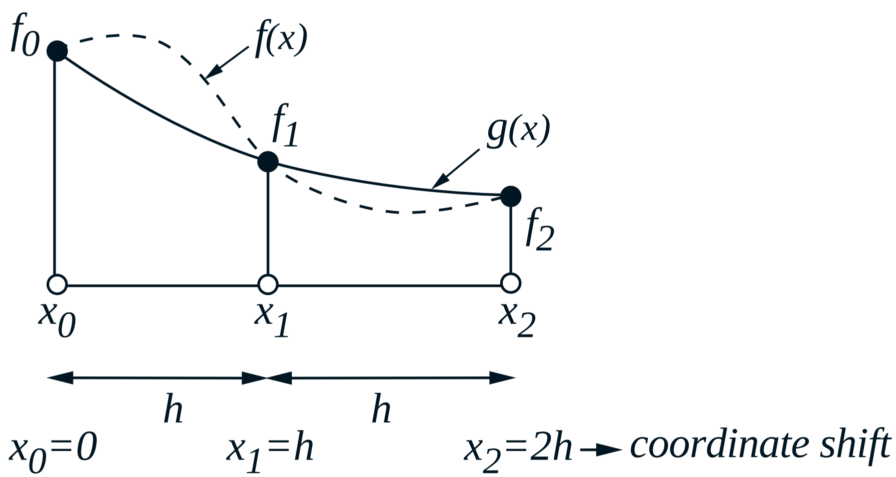
LECTURE 18

NUMERICAL INTEGRATION CONTINUED

Simpson's 1/3 Rule

- Simpson's 1/3 rule assumes 3 equispaced data/interpolation/integration points
- The integration rule is based on approximating $f(x)$ using ***Lagrange quadratic*** (second degree) interpolation.
- The sub-interval is defined as $[x_o, x_2]$ and the integration point to integration point spacing equals $h \equiv \frac{x_2 - x_o}{2}$



- Lagrange quadratic interpolation over the sub-interval:

$$g(x) = f_o V_o(x) + f_1 V_1(x) + f_2 V_2(x)$$

where

$$V_o(x) = \frac{(x - x_1)(x - x_2)}{(x_o - x_1)(x_o - x_2)} \Rightarrow$$

$$V_o(x) = \frac{x^2 - 3hx + 2h^2}{2h^2}$$

$$V_1(x) = \frac{(x - x_o)(x - x_2)}{(x_1 - x_o)(x_1 - x_2)} \Rightarrow$$

$$V_1(x) = \frac{4hx - 2x^2}{2h^2}$$

$$V_2(x) = \frac{(x - x_o)(x - x_1)}{(x_2 - x_o)(x_2 - x_1)} \Rightarrow$$

$$V_2(x) = \frac{x^2 - hx}{2h^2}$$

- Integration rule is obtained by integrating $g(x)$

$$I = \int_{x_o}^{x_2} f(x) \quad \Rightarrow \quad I = \int_{x_o}^{x_2} g(x)dx + E \quad \Rightarrow$$

$$I = \int_{x_o=0}^{x_2=2h} \left\{ f_o\left[\frac{x^2 - 3hx + 2h^2}{2h^2}\right] + f_1\left[\frac{4hx - 2x^2}{2h^2}\right] + f_2\left[\frac{x^2 - hx}{2h^2}\right] \right\} dx + E \quad \Rightarrow$$

$$I = \frac{1}{2h^2}\left[f_o\left(\frac{x^3}{3} - \frac{3hx^2}{2} + 2h^2x\right) + f_1\left(\frac{4hx^2}{2} - \frac{2x^3}{3}\right) + f_2\left(\frac{x^3}{3} - h\frac{x^2}{2}\right)\right]_0^{2h} + E \quad \Rightarrow$$

$$I = \frac{1}{2h^2}\left[f_o\left(8\frac{h^3}{3} - \frac{12h^3}{2} + 4h^3 - 0\right) + f_1\left(8h^3 - \frac{16}{3}h^3\right) + f_2\left(\frac{8h^3}{3} - h\frac{4h^2}{2}\right)\right] + E \quad \Rightarrow$$

