Simulations / Monte Carlo methods

Q: What is the probability of winning Solitaire?

$$p = \frac{\#\text{ permutations where player wins}}{52!} \quad ?$$

It is virtually impossible to solve this with "pure mathematics."

A: But we can use computer-assisted simulations to estimate p.

$$X_i = \begin{cases} 1 & \text{if } i\text{th simulation results in a win} \\ 0 & \text{otherwise} \end{cases}$$

$E(X_i) = p$ ← want to estimate

By LLN, we know that, for very large $n \in \mathbb{N}$,

$$\overline{X}_n = \frac{X_1 + \cdots + X_n}{n} \approx p.$$

Essential input: Randomness generator.

"Pseudo-random" number generator ← routine in your computer to produce a sequence of numbers that is almost indistinguishable from a truly random sequence.

$X_0 = \text{seed}.$

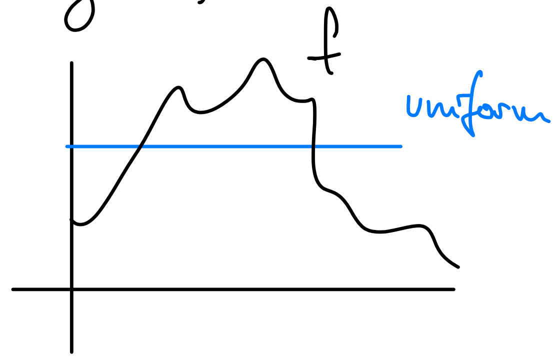
$X_{n+1} = (a X_n + c) \bmod m \qquad a, c, m \in \mathbb{Z}.$

$X_0, X_1, X_2, X_3, \ldots$

This can be used to produce a simulation of $U \sim \text{Uniform}([0,1])$

$$\frac{X_1}{m}, \frac{X_2}{m}, \frac{X_3}{m}, \dots \quad \in [0,1] \cap \mathbb{Q}$$

<u>Q</u>: Given a p.d.f. $f(x)$, how to simulate a random variable X with such p.d.f. (using U)?



<u>Prop</u>: Let $F(x) = \int_{-\infty}^{x} f(t)\,dt$ be the corresponding prescribed c.d.f., set $X = F^{-1}(U)$, where $U \sim \text{Uniform}([0,1])$. Then the pdf of X is $f(x)$.

F is increasing

<u>Pf</u>: $F_X(x) = P(X \leq x) = P(F^{-1}(U) \leq x) \overset{}{=} P(F(F^{-1}(U)) \leq F(x))$

$$= P(U \leq F(x)) = F(x).$$

$U \sim$ Uniform

Therefore, differentiating in x, we have $f_X(x) = f(x)$. $\square$

<u>Example</u>: Simulate an exponential random variable with $\lambda = 1$.

$$f(x) = \begin{cases} e^{-x} & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \longleftarrow \text{prescribed p.d.f.}$$

<u>input</u>: $U \sim \text{Unif}([0,1])$

$$F(x) = \int_{-\infty}^{x} f(t)\,dt = \int_0^x e^{-t}\,dt = \left(-e^{-t}\right)\Big|_0^x = -e^{-x} + 1$$

$$= 1 - e^{-x}$$ ← prescribed c.d.f.

$F^{-1}(y) = x$ where $y = F(x) = 1 - e^{-x}$. Solving for x:

$$y - 1 = -e^{-x} \Rightarrow 1 - y = e^{-x} \Rightarrow \log(1-y) = -x$$

$$\Rightarrow x = -\log(1-y) = \log\frac{1}{1-y}$$

$$\boxed{F^{-1}(y) = \log\frac{1}{1-y}}$$

$X = F^{-1}(U) = \log\dfrac{1}{1-U}$ has the desired p.d.f. $f(x)$.

<u>Q</u>: What if I can't solve for $F^{-1}(y)$?

