A short tutorial of random numbers generation

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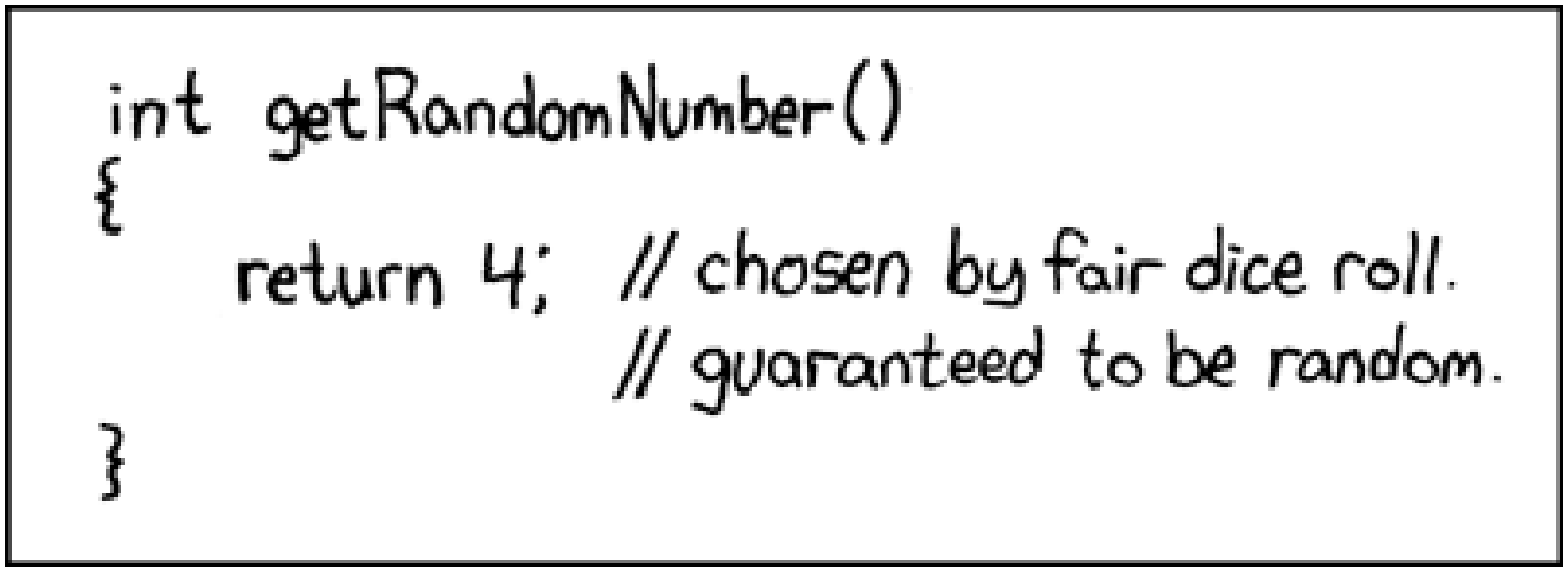


https://xkcd.com/221/

U[0,1]-distributed random numbers

- A good uniform random generator on the interval $[0, 1]$ is a major component of any good random generator library.
- Draws from other distributions are usually obtained by adequately transform an uniformly distributed sample.

Define a transition function $f : \mathcal{S} \to \mathcal{S}$, where $\mathcal{S}$ is the state space. The cardinality of $\mathcal{S}$ is assumed to be finite.

