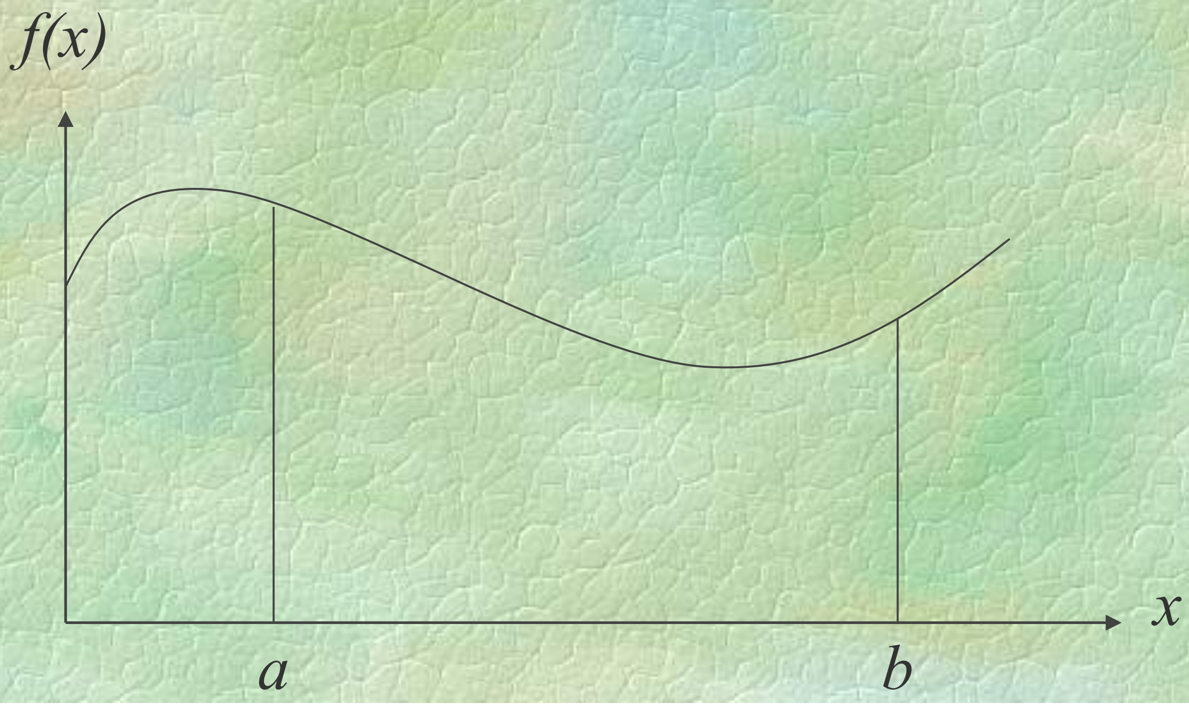
Numerical Integration

One-dimensional integrals

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

The objective of one-dimensional integral is to calculate the area under the curve *f(x)*.



Classical method

1. Rectangular approximation

2. Trapezoidal approximation

3. Simpson's rule

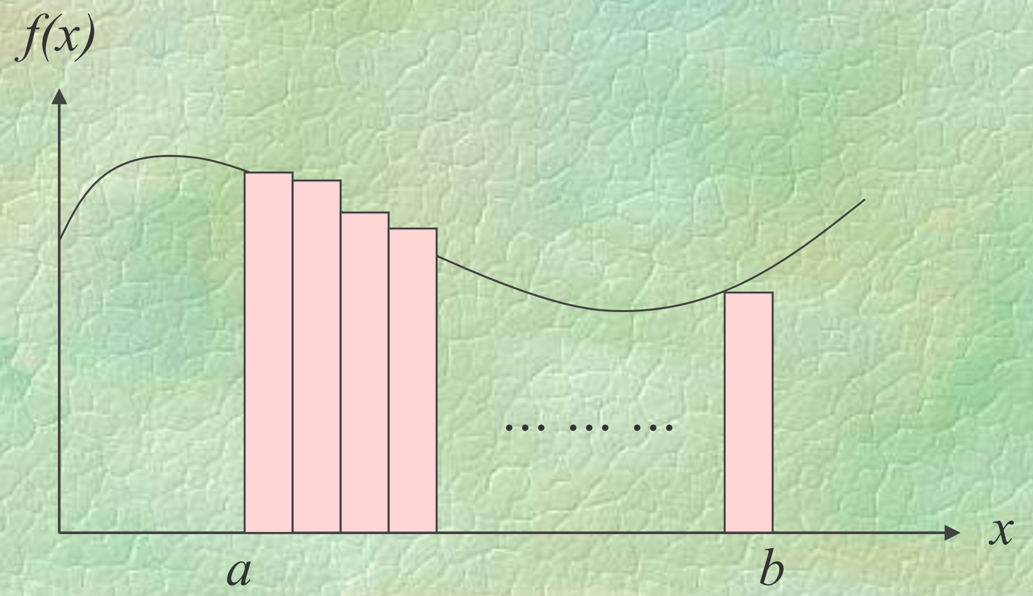
First divided the regions into many intervals

