Random processes and Monte Carlo Simulation

- Monte Carlo integration.

Monte Carlo integration – basic idea

- Normally when we are interested in some physical phenomenon that has some random element, we write down an exact, non-random description that gives the answer for the average behaviour.

Monte Carlo integration – basic idea

- Normally when we are interested in some physical phenomenon that has some random element, we write down an exact, non-random description that gives the answer for the average behaviour.
- In principle, we can reverse the argument: we can start with an exact problem – such as the calculation of an integral – and find an approximate solution to it by running a suitable random process on the computer!

Monte Carlo integration – basic idea

- Normally when we are interested in some physical phenomenon that has some random element, we write down an exact, non-random description that gives the answer for the average behaviour.
- In principle, we can reverse the argument: we can start with an exact problem – such as the calculation of an integral – and find an approximate solution to it by running a suitable random process on the computer!
- This leads to novel ways of performing integrals..

General idea

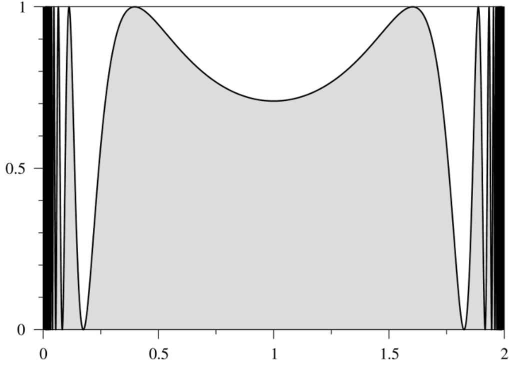
Suppose we want to evaluate the integral:

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)}\right] dx$$

General idea

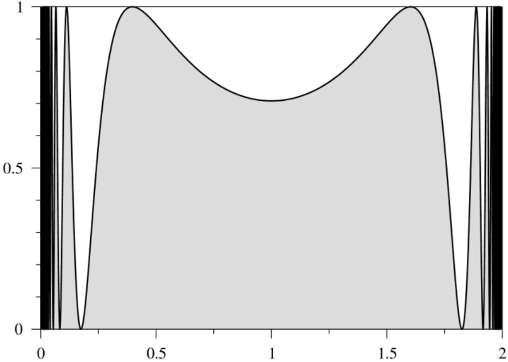
Suppose we want to evaluate the integral:

$$I = \int_0^2 \sin^2\left[\frac{1}{x(2-x)}\right]dx$$



Suppose we want to evaluate the integral:

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)} \right] dx$$



It is perfectly well behaved in the middle of its range – but varies infinitely fast at the edges.

General idea

- On the other hand since the entire function fits in a rectangle of size 2×1, the integral – the shaded area under the curve – is finite and less than 2.

General idea

- On the other hand since the entire function fits in a rectangle of size 2×1, the integral – the shaded area under the curve – is finite and less than 2.
- Methods such as trapezoidal rule or Simpson's rule or Gaussian quadrature are not likely to work well as they will not capture the infinitely fast variation of the function at the edges.

General idea

- On the other hand since the entire function fits in a rectangle of size 2×1, the integral – the shaded area under the curve – is finite and less than 2.
- Methods such as trapezoidal rule or Simpson's rule or Gaussian quadrature are not likely to work well as they will not capture the infinitely fast variation of the function at the edges.
- Monte carlo integration offers a simple way to tackle this integral.

General idea

- The shaded area under the curve is I and given that the area of the rectangle is $A = 2$.

General idea

- The shaded area under the curve is I and given that the area of the rectangle is $A = 2$.
- If we choose a point randomly in the rectangle, the probability that the point falls under the curve rather than over it is $p = I/A$.

General idea

- The shaded area under the curve is I and given that the area of the rectangle is $A = 2$.
- If we choose a point randomly in the rectangle, the probability that the point falls under the curve rather than over it is $p = I/A$.
- We generate a large number, N, of random points in the bounding rectangle and check each one to see if it is below the curve and keep a count of the number that are – k.

