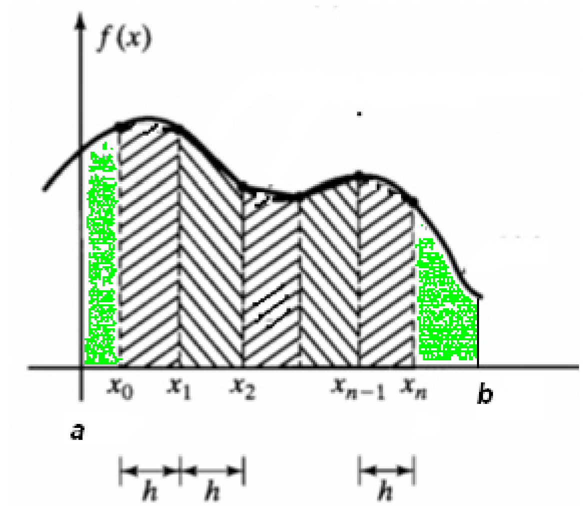
Open and Semi-open Integration

- 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:

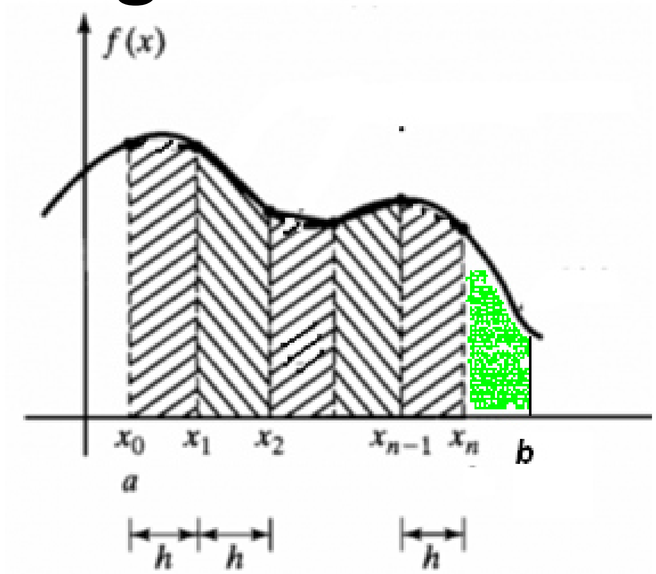
$$a < x_0 \ \text{ AND } \ b > x_n$$

- Semi-open integration:

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

Semi-open Integration

- We discuss only semi-open integration



- Assume $a = x_0\ ;\ b = x_n + h$

- Trapezoidal rule:
  - Linear interpolation in the last segment
  - Integrate by extrapolating up to *b*

$$\widetilde{I}_{n+1} = \int_h^{2h} \left[f_{n-1} + x\frac{f_n - f_{n-1}}{h} \right] dx = \frac{h}{2}\left(3f_n - f_{n-1}\right)$$

Semi-open Integration

- The estimate of I is, therefore,

$$\tilde{I} = \sum_{i=1}^{n+1} \tilde{I}_i = \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n + 3f_n - f_{n-1} \right)$$

$$= \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-2} f_i + f_{n-1} + 4f_n \right)$$

- The error in the *extrapolated segment* is

$$E_{n+1} = \int_h^{2h} x(x-h)\frac{f''(\zeta^*)}{2}dx = \frac{5h^3 f''(\zeta)}{12}; \zeta \in (x_{n-1}, b)$$

(larger than that in the *interpolated segment* and opposite in sign)

