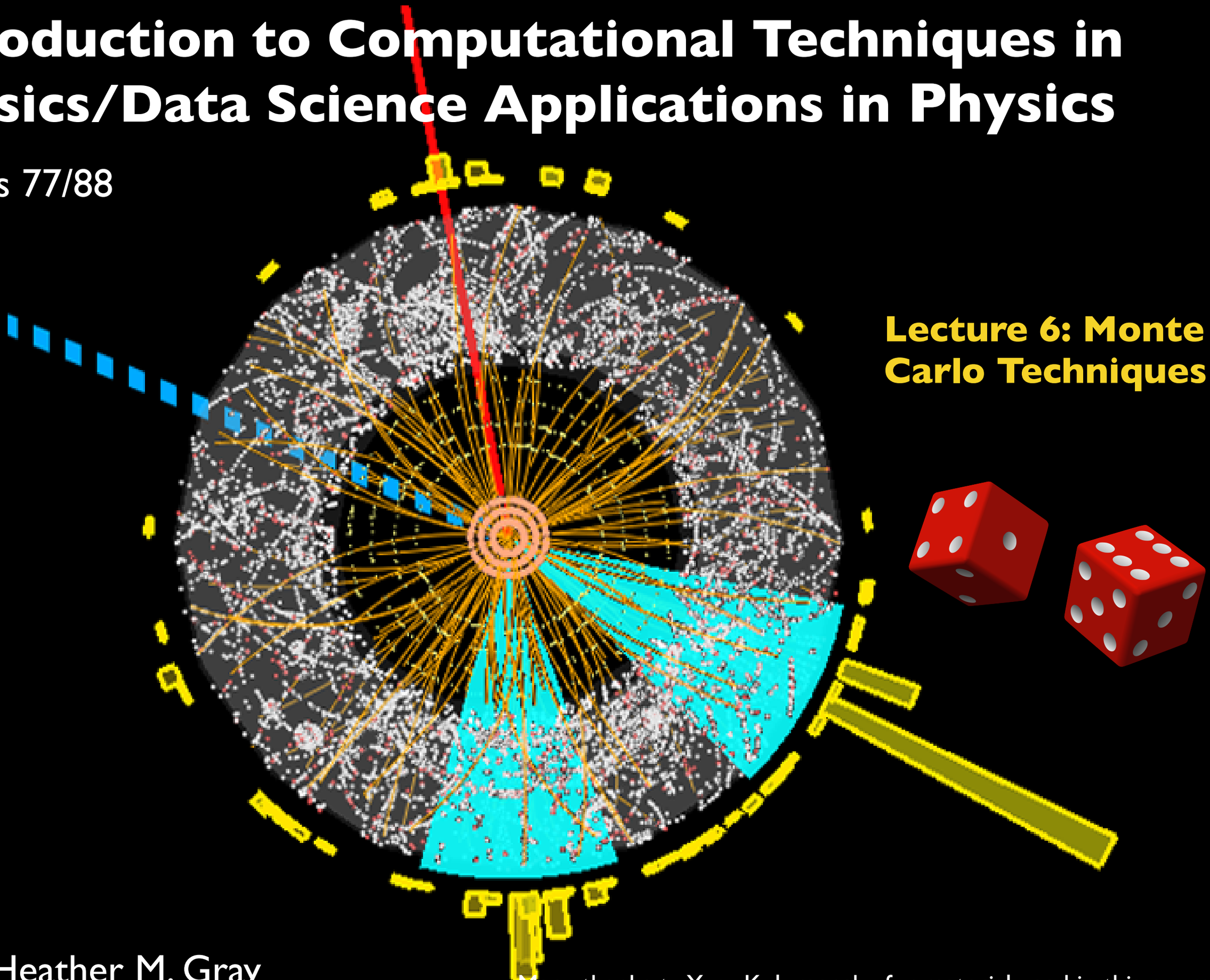
Introduction to Computational Techniques in Physics/Data Science Applications in Physics

Physics 77/88



Lecture 6: Monte Carlo Techniques

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Many thanks to Yury Kolomensky for material used in this course

Monte Carlo Techniques: Outline

- Introduction
- Random number generators
- Random number distributions
- Applications: integration

Monte Carlo Simulation

- technique
  - Applicable when an to a problem is too or
  - Applicable when the problem has
    - e.g. an of a
  - Involves repeated of the to obtain approximate (usually) result
- Applications
  - Most
  - Engineering, finance:
  -
  - And of course,

