NE 255
Numerical Simulations in Radiation Transport
Introduction to Monte Carlo

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Learning Objectives

1. Define Monte Carlo simulation
2. Justify the choice of Monte Carlo for radiation transport
3. Understand the mathematical validity of Monte Carlo for radiation
4. Understand the major components of Monte Carlo methods transport

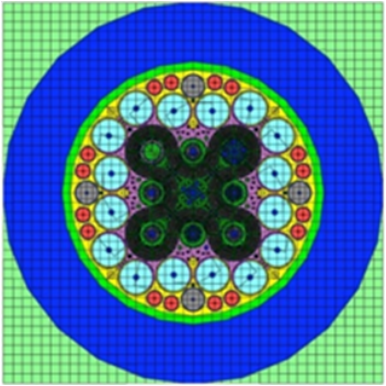


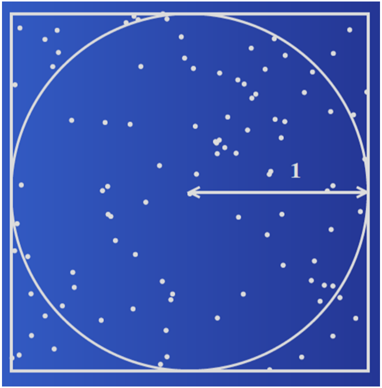
Figure 1 : ATR reactor geometry

Notes derived from Jasmina Vujic and Paul Wilson

What is Monte Carlo?

- The use of *random processes* to determine a *statistically-expected* solution to a problem
- Random processes can fulfill two roles:
  - Statistical approximation to mathematical equations
  - Statistical approximations to physical processes
- Construct a random process for a problem,
- Carry out a numerical simulation by N-fold sampling from a random # sequence

Evaluate π by Random Sampling



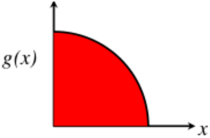
- Area of square, $A_s = 4$
- Area of circle, $A_c = \pi$
- Fraction of random points in circle

$$p = \frac{A_c}{A_s} = \frac{\pi}{4}$$

- Random points = N
- Random points in circle = N_c, $\therefore$

$$p = \frac{N_c}{N}\,; \quad \pi = \frac{4N_c}{N}$$

Evaluate π by Random Sampling (math)



$$g(x) = \sqrt{1 - x^2} \qquad G = \int_0^1 g(x)dx = \frac{\pi}{4}$$

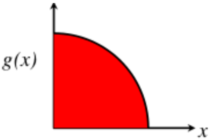
$$G = \int_0^1 g(x)dx = (1 - 0)\overline{g(x)}$$

Determine $\overline{g(x)}$ by random sampling:

for $k = 1, \ldots, N$, choose $\hat{x}_k$ randomly on the interval $(0, 1)$,

$$\overline{g(x)} \equiv \frac{1}{N}\sum_{k=1}^{N} g(\hat{x}_k) = \frac{1}{N}\sqrt{1 - \hat{x}_k^2}$$

EVALUATE π BY RANDOM SAMPLING (PHYSICS)



$$g(x) = \sqrt{1 - x^2} \qquad G = \int_0^1 g(x)dx = \frac{\pi}{4}$$

G = area under curve,

= fraction of unit square under curve

for $k = 1, \ldots, N$, chose $\hat{x}_k, \hat{y}_k$ randomly on the interval $[0, 1]$,

m_N = # of times in N trials that $\hat{x}_k^2 + \hat{y}_k^2 \leq 1$,

$$G = \frac{m_N}{N}$$

Manhattan Project

- The first human engineered nuclear detonation, the Trinity Test in New Mexico.
- Active: 1942–1945
- Branch: U.S. Army Corps of Engineers
- Monte Carlo Pioneers:
  - Enrico Fermi,
  - Stanislaw Ulam,
  - John von Neumann,
  - Robert Richtmeyer,
  - Nicholas Metropolis

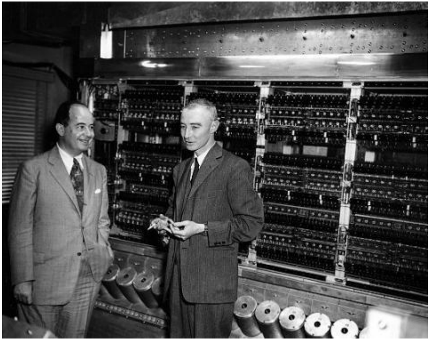


Figure 2 : Oppenheimer, von Neumann, MANIAC

Nicholas Metropolis, S. Ulam. "The Monte Carlo Method," *Journal of the American Statistical Association*, **44**, No. 247, 335-341 (Sep. 1949).

