# Random processes and Monte Carlo Simulation

- Monte Carlo integration.
- Non-uniform distributions.
- Random walk.

### Mean value method

■ There are better ways of evalutating this integral:

$$I = \int_{a}^{b} f(x)dx$$

#### Mean value method

■ There are better ways of evalutating this integral:

$$I = \int_{a}^{b} f(x)dx$$

■ Average value  $\langle f \rangle$  in range a to b is:

$$\langle f \rangle = \frac{1}{b-a} \int_{a}^{b} f(x) dx = \frac{I}{b-a}$$

### Mean value method

■ There are better ways of evalutating this integral:

$$I = \int_{a}^{b} f(x)dx$$

■ Average value  $\langle f \rangle$  in range a to b is:

$$\langle f \rangle = \frac{1}{b-a} \int_{a}^{b} f(x) dx = \frac{I}{b-a}$$

■ A simple way to estimate  $\langle f \rangle$  is to just measure f(x) at N points,  $x_1, x_2, \ldots, x_N$  chosen uniformly between a and b:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

$$I \simeq \frac{b-a}{N} \sum_{i=1}^{N} f(x_i)$$

lacktriangle Variance of the sum on N independent random numbers is equal to N times the variance of a single one.

- lacksquare Variance of the sum on N independent random numbers is equal to N times the variance of a single one.
- Random numbers in this case are the values  $f(x_i)$  and we can estimate the variance of a single one of them  $var f = \langle f^2 \rangle \langle f \rangle^2$  with:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

- lacksquare Variance of the sum on N independent random numbers is equal to N times the variance of a single one.
- Random numbers in this case are the values  $f(x_i)$  and we can estimate the variance of a single one of them  $var f = \langle f^2 \rangle \langle f \rangle^2$  with:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

■ Variance on the sum is N times the variance on a single term or N var f.

- lacktriangle Variance of the sum on N independent random numbers is equal to N times the variance of a single one.
- Random numbers in this case are the values  $f(x_i)$  and we can estimate the variance of a single one of them  $var f = \langle f^2 \rangle \langle f \rangle^2$  with:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

- Variance on the sum is N times the variance on a single term or N var f.
- Error/standard deviation on the integral:

$$\sigma = \frac{b - a}{N} \sqrt{N \operatorname{var} f} = (b - a) \frac{\sqrt{\operatorname{var} f}}{\sqrt{N}}$$

which goes as  $1/\sqrt{N}$  but the variance is smaller!

# Non-uniform sampling

In a large number of situations, random numbers with nonuniform distribution are needed (rather than uniform distribution)

# Non-uniform sampling

In a large number of situations, random numbers with nonuniform distribution are needed (rather than uniform distribution)

Radioactive decay

# Non-uniform sampling

In a large number of situations, random numbers with nonuniform distribution are needed (rather than uniform distribution)

- Radioactive decay
- Experiments with different types of distributions

How does one generate non-uniform random number distributions with a uniform random number generators?

Generating a non-uniform distribution with a probability distribution w(x):

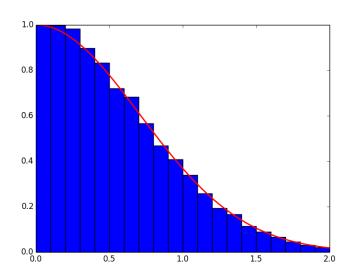
■ Generate two random numbers  $x_i$  on  $[x_{min}, x_{max}]$  and  $y_i$  on  $[y_{min}, y_{max}]$ 

- Generate two random numbers  $x_i$  on  $[x_{min}, x_{max}]$  and  $y_i$  on  $[y_{min}, y_{max}]$
- If  $y_i < w(x_i)$  accept  $x_i$ .

- Generate two random numbers  $x_i$  on  $[x_{min}, x_{max}]$  and  $y_i$  on  $[y_{min}, y_{max}]$
- If  $y_i < w(x_i)$  accept  $x_i$ .
- If  $y_i > w(x_i)$  reject  $x_i$ .

