Numerical Methods

Numerical Differentiation and Integration

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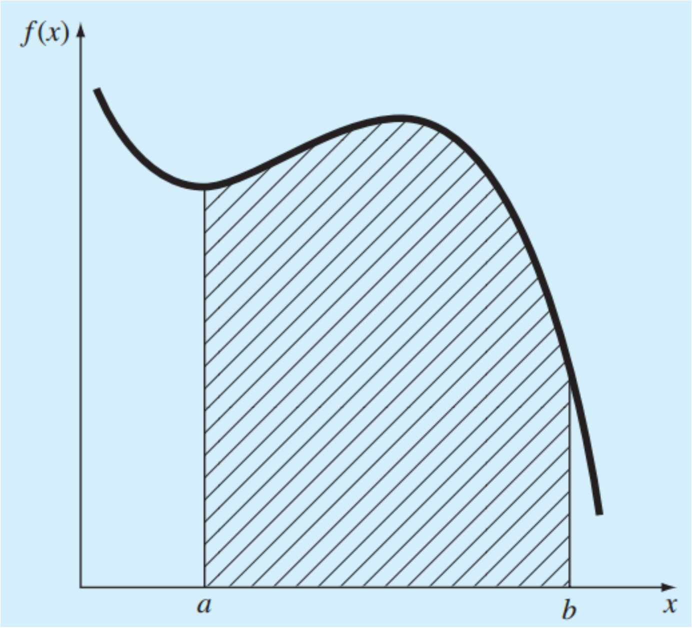
❖ Integration

Mathematically, definite integration is represented by

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

which stands for the integral of the function *f(x)* with respect to the independent variable x, evaluated between the limits x = a to x = b

numerical quadrature (often abbreviated to quadrature) is more or less a synonym for numerical integration



The integral is equivalent to the area under the curve

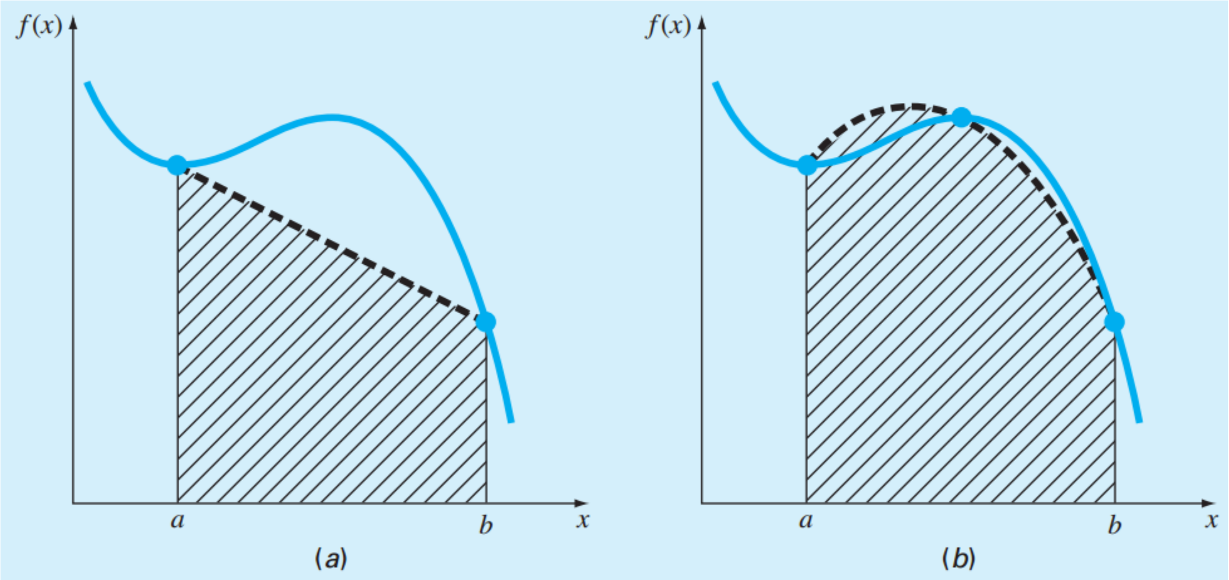
Newton-Cotes formulas

The Newton-Cotes formulas are the most common numerical integration schemes. They are based on the strategy of replacing a complicated function or tabulated data with a polynomial that is easy to integrate:

