MATH 556: MATHEMATICAL STATISTICS I

RANDOM NUMBER GENERATION AND MONTE CARLO

Many functions exist in R to produce random samples from probability distributions.

```
n<-10
args(rnorm)

+ function (n, mean = 0, sd = 1)
+ NULL

rnorm(n,5,sqrt(4))     #sample from Normal(5,4)

+  [1] 7.223009 5.240500 4.715339 4.594866 4.236323 5.163522 5.529968
+  [8] 6.540460 6.992879 8.077577

args(rgamma)

+ function (n, shape, rate = 1, scale = 1/rate)
+ NULL

rgamma(n,2,0.5)        #sample from Gamma(2,0.5)

+  [1] 1.0254782 0.5505856 0.9760013 2.9239228 1.2410966 2.3960980 3.8044358
+  [8] 8.9222620 2.8087903 1.8083036

args(rpois)

+ function (n, lambda)
+ NULL

rpois(n,3.5)           #sample from Poisson(3.5)

+  [1] 7 3 3 5 0 4 1 4 2 1

args(sample)

+ function (x, size, replace = FALSE, prob = NULL)
+ NULL

sample(c(1:100),n,replace=T)    #sample discrete uniform on {1,2,...,100} with replacement

+  [1]  2 50  7 36 41 99  5 25 79 30

sample(c(1:100),n,replace=F)    #sample discrete uniform on {1,2,...,100| without replacement

+  [1] 99 48 26 98 75 70 36 68 17 61

sample(c(1:5),n,replace=T,prob=c(0.2,0.1,0.4,0.1,0.2))  #sample discrete distn on {1,2,...,5}

+  [1] 2 3 5 3 3 5 1 3 2 2
```

The `set.seed()` function can be used to make the random draws reproducible

```
set.seed(8910)
rnorm(5);rnorm(5)

+ [1]  0.8214213  0.6982410 -0.3845740  1.3006786  1.4397298
+ [1]  0.02488985  0.69435700  0.32589669 -1.19616616  0.61756331

set.seed(8910)
rnorm(5)

+ [1]  0.8214213  0.6982410 -0.3845740  1.3006786  1.4397298
```

Random samples can be used for several purposes in basic distribution theory.

- **Visualization:** $X \sim Weibull(\alpha, \beta)$

$$f_X(x) = \alpha\beta x^{\alpha-1}\exp\{-\beta x^{\alpha}\} \qquad x > 0$$

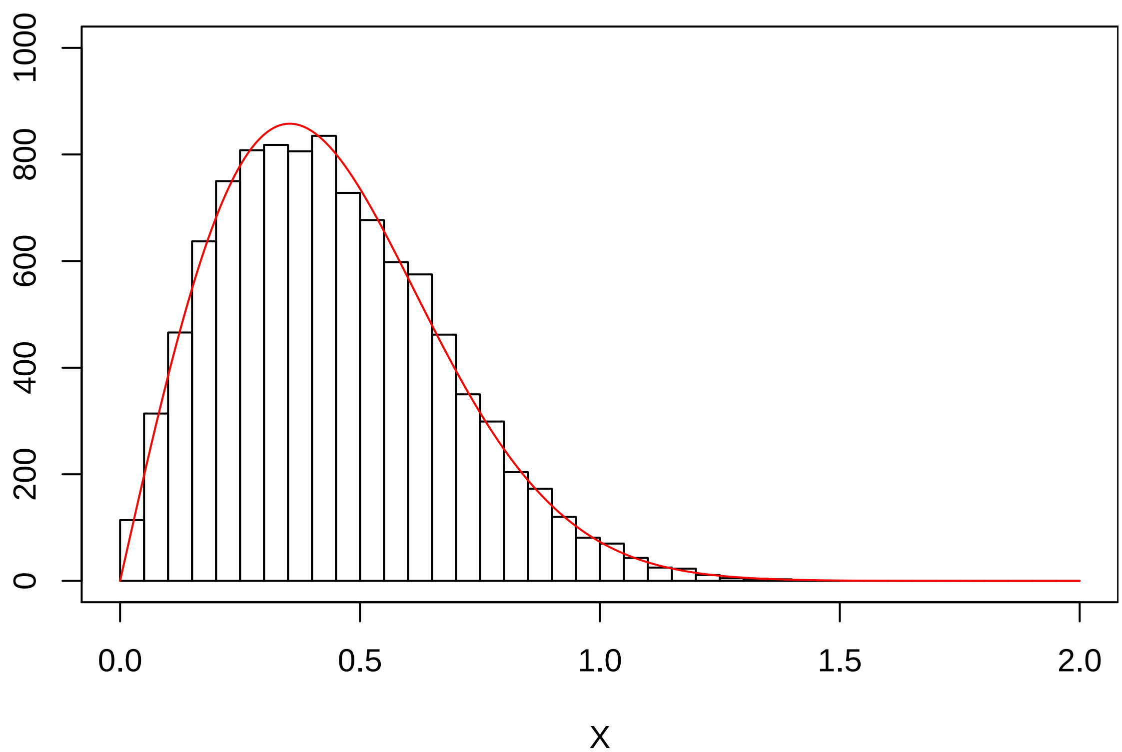
and zero otherwise, for $\alpha > 0$ and $\beta > 0$. Parameter α is the *shape* parameter, and β controls the dispersion of the distribution. An alternative parameterization utilizes the *scale* parameter $\sigma = 1/\beta^{1/\alpha}$ yielding pdf