General Purpose MC Codes

- MCNP: developed at LANL, distributed via RSICC, http://rsicc.ornl.gov
- Geant4: developed by a large collaboration in the HEP community, http://geant4.web.cern.ch/geant4/
- EGSnrc: developed at NRC (Canada), http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html
- SERPENT: Developed by Dr. Jaakko Leppanen, VTT, Finland, http://montecarlo.vtt.fi/
- Shift: developed at ORNL, distributed via RSICC, http://rsicc.ornl.gov
- Capsaicin: developed at LANL, http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-11-01410

Why/When Monte Carlo?

- Applications that are mathematically equivalent to *integration over many dimensions*
  - Analytic integration may be impossible
  - Deterministic numerical integration may be slow and/or require error prone approximations
- However, statistically accurate results can require **significant computer time**
- Fortunately, Monte Carlo and parallel computing go well together
- and we also have Variance Reduction methods

What is MC Radiation Transport?

Simulate many independent particles in a system

- Treat each physical process as a *probabilistic process*
- *Randomly sample* each process using an independent stream of random numbers
- Follow each particle from birth until it no longer matters
- Accumulate the contributions of each particle to find the statistically-expected mean behavior and variance

Mathematical Validity

- Consider particles with a phase space describing position, $\vec{r}$, and velocity, $\vec{v}$
- A neutral particle can be transmitted from one position to another at a constant velocity
$$T(\vec{r}\,' \to \vec{r}, \vec{v})$$
- A particle can undergo a collision at a single position that changes its velocity
$$C(\vec{r}, \vec{v}\,' \to \vec{v})$$

Contributions After 0 Collisions

- Consider a particle born from a source described by

$$Q(\vec{r}\,', \vec{v}\,')$$

- This particle will contribute to the flux at $(\vec{r}, \vec{v})$ before any collisions

$$\psi_0(\vec{r}, \vec{v}) = \int_{\vec{r}\,'} Q(\vec{r}\,', \vec{v}\,') T(\vec{r}\,' \to \vec{r}, \vec{v}) d\vec{r}\,'$$

Contributions After 1 Collision

- The uncollided particles, $\psi_0(\vec{r}\,', \vec{v}\,')$, could undergo 1 collision and then be transmitted to the point $(\vec{r}, \vec{v})$

$$\psi_1(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}\,'} \Bigg[\underbrace{\int_{\vec{v}\,'} \psi_0(\vec{r}\,', \vec{v}\,') C(\vec{r}\,', \vec{v}\,' \to \vec{v}) d\vec{v}\,'}_{\textit{collision}} \Bigg] T(\vec{r}\,' \to \vec{r}, \vec{v}) d\vec{r}\,'}_{\textit{transmission}}$$

Contributions After k Collisions

- Particles that have undergone k collisions, $\psi_k(\vec{r}\,', \vec{v}\,')$, could undergo another collision and then be transmitted to the point $(\vec{r}, \vec{v})$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}\,'} \Bigg[\underbrace{\int_{\vec{v}\,'} \psi_k(\vec{r}\,', \vec{v}\,') C(\vec{r}\,', \vec{v}\,' \to \vec{v}) d\vec{v}\,'}_{\textit{collision}} \Bigg] T(\vec{r}\,' \to \vec{r}, \vec{v}) d\vec{r}\,'}_{\textit{transmission}}$$

Combine Collision and Transmission Kernels

$$\vec{p} = (\vec{r}, \vec{v}) \quad \text{and}$$
$$R(\vec{p}\,' \to \vec{p}) \equiv C(\vec{r}\,', \vec{v}\,' \to \vec{v})T(\vec{r}\,' \to \vec{r}, \vec{v})$$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \psi_k(\vec{p}_k) R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \left[\int_{\vec{p}_{k-1}} \psi_{k-1}(\vec{p}_{k-1}) R(\vec{p}_{k-1} \to \vec{p}_k) d\vec{p}_{k-1} \right] R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

…and so on …

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \int_{\vec{p}_{k-1}} \cdots \int_{\vec{p}_0} \psi_0(\vec{p}_0) R(\vec{p}_0 \to \vec{p}_1) d\vec{p}_0 \cdots$$
$$\psi_{k-1}(\vec{p}_{k-1}) R(\vec{p}_{k-1} \to \vec{p}_k) d\vec{p}_{k-1} R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

Sum Over All Collisions

$$\psi(\vec{p}) = \sum_{k=0}^{\infty} \psi_k(\vec{p})$$

Arriving at the *integral form* of the transport equation

$$\psi(\vec{r}, \vec{v}) = \int_{\vec{r}\,'} \left[\int_{\vec{v}\,'} \psi(\vec{r}\,', \vec{v}\,') C(\vec{r}\,', \vec{v}\,' \to \vec{v}) d\vec{v}\,' \right] T(\vec{r}\,' \to \vec{r}, \vec{v}) d\vec{r}\,'$$

