

## 8. Numerical integration

- differentiation and integration
- Newton-Cotes integration
- Trapezoidal method
- Simpson 1/3 & 3/8 rules
- Romberg integration

# Derivatives

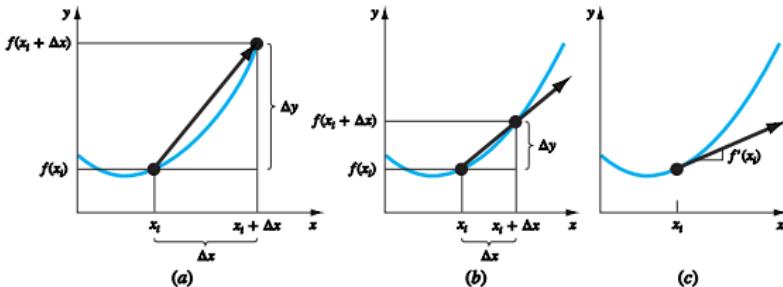
## Difference approximation

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

## Derivative

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

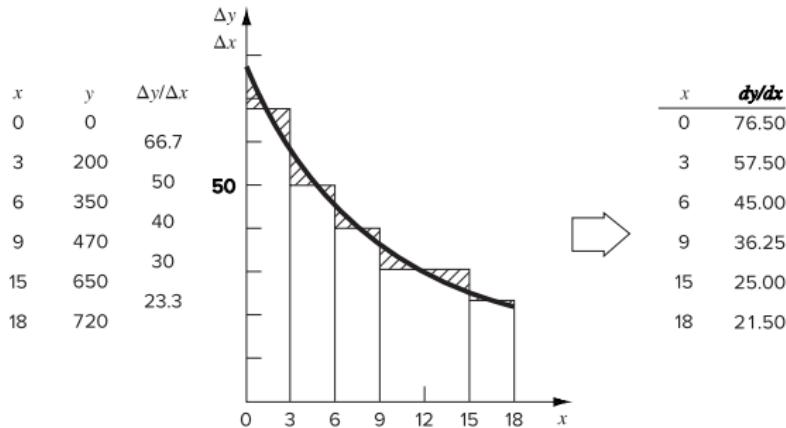
- $\frac{dy}{dx}$  (also  $y'$  or  $f'(x_i)$ ) is the slope of the tangent to the curve at  $x_i$



- *second derivative:*  $\frac{d^2 y}{dx^2} = \frac{d}{dx} \left( \frac{dy}{dx} \right)$  measures how fast slope changes (*curvature*)

# Equal-area graphical differentiation

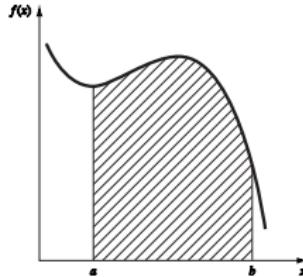
- compute divided differences  $\Delta y / \Delta x$
- plot as a step curve versus  $x$
- sketch a smooth curve balancing positive and negative areas
- read  $dy/dx$  values from the smooth curve



# Integration

**Integration:** the inverse process to differentiation written as

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



- $f(x)$  is the *integrand*
- $\int$  is a stylized  $S$  symbolizing *summation*
- integral corresponds to **area under the curve** of  $f(x)$  between  $x = a$  and  $x = b$
- definite integration: limits  $a, b$  specified
- indefinite integration: limits not specified, result is a family of functions

# Relationship between differentiation and integration

differentiation and integration are inversely related processes

**General link:** integration

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

is equivalent to solving the differential equation

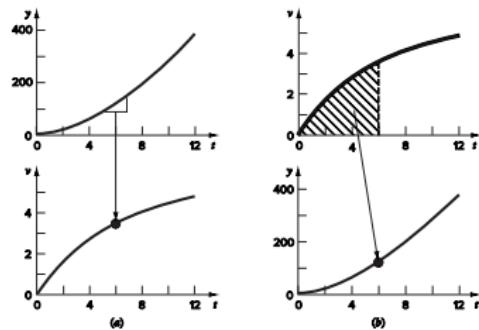
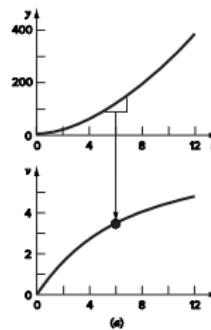
$$\frac{dy}{dx} = f(x), \quad y(a) = 0$$

for  $y(b)$

**Example:** if  $y(t)$  is position and  $v(t)$  is velocity, then

$$v(t) = \frac{d}{dt}y(t), \quad y(0) = 0$$

$$\iff y(t) = \int_0^t v(t) dt$$



## **Noncomputer methods for differentiation and integration**

the function to be differentiated or integrated will usually be one of three forms:

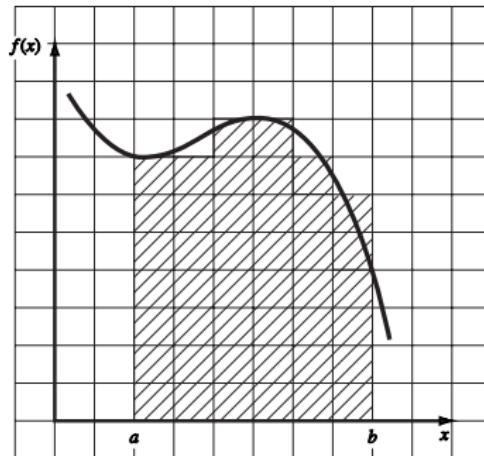
1. simple continuous function (polynomial, exponential, trigonometric)
2. complicated continuous function (difficult or impossible to handle analytically)
3. tabulated function, values given at discrete points (e.g., experimental data)

### **Approaches**

- for case 1: analytic calculus works well
- for cases 2 and 3: approximate methods must be employed

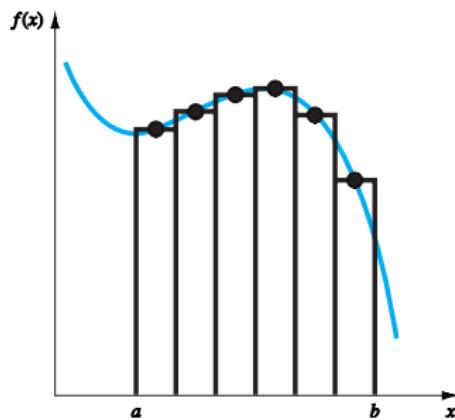
## Graphical integration: grid method

- grid method: sum area of boxes under the curve
- finer grids → improved estimates



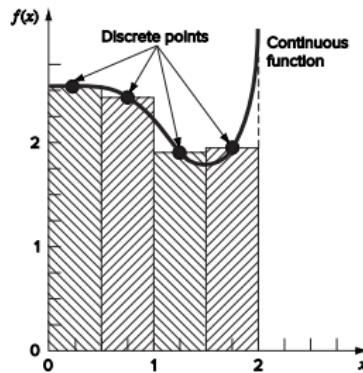
## Graphical integration: strip method

- strip method: sum of rectangles area with height at strip midpoints
- finer strips → improved estimates



$$\int_0^2 \frac{2 + \cos(1 + x^{3/2})}{\sqrt{1 + 0.5 \sin x}} e^{-0.5x} dx$$

x	f(x)
0.25	2.599
0.75	2.414
1.25	1.945
1.75	1.993



## Outline

- differentiation and integration
- **Newton-Cotes integration**
- Trapezoidal method
- Simpson 1/3 & 3/8 rules
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# Newton-cotes formulas

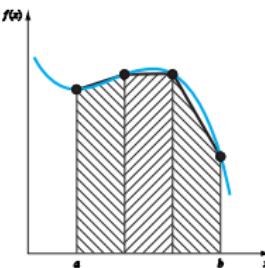
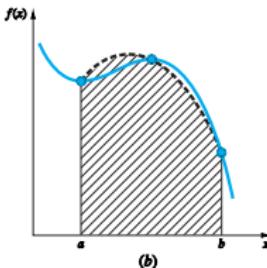
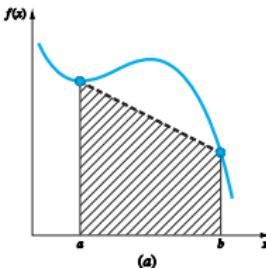
replace a complicated function or data with an approximating polynomial:

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

where  $f_n(x) = a_0 + a_1x + \cdots + a_{n-1}x^{n-1} + a_nx^n$

examples:

- the “strip method” corresponds to piecewise zero-order polynomials (constants)
- first-order polynomial: straight line connecting endpoints (trapezoidal rule)
- second-order polynomial: parabola (Simpson rule)
- straight line segments (composite trapezoidal rule)



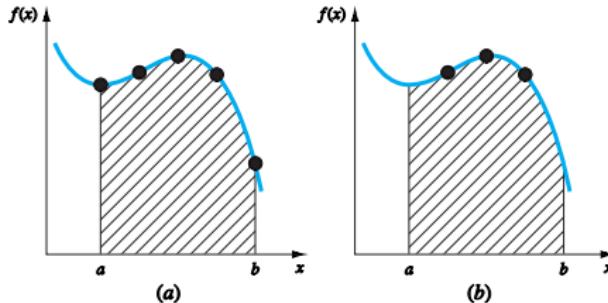
# Closed and open Newton–Cotes formulas

## Closed form

- data points at the beginning and end of the limits of integration are known
- commonly used for definite integration
- trapezoid and Simpson rules are closed forms