$$f_X(x) = \frac{\alpha}{\sigma}\left(\frac{x}{\sigma}\right)^{\alpha-1}\exp\left\{-\left(\frac{x}{\sigma}\right)^{\alpha}\right\} \qquad x > 0$$

This is the parameterization that `R` uses. The expectation of this distribution is

$$\mathbb{E}_X[X] = \frac{\Gamma\left(1+\dfrac{1}{\alpha}\right)}{\beta^{1/\alpha}} = \sigma\Gamma\left(1+\frac{1}{\alpha}\right).$$

```
set.seed(8910)
n<-10000
args(rweibull)
+ function (n, shape, scale = 1)
+ NULL
al<-2;be<-4
sig<-1/be^{1/al}
X<-rweibull(n,al,sig)
par(mar=c(4,3,1,0))
hist(X,breaks=seq(0,2,by=0.05),main='',ylim=range(0,1000));box()
x<-seq(0,2,by=0.001)
fx<-dweibull(x,al,sig)
lines(x,fx*n*0.05,col='red')
```



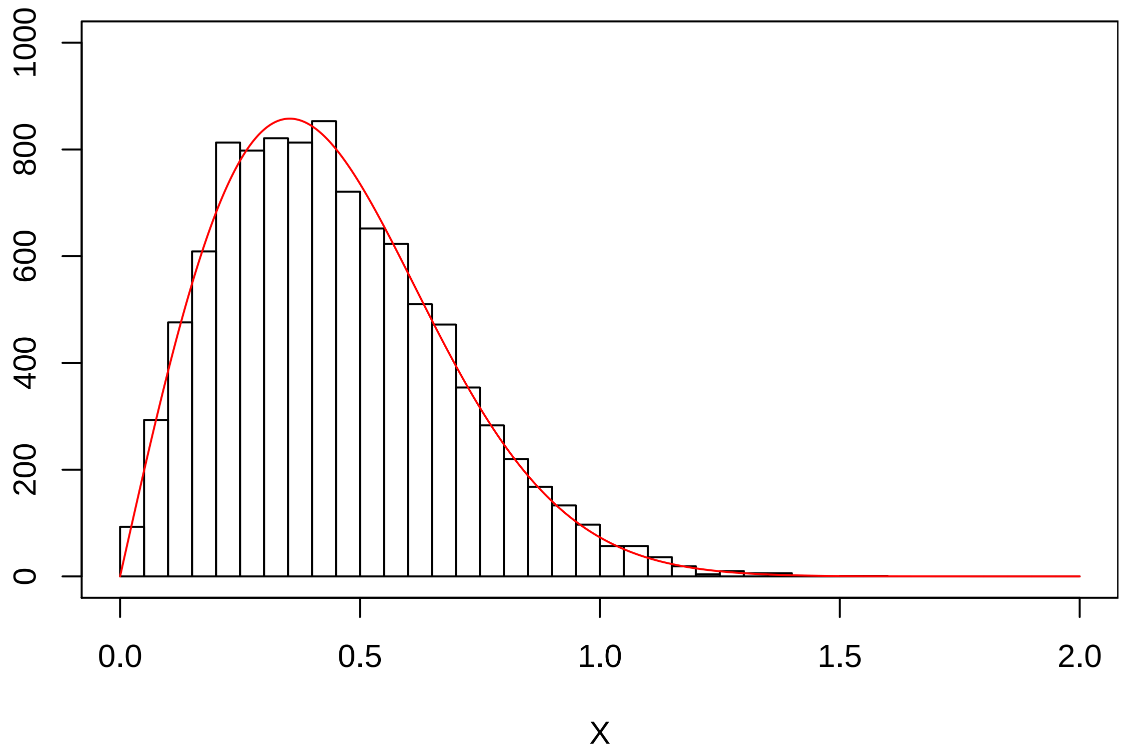

```
