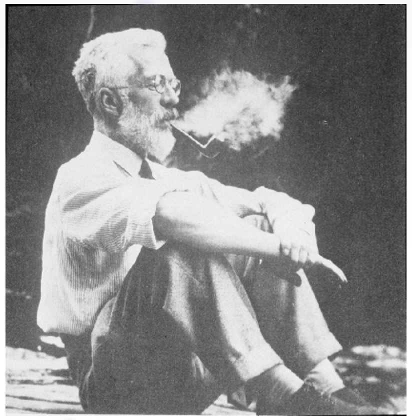
Applied Statistics

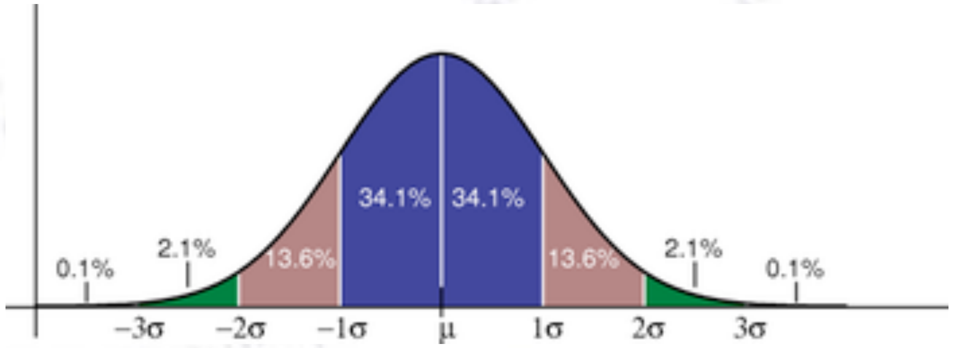
Monte Carlo Simulations







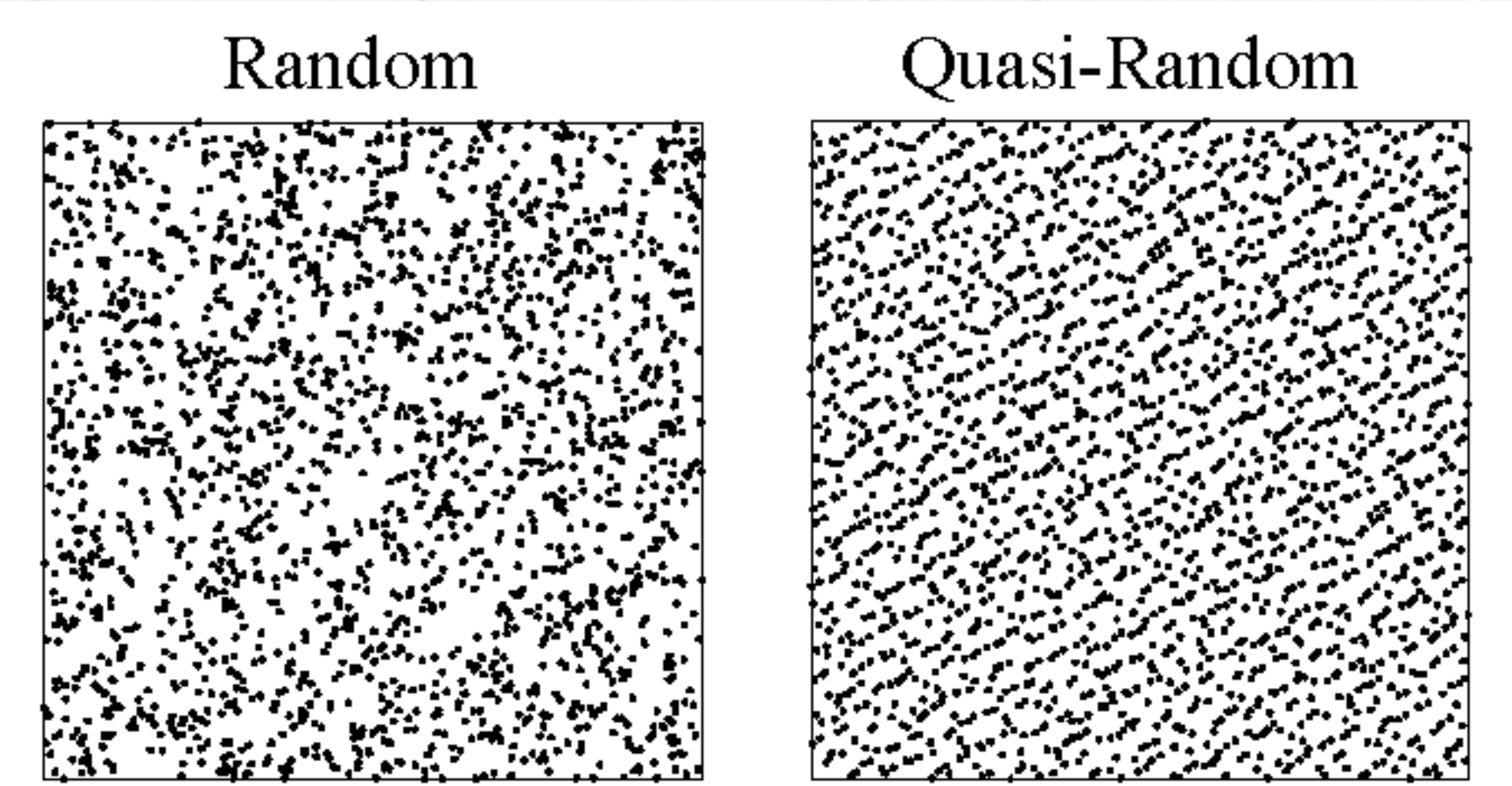

Troels C. Petersen (NBI)



"Statistics is merely a quantisation of common sense"

