Numerical Methods

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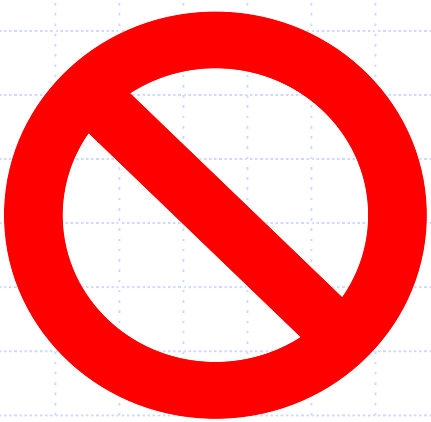
Numerical integration

We calculate the integral $\int_a^b f(x)dx$

1. Constant approximation - the rectangle rule

$$h = \frac{b-a}{n}$$

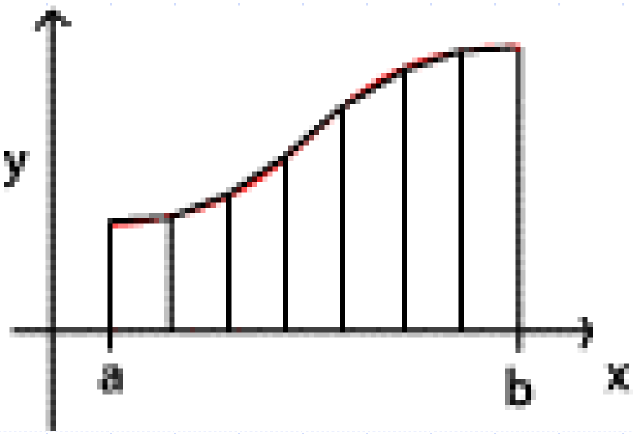


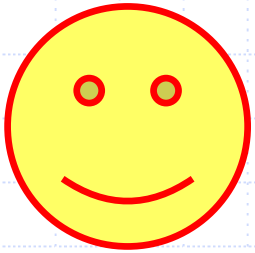
$$\int_a^b f(x)dx \cong h\sum_{i=1}^{n} f_i \cong h\sum_{i=1}^{n} f_{i+1}$$

$$\int_a^b f(x)dx \cong h\sum_{i=1}^{n} f\left(\frac{x_i + x_{i+1}}{2}\right)$$

Numerical integration

2. Linear approximation - the trapezium rule





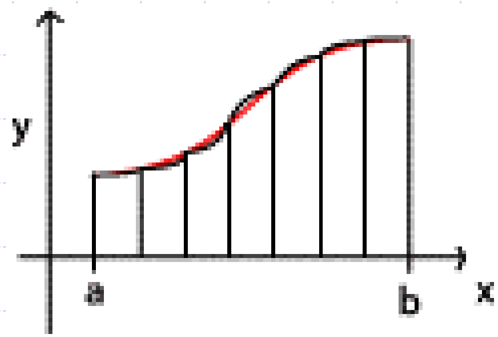
$$h = \frac{b-a}{n}$$

$$\int_a^b f(x)dx \cong \frac{1}{2}h\sum_{i=1}^{n}\left(f_i + f_{i+1}\right) = h\left(\frac{f(a)+f(b)}{2} + \sum_{i=2}^{n} f_i\right)$$

$$\tfrac{1}{12}h^3 \min_{x\in[a,b]}\left|f''(x)\right| \le \varepsilon \le \tfrac{1}{12}h^3 \max_{x\in[a,b]}\left|f''(x)\right|$$

Numerical integration

3. Quadratic approximation - the Simpson rule



$$\int_a^b f(x)dx \cong \frac{1}{3}h\sum_{i=1}^{(n+1)/2}\left(f_{2i-2}+4f_{2i-1}+f_{2i}\right)=$$

$$=\frac{1}{3}h\left(f(a)+f(b)+4\sum_{i=1}^{(n+1)/2}f_{2i-1}+\sum_{i=1}^{(n+1)/2}f_{2i}\right)$$

$$\tfrac{1}{90}h^5\min_{x\in[a,b]}\left|f^{IV}(x)\right|\le\varepsilon\le\tfrac{1}{90}h^5\max_{x\in[a,b]}\left|f^{IV}(x)\right|$$

Calculatng integrals by Monte Carlo method

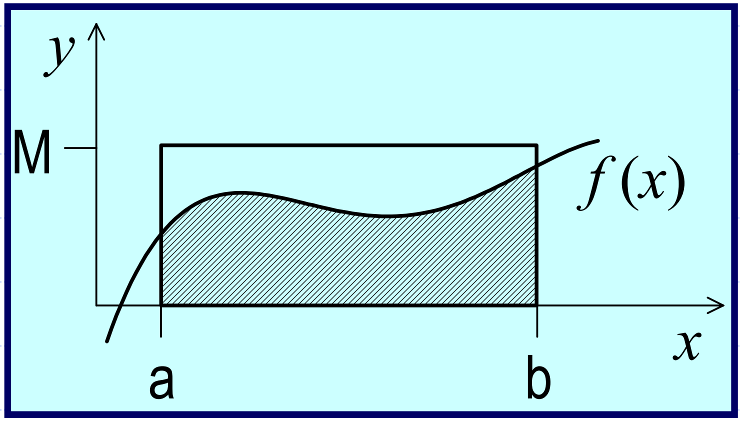
The hit-and-miss method

$$\int_a^b f(x)dx = \frac{n}{N} M(b-a); \qquad 0 \le f(x) \le M$$

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} \dots \int_{a_K}^{b_K} f(\mathbf{X})d\mathbf{X} = \frac{n}{N} V_K$$

N – the total number of hits within the area *M*(*b*-*a*)

n – the number of hits under *f*(*x*) curve (shadowed area)



Calculatng integrals by Monte Carlo method

The sample mean method

$$\int_a^b f(x)dx = (b-a)\langle f \rangle = \frac{(b-a)}{N}\sum_{i=1}^{N} f(x_i)$$

The general (n-D) rule

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty} f(\mathbf{X})d\Phi(\mathbf{X}) = \langle f \rangle = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{X}_i)$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty} f(x^1,x^2,\dots,x^K)d\Phi(x^1,x^2,\dots,x^K) = \langle f \rangle = \frac{1}{N}\sum_{i=1}^{N} f(x_i^1,x_i^2,\dots,x_i^K)$$

where: $d\Phi(\mathbf{X}) = \varphi(\mathbf{X})d\mathbf{X}$ e.g. $d\Phi(x) = \frac{1}{b-a}dx$ (for 1-D)

How accurate is my integral?

Two methods of error estimation:

- analytical (requires the function to be known)
- numerical, based on a series of calculations

Possible improvement of the results:

Richardson extrapolation!

Exercise 7

Calculate the integral

$$S = \int_0^3 \frac{1+\sin^2(x)}{\sqrt{\pi + \cos(x)}}\,dx$$

with accuracy of at least 5 significant digits, using three methods:

- trapezium rule
- *Simpson rule
- sample mean method

Compare the necessary number of intervals (*and calculation times).