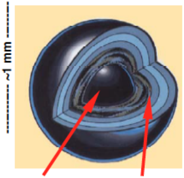
Mathematical Validity

$$\Psi_k(\vec{p}) = \int\int\cdots\int \Psi_0(\vec{p}_0)R(\vec{p}_0 \rightarrow \vec{p}_1)R(\vec{p}_1 \rightarrow \vec{p}_2) \cdots R(\vec{p}_{k-1} \rightarrow \vec{p}_k)d\vec{p}_0 d\vec{p}_1 \cdots d\vec{p}_{k-1}$$

- Integration over many variables
- Generate a "history" (sequence of states $\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_k$)
  - Randomly sample from source: $\Psi_0(\vec{p}_0)$
  - Randomly sample for each of k transitions: $R(\vec{p}_{k-1} \rightarrow \vec{p}_k)$
- Average for result A by averaging of M histories

$$\langle A \rangle = \int A(\vec{p})\Psi(\vec{p})d\vec{p} = \frac{1}{M}\sum_{m=1}^{M}\left[\sum_{k=1}^{\infty} A(\vec{p}_{k,m})\Psi(\vec{p}_{k,m})\right]$$

CAN MODEL VERY COMPLEX THINGS

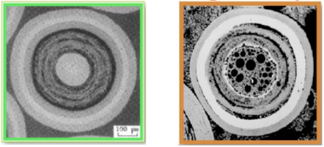


TRISO Fuel Particles:

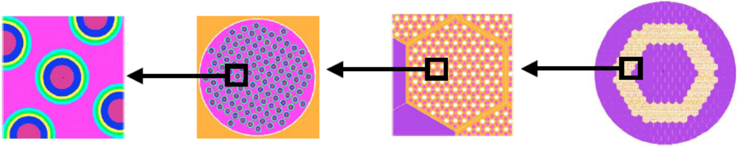
- Fission product gases trapped within coatings
- Coatings remain intact, even with high T & burnup

Fuel concept is same for block or pebble bed

Fresh Fuel | High Burnup



(From General Atomics)

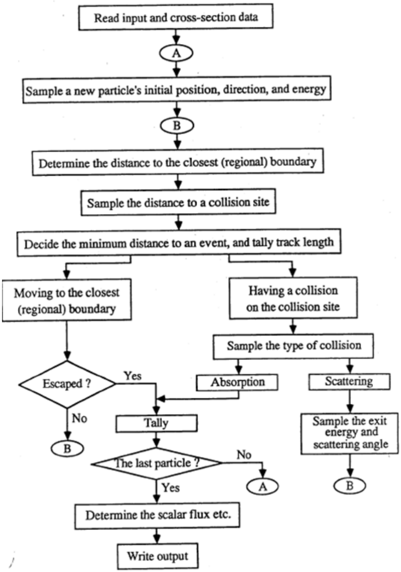


Accurate & explicit modeling at multiple levels

Major Components of MC Algorithm

- **PDFs**: the physical/mathematical system must be described by a set of pdfs.
- **Random number generator**: a source of random #s uniformly distributed on the unit interval.
- **Sampling rule**: prescription for sampling the pdf (given having random #s)
- **Scoring**: the outcomes must be accumulated/tallied for quantities of interest
- **Error estimation**: an estimate of the statistical error (variance) of the solution
- **Variance Reduction**: methods for reducing the variance and computation time simultaneously
- **Parallelization**: efficient use of computers

Basic Event-Based Algorithm



LET'S GET STARTED WITH

1. Physics as Probability
2. Definitions: PDF & CDF
3. Motivation & Goal of Random Sampling
4. Basic Random Sampling Techniques
    - Direct Discrete Sampling
    - Direct Continuous Sampling
    - Rejection Sampling

Notes derived from Jasmina Vujic and Paul Wilson

Learning Objectives

1. Provide examples of probabilistic representations of physics
2. Distinguish between a PDF and CDF
3. Distinguish between a *discrete* PDF (CDF) and a *continuous* PDF (CDF)
4. Describe the goal of random sampling
5. Identify and implement the best random sampling technique for a given distribution

Physics as Probability

Various physical phenomena can be represented by probability distributions

- Photon emission energy
  - Each possible energy has a different probability (intensity)
- Scattering cross-sections
  - Each possible scattering angle has a different probability as a function of the energy
- Transmission through a medium
  - Probability of reaching a particular position depends on the cross-section

Probability Density Functions

All variables, x, have a Probability Density Function (PDF), $p(x)$, with the following characteristics:

Continuous

$$p\{a \le x \le b\} = \int_a^b p(x)dx$$

$$p(x) \ge 0$$

$$\int_{-\infty}^{\infty} p(x)dx = 1$$

Discrete

$$p(x = x_k) = p_k \equiv p(x_k)$$

$$k = 1, \ldots, N$$

$$p_k \ge 0$$

$$\sum_{k=1}^{N} p_k = 1$$

Cumulative Distribution Functions

All PDFs, $p(x)$, have an associated
Cumulative Distribution Function (CDF), $P(x)$, with the following properties:

Continuous

$$P\left\{x' \leq x\right\} = P(x) = \int_{-\infty}^{x} p(x')dx'$$

$$P(-\infty) = 0\,, \quad P(\infty) = 1$$

$$0 \leq P(x) \leq 1$$

$$\frac{dP(x)}{dx} \geq 0$$

Discrete

$$P\left\{x' \leq x\right\} = P_k \equiv P(x_k) = \sum_{j=1}^{k} p_j$$

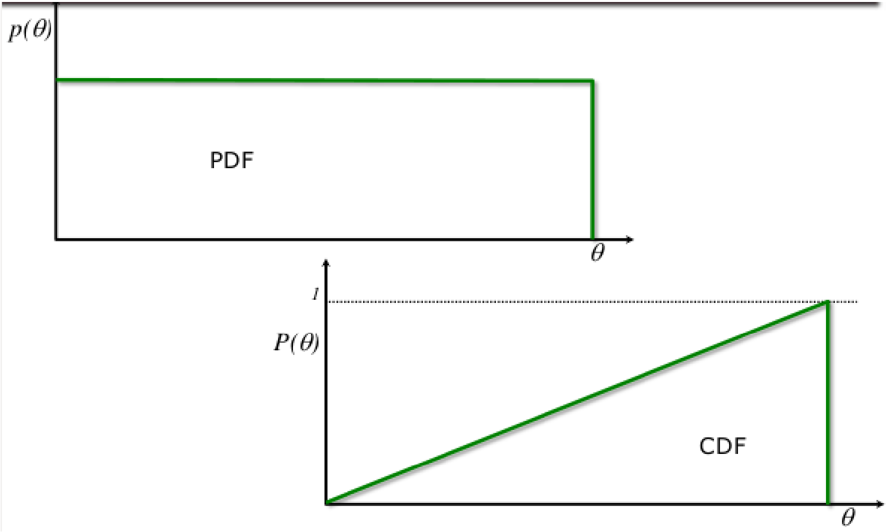
$$k = 1, \ldots, N$$

$$P_0 = 0\,, \quad P_N = 1$$

$$0 \leq P_k \leq 1$$

$$P_k \geq P_{k-1}$$

Random Sampling Basics



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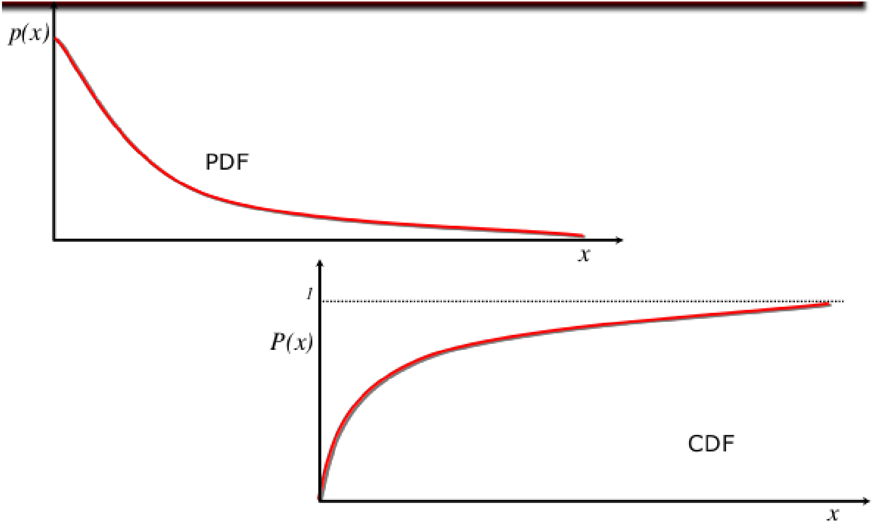
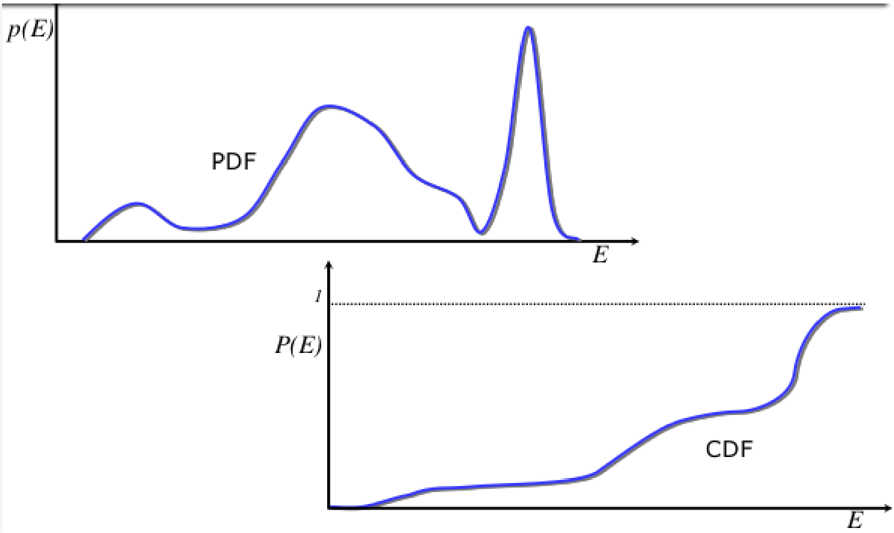