The initial state is denoted by s_0, and we will write

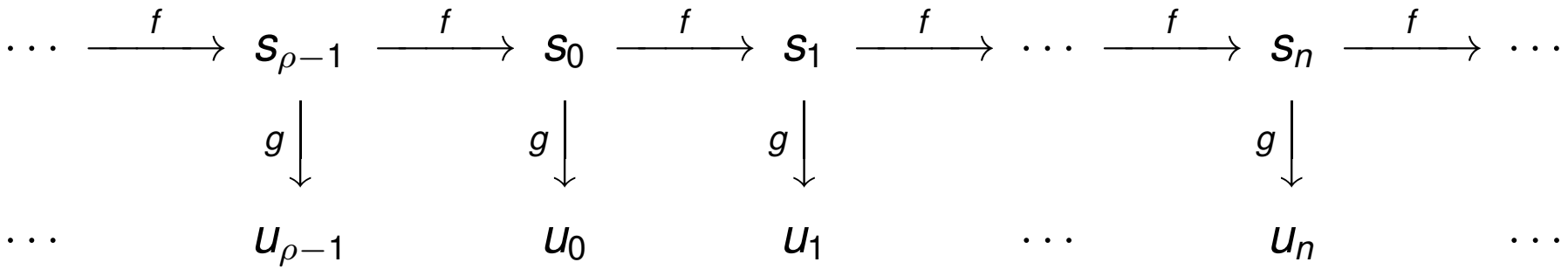
$$s_n = f(s_{n-1}).$$

We will furthermore assume that f is periodic for all n greater of equal to some known τ (often equal to 0), with period ρ:

$$s_{n+\rho} = s_n, \ \forall\, n \geq \tau.$$

U[0,1]-distributed random numbers (cont'd)

- Output space: $\mathcal{U}$.
- We assume here that $\mathcal{U} = (0, 1)$.
- Output function $g : \mathcal{S} \to \mathcal{U}$.
  It transforms the state s_n into an output value u_n.



How to choose f and g?

Goals: large ρ, good uniformity, "random" behavior.

Linear congruential generators (LCGs)

- Introduced by Lehmer (1951).
- State $s = x \in \mathbb{N}_{\geq 0}$.
- Recursive formula:

$$x_i = f(x_{i-1}) = (ax_{i-1} + c) \mod m,$$

where mod is the modulo operator.
Given two numbers, a (the dividend) and n (the divisor),

$$a \mod n = a - n \left\lfloor \frac{a}{n} \right\rfloor .$$

- If $c = 0$, the generator is often called a multiplicative congruential generator, or "Lehmer RNG"

Linear congruential generators: full period?

Full period: m is $c \neq 0$, $m-1$ otherwise (if $c = 0$, 0 is a fixed point for the recurrence). Consider the case $c \neq 0$.

Theorem (Period)

The LCG has full period iff the following three conditions hold:

1. *the only positive integer that (exactly) divides both m and c is 1;*
2. *if q is a prime number that divides m, then q divides $a-1$;*
3. *if 4 divides m, then 4 divides a-1.*

"Standard minimal" (Park and Miller, 1988):

$$x_{n+1} = 16807 x_n \bmod 2147483647.$$

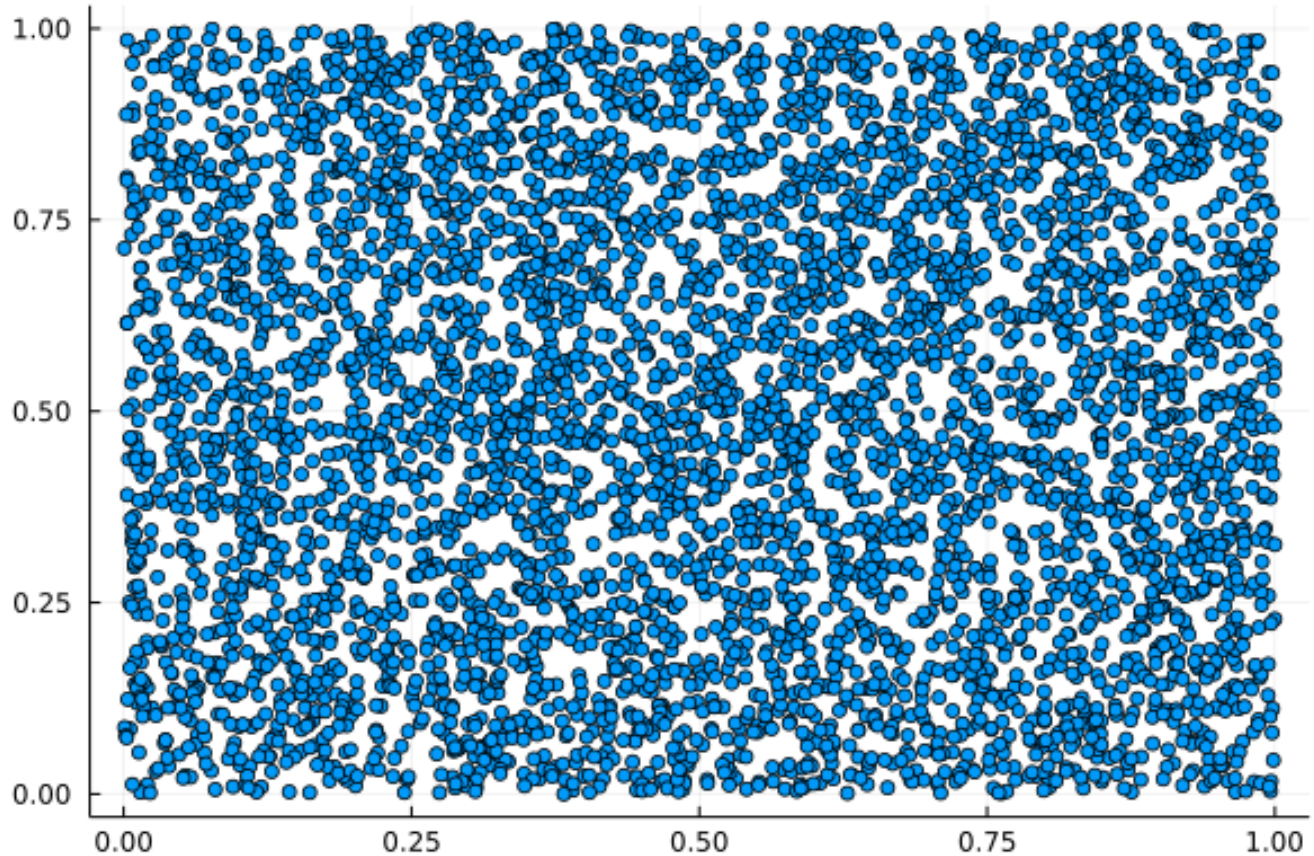
Observe that $2147483647 = 2^{31} - 1$; on 32-bit architectures, the largest representable (signed) integer is 2^{31}.

