# NE 155/255
# Numerical Simulations in Radiation Transport
## Introduction to Monte Carlo

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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: $\xi$
  - Pair of random variables: $(\xi, \eta)$
- PDF for random variables:

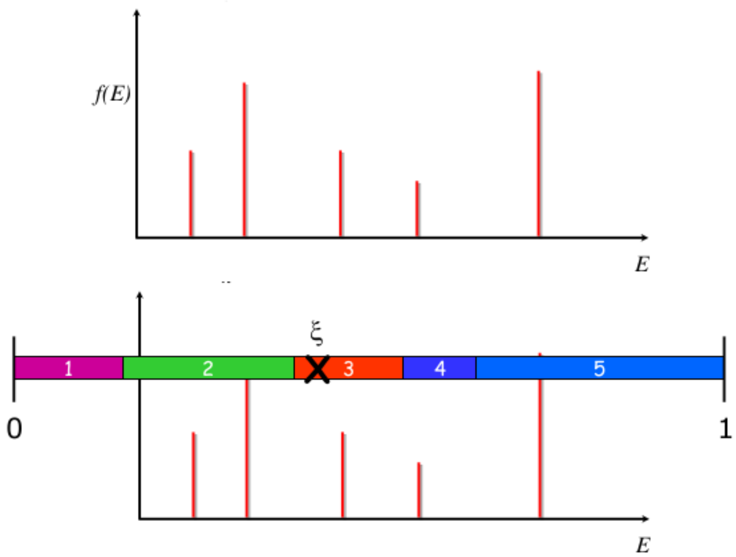
$$p(\xi) = \begin{cases} 1 & 0 \leq \xi < 1 \\ 0 & \text{otherwise} \end{cases}$$




