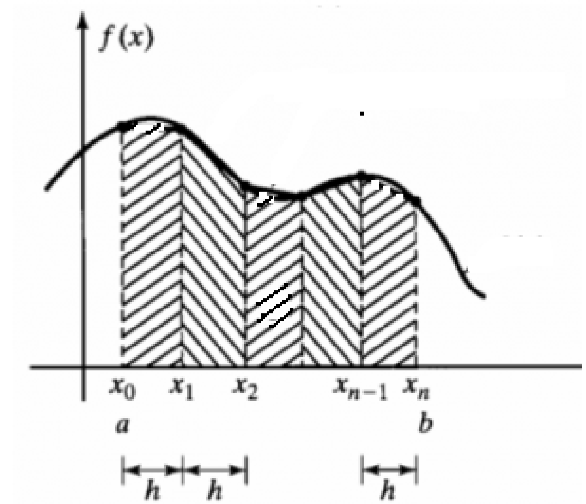
Numerical Integration

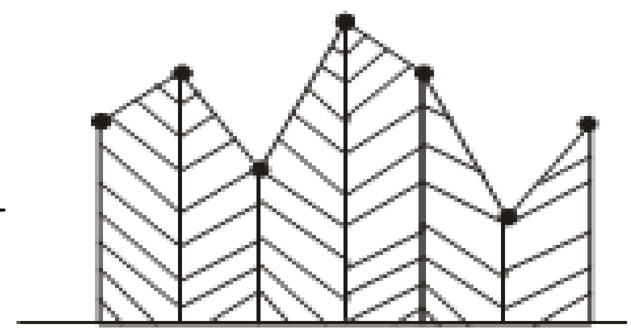
- Given data $\left(x_k, f\left(x_k\right)\right) \quad k = 0,1,2,\ldots,n$



