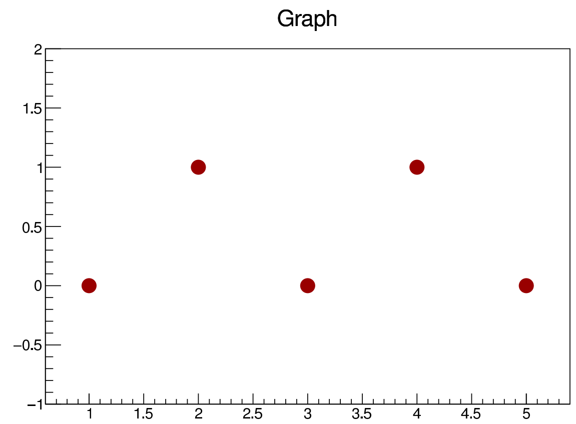
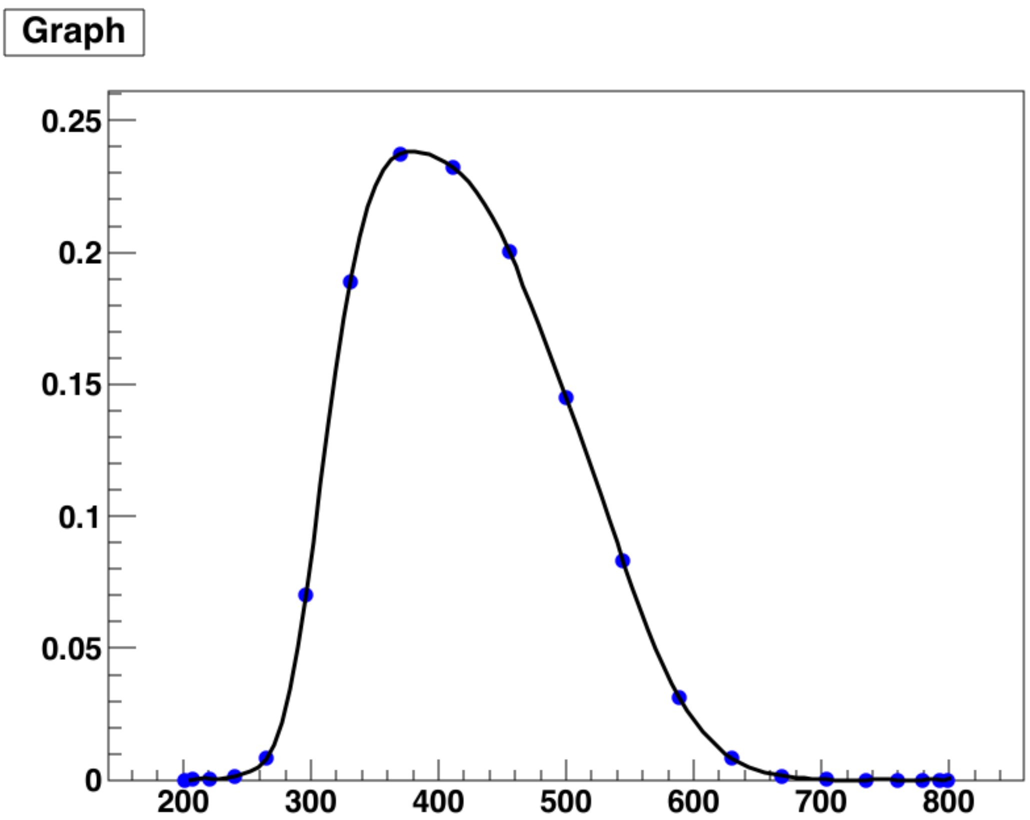
Cubic spline: Problem

Utilizar o método do "cubic spline"para determinar o valor de $y(1.5)$, dados os seguintes valores:

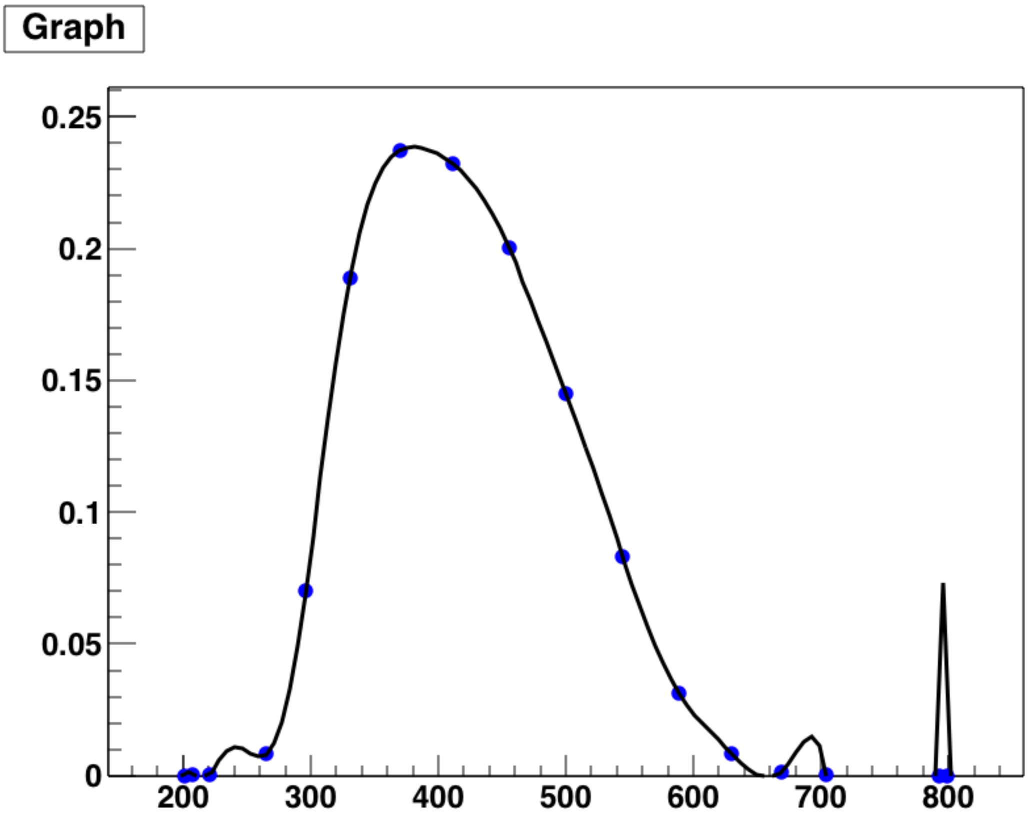
x	1	2	3	4	5
y	0	1	0	1	0



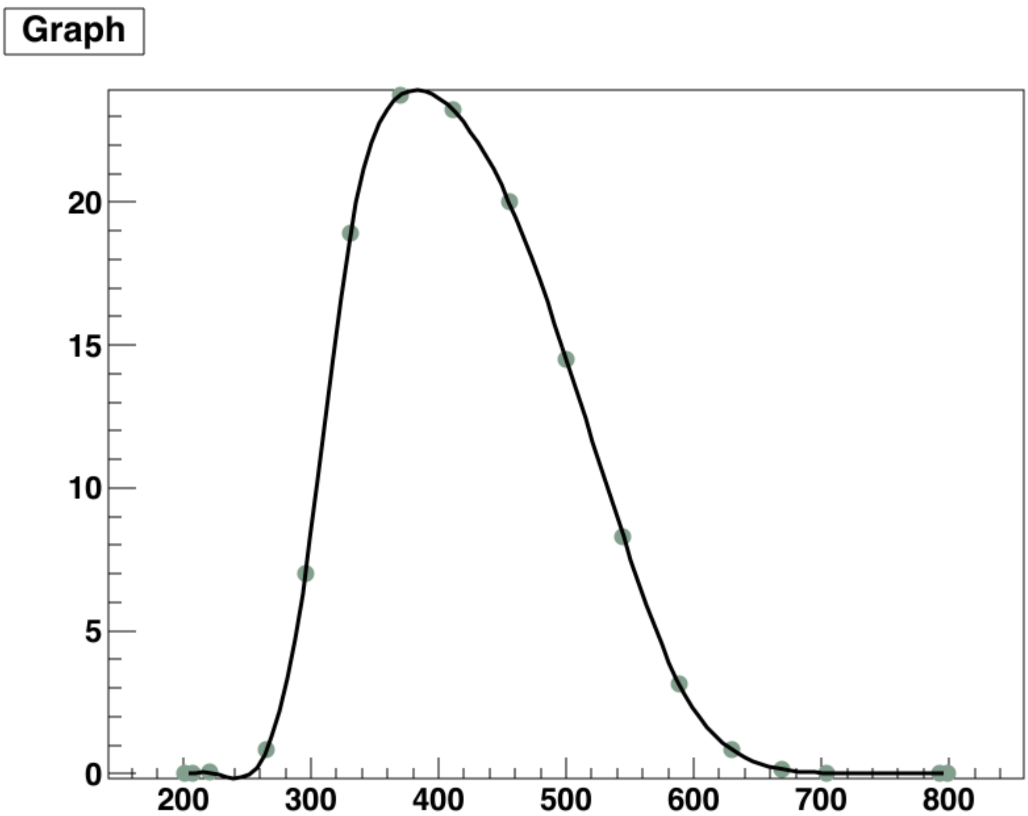
polynomial



polynomial with too many points



the same polynomial with spline3



Computational Physics

Numerical derivatives

Fernando Barao, Phys Department IST (Lisbon)

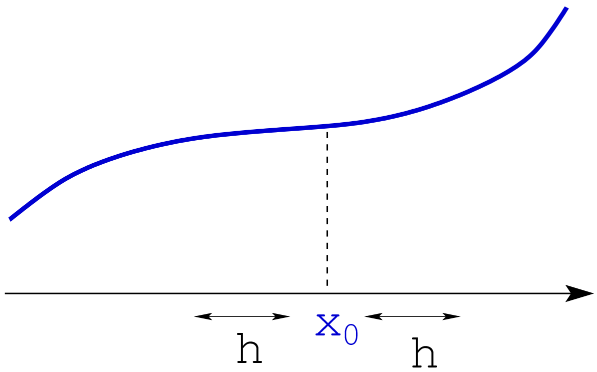
Numerical methods

- System of linear equations
  - Gauss elimination
  - LU decomposition
  - Gauss-Seidel method
- Interpolation
  - Lagrange interpolation
  - Newton method
  - Neville method
  - Cubic spline
- Numerical derivatives
  - First derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - Second derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - Derivative by interpolation
- Numerical integration
  - Newton-Cotes: trapezoidal and Simpson rules
  - Gaussian quadrature
- Monte-Carlo methods

functions: Taylor expansion

- A function can be approximated by a polynomial of order n

$$f(x_0+h) = a_0 + a_1 h + a_2 h^2 + \cdots + a_n h^n$$



- coefficients ($h=0$)

$$f(x_0) = a_0$$
$$f'_h(x_0) = a_1$$
$$f''_h(x_0) = 2a_2 \Rightarrow a_2 = \frac{f''_h(x_0)}{2}$$

$$\begin{aligned} f(x_0+h) &= f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \cdots + \frac{f^{(n)}(x_0)}{n!}h^n \\ f(x_0-h) &= f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \cdots + (-1)^n\frac{f^{(n)}(x_0)}{n!}h^n \end{aligned}$$

