# 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:

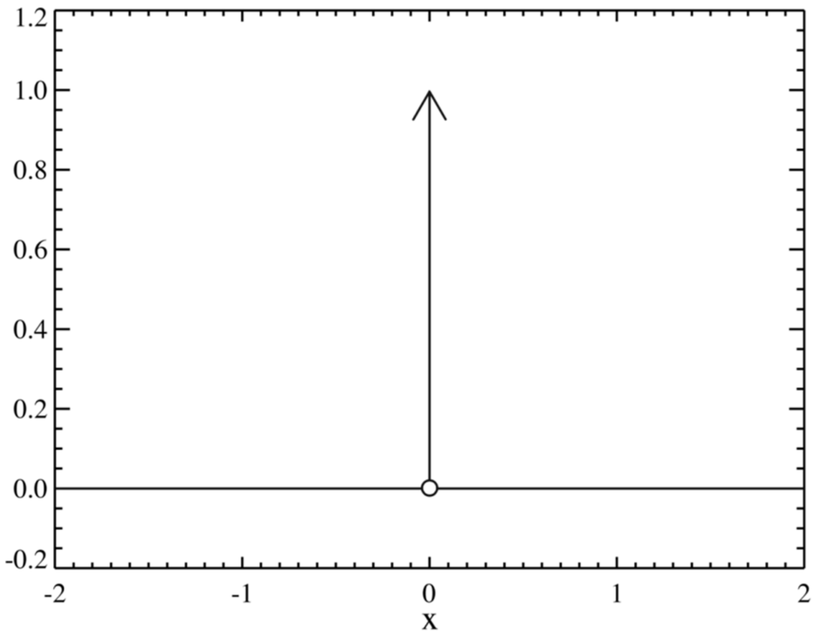
$$f(x) = \sum_{i=1}^{N} p_i \delta(x - x_i) \qquad (1)$$

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

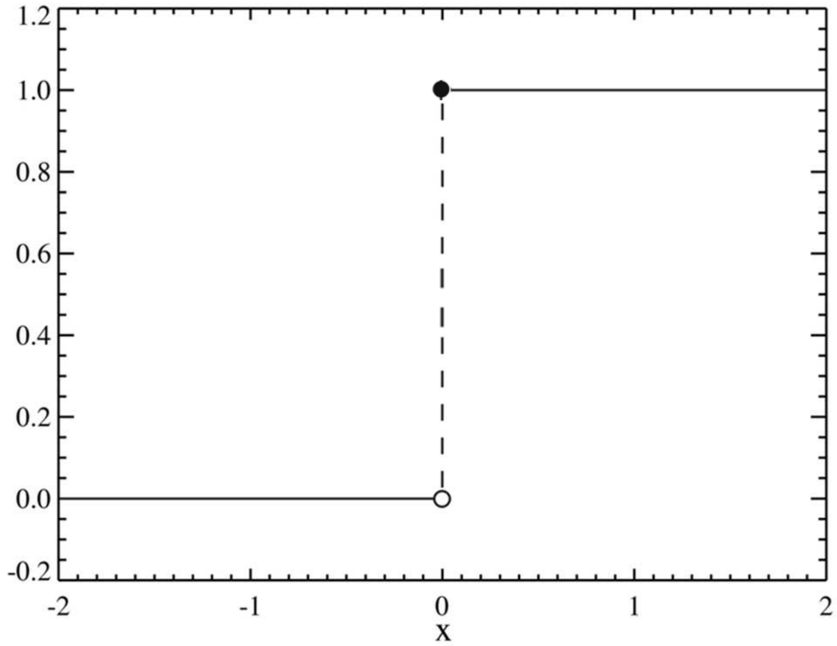
$$\int_{-\infty}^{\infty} \delta(x - x_i) dx = 1 \qquad (2)$$