- Simpson's 1/3 Rule

$$\boldsymbol{I = \frac{h}{3}[f_o + 4f_1 + f_2] + E}$$

Evaluation of the Error for Simpson's 1/3 Rule

- Error is defined as:

$$E = I - \frac{h}{3}(f_o + 4f_1 + f_2) \quad \Rightarrow$$

$$E = \int_0^{2h} f(x)dx - \frac{h}{3}(f_o + 4f_1 + f_2)$$

- We develop Taylor series expansions for $f(x)$, f_o, f_1 and f_2 about $x_1 = h$

$$f(x) = f_1 + (x-h)\ f_1^{(1)} + \frac{1}{2}(x-h)^2\ f_1^{(2)} + \frac{1}{6}(x-h)^3\ f_1^{(3)} + \frac{1}{24}(x-h)^4\ f_1^{(4)} + O(x-h)^5$$

$$f_o = f_1 - h\ f_1^{(1)} + \frac{1}{2}h^2\ f_1^{(2)} - \frac{h^3}{6}\ f_1^{(3)} + \frac{1}{24}h^4\ f_1^{(4)} + O(h)^5$$

$$f_1 = f_1$$

$$f_2 = f_1 + h\ f_1^{(1)} + \frac{1}{2}h^2\ f_1^{(2)} + \frac{h^3}{6}\ f_1^{(3)} + \frac{1}{24}h^4\ f_1^{(4)} + O(h)^5$$

- Substituting into the expression for E

$$E = \int_0^{2h}\left(f_1 + (x-h)\, f_1^{(1)} + \frac{1}{2}(x-h)^2\, f_1^{(2)} + \frac{1}{6}(x-h)^3\, f_1^{(3)} + \frac{1}{24}(x-h)^4\, f_1^{(4)} + O(x-h)^5\right)dx$$

$$-\frac{h}{3}\left(f_1 - h\, f_1^{(1)} + \frac{1}{2}h^2\, f_1^{(2)} - \frac{h^3}{6}\, f_1^{(3)} + \frac{1}{24}h^4\, f_1^{(4)} + O(h)^5 + 4f_1 + f_1 + h\, f_1^{(1)} + \frac{1}{2}h^2\, f_1^{(2)}\right.$$

$$\left. + \frac{h^3}{6}\, f_1^{(3)} + \frac{1}{24}h^4\, f_1^{(4)} + O(h)^5\right)$$

$$\Rightarrow$$

$$E = (2h)f_1 + \frac{1}{2}(h^2 - h^2)\, f_1^{(1)} + \frac{1}{6}(h^3 + h^3)f_1^{(2)} + \frac{1}{24}(h^4 - h^4)f_1^{(3)}$$

$$+ \frac{1}{120}(h^5 + h^5)f_1^{(4)} + O(h)^6 - \frac{h}{3}\left[6f_1 + h^2 f_1^{(2)} + \frac{1}{12}h^4 f_1^{(4)} + O(h)^5\right]$$

$$\Rightarrow$$

$$E = (2h - 2h)f_1 + \left(\frac{2}{6}h^3 - \frac{h^3}{3}\right) f_1^{(2)} + \left(\frac{h^5}{60} - \frac{h^5}{36}\right) f_1^{(4)} + O(h)^6$$

- Error for Simpson's 1/3 Rule

$$E = -\frac{1}{90} h^5 f_1^{(4)}$$

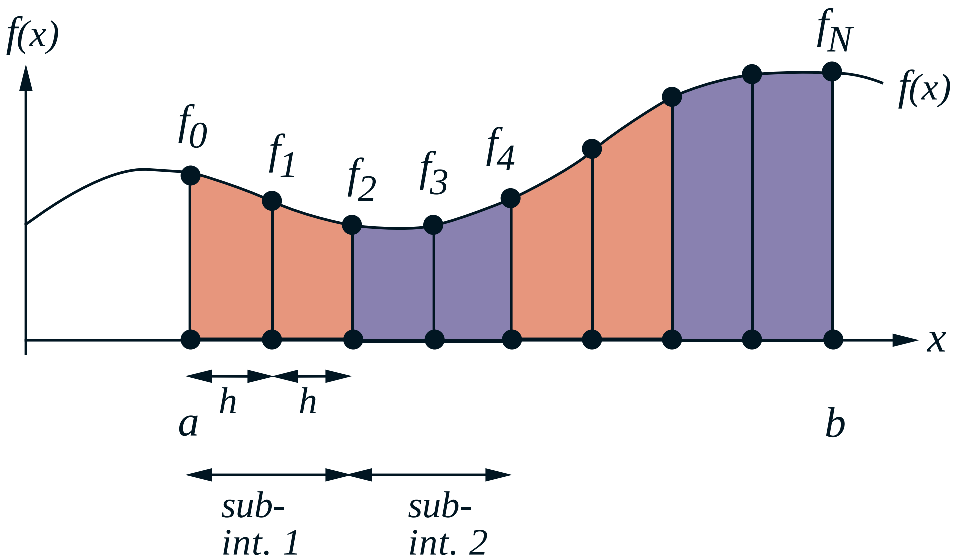
  - This is the error for integration over one sub-interval of width $2h$!
  - Fifth order accurate.
  - Simpson's 1/3 Rule is exact for any cubic polynomial function

