8. Numerical integration

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

Derivatives

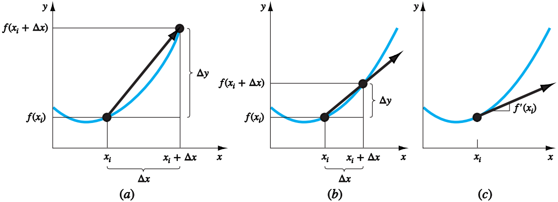
Difference approximation

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

Derivative

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

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

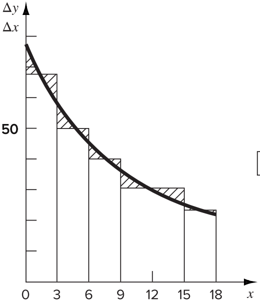


- *second derivative*: $\frac{d^2 y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right)$ measures how fast slope changes (*curvature*)

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

x	y	$\Delta y/\Delta x$
0	0	
		66.7
3	200	
		50
6	350	
		40
9	470	
		30
15	650	
		23.3
18	720	



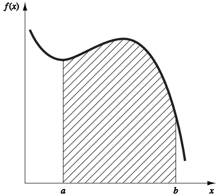
x	dy/dx
0	76.50
3	57.50
6	45.00
9	36.25
15	25.00
18	21.50

Integration

the inverse process to differentiation in calculus is **integration**

Integration

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



- $f(x)$ 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

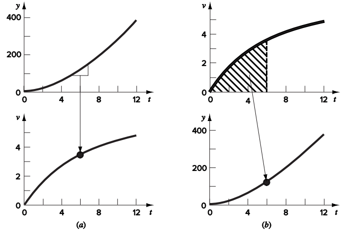
Relationship between differentiation and integration

differentiation and integration are inversely related processes

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

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

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



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 $y(b)$

Noncomputer methods for differentiation and integration

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

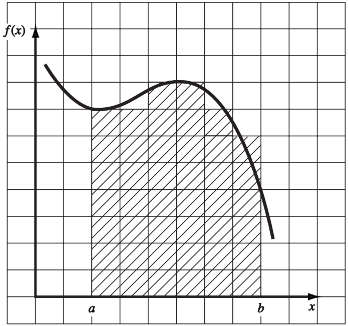
1. simple continuous function (polynomial, exponential, trigonometric)
2. complicated continuous function (difficult or impossible to handle analytically)
3. tabulated function, values given at discrete points (*e.g.*, experimental data)

Approaches

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

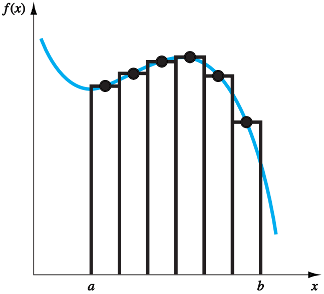
Graphical integration: grid method

- grid method: sum area of boxes under the curve
- finer grids $\longrightarrow$ improved estimates



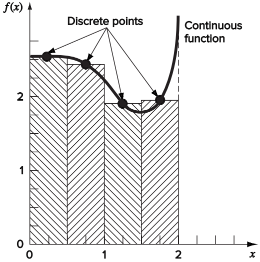
Graphical integration: strip method

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



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

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
- Romberg integration

Newton-cotes formulas

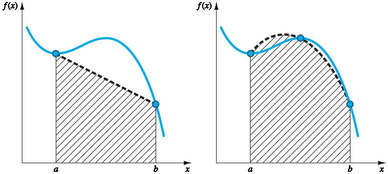
replace a complicated function or data with an approximating polynomial:

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

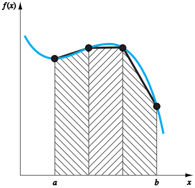
where $f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$

examples:

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



(a) (b)



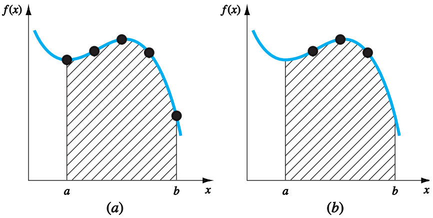
Closed and open Newton–Cotes formulas

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:

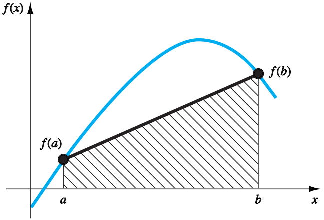
$$I = \int_a^b f(x)\,dx \approx \int_a^b f_1(x)\,dx$$

- 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**:

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

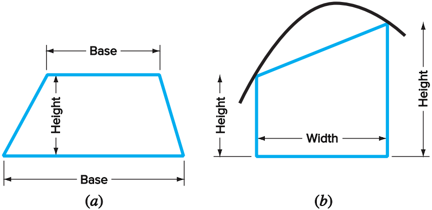


geometrically: $I \approx$ trapezoid area formed by straight line connecting $f(a)$, $f(b)$

Geometric interpretation of the trapezoidal rule

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

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

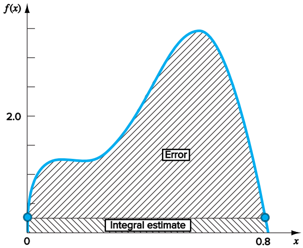


- in the trapezoidal rule, the trapezoid is rotated on its side, thus,

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

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
- for functions with nonzero second derivatives (curvature), error will occur
- the magnitude of the error depends on:
  - the size of the interval $(b-a)$ cubed
  - the curvature of the function, as reflected by $f''(\xi)$

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:

$$I \approx 0.8 \times \frac{0.2 + 0.232}{2} = 0.1728$$

- 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

- second derivative:

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

- average value:

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

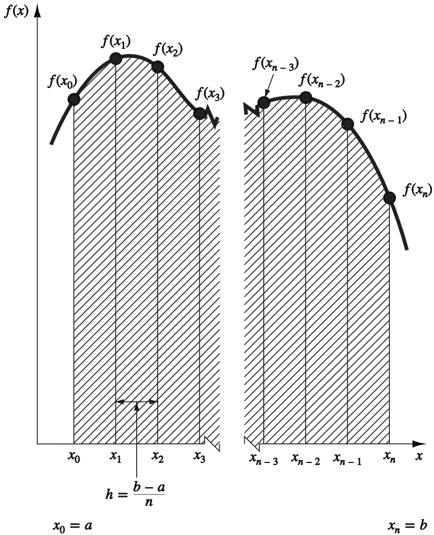
- approximate error:

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

  - 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



Multiple-application trapezoidal rule

- consider $n+1$ equally spaced base points $x_0, x_1, \ldots, x_n$ with step size $h = \frac{b-a}{n}$
- if a and b are designated as x_0 and x_n, 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

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

- grouping terms gives

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

Error of the multiple-application 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 ξ_i located in segment i

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

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

- 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

$$\int_0^{0.8} \left(0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5\right) dx, \quad \text{true value: } 1.640533$$

- $n = 2$, $h = 0.4$; function values:

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

- apply rule:

$$I = \frac{0.8}{4}\left[0.2 + 2(2.456) + 0.232\right] = 1.0688$$

- 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 $n = 2, \ldots, 10$, we get the result shown

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

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:

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

- 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

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

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

$$I = 0.12\frac{1.309729+0.2}{2} + 0.10\frac{1.305241+1.309729}{2} + \cdots + 0.10\frac{0.232+2.363}{2} = 1.594801$$

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

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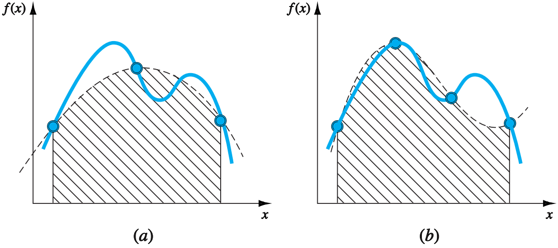
- Trapezoidal method
- **Simpson 1/3 & 3/8 rules**
- Romberg integration

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
- 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:

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

Simpson 1/3 rule: integrating yields

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

where $h = \dfrac{b-a}{2}$ (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