Random numbers

"Any one who considers arithmetical methods of producing random digits is, of course, in a state of sin." [John Von Neumann]

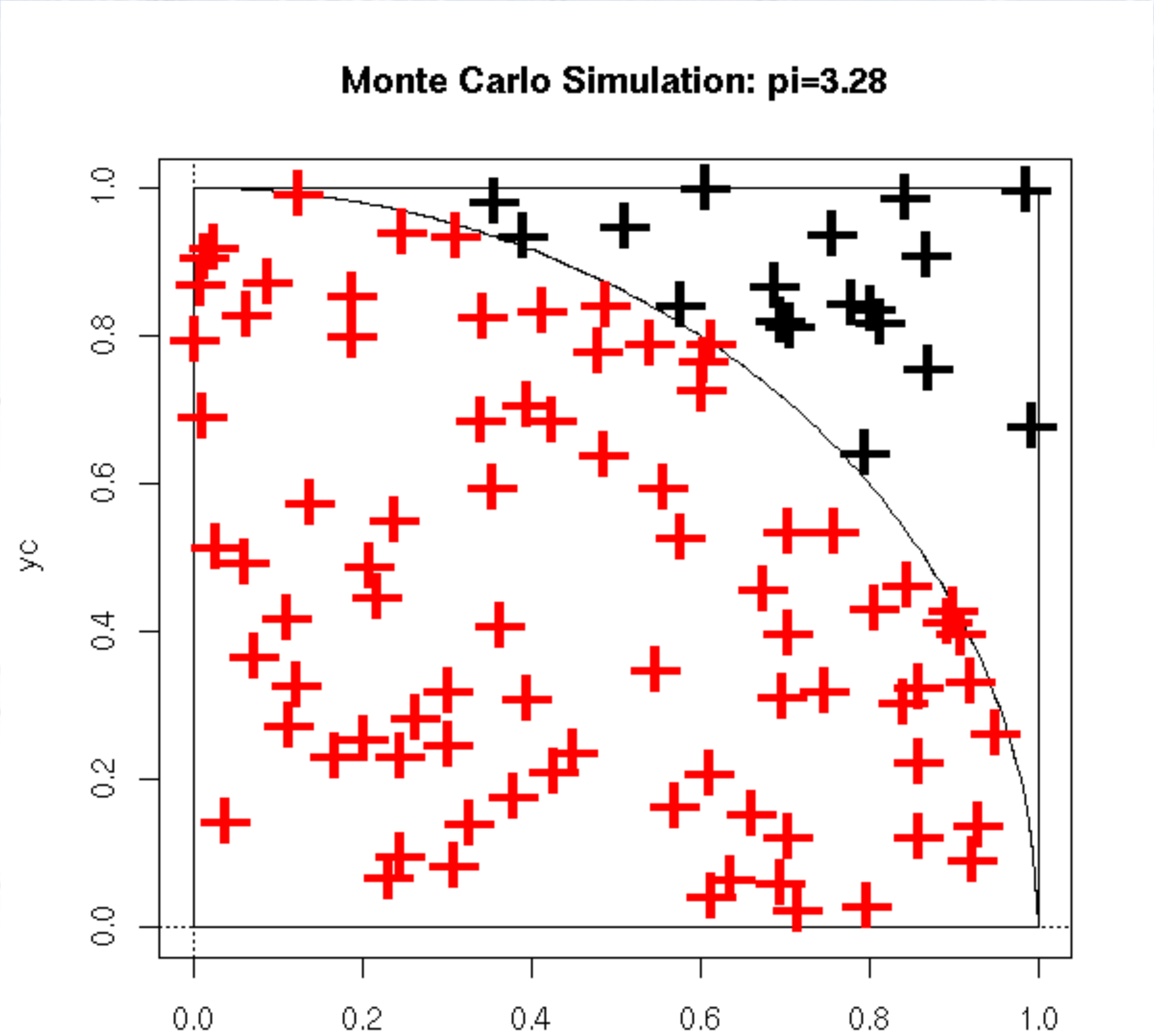


The Monte Carlo method?