General idea

- The shaded area under the curve is I and given that the area of the rectangle is $A = 2$.
- If we choose a point randomly in the rectangle, the probability that the point falls under the curve rather than over it is $p = I/A$.
- We generate a large number, N, of random points in the bounding rectangle and check each one to see if it is below the curve and keep a count of the number that are – k.
- Then the fraction of points below the curve is k/N. This should be equal to the probabilitly, $p = I/A$

$$I \simeq \frac{kA}{N}$$

Example

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)} \right] dx$$

N	I
10^4	1.4542
10^5	1.45252
10^6	1.452492
10^7	1.4513378
10^8	1.45123546

Error Analysis

- For simple integrals – monte carlo methods are not as accurate as trapezoidal rule or Simpson's rule!

Error Analysis

- For simple integrals – monte carlo methods are not as accurate as trapezoidal rule or Simpson's rule!

Probability that a single random point falls below the curve is $p = I/A$ and that it falls above the curve is $(1 - p)$.

Error Analysis

- For simple integrals – monte carlo methods are not as accurate as trapezoidal rule or Simpson's rule!

Probability that a single random point falls below the curve is $p = I/A$ and that it falls above the curve is $(1 - p)$.

Probability that a particular k points fall below the curve and $(N - k)$ fall above the curve is $p^k(1 - p)^{N-k}$.

- For simple integrals – monte carlo methods are not as accurate as trapezoidal rule or Simpson's rule!

Probability that a single random point falls below the curve is $p = I/A$ and that it falls above the curve is $(1 - p)$.

Probability that a particular k points fall below the curve and $(N - k)$ fall above the curve is $p^k(1 - p)^{N-k}$.

But there are $\binom{N}{k}$ ways of choosing k points from a list of N.

- For simple integrals – monte carlo methods are not as accurate as trapezoidal rule or Simpson's rule!

Probability that a single random point falls below the curve is $p = I/A$ and that it falls above the curve is $(1 - p)$.

Probability that a particular k points fall below the curve and $(N - k)$ fall above the curve is $p^k(1-p)^{N-k}$.

But there are $\binom{N}{k}$ ways of choosing k points from a list of N.

Total probability that we get k points below:

$$P(k) = \binom{N}{k} p^k (1-p)^{N-k}$$

Binomial distribution!

Mean of this distribution:

$$
\begin{aligned}
< k > &= \sum_{k=0}^{N} kP(k) \\
&= \sum_{k=1}^{N} k \binom{N}{k} p^k (1-p)^{N-k} \\
&= Np \sum_{k=1}^{N} \binom{N-1}{k-1} p^{k-1} (1-p)^{(N-1)-(k-1)}
\end{aligned}
$$

$$\text{Subsitute} \quad j = k-1 \quad \& \quad M = N-1$$

$$
\begin{aligned}
&= Np \sum_{j=0}^{M} \binom{M}{j} p^j (1-p)^{M-j} \\
&= Np
\end{aligned}
$$

$< k^2 >$ of this distribution:

$$< k(k-1) > = \sum_{k=0}^{N} k(k-1)P(k)$$

$$= \sum_{k=2}^{N} k(k-1)\binom{N}{k} p^k (1-p)^{N-k}$$

$$= N(N-1)p^2 \sum_{k=2}^{N} \binom{N-2}{k-2} p^{k-2} (1-p)^{(N-2)-(k-2)}$$

$$\text{Subsitute} \quad j = k-2 \quad \& \quad M = N-2$$

$$= N(N-1)p^2 \sum_{j=0}^{M} \binom{M}{j} p^j (1-p)^{M-j}$$

$$= N(N-1)p^2$$

$$< k^2 > = < k(k-1) > + < k > = N(N-1)p^2 + Np$$

Variance of this distribution:

$$\mathrm{var}k = Np(1-p) = N\frac{I}{A}\left(1 - \frac{I}{A}\right)$$

Variance of this distribution:

$$\mathrm{var}k = Np(1-p) = N\frac{I}{A}\left(1 - \frac{I}{A}\right)$$

Expected error in the integral:

$$\sigma = \sqrt{\mathrm{var}k}\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}}$$

Variance of this distribution:

$$\mathrm{var}k = Np(1-p) = N\frac{I}{A}\left(1 - \frac{I}{A}\right)$$

Expected error in the integral:

$$\sigma = \sqrt{\mathrm{var}k}\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}}$$

The error varies with N as $N^{-1/2}$ which means the accuracy improves as we increase N.