The Standard Minimal Generator

```
function getlcg(seed::Integer, a::Integer,
                c::Integer, m::Integer)
    state = seed
    am_mil = 1.0/m
    return function lcgrand()
        state = mod(a * state + c, m)
        # produce a number in (0,1)
        return state*am_mil
    end
end

stdmin = getlcg(1234, 16807, 0, 2^31-1)
```

Standard minimal generator: illustration



10000 generated points on the unit square.

Multiple Recursive Generator (MRG)

But we want better! Generalize the LCG:

$$x_n = (a_1 x_{n-1} + \cdots + a_k x_{n-k}) \mod m, \quad u_n = x_n/m.$$

In practice, take $u_n = (x_n + 1)/(m + 1)$, or $u_n = x_n/(m + 1)$ if $x_n > 0$ and $u_n = m/(m+1)$ otherwise, but the structure remains the same, and is easier when studying theoretical properties.

State at step n:

$$s_n = (x_{n-k+1}, \ldots, x_n)^T.$$

State space: $\mathcal{Z}_m^k$, of cardinality m^k.

The maximal period if $\rho = m^k - 1$.

Period of MRG's

It can be shown that for $k > 1$, it is sufficient to have at least two non-zero coefficients, including a_k, in order to get the maximal period.

The cheapest recurrence has therefore the form

$$x_n = (a_r x_{n-r} + a_k x_{n-k}) \mod m.$$

But how to choose a_r and a_k?

It is possible to study theoretical properties of MRG's, and exclude directly some generators that have known strong deficiencies.

Choosing a good MRG's

Example: Lagged-Fibonacci

$$x_n = (\pm x_{n-r} \pm x_{n-k}) \mod m.$$

It can be shown the vectors $(u_n, u_{n+k-r}, u_{n+k})$ are all contained in two plans! We therefore know without additional tests that the numbers cannot be considered as random.

In practice, we can impose various conditions on the coefficients, and compute theoretically appealing generators by maximizing some quality measure. This maximization is numerically expensive.

Combined MRG's

Consider two (or more) MRG's working in parallel:

$$\begin{aligned} x_{1,n} &= (a_{1,1}x_{1,n-1} + \cdots + a_{1,k}x_{1,n-k}) \mod m_1, \\ x_{2,n} &= (a_{2,1}x_{2,n-1} + \cdots + a_{2,k}x_{2,n-k}) \mod m_2. \end{aligned}$$

We define the two combinations

$$\begin{aligned} z_n &:= (x_{1,n} - x_{2,n}) \mod m_1; \qquad & u_n &:= z_n/m_1; \\ w_n &:= (x_{1,n}/m_1 - x_{2,n}/m_2) \mod 1. \end{aligned}$$

The sequence $\{w_n,\ n \geq 0\}$ is the output of another MRG, of module $m = m_1 m_2$, and $\{u_n,\ n \geq 0\}$ is nearly the same sequence if m_1 and m_2 are close.
We can achieve the period $(m_1^k - 1)(m_2^k - 1)/2$.