No text book definition, but here is an attempt:

"Using random numbers
(hence reference to the Monte Carlo casino)
to solve problems,
typically without known
(analytic) solutions and/or
of high dimensionality"

Calculating Pi



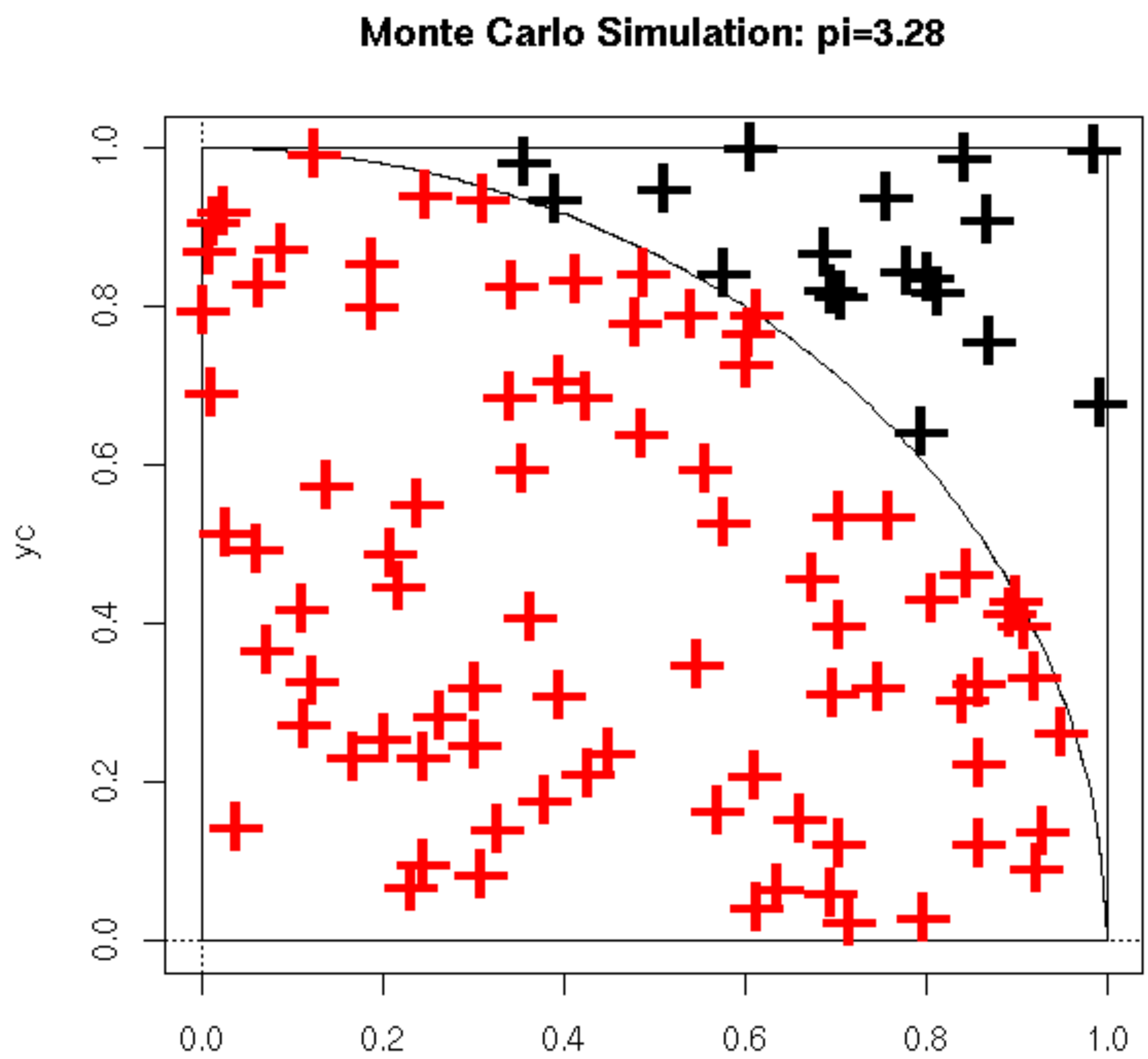
Calculating Pi

Many problems and calculations can be done using random numbers.

In this example, it is the estimate of pi, which is the target.