sig*gamma(1+1/al)   #Expectation
+ [1] 0.4431135
mean(X)             #Sample mean
+ [1] 0.4425448
```

- **Transformations:** If $U \sim Uniform(0,1)$, then

$$X = \left(-\frac{1}{\beta}\log(1-U)\right)^{1/\alpha}$$

ensures that $X \sim Weibull(\alpha, \beta)$

```
set.seed(8910)
n<-10000
U<-runif(n)
X<-(-log(1-U)/be)^(1/al)
par(mar=c(4,3,1,0))
hist(X,breaks=seq(0,2,by=0.05),main='',ylim=range(0,1000));box()
lines(x,fx*n*0.05,col='red')
```




```
sig*gamma(1+1/al)   #Expectation
+ [1] 0.4431135
mean(X)             #Sample mean
+ [1] 0.4448699
```

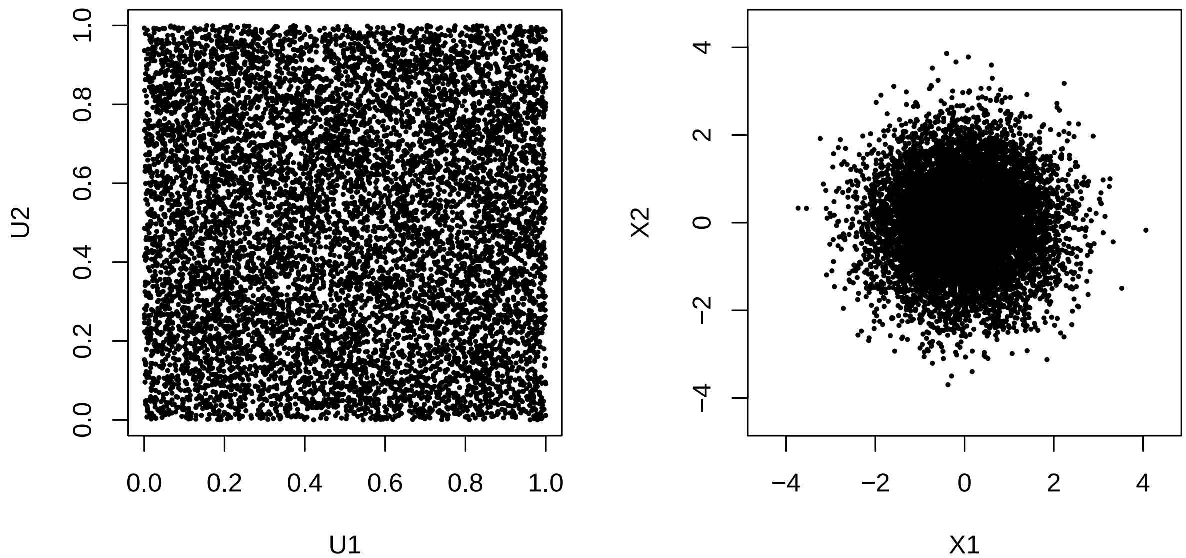
Multivariate transformations can also be studied. Suppose that U_1 and U_2 are independent $Uniform(0,1)$ variables, and consider

