TMA4300 Computer Intensive Statistical Methods

Why simulations?

Frequentist statistics (θ fixed, X (and $\hat{\theta}$) random) — Included in Part 3

Properties of MLEs $\hat{\theta} = \arg\max_{\theta} L(\theta; X)$ such as $E(\hat{\theta})$, $\mathrm{Var}[\hat{\theta})$ and its distribution often impossible to obtain analytically.

Instead simulate many realizations $\hat{\theta}_1^*, \hat{\theta}_2^*, \ldots, \hat{\theta}_n^*$ from an estimated model and estimate $E(\hat{\theta})$ by

$$\widehat{E(\hat{\theta})} = \frac{1}{n}\sum_{i=1}^{n} \hat{\theta}_i^*$$

Bayesian statistics (X fixed, θ random) — Included in Part 2

Joint posterior density

$$\pi(\underline{\theta} \mid \underline{x}) \propto L(\theta; \underline{x})\,\pi(\underline{\theta})$$

difficult to deal with analytically.

Instead sample from $\pi(\underline{\theta} \mid \underline{x})$ using MCMC.

Sanity checking: Analytic results $\rightleftharpoons$ Simulations

Part 1: The basics

Methods for simulating from common continuous and discrete distributions.

Pseudorandom number generators

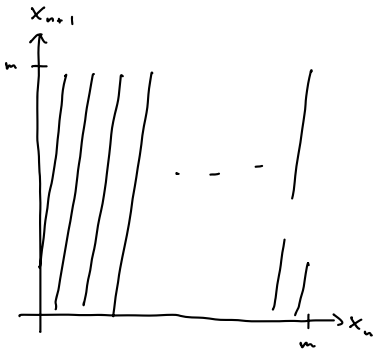
von Neumann (1946). Square X_n and take 4 middle digits as the next "random" number X_{n+1}

Ex. $X_n = 1112$

$X_n^2 = 01\underbrace{2365}_{X_{n+1}}44$

Linear congruential generators (e.g. Lehmer 1951, glibc, gcc)

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



Sinclair ZX81 computer (1981)

$$X_{n+1} = (75 X_n + 74) \bmod (2^{16} + 1)$$

R demo

R default: Mersienne-Twister (1998)

Period of $2^{19937} - 1$

To change:

```
> RNG( kind = "..." )
```

To repeat same sequence many times (e.g. for reproducability):

```
> set.seed(7)
```

Inversion method (Probability integral transform (PIT)-method)

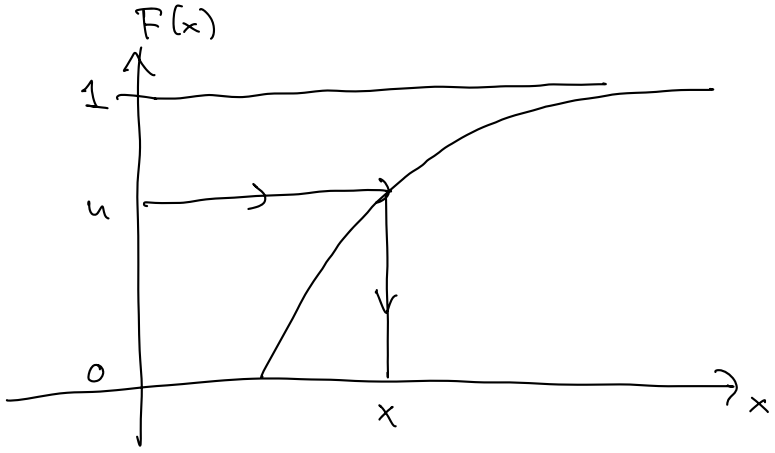
Aim: Simulate $X \sim F_\theta(x)$ given $U \sim unif(0, 1)$ where $F_\theta(x) = P(X \le x)$ is the cdf of X.

Alg.:

$u \sim Unif(0, 1)$

$x = F_\theta^{-1}(u)$

return x



Proof: The cdf of X becomes

$$\begin{aligned} F_X(x) &= P(X \le x) \\ &= P(F^{-1}(U) \le x) \\ &= P(U \le F(x)) \quad \text{if } F \text{ has an inverse } F^{-1} \\ &= F_U(F(x)) \\ &= F(x) \end{aligned}$$

Ex.: If $X \sim \exp(\lambda)$, then $f(x) = \lambda e^{-\lambda x}$, $F(x) = 1 - e^{-\lambda x}$

If

$$x = F^{-1}(u)$$

then

$$u = F(x) = 1 - e^{-\lambda x}$$

$$\ln(1-u) = -\lambda x$$

$$x = -\frac{1}{\lambda}\ln(1-u) = F^{-1}(u)$$

R demo

For continuous random variables F^{-1} is known as the quantile function.

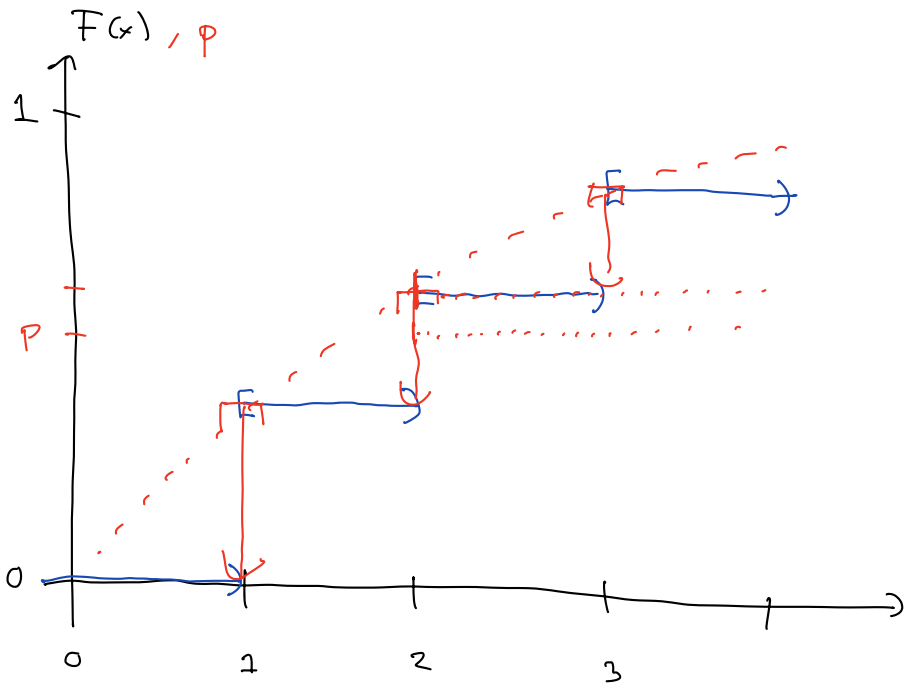
Generally (including for discrete random variables) we usually define the quantile function as

$$F^{-1}(p) = \inf(x \in \mathbb{R} : p \le F(x)) \qquad (1)$$

(convention followed by q.... - functions in R)

Ex.: If $X \sim \text{geom}(q)$ then the pmf is $p(x) = (1-q)^{x-1}$ for $x = 1, 2, \ldots$ and $F(x) = P(X \le x) = 1 - P(X > x)$

$= 1 - P(\text{No failures in first } x \text{ trials}) = 1 - (1-q)^{\lfloor x \rfloor}$ (right continuous)



$p = 1 - (1-q)^x$

$\ln(1-p) = x \ln(1-q)$

$x = \dfrac{\ln(1-p)}{\ln(1-q)}$

$F^{-1}(p) = \inf\{x \in \mathbb{R} : p \le F(x)\} = \ldots = \left\lceil \dfrac{\ln(1-p)}{\ln(1-q)} \right\rceil$ (left continuous)

Alg: $u \sim \text{Unif}[0, 1)$

$x = \left\lceil \dfrac{\ln(1-u)}{\ln(1-q)} \right\rceil$

The quantile function F^{-1} defined by (1) almost surely a left inverse of F in that $F^{-1}(F(X)) = X$ almost surely.

(but $F(F^{-1}(U)) \neq U$ almost surely)

Inversion method only using pmf.

$p(x) = p_i$ for $x = x_i$, $i = 1, 2, \ldots, k$, $x_1 < x_2 < \ldots < x_k$

Alg.