# Direct Discrete Sampling

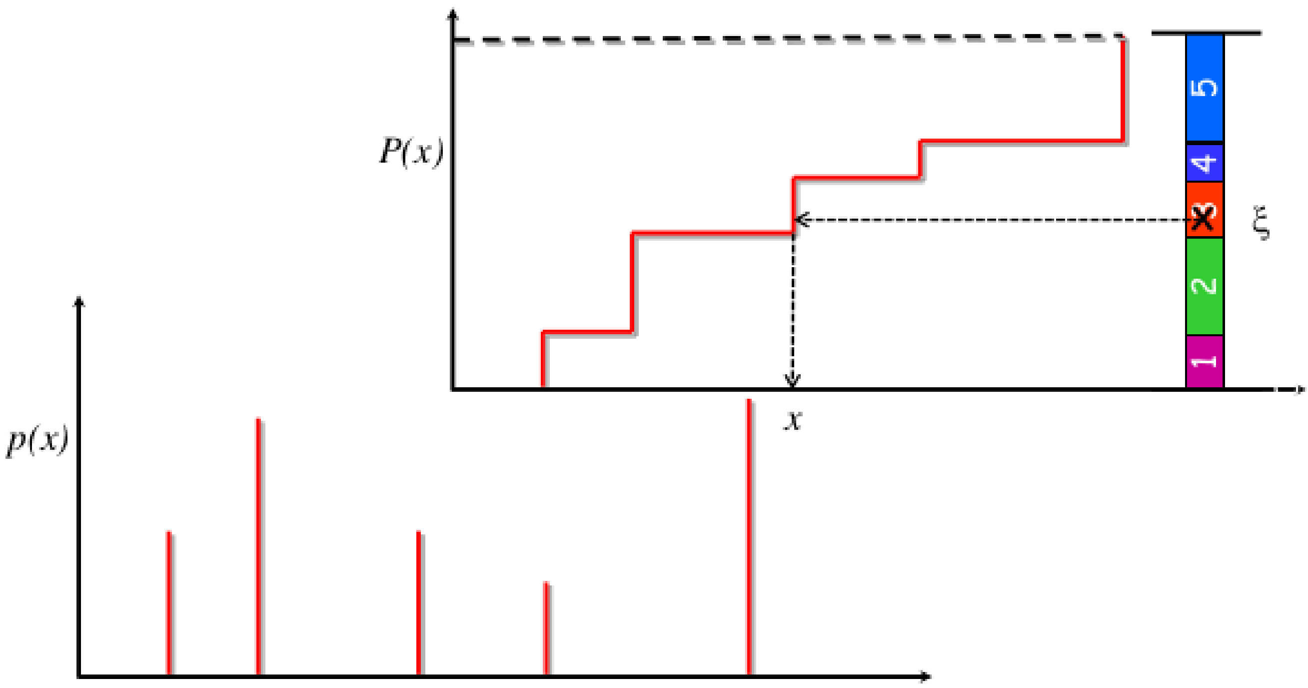
Sampling Procedure

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



# Direct Discrete Sampling

Consider the CDF





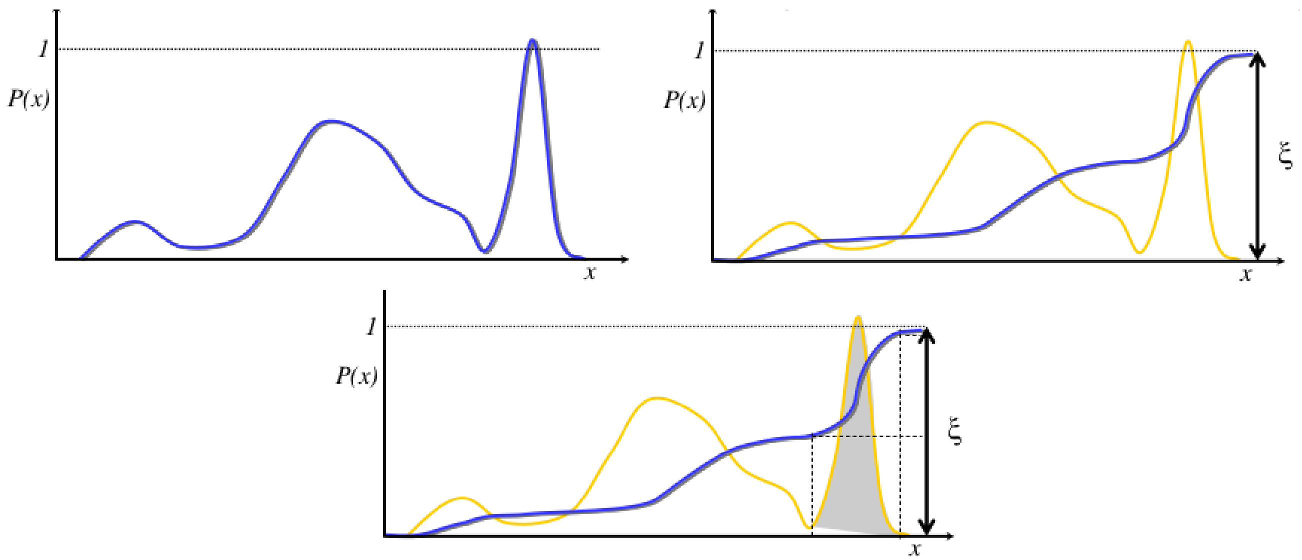

# Direct Discrete Sampling

- 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:

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






# 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~~
- 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

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

$$G(x) = \int_{-\infty}^{x} g(x')dx' = C\int_{a}^{x} dx' = C\left[x'\right]_a^x = C\left(x - a\right)$$

$$G(\infty) = G(b) = C(b - a)$$

$$p(x) = \frac{g(x)}{G(\infty)} = \frac{C}{C(b-a)} = \frac{1}{b-a} \quad a \leq x < b$$

