

UNIT 3

Numerical Differentiation and Integration

(5 Hours) — Numerical Methods (CACS252)

3.1 Introduction to Numerical Differentiation

Numerical differentiation estimates $f'(x)$, $f''(x)$, ... from a table of values of f , or when f is known but too complicated to differentiate analytically. The basic idea is: **fit an interpolating polynomial to the data and differentiate the polynomial**. Differentiation is an *ill-conditioned* process: small errors in the data (or a very small step h) can produce large errors in the derivative, because differences of nearly equal numbers are divided by a small h .

3.1.1 Basic Difference Formulas

From the Taylor series $f(x + h) = f(x) + h f'(x) + (h^2/2) f''(x) + (h^3/6) f'''(x) + \dots$ we obtain:

Formula	Expression	Error
Forward difference	$f'(x) \approx [f(x + h) - f(x)] / h$	$O(h)$
Backward difference	$f'(x) \approx [f(x) - f(x - h)] / h$	$O(h)$
Central difference	$f'(x) \approx [f(x + h) - f(x - h)] / (2h)$	$O(h^2)$
Central, 2nd derivative	$f''(x) \approx [f(x + h) - 2f(x) + f(x - h)] / h^2$	$O(h^2)$

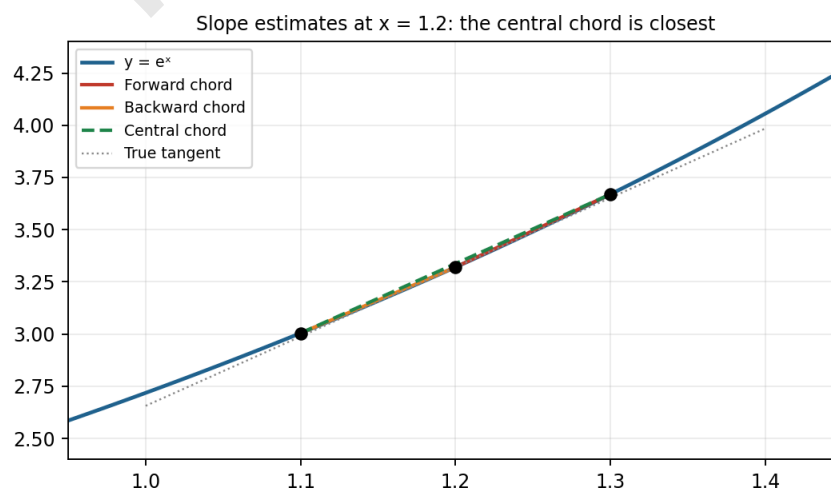


Figure 3.1 — Forward, backward and central chords approximating the tangent slope of $y = e^x$ at $x = 1.2$.

3.2 Newton's Differentiation Formulas

Differentiating Newton's forward interpolation formula $y = y_0 + p\Delta y_0 + [p(p-1)/2!]\Delta^2 y_0 + \dots$ with respect to x , where $p = (x - x_0)/h$ and $dp/dx = 1/h$, gives

$$dy/dx = (1/h) [\Delta y_0 + (2p-1)/2 \cdot \Delta^2 y_0 + (3p^2 - 6p + 2)/6 \cdot \Delta^3 y_0 + (4p^3 - 18p^2 + 22p - 6)/24 \cdot \Delta^4 y_0 + \dots]$$

$$d^2y/dx^2 = (1/h^2) [\Delta^2 y_0 + (p-1) \Delta^3 y_0 + (6p^2 - 18p + 11)/12 \cdot \Delta^4 y_0 + \dots]$$

At a tabulated point $x = x_0$ ($p = 0$) these simplify to

$$y'(x_0) = (1/h) [\Delta y_0 - \Delta^2 y_0/2 + \Delta^3 y_0/3 - \Delta^4 y_0/4 + \dots]$$

$$y''(x_0) = (1/h^2) [\Delta^2 y_0 - \Delta^3 y_0 + (11/12) \Delta^4 y_0 - \dots]$$

Similarly, from Newton's backward formula ($p = (x - x_n)/h$), at the last tabulated point $x = x_n$:

$$y'(x_n) = (1/h) [\nabla y_n + \nabla^2 y_n/2 + \nabla^3 y_n/3 + \nabla^4 y_n/4 + \dots]$$

$$y''(x_n) = (1/h^2) [\nabla^2 y_n + \nabla^3 y_n + (11/12) \nabla^4 y_n + \dots]$$

Note: Use the forward formula near the start of the table, the backward formula near the end, and central-difference formulas (or Stirling's formula) near the middle. For a non-tabulated point keep p in the general formula.