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

- Trapezoidal Rule: Linear interpolation in each segment

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



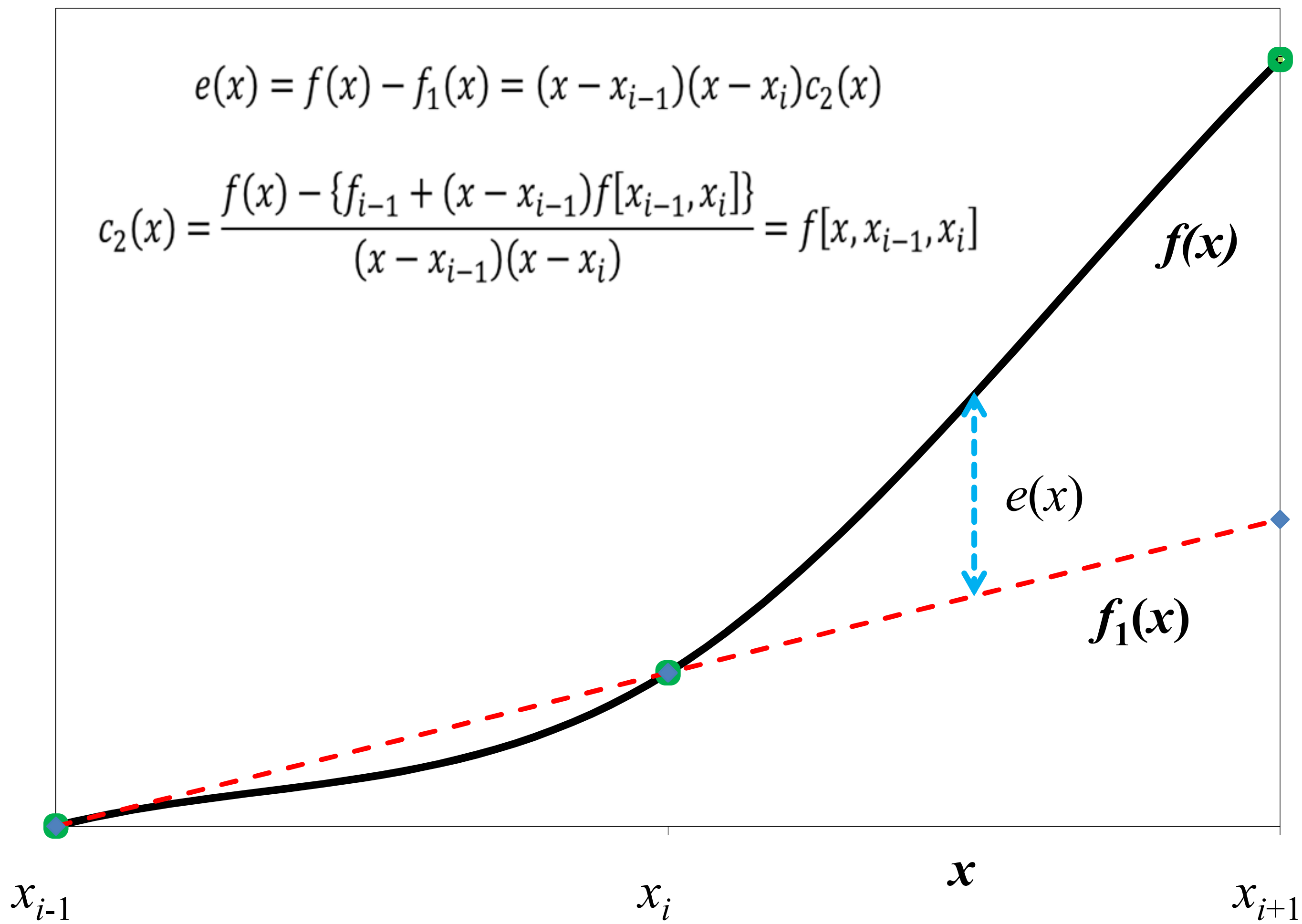
Trapezoidal Rule

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

- Error in the i^th segment:

$$E_i = I_i - \widetilde{I}_i = \int_{x_{i-1}}^{x_i} \left[f(x) - \left(f_{i-1} + (x - x_{i-1}) \frac{f_i - f_{i-1}}{h} \right) \right] dx$$