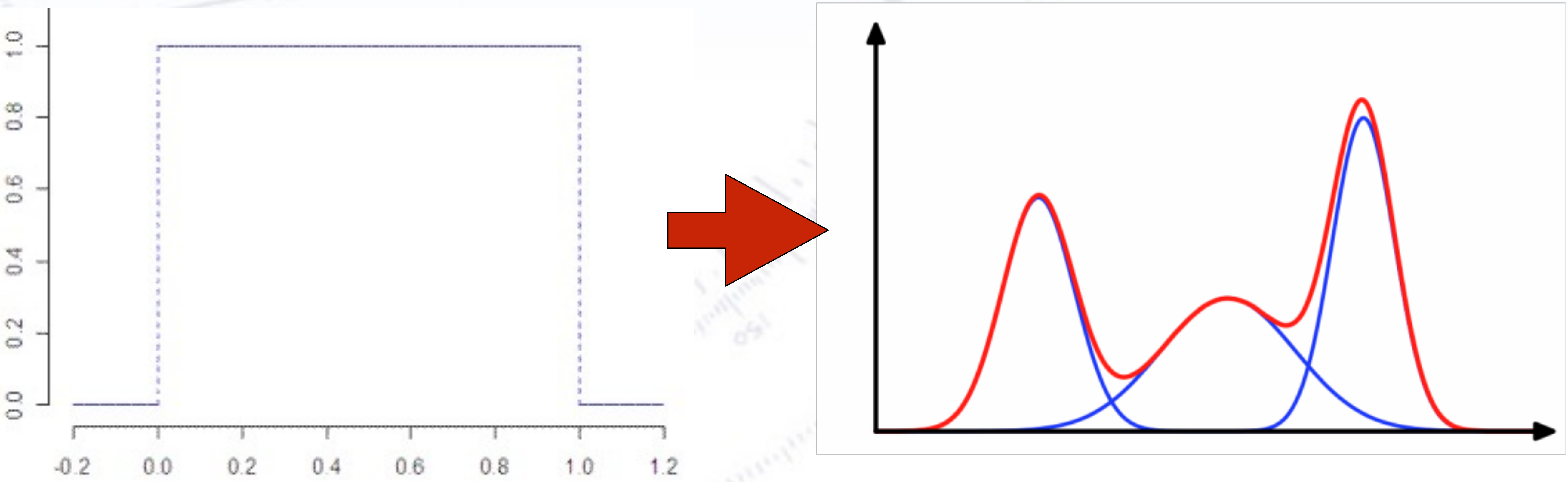
<u>Recipe</u>:

- Find min and max in both x and y.
- Generate uniform random numbers (x,y) in these ranges.
- Accept x, if y < f(x).
- Reject x, if y > f(x).