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

where $f_n(x)$ = a polynomial of the form

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$



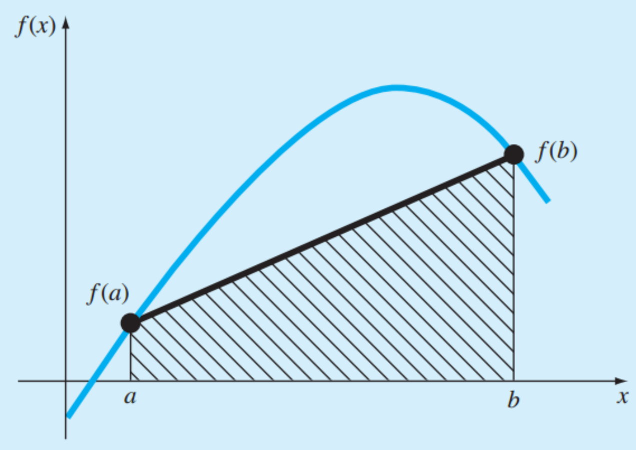
The approximation of an integral by the area under (a) a straight line and (b) a parabola

A series of polynomials: The approximation of an integral by the area under three straight-line segments

trapezoidal rule

The trapezoidal rule is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial is first-order:

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx$$



The result of the integration is

$$I = (b - a)\frac{f(a) + f(b)}{2}$$

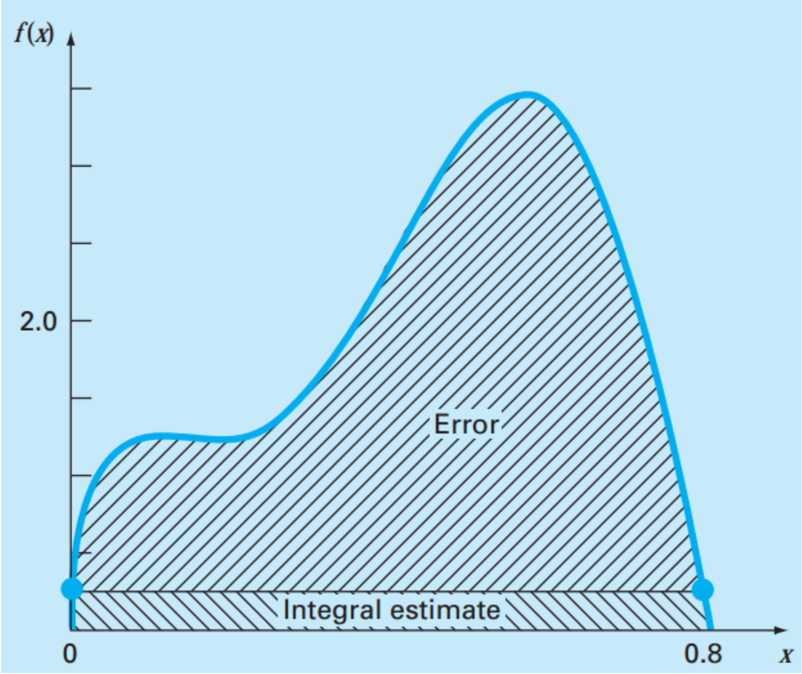
which is called the trapezoidal rule

trapezoidal rule

- If the function being integrated is linear, the trapezoidal rule will be exact
- Otherwise, for functions with second- and higher-order derivatives (that is, with curvature), some error can occur

Error of the Trapezoidal Rule $E_t = -\frac{1}{12} f''(\xi)(b-a)^3$

where ξ lies somewhere in the interval from a to b



Case study

Application of the Trapezoidal Rule

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Numerical Differentiation and Integration

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Solution

The function values $f(0) = 0.2$, $f(0.8) = 0.232$

$$\Rightarrow \boxed{I = (b-a)\frac{f(a) + f(b)}{2}} \Rightarrow I \cong 0.8\frac{0.2 + 0.232}{2} = 0.1728$$

which represents an error of $E_t = 1.640533 - 0.1728 = 1.467733$ $\qquad \varepsilon_t = 89.5\%$