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

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




pdf




cdf

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

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

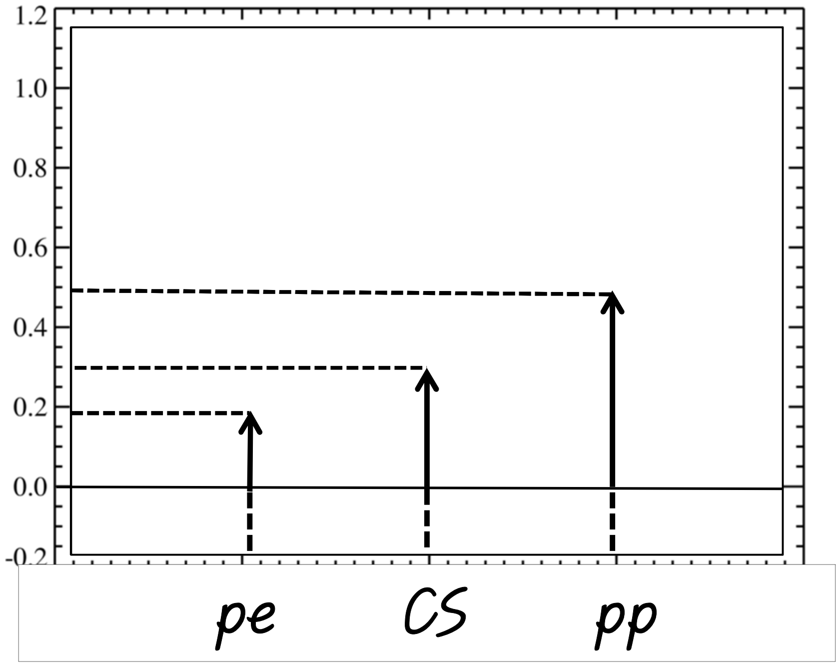
$$= \sum_{i=1}^{N} p_i \int_{-\infty}^{x_J} \delta(x - x_i)\, dx$$

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

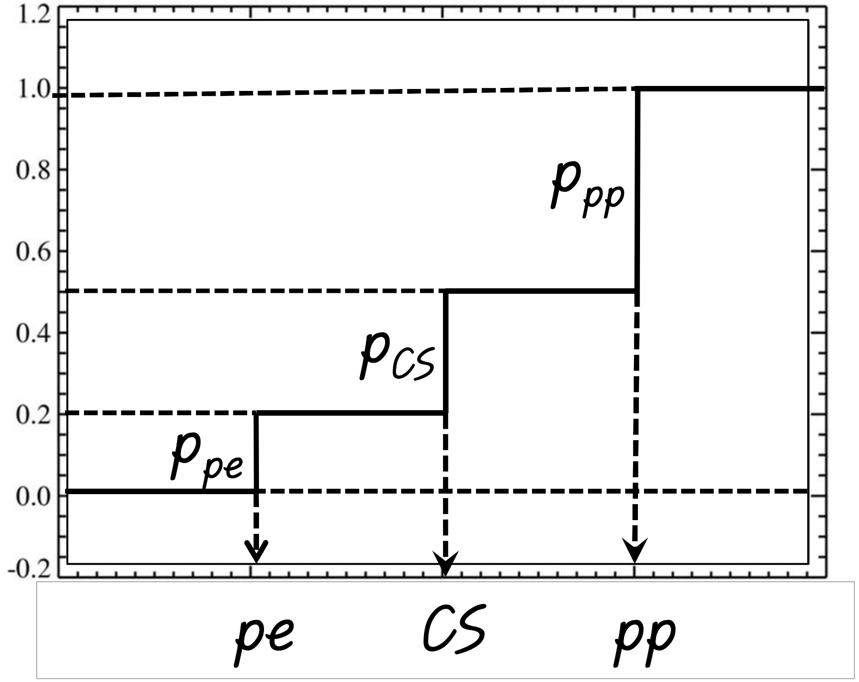
$$= \sum_{i=1}^{i \le J} p_i \Delta(x_J - x_i) + \sum_{i>J}^{N} p_i \Delta(x_J - x_i)$$

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

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




pdf : f(x)



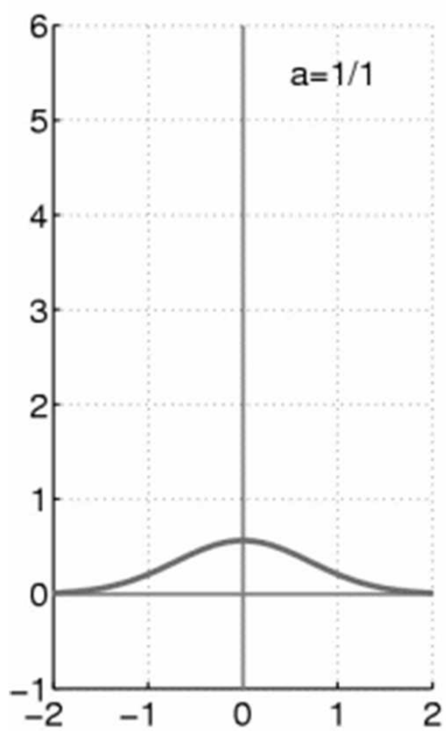

cdf : F(x)

