Lecture 3: What have we learned..

Sampling from random distribution

- Inversion Method:
  - Discrete RV
  - Continuous RV (where it is possible to compute $F^{-1}(x)$)
- Use known relationship between RV
  - Examples: Gamma, χ^2 distributions
- Change of variables
  - Univariate: scale and location parameters
  - Bivariate: Box-Muller algorithm
- Ratio of uniforms method
  - Don't need to know the normalising constant
  - Example: Cauchy distribution

Inversion method

Let F be a distribution, and let $U \sim \mathcal{U}[0,1]$.

a) Let F be the distribution function of a random variable taking non-negative integer values. The random variable X given by

$$X = x_i \quad \text{if and only if} \quad F_{i-1} < u \leq F_i$$

has distribution function F.

b) If F is a continuous function, the random variable $X = F^{-1}(u)$ has distribution function F.

Change of variables

- Can sample from $X \sim \text{Exp}(1)$.
- Interested in $Y = \frac{1}{\lambda}X$
- Method: sample $X \sim \exp(1)$, return $Y = \frac{1}{\lambda}X$

Why does it work?? We have that: $y = g(x) = \frac{1}{\lambda}x$. Application of the change of variables formula leads to:

$$f_Y(y) = f_X(g^{-1}(x))|\frac{d\ g^{-1}(x)}{d\ x}| = \exp(-\lambda y)\lambda$$

It follows: $Y \sim \text{Exp}(\lambda)$.

Bivariate techniques

Generalization of the previous technique

- $(x_1, x_2) \sim f_X(x_1, x_2)$
- $(y_1, y_2) = g(x_1, x_2) \Leftrightarrow (x_1, x_2) = g^{-1}(y_1, y_2)$
- $f_Y(y_1, y_2) = f_X(g^{-1}(y_1, y_2)) \cdot |\mathrm{J}|$

Example: Box-Muller to simulate from $\mathcal{N}(0, 1)$

Box-Muller algorithm

Let

$$X_1 \sim \mathcal{U}[0, 2\pi] \text{ and } X_2 \sim \text{Exp}\left(\frac{1}{2}\right)$$

independently (We already know how to do this).

Let

$$\left.\begin{aligned} y_1 &= \sqrt{x_2}\cos x_1 \\ y_2 &= \sqrt{x_2}\sin x_2 \end{aligned}\right\} \Leftrightarrow \begin{cases} x_1 = \tan^{-1}\left(\frac{y_2}{y_1}\right) \\ x_2 = y_1^2 + y_2^2 \end{cases}$$

This defines a one-to-one function g.

Then hat $y_1 \sim \mathcal{N}(0, 1)$ and $y_2 \sim \mathcal{N}(0, 1)$ independently.

Graphical interpretation:

Relationship between polar and Cartesian coordinates.

Box-Muller algorithm

Generate

$x_1 \sim U(0, \pi)$

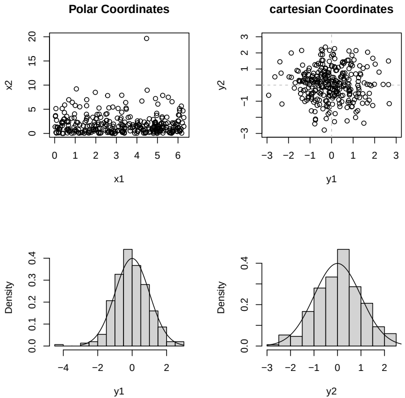
Generate

$x_2 \sim \exp(0.5)$

$y_1 \leftarrow \sqrt{(}x_2) \cos(x_1)$

$y_2 \leftarrow \sqrt{(}x_2) \sin(x_1)$

return (y_1, y_2)



Ratio-of-uniforms method

- $f^\star(x)$ non-negative function with $\int_{-\infty}^{\infty} f^\star(x)dx < \infty$
- $C_f = \{(x_1, x_2)|0 \leq x_1 \leq \sqrt{f^\star(x_2/x_1)}\}$

Thus

a) then C_f has finite area.