Semi-open Integration

- Similarly, quadratic interpolation results in

$$\tilde{I}_{n+1} = \int_{h}^{2h} \left[f_{n-2} + (x+h)\frac{f_{n-1} - f_{n-2}}{h} + (x+h)x \frac{\frac{f_n - f_{n-1}}{h} - \frac{f_{n-1} - f_{n-2}}{h}}{2h} \right] dx$$

$$= \frac{h}{12}\left(5 f_{n-2} - 16 f_{n-1} + 23 f_n\right)$$

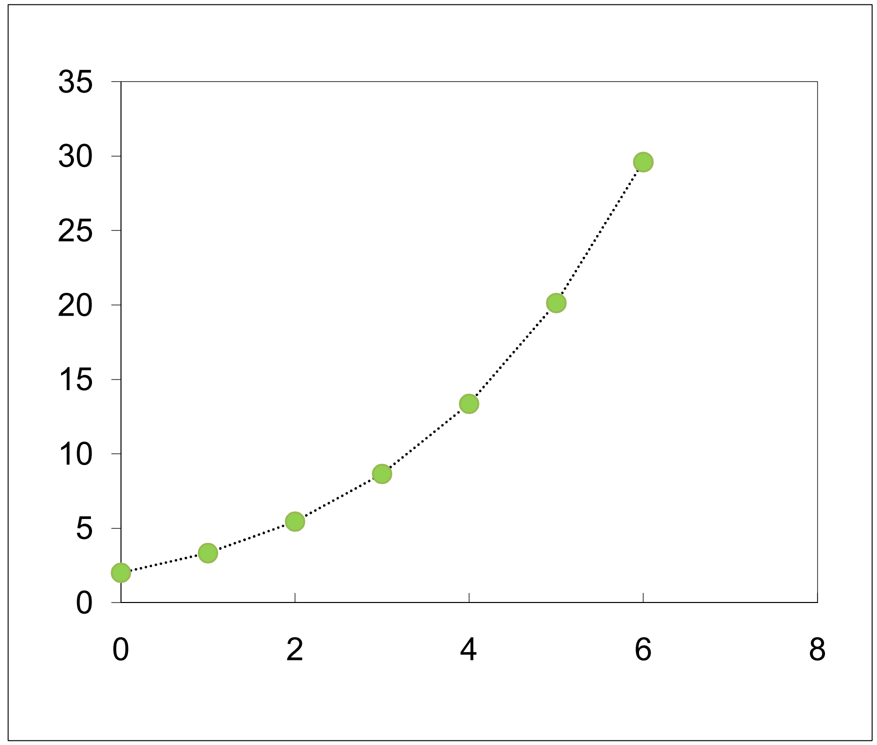
- The error in the *extrapolated segment* is

$$E_{n+1} = \int_{h}^{2h} x(x-h)(x-2h)\frac{f'''(\zeta^*)}{6}dx = \frac{9h^4 f'''(\zeta)}{24}; \zeta \in (x_{n-2}, b)$$

Trapezoidal Rule: Semi-open

- 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 location after 7 seconds (101.61 cm)

$$\tilde{I} = \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-2} f_i + f_{n-1} + 4 f_n \right) = 101.05$$

Numerical Integration: Function given

- Estimate $I = \int_a^b f(x)dx$ for a known function

- One option: Generate $\left(x_k, f\left(x_k\right)\right) \quad k = 0,1,2,\ldots,n$

  and then use any of the methods discussed

- Since the function is known, we could choose any spacing, *h*, and generate the data
- Romberg integration would work well
- Other option: Since function evaluation may require large computational effort, can we "optimize" the number of points?

Numerical Integration of a Function

- We start with the question: If we evaluate the function at 2 points, what should be the location of these points such that the error is minimized?
- Let us write $$\int_a^b f(x)dx \approx \tilde{I} = c_0 f(x_0) + c_1 f(x_1)$$
- Having two additional degrees of freedom, i.e., x_0 and x_1, enables us to integrate polynomials of degree 0, 1, 2, and 3, exactly.

