Exact "combinatorial" simulation of continuous random variables

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- Exact simulation algorithms are known for many distributions, usually assuming exact computations over the reals
- The reference : Devroye (1986)



Basic simulation tricks

► Distribution function inversion : if U is uniform and F(x) is the (continuous, strictly increasing) distribution function (F(x) = P(X ≤ x)) for some distribution, X = F⁻¹(U) has repartition function F

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- ▶ **Distribution function inversion :** if *U* is uniform and F(x) is the (continuous, strictly increasing) distribution function $(F(x) = \mathbb{P}(X \le x))$ for some distribution, $X = F^{-1}(U)$ has repartition function *F*
- **Rejection :** if g is the density of some distribution (that one knows how to simulate), f is some other density with $f(x) \le c.g(x)$ for some c and all x, the following rejection algorithm loops, on average, 1/c times, and simulates density f :
 - draw X (g-distributed)
 - with probability f(X)/(c.g(X)), output X; otherwise, restart

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 - draw X (g-distributed)
 - with probability f(X)/(c.g(X)), output X; otherwise, restart
- ▶ Rejection can be used when densities are only proportional to functions f and g with, say, f ≤ g, without identifying/computing the multiplicative constant

Typical basic examples

► If U is uniform over [0, 1], -ln(1 - U) is exponentially distributed (distribution function inversion)

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- (Kahn 1954; rejection) For the (absolute value of) a normal variable :

- draw E and X, independent exponentials
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(conditioned on X, the acceptance probability is $\exp(-(X-1)^2/2) = \exp(-x^2/2)/\exp(-x))$

- All the previous techniques require
 - 1. a generator of independent, uniform variables on [0,1]
 - 2. exact evaluation of transcendental functions and constants, integrals, etc.

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- For many *discrete* distributions, the *Buffon machines* of [Flajolet, Pelletier, Soria 2011] allow to only use
 - flip() (Bernoulli with parameter 1/2; "coin flips")
 - ▶ Bern[p]() (Bernoulli with parameter p, for unknown parameters p ∈ (0, 1))
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- All the previous techniques require
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 - basic integer arithmetic and bookkeeping (small counters)
- Can we do the same for a variety of continuous distributions? In a more or less systematic way?

Precursor : von Neumann's algorithm

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- describes an exact algorithm for the exponential distribution, using only
 - independent uniforms on [0, 1]
 - comparisons of reals
 - (small) integer counters

The algorithm

- 1. Initialize counter K to 0
- 2. Draw a sequence $X_1, X_2, ..., X_n$ of independent uniforms on [0, 1], until the **first ascent** $(X_n > X_{n-1})$
- 3. If n is odd : failure; increment failure counter K, and go to 2.

4. (Otherwise) *n* is even : success, return $K + X_1$

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Proposition (von Neumann) : This algorithm terminates with probability 1, and its output follows the exponential distribution (density $f(x) = \exp(-x)\mathbf{1}_{x>0}$). The expected number of uniforms used is $\frac{e+e^2}{e-1} \simeq 5.88$.

▶ Uniform sequence : 0.78, 0.04, 0.92, 0.01, 0.83, 0.22...

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- Second attempt : 0.01 < 0.83 : even length, stop
- The output value is 1 + 0.01 = 1.01

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- Summing again : the probability of "success" with X₁ ≤ x, is 1 − e^{-x} (the distribution function for an exponential on [0, 1])
- For the algorithm : the final value of K follows the geometric distribution with parameter 1 − e⁻¹, and the (independent) value of X₁ conditioned on success is distributed as an exponential, conditioned on being ≤ 1; the sum is exponentially distributed.

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- If we allow arbitrary products, then Kahn's method (and von Neumann's algorithm for the exponential) shows that the normal distribution admits such a restricted simulation algorithm.
- [Karney, 2013] describes such a product-less algorithm.

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- This is essentially the interpretation of [Forsythe, 1972]; but the described method involves computing integrals based on solving the equation (to tabulate the probability that the target random variable takes values in a collection of disjoint intervals)
- Today : description of an exact simulation method that is slightly more involved, but does not require the evaluation of any integrals or transcendental functions not in g.

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- Suppose our target distribution (over the positive reals) has a density *f*, satisfying differential equation y'(t) = −g(t).y(t) for some given function g (at most one solution is a probability density)
- Assume g satisfies some "quadrant" condition : there should exist some a ≥ 0 with m = g(a) > 0, such that

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- ▶ **Then** we provide an exact simulation algorithm, using only uniform reals, additions, division by *m*, comparisons, and evaluations of *g* and *h*

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- ▶ **Then** we provide an exact simulation algorithm, using only uniform reals, additions, division by *m*, comparisons, and evaluations of *g* and *h*
- (Notice that the conditions reduce to g as a black box if g is known to be nondecreasing)

The "quadrant condition"



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► The differential equation has solutions
f(t) = f(t₀)e^{-∫_{t₀}^tg(u)du}; initial condition f(t₀) would be determined by condition ∫₀[∞] f(t)dt = 1 (but we will be proceeding by rejection and thus need not compute them)