- Generate two random numbers  $x_i$  on  $[x_{min}, x_{max}]$  and  $y_i$  on  $[y_{min}, y_{max}]$
- If  $y_i < w(x_i)$  accept  $x_i$ .
- If  $y_i > w(x_i)$  reject  $x_i$ .
- The  $x_i$  so accepted will have the weighting  $w(x_i)$ .

$$w(x) = e^{-x^2}$$
  $x \in [0, 2]$ 



■ Suppose we have a source of random numbers z drawn from a distribution with probability density q(z) – the probability of generating a number between z and z+dz is q(z)dz.

- Suppose we have a source of random numbers z drawn from a distribution with probability density q(z) the probability of generating a number between z and z+dz is q(z)dz.
- Suppose we have a function x = x(z).

- Suppose we have a source of random numbers z drawn from a distribution with probability density q(z) the probability of generating a number between z and z+dz is q(z)dz.
- Suppose we have a function x = x(z).
- If z is random, x(z) will also be random, with a different distribution p(x).

- Suppose we have a source of random numbers z drawn from a distribution with probability density q(z) the probability of generating a number between z and z+dz is q(z)dz.
- Suppose we have a function x = x(z).
- If z is random, x(z) will also be random, with a different distribution p(x).
- Our goal is to choose the function x(z) such that x has the distribution we want.

■ The probability of generating a value of x between x and x + dx is by definition equal to the probability of generating a value of z in the corresponding z interval:

$$p(x)dx = q(z)dz$$

■ The probability of generating a value of x between x and x + dx is by definition equal to the probability of generating a value of z in the corresponding z interval:

$$p(x)dx = q(z)dz$$

■ In most common cases, q(z) = 1 in the interval [0,1]. Then integrating both sides:

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_{0}^{z} dz' = z$$

■ The probability of generating a value of x between x and x + dx is by definition equal to the probability of generating a value of z in the corresponding z interval:

$$p(x)dx = q(z)dz$$

■ In most common cases, q(z) = 1 in the interval [0,1]. Then integrating both sides:

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_{0}^{z} dz' = z$$

• If we can do the integral on the left and solve the equation, we will have the required x(z)!

Example: Suppose we want to generate real random numbers x in the interval  $[0,\infty]$  with the exponential probability distribution:

$$p(x) = \frac{1}{\mu}e^{-\mu x}$$

Example: Suppose we want to generate real random numbers x in the interval  $[0,\infty]$  with the exponential probability distribution:

$$p(x) = \frac{1}{\mu}e^{-\mu x}$$

$$\mu \int_0^{x(z)} e^{-\mu x'} dx' = 1 - e^{-\mu x} = z$$
$$x = -\frac{1}{\mu} \ln(1 - z)$$

Example: Suppose we want to generate real random numbers x in the interval  $[0,\infty]$  with the exponential probability distribution:

$$p(x) = \frac{1}{\mu}e^{-\mu x}$$

$$\mu \int_0^{x(z)} e^{-\mu x'} dx' = 1 - e^{-\mu x} = z$$
$$x = -\frac{1}{\mu} \ln(1 - z)$$

Thus if we feed the above equation uniformly distributed z in interval [0,1], it will generate the exponential distribution x for us.

A common problem in physics calculations is the generation of random numbers drawn from a Gaussian (or normal) distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

A common problem in physics calculations is the generation of random numbers drawn from a Gaussian (or normal) distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

■ This does not allow inversion! As the integral is not analytic...

A common problem in physics calculations is the generation of random numbers drawn from a Gaussian (or normal) distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

- This does not allow inversion! As the integral is not analytic...
- However, consider two independent random numbers x and y drawn from a Gaussian distribution with the same  $\sigma$ . The probability that a point (x,y) falls in an element dxdy of the xy plane:

$$p(x)dx \times p(y)dy = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right) dxdy$$

In polar coordinates:

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) dr \times \frac{d\theta}{2\pi} \equiv p(r)dr \times p(\theta)d\theta$$

In polar coordinates:

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) dr \times \frac{d\theta}{2\pi} \equiv p(r)dr \times p(\theta)d\theta$$

lacktriangleright In this expression, heta is just a uniform distribution

$$p(\theta) = \frac{1}{2\pi}$$

In polar coordinates:

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2} \exp{\left(-\frac{r^2}{2\sigma^2}\right)} dr \times \frac{d\theta}{2\pi} \equiv p(r) dr \times p(\theta) d\theta$$