Numerical 1st derivative

- The differentiation of a function is one of the most basic tasks in physics: $\frac{d\vec{v}}{dt} = \frac{\vec{F}}{m}$
- **forward difference**

$$f(x_0+h) - f(x_0) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \cdots - f(x_0)$$

$$f'(x_0) \simeq \frac{f(x_0+h) - f(x_0)}{h} + O(h)$$

- **central difference**

$$\begin{aligned} & f(x_0+h) - f(x_0-h) \\ = & f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \cdots \\ & -\left[f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) + \cdots\right] \\ = & 2hf'(x_0) + \frac{2}{3!}h^3 f^{(3)}(x_0) + \cdots \end{aligned}$$

$$f'(x_0) \simeq \frac{f(x_0+h) - f(x_0-h)}{2h} + O(h^2)$$

the accuracy of the derivative increased by one order!

what h step?

truncation error:

$$\delta(\Delta f) = \frac{2}{3!}h^3 f^{(3)} \geq \varepsilon_M$$

$$\varepsilon_M \sim \begin{cases} 10^{-7} & \text{float} \\ 10^{-15} & \text{double} \end{cases}$$

$$\frac{\delta(\Delta f)}{f^{(3)}} = \frac{2}{3!}h^3 \sim \varepsilon_M$$

$$h^3 \sim 3/2\varepsilon_M$$

$$h \sim (10^{-15})^{1/3} \sim 10^{-5}$$

Numerical 1st derivative (cont.)

- For deriving a higher-order first-derivative expression we can use the function values at $[x_0 - 2h, x_0 - h, x_0 + h, x_0 + 2h]$ for eliminating the next order term (f''').

$$\begin{aligned} f(x_0 \pm h) &= f(x_0) \pm hf'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{3!} f'''(x_0) + \cdots \\ f(x_0 \pm 2h) &= f(x_0) \pm 2hf'(x_0) + \frac{4h^2}{2} f''(x_0) \pm \frac{(2h)^3}{3!} f'''(x_0) + \cdots \end{aligned}$$

- We can start by eliminating the f'' from combining $f(x_0 \pm h)$ and $f(x_0 \pm 2h)$

$$\begin{aligned} f(x_0 + h) - f(x_0 - h) &= 2hf'(x_0) + \frac{2h^3}{3!} f'''(x_0) + \mathcal{O}(h^5) \\ f(x_0 + 2h) - f(x_0 - 2h) &= 4hf'(x_0) + \frac{16h^3}{3!} f'''(x_0) + \mathcal{O}(h^5) \end{aligned}$$

- Combining these two expressions to eliminate $f'''(x_0)$

$$(-8) \times [f(x_0 + h) - f(x_0 - h)] + [f(x_0 + 2h) - f(x_0 - 2h)] = -12hf'(x_0) + \mathcal{O}(h^5)$$

Numerical 1st derivative (cont.)

- The five-point formula for first-derivative:

$$f'(x_0) = \frac{1}{12h} [f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \mathcal{O}(h^4)$$

the truncation error goes as $\mathcal{O}(h^4)$

- Numerically the expression above can be improved by decreasing the number of subtractions!

$$f'(x_0) = \frac{1}{12h} [[f(x_0 - 2h) + 8f(x_0 + h)] - [8f(x_0 - h) + f(x_0 + 2h)]]$$

- Notes
  - supposing we have a set of discrete points $x_i = x_0, x_1, \cdots, x_n$ and their respective function values, the central difference cannot be computed in the extreme abcissa values x_0 and x_n, because we would need the function values on both sides
  - in that case, the backward and forward difference can be used to estimate the derivatives

Forward and backward: higher order

✔ We can also derive expressions for computing the 1st derivative of $O(h^2)$ using *forward* and *backward* differences. We will just combine the Taylor series computed at $(x+h)$ and $(x+2h)$ for forward difference and $(x-h)$ and $(x-2h)$ for backward difference.

