Numerical Differentiation: Finite Difference

Amplitude Error and Phase Error analysis

Consider the periodic basis function:

$f(x) = a\sin(kx+\varphi) \qquad f'(x) = ak\cos(kx+\varphi)$

True derivative at the node $x = x_j$:

$$f'(x_j) = ak\cos(kx_j+\varphi)$$

Numerical derivative using the 2nd order central difference scheme:

$$f_j' = \frac{f_{j+1}-f_{j-1}}{2h} = \frac{a\sin(kx_j+kh+\varphi) - a\sin(kx_j-kh+\varphi)}{2h}$$

$$= a\frac{\sin kh}{h}\cos(kx_j+\varphi) = ak'\cos(kx_j+\varphi)$$

Modified Amplitude = ak'

Numerical Differentiation: Finite Difference

Amplitude Error and Phase Error analysis

Consider the periodic function:

$f(x) = a\sin(kx + \varphi)$ $\qquad$ $f'(x) = ak\cos(kx + \varphi)$

True derivative at the node $x = x_j$:

$$f'(x_j) = ak\cos(kx_j + \varphi)$$

Numerical derivative using the 1st order forward difference scheme:

$$f_j' = \frac{f_{j+1} - f_j}{h} = \frac{a\sin(kx_j + kh + \varphi) - a\sin(kx_j + \varphi)}{h}$$

$$= a\frac{\sin {}^{kh}\!/_2}{{}^{h}\!/_2}\cos\left(kx_j + \frac{kh}{2} + \varphi\right) = ak'\cos(kx_j + \varphi')$$

Modified Amplitude: $ak' = a\frac{\sin {}^{kh}\!/_2}{{}^{h}\!/_2}$; Modified Phase: $\varphi' = \frac{kh}{2} + \varphi$

For Homework: $f(x) = a\cos(kx + \varphi)$

General Technique for Construction of Finite Difference Scheme of Arbitrary Order

General finite difference scheme for uniform grid size *h*:

$$f_i' = \sum_{k=-m}^{n} a_k f_{i+k} + O(h^p)$$

or

$$f_i'' = \sum_{k=-m}^{n} a_k f_{i+k} + O(h^p)$$

or

$$f_i^q = \sum_{k=-m}^{n} a_k f_{i+k} + O(h^p)$$

Let us take an example with $q = 1$, $m = 2$ and $n = 0$

General Technique for Construction of Finite Difference Scheme of Arbitrary Order: Example

General finite difference scheme for uniform grid size h:

$$f_i' = a_{-2} f_{i-2} + a_{-1} f_{i-1} + a_0 f_i + O(h^p)$$

Expand all the function values evaluated at nodes other than i using Taylor's series:

$$f_{i-1} = f_i - h f_i' + \frac{h^2}{2!} f_i'' - \frac{h^3}{3!} f_i''' + \frac{h^4}{4!} f_i^{IV} - \frac{h^5}{5!} f_i^{V} + \frac{h^6}{6!} f_i^{VI} \cdots$$

$$f_{i-2} = f_i - 2h f_i' + \frac{(2h)^2}{2!} f_i'' - \frac{(2h)^3}{3!} f_i''' + \frac{(2h)^4}{4!} f_i^{IV} - \frac{(2h)^5}{5!} f_i^{V} + \frac{(2h)^6}{6!} f_i^{VI} \cdots$$

$$f_i' = a_{-2} f_{i-2} + a_{-1} f_{i-1} + a_0 f_i$$

$$= (a_{-2} + a_{-1} + a_0) f_i + (-2h a_{-2} - h a_{-1}) f_i' + \left(2h^2 a_{-2} + \frac{h^2}{2} a_{-1}\right) f_i''$$

$$+ \left(-\frac{4h^3}{3} a_{-2} - \frac{h^3}{6} a_{-1}\right) f_i''' + \left(\frac{2h^4}{3} a_{-2} + \frac{h^4}{24} a_{-1}\right) f_i^{IV} + \cdots$$

General Technique for Construction of Finite Difference Scheme of Arbitrary Order: Example

$$f_i' = a_{-2}f_{i-2} + a_{-1}f_{i-1} + a_0 f_i$$

$$= (a_{-2} + a_{-1} + a_0)f_i + (-2ha_{-2} - ha_{-1})f_i' + \left(2h^2 a_{-2} + \frac{h^2}{2}a_{-1}\right)f_i''$$

$$+ \left(-\frac{4h^3}{3}a_{-2} - \frac{h^3}{6}a_{-1}\right)f_i''' + \left(\frac{2h^4}{3}a_{-2} + \frac{h^4}{24}a_{-1}\right)f_i^{IV} + \cdots$$

$$a_{-2} + a_{-1} + a_0 = 0$$

$$-2ha_{-2} - ha_{-1} = 1$$

$$2h^2 a_{-2} + \frac{h^2}{2}a_{-1} = 0$$

$$a_0 = \frac{3}{2h}; a_{-1} = -\frac{4}{2h}; a_{-2} = \frac{1}{2h}; \qquad f_i' = \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h}$$

$$TE = -\frac{4h^3}{3}a_{-2} - \frac{h^3}{6}a_{-1} = -\frac{h^2}{3} = O(h^2)$$

General Technique for Construction of Finite Difference Scheme of Arbitrary Order: Example

$$f_i'' = a_{-2}f_{i-2} + a_{-1}f_{i-1} + a_0 f_i$$

$$= (a_{-2} + a_{-1} + a_0)f_i + (-2ha_{-2} - ha_{-1})f_i' + \left(2h^2 a_{-2} + \frac{h^2}{2}a_{-1}\right)f_i''$$

$$+ \left(-\frac{4h^3}{3}a_{-2} - \frac{h^3}{6}a_{-1}\right)f_i''' + \left(\frac{2h^4}{3}a_{-2} + \frac{h^4}{24}a_{-1}\right)f_i^{IV} + \cdots$$

$$a_{-2} + a_{-1} + a_0 = 0$$

$$-2ha_{-2} - ha_{-1} = 0$$

$$2h^2 a_{-2} + \frac{h^2}{2}a_{-1} = 1$$

$$a_0 = \frac{1}{h^2}; a_{-1} = -\frac{2}{h^2}; a_{-2} = \frac{1}{h^2}; \qquad f_i' = \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2}$$

$$TE = -\frac{4h^3}{3}a_{-2} - \frac{h^3}{6}a_{-1} = -h = O(h)$$

General Technique for Construction of Finite Difference Scheme of Arbitrary Order: Example

General finite difference scheme for uniform grid size h:

$$f_i' = a_{-2}f_{i-2} + a_{-1}f_{i-1} + a_0 f_i + O(h^p)$$

		f_i	f_i'	f_i''	f_i'''	f_i^{IV}
LHS	f_i'	0	1	0	0	0
RHS	$a_0 f_i$	a_0	0	0	0	0
RHS	$a_{-1}f_{i-1}$	a_{-1}	$-ha_{-1}$	$\frac{h^2}{2}a_{-1}$	$-\frac{h^3}{6}a_{-1}$	$\frac{h^4}{24}a_{-1}$
RHS	$a_{-2}f_{i-2}$	a_{-2}	$-2ha_{-2}$	$2h^2a_{-2}$	$-\frac{4h^3}{3}a_{-2}$	$\frac{2h^4}{3}a_{-2}$

Richardson's Extrapolation

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - f_i}{h} = f_i' + \frac{h}{2!}f_i'' + \frac{h^2}{3!}f_i''' + \frac{h^3}{4!}f_i^{IV} + \frac{h^4}{5!}f_i^{V} \cdots$$

$$\widetilde{D}_h = \frac{f_{i+1} - f_i}{h} = f_i' + c_1 h + c_2 h^2 + c_3 h^3 + c_4 h^4 \cdots$$

$$\widetilde{D}_{h/2} = f_i' + c_1\frac{h}{2} + c_2\frac{h^2}{4} + c_3\frac{h^3}{8} + c_4\frac{h^4}{16} \cdots$$

$$\widetilde{D}_{h/4} = f_i' + c_1\frac{h}{4} + c_2\frac{h^2}{16} + c_3\frac{h^3}{64} + c_4\frac{h^4}{256} \cdots$$

$$\widetilde{D}_{h/8} = f_i' + c_1\frac{h}{8} + c_2\frac{h^2}{64} + c_3\frac{h^3}{512} + c_4\frac{h^4}{4096} \cdots$$

Richardson's Extrapolation

$$\widetilde{D}_h = f_i' + c_1 h + c_2 h^2 + c_3 h^3 + c_4 h^4 \cdots$$

$$\widetilde{D}_{h/2} = f_i' + c_1 \frac{h}{2} + c_2 \frac{h^2}{4} + c_3 \frac{h^3}{8} + c_4 \frac{h^4}{16} \cdots$$

$$\widetilde{D}_{h/4} = f_i' + c_1 \frac{h}{4} + c_2 \frac{h^2}{16} + c_3 \frac{h^3}{64} + c_4 \frac{h^4}{256} \cdots$$

$$\widetilde{D}_{h/8} = f_i' + c_1 \frac{h}{8} + c_2 \frac{h^2}{64} + c_3 \frac{h^3}{512} + c_4 \frac{h^4}{4096} \cdots$$

$$\widetilde{D}_{h,h/2} = 2\widetilde{D}_{h/2} - \widetilde{D}_h = f_i' - c_2 \frac{h^2}{2} - c_3 \frac{3h^3}{4} - c_4 \frac{7h^4}{8} \cdots$$

$$\widetilde{D}_{h/2,h/4} = 2\widetilde{D}_{h/4} - \widetilde{D}_{h/2} = f_i' - c_2 \frac{h^2}{8} - c_3 \frac{3h^3}{32} - c_4 \frac{7h^4}{128} \cdots$$

$$\widetilde{D}_{h/4,h/8} = 2\widetilde{D}_{h/8} - \widetilde{D}_{h/4} = f_i' - c_2 \frac{h^2}{32} - c_3 \frac{3h^3}{256} - c_4 \frac{7h^4}{2048} \cdots$$