## Open form

- integration limits extend beyond available data points
- does not use endpoints
- mainly applied to improper integrals and in solving ordinary differential equations



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## Trapezoidal rule

- use a first-order polynomial as the approximation:

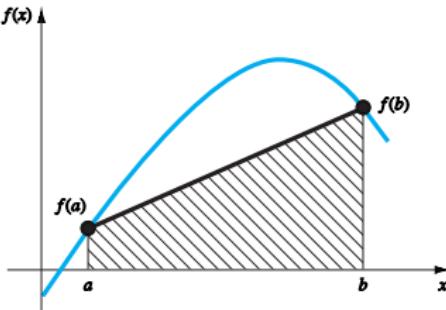
$$I = \int_a^b f(x) dx \approx \int_a^b f_1(x) dx$$

- recall, Newton linear interpolation between  $(a, f(a))$  and  $(b, f(b))$  is

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a} (x - a)$$

- the integral of the straight line approximation yields the **trapezoidal rule**:

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

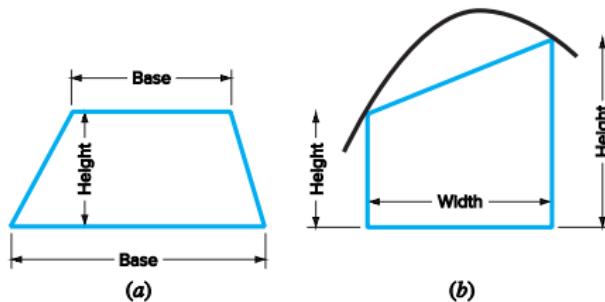


## Geometric interpretation of the trapezoidal rule

geometrically:  $I_{\text{trap}} \approx$  trapezoid area formed by straight line connecting  $f(a), f(b)$

- from geometry, the area of a trapezoid is computed as

$$\text{area} = \text{height} \times \frac{\text{sum of bases}}{2}$$

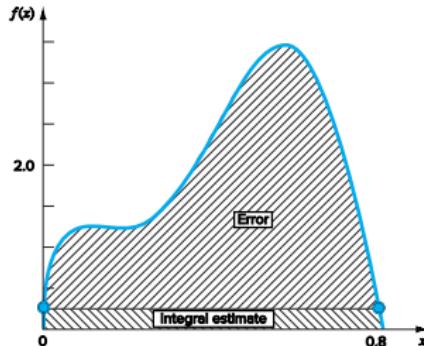


- in the trapezoidal rule, the trapezoid is rotated on its side, thus,

$$I_{\text{trap}} \approx \text{width} \times \text{average height} = (b - a) \frac{f(a) + f(b)}{2}$$

## Error of the trapezoidal rule

error can be substantial



- an estimate of the local truncation error for a single application of trapezoidal rule:

$$E_t = -\frac{1}{12}f''(\xi)(b-a)^3, \quad \xi \in [a, b]$$

- if  $f(x)$  is linear, then  $f''(x) = 0$  and the trapezoidal rule is exact
- error will occur for functions with nonzero second derivatives (curvature)
- to estimate error, replace  $f''(\xi)$  by average over interval:

$$E_a = -\frac{1}{12}\bar{f}''(x)(b-a)^3, \quad \bar{f}''(x) = \frac{1}{b-a} \int_a^b f''(x)dx = \frac{f'(b)-f'(a)}{b-a}$$

## Example

numerically integrate

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

from  $a = 0$  to  $b = 0.8$ ; the exact value of the integral is 1.640533

- the function values are

$$f(0) = 0.2, \quad f(0.8) = 0.232$$

thus:

$$I_{\text{trap}} \approx 0.8 \times \frac{0.2 + 0.232}{2} = 0.1728$$

- error:

$$E_t = 1.640533 - 0.1728 = 1.467733$$

percent relative error:

$$\varepsilon_t = 89.5\%$$

large error results because the straight line neglects much of the area above it

## Example: approximate error estimate

- to estimate error, replace  $f''(\xi)$  by average over interval  $\frac{1}{a-b} \int_a^b f''(x) dx$
- second derivative:

$$f''(x) = -400 + 4050x - 10800x^2 + 8000x^3$$

- average value:

$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4050x - 10800x^2 + 8000x^3) dx}{0.8} = -60$$