- We note that E can also be derived by
  - Estimating the error for Lagrange quadratic interpolation, $e(x) = f(x) - g(x)$, ***in series form***
  - Integrating *e(x)* over the integration interval $[x_o, x_2]$

$$E = \int_{x_o=0}^{x_2=2h} e(x)dx$$

Extended Simpson's 1/3 Rule

- Simply add up integrated values obtained using Simpson's 1/3 rule over each sub-interval.



- Sub-interval size = $2h$
- Number of sub-intervals = $\frac{N}{2}$
- Sub-interval width is $2h$ while the integration point to integration point spacing is equal to $h = \frac{b-a}{N}$

- Again we integrate over N points (the same as extended trapezoidal rule). Therefore

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

$$\Rightarrow$$

$$I = \frac{h}{3}((f_o + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + (f_4 + 4f_5 + f_6)$$

$$+ \dots + (f_{N-4} + 4f_{N-3} + f_{N-2}) + (f_{N-2} + 4f_{N-1} + f_N)) + E_{[a,b]}$$

$$\Rightarrow$$

$$I = \frac{h}{3}[f_o + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + \dots + 2f_{N-2} + 4f_{N-1} + f_N] + E_{[a,b]}$$

- In general we can write

$$I = \frac{h}{3}\left[f(a) + f(b) + 4\sum_{i=1,2}^{N-1} f(a+ih) + 2\sum_{i=2,2}^{N-2} f(a+ih)\right] + E_{[a,b]}$$

- Note that the total number of integration points $N + 1$ must be odd and therefore N must be even!

- The error term is also summed over the sub-intervals and each sub-interval term is evaluated at the mid node of the sub-interval.

$$E_{[a, b]} \approx \sum_{i=1}^{\frac{N}{2}} \left(-\frac{h^5}{90} f_{2i-1}^{(4)} \right)$$

$$\Rightarrow$$

$$E_{[a, b]} \approx -\frac{h^5}{90}\left(\frac{N}{2}\right)\left(\frac{2}{N}\sum_{i=1}^{\frac{N}{2}} f_{2i-1}^{(4)}\right)$$

$$\Rightarrow$$

$$E_{[a, b]} \approx -\frac{h^5}{90} \frac{N}{2} \overline{f^{(4)}}$$

where $\overline{f^{(4)}}$ = average of the 4th derivative over each sub-interval in the interval $[a, b]$.

- However we wish dependence on error to be expressed in terms of h, ***not*** in terms of the number of integration points.

- Noting that for the interval $[a, b]$

$$h = \frac{b-a}{N} \quad \Rightarrow \quad N = \frac{b-a}{h}$$

- Therefore

$$E_{[a,b]} = -\frac{h^5}{90} \cdot \frac{b-a}{h} \cdot \frac{1}{2} \overline{f^{(4)}}$$