Examples

- Let's start with some examples in the jupyter notebook
  -
  -
  -

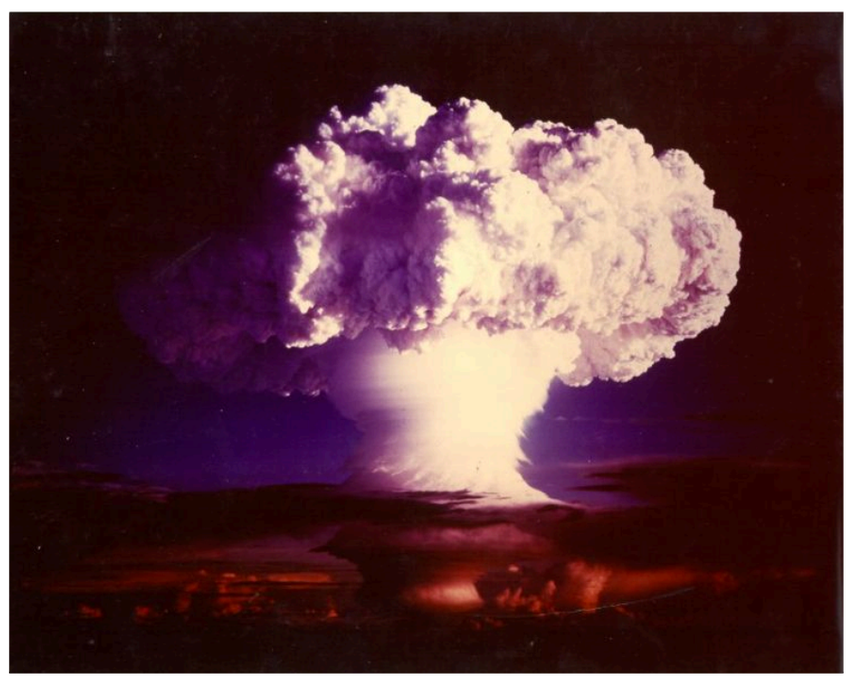
From: https://en.wikipedia.org/wiki/Coin_flipping#/media/File:Coin_Toss_(3635981474).jpg

From: https://en.wikipedia.org/wiki/Dice

From: https://en.wikipedia.org/wiki/File:AcetoFive.JPG

More examples

- Professional packages
  - Particle physics:
    - JETSET
    - Pythia
    - GEANT
  - Many ray-tracing/optics packages
  - First (documented) use: Manhattan project
- Possible Final Projects
  - Tournament simulator (e.g. March Madness, NHL playoffs, etc)
  - Program a game ( )
    - Incorporate some
      - e.g. betting odds, strategy



The Monte Carlo Technique

- What Monte Carlo simulation can not do:
  - Predict of a (measurement, process, …) or of
- What Monte Carlo simulation can do:
  - Compute for a outcome
  - Determine probability , correlations between , … that resemble those observed in the
- Precision limited by:
  - sampling ( )
  - Modeling of the
    - e.g. in describing (systematics)

Overview of the technique

- Split the process into , such that probability density functions for each could be
- For each step:
  - Identify and their
  - Generate
  - Evaluate outcome of the step
  - Repeat for the
  - At the end,
  - Repeat , build up a of the

Example

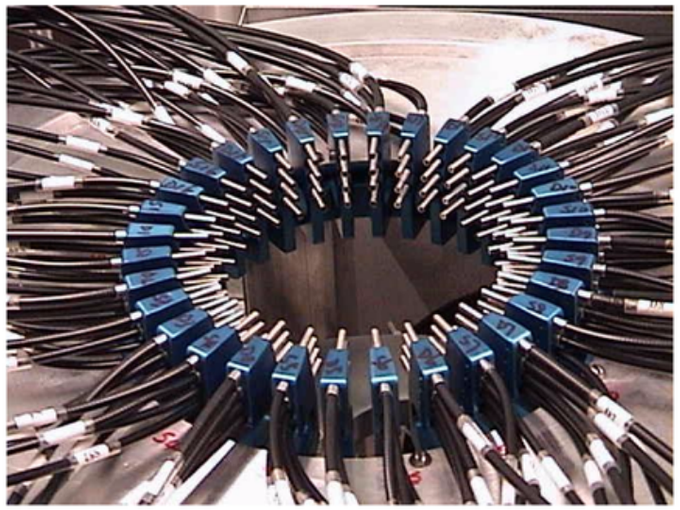
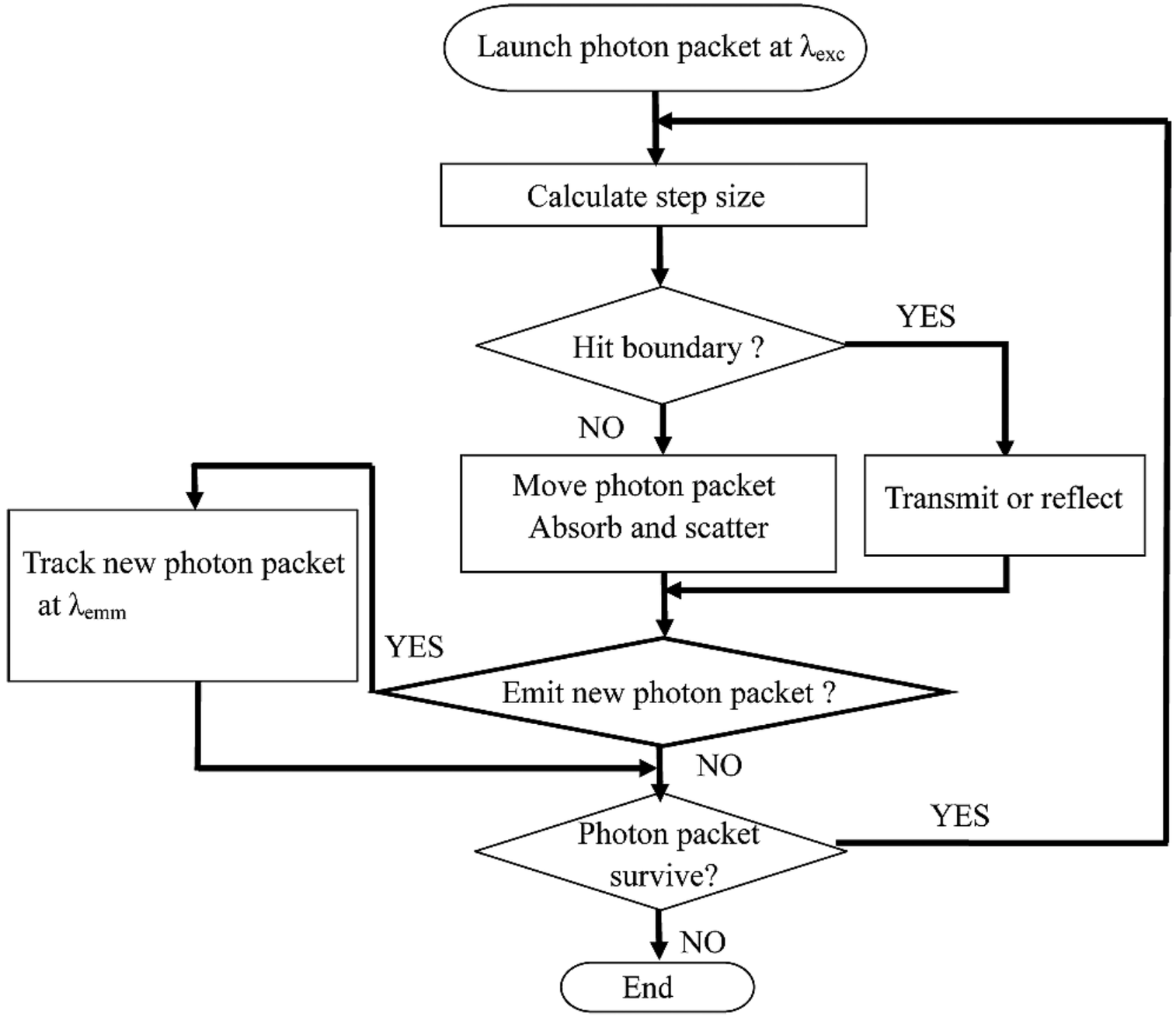