Richardson's Extrapolation

$$\widetilde{D}_{h,h/2} = f_i' - c_2\frac{h^2}{2} - c_3\frac{3h^3}{4} - c_4\frac{7h^4}{8}\cdots$$

$$\widetilde{D}_{h/2,h/4} = f_i' - c_2\frac{h^2}{8} - c_3\frac{3h^3}{32} - c_4\frac{7h^4}{128}\cdots$$

$$\widetilde{D}_{h/4,h/8} = f_i' - c_2\frac{h^2}{32} - c_3\frac{3h^3}{256} - c_4\frac{7h^4}{2048}\cdots$$

$$\widetilde{D}_{h,h/2,h/4} = \frac{4\widetilde{D}_{h/2,h/4} - \widetilde{D}_{h,h/2}}{3} = f_i' + c_3\frac{h^3}{8} + c_4\frac{7h^4}{32}\cdots$$

$$\widetilde{D}_{h/2,h/4,h/8} = \frac{4\widetilde{D}_{h/4,h/8} - \widetilde{D}_{h/2,h/4}}{3} = f_i' + c_3\frac{h^3}{64} + c_4\frac{7h^4}{512}\cdots$$

$$\widetilde{D}_{h,h/2,h/4,h/8} = \frac{8\widetilde{D}_{h/2,h/4,h/8} - \widetilde{D}_{h,h/2,h/4}}{7} = f_i' - c_4\frac{h^4}{64}\cdots$$

Richardson's Extrapolation

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - f_i}{h} = f_i' + \frac{h}{2!}f_i'' + \frac{h^2}{3!}f_i''' + \frac{h^3}{4!}f_i^{IV} + \frac{h^4}{5!}f_i^{V} \cdots$$

$$\widetilde{D}_h = \frac{f_{i+1} - f_i}{h} = f_i' + c_1 h + c_2 h^2 + c_3 h^3 + c_4 h^4 \cdots$$

$$\widetilde{D}_{2h} = f_i' + 2c_1 h + 4c_2 h^2 + 8c_3 h^3 + 16c_4 h^4 \cdots$$

$$\widetilde{D}_{4h} = f_i' + 4c_1 h + 16c_2 h^2 + 64c_3 h^3 + 256c_4 h^4 \cdots$$

$$\widetilde{D}_{8h} = f_i' + 8c_1 h + 64c_2 h^2 + 512c_3 h^3 + 4096c_4 h^4 \cdots$$

Richardson's Extrapolation

$$\widetilde{D}_h = f_i' + c_1 h + c_2 h^2 + c_3 h^3 + c_4 h^4 \cdots$$

$$\widetilde{D}_{2h} = f_i' + 2c_1 h + 4c_2 h^2 + 8c_3 h^3 + 16c_4 h^4 \cdots$$

$$\widetilde{D}_{4h} = f_i' + 4c_1 h + 16c_2 h^2 + 64c_3 h^3 + 256c_4 h^4 \cdots$$

$$\widetilde{D}_{8h} = f_i' + 8c_1 h + 64c_2 h^2 + 512c_3 h^3 + 4096c_4 h^4 \cdots$$

$$\widetilde{D}_{h,2h} = 2\widetilde{D}_h - \widetilde{D}_{2h} = f_i' - 2c_2 h^2 - 6c_3 h^3 - 14c_4 h^4 \cdots$$

$$\widetilde{D}_{2h,4h} = 2\widetilde{D}_{2h} - \widetilde{D}_{4h} = f_i' - 8c_2 h^2 - 48c_3 h^3 - 224c_4 h^4 \cdots$$

$$\widetilde{D}_{4h,8h} = 2\widetilde{D}_{4h} - \widetilde{D}_{8h} = f_i' - 32c_2 h^2 - 384c_3 h^3 - 3584c_4 h^4 \cdots$$

$$\widetilde{D}_{h,2h,4h} = \frac{4\widetilde{D}_{h,2h} - \widetilde{D}_{2h,4h}}{3} = f_i' + 8c_3 h^3 + 56c_4 h^4 \cdots$$

$$\widetilde{D}_{2h,4h,8h} = \frac{4\widetilde{D}_{2h,4h} - \widetilde{D}_{4h,8h}}{3} = f_i' + 64c_3 h^3 + 896c_4 h^4 \cdots$$

$$\widetilde{D}_{h,2h,4h,8h} = \frac{8\widetilde{D}_{h,2h,4h} - \widetilde{D}_{2h,4h,8h}}{7} = f_i' - 64c_4 h^4 \cdots$$

Richardson's Extrapolation

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2!}f_i'' - \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} - \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - f_{i-1}}{2h} = f_i' + \frac{h^2}{3!}f_i''' + \frac{h^4}{5!}f_i^{V} + \frac{h^6}{7!}f_i^{VII} + \frac{h^8}{9!}f_i^{IX} \cdots$$

$$\widetilde{D}_h = \frac{f_{i+1} - f_{i-1}}{2h} = f_i' + c_1 h^2 + c_2 h^4 + c_3 h^6 + c_4 h^8 \cdots$$

$$\widetilde{D}_{h/2} = f_i' + c_1 \frac{h^2}{4} + c_2 \frac{h^4}{16} + c_3 \frac{h^6}{64} + c_4 \frac{h^8}{256} + \cdots$$

$$\widetilde{D}_{h/4} = f_i' + c_1 \frac{h^2}{16} + c_2 \frac{h^4}{256} + c_3 \frac{h^6}{4096} + c_4 \frac{h^8}{65536} + \cdots$$

Richardson’s Extrapolation

$$\widetilde{D}_h = f_i' + c_1 h^2 + c_2 h^4 + c_3 h^6 + c_4 h^8 \cdots$$

$$\widetilde{D}_{h/_2} = f_i' + c_1 \frac{h^2}{4} + c_2 \frac{h^4}{16} + c_3 \frac{h^6}{64} + c_4 \frac{h^8}{256} + \cdots$$

$$\widetilde{D}_{h/_4} = f_i' + c_1 \frac{h^2}{16} + c_2 \frac{h^4}{256} + c_3 \frac{h^6}{4096} + c_4 \frac{h^8}{65536} + \cdots$$

$$\widetilde{D}_{h,h/_2} = \frac{4\widetilde{D}_{h/_2} - \widetilde{D}_h}{3} = f_i' - c_2 \frac{h^4}{4} - c_3 \frac{5h^6}{16} - c_4 \frac{21h^8}{64} \cdots$$

$$\widetilde{D}_{h/_2,h/_4} = \frac{4\widetilde{D}_{h/_4} - \widetilde{D}_{h/_2}}{3} = f_i' - c_2 \frac{h^4}{64} - c_3 \frac{5h^6}{1024} - c_4 \frac{21h^8}{16384} \cdots$$

$$\widetilde{D}_{h,h/_2,h/_4} = \frac{16\widetilde{D}_{h/_2,h/_4} - \widetilde{D}_{h,h/_2}}{15} = f_i' + c_3 \frac{h^6}{64} + c_4 \frac{21h^8}{1024} + \cdots$$

Richardson’s Extrapolation

In order to cancel the term of order h^p from the truncation errors of two successive interval halving or doubling, the general formula is given by:

$$\frac{2^p \widetilde{D}_{fine\ grid} - \widetilde{D}_{coarse\ grid}}{2^p - 1}$$

Order of the resulting approximation may be $(p + 1)$ or $(p + 2)$ depending on the sequence of terms in the truncation error of the original approximation!

