## Lecture 4

Numerical methods: Integration

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# Content

# Introduction

# Introduction i

Numerical integration (or quadtrature) provides an approximation to an integral and it is useful or necessary in many cases. For example:

- $\rightarrow$ experimental data points
- $\rightarrow$ the integral has no simple analytical form
- $\rightarrow$ easier to compute the approximate integral than finding the analytical expression.

**Note**

As in most areas of numerical physics, the choice of the algortithm depends on the problem. In this case, the choice of the algorithm to carry out the numerical integration depends the behaviour of the function $f(x)$ over the interval of integration.

The integral may also need to be recast in a different form, for example to use "simple" functions:

$$\int_{-1}^{1} |x| f(x) dx = \int_{-1}^{0} -x f(x) dx + \int_{0}^{1} x f(x) dx$$

slowly-rapidly varying functions:

$$\int_{0}^{1} x^{1/3} dx = \int_{0}^{1} 3y^3 dy \quad \text{with} \quad y := x^{1/3}$$

removing singularities:

$$\int_{0}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} = 2 \int_{0}^{1} \frac{f(1-y^2)dy}{\sqrt{2-y^2}} \quad \text{with} \quad y := \sqrt{1-x}$$

# "Classical" deterministic numerical integration techniques

# Riemann Sum i

Let $f : [a, b] \to \mathbb{R}$ be a function defined on the interval $[a, b]$.

The interval is partioned into $n$ sub-intervals

$$P = \{[x_0, x_1], [x_1, x_2], \ldots, [x_{n-1}, x_n]\}$$

where the $n + 1$ points are ordered according to

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b$$

or more conveniently

$$x_j = a + \sum_{i=1}^{j} \delta x_i, \quad j = 0 \ldots n$$

and

$$\delta x_i = x_i - x_{i-1}, \quad i = 1 \ldots n$$

# Riemann Sum ii

A **Riemann sun** of the function $f$ over the partition $P$ is defined as

$$S = \sum_{i=1}^{n} f(x_i^*)\ \delta x_i$$

and different Riemann sums can be constructed depending on the choice of

$$x_i^* \in [x_{i-1}, x_i]$$

As the norm of the partition goes to zero (i.e. the length of the longest sub-interval goes to zero), the Riemann sums will converge to the value of the Riemann integral of the function over the interval (if the limit exist).

$$\int_a^b f(x)dx = \lim_{||\delta x|| \to 0} \left[ \sum_{i=1}^{n} f(x_i^*)\delta x_i \right]$$

where $||\delta x|| = max(\delta x_i), \quad i \in [1, n]$

# Simple quadrature rules

Divide the interval [a,b] in $n$ identical sub-intervals of size

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

there are $n+1$ evenly space points over the interval $[a, b]$

$$x_i = a + i\,h \;\text{ with }\; i = 0 \ldots n$$

The integral of the function $f(x)$ is then approximated as

→ **left rule** $x_i^* = x_{i-1}$

$$I_l = h \sum_{i=1}^{n} f(x_{i-1})$$

→ **right rule** $x_i^* = x_i$

$$I_r = h \sum_{i=1}^{n} f(x_i)$$

→ **mid-point rule** $x_i^* = (x_{i-1} + x_i)/2$

$$I_m = h \sum_{i=1}^{n} f\left(\frac{x_{i-1} + x_i}{2}\right)$$

# The left, right and the midpoint rules

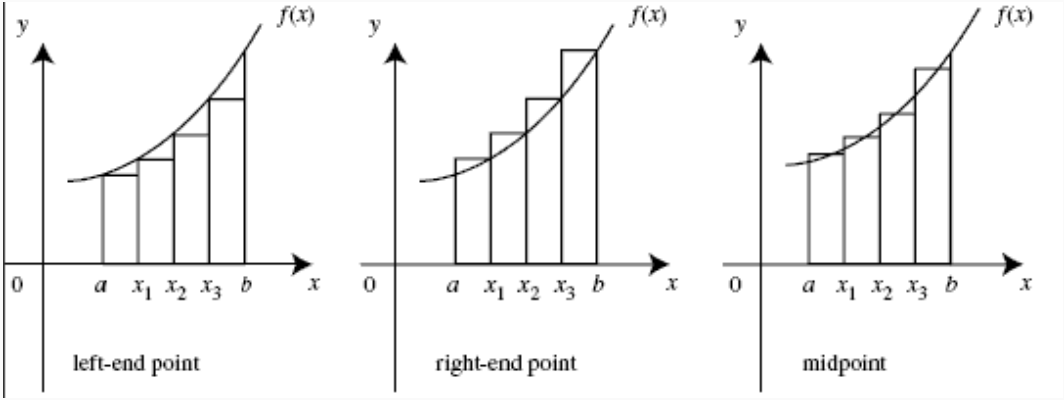


**Figure 1:** Left, right and midpoint rules

# Trapezoidal rule

The trapezoidal rule approximates the function over each sub-interval with a straight line. The area corresponding to a sub-interval is its width, $h$, times the average height, $(f_{i-1} + f_i)/2$. It can also be defined as the average of the left and right Riemann sums:

$$\frac{1}{2}\left[h\sum_{i=1}^{n} f(x_{i-1}) + h\sum_{i=1}^{n} f(x_i)\right] = h\sum_{i=1}^{n}\left[\frac{f(x_{i-1}) + f(x_i)}{2}\right]$$

For computational efficiency (fewer evaluations of the function) the trapezoidal rule is written as

$$I_t = h\left[\frac{f(a) + f(b)}{2} + \sum_{i=1}^{n-1} f(x_i)\right]$$

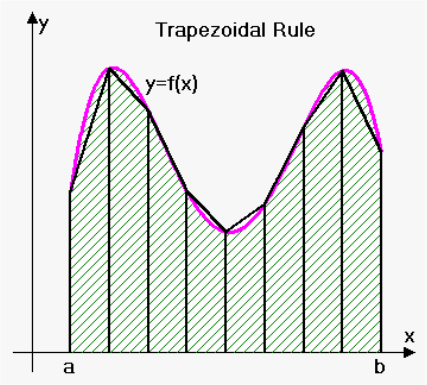


**Figure 2:** The trapezoidal rule

# Simpson's rule

Simpson's rule is one of the most common numerical integration algorithms.
It approximates (interpolates) the function $f(x)$ to be integrated with a quadratic polynomial $P(x)$.
Using Lagrange polynomial interpolation we have:

$$P(x) = f(a)\frac{(x-m)(x-b)}{(a-m)(a-b)} + f(m)\frac{(x-a)(x-b)}{(m-a)(m-b)} + f(b)\frac{(x-a)(x-m)}{(b-a)(b-m)}$$

which gives for the integral:

$$\int_a^b f(x)dx \approx \int_a^b P(x)\,dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

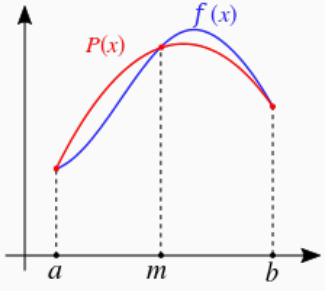


**Figure 3:** The trapezoidal rule

# The composite Simpson's rule

For $n$ sub-intervals, Simpson's rule is applied to each sub-interval as

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx \frac{h}{3}\left[f(x_{i-1}) + 4f\left(\frac{x_{i-1}+x_i}{2}\right) + f(x_i)\right]$$

The integral over the interval $[a, b]$ is then given by

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n}\int_{x_{i-1}}^{x_i} f(x)dx = \sum_{i=1}^{n}\frac{h}{3}\left[f(x_{i-1}) + 4f\left(\frac{x_{i-1}+x_i}{2}\right) + f(x_i)\right]$$

This expression can be rearranged to show that Simpson's rule is the weighted average of the trapezoidal and midpoint rules:

$$I_S = \frac{2h}{3}\sum_{i=1}^{n} f\left(\frac{x_{i-1}+x_i}{2}\right) + \frac{h}{3}\sum_{i=1}^{n}\frac{f(x_{i-1}) + f(x_i)}{2} = \frac{2I_m + I_t}{3}$$

**Different form of Simpson's rule**

The composite Simpson's rule is usually written for an interval $[a, b]$ divided in $n/2$ equal sub-interval, with $n$ even. The rule is applied to each sub-interval $[x_{2i-2}, x_{2i}]$ for $i = 1 \ldots n/2$:

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

# Errors

The errors or a bound on the error associated with numerical integration can be estimated. For large enough $n$ the asymptotic error estimate (see Euler-Mclaurin formula) gives

→ Midpoint rule

$$E_m = \frac{(b-a)^2}{24n^2}\left[f'(b) - f'(a)\right] + \mathcal{O}\left(\frac{1}{n^4}\right)$$

→ Trapezoidal rule

$$E_t = -\frac{(b-a)^2}{12n^2}\left[f'(b) - f'(a)\right] - \mathcal{O}\left(\frac{1}{n^4}\right)$$

→ Simpson's rule

$$E_S = -\frac{(b-a)^4}{180n^4}\left[f'''(b) - f'''(a)\right] + \mathcal{O}\left(\frac{1}{n^6}\right)$$

→ In general the error has the form

$$E \propto \frac{1}{n^\alpha}$$

**Newton-Cotes formulas**

The midpoint, trapezoidal and Simpson rules are special cases of Newton-Cotes formulas for uniform sub-intervals.

