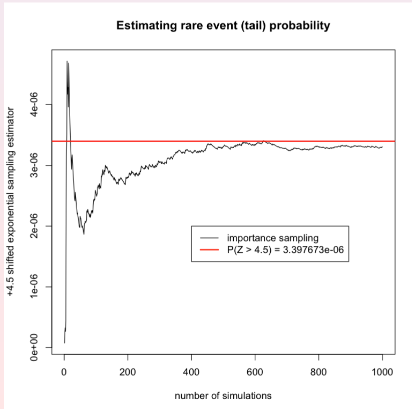
$$g(x)=\frac{e^{-x}}{\int_{4.5}^{\infty} e^{-(x-4.5)}},$$

Example of importance sampling

In the example above, the importance sampling estimator of the tail probability becomes:

$$\frac{1}{n}\sum_{i=1}^{n}\frac{f(X^{(i)})}{g(X^{(i)})} \;=\; \frac{1}{n}\sum_{i=1}^{n}\frac{e^{-X_i^2/2+X_i-4.5}}{\sqrt{2\pi}}$$

```
> pnorm(-4.5)
[1] 3.397673-06
> Nsim=10^3
> x = rexp(Nsim) + 4.5
> isest = cumsum(dnorm(x)/
+           dexp(x-4.5))/1:Nsim
> plot(isest,type="l")
> abline(a=pnorm(-4.5),b=0,
+           col="red")
```



Content of Lecture

Accept-reject principle

Accept-reject Monte Carlo methods are the most powerful and may simulate virtually any integral or density distribution.
We only need to know the target density function f up to a multiplicative constant. We use a simpler instrumental density g verifying the following two conditions:

(i) f and g have a compatible support $[low, high]$, i.e. $g(x) > 0$ when $f(x) > 0$ and $x \in [low, high]$;

(ii) There is a constant M with $f(x)/g(x) \leqslant M$ for all $x \in [low, high]$.

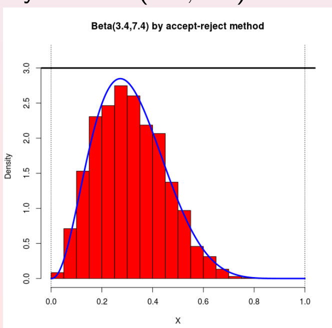
In this case, we proceed like this:

1. Generate independently $Y \sim g$ and $U \sim \mathcal{U}(low, high)$.
2. If $MY \leqslant f(U)$, we set $X = Y$.

Generating a Beta random variable

The support of the beta density is the interval $[0, 1]$. We suppose that $\alpha > 1$ and $\beta > 1$. The upper bound M of the acceptance domain is the highest density observed for $\mathcal{B}eta(a, b)$. For $a = 3.4$ and $b = 7.4$ we notice that $dbeta(3.4, 7.4) < M = 3$. With $U \sim \mathcal{U}(low = 0, high = 1)$, and a uniform intrumental density $Y \sim \mathcal{U}(0, 1)$, we may generate the beta random variable $X \sim \mathcal{B}eta(a = 3.4, b = 7.4)$, by accepting all pairs (U, Y) where MY is strictly below the density of $\mathcal{B}eta(3.4, 7.4)$:

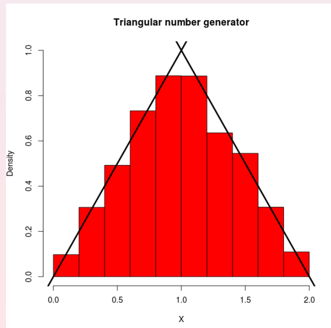
```
> Nsim = 10^4
> low = 0; high = 1
> U = runif(Nsim,low,high)
> Y = runif(Nsim)
> a = 3.4; b = 7.4,M = 3
> X = U[M*Y < dbeta(U,a,b)]
> hist(X,freq=F,xlim=c(0,1),ylim=c(0,3),
+ main="Beta(3.4,7.4)
+       by accept-reject method")
```



Simulating a triangular density function

We may use as well this accept-reject method for simulating a random number generator with a triangular density function$f(x) = 1 - |1 - x|$ for x taking values in the interval $[0, 2]$. The intrumental density may be uniform again. The triangular density being bounded by 1.0, we can set M equal to 1:

```
> Nsim = 10^4
> low = 0 ; high = 2
> U = runif(Nsim,low,high)
> Y = runif(Nsim)
> M = 1
> X = U[M*Y < 1-abs(1-U)]
> hist(X,freq=F,xlim=c(0,2),ylim=c(0,1),
+ main="Triangular number generator")
> abline(0,1);abline(2,-1)
```