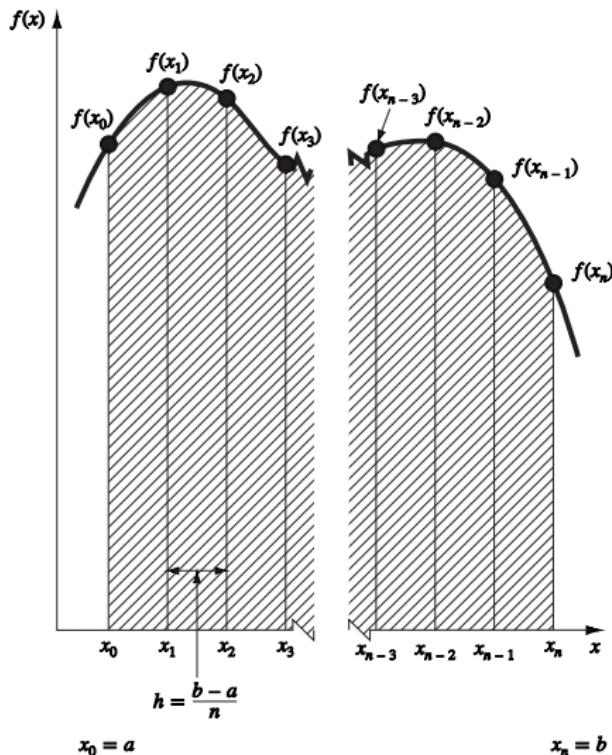
- approximate error:

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

- this is of the same order of magnitude and sign as the true error
- but not exact because  $\bar{f}''$  is not necessarily equal to  $f''(\xi)$

## Multiple-application trapezoidal rule

divide interval  $[a, b]$  into  $n$  equal segments  $[x_{i-1}, x_i]$  and integrate each segment



## Composite trapezoidal rule

- consider  $n + 1$  *equally spaced* base points  $x_0, x_1, \dots, x_n$  with stepsize  $h = \frac{b-a}{n}$
- with  $x_0 = a$  and  $x_n = b$ , the total integral is

$$I = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \cdots + \int_{x_{n-1}}^{x_n} f(x) dx$$

- substituting the trapezoidal rule for each integral yields

$$I_{\text{trap}} = \frac{h}{2} [f(x_0) + f(x_1)] + \frac{h}{2} [f(x_1) + f(x_2)] + \cdots + \frac{h}{2} [f(x_{n-1}) + f(x_n)]$$

- grouping terms gives the *composite trapezoidal rule*:

$$I_{\text{trap}} = \frac{b-a}{2n} \left[ f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$$

## Error of the composite trapezoidal rule

- summing the individual errors for each segment gives

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

where  $f''(\xi_i)$  is the second derivative at a point  $\xi_i$  located in segment  $i$

- result can be simplified by estimating the mean or value of second derivative
- for the entire interval as:

$$\frac{1}{n} \sum_{i=1}^n f''(\xi_i) \approx \bar{f}'' = \frac{1}{b-a} \int_a^b f''(x) dx = \frac{f'(b) - f'(a)}{b-a}$$

- therefore,  $\sum f''(\xi_i) \approx n\bar{f}''$  and approximate error is

$$E_a = -\frac{(b-a)^3}{12n^2} \bar{f}''$$

- if the number of segments is doubled, the truncation error will be quartered

## Example

use the two-segment trapezoidal rule to estimate

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5) dx = 1.640533$$

- $n = 2, h = (0.8 - 0)/2 = 0.4$ ; function values:

$$f(0) = 0.2, \quad f(0.4) = 2.456, \quad f(0.8) = 0.232$$

- apply rule:

$$I_{\text{trap}} = \frac{0.8}{4} [0.2 + 2(2.456) + 0.232] = 1.0688$$

- true error:

$$E_t = 1.640533 - 1.0688 = 0.57173, \quad \varepsilon_t = 34.9\%$$

- approximate error with  $\bar{f}'' = -60$  (from page 8.15):

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

## Example

using  $n = 2, \dots, 10$ , we get the result shown

$n$	$h$	$I_{\text{trap}}$	$\varepsilon_t$ (%)
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

as  $n$  increases, error decreases, but at a gradual rate since  $E_a \propto 1/n^2$

## Trapezoidal rule with unequal segments

consider **unevenly spaced** segments  $h_i = x_i - x_{i-1}$

the trapezoidal rule can be applied segment by segment:

$$\begin{aligned} I_{\text{trap}} &= \frac{1}{2} \sum_{i=1}^{n-1} h_i (f(x_{i-1}) + f(x_i)) \\ &= h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2} \end{aligned}$$

