

NE 255

Numerical Simulations in Radiation Transport

Introduction to Monte Carlo

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November 17, 2016

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

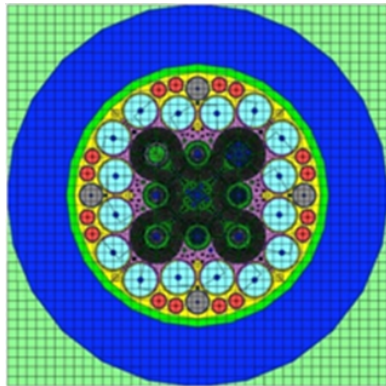


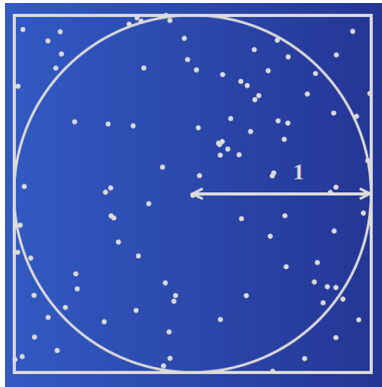
Figure 1 : ATR reactor geometry

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



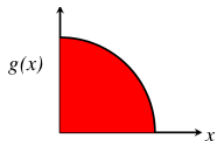
- Area of square, $A_s = 4$
- Area of circle, $A_c = \pi$
- Fraction of random points in circle

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

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

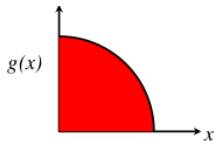
$$p = \frac{N_c}{N} ; \quad \pi = \frac{4N_c}{N}$$

EVALUATE π BY RANDOM SAMPLING (MATH)



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

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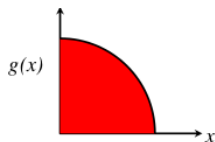
$$G = \int_0^1 g(x) dx = (1 - 0) \overline{g(x)}$$

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

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

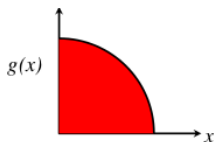
$$\overline{g(x)} \equiv \frac{1}{N} \sum_{k=1}^N g(\hat{x}_k) = \frac{1}{N} \sqrt{1 - \hat{x}_k^2}$$

EVALUATE π BY RANDOM SAMPLING (PHYSICS)



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EVALUATE π BY RANDOM SAMPLING (PHYSICS)



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

G = area under curve,
= fraction of unit square under curve

for $k = 1, \dots, N$, 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

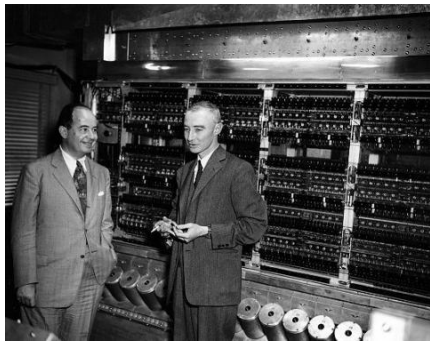


Figure 2: Oppenheimer, von Neumann, MANIAC

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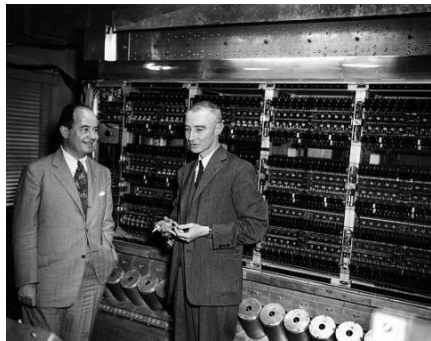


Figure 2: Oppenheimer, von Neumann, MANIAC

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>
- **Mercury**: developed at LLNL, <https://wci.llnl.gov/simulation/computer-codes/mercury>

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

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*

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- Follow each particle from birth until it no longer matters

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

$$T(\vec{r}' \rightarrow \vec{r}, \vec{v})$$

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

$$T(\vec{r}' \rightarrow \vec{r}, \vec{v})$$

- A particle can undergo a collision at a single position that changes its velocity

$$C(\vec{r}, \vec{v}' \rightarrow \vec{v})$$

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

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

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})

$$\psi_1(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}'} \left[\underbrace{\int_{\vec{v}'} \psi_0(\vec{r}', \vec{v}') C(\vec{r}', \vec{v}' \rightarrow \vec{v}) d\vec{v}'}_{\text{collision}} \right] T(\vec{r}' \rightarrow \vec{r}, \vec{v}) d\vec{r}'}_{\text{transmission}}$$