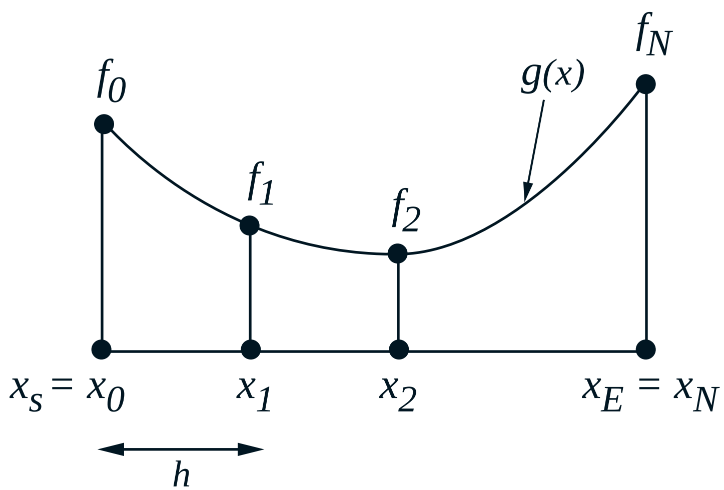
$$\Rightarrow$$

$$\boldsymbol{E_{[a,b]} \approx -\frac{h^4}{180}(b-a)\overline{f^{(4)}}}$$

- Overall the error is 4th order

Newton Cotes Closed Formulae

- Derived by integrating Lagrange approximating polynomials (or equivalently Newton Interpolating formulae) using equispaced integration points (interpolating points, nodes, etc.) over the sub-interval defined by the interpolating data points



- The general form of Newton-Cotes closed formulae:

$$\int_{x_S}^{x_E} f(x)dx = \alpha h[w_o f_o + w_1 f_1 + w_2 f_2 + \ldots + w_N f_N] + E$$

where $f_i = f(x_i)$ $x_i = x_S + ih$ $h \equiv \frac{x_N - x_o}{N}$

- Closed formulae: The sub-interval is closed by the first and last integration points.

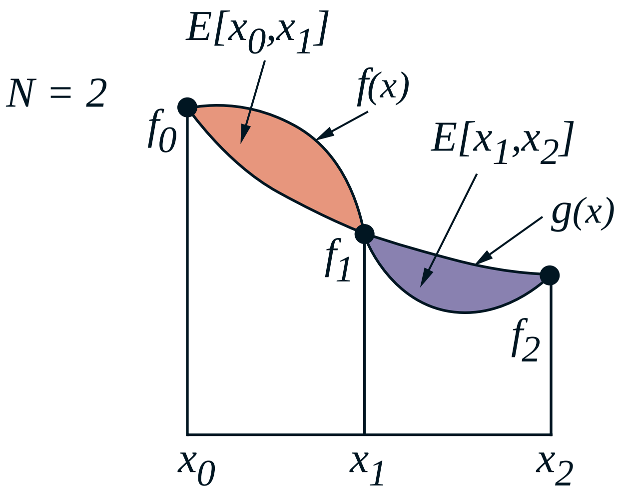
N	α	w_i , $i = 0, 1, 2, \ldots, N$	E	$Note$
1	$\frac{1}{2}$	1 1	$-\frac{1}{12}h^3 f^{(2)}$	Trapezoidal Rule
2	$\frac{1}{3}$	1 4 1	$-\frac{1}{90}h^5 f^{(4)}$	Simpson's $\frac{1}{3}$ Rule
3	$\frac{3}{8}$	1 3 3 1	$-\frac{3}{80}h^5 f^{(4)}$	Simpson's $\frac{3}{8}$ Rule
4	$\frac{2}{45}$	7 32 12 32 7	$-\frac{8}{945}h^7 f^{(6)}$	
10	$\frac{5}{299376}$	16067 106300 -48525 272400 -260550 427368 -260550 272400 -48525 106300 16067	$-0.00412\ h^{13} f^{(12)}$	Round off error tends to become a serious problem!

- Notes
  - All these formulae integrate over one sub-interval only. They can be extended over $[a, b]$ simply by summing up integrals over each sub-interval.
  - In addition the error is summed resulting in one less order of accuracy than the error over the individual sub-interval!
  - Accuracy for Simpson's $\frac{3}{8}$ rule is very similar to accuracy of Simpson's $\frac{1}{3}$ rule.
  - In general each formula will be ***exact*** for polynomials of one degree less than the order of the derivatives in the error terms.

N	$g(x)$	E	$Exact\ for$
1	linear	$\overline{f^{(2)}}$	linear
2	quadratic	$\overline{f^{(4)}}$	cubic
3	cubic	$\overline{f^{(4)}}$	cubic
4	quartic	$\overline{f^{(6)}}$	quintic

- It appears that for N even, the integration is exact for polynomials one degree greater than the interpolation function.

