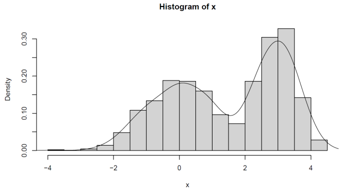
Algorithms and Data Structures

Random Numbers
Methods for other Distributions



Learning goals

- Inverse transform sampling
- Transformations
- Mixture distribution
- Sampling multivariate Gaussian

INVERSE TRANSFORM SAMPLING

Let X be a continuous RV with distribution function $F_X(x)$. Then

$$F_X(X) \sim \mathrm{U}(0,1)$$

Therefore, if $U \sim \mathrm{U}(0,1)$ then the RV $F_X^{-1}(U)$ has the same distribution as X with distribution function $F_X(x)$.

Proof: Define

$$F_X^{-1}(u) := inf\{x : \; F_X(x) \geq u\}, \quad 0 < u < 1$$

If $U \sim \mathrm{U}(0,1)$, then for all $x \in \mathbb{R}$ it holds

$$\begin{aligned} P(F_X^{-1}(U) \leq x) &= P(inf\{t : \; F_X(t) = U\} \leq x) \\ &= P(U \leq F_X(x)) \\ &= F_{\mathrm{U}}(F_X(x)) = F_X(x). \end{aligned}$$

Thus, $F_X^{-1}(U)$ has the same distribution as X.

INVERSE TRANSFORM SAMPLING / 2

Algorithm

1. Calculate inverse function $F_X^{-1}(u)$.
2. For each random number:
   - Generate random u from $\mathrm{U}(0, 1)$.
   - Calculate $x = F_X^{-1}(u)$.

This theoretically solves the problem of simulating continuous random numbers. However, if F^{-1} is difficult to compute, other methods are often preferred.

EX. INVERSION: UNIFORM DISTRIBUTION

$$\text{Be } U \sim \mathrm{U}(0,1)$$

$$\text{Aim: } X \sim \mathrm{U}(a,b)$$

$$F(x) = \begin{cases} 0 & x < a \\ \frac{x-a}{b-a} & x \in [a,b] \\ 1 & x > b \end{cases}$$

$$\frac{x-a}{b-a} \overset{!}{=} u$$

$$\Leftrightarrow x - a = u(b-a)$$

$$\Leftrightarrow x = u(b-a) + a$$

EX. INVERSION: EXPONENTIAL DISTRIBUTION

$$\text{Be } U \sim \mathrm{U}(0,1)$$

$$\text{Aim: } X \sim \mathrm{Exp}(\lambda)$$

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

$$\Leftrightarrow -x\lambda = \log(1-u)$$

$$\Leftrightarrow x = \frac{-\log(1-u)}{\lambda}$$

Since

$$U \sim \mathrm{U}(0,1) \quad \Rightarrow \quad 1 - U \sim \mathrm{U}(0,1)$$

RV can be generated from $F_X^{-1*}(u) = \frac{-\log(u)}{\lambda}$.

INVERSION FOR DISCRETE RANDOM VARIABLES

X is a discrete random variable and

$$\ldots < x_{i-1} < x_i < x_{i+1} < \ldots$$

are steps in $F_X(x)$. Then the inversion is $F_X^{-1}(u) = x_i$, with $F_X(x_{i-1}) < u \leq F_X(x_i)$.

Algorithm

1. Draw random u from $\mathrm{U}(0, 1)$.
2. Output x_i with $F_X(x_{i-1}) < u \leq F_X(x_i)$.

Solving $F(x_{i-1}) < u \leq F(x_i)$ in (2.) can be difficult.

EX. INVERSION: GEOMETRIC DISTRIBUTION

Aim: Generate random numbers from $Geom(p = \frac{1}{4})$.

At points of discontinuity ($x = 0, 1, 2, ...$) the density function is $f_X(x) = pq^x$, with $q = 1 - p$ and distribution function is $F_X(x) = 1 - q^{x+1}$.

Solve $1 - q^x < u \leq 1 - q^{x+1}$, with u from $\mathrm{U}(0, 1)$.

Equation system corresponds to $x < log(1 - u)/log(q) \leq x + 1$.

Solution: $x + 1 = \lceil log(1 - u)/log(q) \rceil$.

LIMITATIONS OF INVERSION SAMPLING

- The quality of the random numbers is heavily dependent on the quality of the quantile function.
- While F is often easy to calculate, the computation of F^{-1} can be difficult:

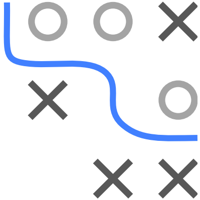
  $\Rightarrow$ Solve numerically $F(X) - U = 0$.
- Especially for quantile functions, which approximate the distribution function numerically in the corresponding integral, the inversion method is inefficient and inaccurate.
- But: in `R` for example, normally distributed random numbers are currently calculated using inverse transform sampling.