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})

$$\psi_{k+1}(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}'} \left[\underbrace{\int_{\vec{v}'} \psi_k(\vec{r}', \vec{v}') C(\vec{r}', \vec{v}' \rightarrow \vec{v}) d\vec{v}'}_{\text{collision}} \right] T(\vec{r}' \rightarrow \vec{r}, \vec{v}) d\vec{r}'}_{\text{transmission}}$$

COMBINE COLLISION AND TRANSMISSION KERNELS

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

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

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

... and so on ...

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

SUM OVER ALL COLLISIONS

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

Arriving at the *integral form* of the transport equation

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

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 $\vec{p}_0, \vec{p}_1, \dots, \vec{p}_k$)
 - Randomly sample from source: $\Psi_0(\vec{p}_0)$
 - Randomly sample for each of k transitions: $R(\vec{p}_{k-1} \rightarrow \vec{p}_k)$

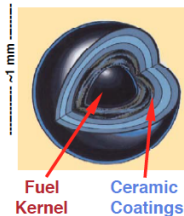
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- Integration over many variables
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 - Randomly sample from source: $\Psi_0(\vec{p}_0)$
 - Randomly sample for each of k transitions: $R(\vec{p}_{k-1} \rightarrow \vec{p}_k)$
- Average for result A 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

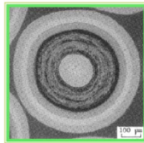


TRISO Fuel Particles:

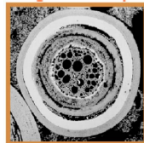
- Fission product gases trapped within coatings
- Coatings remain intact, even with high T & burnup

Fuel concept is same for block or pebble bed

Fresh Fuel



High Burnup



(From General Atomics)



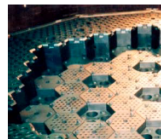
PARTICLES



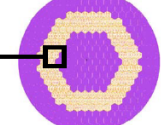
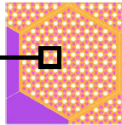
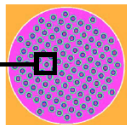
COMPACTS



FUEL BLOCK



CORE



Accurate & explicit modeling at multiple levels

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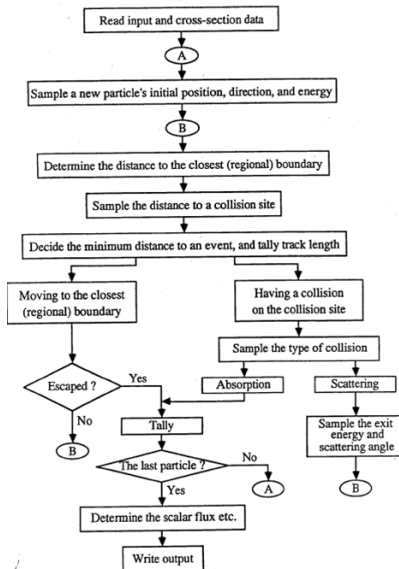
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- **Variance Reduction:** methods for reducing the variance and computation time simultaneously
- **Parallelization:** efficient use of computers

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

- ➊ Provide examples of probabilistic representations of physics
- ➋ Distinguish between a PDF and CDF
- ➌ Distinguish between a *discrete* PDF (CDF) and a *continuous* PDF (CDF)
- ➍ Describe the goal of random sampling
- ➎ Identify and implement the best random sampling technique for a given distribution

PHYSICS AS PROBABILITY

Various physical phenomena can be represented by probability distributions

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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