Partial Derivatives

- ✓ Same expressions can be used for partial derivatives as well.
- ✓ Example: a function of two variables $f(x, y)$, use indices i and j, grid sizes h_x and h_y for x and y:

$$f\left(x_i, y_j\right) = f_{i,j}$$

- ✓ 1st order accurate forward difference at (x_i, y_j):

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1,j} - f_{i,j}}{h_x} \qquad \frac{\partial f}{\partial y} \approx \frac{f_{i,j+1} - f_{i,j}}{h_y}$$

- ✓ 2nd order accurate forward difference at (x_i, y_j):

$$\frac{\partial f}{\partial x} \approx \frac{-3f_{i,j} + 4f_{i+1,j} - f_{i+2,j}}{2h_x} \qquad \frac{\partial f}{\partial y} \approx \frac{-3f_{i,j} + 4f_{i,j+1} - f_{i,j+2}}{2h_y}$$

Partial Derivatives

- ✓ 2nd order accurate central difference at (x_i, y_j):

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1,j} - f_{i-1,j}}{2h_x} \qquad \frac{\partial f}{\partial y} \approx \frac{f_{i,j+1} - f_{i,j-1}}{2h_y}$$

- ✓ 2nd order accurate central difference at (x_i, y_j):

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{{h_x}^2} \qquad \frac{\partial^2 f}{\partial y^2} \approx \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{{h_y}^2}$$

- ✓ 2nd order accurate backward difference at (x_i, y_j):

$$\frac{\partial f}{\partial x} \approx \frac{3f_{i,j} - 4f_{i-1,j} + f_{i-2,j}}{2h_x} \qquad \frac{\partial f}{\partial y} \approx \frac{3f_{i,j} - 4f_{i,j-1} + f_{i,j-2}}{2h_y}$$

ESO 208A: Computational Methods in Engineering

Numerical Integration

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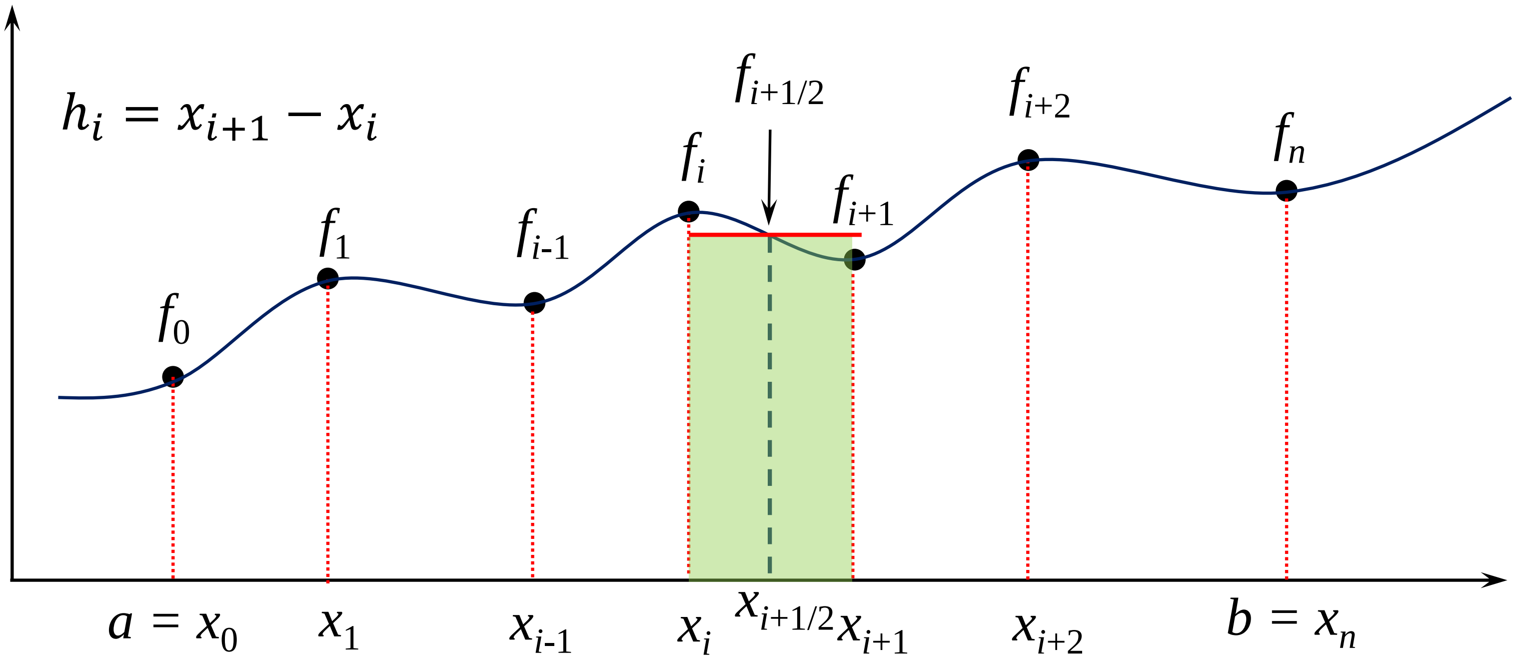
Numerical Integration

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

- ✓ Partition x as: $x = \{a = x_0, x_1, x_2, \cdots x_n = b\}$
- ✓ If $f(x)$ is known, the user or the algorithm will determine the partition or mesh or locations of x_i's
- ✓ If tab(f) is known, the location of the nodes are also known *apriori*
- ✓ General approach: approximate $f(x)$ with one or a piece-wise continuous set of polynomials $p(x)$ and evaluate:

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

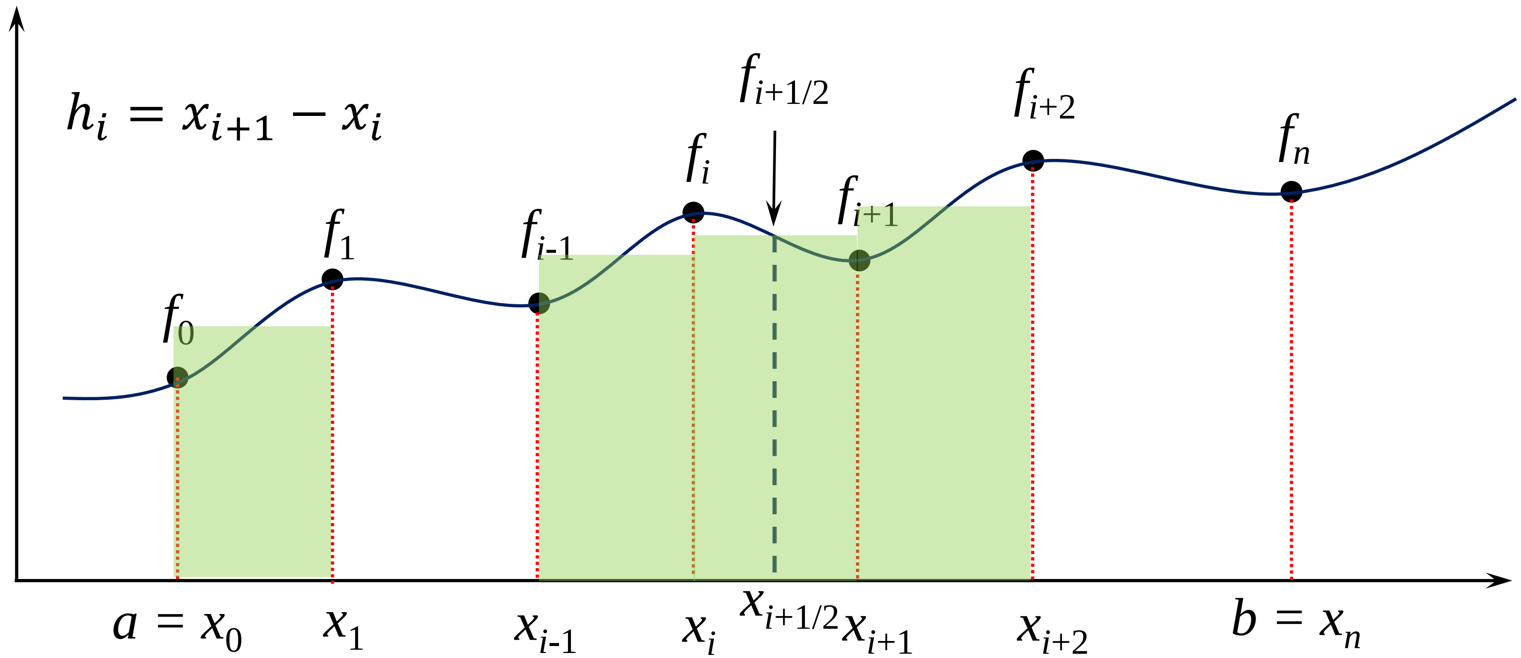
Numerical Integration: Rectangular Rule



Polynomial $p(x)$ is piecewise constant function: $p_i(x) = f_{i+1/2}$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \int_{x_i}^{x_{i+1}} f_{i+1/2}\,dx = h_i f_{i+1/2}$$

