8. Numerical integration

- differentiation and integration

- Newton-Cotes integration

- Trapezoidal method

- Simpson 1/3 & 3/8 rules

- Romberg integration

Derivatives
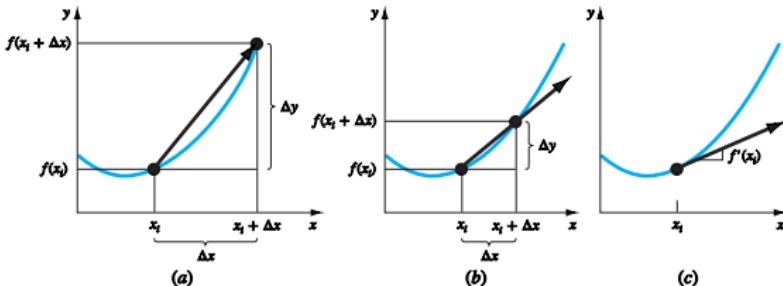
Difference approximation

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

Derivative

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$
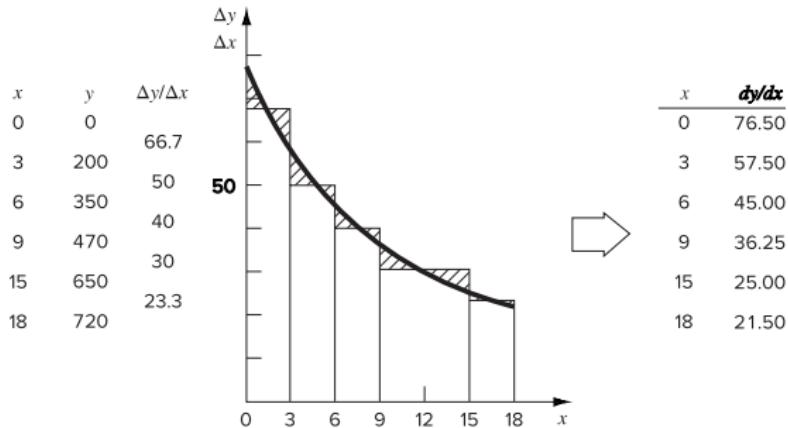
- $\frac{dy}{dx}$ (also y' or $f'(x_i)$) is the slope of the tangent to the curve at x_i

- *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
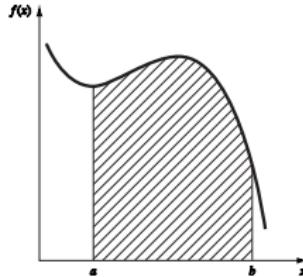
- compute divided differences $\Delta y / \Delta x$

- 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

Integration: the inverse process to differentiation written as

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

- $f(x)$ is the *integrand*
- $\int$ is a stylized $\mathcal{S}$ 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
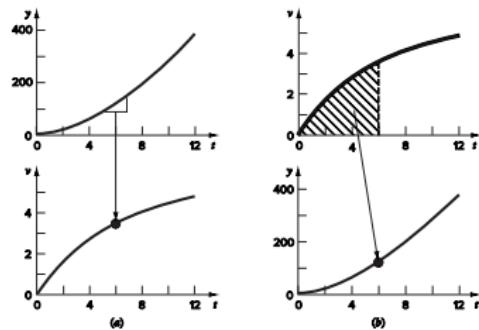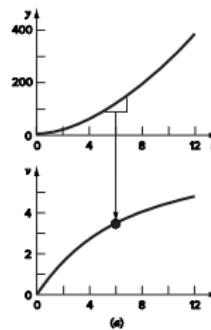
$$\frac{dy}{dx} = f(x), \quad y(a) = 0$$

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:
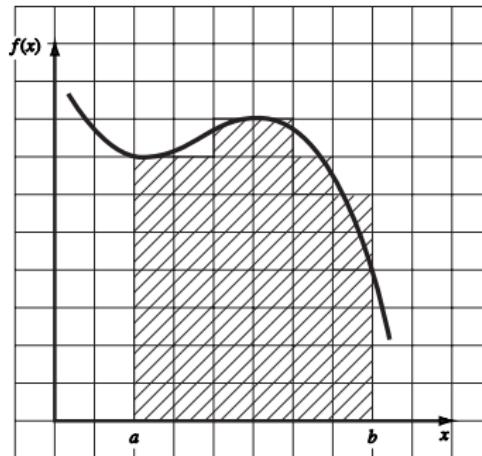
1. simple continuous function (polynomial, exponential, trigonometric)