Numerical Integration of a Function

- For $f(x)$=1, $\int_a^b f(x)dx = c_0 f\left(x_0\right) + c_1 f\left(x_1\right) \Rightarrow c_0 + c_1 = b - a$

- For $f(x)$=x,

$$\int_a^b f(x)dx = c_0 f\left(x_0\right) + c_1 f\left(x_1\right) \Rightarrow c_0 x_0 + c_1 x_1 = \frac{b^2 - a^2}{2}$$

- Similarly, using $f(x)$=x^2, and $f(x)$=x^3,

$$c_0 x_0^2 + c_1 x_1^2 = \frac{b^3 - a^3}{3}$$

$$c_0 x_0^3 + c_1 x_1^3 = \frac{b^4 - a^4}{4}$$

Numerical Integration of a Function

- These 4 equations could be solved to obtain the 4 parameters: c_0, c_1, x_0, x_1
- However, it is more convenient to transform the variable, from x to z, such that the domain (a,b) becomes (-1,1):

$$z = \frac{2}{b-a}\left(x - \tfrac{b+a}{2}\right)$$

$$\Rightarrow \int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f(z)\,dz$$

$$I_x = \frac{b-a}{2} I_z$$

- In subsequent analysis, we find I_z, not I_x

Numerical Integration of a Function

- The four equations then become:

$$c_0 + c_1 = 2; c_0 z_0 + c_1 z_1 = 0; c_0 z_0^2 + c_1 z_1^2 = \frac{2}{3}; c_0 z_0^3 + c_1 z_1^3 = 0$$

resulting in

$$z_0 = -\frac{1}{\sqrt{3}}; z_1 = \frac{1}{\sqrt{3}}; c_0 = 1; c_1 = 1$$

- This technique is known as Gauss Quadrature
  (Numerical evaluation of integration is known as quadrature)