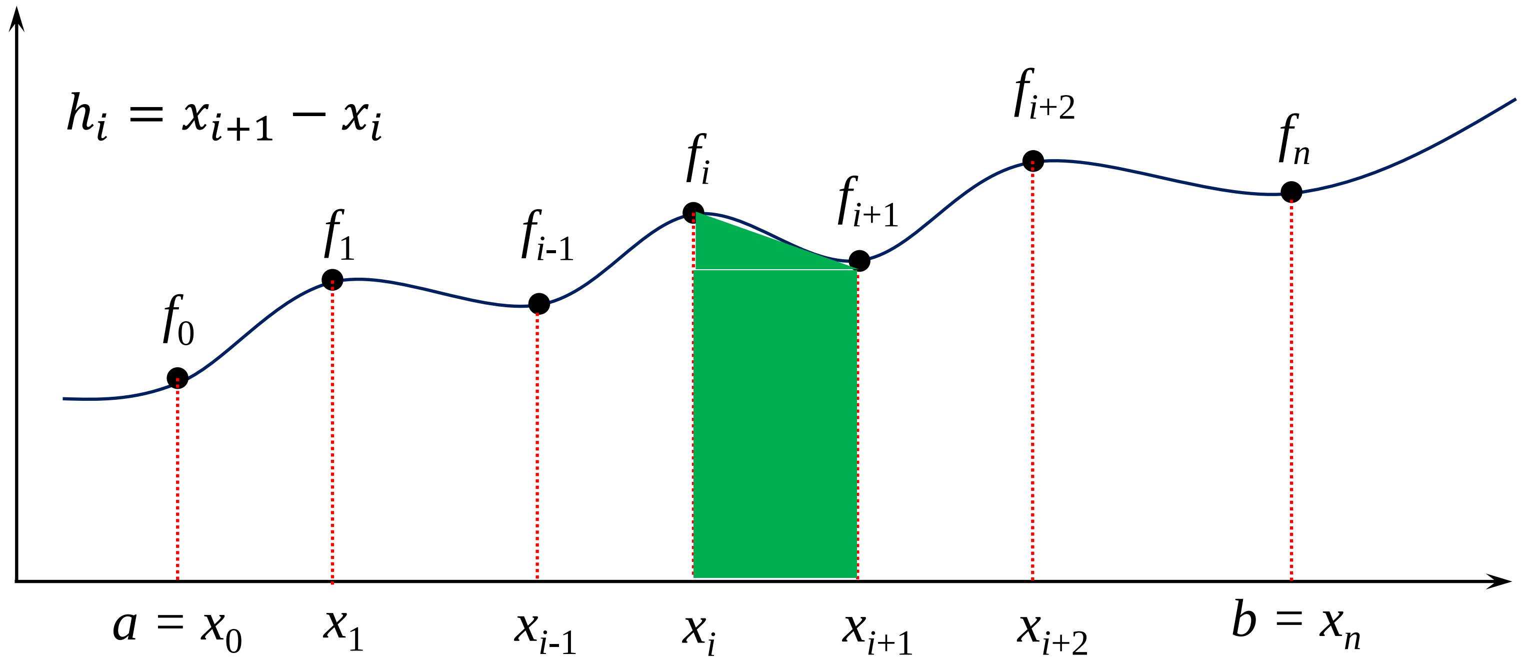
Numerical Integration: Rectangular Rule



$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h_i f_{i+1/2}$$

$$I = \int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} h_i\, f_{i+1/2}$$

Numerical Integration: Trapezoidal Rule



Polynomial $p(x)$ is piecewise linear function:

$$f(x) \approx p(x) = \frac{x - x_i}{x_{i+1} - x_i} f_{i+1} + \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i = \frac{f_{i+1}}{h_i}(x - x_i) - \frac{f_i}{h_i}(x - x_{i+1})$$

Numerical Integration: Trapezoidal Rule

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \int_{x_i}^{x_{i+1}} p(x)dx = \frac{f_{i+1}}{h_i}\int_{x_i}^{x_{i+1}} (x - x_i)dx - \frac{f_i}{h_i}\int_{x_i}^{x_{i+1}} (x - x_{i+1})dx$$

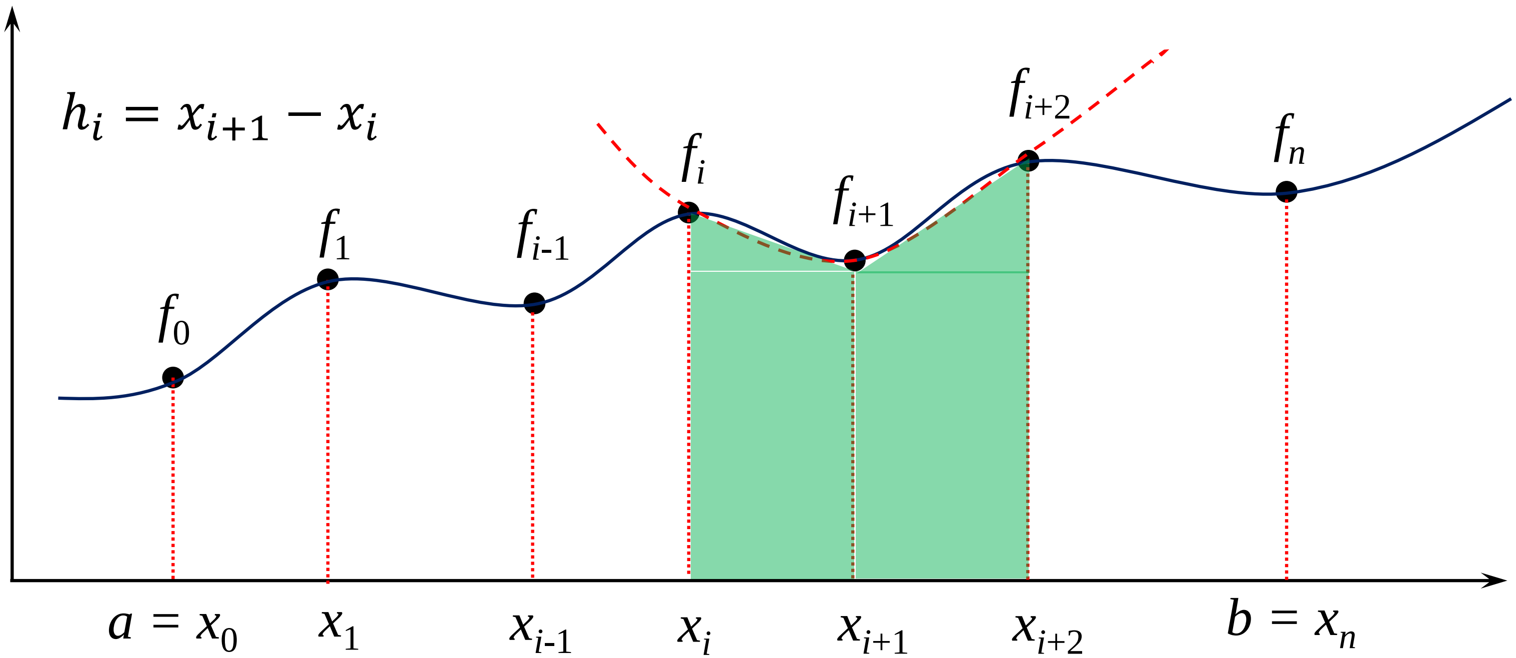
$$= \frac{f_{i+1}}{h_i}\left[\frac{h_i^2}{2}\right] - \frac{f_i}{h_i}\left[-\frac{h_i^2}{2}\right] = h_i\left(\frac{f_{i+1}}{2} + \frac{f_i}{2}\right)$$

$$I = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx \approx \sum_{i=0}^{n-1} h_i\left(\frac{f_{i+1}}{2} + \frac{f_i}{2}\right)$$

If the mesh is uniform, $h_i = h$ for all i:

$$I = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx \approx h\left[\frac{f_0}{2} + \frac{f_n}{2} + \sum_{i=1}^{n-1} f_i\right] = h\sum_{i=0}^{n}\omega_i f_i$$

Numerical Integration: Simpson's Rules



Polynomial $p(x)$ is piecewise quadratic function:

$$f(x) \approx p(x)$$
$$= \frac{(x - x_{i+2})(x - x_{i+1})}{(x_i - x_{i+2})(x_i - x_{i+1})} f_i + \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} f_{i+1} + \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f_{i+2}$$

Numerical Integration: Simpson's Rules

Polynomial $p(x)$ is piecewise quadratic function:

$$f(x) \approx p(x)$$
$$= \frac{(x - x_{i+2})(x - x_{i+1})}{(x_i - x_{i+2})(x_i - x_{i+1})} f_i + \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} f_{i+1}$$
$$+ \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f_{i+2}$$

$$\int_{x_i}^{x_{i+2}} f(x)dx \approx \int_{x_i}^{x_{i+2}} p(x)dx$$

$$= f_i \int_{x_i}^{x_{i+2}} \frac{(x - x_{i+2})(x - x_{i+1})}{(x_i - x_{i+2})(x_i - x_{i+1})} dx + f_{i+1} \int_{x_i}^{x_{i+2}} \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} dx$$
$$+ f_{i+2} \int_{x_i}^{x_{i+2}} \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} dx$$

Assume, $h_i = h_{i+1} = h$ and substitute $z = (x - x_i)$

Numerical Integration: Simpson's Rules

$$\int_{x_i}^{x_{i+2}} f(x)dx \approx \int_{x_i}^{x_{i+2}} p(x)dx$$

$$= f_i \int_{x_i}^{x_{i+2}} \frac{(x - x_{i+2})(x - x_{i+1})}{(x_i - x_{i+2})(x_i - x_{i+1})} dx + f_{i+1} \int_{x_i}^{x_{i+2}} \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} dx$$

$$+ f_{i+2} \int_{x_i}^{x_{i+2}} \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} dx$$

Assume, $h_i = h_{i+1} = h$ and substitute $z = (x - x_i)$

$$\int_{x_i}^{x_{i+2}} f(x)dx \approx \int_{x_i}^{x_{i+2}} p(x)dx$$

$$= \frac{f_i}{2h^2} \int_0^{2h} (z - 2h)(z - h)dz - \frac{f_{i+1}}{h^2} \int_0^{2h} (z - 2h)z dz + \frac{f_{i+2}}{2h^2} \int_0^{2h} (z - h)z dz$$