$$X_1 = \sqrt{-2\log U_1}\cos(2\pi U_2) \qquad X_2 = \sqrt{-2\log U_1}\sin(2\pi U_2).$$

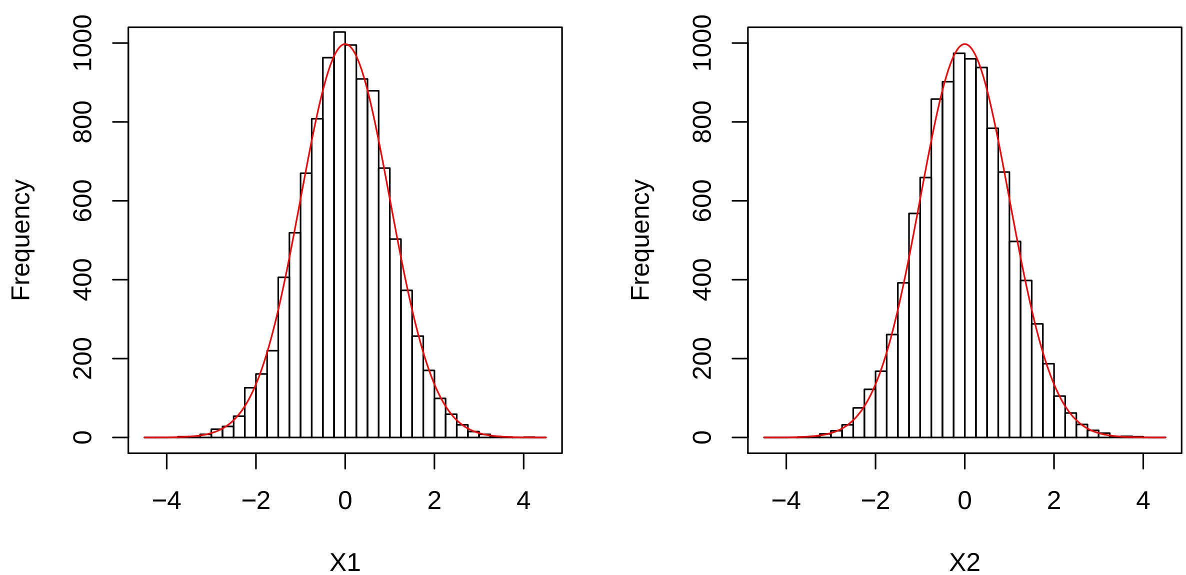
We may use the multivariate transformation theorem to demonstrate that X_1 and X_2 are independent $Normal(0,1)$ variables.

```
set.seed(8910)
n<-10000
U1<-runif(n);U2<-runif(n)
X1<-sqrt(-2*log(U1))*cos(2*pi*U2)
X2<-sqrt(-2*log(U1))*sin(2*pi*U2)
par(mar=c(4,3,1,0))
mean(X1);var(X1)
+ [1] -0.0005129991
+ [1] 0.9711766
```

```
mean(X2);var(X2)
+ [1] -0.007057369
+ [1] 1.029527
cov(X1,X2)
+ [1] 0.001159726
par(mar=c(4,4,1,2),mfrow=c(1,2))
plot(U1,U2,xlim=range(0,1),ylim=range(0,1),pch=19,cex=0.3)
plot(X1,X2,xlim=range(-4.5,4.5),ylim=range(-4.5,4.5),pch=19,cex=0.3)
```




```
x<-seq(-4.5,4.5,by=0.001)
fx<-dnorm(x)
hist(X1,breaks=seq(-4.5,4.5,by=0.25),main='',ylim=range(0,1000));box()
lines(x,fx*n*0.25,col='red')
hist(X2,breaks=seq(-4.5,4.5,by=0.25),main='',ylim=range(0,1000));box()
lines(x,fx*n*0.25,col='red')
```