- We first find the error of interpolation and then integrate it to find the error in integral



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

Trapezoidal Rule: Error estimate

- Therefore,

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

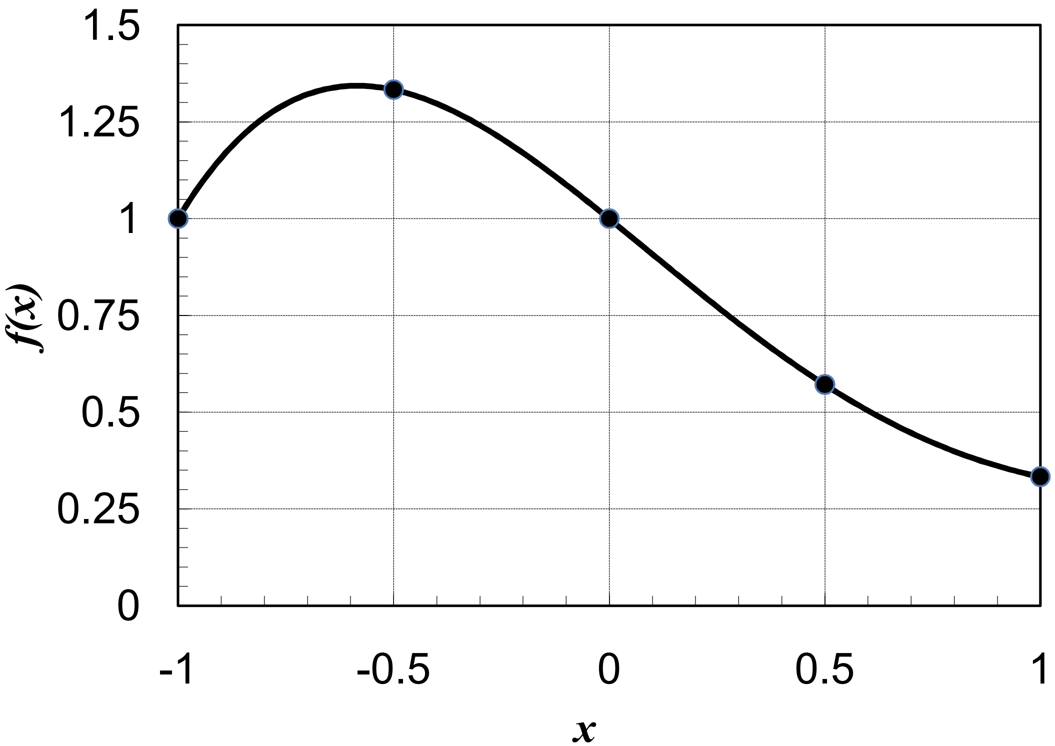
- A relation between divided differences and the function derivatives will be useful
- Use Rolle's theorem (if a function has equal values at the ends of an interval, its derivative must be zero at some point in the interval)