MRG32k3a

The following combined MRG was proposed by L'Ecuyer, and is amongst the most popular and efficient known generators. It combines 2 MRG's.

$k = 3$,
$m_1 = 2^{32} - 209$, $a_{11} = 0$, $a_{12} = 1403580$, $a_{13} = -810728$,
$m_2 = 2^{32} - 22853$, $a_{21} = 527612$, $a_{22} = 0$, $a_{23} = -1370589$.

Combination: $z_n = (x_{1,n} - x_{2,n}) \bmod m_1$.

Corresponding MRG: $k = 3$,
$m = m_1 m_2 = 18446645023178547541$,
$a_1 = 1816966847125289255 7$,
$a_2 = 3186860506199273833$,
$a_3 = 8738613264398222622$.

Période $\rho = (m_1^3 - 1)(m_2^3 - 1)/2 \approx 2^{191}$.

MRG32k3a: basic implementation

```
function rand(rng::MRG32k3a)

p1::Int64 = (a12 * rng.Cg[2] + a13 * rng.Cg[1]) % m1
p1 += p1 < 0 ? m1 : 0

rng.Cg[1] = rng.Cg[2]
rng.Cg[2] = rng.Cg[3]
rng.Cg[3] = p1

p2::Int64 = (a21 * rng.Cg[6] + a23 * rng.Cg[4]) % m2
p2 += p2 < 0 ? m2 : 0

rng.Cg[4] = rng.Cg[5]
rng.Cg[5] = rng.Cg[6]
rng.Cg[6] = p2

u::Float64 = p1 > p2 ? (p1 - p2) * norm :
    (p1 + m1 - p2) * norm
end
```

MRG32k3a: implementations

Note: more efficient implementations exist.
See for instance `https://github.com/vigna/MRG32k3a`.

Random numbers generators on $\mathcal{F}_2$

Alternatives to MRG's: random numbers generators based on linear recurrences in $\mathcal{F}_2$.

Galois field $\mathcal{F}_2$: set $\{0, 1\}$ equipped with addition and multiplication modulo 2.

We construct two sequences of bits vectors $\boldsymbol{x}_n$ and $\boldsymbol{y}_n$ with the linear recurrences

$$\begin{aligned} \boldsymbol{x}_n &= A\boldsymbol{x}_{n-1} && \text{(state vector, } k \text{ bits)}, \\ \boldsymbol{y}_n &= B\boldsymbol{x}_n && \text{(output vector, } w \text{ bits)}, \end{aligned}$$

Output:

$$u_n = \sum_{j=1}^{w} y_{n,j-1} 2^{-j} = .y_{n,0}\ y_{n,1}\ y_{n,2}$$

LFSR

Implementation is often quite complex, but it is possible to operate bitwise, and these RNGs are numerically very fast.

The LFSR (linear feedback shift register), while known to have important deficiencies, gives an illustration of such generators.

We use the relations (with $a_k \neq 0$)

$$u_n = \sum_{\ell=1}^{w} x_{n\nu+j-1} 2^{-\ell} = .x_{n\nu} x_{n\nu+1} x_{n\nu+2} \cdots x_{n\nu+\ell-1}$$

$$X = \begin{pmatrix} & 1 & & \\ & & \ddots & \\ & & & 1 \\ a_k & a_{k-1} & \cdots & a_1 \end{pmatrix}^{\nu}, \qquad B = I.$$

Tausworthe generator

Maximum period: $\rho = 2^k - 1$ iff $\gcd(\nu, 2^k - 1) = 1$ and $Q(z) = z^k - a_1 z^{k-1} - \cdots - a_{k-1} z - a_k$ is primitive.

In most applications, only two coefficients are nonzero:

$$Q(z) = z^k - a_r z^{k-r} - a_k.$$

Since we are working in $\mathcal{F}_2$, the recurrence on x_n becomes

$$x_n = (x_{n-r} + x_{n-k}) \mod 2.$$

The addition modulo 2 is equivalent to the instruction exclusive-or (xor) on the bits:

$$x_n = \begin{cases} 0 & \text{si } x_{n-r} = x_{n-k}, \\ 1 & \text{si } x_{n-r} \neq x_{n-k}. \end{cases}$$

Implementations

More generally, we construct a fast implementation by using shifts, xor's, masks,.... We can also combine them.