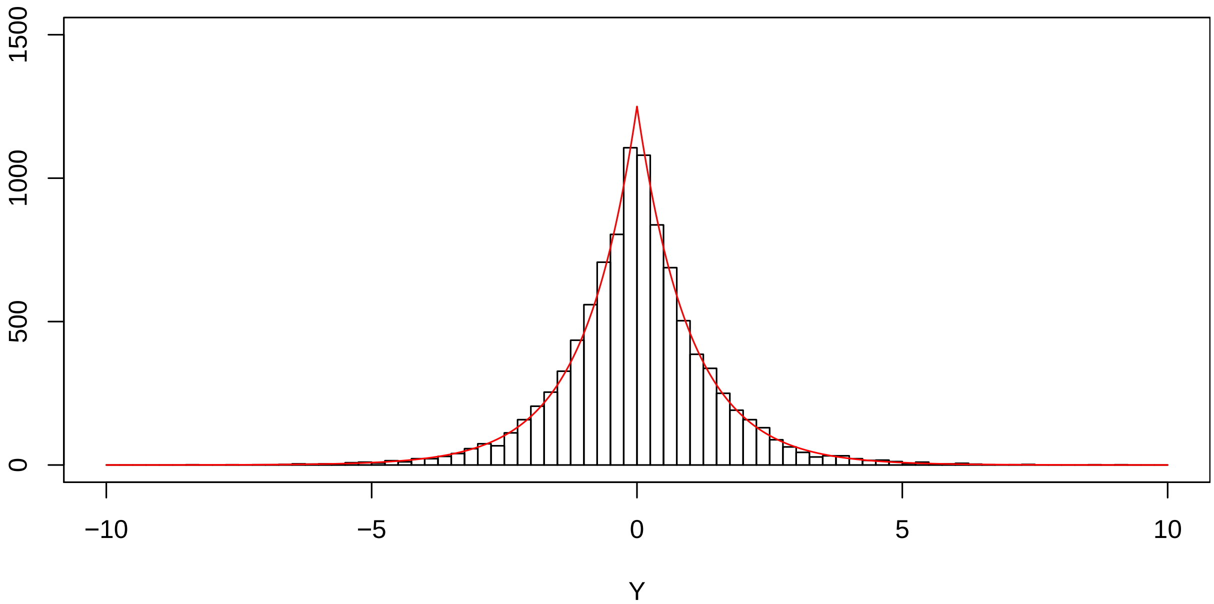
It is also straightforward to study non 1-1 transformations: suppose $X_1, X_2 \sim \mathit{Exponential}(1)$ are independent. We have seen that

$$Y = X_1 - X_2$$

has a Double Exponential (or Laplace) distribution, with

$$f_Y(y) = \frac{1}{2}\exp\{-|y|\} \qquad y \in \mathbb{R}.$$

```
set.seed(8910)
n<-10000
X1<-rexp(n)
X2<-rexp(n)
Y<-X1-X2
par(mar=c(4,3,1,0))
y<-seq(-10,10,by=0.001)
fy<-0.5*exp(-abs(y))
hist(Y,breaks=seq(-10,10,by=0.25),main='',ylim=range(0,1500));box()
lines(y,fy*n*0.25,col='red')
```