$u \sim \text{Unif}(0, 1)$

$i \leftarrow 1$

$F \leftarrow p_1$

while $u > F$ } Find i such that $F(x_{i-1}) < u \leq F(x_i)$

$i \leftarrow i + 1$

$F \leftarrow F + p_i$

end while

return x_i

Ex: $X \sim \text{Bern}(p)$

$u \sim \text{Unif}(0, 1)$

if $(u < p)$

$x \leftarrow 1$

else

$x \leftarrow 0$

return x

Simulating the generating process:

Ex.: $X \sim \text{negbin}(r, p)$

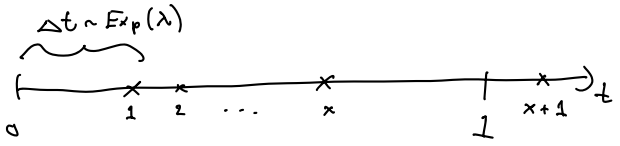
FFFSFFFSFSF . . . FFS
1 2 3 . . . r

```
s <- 0
x <- 0
while (s < r)
    u ~ Unif(0, 1)
    x <- x + 1
    if (u < p)
        s <- s + 1
    end if
end while
return x
```

Ex.: $X \sim \text{bin}(n, p)$

```
x <- 0
for (i = 1, 2, ..., n)
    u ~ Unif(0, 1)
    if (u < p)
        x <- x + 1
    end if
end for
return x
```

Ex.: $X \sim \text{Poisson}(\lambda)$

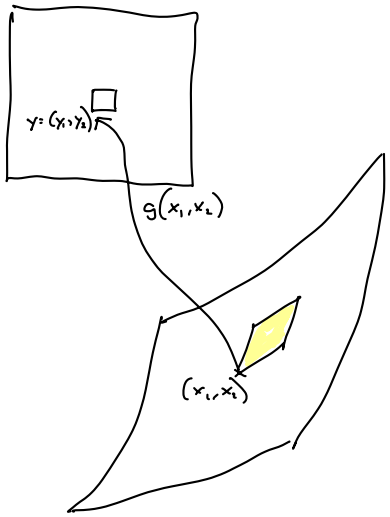



```
x <- 0
t <- 0
do
    Δt ~ Exp(λ)
    t <- t + Δt
    if (t > 1)
        break
    x <- x + 1
end do
return x
```

Transformation formula for joint densities

Suppose that $X = (X_1, X_2)$ has joint pdf $f_X(x_1, x_2)$ and that $Y = (Y_1, Y_2) = g(X_1, X_2)$ is a one-to-one differentiable function with inverse g^{-1}. Then

$$f_Y(y_1, y_2) = \underbrace{f_X\left(g^{-1}(y_1, y_2)\right)}_{= f_X(x_1, x_2)} \underbrace{\left| \begin{matrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_2}{\partial y_1} \\ \frac{\partial x_1}{\partial y_2} & \frac{\partial x_2}{\partial y_2} \end{matrix} \right|}_{|J|}$$



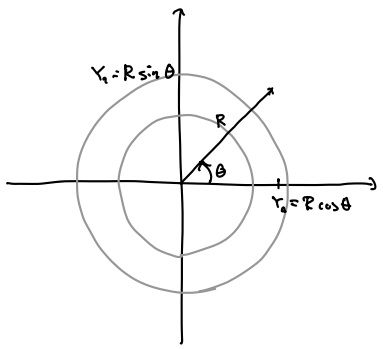
Box-Muller method

Aim: Simulate from the standard normal

Inversion method? $Y_1 = \Phi^{-1}(U)$?

Consider instead

$Y_1, Y_2 \overset{iid}{\sim} N(0,1)$. Then $f_Y(y_1, y_2) = \frac{1}{2\pi} e^{-\frac{y_1^2 + y_2^2}{2}}$



Joint pdf of corresponding polar coordinates

$$f_{R,\theta}(r, \theta) = f_{Y_1, Y_2}(y_1, y_2) \left| \begin{matrix} \frac{\partial y_1}{\partial r} & \frac{\partial y_2}{\partial r} \\ \frac{\partial y_1}{\partial \theta} & \frac{\partial y_2}{\partial \theta} \end{matrix} \right|$$

$y_1 = r\cos\theta$

$y_2 = r\sin\theta$

$$= \frac{1}{2\pi} e^{-\frac{1}{2}(y_1^2 + y_2^2)} \left| \begin{matrix} \cos\theta & \sin\theta \\ -r\sin\theta & r\cos\theta \end{matrix} \right|$$

$$= \frac{1}{2\pi} e^{-\frac{r^2}{2}} \left(r\cos^2\theta + r\sin^2\theta \right)$$

$$= \underbrace{\frac{1}{2\pi}}_{f_\theta(\theta)} \underbrace{r e^{-\frac{r^2}{2}}}_{f_R(r)}$$

i.e. $\theta \sim \text{Unif}(0, 2\pi)$, and $f_R(r) = r e^{-\frac{r^2}{2}}$.

R has cdf

$$F_R(r) = \int_0^r x e^{-\frac{x}{2}} dx = \left[-e^{-\frac{x^2}{2}} \right]_0^r = 1 - e^{-\frac{r^2}{2}}$$

with inverse

$$u = 1 - e^{-\frac{r^2}{2}}$$

$$\sqrt{-2\ln(1-u)} = F_R^{-1}(u) = r$$

Alg. (Box-Muller):

$u \sim \text{Unif}(0,1)$

$\theta \sim \text{Unif}(0, 2\pi)$

$r \leftarrow \sqrt{-2\ln u}$

$y_1 \leftarrow r\cos\theta$

$y_2 \leftarrow r\sin\theta$

return y_1, y_2

But rnorm uses slightly slower inversion method based on minimax rational function approximations of $\Phi^{-1}(\ )$ obtained via Remez-algorithm.

Marsaglia polar method

Alg.: repeat

$x_1 \sim \text{unif}(-1, 1)$

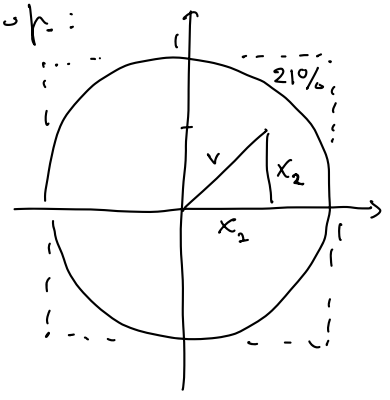
$x_2 \sim \text{unif}(-1, 1)$

$u \leftarrow x_1^2 + x_2^2$

until $u < 1$

return $\sqrt{-\frac{2 \ln u}{u}}\,(x_1, x_2)$

Proof:



Let $V^2 = X_1^2 + X_2^2$

$$f_{V,\theta}(v, \theta) = \underbrace{f_{X_1, X_2}(x_1, x_2)}_{= \frac{1}{\pi}} \cdot \underbrace{|J|}_{v}$$

$$= \underbrace{\frac{1}{2\pi}}_{f_\theta(\theta)} \cdot \underbrace{2v}_{f_V(v)}$$

Thus, $F_V(v) = v^2$ and so $U = X_1^2 + X_2^2 = V^2 = F_V(V) \sim \text{Unif}(0, 1)$

From Box-Muller method we know that

$$N(0,1) \overset{iid}{\sim} (Y_1, Y_2) = R(\cos\theta, \sin\theta) = \sqrt{-2 \ln U}\left(\frac{X_1}{V}, \frac{X_2}{V}\right)$$

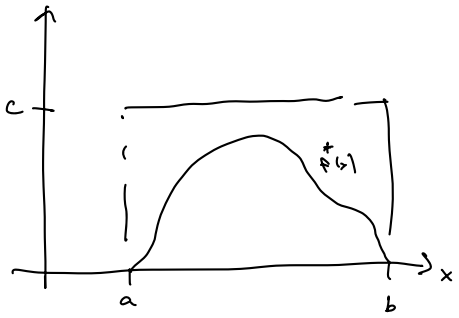
$$= \sqrt{-\frac{2 \ln U}{U}}\,(X_1, X_2)$$

(simplified version)

$k f^*(x)$
$\|$
$f(x)$

Rejection samp. . Aim: Simulate $X \sim f(x)$ where the support of f is (a, b) and c is an upper-bound of f^*.

Alg.: repeat
  $x \leftarrow$ Unif (a, b)
  $u \leftarrow$ Unif $(0, c)$
until $u < f^*(x)$
return x



Proof: Bayes theorem:

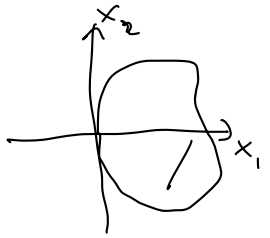
$$f_{X|A}(x) = \frac{P(A|X=x)\frac{1}{b-a}}{P(A)} = \frac{\frac{1}{c} f^*(x)\frac{1}{b-a}}{\int \frac{1}{c} f^*(x)\frac{1}{b-a}\,dx} = \frac{f^*(x)}{\int f^*(x)\,dx} = f(x)$$

Ratio-of-uniforms method

Idea: Transform problems where support of f^* is unbounded. into bivariate density with bounded support.

Alg.: Simulate $(X_1, X_2) \sim$ Unif (C) where $C = \{(x_1, x_2): 0 \le x_1 \le \sqrt{f^*\left(\frac{x_2}{x_1}\right)}\}$
$\|$ z $\quad$ $\|$ y

$y \leftarrow x_2 / x_1$
return y



Proof: Joint density of

$$y = \frac{x_2}{x_1}, \quad z = x_1 \iff x_1 = z \quad x_2 = yz$$

becomes

$$f(y, z) = f(x_1, x_2) \begin{vmatrix} \frac{\partial x_1}{\partial y} & \frac{\partial x_1}{\partial z} \\ \frac{\partial x_2}{\partial y} & \frac{\partial x_2}{\partial z} \end{vmatrix}$$

$$= k \cdot \begin{vmatrix} 0 & 1 \\ z & y \end{vmatrix} = kz.$$

Thus, $\sqrt{f^*(y)}$

$$f(y) = \int_0^{\sqrt{f^*(y)}} \underbrace{f(y,z)}_{kz}\, dz = \frac{kz^2}{2}\Big|_0^{\sqrt{f^*(y)}} = \frac{k}{2} f^*(y)$$

If $x^2 f^*(x)$ and $f^*(x)$ are bounded

then $G^1 \subset [0,a] \times [b_-, b_+]$ where

$$a = \sup_x \sqrt{f^*(x)} = \sqrt{\sup_x f^*(x)}, \quad (1)$$

$$b_- = -\sqrt{\sup_{x\le 0} x^2 f^*(x)}, \quad (2)$$

$$b_+ = \sqrt{\sup_{x\ge 0} x^2 (x)} \quad (3)$$

Proof: $x_1 = z \le \sqrt{f^*\left(\frac{x_2}{x_1}\right)} \le \sup_x \left(\sqrt{f^*(x)}\right) = \sqrt{\sup_x f^*(x)} = a$