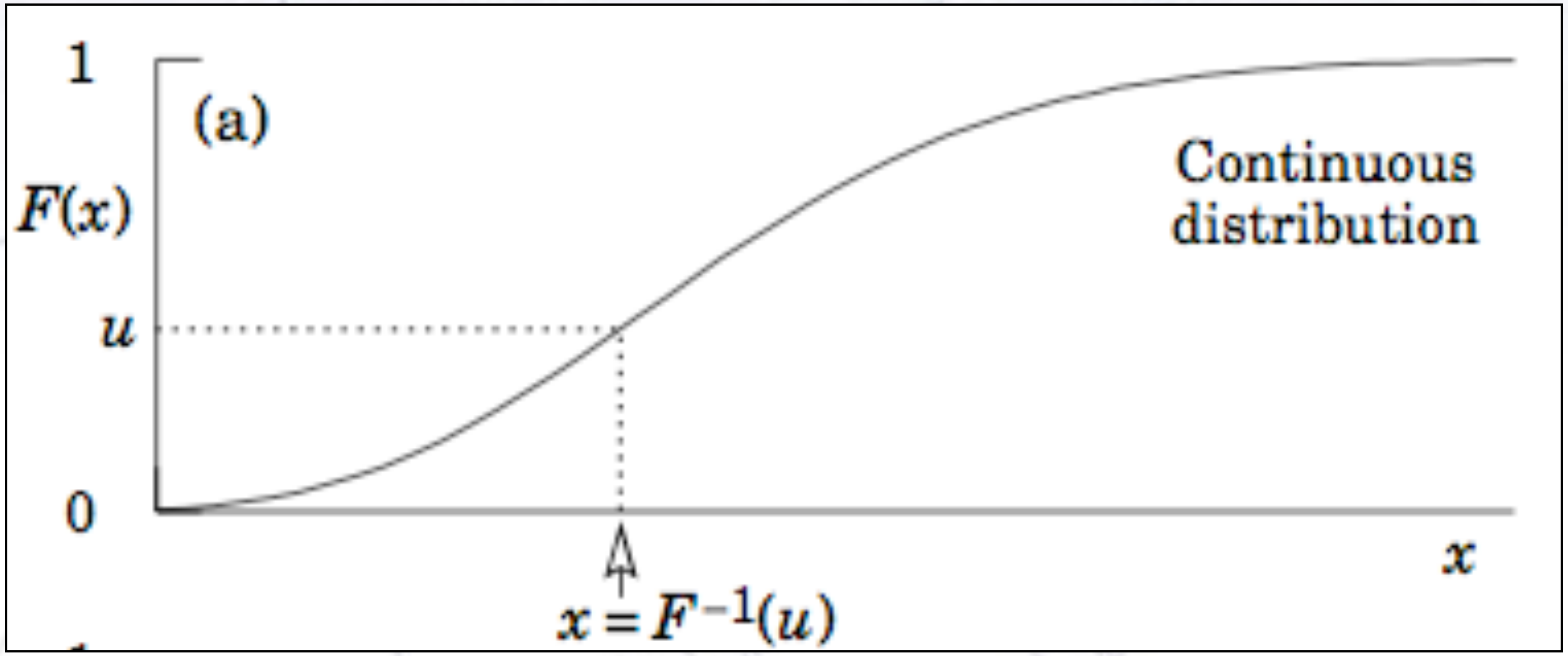
Challenge

How to produce random numbers according to an arbitrary PDF from uniform numbers?



Transformation method

We have uniformly distributed random numbers r.
We want random numbers x according to some distribution.
Can we find a function x(r), such that r (uniformly distributed numbers) will be transformed into the desired distribution f(x)? Well, maybe…



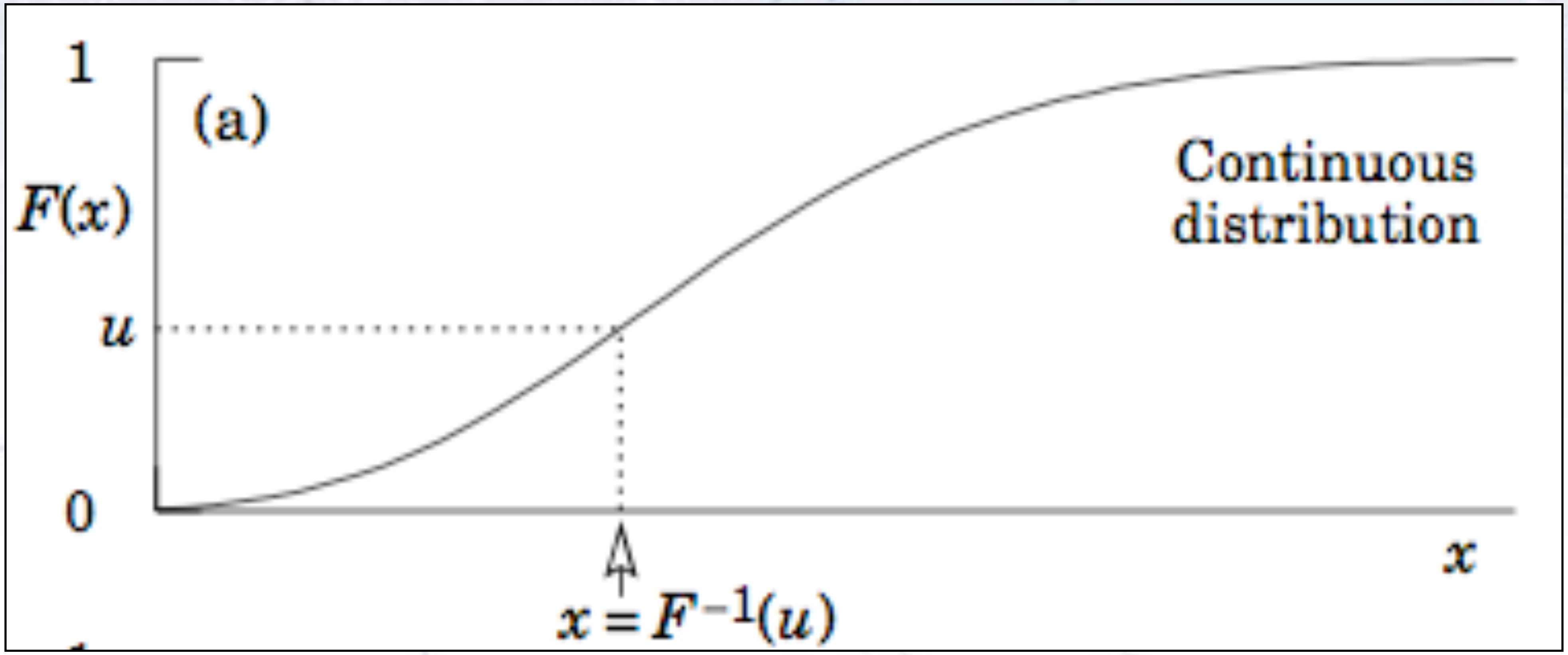
It turns out, that this is only possible, if one can (in this order):

- Integrate f(x), and then…
- Invert F(x)

As this is rare, this method can not often be used by itself. However, in combination with the Hit-and-Miss method, it can pretty much solve all problems.

