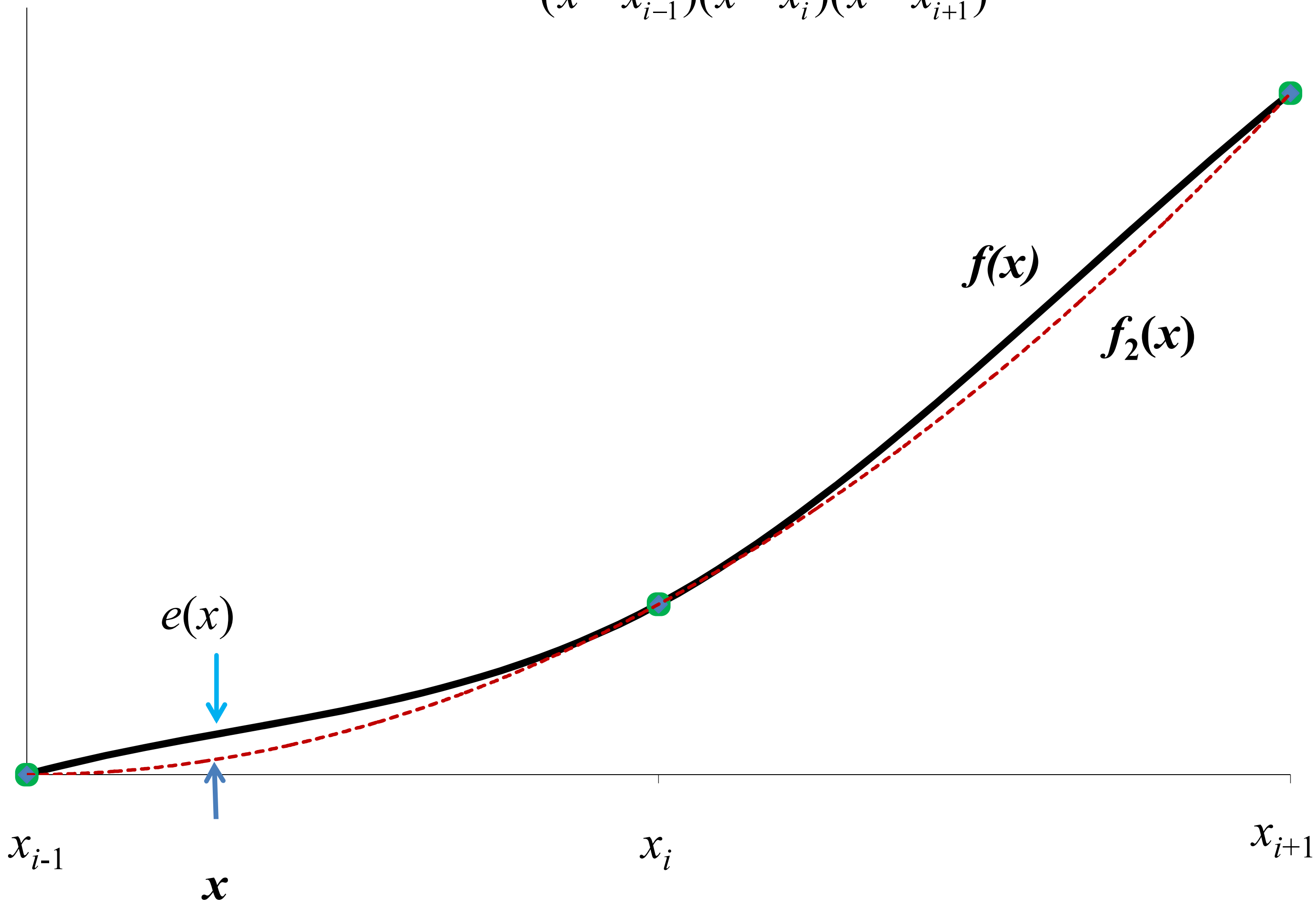
Simpson's Rule: Error Estimate

$$e(x) = f(x) - f_2(x) = (x - x_{i-1})(x - x_i)(x - x_{i+1})c_3(x)$$

$$c_3(x) = \frac{f(x) - \{f_{i-1} + (x - x_{i-1}) f[x_{i-1}, x_i] + (x - x_{i-1})(x - x_i) f[x_{i-1}, x_i, x_{i+1}]\}}{(x - x_{i-1})(x - x_i)(x - x_{i+1})}$$



$$e(x) = (x - x_{i-1})(x - x_i)(x - x_{i+1}) f[x, x_{i-1}, x_i, x_{i+1}]$$

Simpson's Rule: Error Estimate

- Error in the ith sub-interval:

$$E_i = \int_{-h}^{h} (x+h)x(x-h) f[x, x_{i-1}, x_i, x_{i+1}] dx$$

$$= \left[f[x, x_{i-1}, x_i, x_{i+1}] \int_{-h}^{x} (x+h)x(x-h) dx \right]_{-h}^{h}$$

$$- \int_{-h}^{h} \frac{df[x, x_{i-1}, x_i, x_{i+1}]}{dx} \int_{-h}^{x} (x+h)x(x-h) dx\, dx$$

$$\frac{df[x, x_{i-1}, x_i, x_{i+1}]}{dx} = \lim_{\varepsilon \to 0} \frac{f[x+\varepsilon, x_{i-1}, x_i, x_{i+1}] - f[x, x_{i-1}, x_i, x_{i+1}]}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} f[x+\varepsilon, x, x_{i-1}, x_i, x_{i+1}] = \frac{f^{iv}(\zeta_i)}{4!}; \quad \zeta_i \in (x_{i-1}, x_{i+1})$$

Simpson's Rule: Error Estimate

- $\int_{-h}^{h}(x+h)x(x-h)dx = 0$ and $\int_{-h}^{x}(x+h)x(x-h)dx$ is nonnegative for x between (−h,h).

$$E_i = \left[f\left[x, x_{i-1}, x_i, x_{i+1}\right] \int_{-h}^{x}(x+h)x(x-h)dx \right]_{-h}^{h}$$

$$-\int_{-h}^{h} \frac{df\left[x, x_{i-1}, x_i, x_{i+1}\right]}{dx} \int_{-h}^{x}(x+h)x(x-h)dx\,dx$$

Simpson's Rule: Error Estimate

$$E_i = -\frac{f^{iv}(\zeta_i)}{4!}\int_{-h}^{h}\int_{-h}^{x}(x+h)x(x-h)dx\,dx$$

$$= -\frac{f^{iv}(\zeta_i)}{4!}\int_{-h}^{h}\frac{x^4}{4}-\frac{x^2h^2}{2}+\frac{h^4}{4}\;dx$$

$$= -\frac{h^5 f^{iv}(\zeta_i)}{90}$$

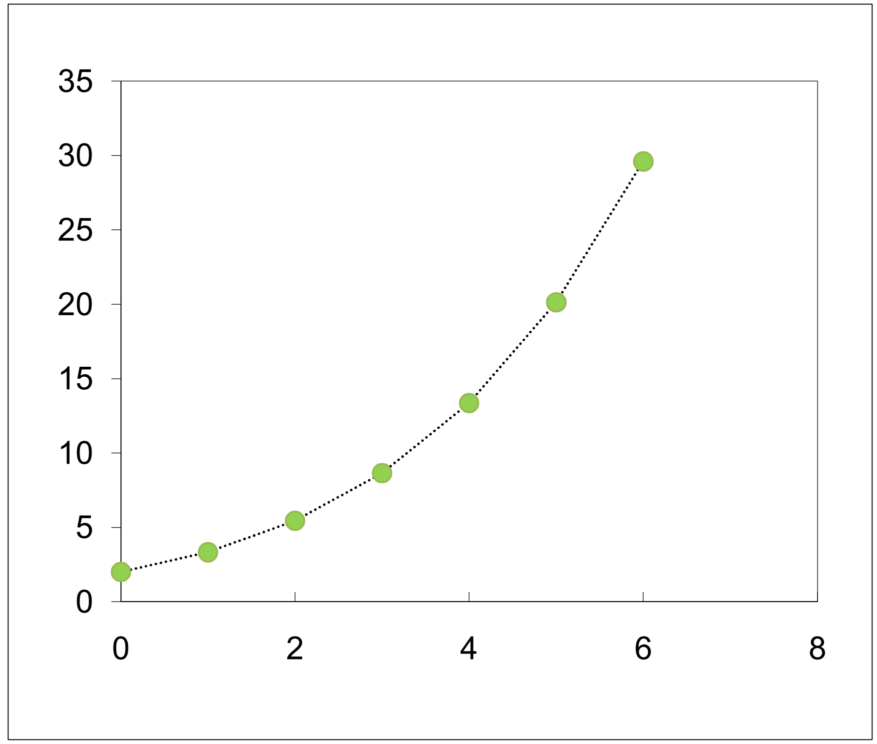
- Sub-interval error is $O(h^5)$
- Total error, $O(h^4)$:

$$E = I - \widetilde{I} = \sum_{i=1,3,5\ldots,n-1} E_i = -\frac{h^5 \sum_{i=1,3,5,\ldots n-1} f^{iv}(\zeta_i)}{90} = -\frac{(b-a)h^4\bar{f}^{iv}}{180}$$