Variance of this distribution:

$$\mathrm{var}k = Np(1-p) = N\frac{I}{A}\left(1 - \frac{I}{A}\right)$$

Expected error in the integral:

$$\sigma = \sqrt{\mathrm{var}k}\,\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}}$$

The error varies with N as $N^{-1/2}$ which means the accuracy improves as we increase N.

Error in Trapezoidal rule went as $\mathcal{O}(h^2) \sim \frac{1}{N^2}$ and in Simpson's rule as $\mathcal{O}(h^4) \sim \frac{1}{N^4}$ – clearly showing that when we can use the regular methods – we should use them. This method is only good for pathological integrands.

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 at random between a and b:

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

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

Error Analysis

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

- 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 $\mathrm{var} f = \langle f^2 \rangle - \langle f \rangle^2$ 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 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 $\mathrm{var} f = \langle f^2 \rangle - \langle f \rangle^2$ 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 $N \mathrm{var} f$.

Error Analysis

- 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 $\mathrm{var} f = \langle f^2 \rangle - \langle f \rangle^2$ 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 $N \mathrm{var} f$.
- Error/standard deviation on the integral:

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

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

Multidimensional integrals

- The error analysis we did for Monte Carlo integration remains the same irrespective of the number of dimensions!!!

Multidimensional integrals

- The error analysis we did for Monte Carlo integration remains the same irrespective of the number of dimensions!!!
- If we have N points then deterministic methods will get $N^{1/d}$ points in each dimension. As a result the overall error in midpoint rule would be $N^{-1/d}$ where as in trapeziodal $N^{-2/d}$.

Multidimensional integrals

- The error analysis we did for Monte Carlo integration remains the same irrespective of the number of dimensions!!!
- If we have N points then deterministic methods will get $N^{1/d}$ points in each dimension. As a result the overall error in midpoint rule would be $N^{-1/d}$ where as in trapeziodal $N^{-2/d}$.
- For higher dimensions – more than 4/5, Monte carlo method becomes faster than any of the deterministic methods!

Importance Sampling

- Monte carlo integration is good for integrating pathological functions but sometimes it does not work very well.

- Monte carlo integration is good for integrating pathological functions but sometimes it does not work very well.
- In particular, if the function to be integrated contains a divergence!

Importance Sampling

- Monte carlo integration is good for integrating pathological functions but sometimes it does not work very well.
- In particular, if the function to be integrated contains a divergence!
- This is because occasionally when the random point is near the divergence, you will get a big change in the sum..

Importance Sampling

- Monte carlo integration is good for integrating pathological functions but sometimes it does not work very well.
- In particular, if the function to be integrated contains a divergence!
- This is because occasionally when the random point is near the divergence, you will get a big change in the sum..
- The variance, σ in such cases is very high.

Importance Sampling

- Monte carlo integration is good for integrating pathological functions but sometimes it does not work very well.
- In particular, if the function to be integrated contains a divergence!
- This is because occasionally when the random point is near the divergence, you will get a big change in the sum..
- The variance, σ in such cases is very high.
- Importance sampling is a way to get around this problem.

Importance Sampling

- For any general function, $g(x)$, we can define a weighted average over the interval from a to b:

$$\langle g \rangle_w = \frac{\int_a^b w(x)g(x)dx}{\int_a^b w(x)dx}$$

where $w(x)$ is any function we choose.

Importance Sampling

- For any general function, $g(x)$, we can define a weighted average over the interval from a to b:

$$\langle g \rangle_w = \frac{\int_a^b w(x)g(x)dx}{\int_a^b w(x)dx}$$

where $w(x)$ is any function we choose.

- Consider the integral:

$$I = \int_a^b f(x)dx$$

Importance Sampling

- For any general function, $g(x)$, we can define a weighted average over the interval from a to b:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx}$$

where $w(x)$ is any function we choose.