Let (x_1, x_2) be uniformly distributed on C_f.

b) Let $y = \frac{x_2}{x_1}$, then $f(y) = \frac{f^\star(y)}{\int_{-\infty}^{\infty} f^\star(u)du}$

Plan for today

- More on ratio of uniform method
- Methods based on mixtures
- The multivariate normal distribution
- Rejection sampling

How to sample from C_f?

- Sometimes we can find an easy way to sample directly from C_f (example: half circle.)
- In general, it can be difficult to sample uniformly from C_f but it is easy in some special cases....

We have $C_f = \{(x_1, x_2) \mid 0 \leq x_1 \leq \sqrt{f^\star\left(\frac{x_2}{x_1}\right)}\}$.

If $f^\star(x)$ and $x^2 f^\star(x)$ are bounded we have

$$C_f \subset [0, a] \times [b_-, b_+], \qquad \text{with}$$

- $a = \sqrt{\sup_x f^\star(x)} > 0$
- $b_+ = \sqrt{\sup_{x\geq 0}(x^2 f^\star(x))}$
- $b_- = -\sqrt{\sup_{x\leq 0}(x^2 f^\star(x))}$

Ratio of uniform method

If $f^{\star}(x)$ and $x^2 f^{\star}(x)$ are bounded we have

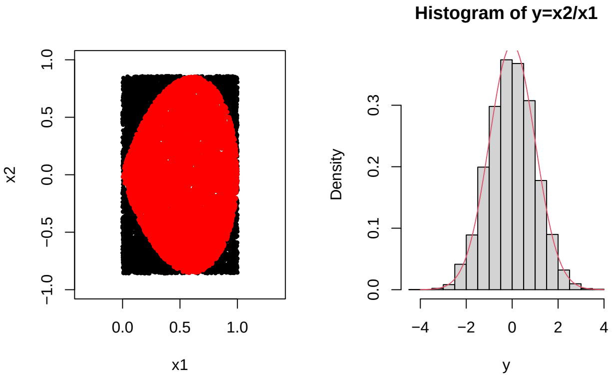
$$C_f \subset [0, a] \times [b_-, b_+], \qquad \text{with}$$

- Proof: see notes from last class
- Use Rejection sampling to sample from C_f.

Example: Normal distribution

see notes from last class

Example: Normal distribution



Methods based on mixtures

Remember: $f(x_1, x_2) = f(x_1|x_2)f(x_2)$

Thus: To generate $(x_1, x_2) \sim f(x_1, x_2)$ we can

- generate $x_2 \sim f(x_2)$
- generate $x_1 \sim f(x_1|x_2)$, where x_2 is the value just generated.

Here x_2 is called the mixing element.

Methods based on mixtures

Note: This mechanism automatically provides a value x_1 from its marginal distribution,

$$x_1 \sim f(x_1) = \int_{-\infty}^{\infty} f(x_1, x_2) dx_2.$$

$\Rightarrow$ We are able to generate a value for x_1 even when its marginal density is awkward to sample from directly.

Example: Simulation from Student-t (I)

The density of a Student t distribution with $n > 0$ degrees of freedom, mean μ and scale σ^2 is

$$f_t(x) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \frac{1}{\sqrt{n\pi\sigma^2}} \left[1 + \frac{1}{n}\left(\frac{x-\mu}{\sigma}\right)^2\right]^{-\frac{n+1}{2}}, \quad -\infty < x < \infty.$$

Let

$$x_1 \sim \text{Ga}\left(\frac{n}{2}, \frac{n}{2}\right)$$
$$x_2 | x_1 \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{x_1}\right)$$

It can be shown that then

$$x_2 \sim t_n(\mu, \sigma^2) \quad \text{(show yourself)}$$

Example: Simulation from Student-t (II)