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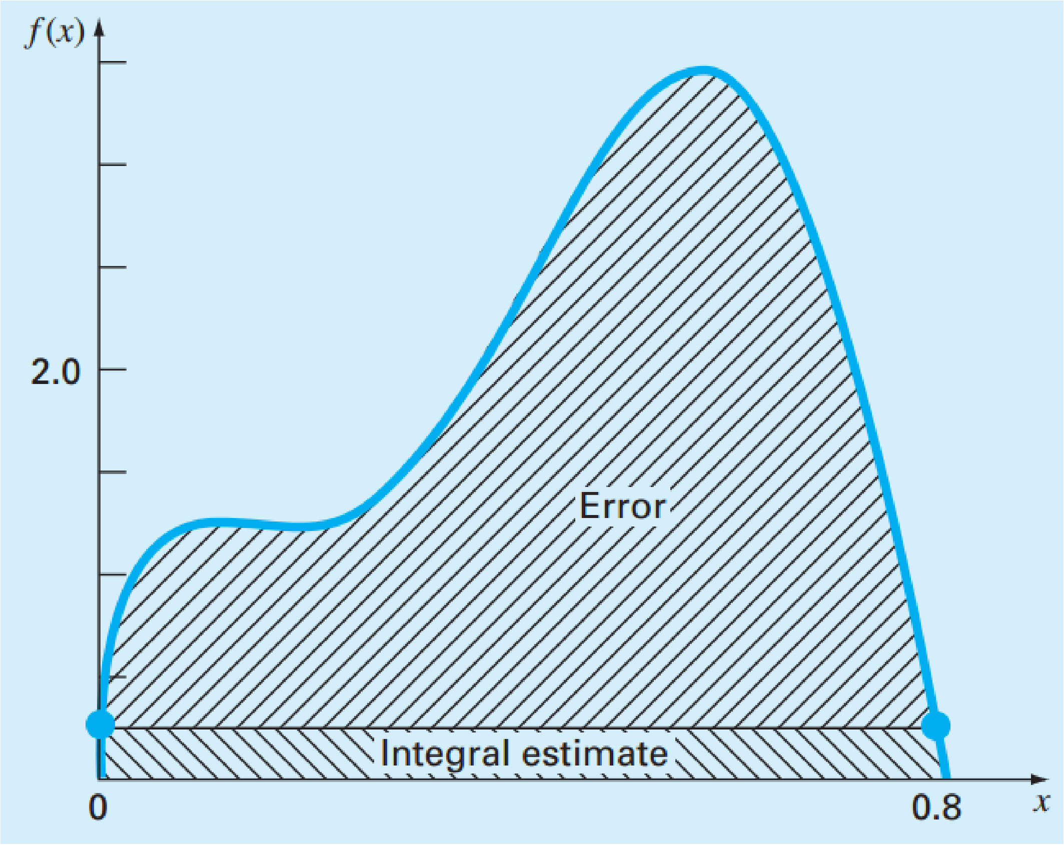


multiple-application trapezoidal rule

The trapezoidal rule :

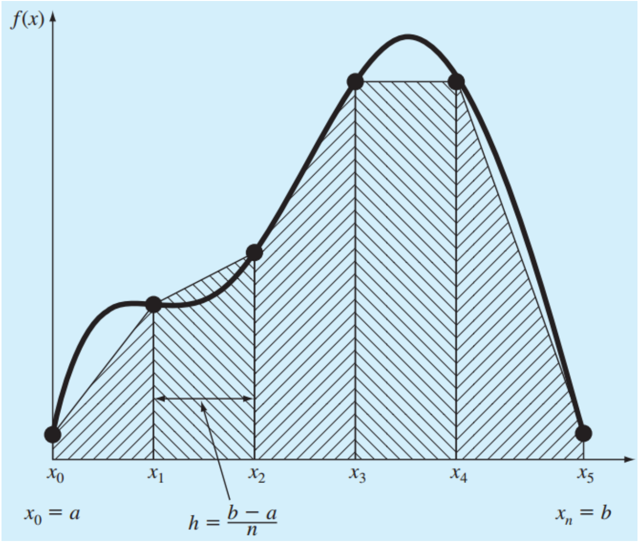
$$I = h\frac{f(x_0) + f(x_1)}{2} + h\frac{f(x_1) + f(x_2)}{2} + \cdots + h\frac{f(x_{n-1}) + f(x_n)}{2}$$

or, grouping terms:

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

Error of the Trapezoidal Rule

$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i=1}^{n} f''(\xi_i)$$



composite trapezoidal rule

Case study

Use the two-segment trapezoidal rule to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Numerical Differentiation and Integration

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Solution

The function values when n= 2 (h= 0.4):

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$$

f(0) = 0.2 , f(0.4) = 2.456, f(0.8) = 0.232

$$\Rightarrow \quad I = 0.8\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

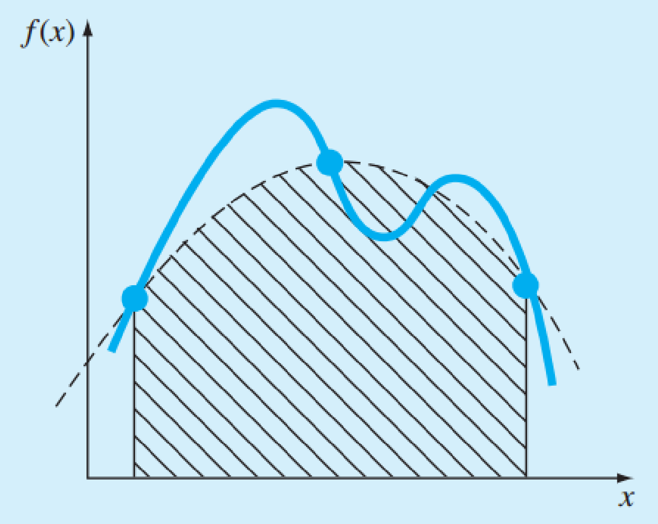
which represents an error of

$$E_t = 1.640533 - 1.0688 = 0.57173 \qquad \varepsilon_t = 34.9\%$$

$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

Simpson's rules

higher-order polynomials: to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points



(a)