Random Sampling Basics



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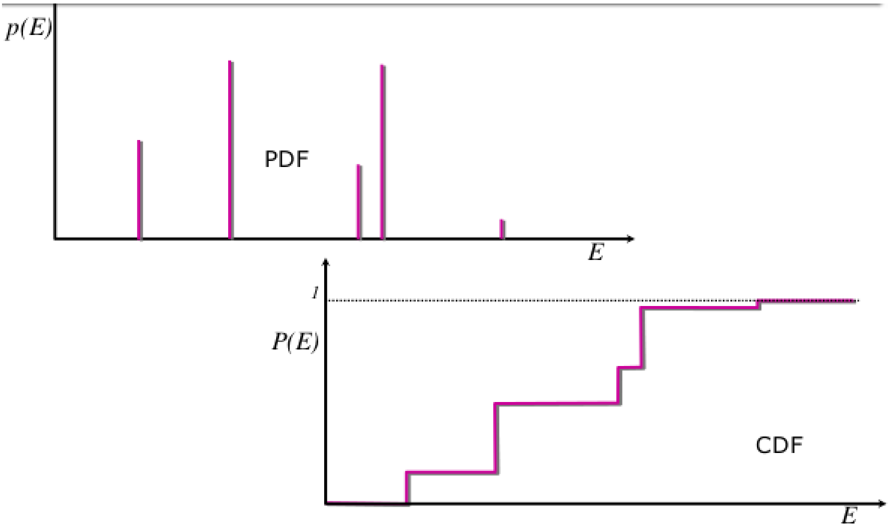


WHY RANDOM SAMPLING

Various physical phenomena can be represented by probabilistic distributions

- The known probability distribution represents the *collective* behavior
- We need to know the behavior at *each* single event
- We need to recreate the collective behavior after many events

Random Sampling Purpose

Use a random process to select a single value with the following requirements

- Each sample should be independent from other samples
- The PDF formed from a large number of samples should converge to the initial PDF
- Recover the full resolution of the initial PDF

Sampling Techniques

Random sampling uses uniformly distributed random variables to choose a value for a variable according to its probability density function

- *Basic* sampling techniques
  - Direct discrete sampling
  - Continuous discrete sampling
  - Rejection sampling

- *Advanced* sampling techniques
  - Histogram
  - Piecewise linear
  - Alias sampling
  - Advanced continuous PDFs

Uniformly-Distributed Random Variable

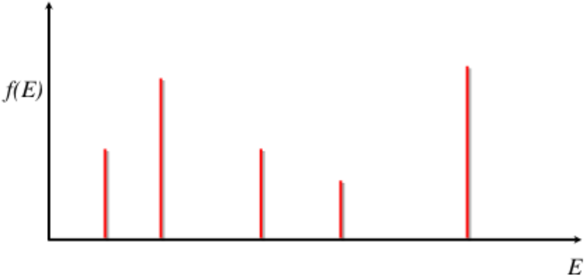
- Standard notation
  - Single random variable: ξ
  - Pair of random variables: (ξ, η)
- PDF for random variables:

$$p(\xi) = \begin{cases} 1 & 0 \leq \xi < 1 \\ 0 & \text{otherwise} \end{cases}$$

Direct Discrete Sampling

Sampling Procedure

- Generate ξ
- Determine k such that $P_{k-1} \leq \xi \leq P_k$
- Return $x = x_k$