If $x_2 \ge 0$ then

$$x_1 \le \sqrt{f^*\left(\frac{x_2}{x_1}\right)}$$

$$x_2 \le \frac{x_2}{x_1}\sqrt{f^*\left(\frac{x_2}{x_1}\right)} = \sqrt{\left(\frac{x_2}{x_1}\right)^2 f^*\left(\frac{x_2}{x_1}\right)} \le \sqrt{\sup_{x\ge 0} x^2 f^*(x)} = b_+$$

If $x_2 \le 0$ then

$$x_2 \ge \frac{x_2}{x_1}\sqrt{f^*\left(\frac{x_2}{x_1}\right)} \ge \sqrt{\inf_{x\le 0} x^2 f^*(x)}$$

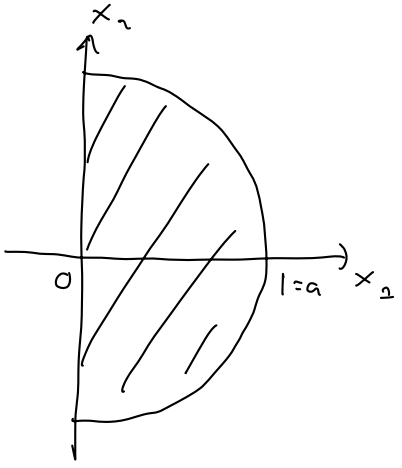
Ex.: $Y \sim \text{Cauchy}(0,1)$ with $f^*(y) = \frac{1}{1+y^2}$

$$a = \sqrt{\sup_x f^*(x)} = 1$$

$$0 \le x_1 \le \sqrt{f^*\left(\frac{x_2}{x_1}\right)} \Rightarrow x_1^2 \le \frac{1}{1+\left(\frac{x_2}{x_1}\right)^2} \Rightarrow 1 \le \frac{1}{x_1^2 + x_2^2}$$

$$\Rightarrow x_1^2 + x_2^2 \le 1$$

$$\sqrt{1-x_2^2} \le x_2 \le \sqrt{1+x_2^2}$$



Alg.:

repeat

$x_1 \sim \text{Unif}(0,1)$

$x_2 \sim \text{Unif}(-1,1)$

until $x_1^2 + x_2^2 \le 1$

$y \leftarrow x_2/x_1$

return x_1

Improvement: If R has density $f(r) = 2r$ for $0 \le r < 1$ and $\theta \sim \text{unif}(-\frac{\pi}{2}, \frac{\pi}{2})$ then $X_1 = R\cos\theta$, $X_2 = R\sin\theta$ has a unif density on C.

But $Y = \frac{X_2}{X_1} = \frac{R\sin\theta}{R\cos\theta}$, $\tan\theta$ (R cancels)

So the alg. simplifies to

$\theta \leftarrow \text{unif}(-\frac{\pi}{2}, \frac{\pi}{2})$

$y \leftarrow \tan(\theta)$

return y

equivalent to the inversion method.

Ex.: $Y \sim N(0,1)$, $f^*(y) = e^{-\frac{y^2}{2}}$

$$a = \sqrt{\sup_x f^*(x)} = 1$$

$$0 \le x_1 \le \sqrt{f^*\left(\frac{x_2}{x_1}\right)}$$

$$x_1^2 \le e^{-\frac{1}{2}\left(\frac{x_2}{x_1}\right)^2}$$

$$2 \ln x_1 \le -\frac{1}{2}\left(\frac{x_2}{x_1}\right)^2$$

$$-4 \ln x_1 \cdot x_1^2 \ge x_2^2$$

$$|x_2| \le 2x_1\sqrt{-\ln x_1} = b(x_1)$$

For $0 \le x_1 \le 1 = a$, $b(x_1)$ has a maximum at

$$2\sqrt{-\ln x_1} - \frac{2x_1}{2\sqrt{-\ln x_1}\, x_1} = 0$$

$$2(-\ln x_1) = 1$$

$$x_1 = e^{-\frac{1}{2}}$$

of $b\left(e^{-\frac{1}{2}}\right) = 2e^{-\frac{1}{2}}\sqrt{\frac{1}{2}} = \sqrt{2}\,e^{-\frac{1}{2}}$ $=$ $b_+ = \sqrt{\sup_x \left(x^2 f^*(x)\right)}$

Alg.:

repeat

$x_1 \sim \text{unif}(0,1)$

$x_2 \sim \text{unif}\left(-\sqrt{2}e^{-\frac{1}{2}}, \sqrt{2}e^{-\frac{1}{2}}\right)$

until $x_2^2 \le -4x_1^2 \ln x_1$

$y \leftarrow x_2/x_1$

return y.

$$\frac{d}{dx}\left(x^2 e^{-\frac{x^2}{2}}\right) = x^2(-x)e^{-\frac{x^2}{2}} + 2xe^{-\frac{x^2}{2}} = 0$$

$$2x - x^3 = 0$$

$$x(2 - x^2) = 0$$

$$x = \pm\sqrt{2}$$

$$\sup\left(x^2 f(x)\right) = 2e^{-\frac{2}{2}} = 2e^{-1}$$

$$b_+ = \sqrt{\sup_x x^2 f(x)} = \sqrt{2}\, e^{-\frac{1}{2}}$$

Ex.: $Y \sim \text{Gamma}(\alpha, \beta)$, $\overset{1}{\text{w.l.o.g.}}$ $f^*(y) = y^{\alpha-1}e^{-y}$

Mode at

$$\frac{d \ln f^*(x)}{dx}: \frac{d}{dx}\left((\alpha-1)\ln x - x\right) = \frac{\alpha-1}{x} - 1 = 0 \Rightarrow x = \alpha - 1$$

if $\alpha \geq 1$. Thus

$$a = \sqrt{\sup_x f^*(x)} = \sqrt{(\alpha-1)^{\alpha-1} e^{-(\alpha-1)}} = \left(\frac{\alpha-1}{e}\right)^{\frac{\alpha-1}{2}}$$

Similarly,

$$\frac{d}{dx}\ln\left(x^{\alpha-1}e^{-x}\right) = \frac{d}{dx}\left[(\alpha+1)\ln x - x\right] = \frac{\alpha+1}{x} - 1 = 0 \Rightarrow x = \alpha+1$$

for all $\alpha > 0$. Thus

$$b_+ = \sqrt{\sup_{x\geq 0} x^2 f^*(x)} = \sqrt{(\alpha+1)^{\alpha+1} e^{-\alpha-1}} = \left(\frac{\alpha+1}{e}\right)^{\frac{\alpha+1}{2}}$$

$$b_- = \sqrt{\inf_{x\leq 0} \underbrace{x^2 f^*(x)}_{=0}} = 0$$

Alg.: repeat

$x_1 \sim \text{Unif}(0, a)$

$x_2 \sim \text{Unif}(0, b_+)$

until $x_1 \le \sqrt{\left(\frac{x_2}{x_1}\right)^{\alpha-1} e^{-\frac{x_2}{x_1}}}$

$y \leftarrow x_2 / x_1$

return y

Ex.: $X \sim \text{Pareto}(\alpha, 1)$, $f^*(x) = \frac{1}{x^{\alpha+1}}$, $x \ge 1$, $\alpha > 0$

$x^2 f^*(x) = \frac{1}{x^{\alpha-1}}$ not bounded for $\alpha < 1$

Ratio-of-uniforms method not suitable

Simulation via mixtures

Many pdfs / pmfs $f(x)$ can be seen as a countable mixture

$$f(x) = \sum_y f(x|y) f(y) = \sum_y f(x,y)$$

or as an uncountable mixture

$$f(x) = \int_{-\infty}^{\infty} f(x|y) f(y)\, dy = \int_{-\infty}^{\infty} f(x,y)\, dy$$

If we can simulate from $f(y)$ and $f(x|y)$ then we can simulate from $f(x)$ using

Alg.: $y \sim f(y)$
$x \sim f(x|y)$
return x

Ex.: If $\lambda \sim \text{Gamma}(\alpha, \beta)$ and $X|\lambda \sim \text{Pois}(\lambda)$ then $X \sim \text{negbin}(\ldots, \ldots)$.

$$M_\lambda(t) = \left(\frac{1}{1-\beta t}\right)^\alpha$$

$$M_{X|\lambda}(t) = e^{\lambda(e^t - 1)}$$

$$M_X(t) = E\left(E e^{tX} \mid \lambda\right)$$

$$= E\, M_{X|\lambda}(t)$$

$$= E\, e^{\lambda(e^t - 1)}$$

$$= M_\lambda(e^t - 1)$$

$$= \frac{1}{\left(1 - \beta(e^t - 1)\right)^\alpha}$$

Alternatively:

$$f_X(x) = \int_0^\infty f_X(x|\lambda)\, f_\lambda(\lambda)\, d\lambda$$

$$= \int_0^\infty \frac{\lambda^x e^{-\lambda}}{x!} \frac{\lambda^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\lambda x}\, d\lambda$$

$$= \ldots$$

$$= \left(\frac{1}{1+\beta-\beta e^t} \right)^\alpha$$

$$= \left(\frac{\frac{1}{1+\beta}}{1-\frac{\beta}{1+\beta}e^t} \right)^\alpha$$

$$= \left(\frac{p}{1-(1-p)e^t} \right)^\alpha,$$

the mgf of $X \sim \text{negbin}(\alpha, p)$ where $p = \frac{1}{1+\beta}$.

Alg. to simulate $X \sim \text{negbin}(\alpha, p)$

$\beta \leftarrow \frac{1}{p} - 1$

$\lambda \sim \text{Gamma}(\alpha, \beta)$

$x \sim \text{pois}(\lambda)$

return x.