Most popular:

- Mersenne Twister MT19937 (Matsumoto and Nishimura); period of $2^{19937} - 1$
- xoshiro: `https://prng.di.unimi.it/`; by default, Julia uses `xoshiro256++`

But even these recent generators are not without flaws! See e.g.

- It Is High Time We Let Go Of The Mersenne Twister
- Unveiling patterns in xorshift128+ pseudorandom number generators

PCGs

- One of the main opponent of the xorshift family is Melissa O'Neil, who proposes the PCGs generators: `https://www.pcg-random.org/`.
- PCG combines a linear congruential generator and permutation functions.
- However, Vigna (the author of xorshift generators) has a lot of critisms regarding PCG: `https://pcg.di.unimi.it/pcg.php`.
- In summary, there are no strong evidence that one should favor a PCG over a MRG. According to Vigna, "there is technically no sensible reason to use a PCG generator: those without flaws are not competitive."

Counter-based generators

- In previously covered RNGs, the transition function does most of the transformation and the output function is very simple.
- Opposite for CBRNGs: the state is a counter, increased by 1, and the output function is complex.
- One popular impletation, Philox, is the default generator in TensorFlow.
- Efficient on a GPU, but their statistical properties are not well studied.
- One strength: easy to jump ahead in the state space.

Jump ahead

- A very useful possibility proposed by some implementation is the possibility to make a jump of m positions in the random number sequences, with m very large.
- This allows to easily define independant random variables.
- Useful in simulation when relying on common random random numbers.

The MRG32k3a implementation proposes functions to generate independent streams and substreams.

RDST library

`https://github.com/JLChartrand/RDST.jl`

This package proposes an implementation of MRG32k3a with streams and substreams.

Non-uniform random variables generation

A good reference: Luc Devroye, *Non-Uniform Random Variate Generation*, `http://luc.devroye.org/rnbookindex.html`.

Assume that we have a good uniform random variates generator, but we want to generate random variables following various probability laws: Normal, Weibull, Poisson, binomial,...

The desired properties are:

- correct method (or good approximation);
- as simple as possible, but as fast as possible;
- low memory consumption;
- robust;
- compatible with variance reduction technique (as quasi-Monte Carlo).

Inversion

Prefered method when applicable: compatible with variance reduction and copulae.

Consider a random variable X with cdf F. Let $U \sim U(0,1)$ and

$$X = F^{-1}(U) = \min\{x : F(x) \geq U\} \quad \text{(Generalized inverse)}.$$

Then

$$P[X \leq x] = P[F^{-1}(U) \leq x] = P[U \leq F(x)] = F(x),$$

i.e., X has the desired distribution. Indeed,

- in the continuous case, $F(X) \sim U[0,1]$;
- in the discrete case, it is easy to prove that $\forall\, i$, $P[X = x_i] = p(x_i)$, and we assume $x_1 < x_2 < \ldots < x_n$;
- The principle still works for mixte distributions.

Inversion (2)

- Advantage: monotone, only one U for all X.
- Weakness: for some laws, F is very difficult to invert. But we can often approximate F^{-1}.

Example: normal law.
If $Z \sim N(0,1)$, then $X = \sigma Z + \mu : N(\mu, \sigma^2)$.
It is therefore sufficient to be able to generate a $N(0,1)$, of density $f(x) = (2\pi)^{-1/2} e^{-x^2/2}$.
We do not have any formula for $F(x)$ or $F^{-1}(x)$. Efficient codes however exist to approximate $F^{-1}(x)$.

Chi-square, gamma, beta, etc.: it is much more complicated since the form of F^{-1} depends of the distribution parameters.

Inversion for discrete distributions

Recall that

$$p(x_i) = P[X = x_i]; \quad F(x) = \sum_{x_i \le x} p(x_i).$$

We have to generate U, search $I = \min\{i | F(x_i) \ge U\}$ and return x_I.

Various algorithms perform this search. Their efficiency depends of the distribution.

Initialization: store the x_i and $F(x_i)$ in arrays, for $i = 1, \ldots, n$.