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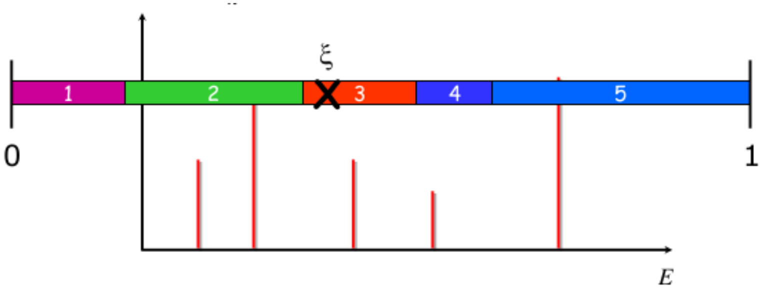
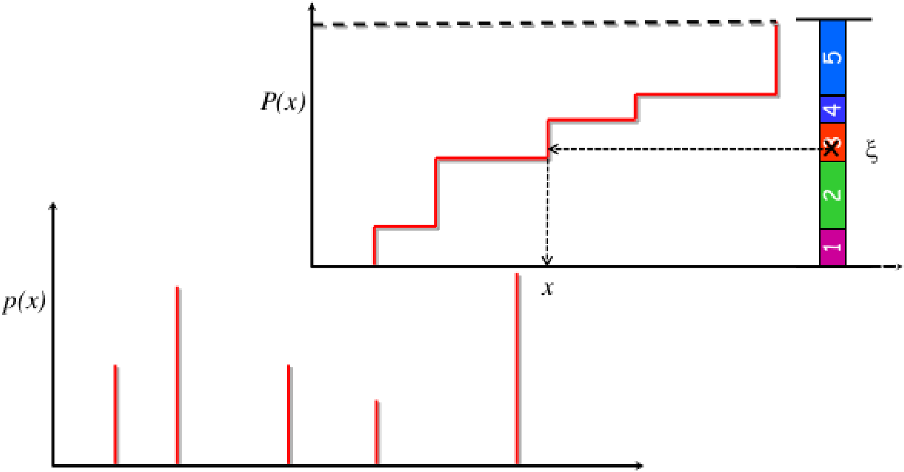


Direct Discrete Sampling

Consider the CDF



Direct Discrete Sampling

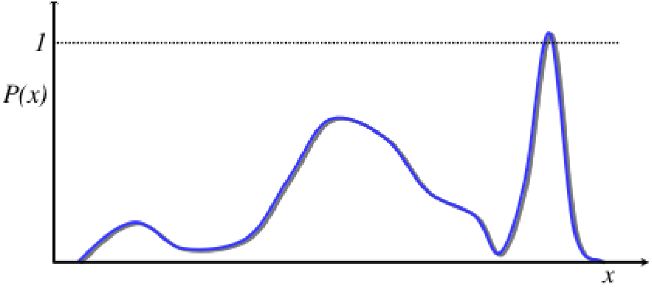
- Requires a table search on P_k
  - Linear search requires $O(N)$ time
  - Binary search requires $O(\log_2 N)$ time

- Special case: Uniform discrete PDF
  - $p_k = 1/N$
  - $P_k = k/N$
  - $k = \lfloor 1 + N\xi \rfloor$ (floor function)

DIRECT CONTINUOUS SAMPLING

- Can only be used if CDF can be inverted
- Direct solution of $P(x) = \xi$
- Sampling Procedure:

$$\text{Generate } \xi \,, \qquad \text{Determine } x = P^{-1}(\xi)$$



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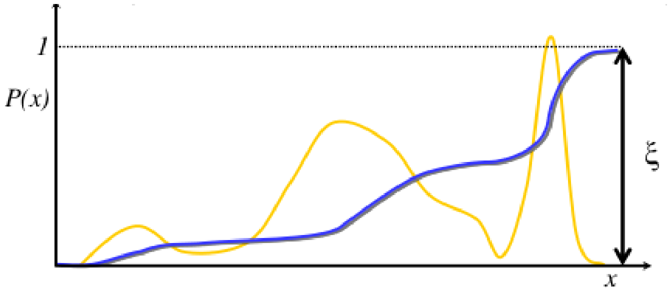

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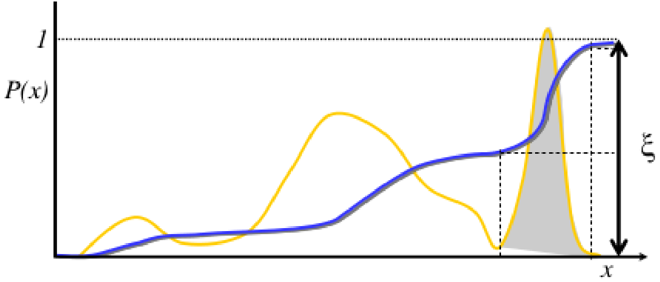


Direct Continuous Sampling

- Advantages:
  - Straightforward math & coding
- Disadvantages:
  - Can involve computationally slow functions
  - Not always possible to invert $P(x)$