Example 3.1

The table gives $y = e^x$ (5 d.p.). Find $y'(1.0)$, $y''(1.0)$ by the forward formula and $y'(1.4)$ by the backward formula. Compare with the exact values.

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
1.0	2.71828	0.28589	0.03006	0.00317	0.00032
1.1	3.00417	0.31595	0.03323	0.00349	
1.2	3.32012	0.34918	0.03672		
1.3	3.66930	0.38590			
1.4	4.05520				

Solution

$h = 0.1$, $x_0 = 1.0$ (forward) and $x_n = 1.4$ (backward).

$$y'(1.0) = (1/0.1)[0.28589 - (0.03006)/2 + (0.00317)/3 - (0.00032)/4] = 2.7184 \text{ (exact } e^1 = 2.7183)$$

$$y''(1.0) = (1/0.01)[0.03006 - 0.00317 + (11/12)(0.00032)] = 2.7183 \text{ (exact } = 2.7183)$$

$$y'(1.4) = (1/0.1)[0.38590 + (0.03672)/2 + (0.00349)/3 + (0.00032)/4] = 4.0550 \text{ (exact } e^{1.4} = 4.0552)$$

Example 3.2 — Simple difference formulas

Using the same table ($h = 0.1$), estimate $y'(1.2)$ and $y''(1.2)$ with forward, backward and central differences.

Solution

Forward: $[y(1.3) - y(1.2)]/0.1 = (3.66930 - 3.32012)/0.1 = 3.4918$

Backward: $[y(1.2) - y(1.1)]/0.1 = (3.32012 - 3.00417)/0.1 = 3.1595$

Central: $[y(1.3) - y(1.1)]/0.2 = (3.66930 - 3.00417)/0.2 = 3.3256$

$$y''(1.2) \approx [y(1.3) - 2y(1.2) + y(1.1)]/0.01 = 3.3230$$

Exact: $y' = y'' = e^{1.2} = 3.3201$. The central difference (error 0.0055) is much more accurate than the one-sided ones (errors 0.1717 and 0.1606).

3.3 Numerical Integration

Numerical integration (*quadrature*) approximates the definite integral $I = \int_a^b f(x) dx$ from a to b when an antiderivative is unavailable or f is given only as a table. We replace f by an interpolating polynomial on equally spaced nodes $x_i = a + i \cdot h$, $h = (b - a)/n$, whose integral is easy. This gives the **Newton–Cotes** formulas.

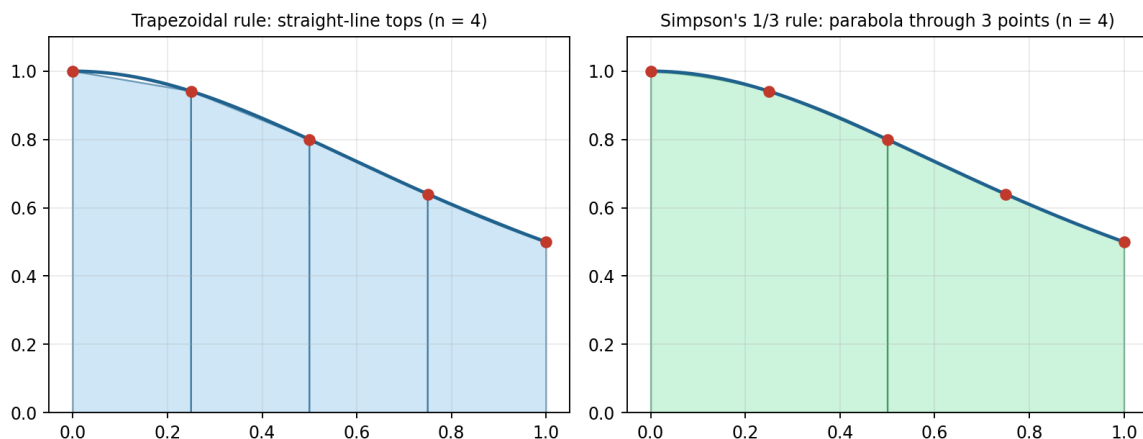


Figure 3.2 — Trapezoidal rule (left) and Simpson's 1/3 rule (right) on $f(x) = 1/(1 + x^2)$, $n = 4$.

