Random Sampling

SNU/NUKE/EHK

Random Sampling for Possible States

- Monte Carlo simulation
  - is applied to some physical and mathematical systems that can be described in terms of probability density functions or pdf's.
  - works on the physical and mathematical system by random sampling from those pdf's and by performing the necessary supplementary computations needed to describe the system evolution.
  - The physical condition and mathematical element are defined by random sampling out of possible choices according to pdf's.

Continuous vs. Discrete pdf's

Table 1. Properties of continuous and discrete pdf's

property	Continuous: $f(x)$	Discrete: $\{p_i\}$
positivity	$f(x) \geq 0, all\ x$	$p_i > 0, all\ i$
normalization	$\int_{-\infty}^{\infty} f(x')dx' = 1$	$\sum_{j=1}^{N} p_j = 1$
interpretation	$f(x)dx = Prob(x \leq x' \leq x' + dx)$	$p_i = prob(i) = prob(x_j = x_i)$
mean	$\bar{x} = \int_{-\infty}^{\infty} xf(x)dx$	$\bar{x} = \sum_{j=1}^{N} x_j \cdot p_j$
variance	$\sigma^2 = \int_{-\infty}^{\infty} (x - \bar{x})^2 f(x)dx$	$\sigma^2 = \sum_{j=1}^{N} (x_j - \bar{x})^2 \cdot p_j$

Equivalent Continuous pdf's

- To express a discrete pdf as a continuous pdf, which simplifies the manipulations for discrete pdf's.

- Given a discrete pdf $\{p_i\}$, associate an event i with the discrete r.v. x_i and then define an equivalent "continuous" pdf as follows:

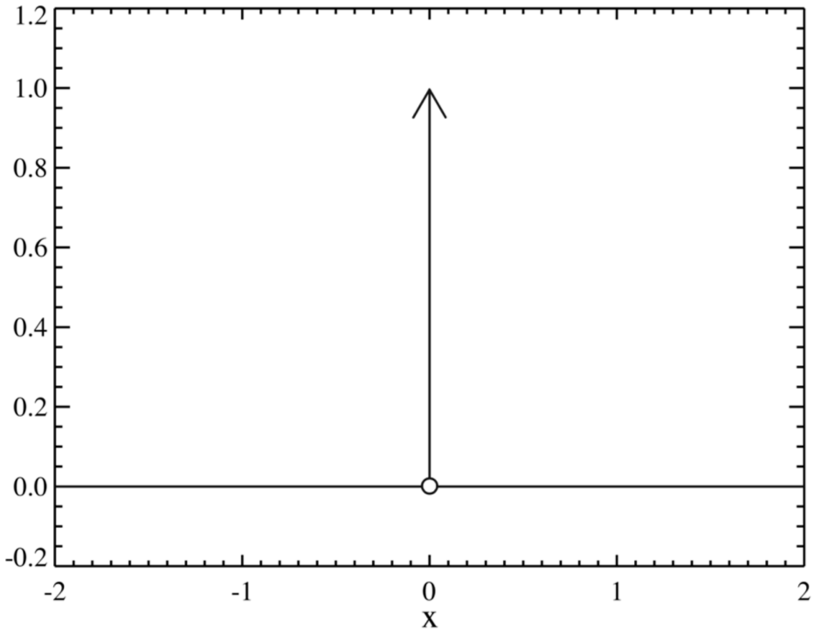
$$f(x) = \sum_{i=1}^{N} p_i \delta(x - x_i) \qquad (1)$$

where $\delta(x-x_i)$ is the "delta" function and it satisfies the following properties: $\delta(x-a) = 0$ for $x \neq a$ and