Ex.: $T \sim \frac{Z}{\sqrt{V/n}} \sim t_n$. Conditional on $V=v$, T is normal with $\text{Var}(T/V=v) = \frac{1}{(\sqrt{v/n})^2} = \frac{n}{v}$ and zero mean, i.e

$$f_{T/V=v}(t) = \frac{1}{\sqrt{2\pi n/v}} e^{-\frac{vt^2}{2n}}$$

Pdf of V $f_V(v) = \frac{2^{n/2}}{\Gamma(n/2)} v^{\frac{n}{2}-1} e^{-\frac{v}{2}}$

Marginal pdf of T is the mixture

$$f_T(t) = \int_0^\infty f_{T/V=v}(t) f_V(v) dv = \ldots \propto \left(1 + \frac{t^2}{n}\right)^{-\frac{v+1}{2}}$$

Multivariate normal

$\underline{x} = (x_1, \dots, x_d) \sim N_d(\underline{\mu}, \Sigma)$ if $f(\underline{x}) = (2\pi)^{-\frac{d}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\underline{x}-\underline{\mu})^T \Sigma^{-1} (\underline{x}-\underline{\mu})\right)$

- Characterization

  Any linear transformation $\underline{y} = A\underline{x} + b$ also (multivariate) normal.

- Marginal and conditional distributions

Let $Q = \Sigma^{-1}$, $\underline{x} = \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \end{bmatrix}$, $\underline{\mu} = \begin{bmatrix} \underline{\mu}_1 \\ \underline{\mu}_2 \end{bmatrix}$, $\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$, $Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}$

Then

$$\underline{x}_1 \sim N(\underline{\mu}_1, \Sigma_{11}), \quad \underline{x}_2 \sim N(\underline{\mu}_2, \Sigma_{22})$$

and

$$\underline{x}_1 | \underline{x}_2 \sim N\left(\underline{\mu}_1 + \Sigma_{12}\Sigma_{22}^{-1}(\underline{x}_2 - \underline{\mu}_2), \ \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)$$

$$\overset{(*)}{=} N\left(\underline{\mu}_1 - Q_{11}^{-1} Q_{12}(x_2 - \underline{\mu}_2), \ Q_{11}^{-1}\right)$$

Proof (*): Suppose w.l.o.g. that $\underline{\mu} = \underline{0}$

$$f_{\underline{x}_1 | \underline{x}_2}(\underline{x}_1) \propto \exp\left(-\frac{1}{2}\begin{pmatrix} \underline{x}_1^T & \underline{x}_2^T \end{pmatrix}\begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}\begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix}\right)$$

$$= \exp\left(-\frac{1}{2}\left(\underline{x}_1^T Q_{11} \underline{x}_1 + \underline{x}_2^T Q_{21} \underline{x}_1 + \underline{x}_1^T Q_{12} \underline{x}_2 + \underline{x}_2^T Q_{22} \underline{x}_2\right)\right)$$

$$\propto \exp\left(-\frac{1}{2}(\underline{x}_1 - \underline{\mu}_{1|2})^T Q_{11} (\underline{x} - \underline{\mu}_{1|2})\right)$$

$$\propto \exp\left(-\frac{1}{2}\left(\underline{x}_1^T Q_{11} \underline{x}_1 - \underline{\mu}_{1|2}^T Q_{11} \underline{x}_1 - \underline{x}_1^T Q_{11} \underline{\mu}_{1|2}\right)\right)$$

Equating coefficients, $-Q_{11}\underline{\mu}_{1|2} = Q_{12}\underline{x}_2$

$$\underline{\mu}_{1|2} = -Q_{11}^{-1} Q_{12} \underline{x}_2$$

- Quadratic forms. If Σ has full rank $p \leq d$ (p nonzero eigenvalues), then

$$(\underline{x}-\underline{\mu})^T \Sigma^{-1} (\underline{x}-\underline{\mu}) \sim \chi^2_p$$

$$\| $$

$$(\underline{x}-\underline{\mu})^T P D^{-1/2} \underbrace{D^{-1/2} P^T (\underline{x}-\underline{\mu})}_{\sim N_d(\underline{0}, \underline{I}_d)}$$

- Simulation:

Let $\underline{x} \sim N_d(0, I_n)$. Then $\underline{y} = \underline{\mu} + A\underline{x} \sim N_d(\underline{\mu}, AA^T)$

Thus, if $AA^T = \Sigma$, then $\underline{y} \sim N_d(\underline{\mu}, \Sigma)$.

Possible choices of A:

$A = PD^{1/2}$ where $PDP^T = \Sigma$ is the eigen decomposition of Σ

$A = \text{chol}(\Sigma) = L$ (lower triangular matrix). (In R chol returns L^T)

Finding L:

We have

$$LL^T = \begin{bmatrix} L_{11}^2 & & \\ L_{21}L_{11} & L_{21}^2 + L_{22}^2 & \\ L_{31}L_{11} & L_{31}L_{21} + L_{32}L_{22} & L_{31}^2 + L_{32}^2 + L_{33}^2 \end{bmatrix} = \begin{bmatrix} \Sigma_{11} & & \\ \Sigma_{21} & \Sigma_{22} & \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{bmatrix}$$

Given Σ, first solve for L_{11}, then L_{21}, L_{22}, L_{31}, L_{32}, L_{33}, ...

Cost $O(n^3)$

Rejection sampling

Aim: Simulate $X \sim f(x) = k f^*(x)$, only $f^*(x)$ known.

Can simulate from proposal $g(x)$.

Let $c \geq 1$ such that $f^*(x) \leq c\, g(x)$ for all $x \in \mathbb{R}$.

Alg.: repeat

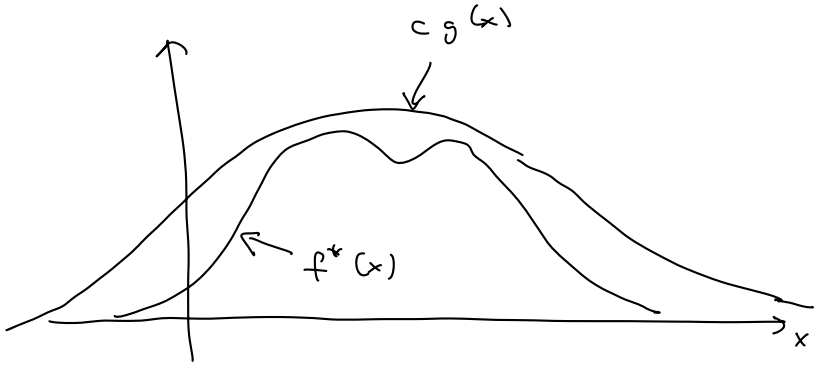
$x \sim g(x)$

$u \sim \text{unif}(0,1)$

$\alpha \leftarrow \frac{1}{c} \frac{f^*(x)}{g(x)}$

until $u < \alpha$

return x.



Proof:

$$f_{X|U<\alpha}(x) = \frac{P(U<\alpha \mid X=x)\, g(x)}{P(U<\alpha)} = \frac{P(U<\alpha \mid X=x)\, g(x)}{\int P(U<\alpha \mid X=x)\, g(x)\, dx}$$

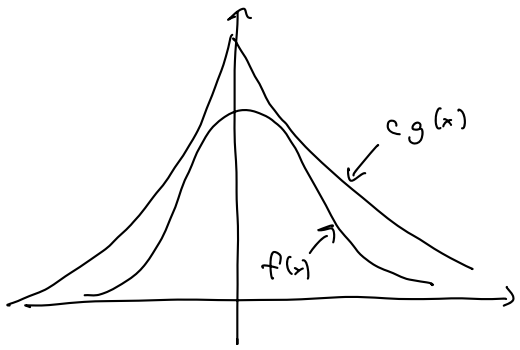
$$= \frac{\frac{1}{c} \frac{f^*(x)}{g(x)}\, g(x)}{\int \frac{1}{c} \frac{f^*(x)}{g(x)}\, g(x)\, dx}$$

$$= \frac{f^*(x)}{\int f^*(x)\, dx} = f(x).$$

Note that overall acceptance probability

$$P(U<\alpha) = \frac{1}{c} \int f^*(x)\, dx = \frac{1}{c} \quad \text{if} \quad f^*(x) = f(x).$$

Ex.: $X \sim N(0,1)$, $f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$



Use $g(x) = \frac{\lambda}{2} e^{-\lambda|x|}$ as proposal.

Optimal choice of c and λ?

Given λ what is $\sup_x \left(\frac{f(x)}{c\,g(x)} \right)$?