Use of Rolle's Theorem

- Newton interpolating polynomial
- ϕ_i is an i^{th}-degree polynomial
- $f(x) - f_n(x)$ is zero at n+1 points

$$f_n(x) = \sum_{j=0}^{n} c_j \phi_j(x)$$

$$\phi_i(x) = \prod_{j=0}^{i-1} (x - x_j)$$

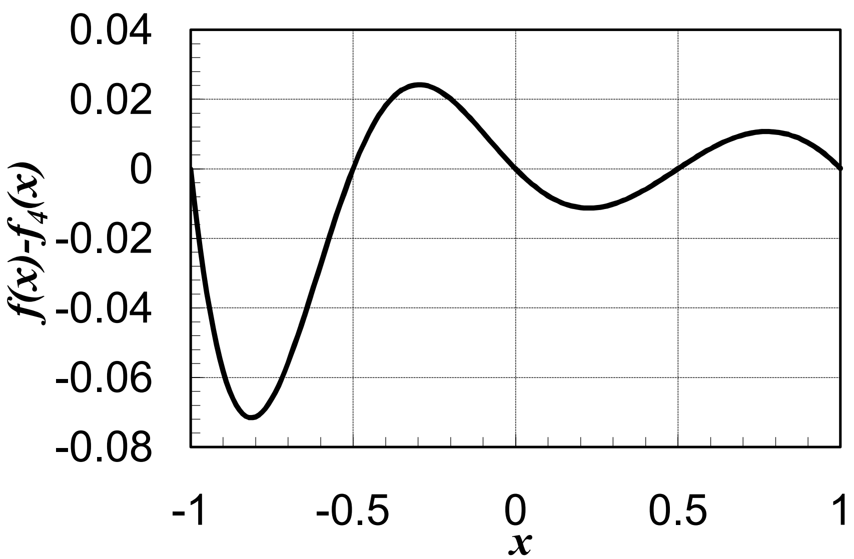


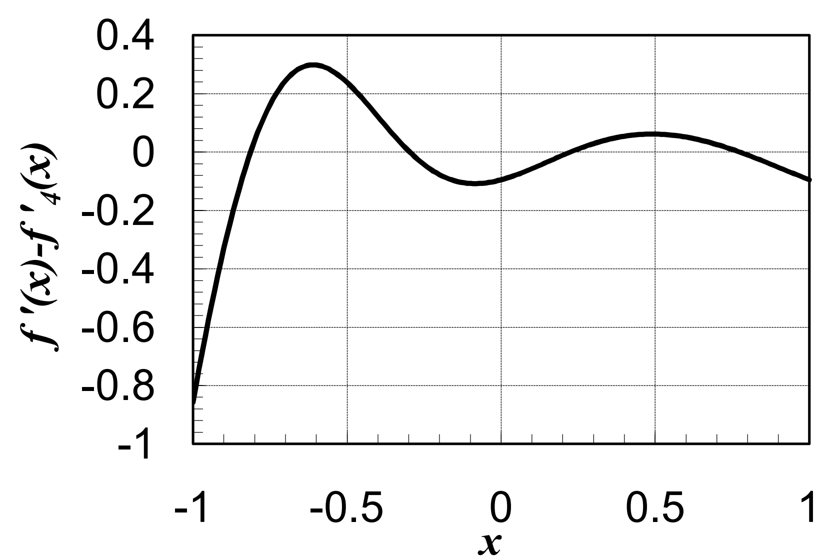
$$f(x) = \frac{1}{1 + x + x^2}$$

$$f_4(x) = 1 - 0.9048x - 0.1429x^2 + 0.5714x^3 - 0.1905x^4$$

Use of Rolle's Theorem

- $f(x) - f_n(x)$ is zero at n+1 points
  - ➢ $f'(x) - f'_n(x)$ is zero at "at least" n points, one within each segment
  - ➢ $f''(x) - f''_n(x)$ is zero at $n-1$ points, one within each of the segments of the previous "bullet"





Proof Outline

- Extending this argument:
  - $f^{[n]}(x) - f_n^{\,[n]}(x)$ is zero at *some* point ζ, within the interval (x_0, x_n)
- Since ϕ_i is an i^{th}-degree polynomial, its n^{th} derivative will be zero for $i<n$
- And n^{th} derivative of ϕ_n is "n!"
- Therefore,

$$f^{[n]}(x) - f[x_n, x_{n-1}, \ldots, x_1, x_0] \frac{d\phi_n(x)}{dx} = 0 \;\text{ at some }\; \zeta \in (x_0, x_n)$$

Trapezoidal Rule: Error estimate

$$\Rightarrow f\left[x_n, x_{n-1}, \ldots, x_1, x_0\right] = \frac{f^{[n]}(\zeta)}{n!}; \quad \zeta \in (x_0, x_n)$$

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

$$= \int_0^h x(x-h) \frac{f''(\zeta_i^*)}{2!} dx \quad \text{where} \quad \zeta_i^* \in (x_{i-1}, x_i)$$

- Use second mean value theorem for integrals

[$\int_a^b f(x)g(x)dx = f(\zeta)\int_a^b g(x)dx$ if $g(x)$ does not change sign over (a, b)]

(note that $x(x-h)$ is uniformly non-positive)

$$E_i = \frac{f''(\zeta_i)}{2!} \int_0^h x(x-h)dx = -\frac{h^3 f''(\zeta_i)}{12}$$

Trapezoidal Rule: Error estimate

The total error is

$$E = I - \widetilde{I} = \sum_{i=1}^{n} E_i = -\frac{h^3 \sum_{i=1}^{n} f''(\zeta_i)}{12} = -\frac{(b-a)h^2 \overline{f''}}{12}$$

where the average value of the second derivative is given by

$$\overline{f''} = \frac{\sum_{i=1}^{n} f''(\zeta_i)}{n} = \frac{\sum_{i=1}^{n} f''(\zeta_i)}{(b-a)/h}$$