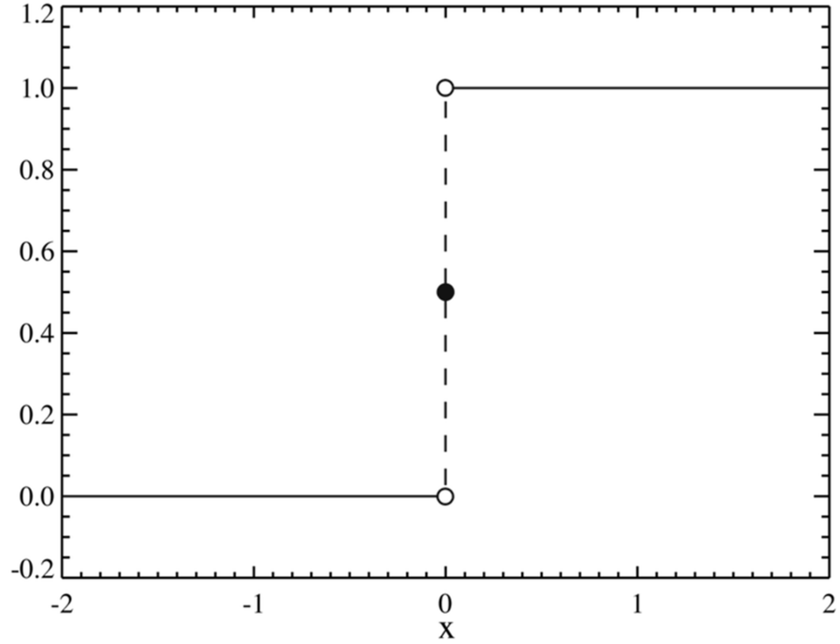
$$\int_{-\infty}^{\infty} \delta(x - x_i) dx = 1 \qquad (2)$$

$$\int_{-\infty}^{\infty} f(x) dx = \int_{-\infty}^{\infty} \sum_{i=1}^{N} p_i \delta(x - x_i) dx = \sum_{i=1}^{N} p_i \int_{-\infty}^{\infty} \delta(x - x_i) dx = \sum_{i=1}^{N} p_i = 1 \qquad (3)$$

Delta function: $\delta(x)$, $\Delta(x)$



pdf



cdf

$$f(x) = \sum_{i=1}^{N} p_i \delta(x - x_i)$$

$$F(x_J) = \int_{-\infty}^{x_J} f(x)\,dx = \int_{-\infty}^{x_J} \sum_{i=1}^{N} p_i \delta(x - x_i)\,dx$$

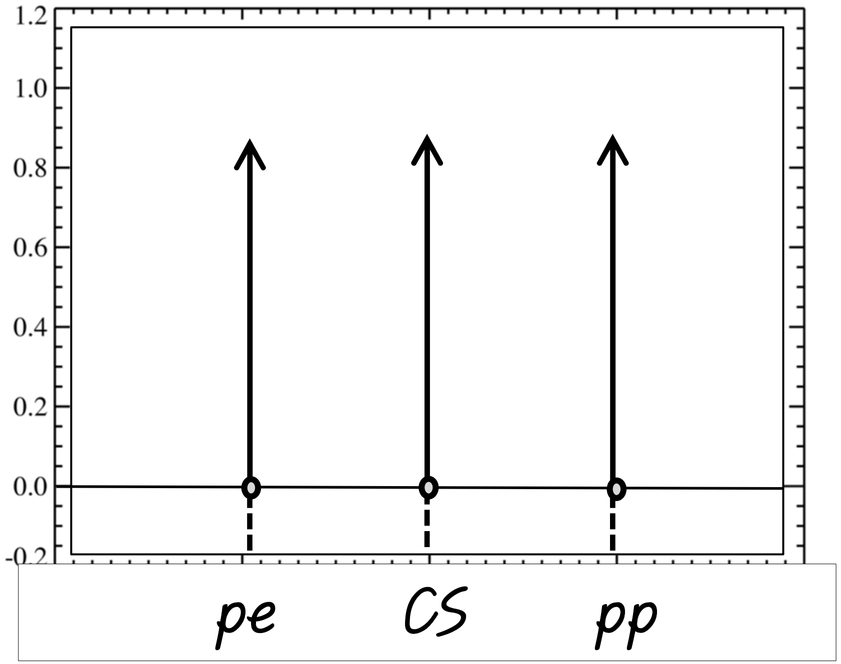
$$= \sum_{i=1}^{N} p_i \int_{-\infty}^{x_J} \delta(x - x_i)\,dx$$