- more practical since data (e.g., experimental measurements) are unevenly spaced
- same as multiple-application trapezoidal rule, except  $h_i$  not fixed
- cannot simplify as before, but easy to implement in computer code

## Example: trapezoidal rule with unequal segments

use trapezoidal rule to integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 = 1.640533$$

for data shown where the exact value of the integral is 1.640533

$x$	$f(x)$	$x$	$f(x)$
0.00	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		

applying the formula gives

$$I_{\text{trap}} = 0.12 \frac{1.309729+0.2}{2} + 0.10 \frac{1.305241+1.309729}{2} + \dots + 0.10 \frac{0.232+2.363}{2} = 1.594801$$

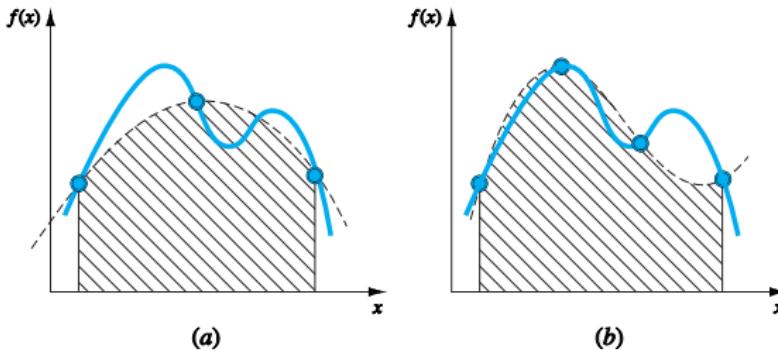
$$\text{with error } \varepsilon_t = \frac{1.640533 - 1.594801}{1.640533} \times 100\% = 2.8\%$$

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- Trapezoidal method
- **Simpson 1/3 & 3/8 rules**
- Romberg integration

## Simpson rules

- use higher-order polynomials to better approximate the integral
- for three points between  $f(a)$  and  $f(b)$ , use parabola
- four points can be connected with a third-order polynomial



- resulting formulas of integrals under these polynomials are called *Simpson rules*

## Simpson 1/3 rule

- we are given three equally spaced data points  $x_0, x_1, x_2$  (two segments)
- Simpson 1/3 rule results when a 2nd-order interpolating polynomial is used

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

if  $a = x_0$  and  $b = x_2$ , and  $f_2(x)$  is represented by a 2nd Lagrange polynomial:

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

**Simpson 1/3 rule:** integrating yields

$$\begin{aligned} I_{1/3} &= (b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \\ &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \end{aligned}$$

where  $h = \frac{b-a}{2}$  (note that the midpoint is  $x_1 = \frac{a+b}{2}$ )

## Error of Simpson 1/3 rule

truncation error for one segment (with  $h = \frac{b-a}{2}$ ):

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \quad \text{for some } \xi \in (a, b)$$

- Simpson 1/3 rule is *third-order accurate* (error  $\propto f^{(4)}$ )
- *i.e., rule exact for all cubic polynomials*
- approximate error for one segment

$$E_a = -\frac{(b-a)^5}{2880} \bar{f}^{(4)}, \quad \bar{f}^{(4)} = \frac{1}{b-a} \int_a^b f^{(4)}(x) dx = \frac{f^{(3)}(b) - f^{(3)}(a)}{b-a}$$

$\bar{f}^{(4)}$  is the average fourth derivative over the interval

## Example

approximate

$$I = \int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5) dx = 1.640533$$

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

- Simpson 1/3 rule:

$$I \approx I_{1/3} = (0.8) \frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

- exact error:

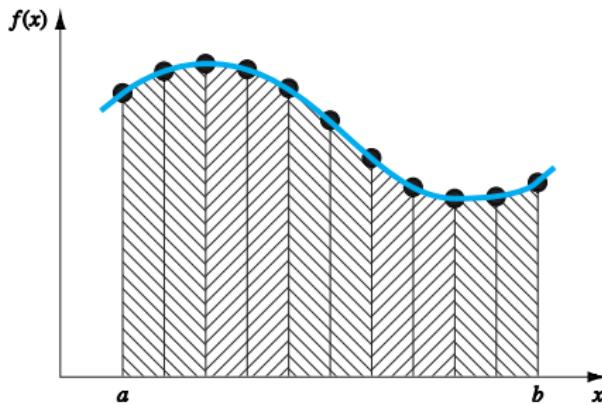
$$E_t = I - I_{1/3} = 1.640533 - 1.367467 = 0.2730667 \quad (\varepsilon_t = 16.6\%)$$