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_2(x)\,dx$$

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

$$\Rightarrow I = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] \qquad \Rightarrow I = (b-a)\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$$

Simpson's 1/3 rule

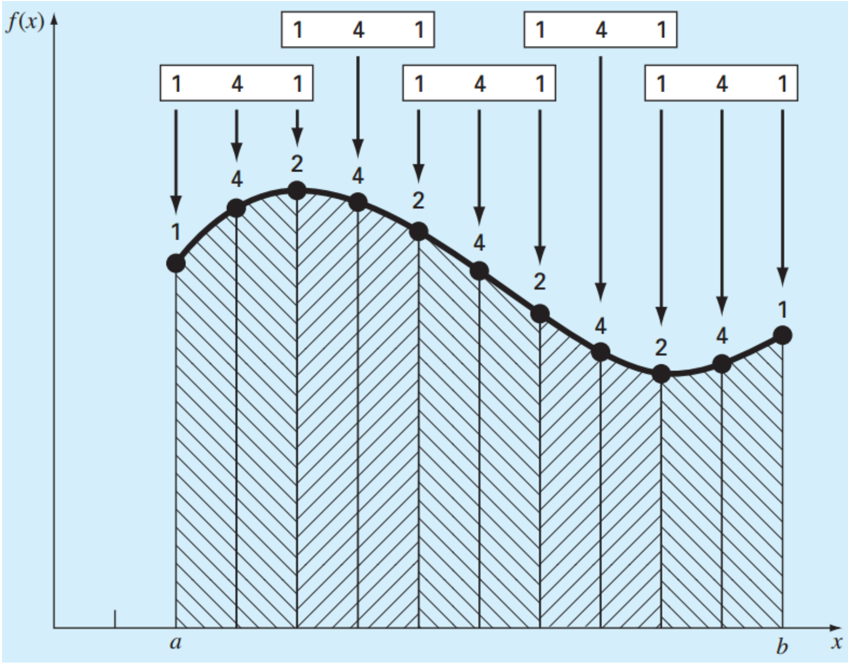
Composite Simpson's rules

Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

The result of the integration is

$$I = (b-a)\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}$$



The Composite Simpson's 1 /3 Rule

Higher-order Newton-Cotes formulas

Segments (n)	Points	Name	Formula
1	2	Trapezoidal rule	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$
2	3	Simpson's 1/3 rule	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$
3	4	Simpson's 3/8 rule	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$
4	5	Boole's rule	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$
5	6		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$

The step size is given by $h = (b - a)/n$

Case study

Use the composite Simson's rule to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Solution

The function values when n= 4 (h= 0.2):

f(0) = 0.2 , f(0.4) = 2.456, f(0.8) = 0.232, f (0.2) = 1.288, f (0.6) = 3.464

$$I = 0.8\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

which represents an error of $E_t = 1.640533 - 1.623467 = 0.017067 \qquad \varepsilon_t = 1.04\%$

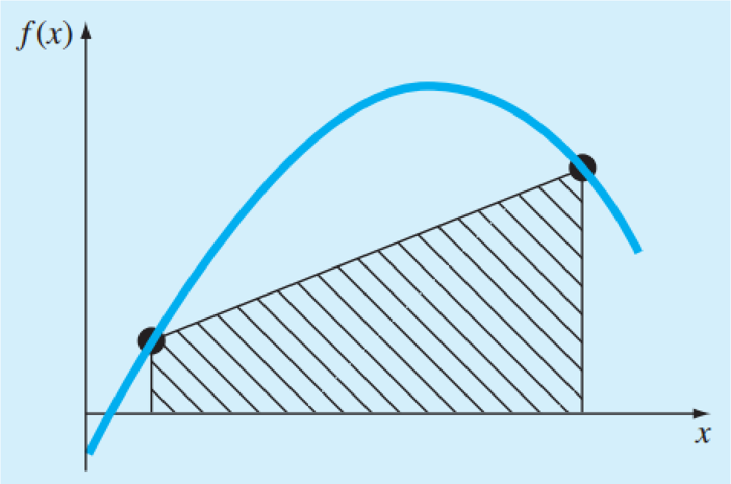
$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

Gauss quadrature

- A characteristic of Newton-cotes formulas was that the integral estimate was based on evenly spaced function values.
- Consequently, the location of the base points used in these equations was predetermined or fixed