Normalization

- Random sampling depends on **shape** and not on ~~magnitude~~
- Normalization for formal definition of PDF/CDF required

$$g(t)dt = e^{-\lambda t}dt\,, \quad t > 0$$

$$G(t) = \int_{-\infty}^{t} g(t')dt' = \int_{0}^{t} g(t')dt' = \left[-\frac{e^{-\lambda t'}}{\lambda}\right]_0^t = \frac{1}{\lambda}\left(1 - e^{-\lambda t}\right)$$

$$G(\infty) = \frac{1}{\lambda}$$

$$p(t) = \lambda g(t) = \lambda e^{-\lambda t}dt\,, \quad t > 0$$

$$P(t) = \int_{-\infty}^{t} p(t')dt' = \int_{0}^{t} \lambda f(t')dt' = \left[e^{-\lambda t'}\right]_0^t = 1 - e^{-\lambda t}$$

$$P(\infty) = 1$$

Shifted Uniform

$$
\begin{aligned}
g(x)dx &= C \quad a \le x < b \\
G(x) &= \int_{-\infty}^{x} g(x')dx' = C \int_{a}^{x} dx' = C\left[x'\right]_a^x = C\left(x - a\right) \\
G(\infty) &= G(b) = C(b - a)
\end{aligned}
$$

$$
\begin{aligned}
p(x) &= \frac{g(x)}{G(\infty)} = \frac{C}{C(b-a)} = \frac{1}{b-a} \quad a \le x < b \\
P(x) &= \int_{-\infty}^{x} p(x')dx' = \frac{1}{b-a} \int_{a}^{x} dx' = \frac{x-a}{b-a}
\end{aligned}
$$

$$
x = P^{-1}(\xi) = \xi\left(b - a\right) + a
$$

Simple Line, Slope = m

$$g(x)dx = mx \qquad 0 \le x < 1$$
$$G(x) = \int_{-\infty}^{x} g(x')dx' = \int_0^x mx'dx' = \frac{m}{2}\left[x'^2\right]_0^x = \frac{m}{2}x^2$$
$$G(\infty) = G(1) = \frac{m}{2}$$

$$p(x) = \frac{mx}{\frac{m}{2}} = 2x \qquad 0 \le x < 1$$
$$P(x) = \int_{-\infty}^{x} p(x')dx' = \int_0^x 2x'dx' = \left[x'^2\right]_0^x = x^2$$

$$x = P^{-1}(\xi) = \sqrt{\xi} \qquad \text{Independent of } m$$

Shifted Line

$$g(x)dx = m(x-a) \qquad a \leq x < b$$

$$G(x) = \int_{-\infty}^{x} g(x')dx' = \int_{a}^{x} m(x'-a)dx' = \frac{m}{2}\left[(x'-a)^2\right]_0^x = \frac{m}{2}(x-a)^2$$

$$G(\infty) = G(1) = \frac{m}{2}(b-a)^2$$

$$p(x) = \frac{m(x-a)}{\frac{m}{2}(b-a)^2} = 2\frac{x-a}{(b-a)^2} \qquad a \leq x < b$$

$$P(x) = \int_{-\infty}^{x} p(x')dx' = \frac{1}{(b-a)^2}\int_{a}^{x} 2(x'-a)dx' = \frac{(x-a)^2}{(b-a)^2}$$

$$x = P^{-1}(\xi) = \sqrt{\xi}(b-a) + a \qquad \text{Independent of } m$$

Rejection Sampling

- Many CDFs cannot be inverted
  - e.g. Klien-Nishina cross-section

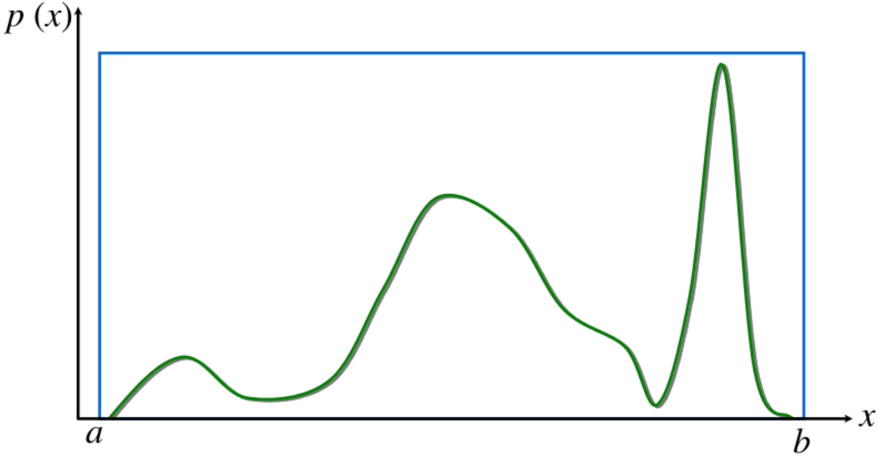
- Use an approach that is more graphical
  - Select a point in a 2-D domain
  - Determine whether that point is above or below the PDF
  - Keep those that are below
  - Start over if above