$$= \sum_{i=1}^{N} p_i \Delta(x_J - x_i)$$

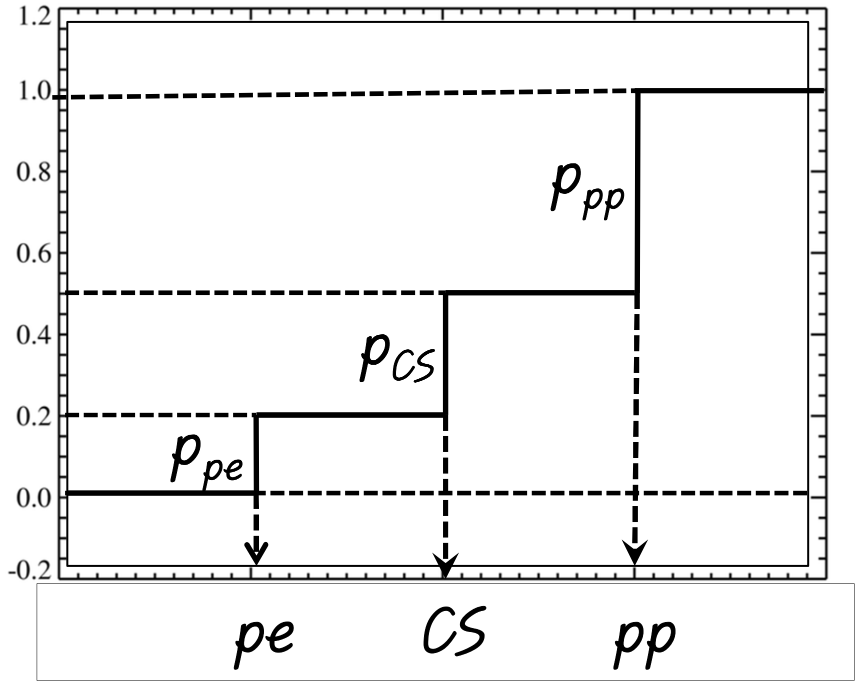
$$= \sum_{i=1}^{i \le J} p_i \Delta(x_J - x_i) + \sum_{i>J}^{N} p_i \Delta(x_J - x_i)$$

$$= \sum_{i=1}^{i \le J} p_i$$

Ex: cdf for selection of photon interaction modes in 20% pe, 30% CS and 50% pp



pdf : f(x)



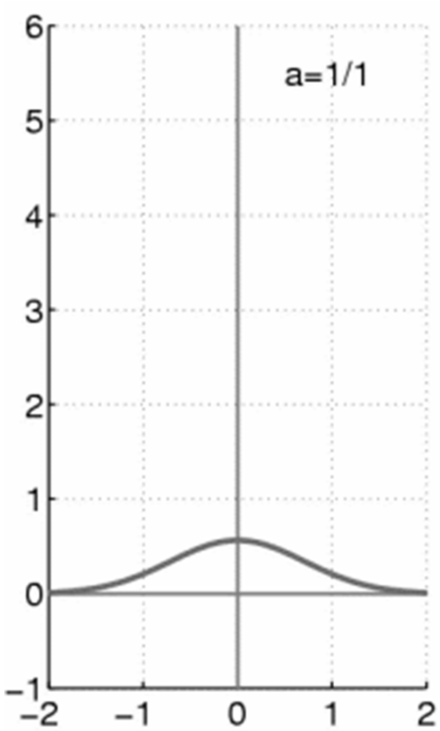
cdf : F(x)