1. Linear search (time in $O(n)$): $U \leftarrow U(0,1)$; $i \leftarrow 1$;
   while $F(x_i) < U$ do $i \leftarrow i + 1$; return x_i.
2. Binary search (time in $O(\log(n))$):
   $U \leftarrow U(0,1)$; $L \leftarrow 0$; $R \leftarrow n$;
   while $L < R - 1$
   $m \leftarrow \lfloor (L + R)/2 \rfloor$;
   if $F(x_m) < U$ then $L \leftarrow m$ otherwise $R \leftarrow m$;
   return x_R.

Other approaches: composition

Assume that F is a convex combination of several cumulative distribution functions:

$$F(x) = \sum_{j=0}^{\infty} p_j F_j(x),$$

and that it is easier to invert F_j, $j = 0, \ldots, \infty$ than F.

Generate $J = j$ with the probability p_j, than generate X following F_J.

The method therefore requires two uniforms for each random variable, and exploit the decomposition

$$P[X \leq x] = \sum_{j=1}^{\infty} P[X \leq x | J = j] P[J = j] = \sum_{j=1}^{\infty} F_j(x) p_j.$$

Convolution

Convolution. Assume that

$$X = Y_1 + Y_2 + \ldots + Y_n,$$

where the Y_i are independent, of given laws. We generate the Y_i, $i = 1, \ldots, n$, and we sum.

Examples: Erlang (sum of exponentials with same mean), binomial.

Acceptance/rejection: the most important technique after inversion.

We consider the case where X is continuous (the discrete cas is analoge). Let $f(x)$ be the density of X, and let t be a "hat" function that majors f, i.e. $f(x) \leq t(x)\ \forall\, x$.

Acceptance/rejection

We can normalize t in a density r:

$$r(x) = t(x)/a, \text{ where } a = \int_{-\infty}^{\infty} t(s)ds.$$

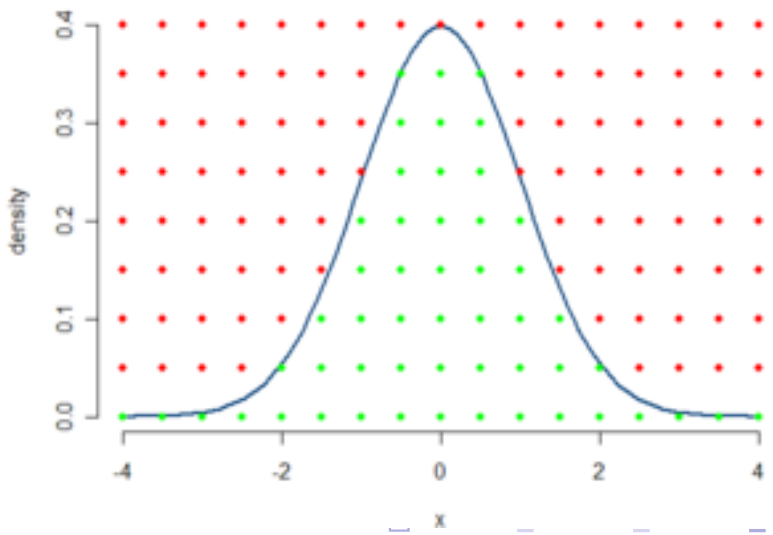
We choose t so that

1. it is easy to generate random variables of density r;
2. a is small (close 1), or in other terms, $t(x)$ is close to $f(x)$.

The choice of t may be automatized.

Algorithm: Repeat

1. generate Y of density $r(x)$;
2. generate $U : U(0,1)$ independantly of Y;
3. until $U \leq f(Y)/t(Y)$;
4. return Y.



Particular cases

Sometimes, we can benefit of mathematical transformations. The main weakness is that they are seldom compatible with variance reduction techniques.

Example: Box-Muller method for the normal law.

Idea: it is easier to generate a point (X, Y) from the bivariate normal law, of density on $\mathbb{R}^2$

$$f(x, y) = \frac{1}{2\pi} e^{-(x^2+y^2)/2}.$$

We change the cartesian coordinates (X, Y) by the polar coordinates (R, Θ):

$$R^2 = X^2 + Y^2; Y = R \sin \Theta.$$

It gives an elegant approach, but incompatible with variance reduction techniques and can be slower than inversion.