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

$$p(x) \geq 0$$
$$\int_{-\infty}^{\infty} p(x)dx = 1$$

Discrete

$$p(x = x_k) = p_k \equiv p(x_k)$$
$$k = 1, \dots, N$$

$$p_k \geq 0$$
$$\sum_{k=1}^N p_k = 1$$

CUMULATIVE DISTRIBUTION FUNCTIONS

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

Continuous

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

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

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

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

Discrete

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

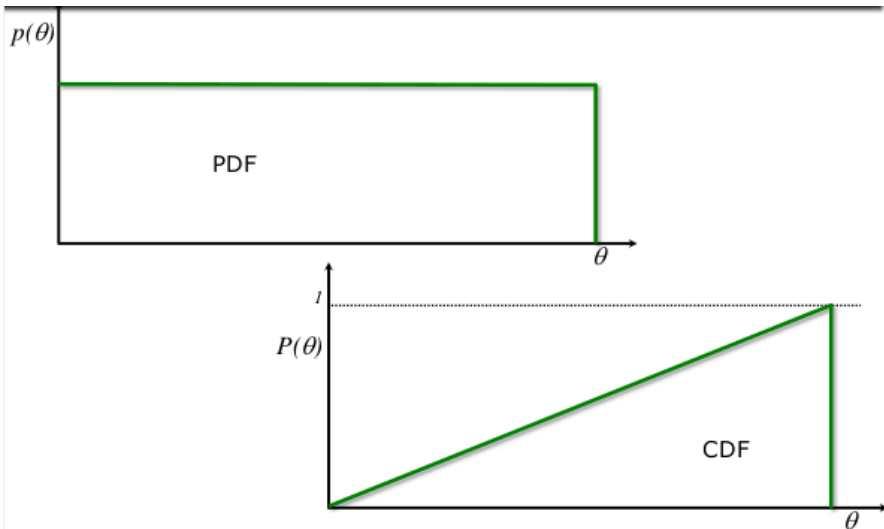
$$k = 1, \dots, N$$

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

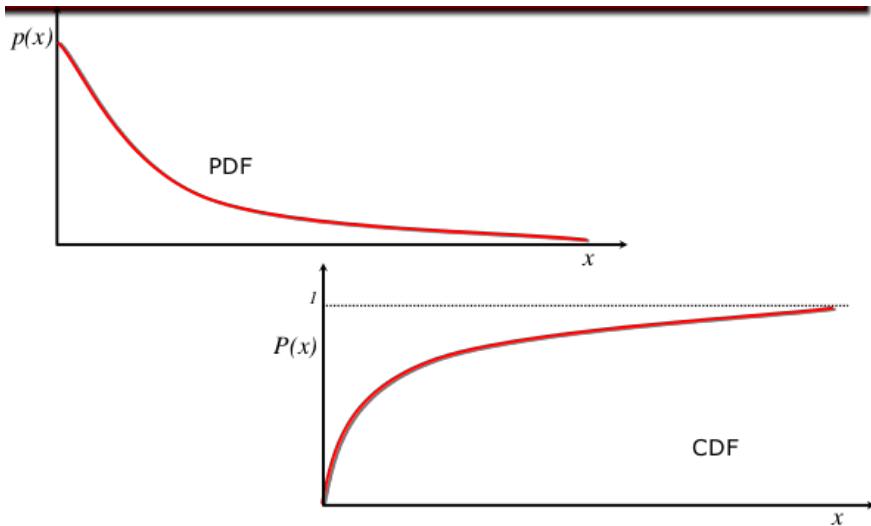
$$0 \leq P_k \leq 1$$

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