$$\Delta x = \frac{b-a}{n}$$

$$x_n = x_0 + n\Delta x$$

For Rectangular approximation

$$F_n \approx \sum_{i=0}^{n-1} f(x_i)\Delta x$$



For Trapezoidal approximation

$$F_n \approx \left[\frac{1}{2} f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} f(x_n)\right] \Delta x$$

For Simpson's rule

$$F_n \approx \frac{1}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots$$
$$2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)]\Delta x$$

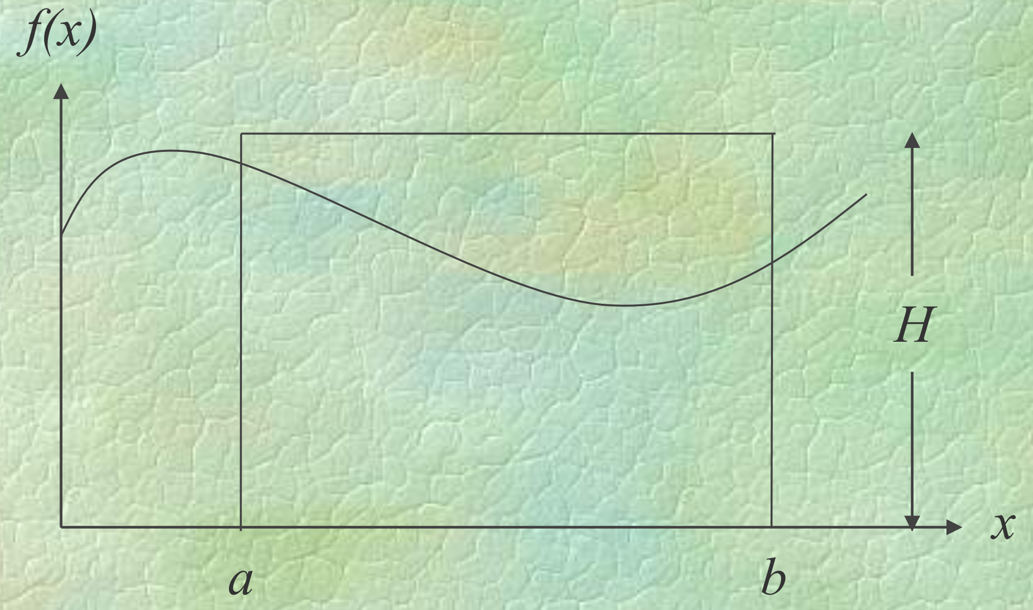
These approximations are adequate for functions f(x) that are reasonably well behaved, e.g. polynomial.

Monte Carlo Integration

1. Hit or Miss method

2. Sample mean method

1. Hit or Miss method



Compute n pairs of random numbers

$$(x_i, y_i) \qquad \textit{where} \qquad a \le x_i \le b, 0 \le y_i \le H$$

$$F_n = H(b-a)\frac{n_s}{n} \qquad n_s = \text{number of points with } y_i \le f(x_i)$$

2. Sample mean method

$$F_n = (b-a)\langle f \rangle = (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

where x_i are random number distributed uniformly in the interval $a \le x_i \le b,$ and n is the number of *trials*.

$$x_i = a + (b-a) * RANDOM(0,1)$$

Is it the same as the Rectangular approximation?

Multidimensional integrals

$$F = \prod_{i=1}^{N} \int_R dx_i \, f(x_1, x_2, \cdots x_N)$$

Classical method

$$F \approx \sum_{i=1}^{N} \sum_{i_k=1}^{n} f(x_{1_k}, x_{2_k}, \cdots, x_{N_k}) W(x_{1_k}, x_{2_k}, \cdots, x_{N_k}) h^N$$

Monte Carlo method

$$F \approx \frac{\Omega}{n} \sum_{i=1}^{n} f(x_{1_i}, x_{2_i}, \cdots, x_{N_i}) W(x_{1_i}, x_{2_i}, \cdots, x_{N_i})$$

Why Monte Carlo?

Error and computation time

Integration => summation of a set of numbers with error due to approximation

Rectangular approximation for 1D

$$\boldsymbol{error} \propto \boldsymbol{n}(\Delta \boldsymbol{x})^2 \propto \boldsymbol{n}[(\boldsymbol{b}-\boldsymbol{a})/\boldsymbol{n}]^2 \propto 1/\boldsymbol{n}$$

Simpson's rule for 1D

$$\boldsymbol{error} \propto \boldsymbol{n}(\Delta \boldsymbol{x})^5 \propto \boldsymbol{n}[(\boldsymbol{b}-\boldsymbol{a})/\boldsymbol{n}]^5 \propto 1/\boldsymbol{n}^4$$

The above error terms are for one dimensional only.