Simpson's Rule: Example

- The velocity of an object is measured (x-direction)

Time (s)	Speed (cm/s)
0	2.00
1	3.33
2	5.44
3	8.65
4	13.36
5	20.13
6	29.60



- Estimate the distance travelled in 6 seconds

(True value = 65.86 cm)

Simpson's Rule: Example

Time (s)	Speed (cm/s)
0	2.00
1	3.33
2	5.44
3	8.65
4	13.36
5	20.13
6	29.60

T.V.=65.86

- Distance travelled

$$d = \int_0^6 v\,dt$$

- Simpson's rule, with h=1 s
  - d=(2+4x(3.33+8.65+20.13)

+2x(5.44+13.36)+29.60)x1/3 = 65.88 cm

- h=3 s
  - d=(2+4x8.65+29.60)x3/3 = 66.20 cm

Simpson's Rule: Example – Error analysis

Time (s)	Speed (cm/s)
0	2.00
1	3.33
2	5.44
3	8.65
4	13.36
5	20.13
6	29.60

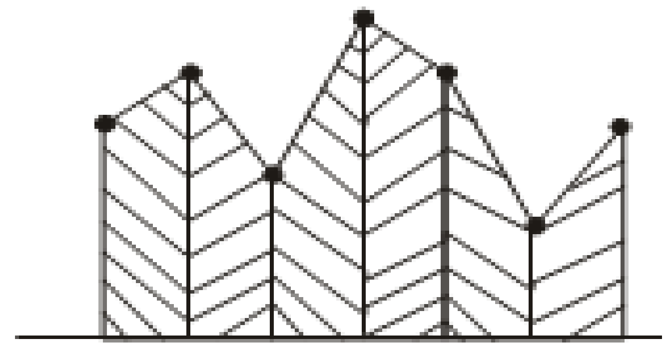
T.V.=65.86

- The fourth derivative is constant at 0.12 cm/s^5
- Error $-\frac{(b-a)h^4 \bar{f}^{iv}}{180}$ should be equal to $-0.004\ h^4$
- For h=1, Error = -0.02 cm
- For h=3, Error = -0.34 cm (nearly 17 times)
- The discrepancy is because of the rounding-off of the measured values.
- If we use more precision, the true value is 65.856, error with h=1 is -0.004 and with h=3, -0.324 (81 times)

Improving accuracy: Other techniques

- Trapezoidal Rule:

$$\widetilde{I}_i = \frac{h}{2}\left(f_{i-1} + f_i\right)$$



- Error: $E_i = -\dfrac{h^3 f''(\zeta_i)}{12}$

- Take two consecutive segments and use the central difference approximation of f”:

$$\widetilde{I}_i = \frac{h}{2}\left(f_{i-1} + f_i\right) - \frac{h^3 f''(\zeta_{i-1,i})}{12} + \frac{h}{2}\left(f_i + f_{i+1}\right) - \frac{h^3 f''(\zeta_{i,i+1})}{12}$$

Improving accuracy: Other techniques

$$\tilde{I}_i = \frac{h}{2}\left(f_{i-1} + 2f_i + f_{i+1}\right) - 2\frac{h^3}{12}\frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$$

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

- Which is the same as Simpson's 1/3 rule
- Another possibility: Assume the form

$$\tilde{I}_i = h\left(c_{i-1}f_{i-1} + c_i f_i + c_{i+1}f_{i+1}\right)$$

- Then use $f(x)$= 1, x and x^2 and obtain the c's

Improving accuracy: Other techniques

- Shift the origin at x_i : Domain (−h,h)
- $f(x) = 1$:

$$I = \int_{-h}^{h} 1dx = 2h = h\left(c_{i-1} + c_i + c_{i+1}\right)$$

$$c_{i-1} + c_i + c_{i+1} = 2$$

- $f(x) = x$:

$$I = \int_{-h}^{h} xdx = 0 = h\left(-c_{i-1}h + c_i.0 + c_{i+1}h\right)$$

$$-c_{i-1} + c_{i+1} = 0$$

- $f(x) = x^2$:

$$I = \int_{-h}^{h} x^2 dx = \frac{2h^3}{3} = h\left(c_{i-1}h^2 + c_i.0 + c_{i+1}h^2\right)$$

$$c_{i-1} + c_{i+1} = \frac{2}{3} \qquad \Rightarrow c_{i-1} = \frac{1}{3}; c_i = \frac{4}{3}; c_{i+1} = \frac{1}{3}$$