Image Credit

fiber-optic array for diffuse optical tomography for breast cancer detection



C. Zhu and Q. Liu, "Review of Monte Carlo modeling of light transport in tissues" J. Biomed. Opt. 18(5), 050902 (May 10, 2013). doi:10.1117/1.JBO.18.5.050902

Random Number Generators

- All MC simulations rely on a
  - Computer , so not
    - Although generators are possible (e.g. Johnson's noise generator — a cute 111A project, random.org)
- The most basic distribution is
  - distributions can be by a transform of a distribution (see below)
- Requirements:
  - Generate with a very long
  - Small within the
  - “Seeded” to produce
  -

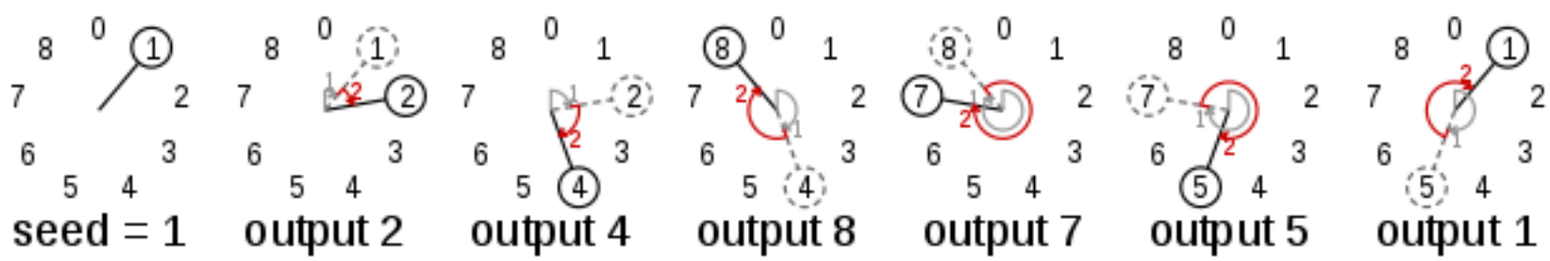
Simplest: Linear Congruent Generator

- $x_{n+1} =$
  - fixed by
  - depends on
  - at most
- So make c , a & b
- E.g. RANDU: a= b= , c=
  - Period of numbers
  - Produces random numbers which are within the
- Modern generator: Mersenne Twister
  - Implemented in Python, ROOT (TRandom3)
    - Period of

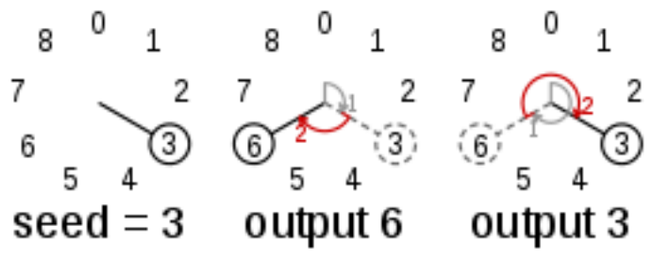
Parameters for LCG

- As we saw, certain sets of can lead to behavior
  - $x_{n+1} = (ax_n + b) \bmod c$