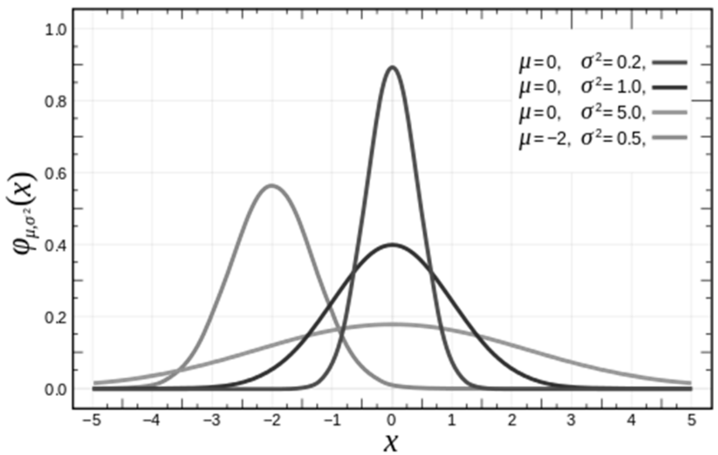
(Dirac) delta function

$$\delta(x) = \begin{cases} \infty, & x = 0 \\ 0, & x \neq 0 \end{cases} \qquad (1)$$

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1, \text{ where } \delta(x) = 0 \text{ for } x \neq 0 \qquad (2)$$

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$





$$\delta(x) = \lim_{a \to 0} \frac{1}{a\sqrt{\pi}} e^{-x^2/a^2}$$

Equivalent Continuous pdf's (cont.)

- *Mean and Variance*

$$\bar{x} = \int_{-\infty}^{\infty} x f(x) dx = \int_{-\infty}^{\infty} x \left[\sum_{i=1}^{N} p_i \delta(x - x_i) \right] dx$$

$$= \sum_{i=1}^{N} p_i \int_{-\infty}^{\infty} x \delta(x - x_i) dx = \sum_{i=1}^{N} p_i x_i \qquad (4)$$

$$var(x) = \int_{-\infty}^{\infty} (x - \bar{x})^2 f(x) dx = \int_{-\infty}^{\infty} (x^2 - 2\bar{x}x + \bar{x}^2) \left[\sum_{i=1}^{N} p_i \delta(x - x_i) \right] dx$$

$$= \sum_{i=1}^{N} p_i \int_{-\infty}^{\infty} (x^2 - 2\bar{x}x + \bar{x}^2) \delta(x - x_i) dx = \sum_{i=1}^{N} p_i (x_i^2 - 2\bar{x}x_i + \bar{x}^2)$$

$$= \sum_{i=1}^{N} p_i (x_i - \bar{x})^2 \qquad (5)$$

- *The equivalent continuous pdf has its mean and variance to be equal to those of the discrete pdf.*

Transformation of pdf's

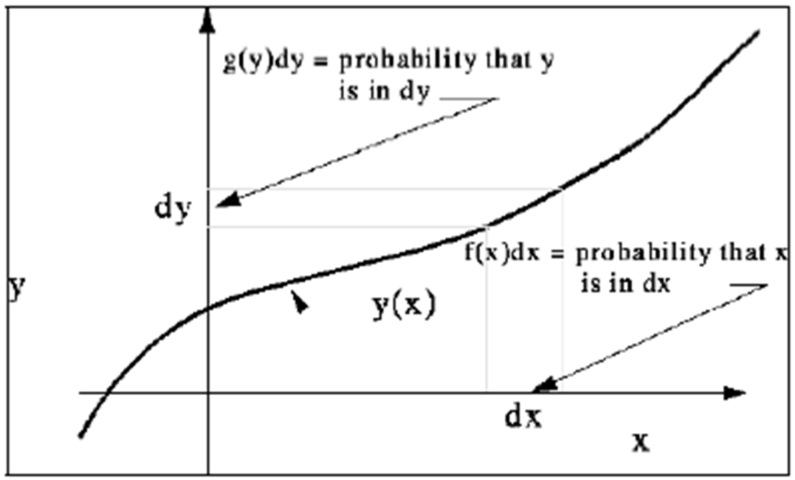
- Given a pdf f(x), one define a new variable y(x) with the goal of finding the pdf g(y).
  - Restrict the transformation y(x) to be a unique transformation, that is, a given value of x corresponds unambiguously to a value of y.
  - Given a 1–to–1 relationship between x and y, y(x) must be strictly monotonically increasing or strictly monotonically decreasing.