Transformation method

So the “recipe” can be summarised as follows:



Steps:

- Ensure that the PDF is normalised!
- Integrate f(x) to get F(x) with the definite integral:
- Invert F(x)

$$F(x) = \int_{-\infty}^{x} f(x')dx'$$

Now you can generate random numbers, x, according to f(x), by choosing $x = F^{-1}(u)$, where u is a random uniform number.

Transformation method: Example

Consider an exponential distribution: $f(x) = \lambda \exp(-\lambda x), \quad x \in [0,\infty]$

Is it normalised? Yes…

Can we integrate f(x) to find F(x)? Yes…
$F(x) = 1 - \exp(-\lambda x), \quad x \in [0,\infty]$

Can we invert F(x) to find $F^{-1}(x)$? Yes…
$F^{-1}(p) = -\log(1-p) \,/\, \lambda, \quad p \in [0,1]$

This is a classic example of how to use the transformation method.
Note that the exponential distribution is not bounded upwards in x.

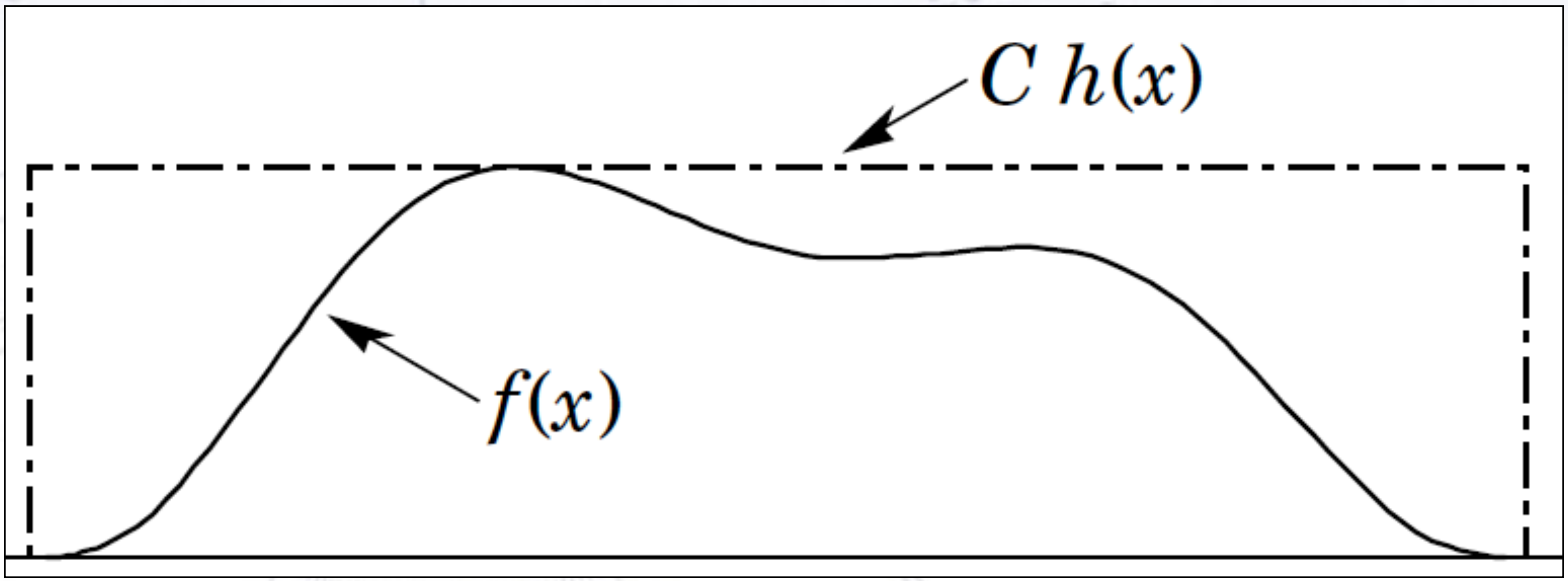
This formula was actually used in the very first exercise (central limit theorem), where some of you noticed it.

Accept-Reject method

(Von Neumann method)

If the PDF we wish to sample from is bounded both in x and y, then we can use the "Accept-Reject" method to select random numbers from it, as follows:

- Pick x and y uniformly without in the range of the PDF.
- If y is below PDF(x), then accept x.