a=2
b=0
c=9



a=2
b=0
c=9



a=4
b=1
c=9

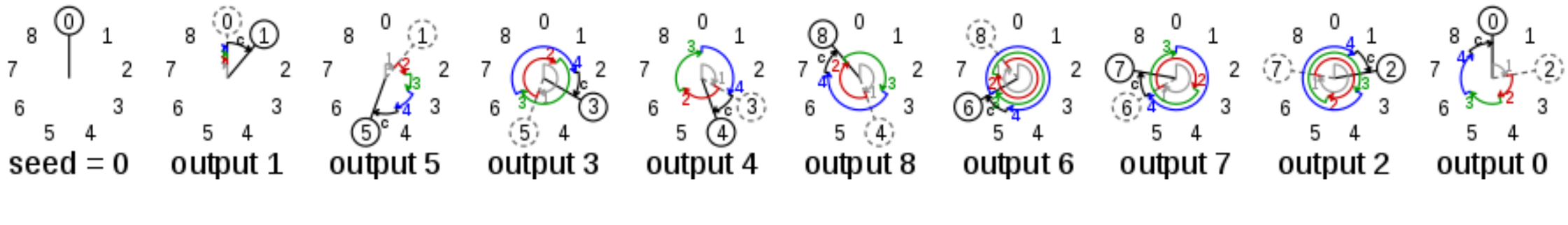


Image Credit

Generating Arbitrary Distributions

- Most frequently, you want a distributed according to some (predefined)
- Since most have a random number generator, derive from a random number :
  -
- Two basic techniques
  - method
  - von Neumann's method