Transformation of pdf's (cont.)

– The mathematical transformation must conserve probability: <u>the probability of x' occurring in dx about x</u> must be the same as <u>the probability of y occurring in dy about y</u>:

$f(x)dx = g(y)dy$ for strictly (monotone) increase: $dy/dx > 0$ (1)

where $f(x)dx = prob(x \le x' \le x+dx)$ and
$g(y)dy = prob(y \le y' \le y+dy)$

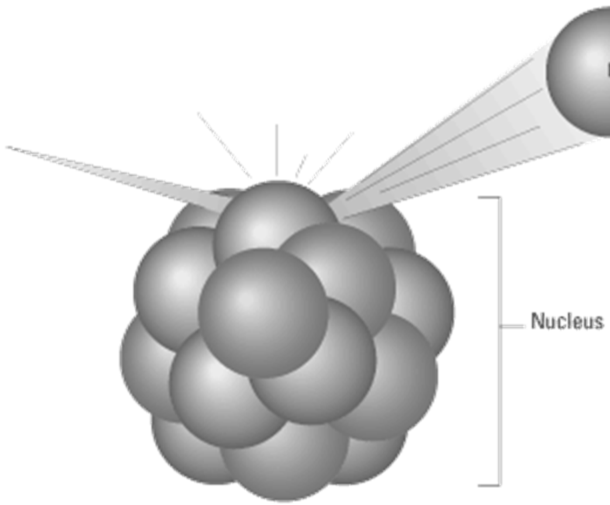


Transformation of pdf's (cont.)

– From (1), $g(y) = f(x)/[dy/dx]$ with <u>strictly</u> monotonous increase in $y(x)$ whereas $g(y) = f(x)/[-dy/dx]$ with <u>strictly</u> monotonous decrease in $y(x)$ due to the fact that <u>$f(x)$ and $g(y)$ are positive</u> by definition of probability.

Ex. Neutron elastic scattering

- *In elastic neutron-scattering, the neutron bounces off the bombarded nucleus without exciting or destabilizing it. With each elastic interaction, the neutron loses energy.*



Ex. Neutron elastic scattering (cont.)

- Consider the elastic scattering of neutrons of energy E_0 from a nucleus of mass A at rest
  - Define $f(E)dE$ as the probability that the final energy of the scattered neutrons is in the energy interval dE about E with the pdf $f(E)$ given by.

$$f(E) = \begin{cases} \dfrac{1}{(1-\alpha)E_0} , & \alpha E_0 \le E \le E_0 \\ 0 , & \text{otherwise} \end{cases}, \quad \text{where } \alpha = \left(\frac{A-1}{A+1}\right)^2 \qquad (2)$$

Ex. Neutron elastic scattering (cont.)