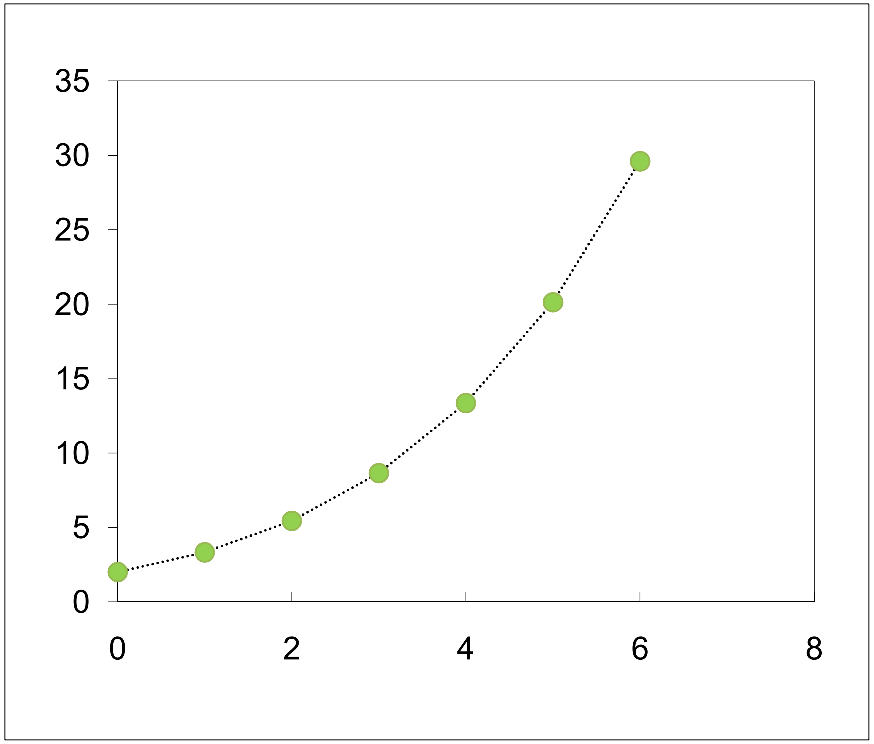
Trapezoidal Rule: Error estimate

- The error in one segment is $O(h^3)$, and the total error over the interval (a,b) is $O(h^2)$
- Implies that if we reduce the step size to half, error in each segment will be reduced to 1/8, but overall error reduces to 1/4 (since the number of segments is doubled!)

Trapezoidal 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)

Trapezoidal Rule: Example

- Distance travelled, $d = \int_0^6 v dt$
- Trapezoidal rule, with h=1 s
  - d=(2/2+3.33+5.44+8.65+13.36+ 20.13+29.60/2)x1 = 66.71 cm
- h=2 s
  - d=(2/2+5.44+13.36+29.60/2)x2 = 69.20 cm
- h=3 s
  - d=(2/2+8.65+29.60/2)x3 = 73.35 cm
- h=6 s
  - d=(2/2+29.60/2)x6 = 94.80 cm

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

Trapezoidal Rule: Example – Error analysis

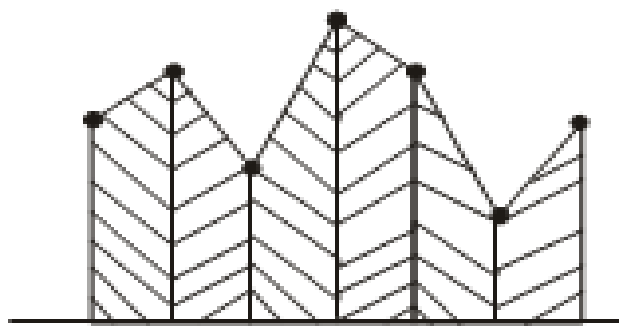
Time (s)	Speed (cm/s)
0	2.00
1	3.33
2	5.44
3	8.65
4	13.36
5	20.13
6	29.60