Inverse Transform Method

- Theorem:
  - If is chosen with , and is a of , then is a random variable distributed between [ ]
  - $F(a) =$
- Therefore can implement with :
  - Generate u:
    - $u \in$ $, f(u) =$
  - Invert :
    - $x =$

Example

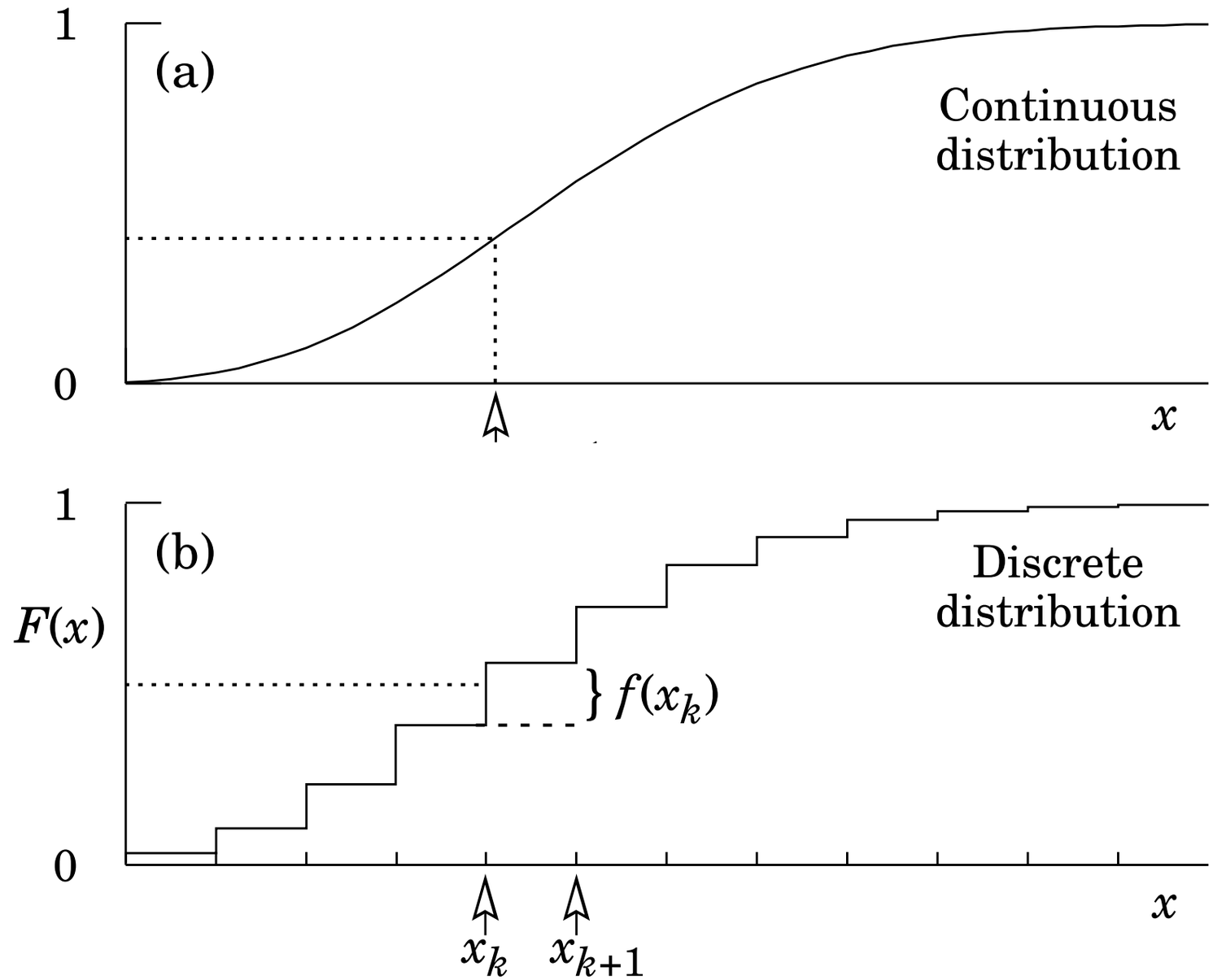
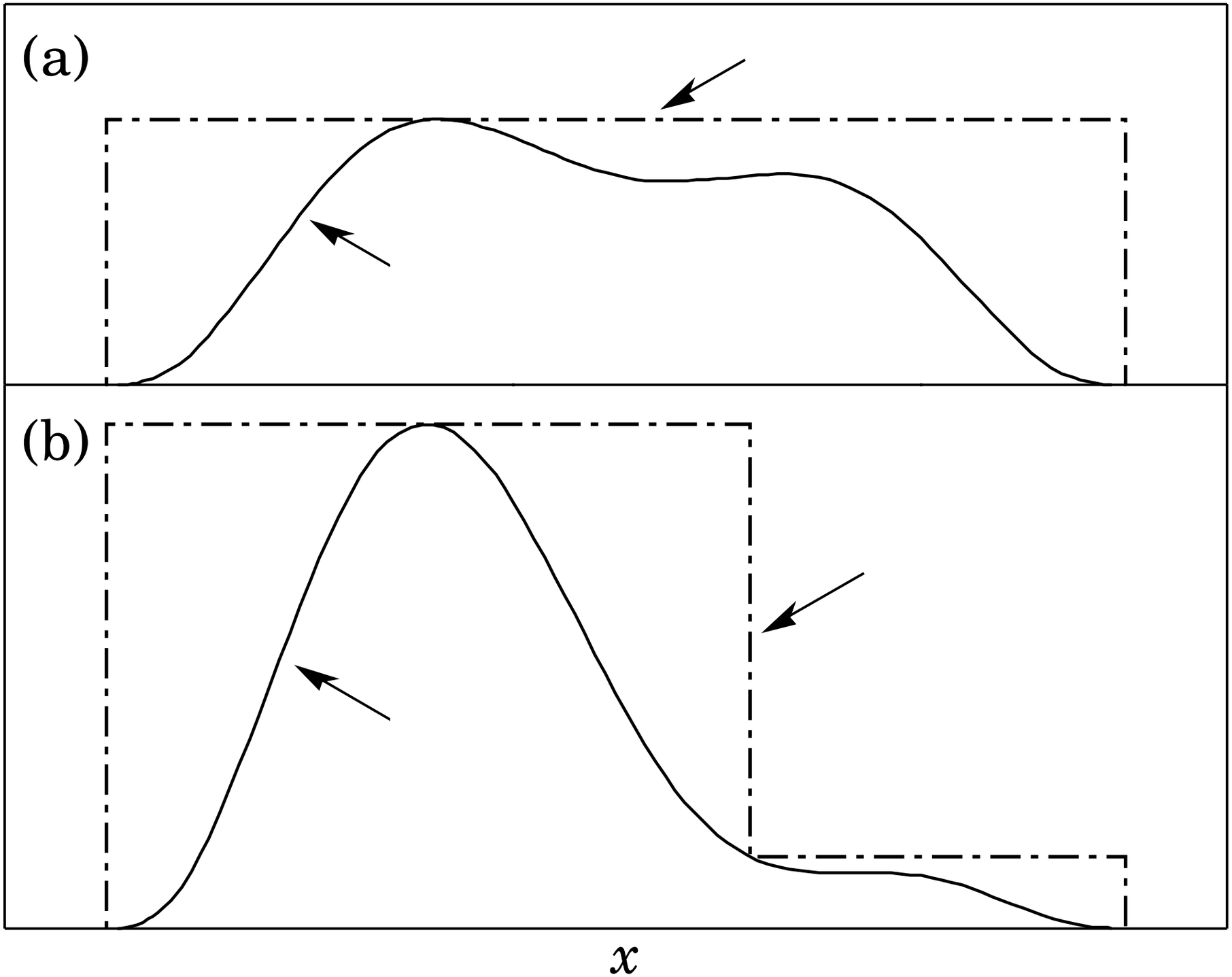