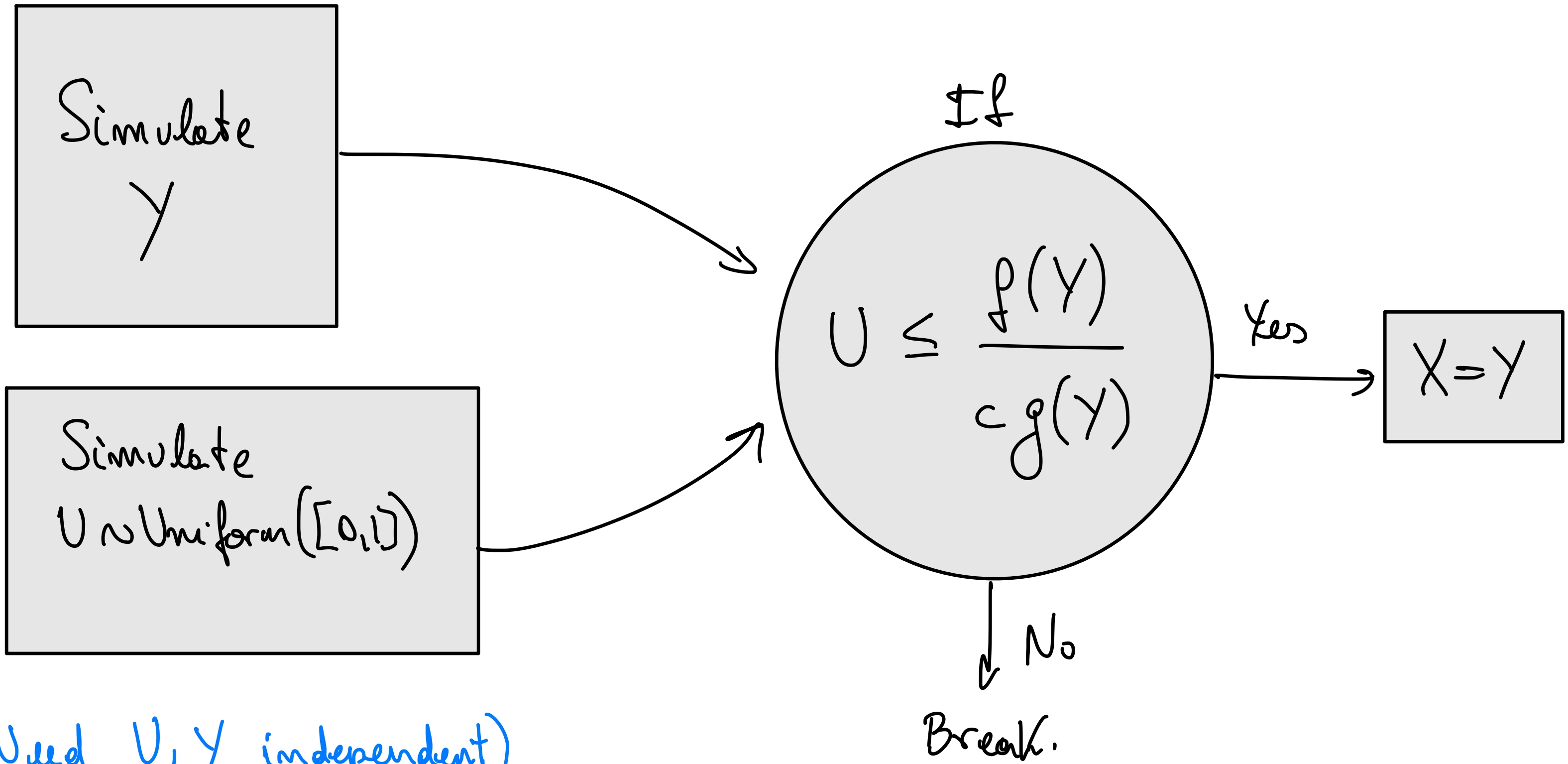
<u>A</u>: Use Rejection Method:

<u>Want</u>: Simulate X with p.d.f $f(x)$

<u>Have</u>: Simulation of Y with p.d.f $g(x)$; and $c \in \mathbb{R}$ such that

$$\frac{f(y)}{g(y)} \leq c \qquad \text{for all } y.$$

Then, proceed as follows:



(Need U, Y independent)

<u>Prop</u>: The random variable X generated as above has p.d.f $f(x)$.

<u>Pf</u>.

N iterations needed for X to be simulated.

$$P(X \le x) = P(Y_N \le x)$$

$$= P\left(Y \le x \,\middle|\, U \le \frac{f(Y)}{c\,g(Y)}\right)$$

$$= \frac{P\left(Y \le x,\ U \le f(Y)/c\,g(Y)\right)}{P\left(U \le f(Y)/c\,g(Y)\right) = K}$$

$$= \frac{1}{K} P\left(Y \le x,\ U \le f(Y)/c\,g(Y)\right).$$

By independence, the above is computed as an integral of the joint p.d.f. for Y and U:

$$f(y,u) = g(y) \qquad \forall\ 0 < u < 1.$$

$$P\left(Y \le x,\ U \le f(Y)/cg(Y)\right) = \iint_{\substack{y \le x \\ 0 \le u \le \frac{f(y)}{cg(y)}}} g(y)\, du\, dy$$

$$= \int_{-\infty}^{x} \left(\int_{0}^{\frac{f(y)}{cg(y)}} 1 \cdot du \right) g(y)\, dy$$

$$= \int_{-\infty}^{x} \frac{f(y)}{c\cancel{g(y)}} \cdot \cancel{g(y)}\, dy = \frac{1}{c} \int_{-\infty}^{x} f(y)\, dy.$$

Thus,

$$P(X \le x) = \frac{1}{cK} \int_{-\infty}^{x} f(y)\, dy.$$

Let $x \to \infty$:

$$1 = P(X \le +\infty) = \frac{1}{cK} \underbrace{\int_{-\infty}^{+\infty} f(y)\, dy}_{1} = \frac{1}{cK}$$

Thus $cK = 1$, so $P(X \le x) = \int_{-\infty}^{x} f(t)\,dt$.

Differentiating in x, we see that $f(x)$ is the p.d.f. of X.

$\square$

<u>Example</u>: Building on what we simulated before:

$U \sim \text{Uniform}([0,1])$

$Y \sim \text{Exponential}(1)$

let us simulate $Z \sim \text{Normal}(0,1)$.

Since Z is symmetric around the origin, it suffices to simulate its absolute value $X = |Z|$, which has p.d.f.

$$f_X(x) = 2 \cdot f_Z(x)\Big|_{(0,+\infty)} = \frac{2}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}.$$

p.d.f. we want to simulate.

Using Rejection Method:

$$g(y) = e^{-y}$$

p.d.f. of $Y \sim Exp(1)$

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

$$= \sqrt{\frac{2}{\pi}}\, e^{-\frac{(x-1)^2}{2}} \cdot e^{\frac{1}{2}} = \sqrt{\frac{2e}{\pi}}\, e^{-\frac{(x-1)^2}{2}} \le \sqrt{\frac{2e}{\pi}}$$

$$c = \sqrt{\frac{2e}{\pi}} \quad \text{so} \quad \frac{f(x)}{c\,g(x)} = e^{-\frac{(x-1)^2}{2}}$$