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

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

Example

evaluate

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

with true value $I_{\text{true}} = 1.640533$ and $f(0) = 0.2$, $f(0.4) = 2.456$, $f(0.8) = 0.232$

- Simpson 1/3 rule:

$$I \approx (0.8)\,\frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

- exact error:

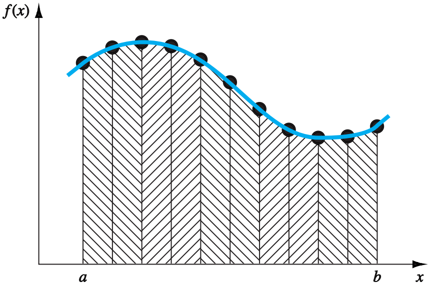
$$E_t = I_{\text{true}} - I = 1.640533 - 1.367467 = 0.2730667 \quad (\varepsilon_t = 16.6\%)$$

- estimated error

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

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

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

Multiple-application Simpson 1/3 rule

- applying Simpson 1/3 rule to each subinterval:

$$I \approx \frac{2h}{6}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{2h}{6}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$
$$+ \cdots + \frac{2h}{6}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

- combining terms and using $h = \frac{b-a}{n}$ yields

$$I \approx \frac{b-a}{3n}\left[f(x_0) + 4\sum_{\substack{i=1 \\ i \text{ odd}}}^{n-1} f(x_i) + 2\sum_{\substack{j=2 \\ j \text{ even}}}^{n-2} f(x_j) + f(x_n)\right]$$

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

Error of multiple-application Simpson 1/3 rule

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

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

where

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

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

- error decreases much faster than trapezoidal rule:
  - trapezoidal: $E \sim \mathcal{O}(n^{-2})$
  - Simpson 1/3: $E \sim \mathcal{O}(n^{-4})$

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 value: 1.640533

- for $n = 4$ ($h = 0.2$):

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

- hence,

$$I = \tfrac{0.8}{12}\,[\,0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232\,] = 1.623467$$

- true error and estimated error:

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

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

Simpson 3/8 rule

- a third-order Lagrange polynomial is fit to four points (3 segments):

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

- resulting formula:

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

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

- truncation error:

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

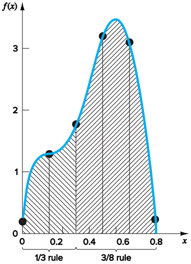
  slightly more accurate than Simpson 1/3 rule, but requires 4 points

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, but has special utility:
  - useful when the number of segments is odd

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

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



Example

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 ($h = \frac{0.8}{3} = 0.2667$)

$$f(0) = 0.2, \quad f(0.2667) = 1.432724,$$
$$f(0.5333) = 3.487177, \quad f(0.8) = 0.232$$

yields

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

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

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

Example

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

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

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

$$I = I_1 + I_2 = 0.380324 + 1.264754 = 1.645077$$
$$E_t = 1.640533 - 1.645077 = -0.004544 \quad (\varepsilon_t = -0.28\%)$$

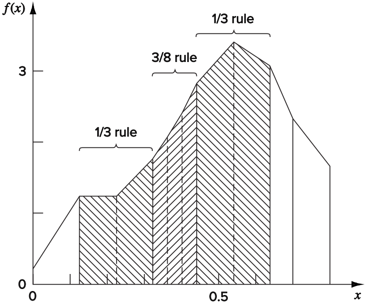
Example: combination of methods for uneven data

using Simpson rules where appropriate integrate

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

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		



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: Simpson $3/8$ rule $I_3 = 0.2727$
- two segments from $x = 0.44$ 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 step sizes to accelerate convergence

Richardson extrapolation

- suppose trapezoidal rule estimate is

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

  - $I(h)$ = the approximation from an n-segment application of the trapezoidal rule
  - $E(h)$ = the truncation error

- for two estimates with step sizes h_1 and h_2:

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

  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 step sizes

- 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

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

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

segments	h	integral	ε_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 $\Rightarrow$ $O(h^8)$

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

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

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

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

Example

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

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)