Figure 39.1: Use of a random number chosen from a uniform distribution (0,1) to find a random number x from a distribution with cumulative distribution function $F(x)$.

http://pdg.lbl.gov

Accept-Reject Method

- If is an , or difficult to compute function, then finding may be
- Let's suppose however that is and , such that for any we can find an easily generated and a constant
  -
- Accept-reject method:
  - Generate according to , and
  - If , accept ;
  - Otherwise and


(a)
(b)
x

Algorithms

- Exponential decay
  - $f(t) =$
  - Generate: $u \in$ $,f(u) =$
  - Define
    - $\alpha =$
    - $\beta =$
      - Then $t =$
- Gaussian distribution
  - If and are on , then
    - $z_1 =$
    - $z_2 =$
- are and with mean and $\sigma =$

Algorithms

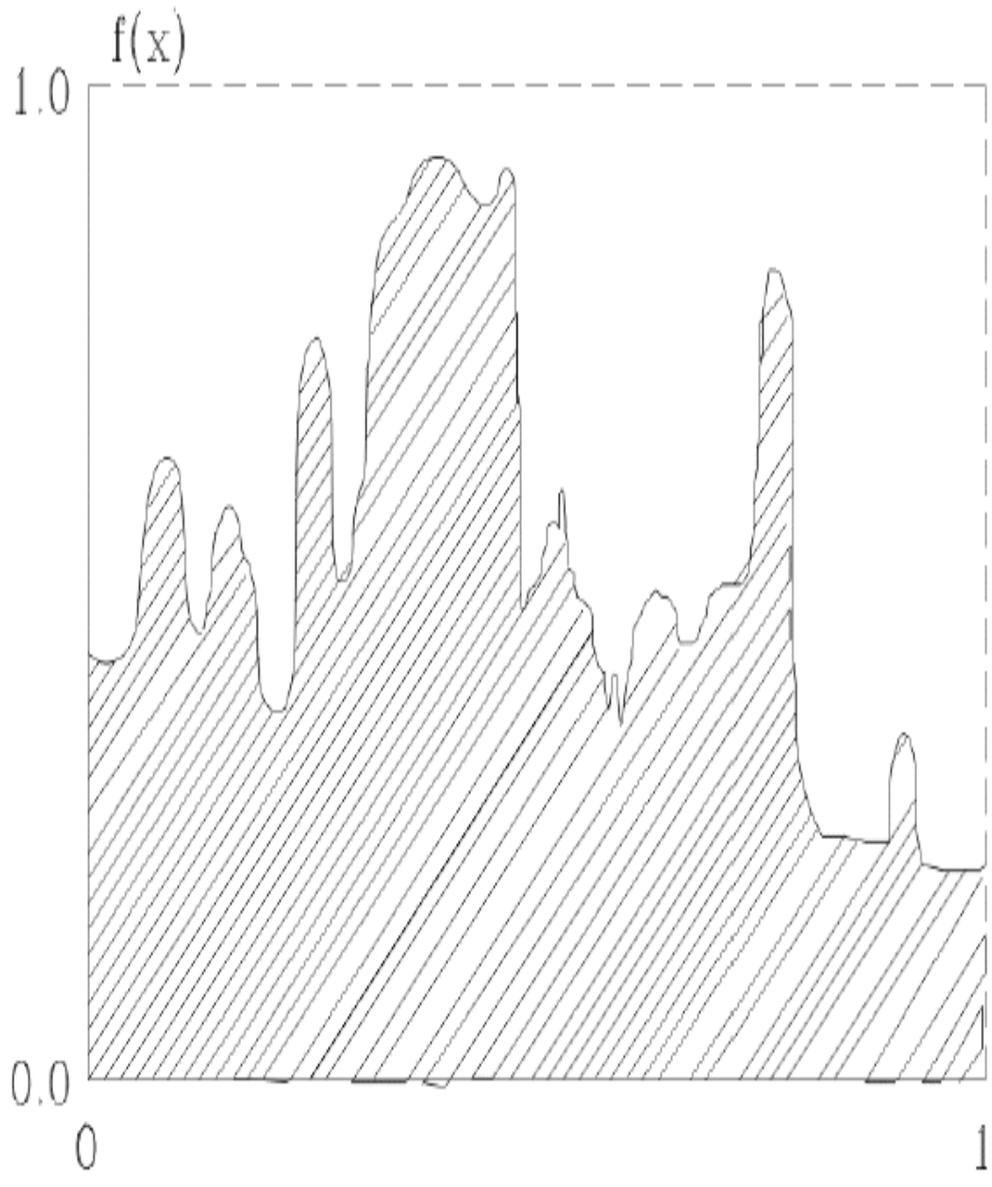
- Poisson Distribution
  - Iterate until a choice
    - Begin with $k =$ and set $A =$
    - Generate
    - Replace A with
    - If A < (where is the parameter)
      - accept $n_k =$ and
- Else increment by and generate a new and repeat
  - Always start with the value of left from the