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
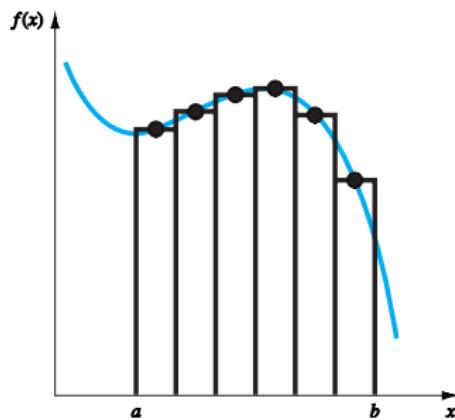
Graphical integration: grid method

- grid method: sum area of boxes under the curve

- finer grids → improved estimates
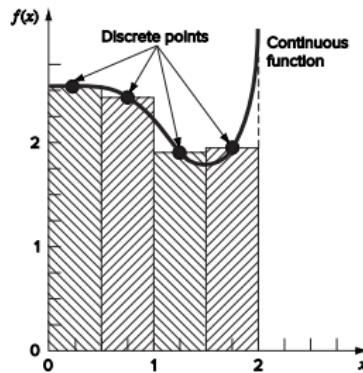
Graphical integration: strip method

- 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
- Romberg integration

Newton-cotes formulas
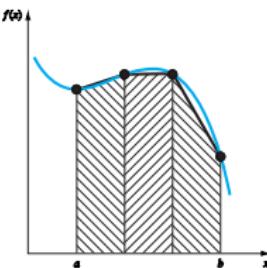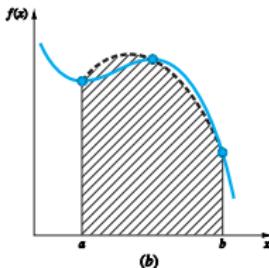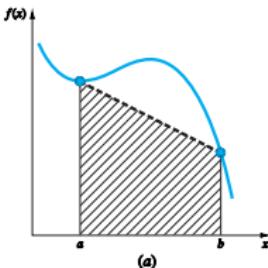
replace a complicated function or data with an approximating polynomial:

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

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 (trapezoidal rule)
- second-order polynomial: parabola (Simpson rule)
- straight line segments (composite trapezoidal rule)
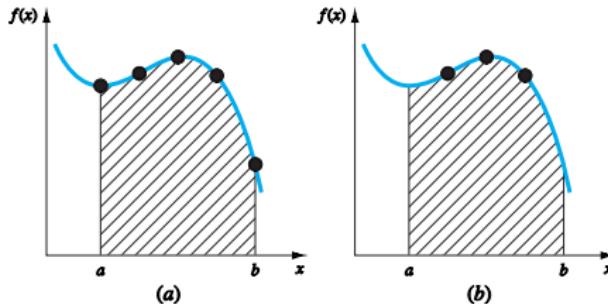
Closed and open Newton–Cotes formulas

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

Outline

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

Trapezoidal rule

- use a first-order polynomial as the approximation:
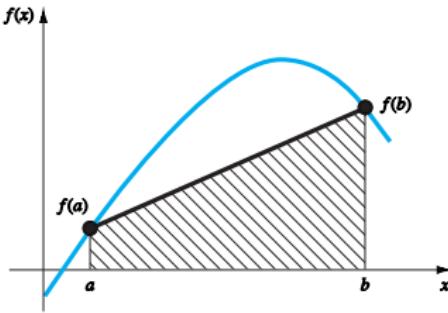
$$I = \int_a^b f(x)\, dx \approx \int_a^b f_1(x)\, dx$$

- 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**:

$$I_{\text{trap}} = (b - a)\,\frac{f(a) + f(b)}{2}$$
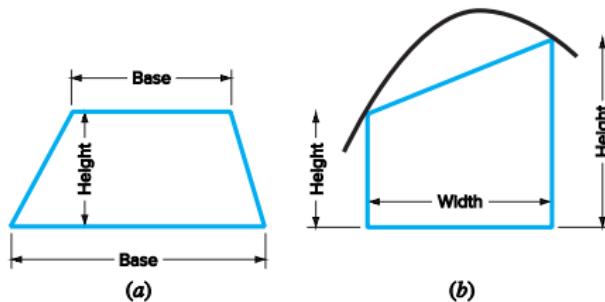
Geometric interpretation of the trapezoidal rule