Improving accuracy: Most common technique

- Richardson Extrapolation:

  - Estimate $I_i = \int_{x_{i-1}}^{x_{i+1}} f(x)dx$

➢ Trapezoidal, with step size h:

$$I_i = \frac{h}{2}\left(f_{i-1} + 2f_i + f_{i+1}\right) + O(h^2) + \text{Higher Order Terms}$$

➢ Trapezoidal, with step size 2h:

$$I_i = \frac{2h}{2}\left(f_{i-1} + f_{i+1}\right) + O(4h^2) + \text{H.O.T.}$$

Richardson Extrapolation: Romberg algorithm

- Eliminate the lowest order terms:

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

- Again getting the Simpson's 1/3 rule, with error of the order h^4, as seen earlier.
- Romberg algorithm: Recursive combination, using integral estimates $\tilde{I}_{h,k}$, of order k and step sizes h and $2h$:

$$\tilde{I}_{h,k+2} = \frac{2^k \tilde{I}_{h,k} - \tilde{I}_{2h,k}}{2^k - 1}$$

Romberg Integration

- Algorithm: Start with trapezoidal rule, with step size of h, 2h, 4h,…
- Since the error is O(h^2), k=2 and $\tilde{I}_{h,4} = \dfrac{4\tilde{I}_{h,k} - \tilde{I}_{2h,k}}{3}$
- Similarly, $\tilde{I}_{2h,4} = \dfrac{4\tilde{I}_{2h,k} - \tilde{I}_{4h,k}}{3}$
- Combine two O(h^4) estimates: $\tilde{I}_{h,6} = \dfrac{16\tilde{I}_{h,4} - \tilde{I}_{2h,4}}{15}$
- Any order of accuracy could be achieved, if we have enough points. We only need to know the Trapezoidal rule!

Romberg Integration: Example

Time (s)	Speed (cm/s)
0	2.00
1	3.33
2	5.44
3	8.65
4	13.36
5	20.13
6	29.60
7	42.56
8	59.92

T.V.=152.45

- Distance travelled in 8 seconds?
- Trapezoidal rule, with h=1 s:
  - ➢ d=(2/2+sum(3.33…42.56)+59.92/2)x1

    = 154.03 cm
  - h=2 s:
  - ➢ d=(2/2+5.44+13.36+29.60+59.90/2)x2 = 158.72 cm
  - h=4 s: d=(2/2+13.36+59.92/2)x4 = 177.28 cm

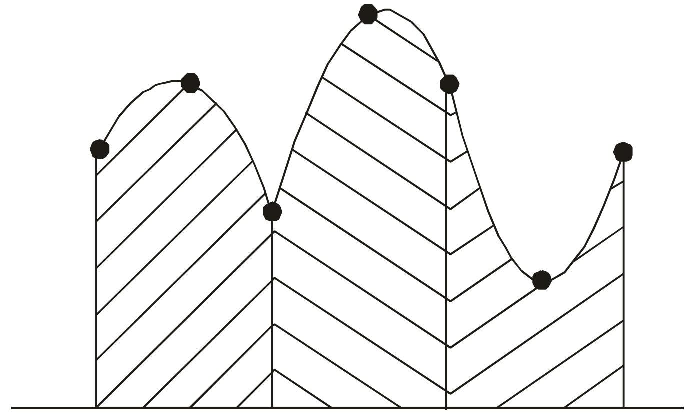
➢ $O(h^4)$ with h,2h: 4/3x154.03-158.72/3 = 152.47 cm

➢ $O(h^4)$ with 2h,4h: 4/3x158.72-177.28/3 = 152.53 cm

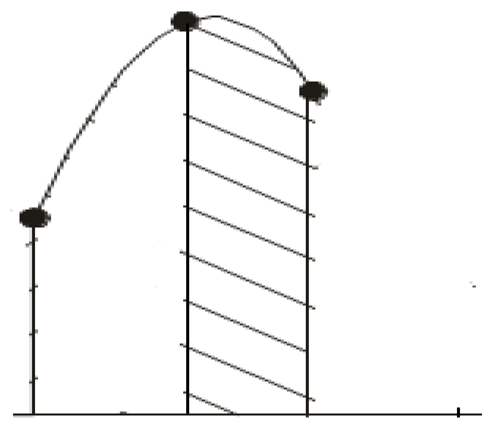
➢ $O(h^6)$ with h,2h,4h: 16/15x152.47-152.53/15 = 152.46 cm