This can be useful when the analytical calculation is less straightforward: suppose $X_1, X_2 \sim Gamma(\alpha, 1)$ are independent. We can study the distribution of

$$Y = X_1 - X_2$$

easily using simulation. By direct but more involved calculation, we can demonstrate that, if α is a positive integer, say $\alpha = r+1$ for $r = 0, 1, 2, \ldots$, then

$$f_Y(y) = \sum_{j=0}^{r} \binom{r}{j} \frac{\Gamma(r+j+1)}{\{\Gamma(r+1)\}^2} \frac{1}{2^{r+j+1}} |y|^{r-j} \exp\{-|y|\} \qquad y \in \mathbb{R}$$

To see this, consider the case $y > 0$ and note that

$$P_Y[Y > y] = P_{X_1,X_2}[X_1 - X_2 > y] = \int_0^{\infty} \int_{x_2+y}^{\infty} f_{X_1}(x_1) f_{X_2}(x_2)\, dx_1 dx_2.$$

From this we compute the density by noting that $F_Y(y) = 1 - P_Y[Y > y]$, and differentiating with respect to y under the first integral: the differentiation is facilitated using the fundamental law of calculus. This yields, for $y > 0$

$$f_Y(y) = \frac{1}{\{\Gamma(\alpha)\}^2} e^{-y} \int_0^{\infty} (x_2(x_2+y))^{\alpha-1} \exp\{-2x_2\}\, dx_2.$$

To compute this integral for $\alpha = r+1$ an integer, we use the binomial expansion

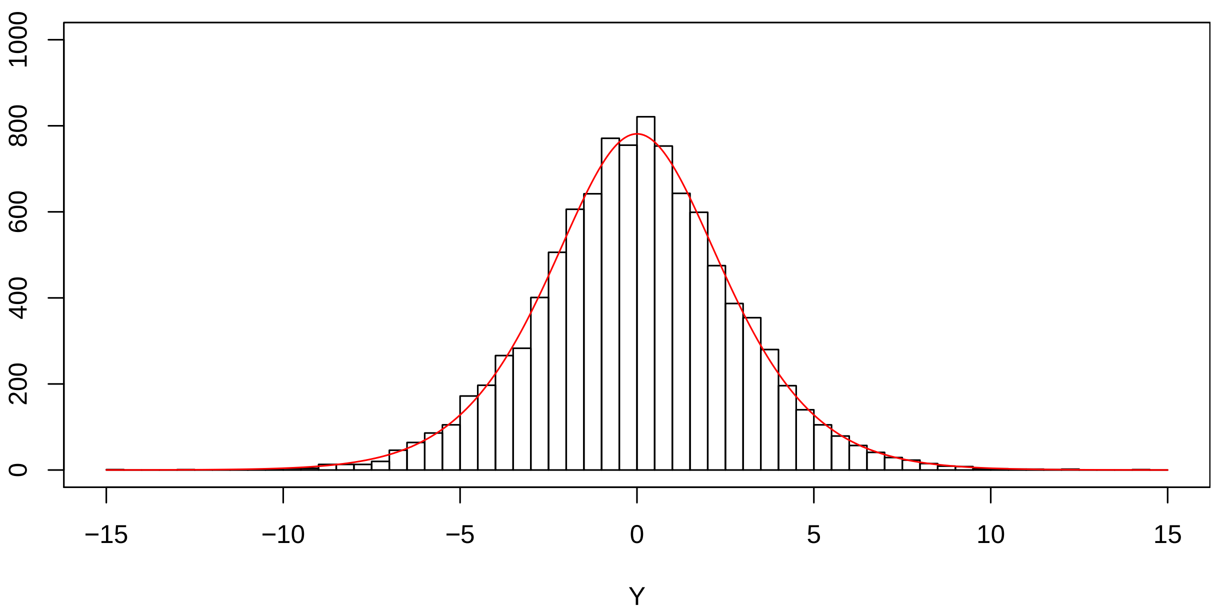
$$(x_2 + y)^r = \sum_{j=0}^{r} \binom{r}{j} x_2^j y^{r-j}$$

and then integrate term-by-term. We have that

$$\int_0^\infty x_2^{r+j} \exp\{-2x_2\}\, dx_2 = \frac{\Gamma(r+j+1)}{2^{r+j+1}}$$