T.V.=65.86

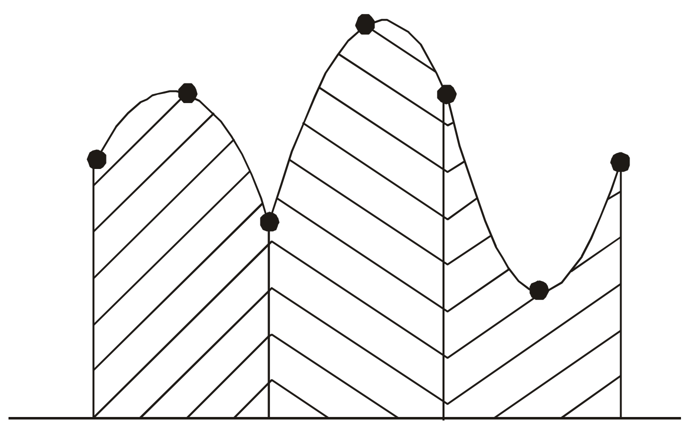
- Here we "know" the function
- The second derivative varies from about 0.6 to 3.5 cm/s^3
- Error $-\dfrac{(b-a)h^2\overline{f}''}{12}$ should vary from about -0.3 h^2 to -1.7 h^2
- For h=1, Error = -0.85 cm
- For h=2, Error = -3.34 cm (nearly 4 times)
- For h=3, Error = -7.49 cm (nearly 9 times)
- For h=6, Error = -28.94 cm (nearly 36 times)

Numerical Integration: Improving accuracy

- Trapezoidal Rule: Linear Interpolation (2 point)



- Quadratic Interpolation: 3 successive points

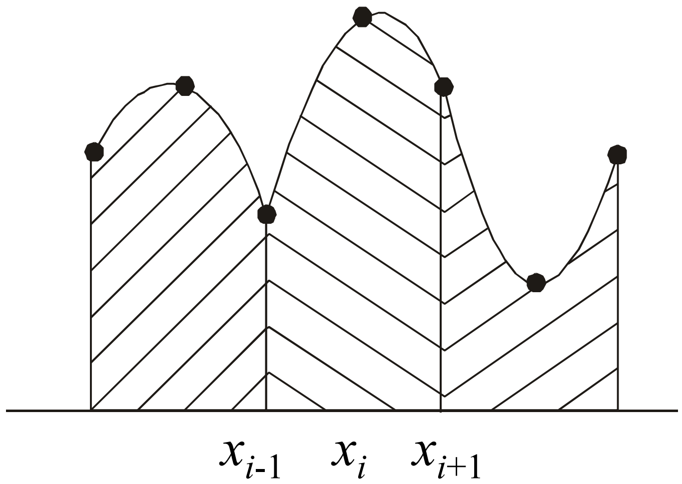


Higher accuracy

- In each sub-interval, comprising 2 segments:

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

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



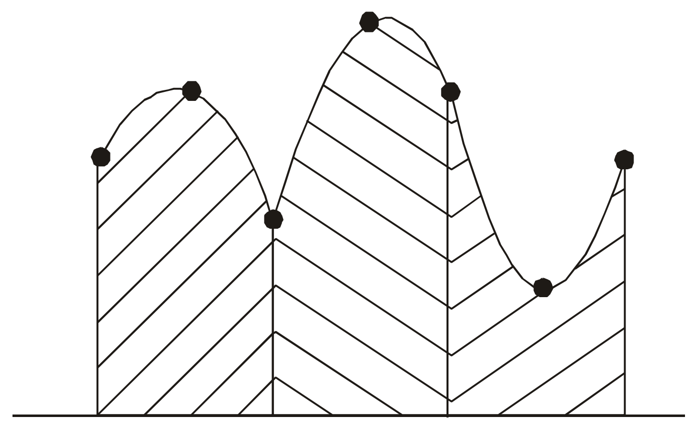
- Simpson's 1/3rd Rule

Simpson's Rule

- Sum over all sub-intervals (assume n is even):

$$\tilde{I} = \sum_{i=1,3,5,\ldots,n-1} \tilde{I}_i = \frac{h}{3}\left(f_{i-1} + 4f_i + f_{i+1}\right)$$

$$= \frac{h}{3}\left(f_0 + 4\sum_{i=1,3,5,\ldots,n-1} f_i + 2\sum_{i=2,4,6,\ldots,n-2} f_i + f_n\right)$$



Simpson's Rule: Error Estimate

- Error in the i[th] sub-interval:

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

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

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

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