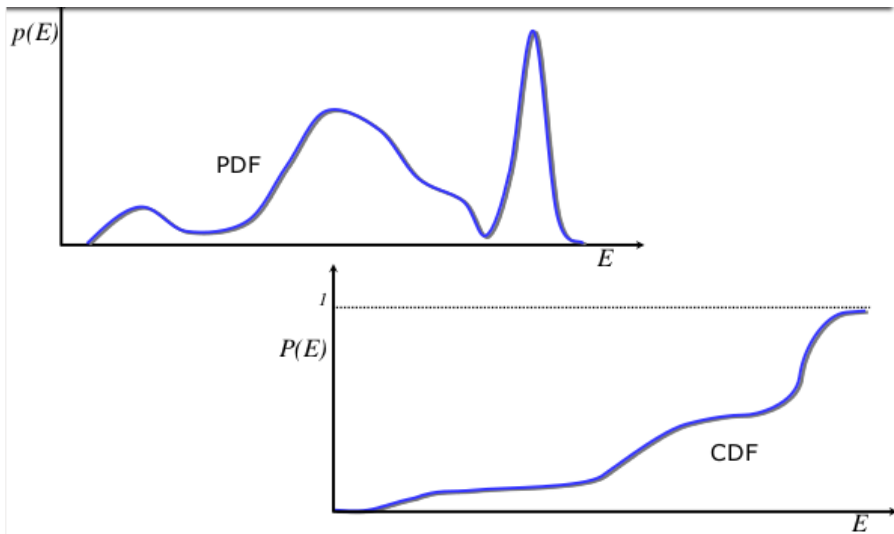
RANDOM SAMPLING BASICS



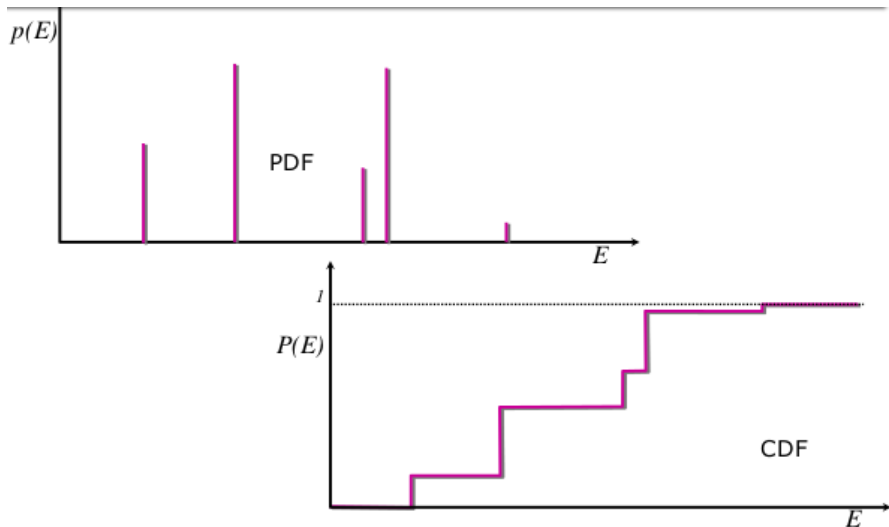
RANDOM SAMPLING BASICS



RANDOM SAMPLING BASICS



RANDOM SAMPLING BASICS



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

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:

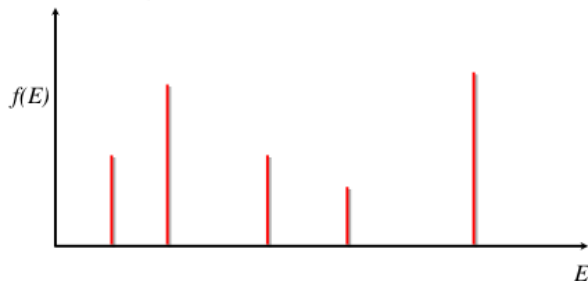
$$p(\xi) = \begin{cases} 1 & 0 \leq \xi < 1 \\ 0 & \text{otherwise} \end{cases}$$



DIRECT DISCRETE SAMPLING

Sampling Procedure

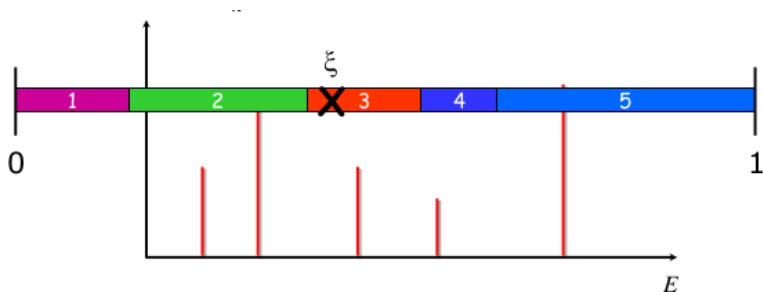
- Generate ξ
- Determine k such that $P_{k-1} \leq \xi \leq P_k$
- Return $x = x_k$



DIRECT DISCRETE SAMPLING

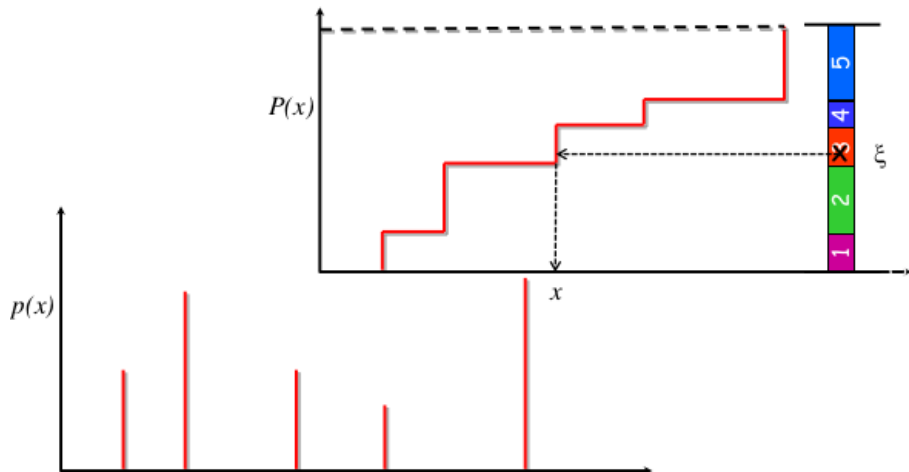
Sampling Procedure

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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