■ In this expression,  $\theta$  is just a uniform distribution

$$p(\theta) = \frac{1}{2\pi}$$

■ The distribution of r can be inverted with z uniformly distributed:

$$r = \sqrt{-2\sigma^2 \ln(1-z)}$$

In polar coordinates:

$$p(r,\theta)drd\theta = \frac{r}{\sigma^2} \exp{\left(-\frac{r^2}{2\sigma^2}\right)} dr \times \frac{d\theta}{2\pi} \equiv p(r) dr \times p(\theta) d\theta$$

■ In this expression,  $\theta$  is just a uniform distribution

$$p(\theta) = \frac{1}{2\pi}$$

■ The distribution of r can be inverted with z uniformly distributed:

$$r = \sqrt{-2\sigma^2 \ln(1-z)}$$

■ Then one can construct x and y as:

$$x = r\cos(\theta)$$
  $y = r\sin(\theta)$ 

#### Random Walk

■ A simple random walk is a sequence of unit steps where each step is taken in the direction of one of the coordinate axis, and each possible direction has equal probability of being chosen.

#### Random Walk

- A simple random walk is a sequence of unit steps where each step is taken in the direction of one of the coordinate axis, and each possible direction has equal probability of being chosen.
- Random walk on a lattice:

- A simple random walk is a sequence of unit steps where each step is taken in the direction of one of the coordinate axis, and each possible direction has equal probability of being chosen.
- Random walk on a lattice:
  - In two dimensions, a single step starting at the point with integer coordinates (x,y) would be equally likely to move to any of one of the four neighbors (x+1,y), (x-1,y), (x,y+1) and (x,y-1).

- A simple random walk is a sequence of unit steps where each step is taken in the direction of one of the coordinate axis, and each possible direction has equal probability of being chosen.
- Random walk on a lattice:
  - In two dimensions, a single step starting at the point with integer coordinates (x,y) would be equally likely to move to any of one of the four neighbors (x+1,y), (x-1,y), (x,y+1) and (x,y-1).
  - In one dimension walk there are two possible neighbors

- A simple random walk is a sequence of unit steps where each step is taken in the direction of one of the coordinate axis, and each possible direction has equal probability of being chosen.
- Random walk on a lattice:
  - In two dimensions, a single step starting at the point with integer coordinates (x,y) would be equally likely to move to any of one of the four neighbors (x+1,y), (x-1,y), (x,y+1) and (x,y-1).
  - In one dimension walk there are two possible neighbors
  - In three dimensions there are six possible neighbors.

■ Brownian motion (answer the question - how many collisions, on average, a particle must take to travel a distance R).

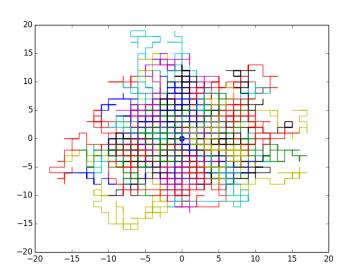
- Brownian motion (answer the question how many collisions, on average, a particle must take to travel a distance R).
- Electron transport in metals

- Brownian motion (answer the question how many collisions, on average, a particle must take to travel a distance R).
- Electron transport in metals
- Polymer simulations.

- Brownian motion (answer the question how many collisions, on average, a particle must take to travel a distance R).
- Electron transport in metals
- Polymer simulations.
- **.**..

# Simple Random walk

In 100 steps,  $\langle r \rangle \sim 8.9$ 



■ Persistent random walk

- Persistent random walk
- Restricted random walk

- Persistent random walk
- Restricted random walk
- Self-avoiding random walk

- Persistent random walk
- Restricted random walk
- Self-avoiding random walk
- **...**

- Persistent random walk
- Restricted random walk
- Self-avoiding random walk
- ...

Examples of applications:

Spread of inflectional diseases and effects of immunization Spreading of fire

# A persistent random walk

■ A persistent random walk in 2 dimensions in a city with n\*n blocks

# A persistent random walk

- A persistent random walk in 2 dimensions in a city with n\*n blocks
- Condition: the walker can not step back

# A persistent random walk

- A persistent random walk in 2 dimensions in a city with n\*n blocks
- Condition: the walker can not step back
- Goal: find average number of steps to get out the city

### Persistent Random walk

To escape  $24 \times 24, \langle n \rangle \sim 92$ 