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 proceeding by rejection and thus need not compute them)
 Taking *t*₀ = *a* for the initial condition, the "quadrant"
 condition implies that the density is upper bounded by the
 solution to *y*'(*t*) = −*m*.*y*(*t*) with the same initial condition :

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for all $t \ge 0$,

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Taking t₀ = a for the initial condition, the "quadrant" condition implies that the density is upper bounded by the solution to y'(t) = −m.y(t) with the same initial condition : for all t ≥ 0,

$$f(t) \leq f(a)e^{-m(t-a)}$$

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We could try a rejection scheme : simulate an exponential E (using the von Neumann algorithm) and set X = E/m, then return X with appropriate probability, or restart.

- ▶ The differential equation has solutions $f(t) = f(t_0)e^{-\int_{t_0}^t g(u)du}$; initial condition $f(t_0)$ would be determined by condition $\int_0^\infty f(t)dt = 1$ (but we will be proceeding by rejection and thus need not compute them)
- Taking t₀ = a for the initial condition, the "quadrant" condition implies that the density is upper bounded by the solution to y'(t) = −m.y(t) with the same initial condition : for all t ≥ 0,

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- We could try a rejection scheme : simulate an exponential E (using the von Neumann algorithm) and set X = E/m, then return X with appropriate probability, or restart.
- Only, the acceptance probability is not something we are allowed to compute :

$$\exp\left(-\int_{a}^{X}g(t)dt+m(X-a)\right)=\exp\left(-\int_{a}^{X}(g(t)-m)dt\right)$$

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► Hypothesis : we can draw uniforms, and have access to a Bernoulli generator with parameter p, for some unknown 0 and 0 with probability 1 − p on each call, with calls being independent)

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- ► Hypothesis : we can draw uniforms, and have access to a Bernoulli generator with parameter p, for some unknown 0 and 0 with probability 1 − p on each call, with calls being independent)
- ► Then we have a von Neumann-like algorithm for a Bernoulli with parameter e^{-p}

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- Draw a sequence of independent **pairs** (X_i, B_i) with X_i uniform on [0, 1], and B_i an independent Bernoulli with parameter p
- Stop at the first n such that B_n = 0 or X_{n−1} < X_n (Bernoulli fails, or ascent in the X sequence)

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(proof along the same line as for von Neumann's algorithm, with powers of p addded, hence the e^{-p} instead of e^{-1})

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- Under suitable conditions, an integral can be interpreted as a probability for an easy-to-simulate event (that a random point falls into some domain)
- If needed, the integral can be written as a sum of integrals on smaller intervals (and the exponential becomes a product of exponentials; the Bernoulli variable becomes a product of Bernoulli variables).

Assume X > a; the case X < a is treated analogously)

▶ We need to split the interval [a, X] into a number of smaller intervals A₁,..., A_K; A_i = [a_{i-1}, a_i].

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▶ Set *a*⁰ = 0.

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- ▶ Set a₀ = 0.
- Assume a_i is known : compute M = h(a_i, 1 + a_i). If M ≤ 1, then set a_{i+1} = 1 + a_i, and repeat.

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- ▶ If M > 1, then let M' denote the smallest power of 2 larger than M, and, for each $1 \le k \le M'$, set $a_{i+k} = a_i + k/M'$ (M' intervals of length 1/M'), and repeat

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• Stop at the first K such that $a_k \ge X$; instead set $a_K = X$

Now the wanted integral is

$$\int_{a}^{X} (g(t) - m) dt = \sum_{i=0}^{K} \int_{A_i} (g(t) - m) dt = \sum_i P_i$$

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- ▶ and in turn, obtain the wanted Bernoulli with parameter $\exp(-\sum_i P_i)$, by taking the product (conjunction) of each individual Bernoulli for each smaller interval : this completes the algorithm.

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• Differential equation : y'(t) = -t.y(t), g(t) = t.

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- (In practice, large values of X are very likely to be rejected; the rejection part should be run after each increment of the K counter for the exponential after K = 1, so as to allow early rejection)
The previous algorithms are very suitable to an adaptation to bit-by-bit computations

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- von Neumann's algorithm was analysed by [Flajolet, Saheb, 1986]; uses on average k + 5.72.. bits to output k bits of the exponential random variable
- In our general differential equation algorithm, we need a bit more than just a black box function g (unless g is known to be increasing)

We obtain exact, "von-Neumann-Buffon-like" algorithms for the simulation of a (not too well-defined) class of distributions that includes the normal distribution

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- In the general case, this is very close to what Devroye described as "the von Neumann-Forsythe method"
- No analysis of the expected (bit) complexity yet (will depend on the quality of upper bound h in the general method)
- The method is unlikely to be competitive with numerical methods (possibly paired with certified floating point calculations), unless one needs very high precision on their random variables

Thank you for your attention

・ロト・日本・ヨト・ヨー うへの