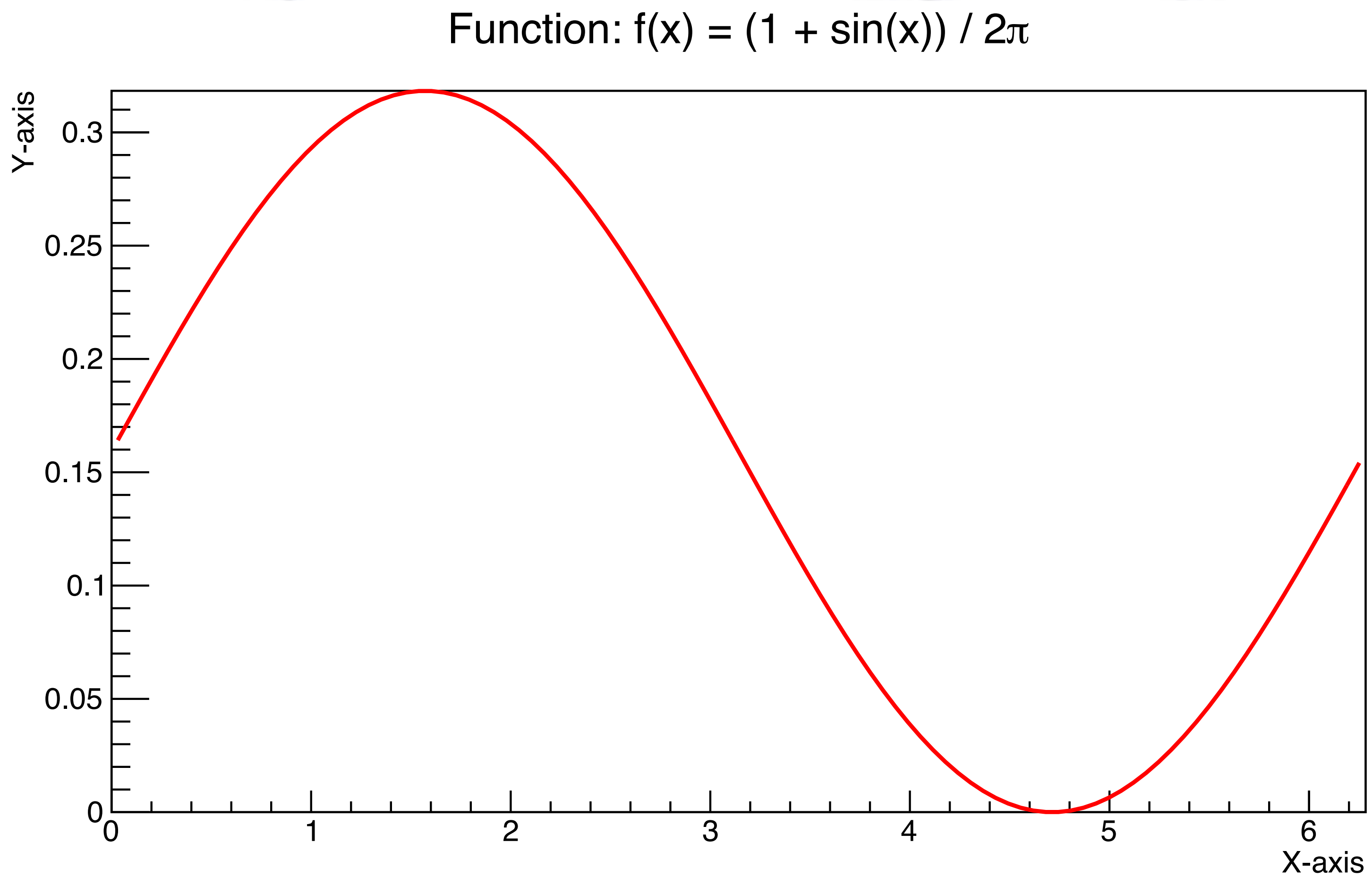
The main advantage of this method is its **simplicity**, without requiring invertible integral. Given modern computers, one does not care much about efficiency. However, it requires **boundaries**!

Accept-Reject method: Example

(Von Neumann method)

Consider an exponential distribution: $f(x) = (1 + \sin(x))/2\pi, \quad x \in [0,2\pi]$
Can we integrate f(x) to find F(x)? Yes… $F(x) = (x - \cos(x))/2\pi, \quad x \in [0,2\pi]$
Can we invert F(x) to find $F^{-1}(x)$? **No!!! So transformation method doesn't work!**

However, the function is bounded in both x and y, and so by generating pairs of random uniform numbers (u,v) in the corresponding x- and y-range, we can get random numbers according to f(x), if we accept those for which $v < f(u)$.