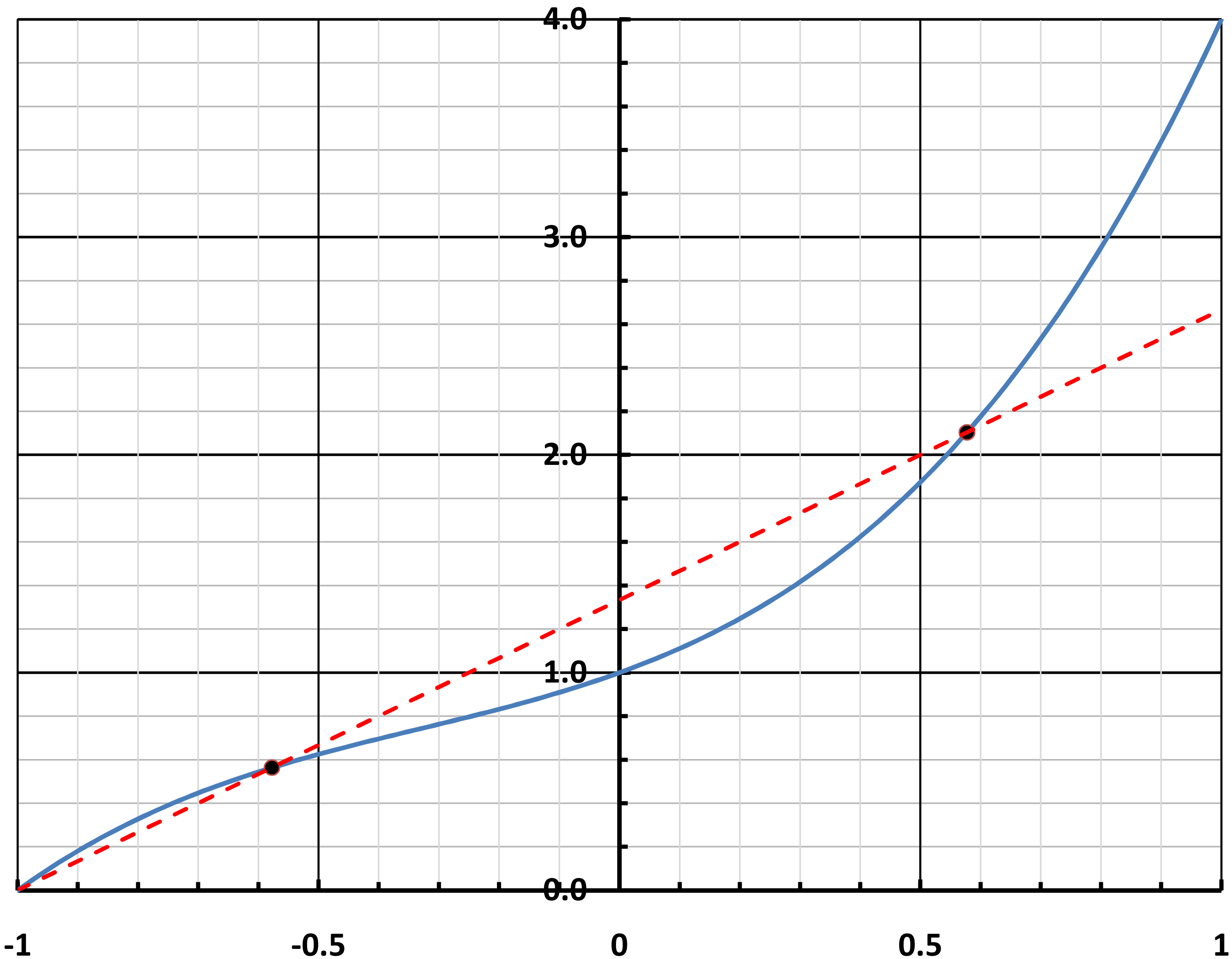
Gauss Quadrature

- With 2 quadrature points, it will be exact for any cubic polynomial, and the error is likely to be proportional to the 4th derivative of $f(z)$
- An estimate of the error may be obtained by using $f(z)=z^4$ (4th derivative = 24) as

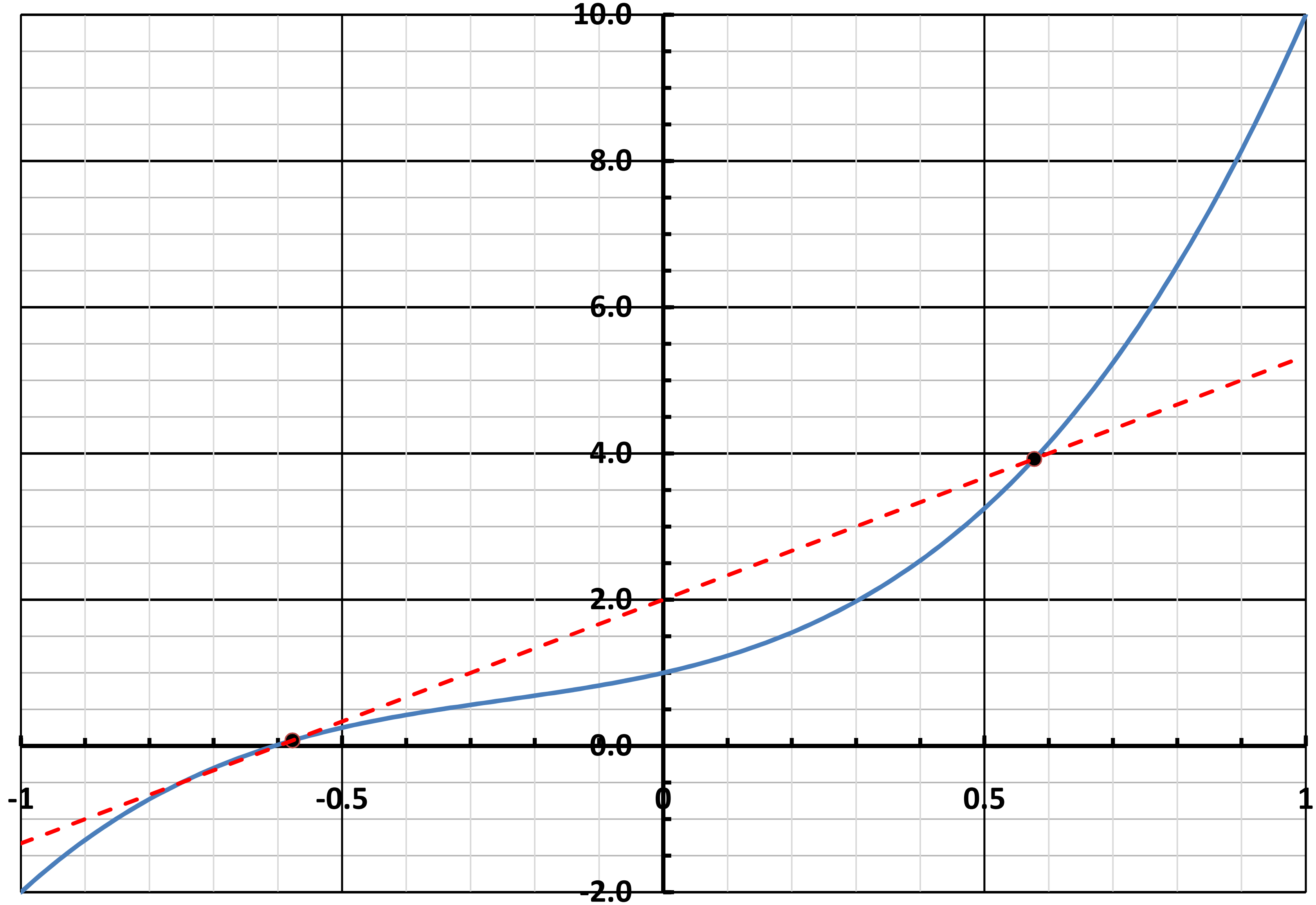
$$E = I - \tilde{I} = \left[\frac{z^5}{5}\right]_{-1}^{1} - \left(\left[-\frac{1}{\sqrt{3}}\right]^4 + \left[\frac{1}{\sqrt{3}}\right]^4\right) = \frac{8}{45}$$