Box-Muller Algorithm

1. Independently draw U_1, U_2 from a $U(0,1)$ distribution.
2. Set

$$R = \sqrt{-2\log(U_1)}$$
$$\theta = 2\pi U_2$$

3. Set

$$X = R\cos(\theta)$$
$$Y = R\sin(\theta)$$

Multivariate distributions

What if we want to draw from $\boldsymbol{X} : \Omega \to \mathcal{X} \subseteq \mathbb{R}^d$?
General approach:

- Generate the marginals
- Combine the marginals as desired.

Multivariate distributions: simple cases

- Ideally, we can explicitly transform the marginals.
- Example: multivariate normal $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$, with

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_d \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,d} \\ \sigma_{1,2} & \sigma_2^2 & \cdots & \sigma_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1,d} & \sigma_{2,d} & \cdots & \sigma_d^2 \end{pmatrix}$$

Then,

$$\boldsymbol{X} = \boldsymbol{\mu} + L\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

with $\Sigma = LL^T$, and L is the Cholesky factor.
Drawing from $\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$: generate d $\mathcal{N}(0, 1)$ independently.

Multivariate distributions: copulae

A d-variate copula $C : [0,1]^d \to [0,1]$is the cdf of a random vector $(U_1, \ldots, U_d)$ with $U(0,1)$ margins:

$$C(u) = P[U_1 \leq u_1, \ldots, U_d \leq u_d]$$

where

$$P[U_j \leq u_j] = u_j$$

for $j = 1, \ldots, d$, and $0 \leq u_j \leq 1$.

Sklar's theorem

Theorem (Sklar's theorem (1959))

- *Let H be a multivariate distribution function with margins $F_1, \ldots, F_d$. There exists a copula C such that*

$$H(x_1, \ldots, x_d) = C\left(F_1(x_1), \ldots, F_d(x_d)\right), \quad x_1, \ldots, x_d \in \overline{\mathbb{R}}.$$

  If F_i, $i = 1, \ldots, d$, are continuous then C is unique. Otherwise C is uniquely determined on the Cartesian product of the range of the marginals $F_1\left(\overline{\mathbb{R}}\right) \times \ldots \times F_d\left(\overline{\mathbb{R}}\right)$.

- *Conversely, if C is a copula and $F_1, \ldots, F_d$ are univariate distribution functions, then the function H defined above is a multivariate distribution function with margins $F_1, \ldots, F_d$.*

Copula

If we know the joint CDF F and the marginals $F_1, \ldots, F_d$, we can find the copula via

$$C(u_1, \ldots, u_d) = F\left(F_1^{-1}(u_1), \ldots, F_d^{-1}(u_d)\right),$$

where $F_j^{-1}(\cdot)$ is the generalized inverse for margin j:

$$F_j^{-1}(u) = \min\{x : F_j(x) \geq u\}.$$

Fréchet–Hoeffding bounds

Any bivariate copula C verifies

$$\max(F_X(x) + F_Y(y) - 1, 0) \leq C(x, y) \leq \min(F_X(x), F_Y(y))$$

Upper bound proof

$$\begin{aligned} C(x, y) &= P[X \leq x \cap Y \leq y] \\ &\leq P[X \leq x]P[Y \leq y] \\ &\leq \min(F_X(x), F_Y(y)) \end{aligned}$$

Fréchet–Hoeffding bounds

Lower bound proof

$$\begin{aligned} 1 - C(x, y) &= P[X > x \cup Y > y] \\ &\leq P[X > x] + P[Y > y] \\ &= 1 - F_X(x) + 1 - F_Y(y) \end{aligned}$$

Thus,

$$C(x, y) \geq F_X(x) + F_Y(y) - 1.$$

Note: this can be viewed as a particular of the Bonferroni inequality

$$P\left[\cap_{i=1}^{d} A_i\right] \geq 1 - d + \sum_{i=1}^{d} P[A_i].$$

Gaussian copula

$$C\left(F_1(x_1), \ldots, F_d(x_d)\right) = \Phi_\Sigma\left(\phi^{-1}\left(F_1(x_1)\right), \ldots, \phi^{-1}\left(F_d(x_d)\right)\right),$$

where

- ϕ is the cdf of a $\mathcal{N}(0,1)$,
- Φ_Σ is the cdf of a d-dimensional $\mathcal{N}(\mathbf{0}, \Sigma)$.

Copulae estimation

- Parametric estimation;
- Non-parametric estimation;
- Machine-learning models (see Jutras et al.: `https://arxiv.org/abs/2302.09193v3`).