# Improper integrals i

An integral $\int_a^b f(x)dx$ is improper if

$\rightarrow$ a or b are $\infty$

$\rightarrow$ $f(x)$ is not defined at a or b

The integral can be convergent

$$\int_1^\infty \frac{1}{x^2}dx = \lim_{t\to\infty}\int_1^t \frac{1}{x^2}dx = \lim_{t\to\infty}\left(1-\frac{1}{t}\right) = 1$$

or divergent

$$\int_1^\infty \frac{1}{x}dx = \infty$$

To integrate numerically a convergent improper integral, it needs to be transformed first (if possible) into a proper integral.

# Improper integrals ii

**Example**

Integrate

$$\int_0^\infty \exp(-x)\, dx = 1$$

1. Split the integral

$$\int_0^\infty \exp(-x)\, dx = \int_0^1 \exp(-x)\, dx + \int_1^\infty \exp(-x)\, dx$$

2. change the variable for the remaining improper integral

$$x = \frac{1}{t}, \quad dx = -\frac{1}{t^2} dt$$

$$\int_0^1 \frac{\exp(-1/t)}{t^2}\, dt$$

3. integrate numerically

$$\int_0^\infty \exp(-x)\, dx = \int_0^1 \exp(-x)\, dx + \int_0^1 \frac{\exp(-1/t)}{t^2}\, dt$$

Be careful in using quadrature rules that use the endpoints! → see exercise in the notebook

# "Monte Carlo" numerical integration technique: basics

# Mean Value Theorem for Integrals i

The mean value theorem for integrals states that a continuous function defined on a closed and bounded interval takes somewhere over the interval its mean value:

$$\int_a^b f(x)dx = (b-a)f(\xi)$$

and from the definition of the mean value of $f(x)$ over the interval:

$$f(\xi) = \langle f \rangle$$

For a proof see here: `https://proofwiki.org/wiki/Mean_Value_Theorem_for_Integrals`

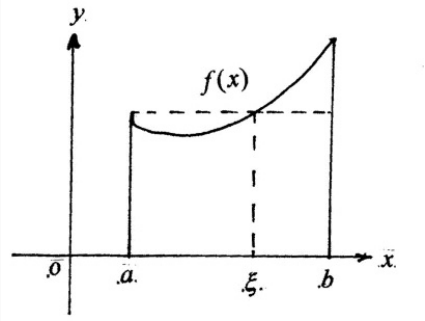


**Figure 4:** Geometrical interpretation of the mean value theorem for integrals

# Mean Value Theorem for Integrals ii

The Monte Carlo integration methods uses random sampling to evaluate the mean $\langle f \rangle$ and thus the integral:

$$I = \int_a^b f(x)dx = (b-a)\langle f \rangle$$

The sample mean

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

is determined from sampling the function $f(x)$ with a sequence of uniform[1] random numbers

$$a \leq x_i \leq b$$

This is easily generalized to multidimensional space. In 2D it becomes:

$$\int_a^b dx \int_c^d dy f(x,y) \simeq (b-a)(d-c)\frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i) = (b-a)(d-c)\langle f \rangle$$

[1] There are also algorithms that use quasi-random sampling, point targeting high-variance regions, non uniform random distributions,...

# Why Monte Carlo integration?

For deterministic integration techniques, in order to maintain the error "small" the number of points that are required for integration needs to grow with the number of dimensions.

If we are sampling a given dimension with $N$ points, then we will require $N^D$ points in $D$ dimensions. This number rapidly becomes prohibitive for problems in high-dimensions.

Similarly, let's say we are limited to use N points in total (e.g. because of limited computational resources). As the number of dimensions increases, we have that for each dimension the number of points decreases, $N/D$, and thus that the error increases.

The interest in Monte Carlo integration is that the error scales as

$$E \sim \frac{1}{\sqrt{N}}$$

and it is independent of the number of dimensions. In general for

$$D \gtrsim 4 - 5$$

Monte Carlo integration is more accurate.