- What is the probability $g(v)dv$ that the neutron scatters in the speed interval dv about v where $E = mv^2/2$?
  - Using Eq. (1), one can find the following:

$$g(v) = \begin{cases} \dfrac{2v}{(1-\alpha)v_0^2}, & \sqrt{\alpha}\, v_0 \le v \le v_0 \\ 0, & \text{otherwise} \end{cases} \qquad (2)$$

  - $\int_{-\infty}^{\infty} g(v)dv = \int_{\sqrt{\alpha}v_0}^{v_0} \dfrac{2v}{(1-\alpha)v_0^2} dv = 1.$

Transformation to cdf's

- Given a cdf $F(x)$

$$y(x) = F(x) \equiv \int_{-\infty}^{x} f(x')dx', \qquad (3)$$

one finds that the pdf $g(y)$

$$g(y) = 1, \quad \text{for } 0 \le y \le 1 \qquad (4)$$

since $g(y) = f(x)(dy/dx)^{-1}$ and $dy/dx = f(x)$.

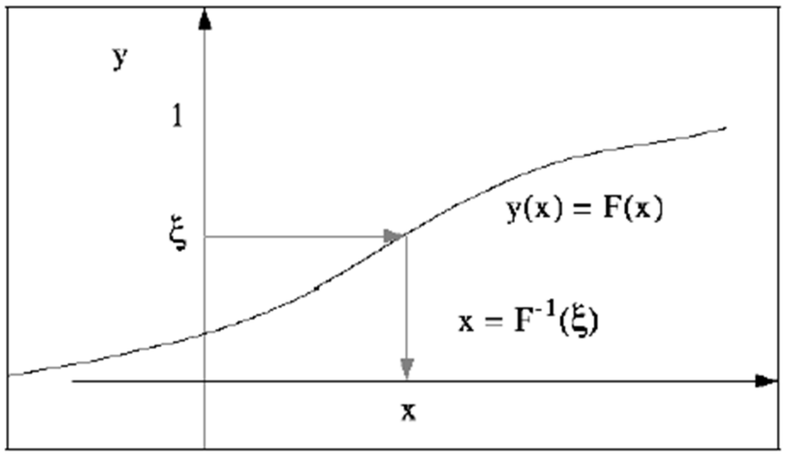
- The cdf $y(x) = F(x)$ always uniformly distributed on [0, 1], <u>independently of the pdf f(x)</u>!
- Any value of y for the cdf $g(y)$ is equally likely on the interval [0, 1].

← We pick up a random number just like that way!

Sampling via Inversion of cdf

- The r.v. x and the cdf $F(x)$ correspond by one-to-one. Hence one can sample $y(x) = F(x)$ and then solve for x by inverting $F(x)$: $x = F^{-1}(y)$.
- Since y is uniformly distributed on [0, 1], as shown in (4), one simply uses a random number generator that gives any number on [0, 1] by uniform chance to generate a sample $y = \xi$ from the cdf $F(x)$. The value x is then $x = F^{-1}(\xi)$

--→ golden rule for sampling



Ex. a pdf f(x) of uniform distribution

- Let the random variable x be uniformly distributed between a and b.

$$f(x) = \begin{cases} 1/(b-a), & a \le x \le b \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

- The cdf F(x) is

$$F(x) = (x-a)/(b-a).$$

- Sample a random number ξ, set it equal to F(x). Then

$$x = a + (b-a)\xi,$$

which yields a sample point x that is uniformly distributed on the interval [a, b].

Ex. An exponential distribution of x

- Consider the penetration of neutrons in a shield. The pdf for the distance x to collision is described by

$$f(x) = \Sigma_t e^{-\Sigma_t x} \; for \; \Sigma_t > 0 \; and \; x \geq 0. \qquad (6)$$

- A distance x to collision is then chosen by sampling a value ξ from the cdf F(x) from [0, 1]:
  - The cdf is $F(x) = 1 - e^{-\Sigma_t x}$.
  - Set $\xi = 1 - e^{-\Sigma_t x}$.
  - Obtain $x = -\frac{\ln(1-\xi)}{\Sigma_t}$ or $x = -\frac{\ln(\xi)}{\Sigma_t}$.

- mean distance ?

$$0 < \; x = -\frac{\ln(\xi)}{\Sigma_t} < \; \infty$$