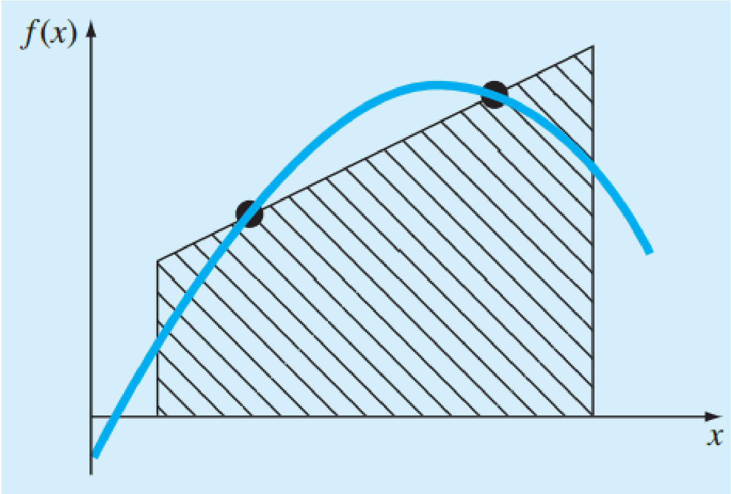
⇨ large error

- Suppose that the constraint of fixed base points was removed and we were free to evaluate the area under a straight line joining any two points on the curve.
- By positioning these points wisely, we could define a straight line that would balance the positive and negative errors. Hence, we would arrive at an improved estimate of the integral



trapezoidal rule

⇩



Gauss quadrature

Basis of the Gaussian Quadrature Rule

Previously, the Trapezoidal Rule was developed by the method of undetermined coefficients. The result of that development is summarized below.

$$\int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$$

$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

Basis of the Gaussian Quadrature Rule

- The two-point Gauss Quadrature Rule is an extension of the Trapezoidal Rule approximation where the arguments of the function are not predetermined as a and b but as unknowns x_1 and x_2.
- In the two-point Gauss Quadrature Rule, the integral is approximated as

$$I = \int_a^b f(x)dx \quad \approx c_1 f(x_1) + c_2 f(x_2)$$

The previous four simultaneous nonlinear Equations have only one acceptable solution,

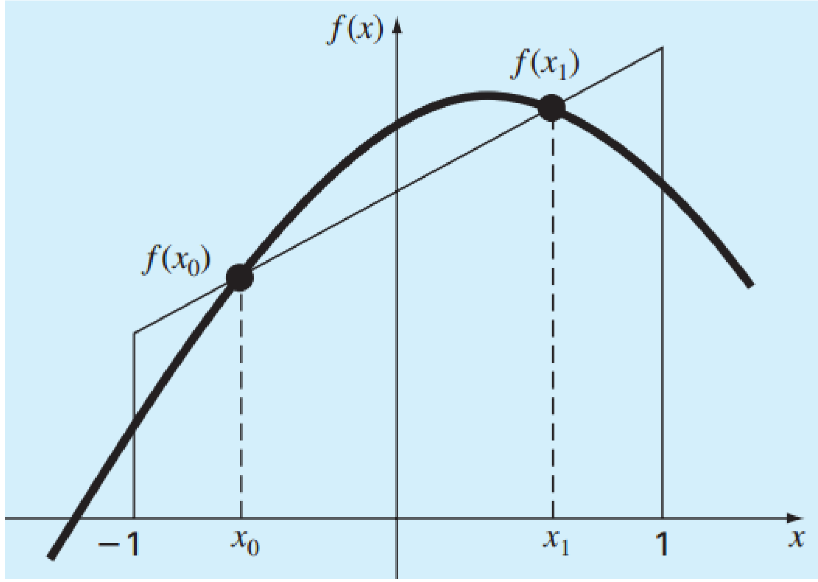
$$x_1 = \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2} \qquad x_2 = \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$$

$$c_1 = \frac{b-a}{2} \qquad c_2 = \frac{b-a}{2}$$

Two-Point Gaussian Quadrature Rule

$$\int_a^b f(x)dx \approx c_1 f\left(x_1\right)+c_2 f\left(x_2\right)$$

$$=\frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right)+\frac{b+a}{2}\right)+\frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)+\frac{b+a}{2}\right)$$



If a = -1, b = 1

$$\int_{-1}^{1} f(x)dx \cong \sum_{i=1}^{2} c_i f(x_i) = f\left(-\frac{1}{\sqrt{3}}\right)+ f\left(\frac{1}{\sqrt{3}}\right)$$

Integration

1D quardrature rule recap

$$\boxed{I = \int_{-1}^{1} f(\xi)\, d\xi \approx \sum_{i=1}^{M} W_i \; f(\xi_i)}$$

Weight   Integration point

Choose the integration points **and** weights to maximize accuracy

$$\int_a^b f(x)\, dx = \boxed{\;?\;}$$

Gauss quadrature

An integral over [a, b] must be changed into an integral over [−1, 1] before applying the Gaussian quadrature rule. This change of interval can be done in the following way:

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)dx$$

avec

$$x = \frac{(b+a)+(b-a)x_d}{2}$$

$$dx = \frac{b-a}{2}dx_d$$

Applying the Gaussian quadrature rule then results in the following approximation

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Gauss quadrature

2 points

$$I = \int_{-1}^{1} f(x)dx \cong f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