Numerical Integration: Simpson's Rules

$$\int_{x_i}^{x_{i+2}} f(x)dx \approx \int_{x_i}^{x_{i+2}} p(x)dx$$

$$= \frac{f_i}{2h^2}\int_0^{2h} (z-2h)(z-h)dz - \frac{f_{i+1}}{h^2}\int_0^{2h} (z-2h)zdz$$

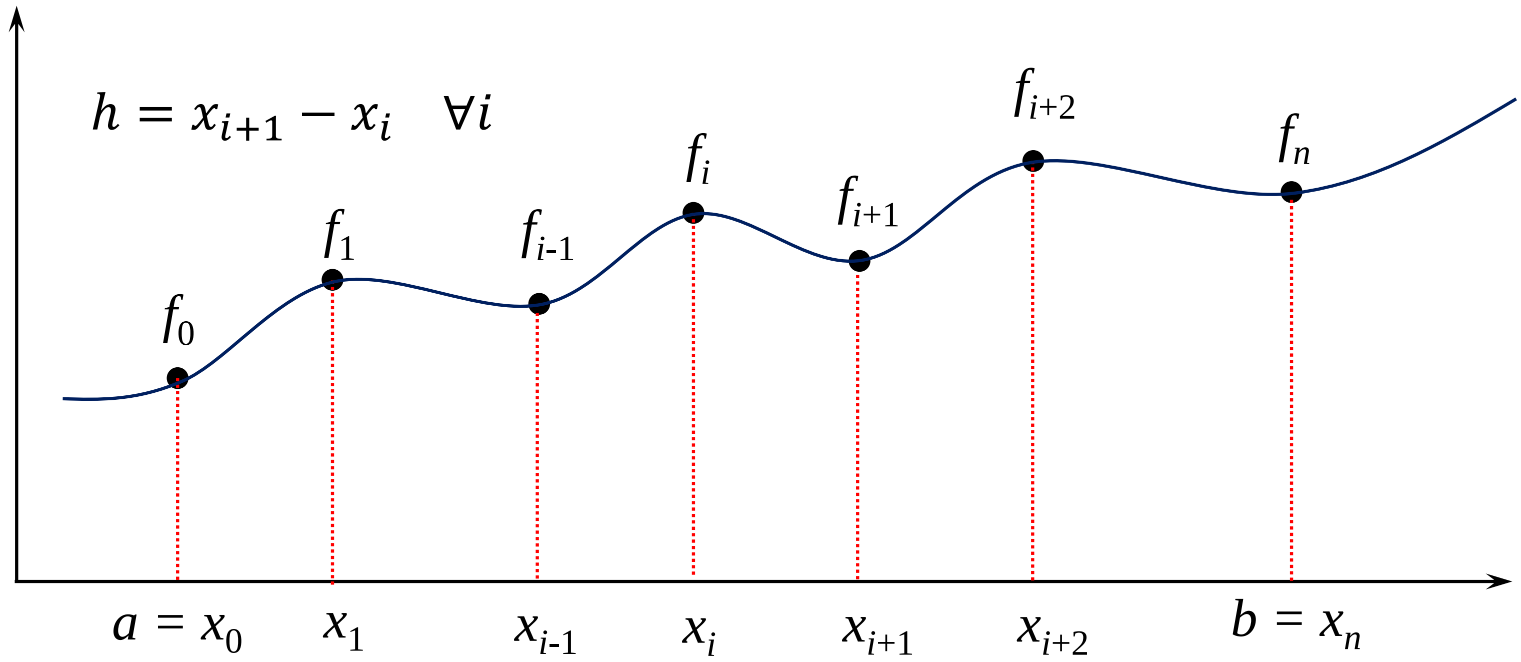
$$+ \frac{f_{i+2}}{2h^2}\int_0^{2h} (z-h)zdz$$

$$= \frac{f_i}{2h^2}\left[\frac{(2h)^3}{3} - 3h\frac{(2h)^2}{2} + 2h^2(2h)\right] - \frac{f_{i+1}}{h^2}\left[\frac{(2h)^3}{3} - 2h\frac{(2h)^2}{2}\right]$$

$$+ \frac{f_{i+2}}{2h^2}\left[\frac{(2h)^3}{3} - h\frac{(2h)^2}{2}\right] = \frac{h}{3}[f_i + 4f_{i+1} + f_{i+2}]$$

This is known as Simpson's 1/3rd Rule

Numerical Integration: Simpson's Rules



If the mesh is uniform, $h_i = h$ for all i:

$$I = \int_a^b f(x)\,dx \approx \frac{h}{3}\left[f_0 + f_n + 4\sum_{\substack{i=1\\i=odd}}^{n-1} f_i + 2\sum_{\substack{i=1\\i=even}}^{n-2} f_i\right] = h\sum_{i=0}^{n} \omega_i f_i$$

$n = 2m$, m integer

Numerical Integration: Simpson's Rules

Polynomial $p(x)$ is piecewise cubic function:

$$f(x) \approx p(x)$$
$$= \frac{(x-x_{i+3})(x-x_{i+2})(x-x_{i+1})}{(x_i-x_{i+3})(x_i-x_{i+2})(x_i-x_{i+1})} f_i + \frac{(x-x_{i+3})(x-x_{i+2})(x-x_i)}{(x_{i+1}-x_{i+3})(x_{i+1}-x_{i+2})(x_{i+1}-x_i)} f_{i+1}$$
$$+ \frac{(x-x_i)(x-x_{i+1})(x-x_{i+3})}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})(x_{i+2}-x_{i+3})} f_{i+2}$$
$$+ \frac{(x-x_i)(x-x_{i+1})(x-x_{i+2})}{(x_{i+3}-x_i)(x_{i+3}-x_{i+1})(x_{i+3}-x_{i+2})} f_{i+3}$$

Assume, $h_i = h_{i+1} = h_{i+2} = h$ and substitute $z = (x - x_i)$

$$\int_{x_i}^{x_{i+3}} f(x)dx \approx \int_{x_i}^{x_{i+3}} p(x)dx$$
$$= -\frac{f_i}{6h^3}\int_0^{3h} (z-3h)(z-2h)(z-h)dz + \frac{f_{i+1}}{2h^3}\int_0^{3h} (z-3h)(z-2h)zdz$$
$$-\frac{f_{i+2}}{2h^3}\int_0^{3h} (z-3h)(z-h)zdz + \frac{f_{i+2}}{6h^3}\int_0^{3h} (z-2h)(z-h)zdz$$

Numerical Integration: Simpson's Rules

$$\int_{x_i}^{x_{i+3}} f(x)dx \approx \int_{x_i}^{x_{i+3}} p(x)dx$$

$$= -\frac{f_i}{6h^3}\int_0^{3h}(z-3h)(z-2h)(z-h)dz + \frac{f_{i+1}}{2h^3}\int_0^{3h}(z-3h)(z-2h)zdz$$

$$-\frac{f_{i+2}}{2h^3}\int_0^{3h}(z-3h)(z-h)zdz + \frac{f_{i+3}}{6h^3}\int_0^{3h}(z-2h)(z-h)zdz$$

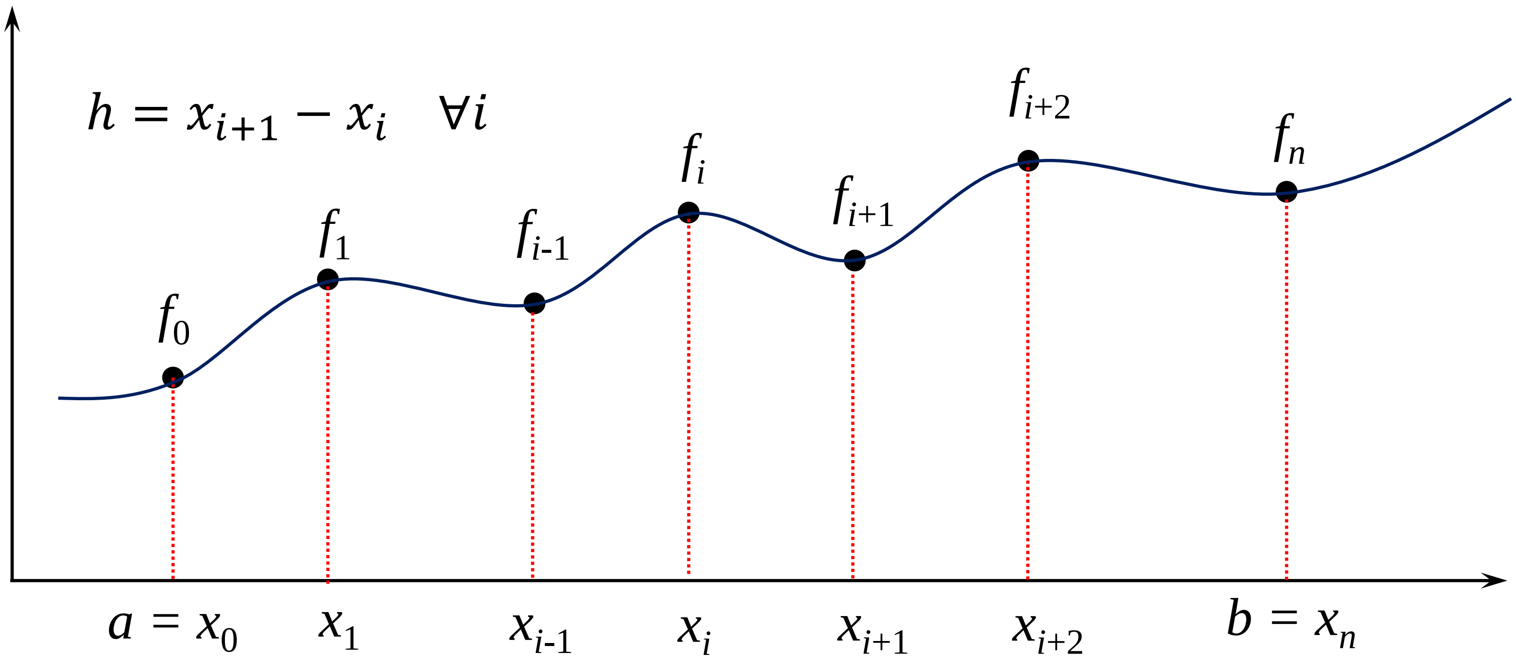
$$= -\frac{f_i}{6h^3}\left[\frac{(3h)^4}{4} - 6h\frac{(3h)^3}{3} + 11h^2\frac{(3h)^2}{2} - 6h^3(3h)\right]$$