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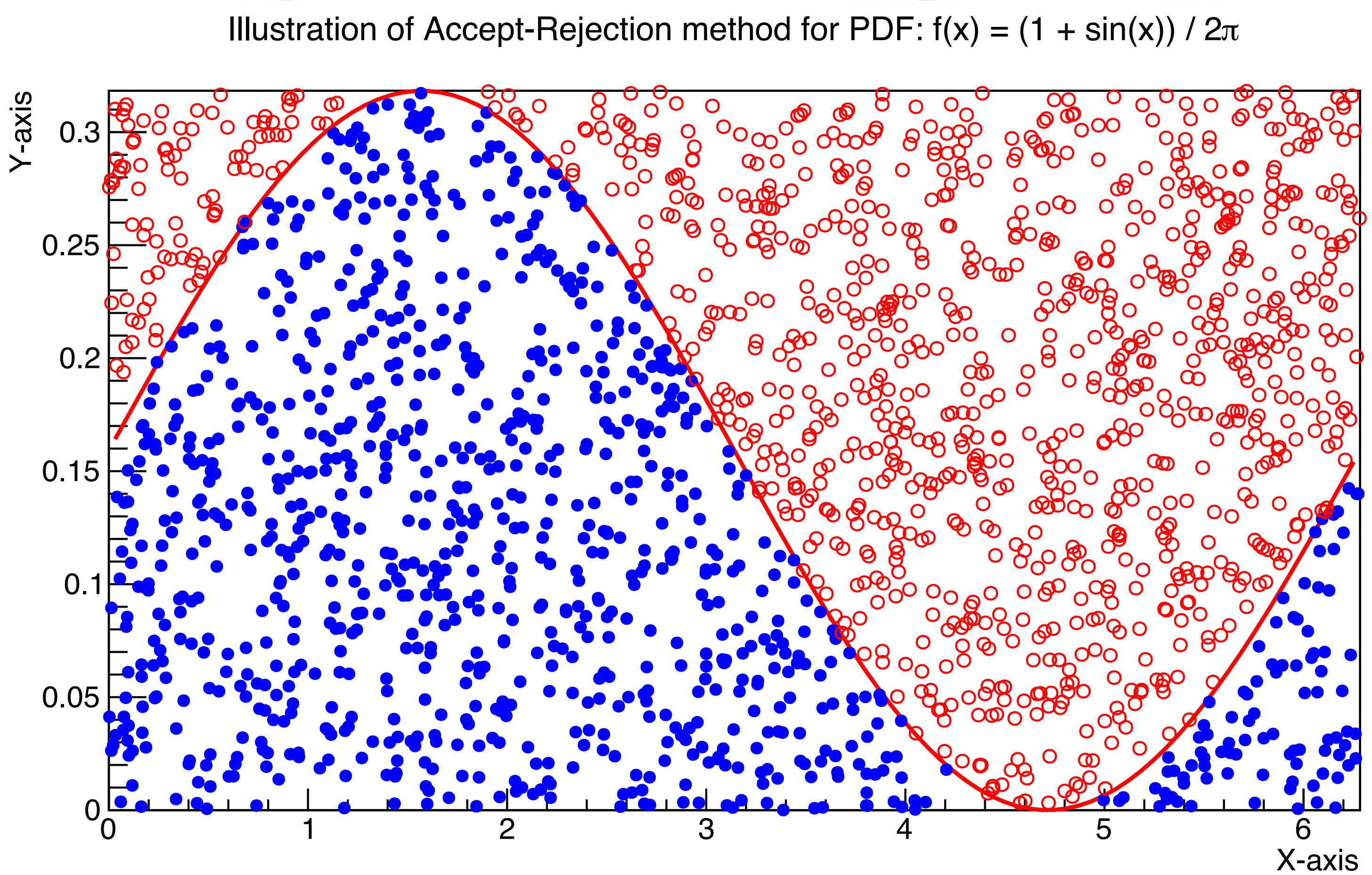

Dimensionality of problems

For simple "low dimensionality" problems, (possibly) numerical integrals are the fastest solution.

However, with increasing complexity, the Monte Carlo method "wins":

- Monte Carlo method: $$\frac{1}{\sqrt{N}}$$
- Numerical (e.g. trapezoidal rule): $$\frac{1}{N^{2/d}}$$

The Monte Carlo method is also easier to get uncertainties from, and usually quicker to implement.

Monte Carlo is simply a great tool for testing/giving insight/integrating into almost all experimental situations. Use it!

History of the Monte Carlo

The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. **The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully?** After spending a lot of time trying to estimate them by pure **combinatorial calculations**, I wondered whether a **more practical method** than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers […]. Later [in 1946], I described the idea to John von Neumann, and we began to plan actual calculations.

[Stanisław Ulam, co-inventer of the hydrogen bomb]

"Stanisław Ulam is probably best known for realising that electronic computers made it practical to apply statistical methods to functions without known solutions, and as computers have developed, the Monte Carlo method has become a ubiquitous and standard approach to many problems." [Wikipedia on Stanislaw Ulam]