3 points

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

Number of points, n	Points, x_i	Weights, w_i
1	0	2
2	$\pm\sqrt{\frac{1}{3}}$	1
3	0	$\frac{8}{9}$
	$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
4	$\pm\sqrt{\frac{3}{7} - \frac{2}{7}\sqrt{\frac{6}{5}}}$	$\frac{18+\sqrt{30}}{36}$
	$\pm\sqrt{\frac{3}{7} + \frac{2}{7}\sqrt{\frac{6}{5}}}$	$\frac{18-\sqrt{30}}{36}$
5	0	$\frac{128}{225}$
	$\pm\frac{1}{3}\sqrt{5 - 2\sqrt{\frac{10}{7}}}$	$\frac{322+13\sqrt{70}}{900}$
	$\pm\frac{1}{3}\sqrt{5 + 2\sqrt{\frac{10}{7}}}$	$\frac{322-13\sqrt{70}}{900}$

Differentiation

Points	Weighting Factors	Function Arguments	Truncation Error
1	$c_0 = 2$	$x_0 = 0.0$	$\cong f^{(2)}(\xi)$
2	$c_0 = 1$	$x_0 = -1/\sqrt{3}$	$\cong f^{(4)}(\xi)$
	$c_1 = 1$	$x_1 = 1/\sqrt{3}$	
3	$c_0 = 5/9$	$x_0 = -\sqrt{3/5}$	$\cong f^{(6)}(\xi)$
	$c_1 = 8/9$	$x_1 = 0.0$	
	$c_2 = 5/9$	$x_2 = \sqrt{3/5}$	
4	$c_0 = (18 - \sqrt{30})/36$	$x_0 = -\sqrt{525 + 70\sqrt{30}}/35$	$\cong f^{(8)}(\xi)$
	$c_1 = (18 + \sqrt{30})/36$	$x_1 = -\sqrt{525 - 70\sqrt{30}}/35$	
	$c_2 = (18 + \sqrt{30})/36$	$x_2 = \sqrt{525 - 70\sqrt{30}}/35$	
	$c_3 = (18 - \sqrt{30})/36$	$x_3 = \sqrt{525 + 70\sqrt{30}}/35$	
5	$c_0 = (322 - 13\sqrt{70})/900$	$x_0 = -\sqrt{245 + 14\sqrt{70}}/21$	$\cong f^{(10)}(\xi)$
	$c_1 = (322 + 13\sqrt{70})/900$	$x_1 = -\sqrt{245 - 14\sqrt{70}}/21$	
	$c_2 = 128/225$	$x_2 = 0.0$	
	$c_3 = (322 + 13\sqrt{70})/900$	$x_3 = \sqrt{245 - 14\sqrt{70}}/21$	
	$c_4 = (322 - 13\sqrt{70})/900$	$x_4 = \sqrt{245 + 14\sqrt{70}}/21$	
6	$c_0 = 0.171324492379170$	$x_0 = -0.932469514203152$	$\cong f^{(12)}(\xi)$
	$c_1 = 0.360761573048139$	$x_1 = -0.661209386466265$	
	$c_2 = 0.467913934572691$	$x_2 = -0.238619186083197$	
	$c_3 = 0.467913934572691$	$x_3 = 0.238619186083197$	
	$c_4 = 0.360761573048131$	$x_4 = 0.661209386466265$	
	$c_5 = 0.171324492379170$	$x_5 = 0.932469514203152$	

Weighting factors and function arguments used in Gauss-Legendre formulas.

Case study

estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from a = 0 to b = 0.8, the exact value: 1.640533

Solution

Before integrating the function, we must perform a change of variable so that the limits are from −1 to +1

$$x = 0.4 + 0.4x_d \qquad \text{and} \qquad dx = 0.4dx_d$$

Both of these can be substituted into the original equation to yield

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\, dx$$

$$= \int_{-1}^{1} [0.2 + 25(0.4 + 0.4x_d) - 200(0.4 + 0.4x_d)^2 + 675(0.4 + 0.4x_d)^3 - 900(0.4 + 0.4x_d)^4 + 400(0.4 + 0.4x_d)^5]0.4dx_d$$