- estimated error

$$-\frac{(b-a)^5}{2880} f^{(4)}(\xi) \approx E_a = -\frac{(0.8)^5}{2880} (-2400) = 0.2730667$$

where  $-2400$  is the average of  $f^{(4)}$  on  $[0, 0.8]$

## Multiple-application Simpson 1/3 rule



- subdivide  $[a, b]$  into **even** number  $n$  of equal segments  $h = \frac{b-a}{n}$
- integrate

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

## Composite Simpson 1/3 rule

- applying Simpson 1/3 rule to each subinterval:

$$\begin{aligned} I_{1/3} &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3} [f(x_2) + 4f(x_3) + f(x_4)] \\ &\quad + \dots + \frac{h}{3} [f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \end{aligned}$$

- combining terms and yields

$$I_{1/3} = \frac{h}{3} \left[ f(x_0) + 4 \sum_{\substack{i=1 \\ i \text{ odd}}}^{n-1} f(x_i) + 2 \sum_{j=2}^{n-2} f(x_j) + f(x_n) \right]$$

where  $h = \frac{b-a}{n}$

- method requires *even* number of segments (odd number of points)

## Error of composite Simpson 1/3 rule

- approximate truncation is sum of errors and average over  $n/2$  integrals:

$$E_a = - \frac{(b-a)^5}{180 n^4} \bar{f}^{(4)}$$

where

$$\bar{f}^{(4)} = \frac{1}{a-b} \int_a^b f^{(4)}(x) dx = \frac{f^{(3)}(b) - f^{(3)}(a)}{b-a}$$

is the average value of the fourth derivative of  $f(x)$  on  $[a, b]$

- error decreases much faster than trapezoidal rule:

- trapezoidal:  $E \sim O(n^{-2})$
- Simpson 1/3:  $E \sim O(n^{-4})$

## Example

use multiple application of Simpson 1/3 rule with  $n = 4$  to estimate the integral

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

from  $a = 0$  to  $b = 0.8$ ; exact (true) value: 1.640533

- for  $n = 4$  ( $h = (0.8 - 0)/4 = 0.2$ ):

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

- hence,

$$I_{1/3} = \frac{0.8}{12} [ 0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232 ] = 1.623467$$

- true error and estimated error:

$$E_t = 1.640533 - 1.623467 = 0.017067, \quad \varepsilon_t = 1.04\%$$

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

## Simpson 3/8 rule

- use a third-order Lagrange polynomial to approximate integral:

$$I = \int_a^b f(x) dx \approx \int_a^b f_3(x) dx$$

require four points  $x_0, x_1, x_2, x_3$  ( $n = 3$  segments)

- resulting formula:

$$\begin{aligned} I_{3/8} &= \frac{b-a}{8} \left[ f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right] \\ &= \frac{3h}{8} \left[ f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right] \end{aligned}$$

where  $h = \frac{b-a}{3}$

- truncation error:

$$E_t = -\frac{3}{80} h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

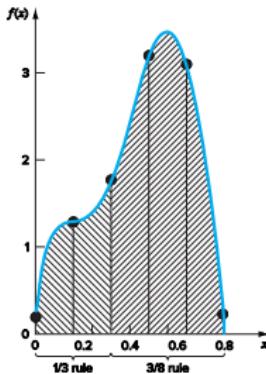
slightly more accurate than Simpson 1/3 rule, but requires 4 points

## Simpson 1/3 versus 3/8 rules

- Simpson 1/3 rule is usually the method of preference:
  - attains third-order accuracy with only 3 points
  - more efficient than 3/8 rule
- Simpson 3/8 rule requires 4 points and useful when the no. of segments is odd

**Example:** suppose we have 5 segments, then we have two options:

- multiple-application trapezoidal rule → large truncation error
- apply Simpson 1/3 rule to the first 2 segments and Simpson 3/8 rule to others



## Example

numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5, \quad a = 0, b = 0.8$$

using (a) Simpson 3/8 rule; (b) 5 segments used with Simpson 1/3 and 3/8 rules

(a) Simpson 3/8 rule with four equally spaced points ( $h = \frac{0.8-0}{3} = 0.2667$ )

$$\begin{aligned} f(0) &= 0.2, & f(0.2667) &= 1.432724, \\ f(0.5333) &= 3.487177, & f(0.8) &= 0.232 \end{aligned}$$

yields

$$I_{3/8} \approx \frac{0.8}{8} [0.2 + 3(1.432724 + 3.487177) + 0.232] = 1.519170$$

$$E_t = 1.640533 - 1.519170 = 0.121363 \quad (\varepsilon_t = 7.4\%)$$

$$E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.121363$$

## Example

(b) five-segment case ( $h = \frac{0.8-0}{5} = 0.16$ )

$$f(0) = 0.2, \quad f(0.16) = 1.296919, \quad f(0.32) = 1.743393,$$
$$f(0.48) = 3.186015, \quad f(0.64) = 3.181929, \quad f(0.80) = 0.232$$