✔ For eliminating the next order term (f'') we do for the *forward difference*:

$$f(x_0+2h) - 4f(x_0+h) = -3f(x_0) - 2hf'(x_0) + \frac{2h^3}{3}f'''(x_0) + \cdots$$

$$\boxed{f'(x_0) = \frac{-f(x_0+2h) + 4f(x_0+h) - 3f(x_0)}{2h} + O(h^2)}$$

✔ For eliminating the next order term (f'') we do for the *backward difference*:

$$f(x_0-2h) - 4f(x_0-h) = -3f(x_0) + 2hf'(x_0) - \frac{2h^3}{3}f'''(x_0) + \cdots$$

$$\boxed{f'(x_0) = \frac{f(x_0-2h) - 4f(x_0-h) + 3f(x_0)}{2h} + O(h^2)}$$

1st derivative: non uniform data points

✔ In case the data grid is composed of uneven intervals of x, the derivative formulas derived before cannot be used
What can we do?

- ☞ Eventually interpolate the data points in order to have an uniform distribution of data points
- ☞ We can approximate the derivative of $f(x)$ by the derivative of an interpolant
- ☞ We can derive finite difference approximations for unevenly spaced data

1st derivative: three-point formulas

- ✔ We can develop the function $f(x)$ at the points $x_i \pm h_{i\pm i}$ where $h_{i\pm i}$ is different for the left and right points
- ✔ Let's combine $f(x_i + h_{i+1})$ and $f(x_i - h_{i-1})$ to eliminate the second order term ($f''(x_i)$)

$$f(x_i + h_{i+1}) \equiv f(x_{i+1}) = f(x_i) + h_{i+1} f'(x_i) + \frac{h_{i+1}^2}{2} f''(x_i) + \mathcal{O}(h^3) \quad (1)$$

$$f(x_i - h_{i-1}) \equiv f(x_{i-1}) = f(x_i) - h_{i-1} f'(x_i) + \frac{h_{i-1}^2}{2} f''(x_i) + \mathcal{O}(h^3) \quad (2)$$

Multiplying (1) by (h_{i-1}^2) and (2) by $(-h_{i+1}^2)$ and adding the eqs we get rid of the second derivative:

$$f'_i = \frac{h_{i-1}^2 f_{i+1} + (h_i^2 - h_{i-1}^2) f_i - h_i^2 f_{i-1}}{h_i h_{i-1}(h_{i-1} + h_i)} + \mathcal{O}(h^2)$$

1st derivative: by interpolation

- ✔ The cubic spline interpolant segment by segment can be used to get the function derivative at any point

$$f_{i,i+1}(x) = \frac{K_i}{6}\left[\frac{(x-x_{i+1})^3}{x_i - x_{i+1}} - (x - x_{i+1})(x_i - x_{i+1})\right] - \frac{K_{i+1}}{6}\left[\frac{(x-x_i)^3}{x_i - x_{i+1}} - (x - x_i)(x_i - x_{i+1})\right] + \frac{y_i(x-x_{i+1}) - y_{i+1}(x-x_i)}{x_i - x_{i+1}}$$

☞ where $K_{i,i+1}$ are the second derivative values

- ✔ The 1st derivative of the function for x belonging to the segment is:

$$f'_{i,i+1}(x) = \frac{K_i}{6}\left[3\frac{(x-x_{i+1})^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] - \frac{K_{i+1}}{6}\left[3\frac{(x-x_i)^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] + \frac{y_i - y_{i+1}}{x_i - x_{i+1}}$$

- ✔ The 2nd derivative of the function for x belonging to the segment is:

$$f''_{i,i+1}(x) = K_i\left(\frac{x - x_{i+1}}{x_i - x_{i+1}}\right) - K_{i+1}\left(\frac{x - x_i}{x_i - x_{i+1}}\right)$$

Numerical 2nd derivative

- Defining the function expansions at $(x_0 + h)$ and $(x_0 - h)$:

$$f(x_0 \pm h) = f(x_0) \pm h f'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{3!} f'''(x_0) + \cdots$$

- Adding the function expansions, make the odd derivatives disappear:

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + h^2 f''(x_0) + \frac{2h^4}{24} f^{(4)}(x_0) + \cdots$$

- The three-point formula:

$$f''(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} + O(h^2)$$

- The five-pont formula:

$$f''(x_0) = \frac{-f(x_0 - 2h) + 16f(x_0 - h) - 30f(x_0) + 16f(x_0 + h) - f(x_0 + 2h)}{12h^2} + O(h^4)$$

Computational Physics
Numerical integration

Fernando Barao, Phys Department IST (Lisbon)

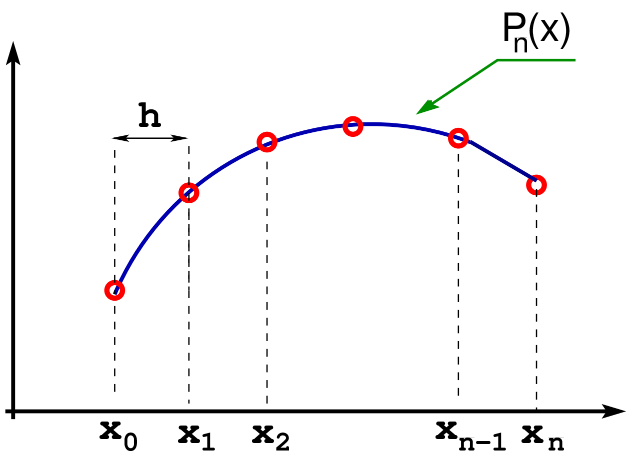
Numerical methods

- ✔ System of linear equations
  - ▶ Gauss elimination
  - ▶ LU decomposition
  - ▶ Gauss-Seidel method
- ✔ Interpolation
  - ▶ Lagrange interpolation
  - ▶ Newton method
  - ▶ Neville method
  - ▶ Cubic spline
- ✔ Numerical derivatives
  - ▶ First derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - ▶ Second derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - ▶ Derivative by interpolation
- ✔ Numerical integration
  - ▶ Newton-Cotes: trapezoidal and Simpson rules
  - ▶ Gaussian quadrature
- ✔ Monte-Carlo methods

Numerical integration: Newton-Cotes

- ✔ Numerical integration consists in replacing the **integral** continous operator by a **sum** of weighted (w_i) function values ($f(x_i)$),

$$F = \boxed{\int_a^b f(x)dx \to \sum_{i=0}^{n} w_i f(x_i)}$$



- ✔ Newton-Cotes formulas are based on local interpolation and they are characterized by equally spaced abcissas
- ✔ They correspond to the **trapezoidal** and **Simpson** methods
- ✔ This approach is generally used when the function can be easily computed at equal intervals

Numerical integration: Newton-Cotes (cont.)

- ✔ Divide the range of integration $[a, b]$ into n intervals of width $h = (b - a)/n$ with the nodes of intervals defined by $x_o, x_1, \cdots, x_n$
- ✔ Next, we approximate the function $f(x)$ by a polynomial of degree n passing through all the nodes. Using the Lagrange form,

$$P_n(x) = \sum_{i=0}^{n} f(x_i)\, \ell_i(x)$$

- ✔ The integral can therefore be expressed as:

$$F = \int_a^b f(x)dx = \sum_{i=0}^{n} \left[f(x_i) \int_a^b \ell_i(x)dx \right] \rightarrow \sum_{i=0}^{n} w_i f(x_i) \qquad (i = 0, 1, \cdots, n)$$