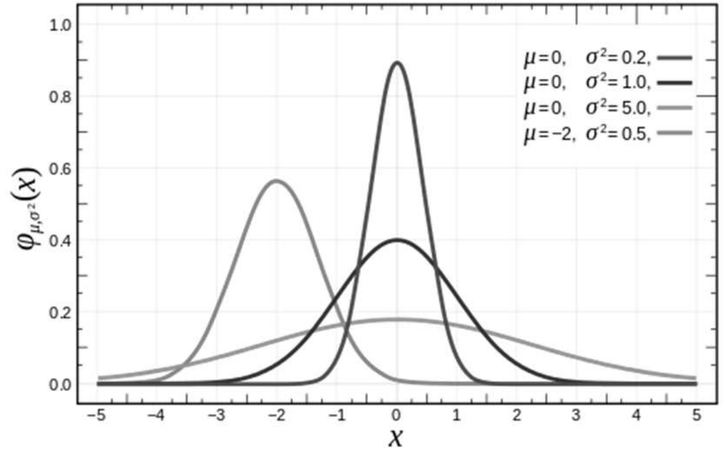
# (Dirac) delta function

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

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

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




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

# Equivalent Continuous pdf's (cont.)

- Mean and Variance

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

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

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

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

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

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

# *Transformation of pdf's*

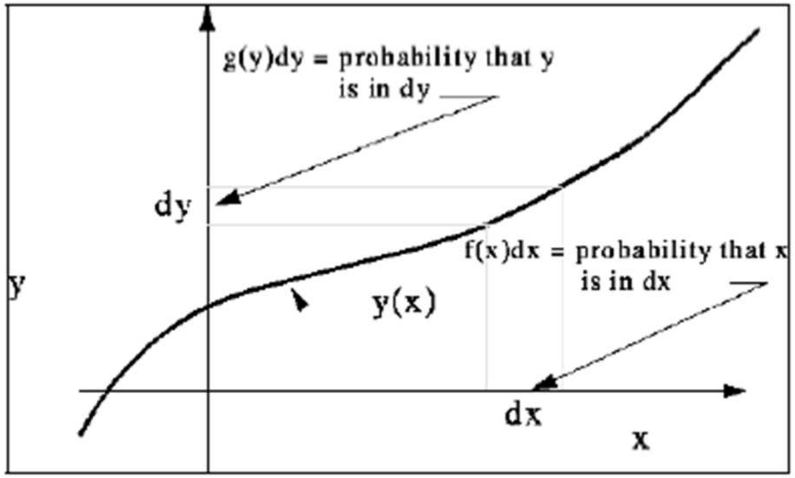
- *Given a <u>pdf</u> f(x), one define a new variable y(x) with the goal of finding the <u>pdf</u> g(y).*
  - *Restrict the transformation y(x) to be a unique transformation, that is, a given value of x corresponds unambiguously to a value of y.*
  - *Given a 1–to–1 relationship between x and y, y(x)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

# Transformation of pdf's (cont.)

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

$$f(x)dx = g(y)dy \quad \text{for strictly (monotone) increase: } dy/dx > 0 \qquad (1)$$