The acceptance probability (conditional on $X = x$) is

$$\frac{f(x)}{cg(x)} = \frac{2e^{-x^2/2}}{\sqrt{2\pi}\, c\, \lambda e^{-\lambda|x|}} \underset{x>0}{=} \frac{1}{\lambda c}\sqrt{\frac{2}{\pi}} e^{-\frac{x^2}{2} + \lambda x}$$

$$= \frac{1}{\lambda c}\sqrt{\frac{2}{\pi}} e^{-\frac{1}{2}\left[(x-\lambda)^2 - \lambda^2\right]}$$

and has its maximum of

$$\frac{1}{\lambda c}\sqrt{\frac{2}{\pi}} e^{\frac{\lambda^2}{2}}$$

at $x = \lambda$. We need

$$\frac{1}{\lambda c}\sqrt{\frac{2}{\pi}} e^{\frac{\lambda^2}{2}} \leq 1$$

and thus

$$c \geq \frac{1}{\lambda}\sqrt{\frac{2}{\pi}} e^{\frac{\lambda^2}{2}} = c(\lambda)$$

The overall acceptance probabity (known since f is known)

$$P(U < \alpha) = \frac{1}{c(\lambda)} = \sqrt{\frac{\pi}{2}}\, \lambda\, e^{-\frac{\lambda^2}{2}} \qquad (*)$$

has its maximum when

$$\frac{d}{d\lambda}\left(\ln\lambda - \frac{\lambda^2}{2} \right) = \frac{1}{\lambda} - \lambda = 0 \quad \Rightarrow \quad \lambda = 1$$

for which $c(\lambda) = \sqrt{\frac{2}{\pi}} e^{\frac{1}{2}} = 1.315$ and $P(U < \alpha) = \frac{1}{c} = 0.7602$

Implementation:

repeat

$u_1 \sim \text{Unif}(0,1)$

$x \leftarrow -\log(u_1)$

$u_2 \leftarrow \text{Unif}(0,1)$

if $(u_2 < \frac{1}{2})$

$x \leftarrow -x$

$\alpha \leftarrow e^{-\frac{x^2}{2} + |x| + \frac{1}{2}}$

$u_2 \leftarrow \text{Unif}(0,1)$

until $(u_2 < \alpha)$

return x

$$\alpha = \frac{f(x)}{c\,g(x)} = \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}\, e^{-|x|+\frac{1}{2}}} = e^{-\frac{x^2}{2} + |x| + \frac{1}{2}}$$

Note: If only f^* was known we would need to maximise $(*)$ by experimental tuning of λ.

Rejection sampling multivariate densities

Ex: Sampling uniformly within a unit n-ball.

$$f(\underline{x}) = f(x_1, \ldots, x_n) = \frac{1}{V_n} \quad \text{for } \|\underline{x}\|_2 \leq 1$$

where $V_n = \dfrac{\pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)}$

Proposal

$$g(\underline{x}) = \frac{1}{2^n} \quad \text{for } -1 \leq x_i \leq 1, \; i = 1, 2, \ldots, n.$$

$$f(\underline{x}) = \frac{1}{V_n} \leq c\, g(\underline{x}) = \frac{c}{2^n} \quad \text{for } c \geq \frac{2^n \Gamma\left(\frac{n}{2}+1\right)}{\pi^{n/2}}$$

Accept with prob. $P(U < \alpha \mid \underline{X} = \underline{x}) = \alpha = \dfrac{f(\underline{x})}{c\, g(\underline{x})} = \begin{cases} 1 & \text{if } \|x\|_2 \leq 1 \\ 0 & \text{otherwise} \end{cases}$

Overall acceptance probability

$$P(U \leq \alpha) = \int_{V_n} \frac{f(\underline{x})}{c\, g(\underline{x})} \cdot g(\underline{x})\, d\underline{x} = \frac{1}{c} = \frac{\pi^{n/2}}{2^n \Gamma\left(\frac{n}{2}+1\right)}$$

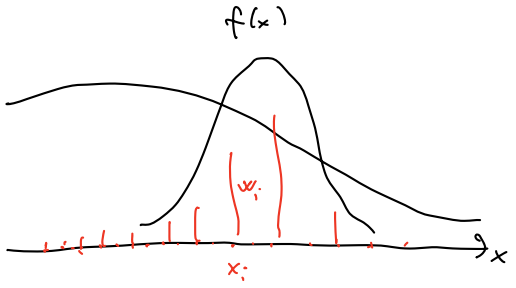
n	$U \leq \alpha$
1	1
2	$\pi/4 = 0.78$
3	$\dfrac{\pi^{3/2}}{2^3 \Gamma\left(\frac{3}{2}+1\right)} = \dfrac{\pi^{3/2}}{2^3 \frac{3}{2} \cdot \frac{1}{2}\sqrt{\pi}} = \dfrac{\pi}{2 \cdot 3} = 0.52$
4	$\dfrac{\pi^2}{2^4 \Gamma(3)} = \dfrac{\pi^2}{2^4 \, 2 \cdot 1} = 0.308$
10	0.0025

Rejection sampling cont.

Difficulties	Alternative method
Finding c	Weighted resampling
Finding good proposal	Adaptive rejection sampling
	Alias method (X discrete, finite support)

Weighted resampling

Aim: Sample from $f^*(x)$.



Alg.:

$$x_1, \ldots, x_n \overset{iid}{\sim} g(x)$$

for $i = 1, \ldots, n$

$$w_i \leftarrow \frac{f^*(x_i)/g(x_i)}{\sum f^*(x_i)/g(x_i)}$$

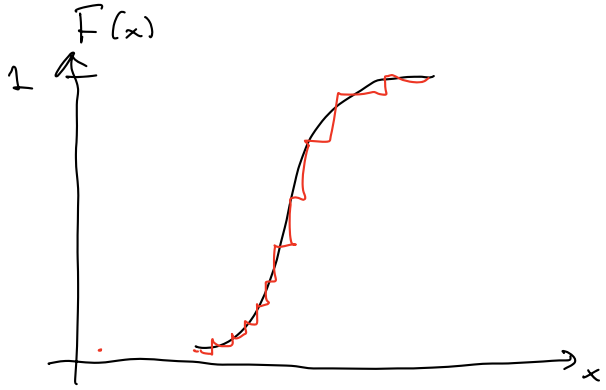
$$y_1, \ldots, y_m \overset{iid}{\sim} f_X(y) \quad \text{where} \quad f_X(y) = \begin{cases} w_i & \text{for } y = x_i,\ i = 1, 2, \ldots, n \\ 0 & \text{elsewhere} \end{cases}$$

return $y_1, \ldots, y_m$

The discrete distribution f_X approximates f in the sense that its cdf

$$F_X(a) = P(X \le a)$$

$$= \sum_{\{i : x_i \le a\}} w_i$$



$$= \frac{\sum_{i=1}^{n} I(x_i \le a) \frac{f(x_i)}{g(x_i)}}{\sum_{i=1}^{n} \frac{f(x_i)}{g(x_i)}} \longrightarrow \frac{\int_{-\infty}^{a} \frac{f^*(x)}{g(x)} \cdot g(x)\, dx}{\int_{0}^{\infty} \frac{f^*(x)}{g(x)} \cdot g(x)\, dx} = \int_{-\infty}^{a} f(x)\, dx$$

$$= F(a),$$

the cdf of X, as $n \to \infty$.

The second sample $y_1, \ldots, y_m$ can be generated using the alias-method (function sample in R)

R demo

Tail behaviours:

$\lim_{x \to \pm\infty} \frac{f^*(x)}{g(x)}$ must be finite

$e^{-\frac{1}{2}\left((x-1)^2 - x^2\right)} = e^{-\frac{1}{2}(-2x+1)} \xrightarrow{x \to \infty} \infty$

Alias method (Walker 1974, 1977)

Aim: Simulate X having pmf $P(X=i)=p_i$, $i=1,2,\dots,n$

Alg.:

Precompute (U_i, K_i), $i=1,2,\dots,n$ — $O(n \ln n)$

$U_i \leftarrow n p_i$, $K_i \leftarrow NA$

While $U_i > 1, U_j < 1, K_j = NA$ for $i \neq j$

$U_i \leftarrow U_i - (1-U_j)$

$K_j \leftarrow i$

Ex.: $n=5$

$p = (p_1, \dots, p_5)$

$= (.25, .3, .1, .2, 0.15)$

i	U_i	K_i
1	~~1.25~~ 0.75	NA ~~2~~
2	~~1.5~~ ~~1.25~~ 1	NA
3	0.5	~~NA~~ 1
4	1	NA
5	0.75	NA 2

Operation — $O(1)$

$u \sim unif(0,1)$

$i \leftarrow \lfloor nu \rfloor + 1$

$y \leftarrow nu - \lfloor nu \rfloor$

if $(y < U_i)$

$x \leftarrow i$

else

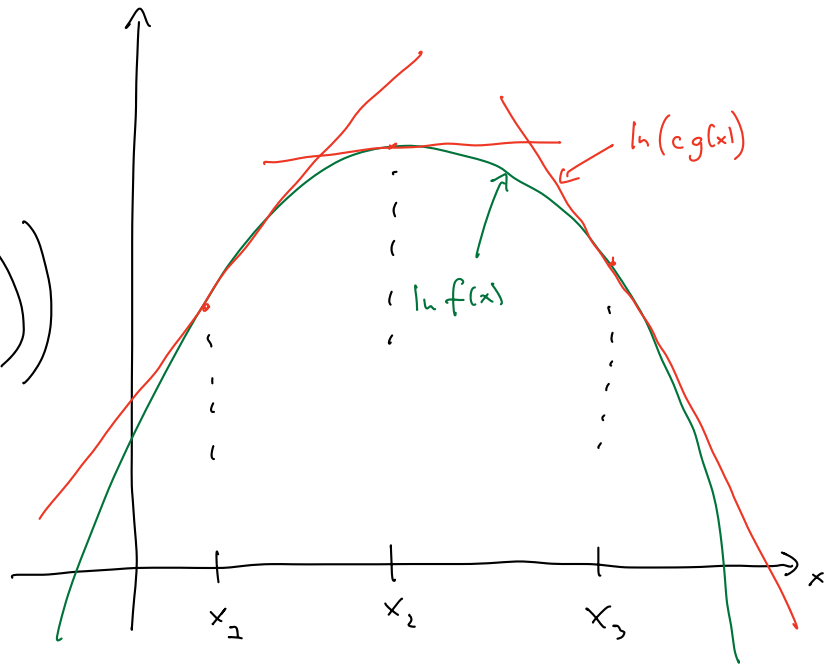
$x \leftarrow K_i$

return x

Adaptive rejection sample

Assuming that $\ln f(x)$ is concave:

- Construct a piecewise linear log proposal $\ln(cg(x))$ from tangents of $\ln f(x)$ at initial grid points $x_1, x_2, \ldots, x_n$.



do

$x \sim g(x)$

(a countable finite mixture of truncated exponentials)

$\alpha \leftarrow \dfrac{f(x)}{cg(x)}$

$u \sim \text{unif}(0,1)$

if $(u < \alpha)$

break

improve $\ln(cg(x))$ by adding x to grid

end do

return x

R-package : ars

Monte Carlo integration

Aim: Estimate $E(h(X))$ where $X \sim f(x)$.