For a total of n data, if the error goes as order n^{-a} in 1D.

Then the error in d dimensions goes as $n^{-a/d}$.

However Monte Carlo errors vary as $n^{-1/2}$, ***independent*** of dimension, it is better for large enough dimension.

Example : $$2^{-7}\int_a^b \cdots \int_a^b (x_1 + x_2 + \cdots + x_8)^2 \, dx_1 \cdots dx_8$$

$$= \frac{8}{3}\left(b^3 - a^3\right)\left(b-a\right)^7 + 14\left(b^2 - a^2\right)^2\left(b-a\right)^6$$

(a,b); n	Classical method (rectangular approximation)	Monte Carlo method
(0,1); 4^8	0.1298771 error = -3.31×10^{-4}	0.1280971 error = -2.11×10^{-3}
(0,1); 8^8	0.1314049 error = -1.20×10^{-3}	0.1294123 error = -7.96×10^{-4}
(0,1); 16^8	0.1303383 error = -1.30×10^{-4}	0.1302604 error = -5.21×10^{-5}
(0,2); 4^8	132.9941 error = –0.34	131.1715 error = –2.16
(0,2); 8^8	134.5586 error = 1.225	132.5182 error = –0.815
(0,2); 16^8	134.0973 error = 0.764	133.2193 error = –0.114

Important sampling

The basic idea is to concentrate the distribution of the sample points in the part of region that are most "importance" instead of spreading them evenly.

We introduce a positive function *p(x)* such that

$$\int_a^b dx\; p(x) = 1$$

$$F = \int_a^b dx\; p(x)\left[\frac{f(x)}{p(x)}\right]$$

$$F = \frac{1}{n}\sum_{i=1}^{n}\frac{f(x_i)}{p(x_i)}$$

Better choice of p(x) will reduce the variance of the integral.

Metropolis algorithm

This method is useful for computing

$$\langle f \rangle = \frac{\int p(x) f(x) dx}{\int p(x) dx}$$

The Metropolis method produces a random walk of points $\{x_i\}$ whose asymptotic probability distribution approcahes $p(x)$ after a large number of steps.

The random walk is defined by specifying a *transition probability* $T(x_i \rightarrow x_j)$ from one value x_i to another value x_j such that the distribution of points $x_0, x_1, x_2,$L converges to $p(x)$.

It is sufficient to satisfy the "detailed balance" condition if

$$p(x_i)T(x_i \rightarrow x_j) = P(x_j)T(x_j \rightarrow x_i)$$

This relation does not uniquely specify $T(x_i \rightarrow x_j)$

A simple choice of $T(x_i \rightarrow x_j)$ is

$$T(x_i \rightarrow x_j) = \min\left[1, \frac{p(x_j)}{P(x_i)}\right]$$

A simple algorithm

Step 1. Randomly pick up a $\boldsymbol{x}$

Step 2. Let $\boldsymbol{x'} = \boldsymbol{x} + \boldsymbol{dx}$, calculate $\boldsymbol{s=p(x')/p(x)}$.

Step 3. If $\boldsymbol{s} > 1$, accept $\boldsymbol{x'}$.

Step 4. If $\boldsymbol{s} < 1$, compare $\boldsymbol{s}$ with $\boldsymbol{r}$=random number (0,1).

If $\boldsymbol{s > r}$, accept $\boldsymbol{x'}$; otherwise, back to step 2.

Continue

Choice of $\boldsymbol{dx}$? Acceptance rate between 1/3 and 2/3.

Example:

Calculate the mean energy for

$$E = \sum_{i=1}^{10} \cos(\theta_i - \theta_{i+1}), \textit{where } \theta_{11} = \theta_1$$

That means we need to calculate

$$\langle E \rangle = \frac{\prod_{i=1}^{10} \int_{-\pi}^{\pi} d\theta_i E \exp(-E)}{\prod_{i=1}^{10} \int_{-\pi}^{\pi} d\theta_i \exp(-E)}$$

Number of points calculated / number of trials	$\langle E \rangle$	
	Uniform sample	Metropolis method **With p=Exp(-E)**
$2^{10} = 1024$	-7.955661	-4.275162
$3^{10} = 59049$	-3.494802	-4.802259
$4^{10} = 1048576$	-4.628727	-4.481805
$5^{10} = 9765625$	-4.448703	-4.476263
$6^{10} = 60466176$	-4.470915	-4.474854