resulting in

$$E = \frac{f^{iv}(\zeta)}{135}$$



$$f(x) = 1 + x + x^2 + x^3$$



$$f(x) = 1 + 2x + 3x^2 + 4x^3$$

Gauss Quadrature: General Form

- Let there be *n*+1 quadrature points: $z_0, z_1, .. z_n$
- We have 2n+2 *adjustable parameters*
- We should be able to *exactly* integrate *all* polynomials of degree 2*n*+1 (and lower)
- All these polynomials must necessarily match the function values at the (*n*+1) z_i's
- We may write these polynomials using a combination of the Lagrange polynomials, L_i, and the Newton polynomial, $\prod_{i=0}^{n}(z - z_i)$

Gauss Quadrature: General Form

- With $p_n(z)$ being an arbitrary polynomial of degree n, we write the *exactly integrable*

$$f_{2n+1}(z) = \sum_{i=0}^{n} L_i(z) f(z_i) + p_n(z) \prod_{i=0}^{n} (z - z_i)$$

- The first term on the RHS is the Lagrange interpolating polynomial, of degree n.
- Clearly, it matches the function at grid points, since the second term is zero at all z_i's.
- The second term on the RHS is a polynomial of degree $2n+1$

Gauss Quadrature: General Form

- If f_{2n+1} is exactly integrable by a quadrature scheme using n+1 Gauss points

$$\int_{-1}^{1} f_{2n+1}(z)dz = \sum_{i=0}^{n} c_i f(z_i)$$

=>

$$\sum_{i=0}^{n} \int_{-1}^{1} L_i(z)dz\ f(z_i) + \int_{-1}^{1} p_n(z) \prod_{i=0}^{n} (z - z_i) dz = \sum_{i=0}^{n} c_i f(z_i)$$

- This is achieved by letting $c_i = \int_{-1}^{1} L_i(z)dz$ and choosing the z_i's as the zeroes of an n+1th degree polynomial which is orthogonal to *ALL* polynomials of degree n: Legendre polynomial