with $w_i = \int_a^b \ell_i(x)dx$ where ℓ_i are the Lagrange cardinal functions

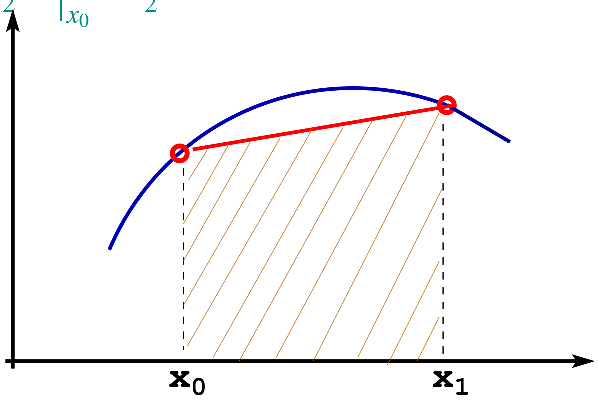
Trapezoidal rule

- ✔ The trapezoidal rule results from $n = 1$, i.e., from defining a linear polynomial passing in two points x_0, x_1 separated of a distance h,

$$F = \int_{x_0}^{x_1} f(x)dx \simeq \sum_{i=0}^{1} f(x_i) \int_{x_0}^{x_1} \prod_{\substack{j=0 \\ (j \neq i)}}^{1} \frac{x - x_j}{x_i - x_j}$$

$$\begin{aligned} w_0 &= \int_{x_0}^{x_1} \ell_0(x)dx = \int_{x_0}^{x_1} \frac{x-x_1}{x_0-x_1} dx = -\frac{1}{h} \left. \frac{(x-x_1)^2}{2} \right|_{x_0}^{x_1} = \frac{h}{2} \\ w_1 &= \int_{x_0}^{x_1} \ell_1(x)dx = \int_{x_0}^{x_1} \frac{x-x_0}{x_1-x_0} dx = -\frac{1}{h} \left. \frac{(x-x_0)^2}{2} \right|_{x_0}^{x_1} = \frac{h}{2} \\ F &= \frac{h}{2} f(x_0) + \frac{h}{2} f(x_1) \\ &= \frac{h}{2} [f(x_0) + f(x_1)] \end{aligned}$$

$$F = \frac{h}{2} [f(x_i) + f(x_{i+1})]$$



Trapezoidal rule error

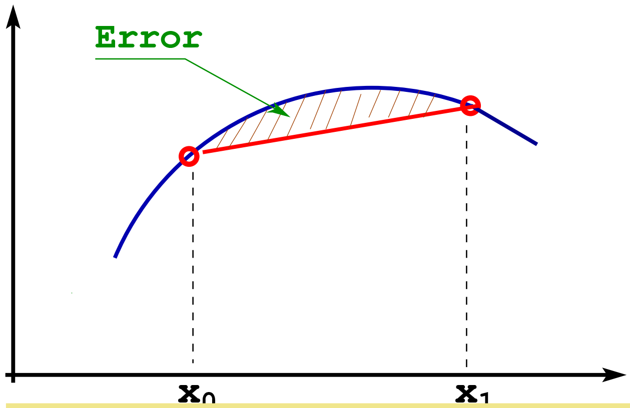
- The error from integrating the function with the **trapezoidal rule** is due to the approximation of the function

$$\Delta F = \int f(x)dx - \int P_n(x)dx$$

- For a given slice $[x_i, x_{i+1}]$, the truncation error associated to the linear approximation is
$f(x) - P_1(x) = \frac{(x-x_i)(x-x_{i+1})}{(n+1)!} f''(\chi)$
(χ, lies in $[x_i, x_{i+1}]$)

- The slice trapezoidal error:

$$\begin{aligned}\Delta F_i &= \int_{x_i}^{x_{i+1}} \frac{(x-x_i)(x-x_{i+1})}{2!} f''(\chi)dx \\ &= \frac{f''(\chi)}{2} \int_{x_i}^{x_{i+1}} (x-x_i)(x-x_{i+1})dx \\ &\simeq -\frac{h^3}{12} f''\left(\frac{(x_i+x_{i+1})}{2}\right) = -\frac{h^3}{12} f''_{i+1/2}\end{aligned}$$



solving the integral:

$$\int_{x_i}^{x_{i+1}} \underbrace{(x-x_i)}_{u} \underbrace{(x-x_{i+1})dx}_{dv} =$$
$$\frac{1}{2}(x-x_i)(x-x_{i+1})^2\Big|_{x_i}^{x_{i+1}} - \frac{1}{2}\int_{x_i}^{x_{i+1}} (x-x_{i+1})^2 dx =$$
$$-\frac{1}{6}(x-x_{i+1})^3\Big|_{x_i}^{x_{i+1}} =$$
$$\frac{1}{6}(x_i - x_{i+1})^3 = -\frac{h^3}{6}$$