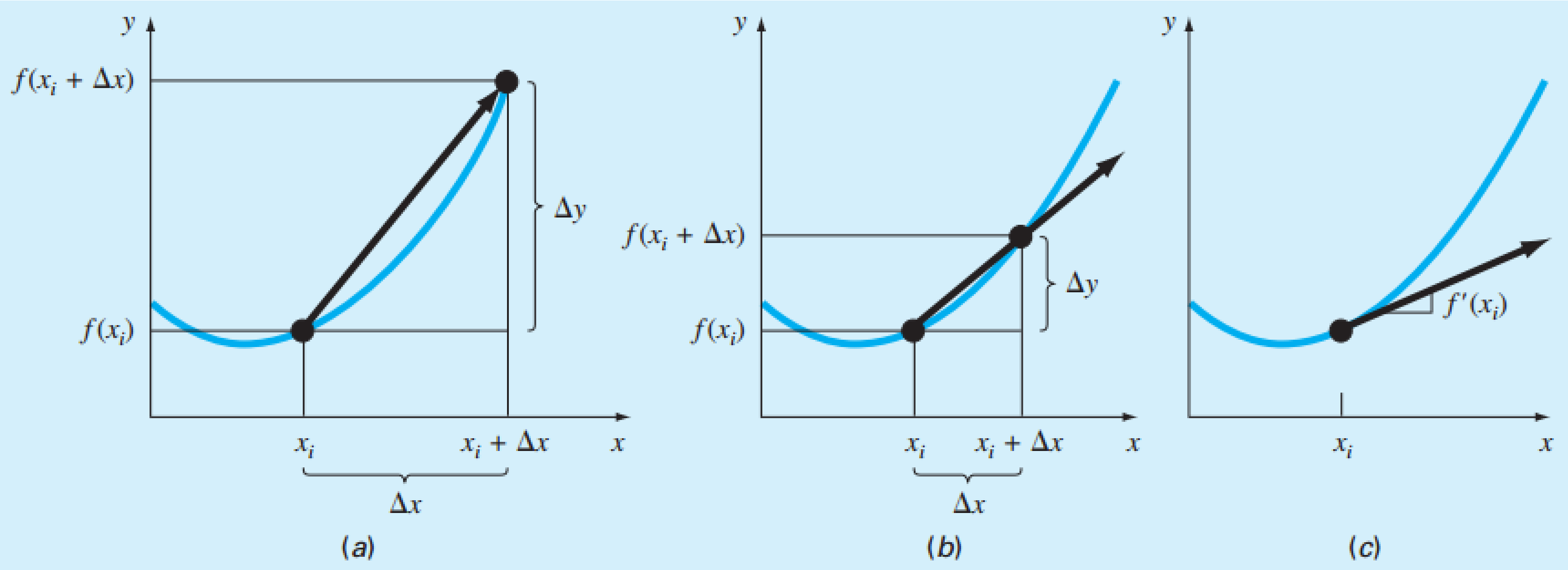
- Topics
  - Numerical Integration
    - Newton-Cotes Formulas: Trapezoidal rule, Simpson’s rule
    - Gauss Quadrature
  - Numerical Differentiation

Differentiation

❖ Notion

➢ the derivative represents the rate of change of a dependent variable with respect to an independent variable

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \qquad \frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



Numerical Differentiation and Integration

Notion

- the derivative can be visualized as the slope of a function.
- Integration is the inverse of differentiation
- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

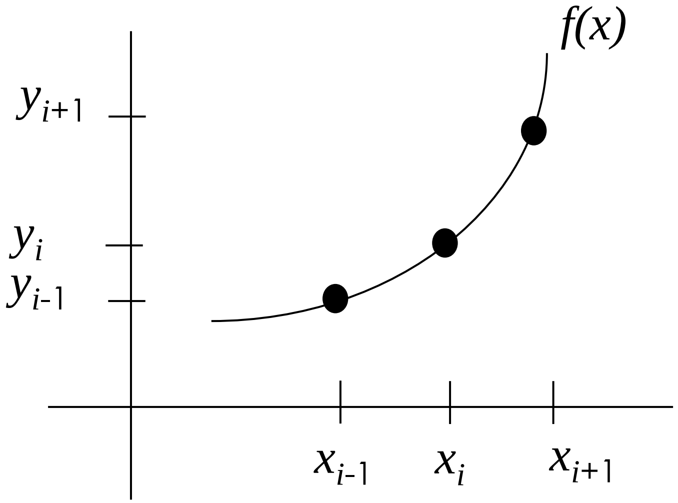
$$\Rightarrow \quad f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h + O(h^2)$$

$$\Rightarrow \quad f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

Differentiation

<u>Forward Differences</u>

$$f'(x_i) \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i} = \frac{y_{i+1} - y_i}{h}$$



<u>Backward Differences</u>

$$f'(x_i) \approx \frac{y_{i-1} - y_i}{x_{i-1} - x_i} = \frac{y_{i-1} - y_i}{h}$$

<u>Central Difference</u>

$$f'(x_i) \approx \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{2h}$$

Differentiation

First Derivative	Error
$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Case study

Use the numerical differentiation to estimate the integral of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5 using finite-differences and a step size of h = 0.25

the true value of f′(0.5) = −0 .9125

Solution

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

$$\begin{aligned}
x_{i-2} &= 0 & f(x_{i-2}) &= 1.2 \\
x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.1035156 \\
x_i &= 0.5 & f(x_i) &= 0.925 \\
x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.6363281 \\
x_{i+2} &= 1 & f(x_{i+2}) &= 0.2
\end{aligned}$$

	Backward $O(h)$	**Centered** $O(h^2)$	**Forward** $O(h)$
Estimate	−0.714	−0.934	−1.155
ε_t	21.7%	−2.4%	−26.5%

Matlab

Exercises

Results for the composite trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8. The exact value is 1.640533.