as the integrand is proportional to a $Gamma(r+j+1,2)$ pdf. The result follows. Note that the pdf is symmetric about zero as we must have that the distribution of $X_1 - X_2$ is identical to the distribution of $X_2 - X_1$.

```
set.seed(8910)
n<-10000
al<-4
r<-al-1
X1<-rgamma(n,al,1)
X2<-rgamma(n,al,1)
Y<-X1-X2
par(mar=c(4,3,1,0))
y<-seq(-15,15,by=0.001)
ay<-abs(y)
fy<-y*0
for(j in 0:r){
    fy<-fy+choose(r,j)*(gamma(r+j+1)/gamma(r+1)^2)*(2^(-(r+j+1)))*ay^(r-j)*exp(-ay)
}
hist(Y,breaks=seq(-15,15,by=0.5),main='',ylim=range(0,1000));box()
lines(y,fy*n*0.5,col='red')
```



- **Monte Carlo:** The general principle of Monte Carlo is that the availability of random samples from a distribution $F_X(x)$ is essentially equivalent to knowledge of F_X itself if the number of samples is large enough. Suppose $X_1, \ldots, X_n$ are independent rvs having the same cdf F_X. We may approximate F_X itself using the *empirical distribution function*, $\widehat{F}_n$, defined by

$$\widehat{F}_n(x) = \frac{1}{n}\sum_{i=1}^n \mathbb{1}_{[x,\infty)}(X_i) \equiv \frac{1}{n}\sum_{i=1}^n \mathbb{1}_{(-\infty,X_i]}(x) \qquad x \in \mathbb{R}$$

which, for any fixed x, records the fraction of the X_is that are greater than or equal to x. If n is large enough, we can show that $\widehat{F}_n(x)$, when computed with simulated sample values $x_1, \ldots, x_n$, closely approximates $F_X(x)$. Thus we may also approximate the expectation

$$\mathbb{E}_X[g(X)] = \int_{-\infty}^{\infty} g(x)\, dF_X(x)$$

by the sample average

$$\widehat{\mathbb{E}}_X[g(X)] = \int_{-\infty}^{\infty} g(x)\, d\widehat{F}_n(x) = \frac{1}{n}\sum_{i=1}^{n} g(x_i).$$

This is the same principle that we use in statistical inference when we use the sample mean, sample variance etc. from a data sample to estimate the theoretical mean and variance etc. The discrete distribution

$$\widehat{f}_n(x) = \sum_{i=1}^{n} \frac{1}{n}\mathbb{1}_{\{x\}}(X_i) = \sum_{i=1}^{n} \frac{1}{n}\mathbb{1}_{\{X_i\}}(x)$$

with masses $1/n$ placed at the X_is is used to approximate the pmf/pdf of X.

In the previous example, with X_1 and X_2 independent $Gamma(\alpha, 1)$, we may compute the variance of $Y = X_1 - X_2$ directly as $\text{Var}_Y[Y] = \text{Var}_{X_1}[X_1] + \text{Var}_{X_2}[X_2] = \alpha + \alpha = 2\alpha$, and approximate it by Monte Carlo as follows:

```
var(Y)  #sample variance
+ [1] 7.809462
2*al     #theoretical variance.
+ [1] 8
```

Note that because the values are randomly drawn, we will get slightly different numerical results each time. For 10 replicate runs, we get

```
vvec<-replicate(10,var(rgamma(n,al,1)-rgamma(n,al,1)))
vvec
+  [1] 8.007298 7.952201 8.030130 8.125803 7.950684 7.839052 7.800716
+  [8] 7.868360 8.265122 8.025022
```

If the sample size is increased, the variation becomes smaller.

```
n<-n*10
vvec<-replicate(10,var(rgamma(n,al,1)-rgamma(n,al,1)))
vvec
+  [1] 7.995375 8.042749 8.109641 7.949860 8.025333 7.962438 8.046584
+  [8] 8.060480 7.964145 7.999656
n<-n*10
vvec<-replicate(10,var(rgamma(n,al,1)-rgamma(n,al,1)))
vvec
+  [1] 7.978249 8.001125 8.017460 7.996612 7.992621 7.995561 7.998518
+  [8] 7.987549 8.002257 8.016414
```