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

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

(a) (b)
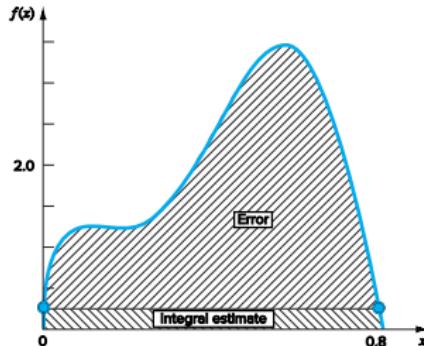
- in the trapezoidal rule, the trapezoid is rotated on its side, thus,

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

Error of the trapezoidal rule

error can be substantial

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

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

- 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:

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

Trapezoidal method

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:

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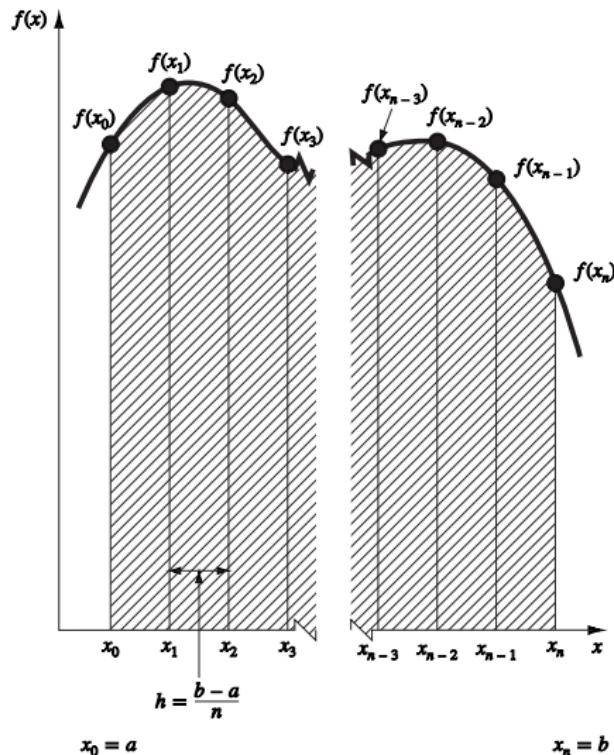
- approximate error:

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

  - 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

Composite trapezoidal rule

- consider $n + 1$ *equally spaced* base points $x_0, x_1, \ldots, x_n$ 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

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

- grouping terms gives the *composite trapezoidal rule:*

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

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 ξ_i located in segment i

- result can be simplified by estimating the mean or value of second derivative

- for the entire interval as:

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

- 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

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

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

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

- apply rule:

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

- 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_{trap}	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:

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

- 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

$$I_{\text{trap}} = 0.12\frac{1.309729+0.2}{2} + 0.10\frac{1.305241+1.309729}{2} + \cdots + 0.10\frac{0.232+2.363}{2} = 1.594801$$
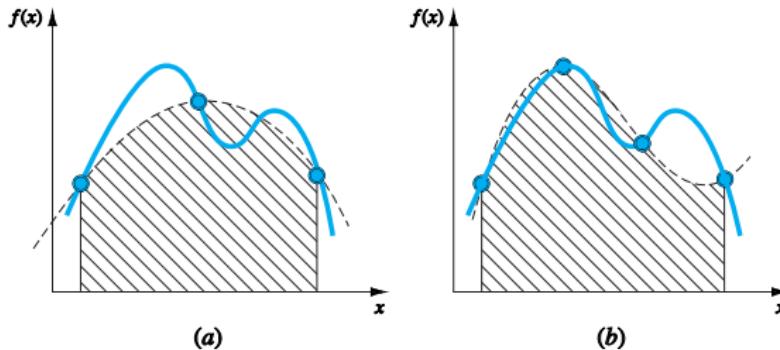
with error $\varepsilon_t = \frac{1.640533-1.594801}{1.640533} \times 100\% = 2.8\%$

Outline

- differentiation and integration

- Newton-Cotes integration

- 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

(a) (b)