Ex.: $E(\underbrace{X}_{h(X)=X})$, $\mathrm{Var}\, X = E(\underbrace{(X-\mu)^2}_{h(X)})$, $P(X>a) = E(\underbrace{I(X>a)}_{h(X)})$

Simulate $X_1, X_2, \ldots, X_n \overset{iid}{\sim} f(x)$ and estimate $E(h(X))$ by

$$\widehat{E(h(X))} = \frac{1}{n}\sum_{i=1}^{n} h(X_i)$$

Unbiased since

$$E\left(\frac{1}{n}\sum_{i=1}^{n} h(X_i)\right) = \frac{1}{n}\sum_{i=1}^{n} E\,h(X_i) = E\,h(X)$$

By strong law of large numbers

$$\frac{1}{n}\sum h(X_i) \xrightarrow{a.s} E\,h(X)$$

as $n \to \infty$

Importance sampling

Aim: Estimate $E(h(X))$, $X \sim f(x)$

Alg:

Sample $x_1, x_2, \ldots, x_n \overset{iid}{\sim} g(x)$.

Compute

$$\widehat{E(h(X))} = \frac{1}{n} \sum_{i=1}^{n} h(x_i) \frac{f(x_i)}{g(x_i)}$$

This estimator is unbiased since

$$E\left(\widehat{E(h(X))}\right) = \frac{1}{n} \sum_{i=1}^{n} E\left(h(X_i) \frac{f(X_i)}{g(X_i)}\right)$$

$$= \int_{-\infty}^{\infty} h(x) \frac{f(x)}{g(x)} g(x)\, dx$$

$$= \int_{-\infty}^{\infty} h(x) f(x)\, dx = E(h(X)).$$

By the law of large numbers $\widehat{E(h(X))} \xrightarrow[n \to \infty]{a.s.} E(h(X))$

Optimal choice of $g(x)$ is

$$g(x) = \frac{h(x) f(x)}{\int h(x) f(x)\, dx}$$

since this leads to

$$Var\left(\frac{h(X) f(X)}{g(X)}\right) = Var\left(\frac{h(X) f(X)}{\frac{h(X) f(X)}{\int h(x) f(x)\, dx}}\right) = Var\left(\int h(x) f(x)\, dx\right) = 0$$

In practice choose $g(x)$ such that it is approximately proportional to $h(x) g(x)$.

R demo

Importance sampling cont. (self-normalizing version):

Given only $f^*(x)$ (unnormalized density of X), the alternative estimator

$$\widetilde{E(h(X))} = \frac{\sum_{i=1}^{n} h(x_i) \frac{f^*(x_i)}{g(x_i)}}{\sum_{i=1}^{n} \frac{f^*(x_i)}{g(x_i)}}$$

is not unbiased (since $E(\frac{U}{V}) \neq \frac{E(U)}{E(V)}$). But, as $n \to \infty$,

$$\sum_{i=1}^{n} \frac{f^*(x_i)}{g(x_i)} \xrightarrow{d} E\left(\frac{f^*(X)}{g(X)}\right) = \int \frac{f^*(x)}{g(x)} g(x)\,dx = \int f^*(x)\,dx$$

and

$$\sum_{i=1}^{n} h(X_i) \frac{f^*(x_i)}{g(x_i)} \xrightarrow{d} E\left(h(X) \frac{f^*(X)}{g(X)}\right) = \ldots = \int h(x) f^*(x)\,dx$$

Thus, using Slutsky's theorem,

$$\widetilde{E(h(X))} \xrightarrow{d} \frac{\int h(x) f^*(x)\,dx}{\int f^*(x)\,dx} = \int h(x) f(x)\,dx = E(h(X)),$$

i.e. $\widetilde{E(h(X))}$ is consistent.

Bayesian inference

Recall: From def. of cond. prob.

$$P(A_i|B) = \frac{P(A_i \cap B)}{P(B)} = \frac{P(B|A_i)P(A_i)}{P(B)} \overset{\text{L.T.P.}}{=} \frac{P(B|A_i)P(A_i)}{\sum P(B|A_i)P(A_i)} \propto P(B|A_i)P(A_i)$$

for $i = 1, 2, \ldots, n$ where $A_1, \ldots, A_n$ is a partition of sample space B.

For discrete random variables,

$$P(X=x|Y=y) = \frac{\overbrace{P(X=x \cap Y=y)}^{\text{joint pmf of } X,Y}}{\underbrace{P(Y=y)}_{\text{marginal pmf of } Y}} = \frac{P(Y=y|X=x)P(X=x)}{P(Y=y)}$$

For continuous random variables, conditional pdf of X given $Y=y$

$$f_{X|Y}(x|y) = \frac{f_{Y|X}(y|x)\, f_X(x)}{f_Y(y)}$$

or

$$f(x|y) = \frac{f(y|x)\, f(x)}{f(y)}$$

Probabilities are extended to include subjective (personal) degree of belief in different values of unknown parameters (fixed constant) and updated via Bayes theorem

$$\underbrace{f(\theta|x)}_{\text{posterior distn.}} \propto \underbrace{f(x|\theta)}_{\text{likelihood}} \underbrace{f(\theta)}_{\text{prior distn.}}$$

Ex.: $X \sim \text{bin}(n, p)$, n known, p unknown. (e.g. proportion of conservative voters in political survey)

Prior beliefs about p modelled by assuming that $p \sim \text{Beta}(\alpha, \beta)$

Thus, the prior (density) is

$$f(p) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1}(1-p)^{\beta-1} \propto p^{\alpha-1}(1-p)^{\beta-1} \quad \text{for } 0 \le p \le 1$$

The likelihood $L(\theta; x) = f(x|\theta) = \binom{n}{x} p^x (1-p)^{n-x}$.

Given the data $X=x$, the posterior density

$$f(p|x) \propto f(x|p) f(p)$$

$$\propto p^{x} (1-p)^{n-x} \; p^{\alpha-1} (1-p)^{\beta-1}$$

$$= p^{\alpha+x-1} (1-p)^{\beta+n-x-1}$$

i.e. $p|X=x \sim \text{Beta}(\alpha+x, \beta+n-x)$.

For $n=10$, $x=0$ and $\alpha=\beta=1$, $p \sim \text{unif}(0,1)$ and

$$p|X=0 \sim \text{Beta}(1, 11)$$

with posterior expectation and standard deviation

$$E(p|X=0) = \frac{1}{1+11} = \frac{1}{12} = 0.083, \quad SD(p|X=0) = \sqrt{\frac{1}{12} \cdot \frac{11}{12} \cdot \frac{1}{13}} = 0.076.$$

In contrast, MLE of p and MLE of its SE is

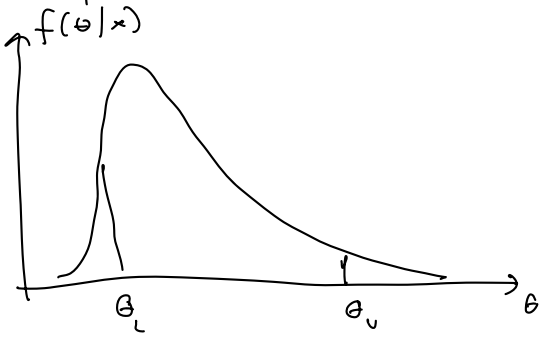
$$\hat{p} = \frac{x}{n} = 0, \quad \widehat{SE}(\hat{p}) = \sqrt{\frac{\hat{p}(1-\hat{p})}{n}} = 0.$$

Other summaries of $f(p|x)$, Bayesian point estimates:

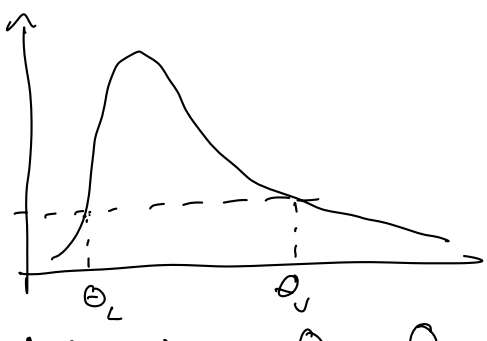
- The mode $\text{Mod}(\theta|x) = \underset{\theta}{\text{argmax}}\, f(\theta|x)$
- The median
- Credible intervals $(\theta_L(x), \theta_U(x))$ s.t.

$$\mathbb{P}(\theta_L(x) < \theta < \theta_U(x) | X=x) = 1-\alpha$$

Equal tail CI:



Higest post. density (HPD) CI



Minimises $\theta_U - \theta_L$

In contrast, a confidence interval $(\hat{\theta}_L(X), \hat{\theta}_U(X))$ is defined s.t.

$$P\left(\hat{\theta}_L(X) < \theta < \hat{\theta}_U(X) \mid \theta\right) = 1-\alpha$$

Note that (LTP)

$$\int \underbrace{P(\theta_L < \theta < \theta_U \mid X=x)}_{=1-\alpha} f(x)\,dx = \int \underbrace{P(\theta_L < \theta < \theta_U \mid \theta)}_{\text{freq. coverage}} f(\theta)\,d\theta$$

i.e. frequentist coverage of Bayesian credible interval is $1-\alpha$ on average

Sequential updating

Step 1: Condition on x_1

$$\underbrace{f(\theta \mid x_1)}_{\text{posterior}} \propto f(x_1 \mid \theta) \underbrace{f(\theta)}_{\text{prior}}$$

Step 2: Condition also on x_2

$$\underbrace{f(\theta \mid x_2, x_1)}_{\text{new posterior}} \propto \underbrace{f(x_2 \mid \theta, x_1)}_{\substack{= f(x_2 \mid \theta) \\ \text{if } x_2, x_1 \mid \theta \\ \text{are indep.}}} f(\theta \mid x_1)$$

old posterior = new prior

Same result as

$$f(\theta \mid x_2, x_1) \propto f(x_2, x_1 \mid \theta) f(\theta)$$

$$= f(x_2 \mid x_1, \theta) f(x_1 \mid \theta) f(\theta)$$

Choice of prior:

Should represent prior beliefs.