Monte Carlo methods are most often used when there are no straightforward analytic results available. Suppose we have that

$$g(x) = \max\{2|x|\log|x|, 5\}.$$

Then

$$\widehat{\mathbb{E}}_X[g(X)] = \frac{1}{n}\sum_{i=1}^{n} \max\{2|x_i|\log|x_i|, 5\}$$

where $x_1, \ldots, x_n$ are drawn from f_X.

```
n<-100000
ecalc<-function(nv,av){
    xv<-rgamma(nv,av,1)-rgamma(nv,av,1)
    gxv<-pmax(2*abs(xv)*log(abs(xv)),5)
    return(mean(gxv))
}
gvec<-replicate(10,ecalc(n,al))
gvec
+  [1] 7.582499 7.545870 7.584154 7.558610 7.548019 7.568509 7.548397
+  [8] 7.592875 7.595055 7.542022
```

An extension to basic Monte Carlo is ***importance sampling***: we have that

$$\mathbb{E}_X[g(X)] = \int_{-\infty}^{\infty} g(x)\frac{dF_X(x)}{dF_0(x)}\, dF_0(x)$$

where F_0 is some other distribution, provided the quantity

$$\frac{dF_X(x)}{dF_0(x)} \equiv \frac{f_X(x)}{f_0(x)}$$

is well-defined and finite on the support of X. Thus we may write

$$\mathbb{E}_X[g(X)] = \mathbb{E}_0\left[g(X)\frac{f_X(X)}{f_0(X)}\right]$$

that is, as an expectation with respect to f_0.

Cautionary note: Monte Carlo is a powerful technique, but it is not suitable for solving all problems. Consider computing the (Riemann) integral

$$\int_0^1 \frac{1}{x}\sin(2\pi/x)\,dx$$

by Monte Carlo. This involves sampling $X_1, \ldots, X_n \sim Uniform(0,1)$ independently, and then computing

$$\frac{1}{n}\sum_{i=1}^{n}\frac{1}{x_i}\sin(2\pi/x_i)$$

The Riemann integral can be computed as

$$\begin{aligned}\int_0^1 \frac{1}{x}\sin(2\pi/x)\,dx = \int_1^\infty \frac{\sin(2\pi t)}{t}\,dt &= \int_0^\infty \frac{\sin(t)}{t}\,dt - \int_0^{2\pi}\frac{\sin(t)}{t}\,dt \\ &= \mathrm{Si}(\infty) - \mathrm{Si}(2\pi)\end{aligned}$$

where Si(.) is a special function (the *sine integral*) with $\mathrm{Si}(\infty) = \pi/2$. The numerical value of the integral is 0.1526.

```
library(pracma)
Si(10^6)-Si(2*pi)  #Riemann integral result

+ [1] 0.1526438

sincalc<-function(nv){
    xv<-runif(nv)
    return(mean(sin(2*pi/xv)/xv))
}
svec<-replicate(20,sincalc(n))  #Monte Carlo replicates
svec

+  [1]  6.2222875 -5.3297809  1.1591927 -1.0311998  1.0686836 -0.2439774
+  [7] -1.5354914  0.4194717  0.9593114 -0.5984831 15.6722360  6.8136477
+ [13]  1.1831975  0.4768715 -1.0018140  1.8673244  0.4550503 -0.0316202
+ [19]  0.3104977 -4.7483663
```

The problem is that if $X \sim Uniform(0,1)$

$$\mathbb{E}_X\left[\frac{1}{X}\sin\left(\frac{2\pi}{X}\right)\right]$$

is not defined. Specifically

$$\mathbb{E}_X\left[\left|\frac{1}{X}\sin\left(\frac{2\pi}{X}\right)\right|\right]$$

is not finite.