Applications: MC Integration

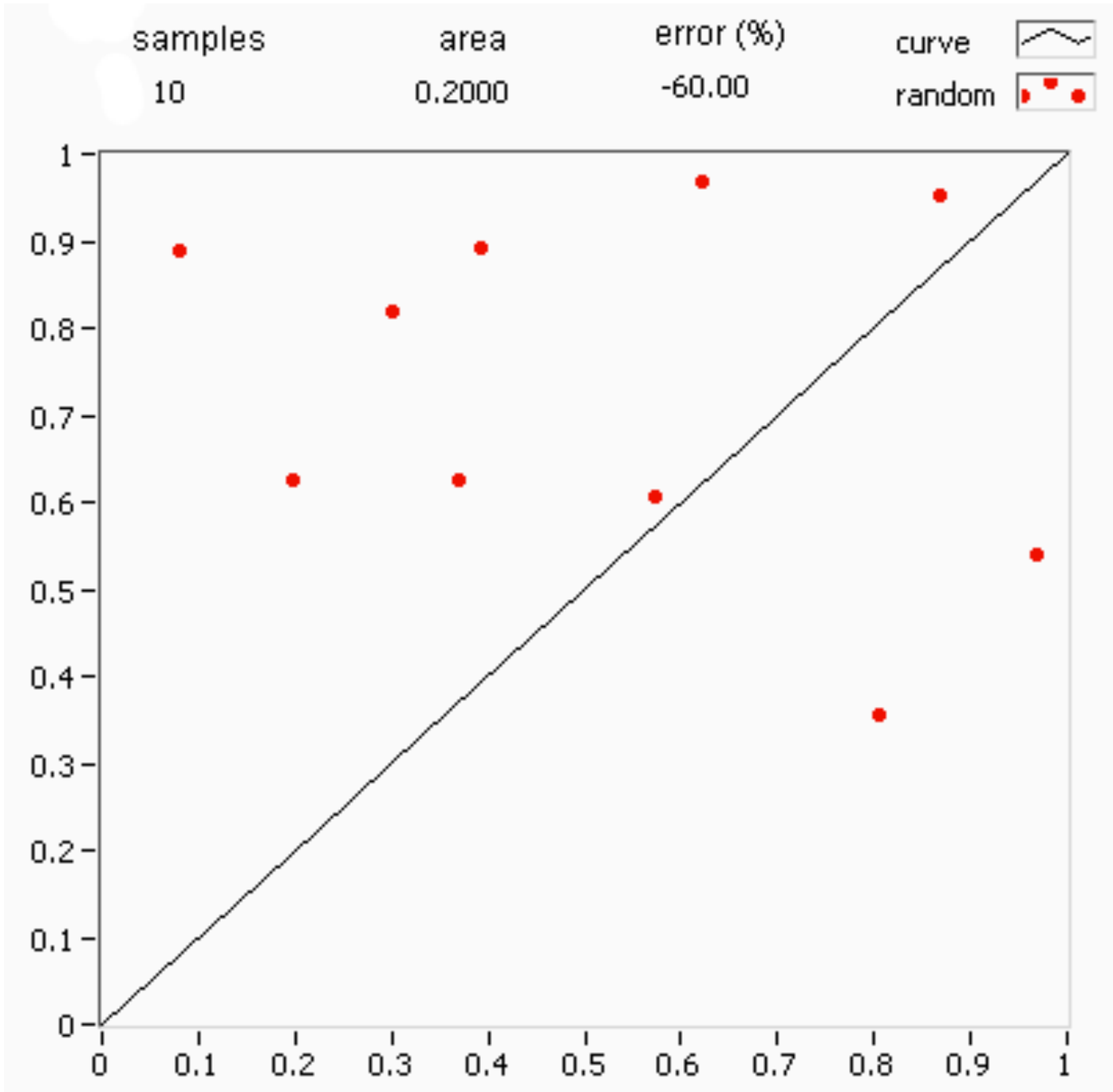
- Suppose we want to compute a
  - $Z = \int$
- Generate a (e.g. distributed in space)
- If is within , increment sum
- Repeat times
- Uncertainty on typically scales as

I-dimensional MC

- Suppose we want to find the under the for $y =$ for a given
- Now let's assume we are at the picture of
- Each will land on a point (,), where and
- If the value of , then we count it as a
- Repeat the for a large number of
- The under the is the /