Trapezoidal rule (cont.)

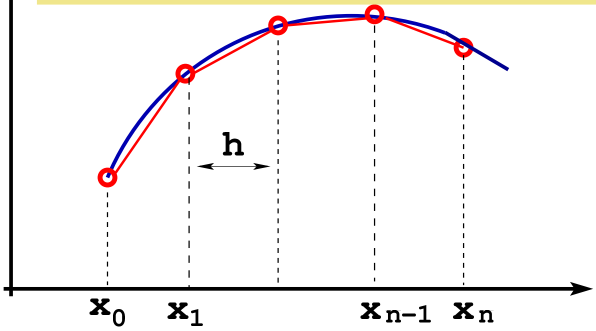
- For extending now the range of integration to the interval [a,b], we divide it in **n** intervals, each with a width **h**

- For every interval

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

- For all the range divided in **n** intervals ($\mathbf{i = 0, 1, , \cdots, n-1}$)

What happens if we double the number of points?



$$F \simeq \frac{h}{2}\sum_{i=0}^{n-1}\left[f(x_i) + f(x_{i+1})\right] = \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)\right]$$

- The truncation error ($n = (b-a)/h$):

$$\Delta F = \sum_{i=0}^{n-1} \Delta F_i = -\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\chi) = -\frac{h^3}{12} n < f''(\chi) >= -\frac{h^2(b-a)}{12} < f''(\chi) >$$

Trapezoidal rule: adaptative scheme

An algorithm for the trapezoidal rule involving the calculation of the integral with an improved accuracy

We will double the number of slices and can keep under control the error of the integral (the difference of the next order with the previous one, provides a good estimation)

Let's use a progressive index $k = 1, 2, 3, \cdots$, that double the number of slices: $n = 2^{k-1} = 1, 2, 4, \cdots$

- ✔ Number of slices = 1 : [a,b] $(k = 1)$

$$F_1 = \frac{b-a}{2}\,[f(a) + f(b)]$$

- ✔ Number of slices = 2 : [a,b] $(k = 2)$

$$F_2 = \frac{b-a}{4}\left[f(a) + 2f\left(a + \frac{b-a}{2}\right) + f(b)\right] = \frac{1}{2}\underbrace{\frac{b-a}{2}\,[f(a) + f(b)]}_{F_1} + \frac{b-a}{2} f\left(a + \frac{b-a}{2}\right)$$

- ✔ Number of slices = 4 : [a,b] $(k = 3)$

$$F_3 = \frac{b-a}{8}\left[f(a) + 2f\left(a + \frac{b-a}{4}\right) + 2f\left(a + 2\frac{b-a}{4}\right) + 2f\left(a + 3\frac{b-a}{4}\right) + f(b)\right]$$
$$= \frac{1}{2}\underbrace{\frac{b-a}{4}\left[f(a) + 2f\left(a + \frac{b-a}{2}\right) + f(b)\right]}_{F_2} + \frac{b-a}{4}\left[f\left(a + \frac{b-a}{4}\right) + f\left(a + 3\frac{b-a}{4}\right)\right]$$

Trapezoidal rule: adaptative scheme

$$F_k = \frac{1}{2} F_{k-1} + \frac{b-a}{2^{k-1}} \sum_{i=1}^{2^{k-2}} f\left(a + (2i-1)\,\frac{b-a}{2^{k-1}}\right)$$