Thus, we can simulate

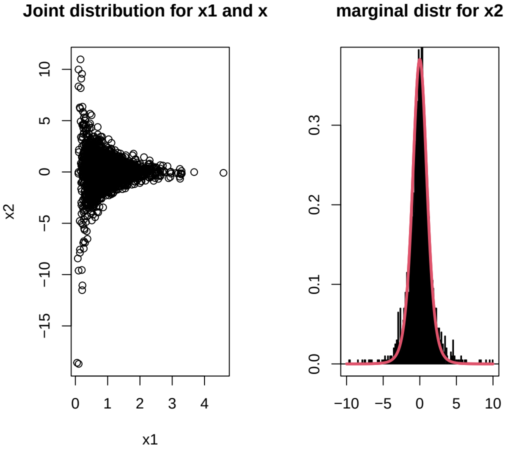
$x_1 \sim t_n(\mu, \sigma^2)$ by

Generate $x_1 \sim \text{Ga}\left(\frac{n}{2}, \frac{n}{2}\right)$

Generate

$x_2 | x_1 \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{x_1}\right)$

return x_2



Another example: Mixture of normal distributions

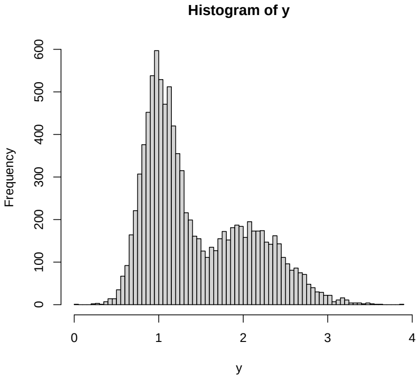
If the mixing element is discrete $f(a_i) = P(X_2 = a_i) = p_i$, $i = 1, \dots, k$, then:

$$f(x_2) = \sum_i f(x_2 | X_1 = a_i) * P(X_1 = a_i)$$

Say we have that $X_1 = \{1, 2\}$ with $p_1 = 0.2$ and $p_2 = 0.8$ and $f(x_2 | X_1 = i) = \mathcal{N}(\mu_i, \sigma_i)$ for $i = 1, 2$

Mixture of normal distribution

Generate $x_1 \sim \text{Binom}(1, p_1)$
if $x_1 = 0$ **then**
  Generate $x_2 \sim \mathcal{N}(\mu_1, \sigma_1)$
else
  Generate $x_2 \sim \mathcal{N}(\mu_2, \sigma_2)$
end if
return x_2



Multivariate normal distribution

$\boldsymbol{x} = (x_1, \ldots, x_d)^\top \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$ if the density is

$$f(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}} \cdot \frac{1}{\sqrt{|\Sigma|}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right)$$

with

- $\boldsymbol{x} \in \mathbb{R}^d$
- $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_d)^\top$
- $\Sigma \in \mathbb{R}^{d \times d}$, Σ must be positive definite.

Important properties (I)

Important properties of $\mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$

(known from "Linear statistical models")

i) Linear transformations:

$\boldsymbol{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma) \Rightarrow \boldsymbol{y} = \mathrm{A}\boldsymbol{x} + \boldsymbol{b} \sim \mathcal{N}_r(\mathrm{A}\boldsymbol{\mu} + \boldsymbol{b}, \mathrm{A}\Sigma\mathrm{A}^\top)$, with $\mathrm{A} \in \mathbb{R}^{r \times d}$, $\boldsymbol{b} \in \mathbb{R}^r$.

ii) Marginal distributions:

Let $\boldsymbol{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$ with $\Sigma^{-1} = \mathrm{Q}$, and:

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix}, \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}, \mathrm{Q} = \begin{bmatrix} \mathrm{Q}_{11} & \mathrm{Q}_{12} \\ \mathrm{Q}_{21} & \mathrm{Q}_{22} \end{bmatrix}.$$

Then

$$\boldsymbol{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \Sigma_{11})$$

$$\boldsymbol{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}_2, \Sigma_{22})$$

Important properties (II)

iii) Conditional distributions:

With the same notation as in ii) we also have,

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

and,

$$\boldsymbol{x}_1|\boldsymbol{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}_1 - \boldsymbol{Q}_{11}^{-1}\boldsymbol{Q}_{12}(\boldsymbol{x}_2 - \boldsymbol{\mu}_2), \boldsymbol{Q}_{11}^{-1}).$$

iv) Quadratic forms:

$\boldsymbol{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma) \Rightarrow (\boldsymbol{x} - \boldsymbol{\mu})^\top \Sigma^{-1}(\boldsymbol{x} - \boldsymbol{\mu}) \sim \chi^2_d$

Simulation from the multivariate normal

How can we simulate from $\mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$?