TRANSFORMATIONS

For the simulation of specifically distributed random variables transformations of other random variables can be used, e.g.:

1. If $Z \sim N(0,1)$, then $V = Z^2 \sim \chi^2(1)$.
2. If $U \sim \chi^2(m)$ and $V \sim \chi^2(n)$ are independent, then $F = \frac{U/m}{V/n} \sim F(m,n)$.
3. If $Z \sim N(0,1)$ and $V \sim \chi^2(n)$ are independent, then $T = \frac{Z}{\sqrt{V/n}} is \sim t(n)$.
4. If $U \sim Gamma(r,\lambda)$ and $V \sim Gamma(s,\lambda)$ are independent, then $X = \frac{U}{U+V} \sim Beta(r,s)$.

MIXTURE DISTRIBUTIONS



Random variable X follows (discrete) mixture distribution, if $X \sim F_X$

$$F_X(x) = \sum_{i=1}^{K} \theta_i F_{X_i}(x)$$

for a set of K random variables $X_1, X_2, ..., X_K$, with $\theta_i > 0$ and $\sum \theta_i = 1$.

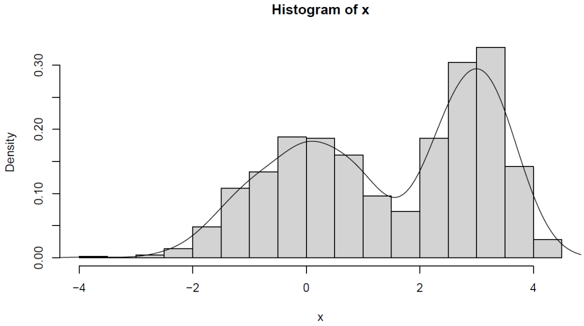
Simulation of mixture distributions:

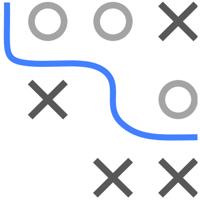
1. Draw integer $k \in \{1, ..., K\}$, with $P(k) = \theta_k$.
2. Draw random number x from F_{X_k}.

MIXTURE DISTRIBUTIONS / 2

Example: Mixture distribution

Draw from a 50%-50% - mixture of $N(0, 1)$ and $N(3, 0.5)$





SAMPLING MULTIVARIATE GAUSSIAN

$X = (X_1, ..., X_d) \sim N_d(\boldsymbol{\mu}, \Sigma)$:

$$f(x) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} exp(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}))$$

with mean $\boldsymbol{\mu} = (\mu_1, ..., \mu_d)^T$ and symmetrical, positive definite covariance matrix Σ.

Sampling from multivariate Gaussian:

1. Generate $Z = (Z_1, ..., Z_d)$, with $Z_i \overset{iid}{\sim} N(0, 1)$.
2. Transform random vector Z to desired mean and covariance.

SAMPLING MULTIVARIATE GAUSSIAN / 2

Derivation of Transformation:

- If $Z \sim N_d(\boldsymbol{\mu}, \Sigma)$, then $CZ + \boldsymbol{b}$ is $\sim N_d(C\boldsymbol{\mu} + \boldsymbol{b}, C\Sigma C^T)$.
- If $Z \sim N_d(0, \boldsymbol{I}_d)$, then $CZ + \boldsymbol{b}$ is $\sim N_d(\boldsymbol{b}, CC^T)$.
- Assuming Σ can be factorized into $\Sigma = CC^T$ for a matrix C, then $CZ + \boldsymbol{\mu} \sim N_d(\boldsymbol{\mu}, \Sigma)$.
- Hence, $CZ + \boldsymbol{\mu}$ is the transformation we are looking for.

SAMPLING MULTIVARIATE GAUSSIAN / 3

- Calculation of the square root $\Sigma^{1/2} = C$ by **spectral decomposition**.

- $\Sigma = P \Lambda P^{-1}$, with Λ being a diagonal matrix of the eigenvalues of Σ and P being a matrix with the orthogonal eigenvectors in the columns space ($P^{-1} = P^T$).

- $\Sigma^{1/2}$ then corresponds to $\Sigma^{1/2} = P \Lambda^{1/2} P^{-1}$, with $\Lambda^{1/2} = diag(\lambda_1^{1/2}, ..., \lambda_d^{1/2})$.

- There are other possibilities to factorize Σ (e.g. Cholesky decomposition) $\rightarrow$ see chapter 7.

SAMPLING MULTIVARIATE GAUSSIAN / 4