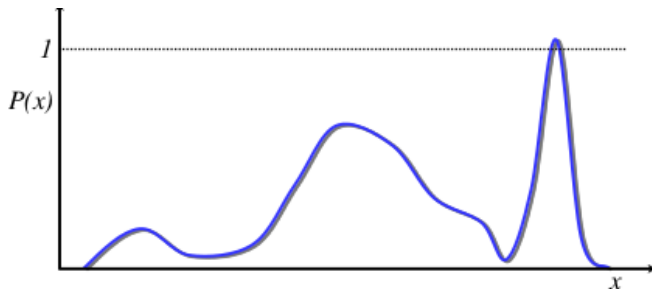
DIRECT DISCRETE SAMPLING

- 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:

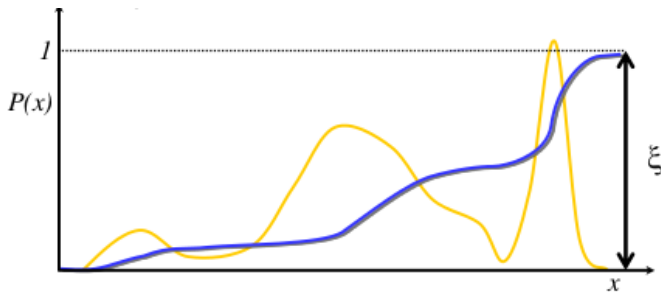
Generate ξ , Determine $x = P^{-1}(\xi)$



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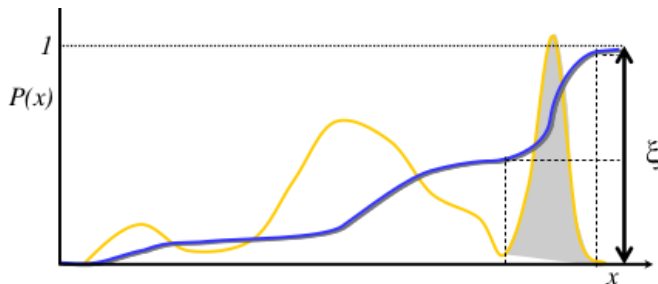
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- Sampling Procedure:

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



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

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

SIMPLE LINE, SLOPE = m

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SHIFTED LINE

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

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

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

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

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

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

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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

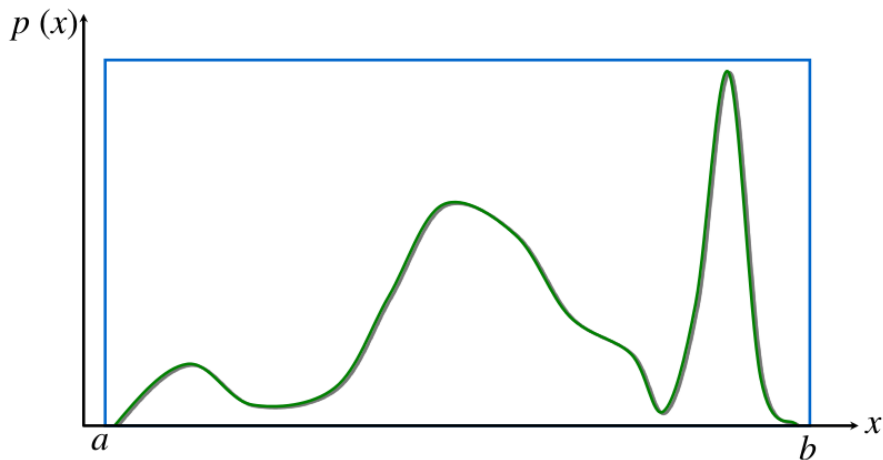
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- Select a bounding function, $g(x)$, such that
 - $g(x) \geq p(x)$ for all x
 - $g(x)$ is easy to sample
- Simplest choice is $g(x) = C$
- May not be best choice