Let $\boldsymbol{x} \sim \mathcal{N}_d(0, \mathrm{I})$

$$\boldsymbol{y} = \boldsymbol{\mu} + \mathrm{A}\boldsymbol{x} \quad \overset{\text{i)}}{\Rightarrow} \quad \boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}, \mathrm{A}\mathrm{A}^\top)$$

Thus, if we choose A so that $\mathrm{A}\mathrm{A}^\top = \Sigma$ we are done.

Note: There are several choices of A. A popular choice is to let A be the Cholesky decomposition of Σ.

Rejection sampling

We discuss a general approach to generate samples from some target distribution with density $f(x)$, called rejection sampling, without actually sampling from $f(x)$.

Rejection sampling

The goal is to effectively simulate a random number $X \sim f(x)$ using two independent random numbers

- $U \sim \mathrm{U}(0,1)$ and
- $X \sim g(x)$,

where $g(x)$ is called proposal density and can be chosen arbitrarily under the assumption that there exists an $c \geq 1$ with

$$f(x) \leq c \cdot g(x) \quad \text{for all } x \in \mathbb{R}\,.$$

Rejection sampling - Algorithm

Let $f(x)$ denote the target density.

1. Generate $x \sim g(x)$
2. Generate $u \sim \mathcal{U}(0,1)$.
3. Compute $\alpha = \frac{1}{c} \cdot \frac{f(x)}{g(x)}$.
4. If $u \leq \alpha$ return x (acceptance step).
5. Otherwise go back to (1) (rejection step).

Note $\alpha \in [0,1]$ and α is called acceptance probability.

Claim: The returned x is distributed according to $f(x)$.

Proof

See blackboard

Rejection sampling

- We want $x \sim f(x)$ (density).
- We know how to generate realisations from a density $g(x)$
- We know a value $c > 1$, so that $\frac{f(x)}{g(x)} \leq c$ for all x where $f(x) > 0$.

Algorithm:

finished $= 0$

while (finished $= 0$)

    generate $x \sim g(x)$

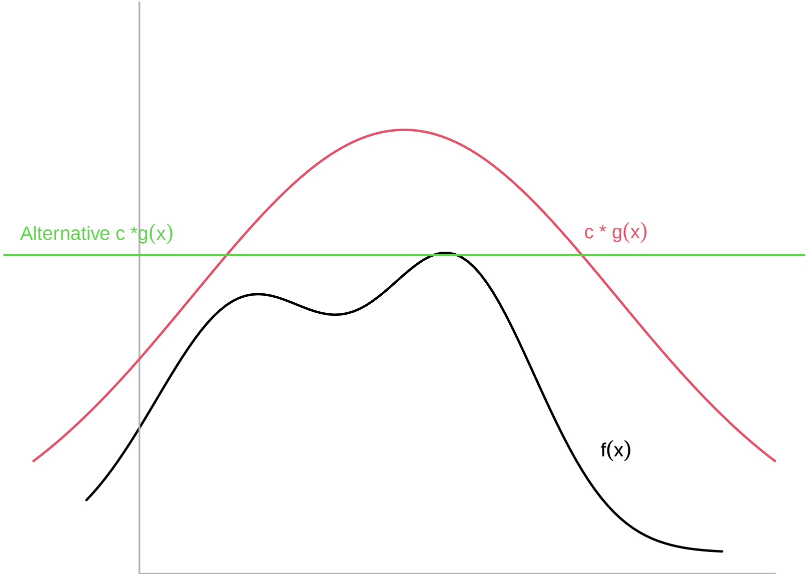
    compute $\alpha = \frac{1}{c} \cdot \frac{f(x)}{g(x)}$

    generate $u \sim U[0, 1]$

    if $u \leq \alpha$ set finished $= 1$

return x

Rejection sampling



Rejection sampling

What is the overall acceptance probability??

$$\mathrm{P}\left(U \leq \frac{1}{c} \cdot \frac{f(X)}{g(X)}\right) = \int_{-\infty}^{\infty} \frac{f(x)}{c \cdot g(x)} g(x)\, dx = \int_{-\infty}^{\infty} \frac{f(x)}{c}\, dx = c^{-1}.$$

The single trials are independent, so the number of trials up to the first success is geometrically distributed with parameter $1/c$.