**First two segments** (Simpson 1/3 rule)

$$I_1 = \frac{0.32}{6} [0.2 + 4(1.296919) + 1.743393] = 0.380324$$

**Last three segments** (Simpson 3/8 rule)

$$I_2 = \frac{0.48}{8} [1.743393 + 3(3.186015 + 3.181929) + 0.232] = 1.264754$$

**Total integral**

$$I_{\text{total}} = I_1 + I_2 = 0.380324 + 1.264754 = 1.645077$$

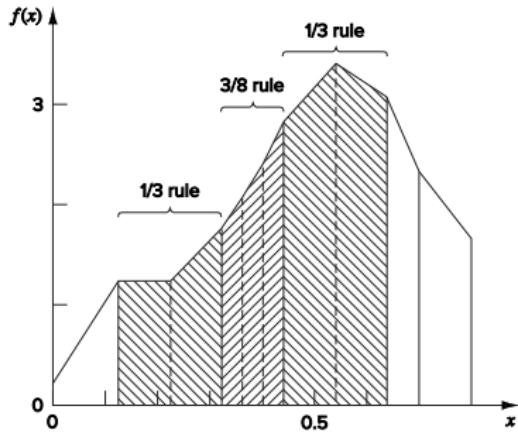
$$E_t = 1.640533 - 1.645077 = -0.004544 \quad (\varepsilon_t = -0.28\%)$$

## Example: combination of methods for uneven data

given the data below, use trapezoidal and Simpson rules where appropriate to find

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

$x$	$f(x)$	$x$	$f(x)$
0.00	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		



## Example: inclusion of Simpson rules for uneven data

- first segment ( $x = 0$  to  $0.12$ ): trapezoidal rule  $I_1 = 0.0906$
- next two segments ( $x = 0.12$  to  $0.32$ ): Simpson 1/3 rule  $I_2 = 0.2758$
- next three segments ( $x = 0.32$  to  $0.44$ ): Simpson 3/8 rule  $I_3 = 0.2727$
- next two segments ( $x = 0.44$  to  $0.64$ ): Simpson 1/3 rule  $I_4 = 0.6685$
- last two unequal segments: trapezoidal rule  $I_5 = 0.1663 + 0.1298$

total integration:

$$I_{\text{total}} = I_1 + I_2 + I_3 + I_4 = 1.603641 \quad \Rightarrow \quad \varepsilon_t = 2.2\%$$

## Outline

- differentiation and integration
- Newton-Cotes integration
- Trapezoidal method
- Simpson 1/3 & 3/8 rules
- **Romberg integration**

## Romberg integration

- Romberg integration is based on successive applications of the trapezoidal rule
- but employs mathematical manipulations to achieve higher accuracy
- key idea: combine results from trapezoidal approximations with different stepsizes to reduce error

## Richardson extrapolation

- suppose composite trapezoidal rule estimate is

$$I = I(h) + E(h), \quad h = (b - a)/n$$

- $I(h)$  = approximation from an  $n$ -segment application of the trapezoidal rule
- $E(h)$  = truncation error
- for two estimates with stepsizes  $h_1$  and  $h_2$  ( $h_2 < h_1$ ):

$$I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

where error is

$$E(h) \approx -\frac{b-a}{12} h^2 \bar{f}''$$

- ratio of errors:

$$\frac{E(h_1)}{E(h_2)} \approx \left(\frac{h_1}{h_2}\right)^2 \Rightarrow E(h_1) \approx \left(\frac{h_1}{h_2}\right)^2 E(h_2)$$

## Error elimination and improved estimate

- substituting and rearranging gives

$$E(h_2) \approx \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}$$

gives estimate of truncation error in terms of integral estimates and stepsizes

- improved estimate of the integral:

$$I \approx I(h_2) + E(h_2) = I(h_2) + \frac{1}{(h_1/h_2)^2 - 1} [I(h_2) - I(h_1)]$$