Improving accuracy: Newton-Cotes and Adams

- Newton-Cotes: Use a higher degree interpolating polynomial and integrate over the entire sub-interval
  - Trapezoidal
  - Simpson's 1/3

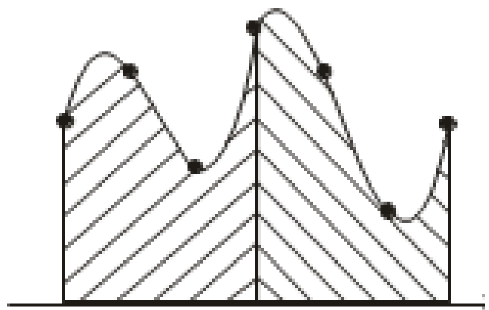


- Adams: Use a higher degree interpolating polynomial and integrate over only one segment



Newton-Cotes : Third-degree polynomial

- Newton-Cotes: Assume that n is a multiple of 3. Use cubic interpolating polynomial in a sub-interval with 4 consecutive points



- Simpson's 3/8 rule

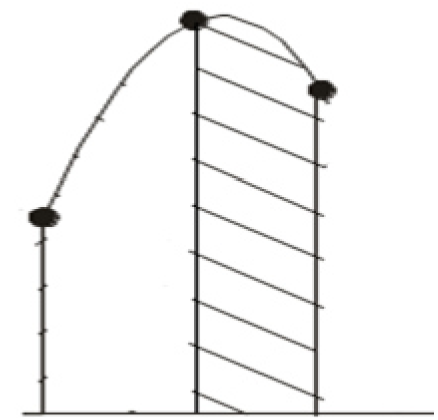
$$\tilde{I}_i = \frac{3h}{8}\left(f_{i-3} + 3f_{i-2} + 3f_{i-1} + f_i\right)$$

$$\tilde{I} = \frac{3h}{8}\left(f_0 + 3\sum_{i=1,4,7,\ldots,n-2}(f_i + f_{i+1}) + 2\sum_{i=3,6,9,\ldots,n-3} f_i + f_n\right)$$

$$E = I - \tilde{I} = \sum_{i=3,6,9\ldots,n} E_i = -\frac{3h^5 \sum\limits_{i=3,6,9,\ldots,n} f^{iv}(\zeta_i)}{80} = -\frac{(b-a)h^4 \bar{f}^{iv}}{80}$$

Adams Method

- Adams: Use a higher degree interpolating polynomial and integrate over only one segment: useful in "open" method
- E.g., quadratic using $x_{i\text{-}1}, x_i, x_{i+1}$



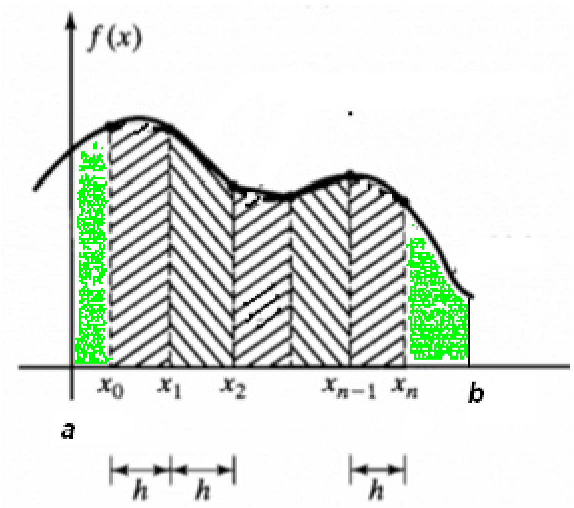
$$\tilde{I}_{i+1} = \int_0^h \left[f_{i-1} + (x+h)\frac{f_i - f_{i-1}}{h} + (x+h)x\frac{\dfrac{f_{i+1}-f_i}{h} - \dfrac{f_i - f_{i-1}}{h}}{2h} \right] dx$$

$$= \frac{h}{12}\left(-f_{i-1} + 8f_i + 5f_{i+1}\right)$$

Open and Semi-open Integration

- Given data $\left(x_k, f\left(x_k\right)\right) \quad k = 0,1,2,\ldots,n$

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



- Open Integration:

$$a < x_0 \ \text{ AND } \ b > x_n$$

- Semi-open integration:

$$a < x_0 \ \text{ OR } \ b > x_n$$