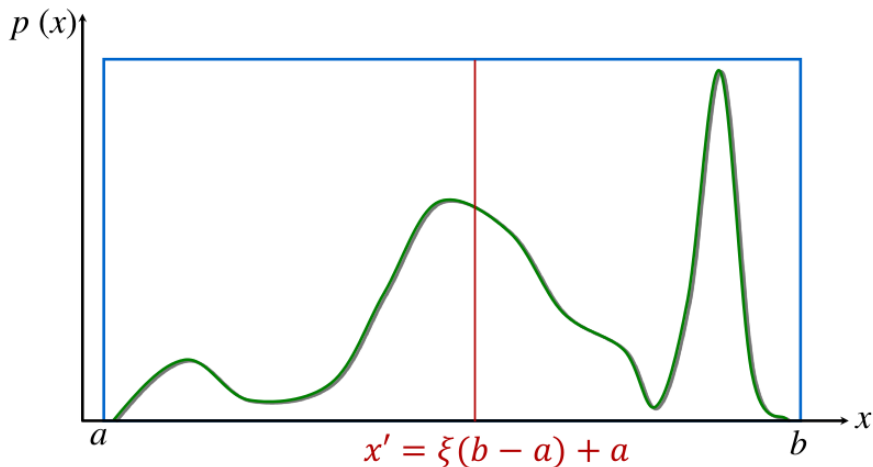
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- Generate pair of random variables, (ξ, η)
 - $x' = G^{-1}(\xi)$
 - If $\eta < p(x')/g(x')$, accept x'
 - Else, reject x'

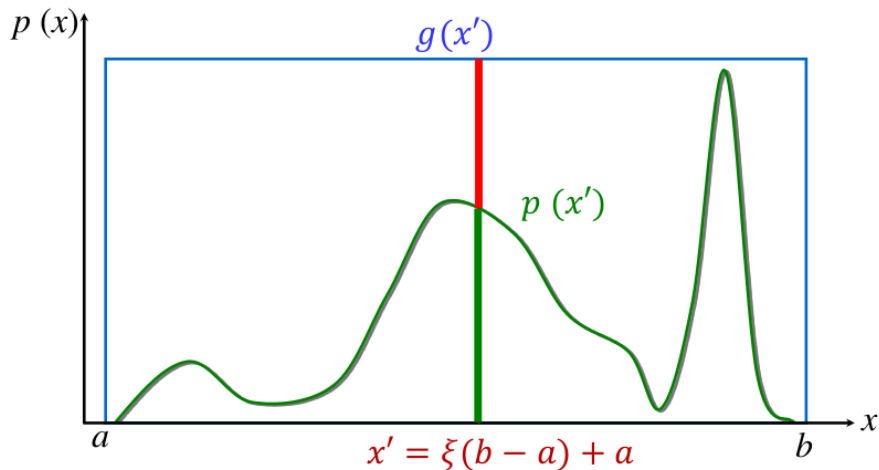
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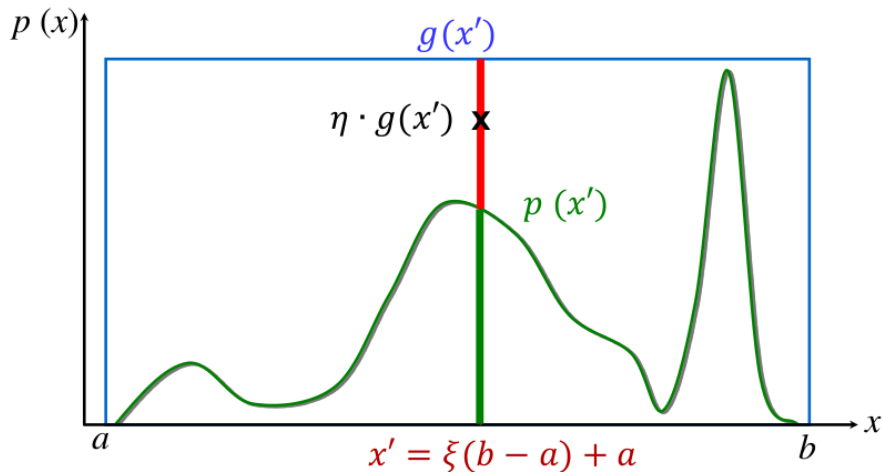
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- Advantages
 - Computationally simple
 - Always works

REJECTION SAMPLING

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

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

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- 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**