- estimate has error  $O(h^4)$ , versus  $O(h^2)$  for trapezoidal rule

### Special case: halved intervals

- if  $h_2 = h_1/2$ , the Romberg formula simplifies to

$$I \approx \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1)$$

- forms the basis of Romberg integration tables

## Example

before, we evaluated

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

by single and multiple applications of the trapezoidal rule, obtaining:

segments	$h$	integral	$\varepsilon_t$ (%)
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
4	0.2	1.4848	9.5

use Richardson extrapolation with halved step ( $h_2 = h_1/2$ ),

$$I \approx \frac{4}{3} I(h/2) - \frac{1}{3} I(h)$$

to compute improved estimates of the integral

## Example

- **combine 1- and 2-segment results**

$$I \approx \frac{4}{3} (1.0688) - \frac{1}{3} (0.1728) = 1.367467$$

$$E_t = 1.640533 - 1.367467 = 0.273067 \quad (\varepsilon_t = 16.6\%)$$

- **combine 2- and 4-segment results**

$$I \approx \frac{4}{3} (1.4848) - \frac{1}{3} (1.0688) = 1.623467$$

$$E_t = 1.640533 - 1.623467 = 0.017067 \quad (\varepsilon_t = 1.0\%)$$

### Takeaway

- a single Richardson step boosts the order from  $O(h^2)$  (trapezoid) to  $O(h^4)$
- significant accuracy gains with no extra function evaluations beyond two trap. runs

## Romberg integration: higher-order error correction

- combine two  $O(h^4)$  results  $\Rightarrow O(h^6)$

$$I \approx \frac{16}{15}I_m - \frac{1}{15}I_l$$

- $I_m$  = more accurate estimate
- $I_l$  = less accurate estimate

- combine two  $O(h^6)$  results  $\Rightarrow O(h^8)$

$$I \approx \frac{64}{63}I_m - \frac{1}{63}I_l$$

### Example

- we used Richardson extrapolation to compute two integral estimates of  $O(h^4)$
- we can combine these estimates to compute an integral with  $O(h^6)$

$$I = \frac{16}{15}(1.623467) - \frac{1}{15}(1.367467) = 1.640533$$

exact to seven significant figures

## Romberg integration: general algorithm

$$I_{j,k} \approx \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

- $I_{j,k}$  = improved integral
- $k$  = level of accuracy ( $k = 1$ : original trapezoid  $O(h^2)$ ,  $k = 2$ :  $O(h^4)$ , ...)
- $j$  = index distinguishing more ( $j + 1$ ) and less ( $j$ ) accurate integrals

**Stopping criterion:**

$$|\varepsilon_a| = \left| \frac{I_{1,k} - I_{2,k-1}}{I_{1,k}} \right| \times 100\%$$

terminate when  $|\varepsilon_a| < \varepsilon_s$

**Interpretation**

- each iteration adds one trapezoidal estimate
- successively better integrals appear along the lower diagonal

## Graphical depiction of Romberg integration

Trapezoid

	$k = 1$ $O(h^2)$	$k = 2$ $O(h^4)$	$k = 3$ $O(h^6)$	$k = 4$ $O(h^8)$	$k = 5$ $O(h^{10})$
$h$	$I_{1,1}$	$I_{1,2}$	$I_{1,3}$	$I_{1,4}$	$I_{1,5}$
$h/2$	$I_{2,1}$	$I_{2,2}$	$I_{2,3}$	$I_{2,4}$	
$h/4$	$I_{3,1}$	$I_{3,2}$	$I_{3,3}$		
$h/8$	$I_{4,1}$	$I_{4,2}$			
$h/16$	$I_{5,1}$				
	$\frac{4I_{j+1,1} - I_{j,1}}{3}$	$\frac{16I_{j+1,2} - I_{j,2}}{15}$	$\frac{64I_{j+1,3} - I_{j,3}}{63}$	$\frac{256I_{j+1,4} - I_{j,4}}{255}$	

the first column contains the trapezoidal rule evaluations that are designated  $I_{j,1}$

- $j = 1 \Rightarrow$  single-segment application (stepsize =  $b - a$ )
- $j = 2 \Rightarrow$  two-segment application (stepsize =  $\frac{b-a}{2}$ )
- $j = 3 \Rightarrow$  four-segment application (stepsize =  $\frac{b-a}{4}$ )
- and so forth

# Example

	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
(a)	0.172800 1.068800	1.367467		
(b)	0.172800 1.068800 1.484800	1.367467 1.623467	1.640533	
(c)	0.172800 1.068800 1.484800 1.600800	1.367467 1.623467 1.639467	1.640533 1.640533	1.640533

## References and further readings

- S. C. Chapra and R. P. Canale. *Numerical Methods for Engineers* (8th edition). McGraw Hill, 2021. (Ch.21, 22)
- S. C. Chapra. *Applied Numerical Methods with MATLAB for Engineers and Scientists* (5th edition). McGraw Hill, 2023. (Ch.19, 20)