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

Using diff for Differentiation

Explore how the MATLAB diff function can be employed to differentiate the function

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

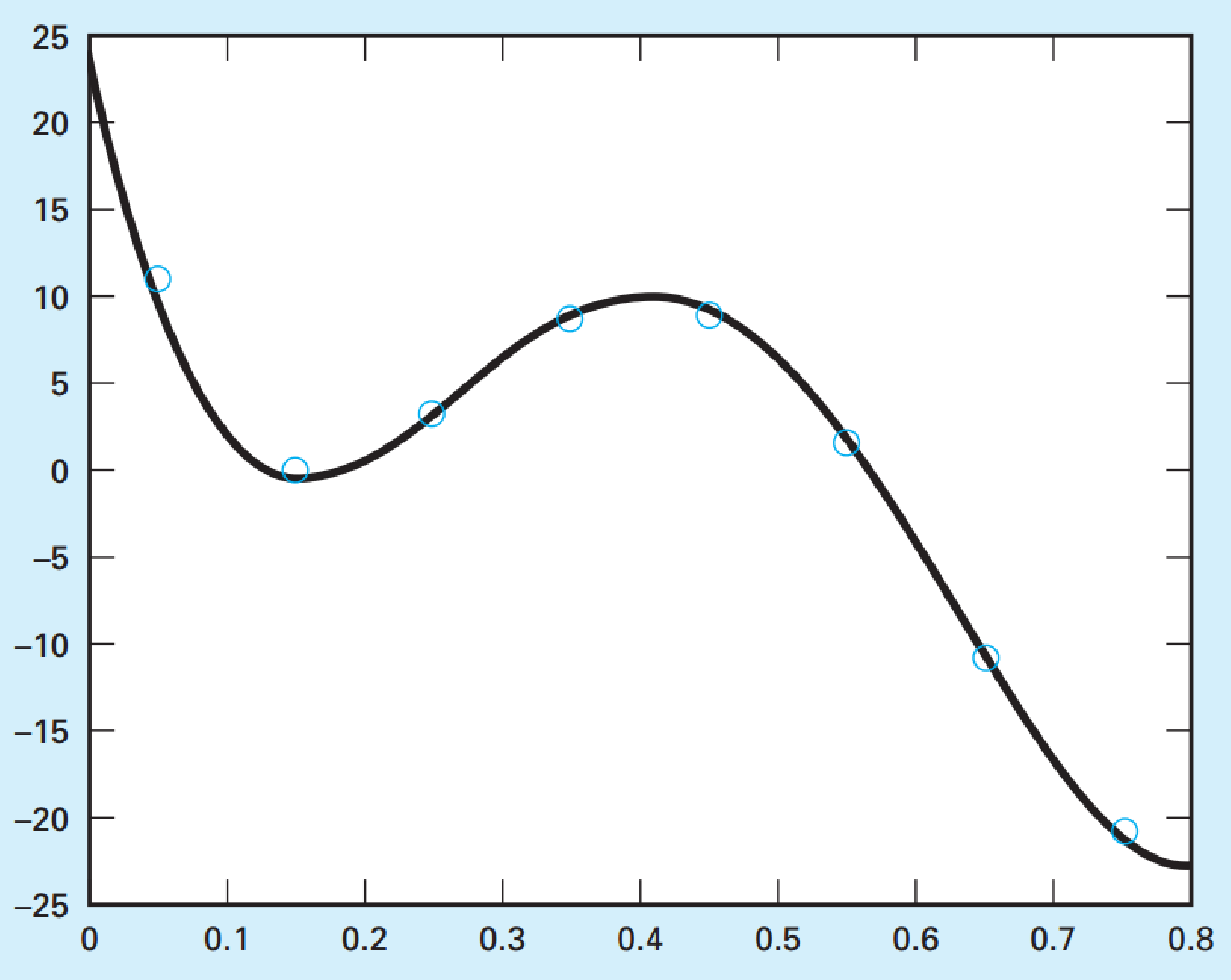
from x = 0 to 0.8. Compare your results with the exact solution

$$f'(x) = 25 - 400x^2 + 2025x^2 - 3600x^3 + 2000x^4$$

Using diff for Differentiation

Comparison of the exact derivative (line) with numerical estimates (circles) computed with MATLAB's diff function

>> plot(xm,d,'o',xa,ya)



Using gradient for Differentiation   fx = gradient(f, h)

Explore how the MATLAB diff function can be employed to differentiate the function

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from x = 0 to 0.8. Compare your results with the exact solution

$$f'(x) = 25 - 400x^2 + 2025x^2 - 3600x^3 + 2000x^4$$

Using gradient for Differentiation

fx = gradient(f, h)