$$+\frac{f_{i+1}}{2h^3}\left[\frac{(3h)^4}{4} - 5h\frac{(3h)^3}{3} + 6h^2\frac{(3h)^2}{2}\right] - \frac{f_{i+2}}{2h^3}\left[\frac{(3h)^4}{4} - 4h\frac{(3h)^3}{3} + 3h^2\frac{(3h)^2}{2}\right]$$

$$+\frac{f_{i+3}}{6h^3}\left[\frac{(3h)^4}{4} - 3h\frac{(3h)^3}{3} + 2h^2\frac{(3h)^2}{2}\right] = \frac{3h}{8}[f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3}]$$

This is known as Simpson's 3/8$^{\text{th}}$ Rule

Numerical Integration: Simpson's Rules



If the mesh is uniform, $h_i = h$ for all i:

$$I = \int_a^b f(x)\,dx \approx \frac{3h}{8}\left[f_0 + f_n + 3\sum_{i=1,4,7,10\ldots}^{n-1}(f_i + f_{i+1}) + 2\sum_{i=3,6,9,\ldots}^{n-3} f_i\right] = h\sum_{i=0}^{n}\omega_i f_i$$

$n = 3m$, m integer

Numerical Integration

- ✓ *Accuracy:* How accurate are the numerical integration schemes with respect to the TRUE integral?
  - ✓ **Truncation Error** analysis: ***local*** and ***global***
- ✓ Recall: True Value (a) = Approximate Value ($\tilde{a}$) + Error (ε)
- ✓ Is it possible to improve the accuracy?
  - ✓ Romberg Integration
  - ✓ Quadrature Methods

Numerical Integration: Rectangular Rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h_i f\left(x_{i+\frac{1}{2}}\right) = h_i f_{i+\frac{1}{2}} \qquad x_{i+\frac{1}{2}} = \frac{x_i + x_{i+1}}{2}$$

Expand $f(x)$ in Taylor's series around $x_{i+1/2}$:

Let us denote $y_i = x_{i+1/2}$

$$f(x)$$
$$= f(y_i) + (x - y_i)f'(y_i) + \frac{(x - y_i)^2}{2} f''(y_i)$$
$$+ \frac{(x - y_i)^3}{6} f'''(y_i) + \frac{(x - y_i)^4}{24} f^{IV}(y_i) + \frac{(x - y_i)^5}{120} f^{V}(y_i)$$
$$+ \frac{(x - y_i)^6}{720} f^{VI}(y_i) + \cdots$$

Numerical Integration: Rectangular Rule

$$f(x)$$

$$= f(y_i) + (x-y_i)f'(y_i) + \frac{(x-y_i)^2}{2}f''(y_i) + \frac{(x-y_i)^3}{6}f'''(y_i)$$

$$+ \frac{(x-y_i)^4}{24}f^{IV}(y_i) + \frac{(x-y_i)^5}{120}f^{V}(y_i) + \frac{(x-y_i)^6}{720}f^{VI}(y_i) + \cdots$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$= f(y_i)\int_{x_i}^{x_{i+1}} dx + f'(y_i)\cancelto{0}{\int_{x_i}^{x_{i+1}} (x-y_i)\,dx} + \frac{f''(y_i)}{2}\int_{x_i}^{x_{i+1}} (x-y_i)^2\,dx$$

$$+ \frac{f'''(y_i)}{6}\cancelto{0}{\int_{x_i}^{x_{i+1}} (x-y_i)^3\,dx} + \frac{f^{IV}(y_i)}{24}\int_{x_i}^{x_{i+1}} (x-y_i)^4\,dx$$

$$+ \frac{f^{V}(y_i)}{120}\cancelto{0}{\int_{x_i}^{x_{i+1}} (x-y_i)^5\,dx} + \frac{f^{VI}(y_i)}{720}\int_{x_i}^{x_{i+1}} (x-y_i)^6\,dx + \cdots$$

Numerical Integration: Rectangular Rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$= f(y_i)\int_{x_i}^{x_{i+1}} dx + f'(y_i)\underbrace{\int_{x_i}^{x_{i+1}} (x-y_i)\,dx}_{\mathbf{0}} + \frac{f''(y_i)}{2}\int_{x_i}^{x_{i+1}} (x-y_i)^2\,dx$$

$$+ \frac{f'''(y_i)}{6}\underbrace{\int_{x_i}^{x_{i+1}} (x-y_i)^3\,dx}_{\mathbf{0}} + \frac{f^{IV}(y_i)}{24}\int_{x_i}^{x_{i+1}} (x-y_i)^4\,dx$$

$$+ \frac{f^{V}(y_i)}{120}\underbrace{\int_{x_i}^{x_{i+1}} (x-y_i)^5\,dx}_{\mathbf{0}} + \frac{f^{VI}(y_i)}{720}\int_{x_i}^{x_{i+1}} (x-y_i)^6\,dx + \cdots$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h_i f(y_i) + \frac{h_i^3 f''(y_i)}{24} + \frac{h_i^5 f^{IV}(y_i)}{1920} + \frac{h_i^7 f^{VI}(y_i)}{138240} + \cdots$$

Numerical Integration: Rectangular Rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$= h_i f(y_i) + \frac{h_i^3 f''(y_i)}{24} + \frac{h_i^5 f^{IV}(y_i)}{1920} + \frac{h_i^7 f^{VI}(y_i)}{138240} + \cdots$$

Rectangular rule is $O(h^3)$ accurate in a single interval. This is also known as *Local Truncation Error*.

We will derive Global Truncation Error later. First, let us derive Local Truncation Errors for Trapezoidal and Simpson's 1/3rd Rule!

Numerical Integration: Trapezoidal Rule

$$f(x_i) = f\left(y_i - \frac{h_i}{2}\right)$$
$$= f(y_i) - \frac{h_i}{2} f'(y_i) + \frac{h_i^2}{8} f''(y_i) - \frac{h_i^3}{48} f'''(y_i) + \frac{h_i^4}{384} f^{IV}(y_i) - \frac{h_i^5}{3840} f^{V}(y_i)$$
$$+ \frac{h_i^6}{46080} f^{VI}(y_i) + \cdots$$
$$f(x_{i+1}) = f\left(y_i + \frac{h_i}{2}\right)$$
$$= f(y_i) + \frac{h_i}{2} f'(y_i) + \frac{h_i^2}{8} f''(y_i) + \frac{h_i^3}{48} f'''(y_i) + \frac{h_i^4}{384} f^{IV}(y_i) + \frac{h_i^5}{3840} f^{V}(y_i)$$
$$+ \frac{h_i^6}{46080} f^{VI}(y_i) + \cdots$$
$$\frac{f(x_{i+1}) + f(x_i)}{2} = f(y_i) + \frac{h_i^2}{8} f''(y_i) + \frac{h_i^4}{384} f^{IV}(y_i) + \frac{h_i^6}{46080} f^{VI}(y_i) + \cdots$$
$$f(y_i) = \frac{f(x_{i+1}) + f(x_i)}{2} - \frac{h_i^2}{8} f''(y_i) - \frac{h_i^4}{384} f^{IV}(y_i) - \frac{h_i^6}{46080} f^{VI}(y_i) + \cdots$$

Numerical Integration: Trapezoidal Rule

$$f(y_i) = \frac{f(x_{i+1}) + f(x_i)}{2} - \frac{h_i^2}{8} f''(y_i) - \frac{h_i^4}{384} f^{IV}(y_i) - \frac{h_i^6}{46080} f^{VI}(y_i) + \cdots$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h_i f(y_i) + \frac{h_i^3 f''(y_i)}{24} + \frac{h_i^5 f^{IV}(y_i)}{1920} + \frac{h_i^7 f^{VI}(y_i)}{138240} + \cdots$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h_i \frac{f(x_{i+1}) + f(x_i)}{2} - \frac{h_i^3 f''(y_i)}{12} - \frac{h_i^5 f^{IV}(y_i)}{480} - \frac{h_i^7 f^{VI}(y_i)}{69120} + \cdots$$

Therefore, the Trapezoidal Rule is $O(h^3)$ accurate in a single interval.