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

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

## Simple Line, Slope $= m$

$$g(x)dx = mx\,dx \qquad 0 \le x < 1$$

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

$$G(\infty) = G(1) = \frac{m}{2}$$

$$p(x) = \frac{mx}{\frac{m}{2}} = 2x \qquad 0 \le x < 1$$

$$P(x) = \int_{-\infty}^{x} p(x')dx' = \int_{0}^{x} 2x'dx' = \left[x'^2\right]_0^x = x^2$$

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



## Shifted Line

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

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

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

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

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

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

# Rejection Sampling

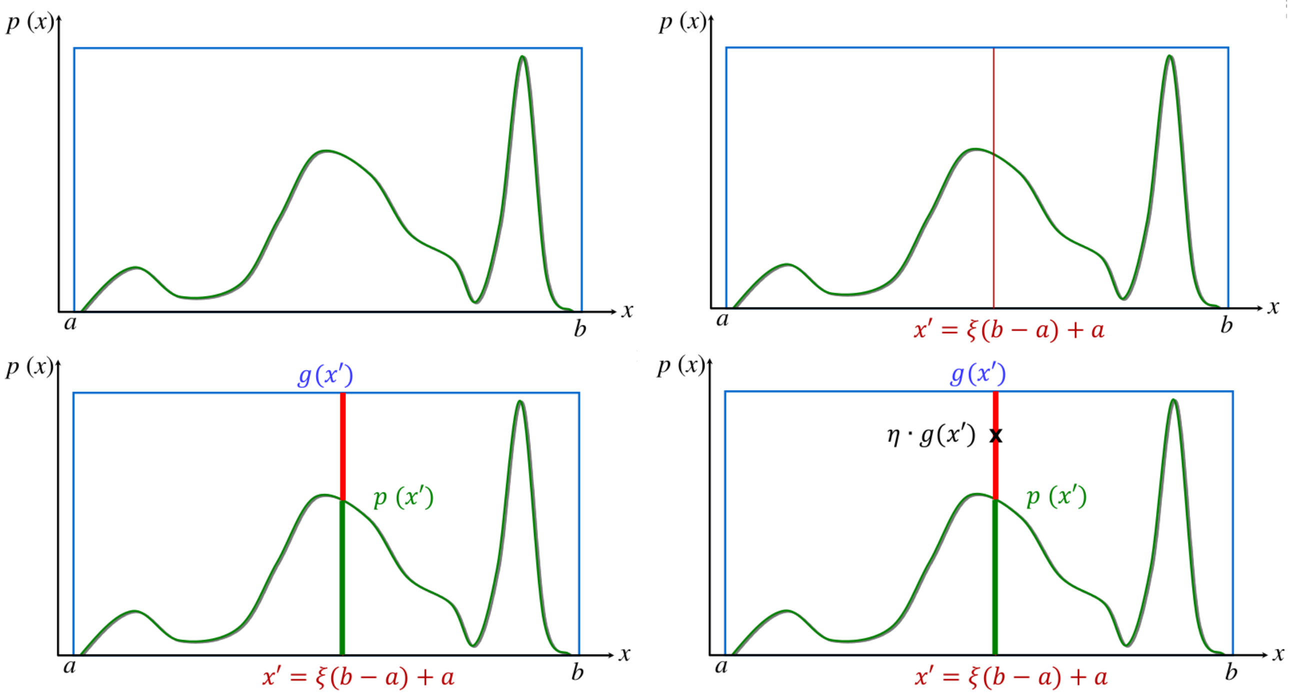
- Many CDFs cannot be inverted
  - e.g. Klein-Nishina cross-section
- Use an approach that is more graphical
  - Select a point in a 2-D domain
  - Determine whether that point is above or below the PDF
  - Keep those that are below
  - Start over if above



# 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, $(\xi, \eta)$
  - $x' = G^{-1}(\xi)$
  - If $\eta < p(x')/g(x')$, accept $x'$
  - Else, reject $x'$

# Rejection Sampling






# 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