- Conjugate priors

  A family G of distributions is conjugate with respect to a likelihood $L(\theta; x) = f(x|\theta)$ if both prior $f(\theta)$ and posterior $f(\theta|x)$ is in G.

Ex. 1: $L(p; x) = \binom{n}{x} p^x (1-p)^{n-x}$, $p \sim Beta(\alpha, \beta)$ is conjugate to $L(p;\theta)$ since $p|x \sim Beta(\alpha + x, \beta + n - x)$ if $p \sim Beta(\alpha, \beta)$.

Note: Simplifies sequential updating.

Ex. 2: $X \sim N(\mu, \sigma^2)$, σ^2 known, μ unknown

$$L(\mu; x) = f(x|\mu) \propto e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Conjugate prior is $\mu \sim N(\mu_0, \sigma_0^2)$

$$f(\mu) \propto e^{-\frac{1}{2\sigma_0^2}(\mu - \mu_0)^2}$$

since the posterior is then

$$f(\mu|x) \propto f(x|\mu) f(\mu)$$

$$= e^{-\frac{1}{2}\left[\frac{1}{\sigma^2}(x-\mu)^2 + \frac{1}{\sigma_0^2}(\mu-\mu_0)^2\right]}$$

$$\propto e^{-\frac{1}{2}\left[\left(\frac{1}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{x}{\sigma^2} + \frac{\mu_0}{\sigma_0^2}\right)\mu + \dots\right]}$$

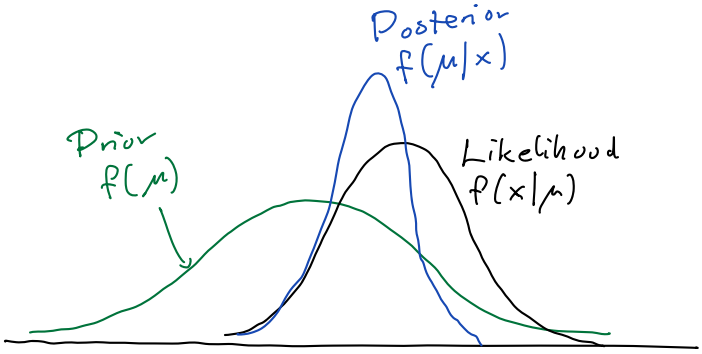
$$\propto e^{-\frac{1}{2}\left(\frac{1}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\left[\left(\mu - \frac{\frac{x}{\sigma^2} + \frac{\mu_0}{\sigma_0^2}}{\frac{1}{\sigma^2} + \frac{1}{\sigma_0^2}}\right)^2 + \dots\right]}$$

(completing the square)

i.e. $\mu|x \sim N(\mu_1, \sigma_1^2)$ where $\underbrace{\frac{1}{\sigma_1^2}}_{\text{posterior precision}} = \underbrace{\frac{1}{\sigma^2}}_{\text{likelihood precision}} + \underbrace{\frac{1}{\sigma_0^2}}_{\text{prior precision}}$ (add precisions)

and $\mu_1 = \dfrac{\frac{1}{\sigma^2}x + \frac{1}{\sigma_0^2}\mu}{\frac{1}{\sigma^2} + \frac{1}{\sigma_0^2}}$ (average of x and μ weighted by respective precisions)

(same family G)



Ex. 3.: $X|\sigma^2 \sim N(\mu, \sigma^2)$, μ known, σ^2 unknown

$$L(\sigma^2; x) \propto (\sigma^2)^{-\frac{1}{2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Reparameterizing in terms of precision $\tau = \frac{1}{\sigma^2}$

$$L(\tau; x) \propto \tau^{\frac{1}{2}} e^{-\frac{(x-\mu)^2}{2}\tau}$$

Conjugate prior is $\tau \sim \text{Gamma}(\alpha, \beta)$ (β = rate)

$$f(\tau) \propto \tau^{\alpha-1} e^{-\beta\tau}$$

since

$$f(\tau|x) \propto \tau^{\alpha+\frac{1}{2}-1} e^{-\left(\beta + \frac{(x-\mu)^2}{2}\right)\tau}$$

i.e.

$$\tau|x \sim \text{Gamma}\left(\alpha + \frac{1}{2}, \beta + \frac{(x-\mu)^2}{2}\right)$$

Accordingly, conjugate family for $\sigma^2 = \frac{1}{\tau}$ is the inverse gamma

Ex. 4–6:

Likelihood	Conjugate
Geom	Beta
Poisson	Gamma
Exp	Gamma

Exponential family likelihoods always have a conjugate prior (GL 2.3.1.)

Improper priors.

Attempt at representing complete lack of prior knowledge about θ ("objectivity") via pdf $f(\theta)$, $\int_{-\infty}^{\infty} f(\theta)\,d\theta = \infty$, e.g. $f(\theta) = 1$ for $-\infty < \theta < \infty$

Ex. 2 cont.: $X|\mu \sim N(\mu, \sigma^2)$, σ^2 known,

$$\mu \sim N(\mu_0, \sigma_0^2) \tag{1a}$$

prior for μ.

As $\sigma_0^2 \to \infty$, the posterior

$$f(\mu|x) \to \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(\mu-x)^2}{2\sigma^2}} \tag{1b}$$

If we instead use the improper prior

$$f(\mu) \propto 1 \tag{2a}$$

as prior for μ, and assume that

$$f(\mu|x) \propto f(x|\mu) f(\mu) \tag{2b}$$

still holds, we obtain

$$f(\mu|x) \propto e^{-\frac{(x-\mu)^2}{2\sigma^2}} \cdot 1 \tag{2c}$$

i.e. the same result as limiting posterior (1b) above.

But note that

$$\lim_{\sigma_0^2 \to \infty} f(\mu; \mu_0, \sigma_0^2) \to 0$$

which differ from $f(\mu)$ in (2a).

If a sequence of proper priors converges g-vaguely (see Bioche & Druilhet, 2016, for def.) to an improper prior $f(\theta)$, then the limiting posterior (as in 1b) can be obtained instead via $f(\theta|x) \propto f(x|\theta) f(\theta)$ (as in 2c) where $f(\theta)$ is the g-vague limiting improper prior.

Some improper priors leads to credible intervals with exact frequentist coverage. (matching priors)

Non-informative "flat" priors

Aim: "Objectivity".

Ex.: $X \sim \text{bin}(n, p)$, Prior on p: $f(p) = 1$ for $0 < p < 1$.

Criticism: Implies that

$$\theta = \ln \frac{p}{1-p} \qquad p = \frac{e^\theta}{1+e^\theta}$$

has a non-uniform density

$$f_\Theta(\theta) = f(p) \left| \frac{dp}{d\theta} \right| = \frac{e^\theta}{(1+e^\theta)^2} \quad \text{for } -\infty < \theta < \infty,$$

i.e. $\theta \sim \text{logistic}(0, 1)$. So in terms of θ the prior is not "non-informative".

An alternative improper prior is $f(\theta) \propto 1$ for $-\infty < \theta < \infty$ which leads to

$$f(p) = f(\theta) \frac{d\theta}{dp} = \frac{1}{p} - \frac{1}{1-p} = \frac{1}{p(1-p)} = p^{-1}(1-p)^{-1}$$

(the Haldane prior) which can be seen as a (improper) limit of a $\text{Beta}(\alpha, \beta)$ as $\alpha, \beta \to 0$. For the $X|p \sim \text{bin}(n, p)$ likelihood this leads to

$$p|X=x \sim \text{Beta}(x, n-x)$$

and thus

$$E(p|X=x) = \frac{x}{x + n - x} = \frac{x}{n}$$

for $0 < x < n$. For $x = 0$ the posterior

$$f(p|x) \propto p^{-1}(1-p)^{n-1}$$

is improper (and similarly for $x = n$).

Jeffreys prior

Aim: Invariance w.r.t. reparameterization

Def.: $f(\theta) \propto |J(\theta)|^{\frac{1}{2}}$

where $J(\theta) = E\left(-\frac{\partial^2}{\partial\theta\,\partial\theta^T} \ln L(\theta; X)\right) = E\left(\frac{\partial}{\partial\theta} \ln L(\theta; X) \frac{\partial}{\partial\theta^T} \ln L(\theta; X)\right)$

is the Fisher information.

alternative equivalent def.