Example



https://en.wikipedia.org/wiki/Monte_Carlo_method

Link to gif

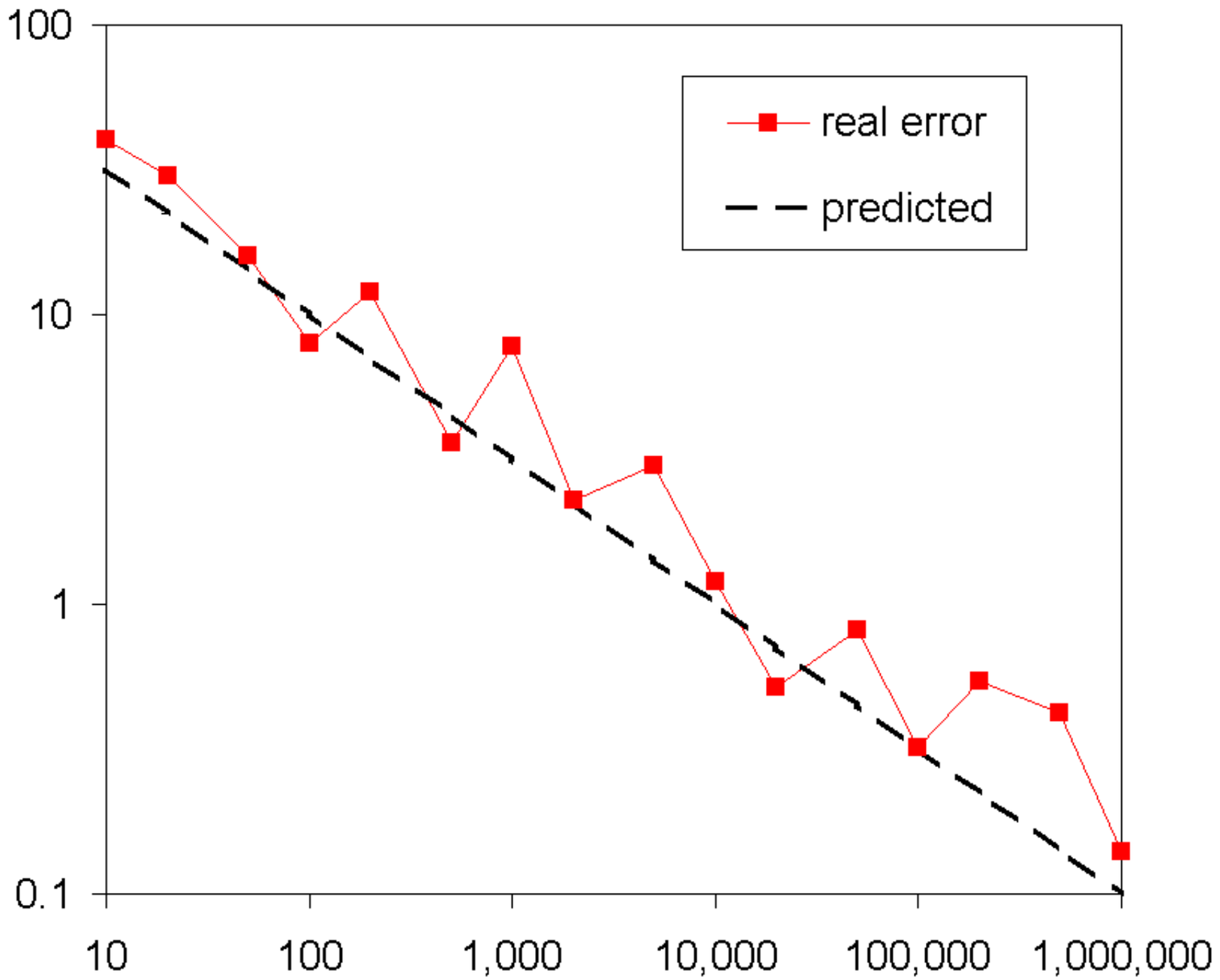
Error Estimate for MC Integrals

- Uncertainties for follow the distribution
  - Let the under the curve be , and the populated by is
  - Let be the number of points , and the number of points
  - Then the estimator of is:
    - $\hat{S} =$
- Define the of as
  - $\epsilon =$
  - $\Rightarrow$

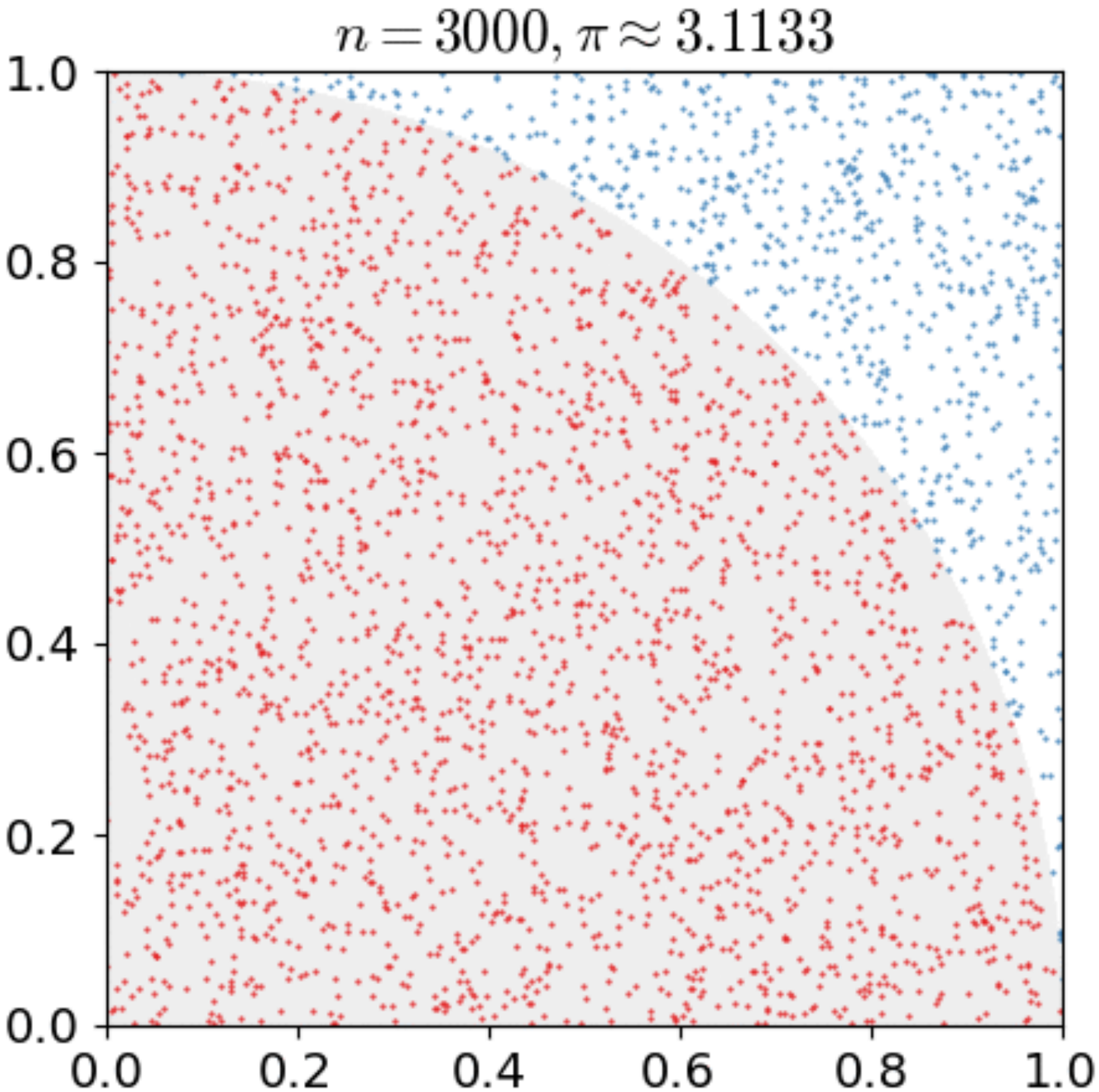
Error Estimate for MC Integrals

- is a variable, which follows a distribution ("choose out of ").
- Estimator of is therefore also a
- Its is given by
  - $\sigma(\hat{\epsilon}) =$
- You can show that in the limit
  - $\sigma(\hat{\epsilon}) \approx$
  - $\sigma(\hat{S}) =$

Error Estimate



Example: Compute π by MC



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