- For Simpson's 1/3 Rule:
  - It turns out that if $f(x)$ is a ***cubic*** and $g(x)$ is quadratic, $E_{[x_o,\, x_1]} = -E_{[x_1,\, x_2]}$



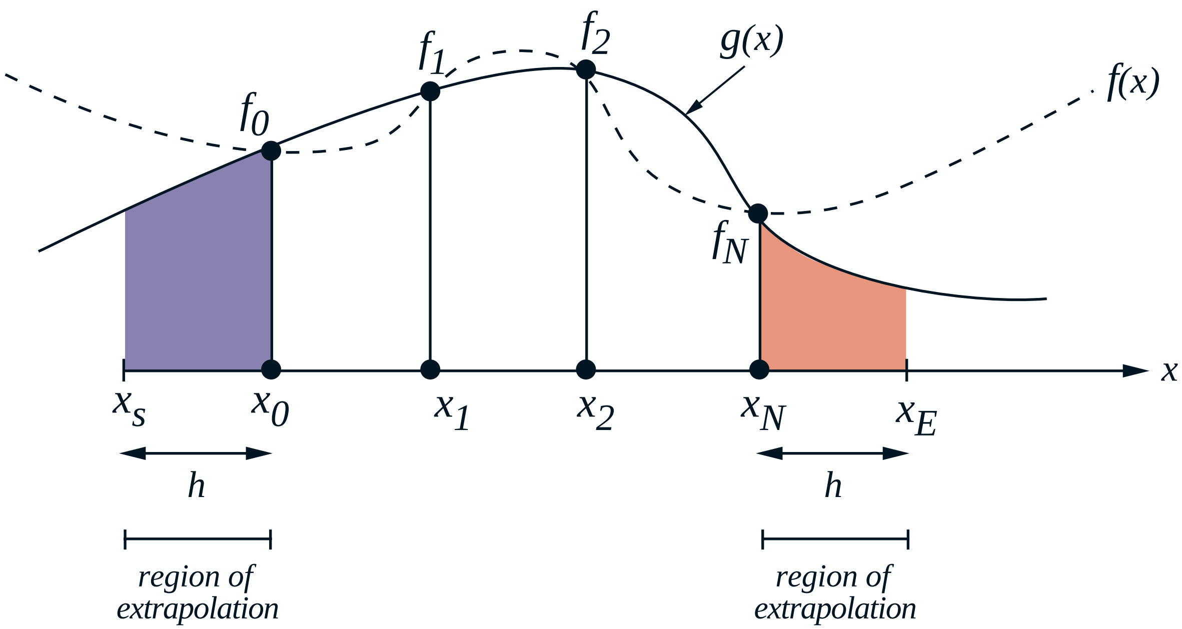
  - The errors cancel over the interval ***due to the location*** of point x_1!

- We can actually improve the accuracy of integration formulae by locating integration points in special locations!

- We do ***not*** experience any improvement in accuracy for N = odd.

Newton-Cotes Open Formulae

- Derived by integrating Lagrange approximating formulae (or equivalently Newton Interpolating formulae) using equispaced data points/nodes/integration points over the sub-interval defined by the interpolating data points ***and*** extended to the left and right by h.



- Note that $x_S = x_o - h \quad x_E = x_N + h$ and $h = \dfrac{x_N - x_o}{N}$

- Note that $g(x)$ does not generally pass through $f(x_S)$ or through $f(x_E)$

- Newton Cotes open formula:

$$\int_{x_S}^{x_E} f(x)dx = \alpha h[w_0 f_0 + w_1 f_1 + \ldots + w_N f_N] + E$$

N	α	$w_i \; i = 0, 1, \ldots, N$	E	Error compared to closed interval	Interval size compared to closed interval
1	3/2	1 1	$\frac{1}{4}h^3 f^{(2)}$	3 ×	3 ×
2	4/3	2 -1 2	$\frac{28}{90}h^5 f^{(4)}$	28 ×	2 ×
3	5/24	11 1 1 11	$\frac{95}{144}h^5 f^{(4)}$	18 ×	1.7 ×

- Notes
  - Each formula and error is for ***one*** sub-interval with $N + 1$ data/node/integration points. We can extend the interval to $[a, b]$ by summing integrals and errors (error increases by one order).
  - Sub-interval errors are greater than closed formulae since
    - sub-interval is larger
    - the error in the interpolation functions tended to be greater near the ends and especially outside of the interpolating region!
  - Higher order formulae involve large coefficients with +/- signs. This leads to roundoff problems.
  - Open formulae can be used when functional values are not available at the integrating limits.