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

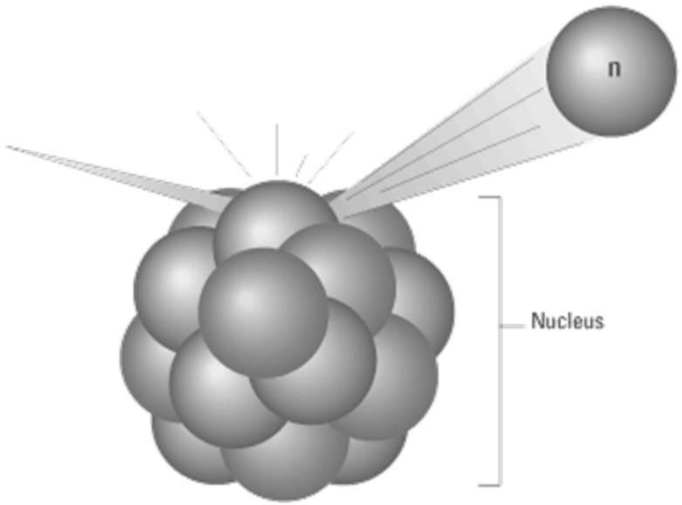


# Transformation of pdf's (cont.)

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

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

# 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:

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

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

# 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 $g(y)$

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

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

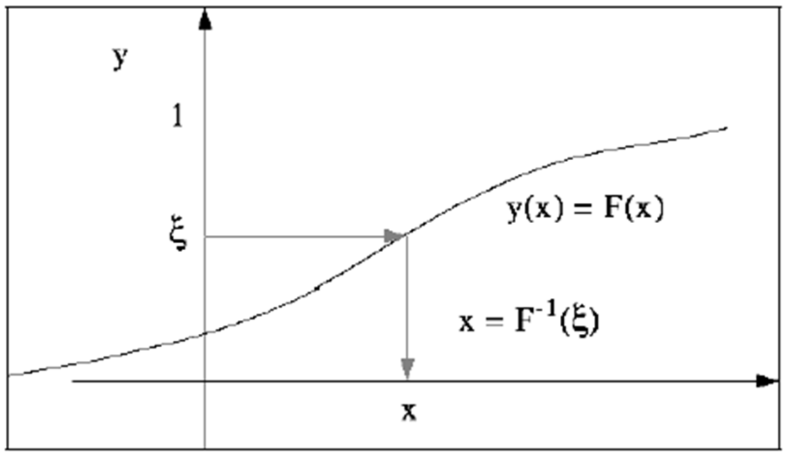
- The cdf $y(x) = F(x)$ always uniformly distributed on [0, 1], independently of the pdf $f(x)$!
- Any value of $y$ for the cdf $g(y)$ is equally likely on the interval [0, 1].

← 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 $b$.

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

- The cdf $F(x)$ is

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

- Sample a random number $\xi$, 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 $[a, b]$.

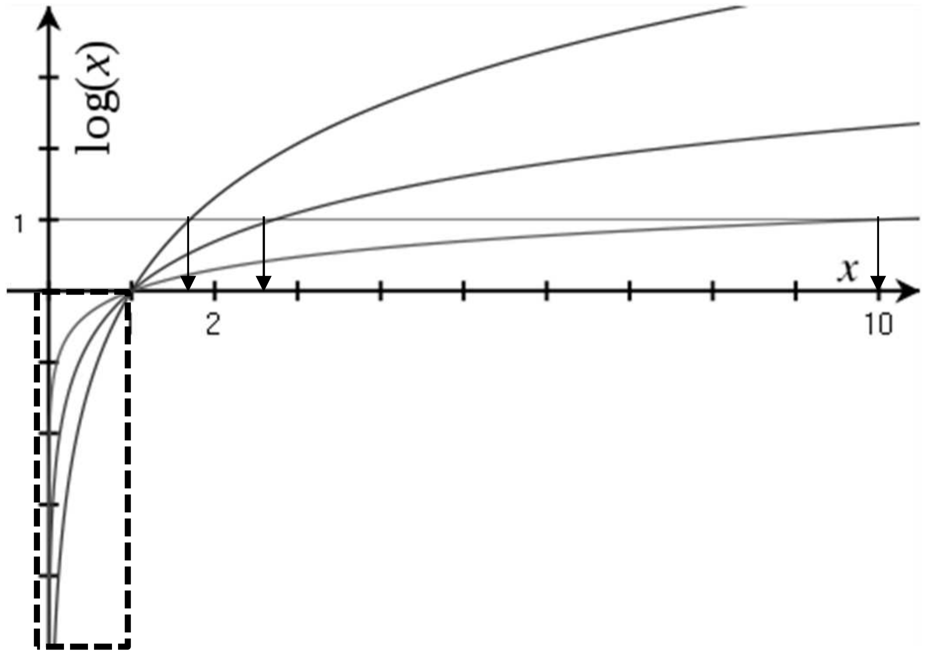
# Ex. An exponential distribution of x

- 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 ?




Logarithm functions, graphed for various bases:
Each tick on the axes is one unit. Logarithms of all bases pass through the point (1,0), because any non-zero number raised to the power 0 is 1, and through the points (b,1) for base b, because a number raised to the power 1 is itself. The curves approach the y-axis but do not reach it because of the singularity at $x = 0$ (a vertical asymptote).

# Homework #1 & #2