- Consider the integral:

$$I = \int_a^b f(x) dx$$

- Setting $g(x) = f(x)/w(x)$ we have:

$$\left\langle \frac{f(x)}{w(x)} \right\rangle_w = \frac{\int_a^b w(x) f(x)/w(x) dx}{\int_a^b w(x) dx} = \frac{I}{\int_a^b w(x) dx}$$

$$I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x) dx$$

Importance Sampling

- This is similar to the mean value method but allows us to calculate the integral from a weighted average rather than a standard uniform average.

Importance Sampling

- This is similar to the mean value method but allows us to calculate the integral from a weighted average rather than a standard uniform average.
- Let us define a probability density function:

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

Importance Sampling

- This is similar to the mean value method but allows us to calculate the integral from a weighted average rather than a standard uniform average.
- Let us define a probability density function:

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

- Let us sample N random points, x_i, non-uniformly with this density. That is the probability of generating a value in the interval between x and $x + dx$ will be $p(x)dx$.

Importance Sampling

- This is similar to the mean value method but allows us to calculate the integral from a weighted average rather than a standard uniform average.
- Let us define a probability density function:

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

- Let us sample N random points, x_i, non-uniformly with this density. That is the probability of generating a value in the interval between x and $x + dx$ will be $p(x)dx$.
- Then the average number of sample that fall in this interval are $Np(x)dx$ and so for any function $g(x)$:

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b Np(x)g(x)dx$$

Importance Sampling

- So using this the general weighted average is given as:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx} = \int_a^b p(x) g(x) dx \simeq \frac{1}{N} \sum_{i=1}^{N} g(x_i)$$

Importance Sampling

- So using this the general weighted average is given as:

$$\langle g \rangle_w = \frac{\int_a^b w(x)g(x)dx}{\int_a^b w(x)dx} = \int_a^b p(x)g(x)dx \simeq \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

- Putting it all together for our integral:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \int_a^b w(x)dx$$

Importance Sampling

- So using this the general weighted average is given as:

$$\langle g \rangle_w = \frac{\int_a^b w(x)g(x)dx}{\int_a^b w(x)dx} = \int_a^b p(x)g(x)dx \simeq \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

- Putting it all together for our integral:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx$$

- The formula allows us to estimate I by calculating not the sum $\sum_{i=1}^{N} f(x_i)$, but instead the modified sum $\sum_{i=1}^{N} f(x_i)/w(x_i)$ where $w(x)$ is any function we choose.

- So using this the general weighted average is given as:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx} = \int_a^b p(x) g(x) dx \simeq \frac{1}{N} \sum_{i=1}^{N} g(x_i)$$

- Putting it all together for our integral:

$$I \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \int_a^b w(x) dx$$

- The formula allows us to estimate I by calculating not the sum $\sum_{i=1}^{N} f(x_i)$, but instead the modified sum $\sum_{i=1}^{N} f(x_i)/w(x_i)$ where $w(x)$ is any function we choose.
- This is useful because it allows us to choose a $w(x)$ that can get rid of the pathologies of $f(x)$.

- So using this the general weighted average is given as:

$$\langle g\rangle_w = \frac{\int_a^b w(x)g(x)dx}{\int_a^b w(x)dx} = \int_a^b p(x)g(x)dx \simeq \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

- Putting it all together for our integral:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx$$

- The formula allows us to estimate I by calculating not the sum $\sum_{i=1}^{N} f(x_i)$, but instead the modified sum $\sum_{i=1}^{N} f(x_i)/w(x_i)$ where $w(x)$ is any function we choose.
- This is useful because it allows us to choose a $w(x)$ that can get rid of the pathologies of $f(x)$.
- The price we pay is that we have to draw our samples from a non-uniform distribution rather than a uniform distribution.

Error Analysis

$$\sigma = \frac{\sqrt{\mathrm{var}_w(f/w)}}{\sqrt{N}} \int_a^b w(x)dx$$

where

$$\mathrm{var}_w g = \langle g^2 \rangle_w - \langle g \rangle_w^2$$