- 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

$$I_{1/3} = (b - a)\, \frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$$

$$= \frac{h}{3}\, [f(x_0) + 4f(x_1) + f(x_2)]$$

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

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

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

Example

approximate

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

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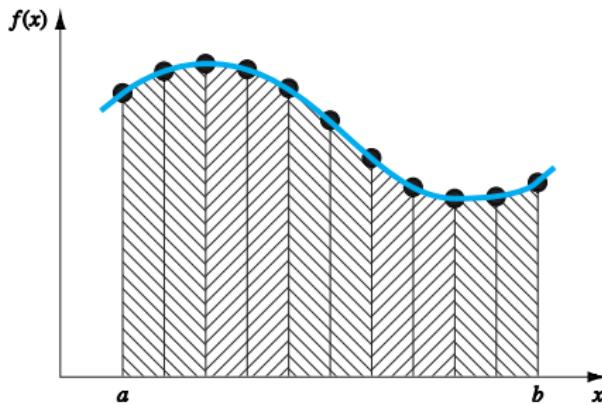
$$E_t = I - I_{1/3} = 1.640533 - 1.367467 = 0.2730667 \quad (\varepsilon_t = 16.6\%)$$

- 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:

$$I_{1/3} = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$

$$+ \cdots + \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

- combining terms and yields

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

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,

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

- 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

- 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:

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

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

- truncation error:

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480}f^{(4)}(\xi), \quad E_a = -\frac{(b-a)^5}{6480}\bar{f}^{(4)}$$
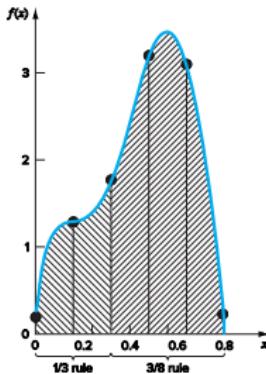
  slightly more accurate than Simpson 1/3 rule, but requires 4 points

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 ($h = \frac{0.8-0}{3} = 0.2667$)

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

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 ($h = \frac{0.8-0}{5} = 0.16$)

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

First two segments (Simpson 1/3 rule)

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

Last three segments (Simpson 3/8 rule)

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

Total integral

$$I_{\text{total}} = I_1 + I_2 = 0.380324 + 1.264754 = 1.645077$$
$$E_t = 1.640533 - 1.645077 = -0.004544 \quad (\varepsilon_t = -0.28\%)$$
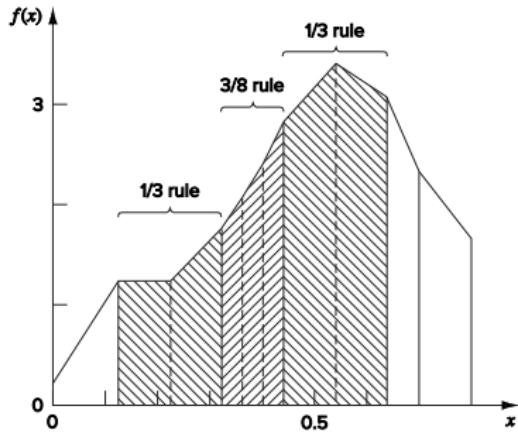
Example: combination of methods for uneven data

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:

$$I_{\text{total}} = I_1 + I_2 + I_3 + I_4 + I_5 = 1.603641 \quad \Rightarrow \quad \varepsilon_t = 2.2\%$$

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

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

  - $I(h)$ = 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:

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

- 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 $\implies O(h^6)$

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

  - I_m = more accurate estimate

  - I_l = less accurate estimate

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

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

Example

- we used Richardson extrapolation to compute two integral estimates of $O(h^4)$

- we can combine these estimates to compute an integral with $O(h^6)$

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

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 with $k = 1$: $I_{j,1}$ original trapezoid $O(h^2)$
- j = index distinguishing more $(j + 1)$ and less (j) accurate integrals
- $k \geq 2$ level of accuracy ($k = 2$: $O(h^4)$, $k = 3$: $O(h^6)$, ...)

Stopping criterion: terminate when

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

Interpretation

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

Graphical depiction of Romberg integration

Trapezoid

	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$
	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$	$O(h^{10})$
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 $I_{j,1}$

- $j=1 \implies$ single-segment application (stepsize $= b-a$)

- $j=2 \implies$ two-segment application (stepsize $= \frac{b-a}{2}$)

- $j=3 \implies$ four-segment application (stepsize $= \frac{b-a}{4}$)

- and so forth

Example

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

	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
(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)