The *Local Truncation Error* of both, Rectangular Rule and Trapezoidal Rule is 3rd order.

Let us apply these two integration techniques over an interval $2h_i$ or $\{x_i, x_{i+2}\}$

In this case: $y_i = x_{i+1}$

Numerical Integration: Simpson's 1/3rd Rule

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = 2h_i f(x_{i+1}) + \frac{h_i^3 f''(x_{i+1})}{3} + \frac{h_i^5 f^{IV}(x_{i+1})}{60} + \frac{h_i^7 f^{VI}(x_{i+1})}{1080} \cdots$$

$$\int_{x_i}^{x_{i+2}} f(x)\,dx$$

$$= h_i[f(x_{i+2}) + f(x_i)] - \frac{2h_i^3 f''(x_{i+1})}{3} - \frac{h_i^5 f^{IV}(x_{i+1})}{15} - \frac{h_i^7 f^{VI}(x_{i+1})}{540} \cdots$$

Weighted sum with weights of 2/3 and 1/3!

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = \frac{h_i}{3}[f(x_{i+2}) + 4f(x_{i+1}) + f(x_i)] - \frac{h_i^5 f^{IV}(x_{i+1})}{90} - \cdots$$

Therefore, the Simpson's 1/3rd Rule is $O(h^5)$ accurate in a single interval or the *Local Truncation Error* of Simpson's 1/3rd Rule is $O(h^5)$

Global Truncation Error: Trapezoidal Rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h_i \frac{f(x_{i+1}) + f(x_i)}{2} - \frac{h_i^3 f''(y_i)}{12} - \frac{h_i^5 f^{IV}(y_i)}{480} - \frac{h_i^7 f^{VI}(y_i)}{69120} + \cdots$$

Recall, if the mesh is uniform, $h_i = h$ for all i:

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx \approx h\left[\frac{f_0}{2} + \frac{f_n}{2} + \sum_{i=1}^{n-1} f_i\right] = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx$$

$$= \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i\right] - \frac{h^3}{12}\sum_{i=0}^{n-1} f''(y_i) - \frac{h^5}{480}\sum_{i=0}^{n-1} f^{IV}(y_i) + \cdots$$

Apply, the first mean value theorem of integrals!

Global Truncation Error: Trapezoidal Rule

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i\right] - \frac{h^3}{12}\sum_{i=0}^{n-1} f''(y_i) - \frac{h^5}{480}\sum_{i=0}^{n-1} f^{IV}(y_i) + \cdots$$

Applying the first mean value theorem for integrals:

$$\sum_{i=0}^{n-1} f''(y_i) = \sum_{i=0}^{n-1} f''\left(x_{i+1/2}\right) = nf''(\xi) = \frac{b-a}{h} f''(\xi); \qquad \xi \in [a,b]$$

$$\sum_{i=0}^{n-1} f^{IV}(y_i) = \sum_{i=0}^{n-1} f^{IV}\left(x_{i+1/2}\right) = nf^{IV}(\eta) = \frac{b-a}{h} f^{IV}(\eta); \qquad \eta \in [a,b]$$

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i\right] - \frac{h^2}{12}(b-a)f''(\xi) - \frac{h^4}{480}(b-a)f^{IV}(\eta)\cdots$$

Global Truncation Error of the Trapezoidal Rule is $O(h^2)$

Similarly, for all the methods, we can derive *GTE* to be one order less than *LTE*!

Order of a method is referred by it's *GTE*!

Romberg Integration

$$I = \int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i\right] - \frac{h^2}{12}(b-a)f''(\xi) - \frac{h^4}{480}(b-a)f^{IV}(\eta)\cdots$$

$$\tilde{I}_h = I + c_1 h^2 + c_2 h^4 + c_3 h^6 + c_4 h^8 \cdots$$

$$\tilde{I}_{h/2} = I + c_1\frac{h^2}{4} + c_2\frac{h^4}{16} + c_3\frac{h^6}{64} + c_4\frac{h^8}{256} + \cdots$$

$$\tilde{I}_{h/4} = I + c_1\frac{h^2}{16} + c_2\frac{h^4}{256} + c_3\frac{h^6}{4096} + c_4\frac{h^8}{65536} + \cdots$$

$$\tilde{I}_{h,h/2} = \frac{4\tilde{I}_{h/2} - \tilde{I}_h}{3} = I - c_2\frac{h^4}{4} - c_3\frac{5h^6}{16} - c_4\frac{21h^8}{64}\cdots$$

$$\tilde{I}_{h/2,h/4} = \frac{4\tilde{I}_{h/4} - \tilde{I}_{h/2}}{3} = I - c_2\frac{h^4}{64} - c_3\frac{5h^6}{1024} - c_4\frac{21h^8}{16384}\cdots$$

$$\tilde{I}_{h,h/2,h/4} = \frac{16\tilde{I}_{h/2,h/4} - \tilde{I}_{h,h/2}}{15} = I + c_3\frac{h^6}{64} + c_4\frac{21h^8}{1024} + \cdots$$

Gauss Quadrature

All integration methods derived so far:

$$I = \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} \omega_i f_i$$

- ✓ The weights ω_i are fixed based on the method chosen!
- ✓ Ability to integrate a function exactly does not depend on the number of nodes (n + 1):
  - ✓ Trapezoidal and Rectangular methods integrate a first order (or straight line) polynomial exactly.
  - ✓ Simpson's 1/3rd rule integrates a quadratic or 2nd order polynomial exactly.
  - ✓ Simpson's 3/8th rule integrates a 3rd order polynomial exactly.
- ✓ For all higher order functions, there will be some error and the error is inversely proportional to n.
- ✓ Goal is to design methods that can integrate a polynomial of order (2n + 1) exactly with (n + 1) nodes!

Gauss Quadrature

Problem: Consider the integral

$$I = \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} \omega_i f_i$$

For a given function $f(x)$, choose $(n + 1)$ - x_i and ω_i such that the above integral is exact for a polynomial of order $(2n + 1)$

Let $f(x)$ be a polynomial of order $(2n + 1)$

Let us approximate $p(x)$ by an n^{th} order Lagrange polynomial:

$$p(x) = \sum_{i=0}^{n} f_i \delta_i(x) \qquad \delta_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

Note:

- ✓ the polynomial matches the function $f(x)$ exactly at the grid points $\{x_0, x_1, \cdots x_n\}$
- ✓ the residual polynomial $f(x) - p(x)$ is a polynomial of order $(2n + 1)$ that has zeroes at the grid points.

Gauss Quadrature

- ✓ Let $g(x)$ be a polynomial of order $(n + 1)$ that has zeroes at the grid points $\{x_0, x_1, \cdots x_n\}$

$$g(x) = (x - x_0)(x - x_1)(x - x_2)\cdots(x - x_n)$$

- ✓ Choose a set of linearly independent basis functions $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ $e.g.$, $\{1, x, x^2, \cdots x^n\}$

We may write:

$$f(x) - p(x) = g(x)\sum_{k=0}^{n} c_k\varphi_k = g(x)\sum_{k=0}^{n} c_k x^k$$

$$\int f(x)dx = \int p(x)dx + \sum_{k=0}^{n} c_k \int g(x)\varphi_k(x)dx$$

$$= \int p(x)dx + \sum_{k=0}^{n} c_k \int g(x)x^k dx$$

Gauss Quadrature

$$\int f(x)dx = \int p(x)dx + \sum_{k=0}^{n} c_k \int g(x)\varphi_k(x)dx$$

$$= \int p(x)dx + \sum_{k=0}^{n} c_k \int g(x)x^k dx$$

If we can choose $g(x)$ such that,

$$\int g(x)\varphi_k(x)dx = \int g(x)x^k dx = 0 \qquad k = 0, 1, 2 \cdots n$$

Then,

$$\int f(x)dx = \int p(x)dx$$

and the *nodes* or grid points are located at the zeroes of $g(x)$

Gauss Quadrature

Then,

$$\int f(x)dx = \int p(x)dx = \int \sum_{i=0}^{n} f_i \delta_i(x)\, dx = \sum_{i=0}^{n} f_i \int \delta_i(x) dx$$

$$= \sum_{i=0}^{n} \omega_i f_i$$

$$\omega_i = \int \delta_i(x) dx$$

We return to choose the polynomial $g(x)$ of order $(n + 1)$ such that,

$$\int g(x)\varphi_k(x)dx \ = \int g(x)x^k dx = 0 \qquad k = 0, 1, 2 \cdots n$$

Therefore, $g(x)$ is a polynomial of order $(n + 1)$ which is orthogonal to all polynomials up to order n.

Two such polynomials are well-known: *Legendre* and *Hermite*

Gauss-Legendre Quadrature

- ✓ We already know the *Legendre* polynomials, let's use it!
- ✓ We choose the Legendre polynomial of order (n + 1) and the zeroes of this polynomial are the nodes or grid points $\{x_0, x_1, \cdots x_n\}$. Recall:

$$P_0(x) = 1; \;\; P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}[(x^2-1)^n]; \;\; P_n(x) = \frac{2n-1}{n} x P_{n-1}(x) - \frac{n-1}{n} P_{n-2}(x)$$

- ✓ Since Legendre polynomials are defined in [-1, 1], that is also the limits of x for integrals.