Accept-reject based generators - Exercises

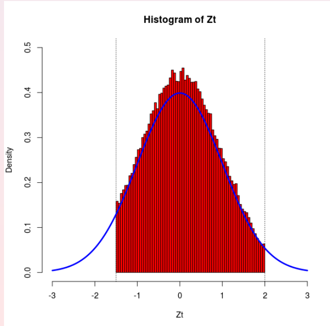
Exercise

1. *Accept-reject methods based generators do not deliver a fixed number of random numbers. Update the method in order to deliver a given number* `Nsim` *of instances.*
2. *Generalize the previous approach to implement a parametric generator for triangular random numbers defined on the real interval* $[m = 0, M = 10]$ *with mode* $x_{mo} = 4$ *and a probability* $r = 0.6$ *to observe a value before or equal* x_{mo} *and* $1 - r = 0.4$ *after it.*

Application: Simulate a truncated Gaussian

We want to simulate the standard normal $Z \sim \mathcal{N}(0,1)$ random variable restricted to the domain $[-1.5, +2]$.
As instrumental distribution we take the standard Z variable and we accept only the observations z that are in the required range. We thus obtain the following truncated Gaussian random variable Zt:

```
> Nsim = 10^5
> low = -1.5; high = 2
> Z = rnorm(Nsim)
> Zt = Z[(Z > low) & (Z < high)]
> hist(Zt,freq=F,breaks=51,
      xlim=c(-3,3),col="red")
> z = seq(-3,3,length=500)
> lines(z,dnorm(z),col="blue")
```

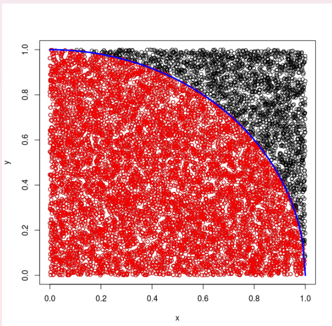


Application: Monte Carlo π estimation

The area of the circle of radius $r = 1$ is πr^2. The area of the square containing this circle is $(2r)^2 = 2^2 = 4$. The ratio of the area of the circle to the area of the square is:

$$\rho = \frac{\pi r^2}{(2r)^2} = \frac{\pi}{4} = \frac{3.141593}{4} = 0.7853982$$

```
> x = runif(Nsim)
> y = runif(Nsim)
> plot(x,y)
> rhox = x[(x^2+y^2)<1]
> rhoy = y[(x^2+y^2)<1]
> points(rhox,rhoy,col="red")
> ax = seq(0,1,0.01)
> lines(ax, sqrt(1-ax^2),
+       lwd=3,col="blue")
> 4*length(rhox)/length(x)
[1] 4 x 0.786 = 3.144
```



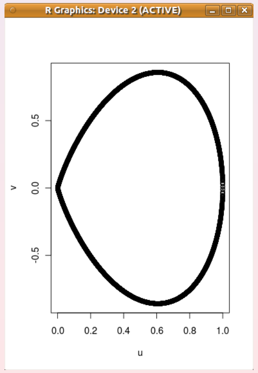
The Box-Muller accept-reject tranform

Recall the Box-Muller algorithm for the centered and reduced normal $Z \sim \mathcal{N}(0,1)$ variable. It is based on the observation that, if U_1 and U_2 are two independent and identically $\mathcal{U}(0,1)$ distributed random variables, then: $X_1 = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$, $\quad X_2 = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$, are two independent and identically $\mathcal{N}(0,1)$ distributed random variables.
Suppose we pick V_1 and V_2 instead as the ordinate and abcissa of a uniform random point in the unit circle around the origin. Then the sum of their squares $R^2 = V_1^2 + V_2^2$ is a uniform variable that can be used for U_1, while the angle that the point (V_1, V_2) defines with respect to the V_1 axis can serve as random angle $2\pi U_2$.
The cosine and sinus in the Box-Muller formula can now be written as $V_1/\sqrt{R^2}$ and $V_2/\sqrt{R^2}$. This implementation can in fact be seen as a kind of acept-reject method for computing trigonometric functions of a uniform random angle.
(See Box-Muller transform)

Ratio-Of-Uniforms Method

Virtually any random variable X can be simulated by the following simple prescription:

1. Construct a region A in the (u, v) plane bounded by $0 \leqslant u \leqslant [p(v/u)]^{1/2}$.
2. Choose a point $P = (u, v)$ distributed uniformly within this region A.
3. If $P(u, v) \in A$, return v/u as a required simulated random variable instance .



Fast generation of Gaussian random variable

In case of a normal $Z \sim \mathcal{N}(0, 1)$ random variable, the region A becomes:

$$A = \{(u, v) \mid v^2 < -4u^2 \ln u\}.$$

This region is entirely contained in the rectangle $R = \{0 < u < 1, -(2/e)^{1/2} < v < (2/e)^{1/2}\}$ and the accept-reject method is used to select the points $P = (u, v)$ such that $z = v/u$ delivers the variable Z.

Exercise

In 1992, Joseph Leva has published a very fast and efficient Z variable generator based on this approach (see his paper in the moodle resources).

1. *Implement this algorithm in C++ (NR), in Python and in R,*
2. *Check the quality of the generator when compared with the standard Python and R generators,*
3. *Compare the respective run times in C++, in Python and R for a sample of 100000 normal random numbers.*