Rejection Sampling

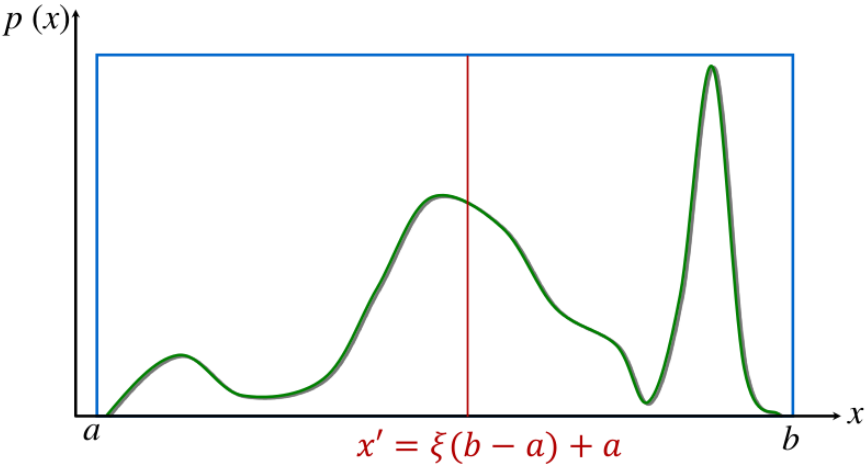
- Select a bounding function, g(x), such that
  - $g(x) \geq p(x)$ for all x
  - $g(x)$ is easy to sample
- Simplest choice is $g(x) = C$
- May not be best choice

- Generate pair of random variables, (ξ, η)
  - $x' = G^{-1}(\xi)$
  - If $\eta < p(x')/g(x')$, accept x'
  - Else, reject x'

Rejection Sampling



Rejection Sampling



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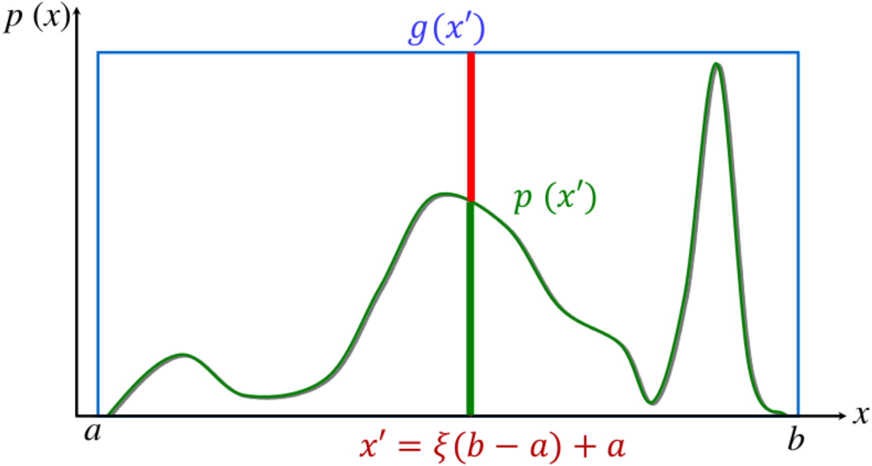

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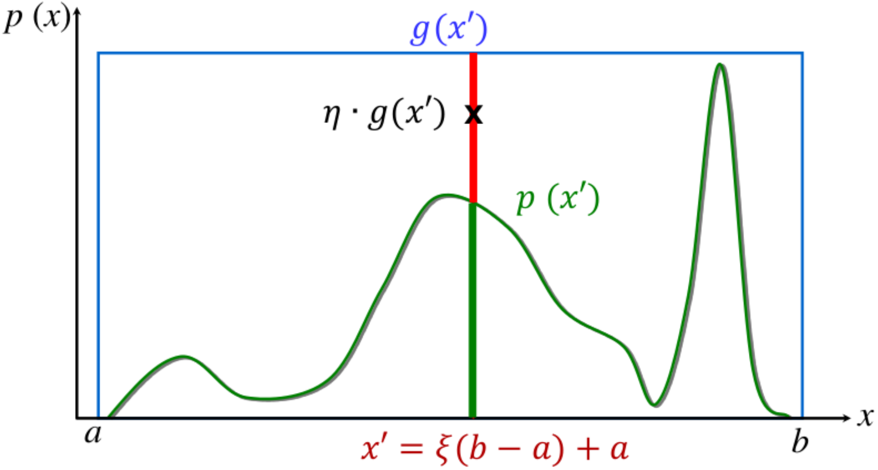

Rejection Sampling

- Advantages
  - Computationally simple
  - Always works
- Disadvantages
  - Will be inefficient if shapes of $g(x)$ and $p(x)$ are not similar

$$\text{Efficiency } = \frac{\int p(x)dx}{\int g(x)dx}$$

Random Sampling Summary

- Physics can be represented *probabilistically*
- We can create PDFs and from those generate CDFs
- These can be either continuous or discrete
- We learned some basic ways to use random numbers to *sample* from these distributions to simulate physics