The expected number of trials up to the first success is therefore c.

Problem:

In high-dimensional spaces c is generally large so many samples will get rejected.

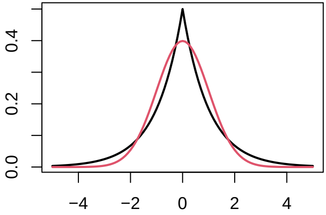
Example: Sample from $N(0,1)$ with rejection sampling

Target distribution:

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right).$$

Proposal distribution:

$$g(x) = \frac{\lambda}{2} \exp(-\lambda|x|), \lambda > 0$$



Sampling from a double exponential

Proposal distribution:

$$g(x) = \frac{\lambda}{2} \exp(-\lambda |x|), \lambda > 0$$

How to sample from $g(x)$:

Sampling from a double exponential

Proposal distribution:

$$g(x) = \frac{\lambda}{2}\exp(-\lambda|x|), \lambda > 0$$

How to sample from $g(x)$:

Simulate $z \sim \exp(\lambda)$

Simulate

$y \sim \text{Bern}(p = 0.5)$

if $y = 0$ **then**

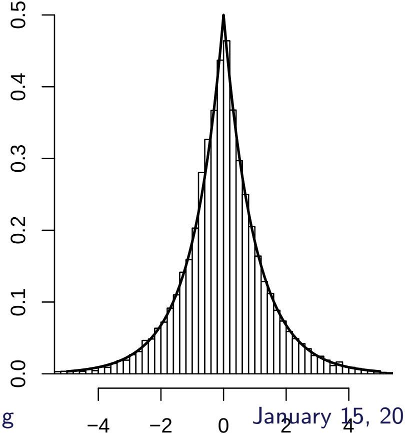
  $x = z$

else

  $x = -z$

end if

return x



Example: Sample from $N(0,1)$ with rejection sampling

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Proposal distribution:

$$g(x) = \frac{\lambda}{2} \exp(-\lambda|x|), \lambda > 0$$

- Need to find c such that $\frac{f(x)}{g(x)} < c$, $\forall x$ where $f(x) > 0$

Example: Find an efficient bound c

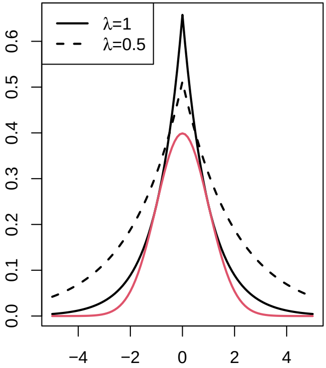
$$\frac{f(x)}{g(x)} \leq \sqrt{\frac{2}{\pi}}\lambda^{-1} \exp\left(\frac{1}{2}\lambda^2\right) \leq c$$

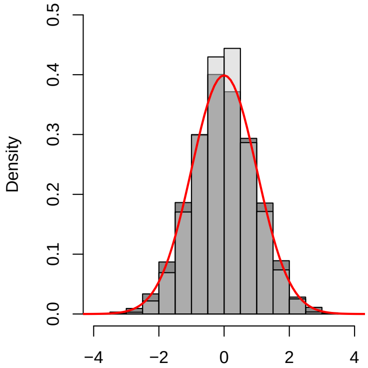
Which value of λ should we choose for proposal density?

We need to choose the smallest possible value for c

Do this yourself

Example: Illustration





- Left: Comparison of $f(x)$ versus $c \cdot g(x)$ when $\lambda \stackrel{\text{x1}}{=} 1$ and $\lambda = 1$.
- Right: Distribution of accepted samples compared to $f(x)$.

  10000 samples were generated and 7582 accepted for $\lambda = 1$.

  10000 samples were generated and 4774 accepted for $\lambda = 0.5$.

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