Proof of invariance (1-dimensional case):

The log-likelihood after reparameterization to $\gamma = h(\theta)$ where h is one-to-one and differentiable is

$$\ell(\gamma; X) = \ell_\theta(\theta(\gamma); X) \quad \text{where} \quad \ell_\theta(\theta; X) = \ln L(\theta; X).$$

Thus

$$\frac{d}{d\gamma}\ell(\gamma; X) = \frac{d}{d\theta}\ell_\theta(\theta(\gamma); X)\frac{d\theta}{d\gamma}$$

$$\frac{d^2}{d\gamma^2}\ell(\gamma; X) = \frac{d^2}{d\theta^2}\ell_\theta(\theta(\gamma); X)\left(\frac{d\theta}{d\gamma}\right)^2 + \frac{d}{d\theta}\ell_\theta(\theta(\gamma); X)\frac{d^2\theta}{d\gamma^2} \quad (*)$$

and

$$J_\gamma(\gamma) = -E\left(\frac{\partial^2}{\partial\gamma^2}\ell_\gamma(\gamma; X)\right)$$

$$= J_\theta(\theta)\left(\frac{\partial\theta}{\partial\gamma}\right)^2$$

since the score function (second term in $(*)$) has zero expectation.

Hence, prior based on $J_\gamma(\gamma)$ for the reparameterized model

$$f_\gamma(\gamma) = \sqrt{J_\theta(\theta)}\left|\frac{d\theta}{d\gamma}\right| = f_\theta(\gamma)\left|\frac{d\theta}{d\gamma}\right|$$

is equal to the prior implied the transformation formula and $J_\theta(\theta)$ in first parameterization.

Proof in p-dimensional case

$\gamma = g(\theta)$, $g: \mathbb{R}^p \to \mathbb{R}^p$

$$\underbrace{\frac{\partial}{\partial \gamma}}_{p\times 1} \ell_\gamma(\gamma; X) = \frac{\partial}{\partial \gamma} \ell_\theta(\theta(\gamma); X) = \underbrace{\frac{\partial \theta}{\partial \gamma}}_{p\times p} \underbrace{\frac{\partial \ell_\theta}{\partial \theta}}_{p\times 1}$$

$$J_\gamma(\gamma) = E\left(\frac{\partial \ell_\gamma}{\partial \gamma} \cdot \frac{\partial \ell_\gamma}{\partial \gamma^T} \right) = E\Big(\underbrace{\frac{\partial \theta}{\partial \gamma}}_{p\times p} \cdot \overbrace{\underbrace{\frac{\partial \ell_\theta}{\partial \theta}}_{p\times 1} \cdot \underbrace{\frac{\partial \ell_\theta}{\partial \theta^T}}_{1\times p}}^{\text{random var.}} \cdot \underbrace{\frac{\partial \theta}{\partial \gamma^T}}_{p\times p} \Big)$$

$$= \frac{\partial \theta}{\partial \gamma} J_\theta(\theta) \frac{\partial \theta}{\partial \gamma^T}$$

$$f_\gamma(\gamma) = \left| J_\gamma(\gamma) \right|^{1/2} = \left| \frac{\partial \theta}{\partial \gamma} \right|^{1/2} \left| J_\theta(\theta) \right|^{1/2} \left| \frac{\partial \theta}{\partial \gamma} \right|^{1/2}$$

$$= \left| \frac{\partial \theta}{\partial \gamma} \right| f_\theta(\theta)$$

Ex.: $X \sim \text{bin}(n, p)$, $\ell(p) = x \ln p + (n-x)\ln(1-p)$

$$\frac{d\ell}{dp} = \frac{x}{p} - \frac{n-x}{1-p}$$

$$\frac{d^2\ell}{dp^2} = -\frac{x}{p^2} - \frac{n-x}{(1-p)^2}$$

$$J(p) = E\left[-\frac{d^2\ell}{dp^2}\right] = \frac{np}{p^2} + \frac{n(1-p)}{(1-p)^2} = \frac{n}{p} - \frac{n}{1-p} = \frac{n}{p(1-p)}$$

Jeffreys prior

$$f(p) = \left(J(p)\right)^{\frac{1}{2}} \propto p^{-\frac{1}{2}}(1-p)^{-\frac{1}{2}} = p^{\frac{1}{2}-1}(1-p)^{\frac{1}{2}-1}$$

i.e.

$p \sim \text{Beta}\left(\frac{1}{2}, \frac{1}{2}\right)$

also called the arcsine distribution. $F(p) = \frac{\sin^{-1}(2p-1)}{\pi} + \frac{1}{2}$

Sanity check of invariance property:

Reparametized model, $\theta = \ln \frac{p}{1-p}$

$$\ell(\theta) = x\theta + n\ln(1-p)$$

$$= x\theta + n\ln\left(\frac{1}{1+e^{\theta}}\right)$$

$$= x\theta - n\ln(1+e^{\theta})$$

$$\frac{d\ell}{d\theta} = x - \frac{n e^{\theta}}{1+e^{\theta}}$$

$$\frac{d^2\ell}{d\theta^2} = -\frac{n e^{\theta}}{(1+e^{\theta})^2}$$

$$f(\theta) = \left(J(\theta)\right)^{\frac{1}{2}} \propto \frac{e^{\theta/2}}{1+e^{\theta}}$$

Via transformation formula:

$$f(\theta) = f(p)\left|\frac{dp}{d\theta}\right| = p^{-\frac{1}{2}}(1-p)^{-\frac{1}{2}}\frac{e^{\theta}}{(1+e^{\theta})^2} = \frac{e^{\theta/2}}{1+e^{\theta}}$$

If we instead were to observe $Y \sim \text{geom}(p)$ (where p is the same parameter), the Jeffrey's prior (our prior beliefs about p) would have needed to be different!

Criticism: Absurd that prior beliefs is determined (via the likelihood) by the type of data we happen to have obtained.

Antithetic sampling

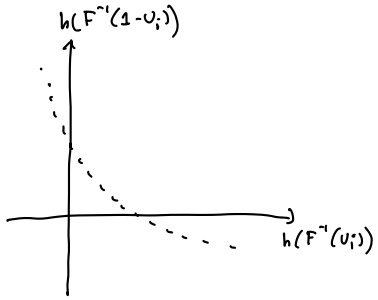
Aim: Reduce variance of Monte Carlo (or importance sampling) estimate $\frac{1}{n}\sum_{i=1}^{n} h(X_i)$ by making terms negatively correlated.

Generate $U_1, U_2, \ldots, U_n \overset{iid}{\sim} \text{Unif}(0,1)$ and compute

$$\widehat{E(h(X))} = \frac{1}{2n}\left(\sum_{i=1}^{n} h(\underbrace{F^{-1}(U_i)}_{X_i}) + \sum_{i=1}^{n} h(\underbrace{F^{-1}(1-U_i)}_{X_i^*}) \right) = \frac{1}{n}\sum_{i=1}^{n} \underbrace{\frac{1}{2}\left(h(F^{-1}(U_i)) + h(F^{-1}(1-U_i)) \right)}_{\text{i.i.d}} \quad (1)$$

It follows that $h(F^{-1}(U_i)) \sim h(F^{-1}(1-U_i))$

Hence, (1) remains unbiased and converges a.s. to $Eh(X)$.



Also, at least if h (and hence $h \circ F^{-1}$) is monotonic,

$$\text{Cov}\left(h(F^{-1}(U_i)),\ h(F^{-1}(1-U_i)) \right) \leq 0.$$

(see GH, p. 187–188 for a proof)

Hence,

$$\text{Var}\left(\widehat{E(h(X))}\right) = \frac{1}{2n}\text{Var}\, h(X_i) + \frac{1}{(2n)^2} \cdot n2\,\text{Cov}\left(h(X_i), h(X_i^*)\right)$$

$$= \frac{1}{2n}\text{Var}\, h(X_i)\,(1+\rho)$$

$$\leq \frac{1}{2n}\text{Var}\, h(X_i),$$

the variance of an ordinary Monte Carlo estimate based on sample of size $2n$, if $\rho = \text{corr}\left(h(X_i), h(X_i^*)\right) \leq 0$

Ex. 1: Find $E(\sqrt{X})$ where $X \sim \exp(1)$.

R demo

Ex. 2. Find $E(h(X))$ where $X \sim N(0,1)$, $h(X) = \frac{x}{2^x - 1}$.

Letting $X_i^* = -X_i$, $X_i^* \sim X_i$ (inversion method not needed)

R demo

Similar ideas can be in conjunction with Markov chain Monte Carlo (MCMC part 2)

Summary part 1, sampling methods

Sampling method	When to use	Normalized $f(x)$	Pros	Cons
Inversion	F^{-1} avail	(yes)	Fast	
	F avail			Need to solve $F(x)=u$ numerically
Transformation from simpler RV.	Normal (Box-Muller), location-scale families	(yes)	Fast	Simple transformation may not exist
Rejection sampling	c and $g(x)$ available	No		Slow in high dimensions Finding $g(x)$ similar to $f(x)$ s.t. $f(x)/g(x)$ is bounded
Weighted resampling	c unknown	No		Only approximate
Adaptive rejection sampling	$f(x)$ log-concave	No	Fast	Only in one dimension
Ratio of uniforms	Support of $f(x)$ unbounded, $f(x)$ and $x^2 f(x)$ bounded	No	Fast	
Mixtures	If sampling from $f(x\|y)$ and $f(y)$ is easy			
Multivariate normal				
Alias method	pmfs with finite support			
Simulating generating process	Sanity checking			Slow

Estimating expectations, $E(h(x))$

Integration method	When to use	Normalized $f(x)$	Pros	Cons
Analytic	Whenever possible	Yes	Exact	
Numerical Adaptive Gauss Hermite quadrature	Integrand approx. Gaussian	Yes	Fast and often very accurate	Difficult in for high-dimensions
Monte Carlo		No	Unbiased	High variance
Importance sampling		Yes	Unbiased, smaller variance	Finding $s(x)$ similar to $h(x)f(x)$
		No	Consistent	Biased
Antithetic sampling				