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} p(x)dx = \sum_{i=0}^{n} f_i \int_{-1}^{1} \delta_i(x)dx = \sum_{i=0}^{n} \omega_i f_i$$

$$\omega_i = \int_{-1}^{1} \delta_i(x)dx$$

For arbitrary limit $\int_a^b f(x)\,dx$, use $x = \frac{b+a}{2} + \frac{b-a}{2} z$

$$x \in [a, b] \quad \rightarrow \quad z \in [-1, 1]$$

Gauss-Legendre Quadrature: Example

- ✓ One-point integration:

$$P_1(x) = x = 0; \quad \omega = 1$$

- ✓ Two-points integration:

$$P_2(x) = \tfrac{1}{2}(3x^2 - 1) = 0; \;\; x = \pm\frac{1}{\sqrt{3}}; x_0 = -\frac{1}{\sqrt{3}}; x_1 = \frac{1}{\sqrt{3}}$$

$$\omega_0 = \int_{-1}^{1} \frac{x - x_1}{x_0 - x_1} dx = -\frac{\sqrt{3}}{2} \int_{-1}^{1} \left(x - \frac{1}{\sqrt{3}}\right) dx = 1$$

$$\omega_1 = \int_{-1}^{1} \frac{x - x_0}{x_1 - x_0} dx = \frac{\sqrt{3}}{2} \int_{-1}^{1} \left(x + \frac{1}{\sqrt{3}}\right) dx = 1$$

Gauss-Legendre Quadrature: Example

✓ Three-points integration:

$$P_3(x) = \tfrac{1}{2}(5x^3 - 3x) = 0; \quad x = 0, \pm\sqrt{\frac{3}{5}}$$

$$x_0 = -\sqrt{\frac{3}{5}}; \qquad x_1 = 0; \qquad x_2 = \sqrt{\frac{3}{5}}$$

$$\omega_0 = \int_{-1}^{1} \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} dx = \frac{5}{6} \int_{-1}^{1} x\left(x - \sqrt{\frac{3}{5}}\right) dx = \frac{5}{9}$$

$$\omega_1 = \int_{-1}^{1} \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} dx = -\frac{5}{3} \int_{-1}^{1} \left(x + \sqrt{\frac{3}{5}}\right)\left(x - \sqrt{\frac{3}{5}}\right) dx = \frac{8}{9}$$

$$\omega_2 = \int_{-1}^{1} \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} dx = \frac{5}{6} \int_{-1}^{1} x\left(x + \sqrt{\frac{3}{5}}\right) dx = \frac{5}{9}$$

Numerical Integration: Example

Evaluate $\int_0^2 x^5 dx$ using 3 points with Trapezoidal, Simpson's 1/3rd and Gauss-Legendre Quadrature. Compare TRUE errors.

- ✓ True integral = $2^6/6$ = 10.6667
- ✓ Trapezoidal (T) and Simpson's 1/3rd Rule (S):

$$x_0 = 0, \qquad x_1 = 1, \qquad x_2 = 2$$
$$f_0 = 0, \qquad f_1 = 1, \qquad f_2 = 32$$
$$T = \frac{1}{2}[0 + 32 + 2 \times 1] = 17 \qquad \varepsilon = 59.4\%$$
$$S = \frac{1}{3}[0 + 4 \times 1 + 32] = 12 \qquad \varepsilon = 12.5\%$$

- ✓ For Gauss-Legendre Quadrature, use transformation $x = (1 + z)$. The integral becomes:

$$\int_0^2 x^5 dx = \int_{-1}^{1} (1 + z)^5 dz$$

Numerical Integration: Example

$$\int_{-1}^{1} (1+z)^5 dz$$

$$z_0 = -\sqrt{\frac{3}{5}}, \qquad z_1 = 0, \qquad z_2 = \sqrt{\frac{3}{5}}$$

$$f_0 = 0.5818 \times 10^{-3}, \qquad f_1 = 1, \qquad f_2 = 17.599$$

$$\omega_0 = 5/9, \qquad \omega_1 = 8/9, \qquad \omega_2 = 5/9$$

$$\int_{-1}^{1} (1+z)^5 dz = \sum_{i=0}^{n} \omega_i f_i = 10.6667 \qquad \varepsilon = 0\%$$

Numerical Integration: Example

Consider the error function:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi$$

Evaluate erf(1) using 3 points with Trapezoidal, Simpson's 1/3rd and Gauss-Legendre Quadrature. Compare true relative errors (%) using the true erf(1) = 0.8427

✓ Trapezoidal (T) and Simpson's 1/3rd Rule (S):

$$\xi_0 = 0, \qquad \xi_1 = 0.5, \qquad \xi_2 = 1$$

$$f_0 = 1, \qquad f_1 = 0.7788, \qquad f_2 = 0.3679$$

$$T = \frac{2}{\sqrt{\pi}} \frac{0.5}{2} [1 + 0.3679 + 2 \times 0.7788] = 0.8253 \qquad \varepsilon = 2.1\%$$

$$S = \frac{2}{\sqrt{\pi}} \frac{0.5}{3} [1 + 4 \times 0.7788 + 0.3679] = 0.8431 \qquad \varepsilon = 0.05\%$$

Numerical Integration: Example

✓ For Gauss–Legendre Quadrature, use transformation $\xi = (1 + z)/2$. The integral becomes:

$$\frac{2}{\sqrt{\pi}}\int_0^1 e^{-\xi^2}d\xi = \frac{1}{\sqrt{\pi}}\int_{-1}^{1} e^{-\left(\frac{1+z}{2}\right)^2}dz$$

$$z_0 = -\sqrt{\frac{3}{5}}, \qquad z_1 = 0, \qquad z_2 = \sqrt{\frac{3}{5}}$$

$$f_0 = 0.9874, \qquad f_1 = 0.7788, \qquad f_2 = 0.4551$$

$$\omega_0 = 5/9, \qquad \omega_1 = 8/9, \qquad \omega_2 = 5/9$$

$$\frac{1}{\sqrt{\pi}}\int_{-1}^{1} e^{-\left(\frac{1+z}{2}\right)^2}dz = \frac{1}{\sqrt{\pi}}\sum_{i=0}^{n}\omega_i f_i = 0.8427 \qquad \varepsilon = 0\%$$

ESO 208A: Computational Methods in Engineering

Ordinary Differential Equation: Initial Value Problems

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ODE: Initial Value Problems

We will consider general problems of the form:

$$\frac{dy}{dt} = f(y,t) \qquad y(t_0) = y_0 \quad t \geq 0$$

- ✓ Solution of this equation is a function $y(t)$
- ✓ Starting from t_0, we shall take discrete time steps $t_1, t_2, \cdots t_n \cdots$ of size h such that, $t_n = t_0 + nh$
- ✓ Starting from the known initial value y_0, we shall compute values of y at each time step, $y_1, y_2, \cdots y_n \cdots$ at each time step, i.e., compute tab(y)
- ✓ An obvious way can be:

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2!}y_n'' + \frac{h^3}{3!}y_n''' + \frac{h^4}{4!}y_n^{IV} + \frac{h^5}{5!}y_n^{V} + \frac{h^6}{6!}y_n^{VI} \cdots$$

- ✓ Neglecting, h^2 and higher order terms:

$$y_{n+1} \approx \tilde{y}_{n+1} = y_n + hy_n' \quad \Longrightarrow \quad y_{n+1} = y_n + hf(y_n, t_n)$$

ODE: Initial Value Problems

$$y_{n+1} = y_n + hf(y_n, t_n) \quad \Longrightarrow \quad \frac{y_{n+1} - y_n}{h} = f(y_n, t_n)$$

- ✓ The method is equivalent to making a *forward* difference approximation of *dy/dt* at the n^{th} node. It is known as the ***Euler Forward Method***.

- ✓ Why not make a *backward* difference approximation of *dy/dt* at the n^{th} node?

$$\frac{y_n - y_{n-1}}{h} = f(y_n, t_n) \Longrightarrow \quad y_{n+1} = y_n + hf(y_{n+1}, t_{n+1})$$

This is known as the ***Euler Backward Method***.

- ✓ Instead of evaluating the function *f* either at the n^{th} node or at the $(n+1)^{\text{th}}$ node, if we take the average of the two:

$$y_{n+1} = y_n + \frac{h}{2}\left[f(y_{n+1}, t_{n+1}) + f(y_n, t_n)\right]$$

ODE: Initial Value Problems

$$y_{n+1} = y_n + \frac{h}{2}[f(y_{n+1}, t_{n+1}) + f(y_n, t_n)]$$

✓ This method may also be seen as follows:

$$\frac{dy}{dt} = f(y,t) \qquad \Longrightarrow \qquad \int_{y_n}^{y_{n+1}} dy = \int_{t_n}^{t_{n+1}} f(y,t)dt$$

✓ Left side integral is straight forward. Use Trapezoidal Method for the right side integral.

$$y_{n+1} - y_n = \frac{h}{2}[f(y_{n+1}, t_{n+1}) + f(y_n, t_n)]$$

This is known as the ***Trapezoidal Method***.