3.3.1 Trapezoidal Rule

Replace f on each sub-interval by a straight line (degree-1 polynomial). The composite rule for n sub-intervals is

$$I \approx (h/2) [y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]$$

Error: $E = -[(b-a)/12] h^2 f''(\xi)$, so the rule is $O(h^2)$ and is exact for polynomials of degree ≤ 1 . It can be used with any number n of sub-intervals.

3.3.2 Simpson's 1/3 Rule

Replace f on each *pair* of sub-intervals by a parabola through three points. It requires an **even** n :

$$I \approx (h/3) [y_0 + 4(y_1 + y_3 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2}) + y_n]$$

Error: $E = -[(b-a)/180] h^4 f'''(\xi)$, so the rule is $O(h^4)$ and is exact for polynomials up to degree 3.

3.3.3 Simpson's 3/8 Rule

Uses a cubic through four points on each group of three sub-intervals. It requires n to be a **multiple of 3**:

$$I \approx (3h/8) [y_0 + 3(y_1 + y_2 + y_4 + y_5 + \cdots) + 2(y_3 + y_6 + \cdots) + y_n]$$

Error: $E = -[(b-a)/80] h^4 f'''(\xi)$; also exact for cubics. Its error constant is larger than that of the 1/3 rule, so the 1/3 rule is preferred when n is even; the 3/8 rule is used when n is a multiple of 3 (for example to finish an odd number of intervals).

Rule	n must be	Weights (pattern)	Error order
Trapezoidal	any $n \geq 1$	1, 2, 2, ..., 2, $1 \times h/2$	$O(h^2)$
Simpson's 1/3	even	1, 4, 2, 4, ..., 4, $1 \times h/3$	$O(h^4)$
Simpson's 3/8	multiple of 3	1, 3, 3, 2, 3, 3, 2, ..., 3, 3, $1 \times 3h/8$	$O(h^4)$

Example 3.3

Evaluate $I = \int_0^1 dx/(1+x^2)$ with $n = 6$ ($h = 1/6$) by the trapezoidal, Simpson's 1/3 and Simpson's 3/8 rules. The exact value is $\pi/4 = 0.785398$.

i	x_i	$y_i = 1/(1+x_i^2)$
0	0.0000	1.000000

i	x_i	$y_i = 1/(1 + x_i^2)$
1	0.1667	0.972973
2	0.3333	0.900000
3	0.5000	0.800000
4	0.6667	0.692308
5	0.8333	0.590164
6	1.0000	0.500000

Solution

Trapezoidal: $(h/2)[y_0 + 2(y_1 + \dots + y_5) + y_6] = (1/12)[1.000000 + 2(3.955445) + 0.500000] = 0.784241$

Simpson 1/3: $(h/3)[y_0 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4) + y_6] = (1/18)[1.000000 + 4(2.363137) + 2(1.592308) + 0.500000] = 0.785398$

Simpson 3/8: $(3h/8)[y_0 + 3(y_1 + y_2 + y_4 + y_5) + 2y_3 + y_6] = (1/16)[1.000000 + 3(3.155445) + 2(0.800000) + 0.500000] = 0.785396$

Rule	Value	Absolute error
Trapezoidal	0.784241	1157×10^{-6}
Simpson's 1/3	0.785398	0.2×10^{-6}
Simpson's 3/8	0.785396	2.3×10^{-6}
Exact ($\pi/4$)	0.785398	—

Note: Simpson's rules are far more accurate than the trapezoidal rule for the same number of function values, and the 1/3 rule beats the 3/8 rule here.

3.4 Romberg Integration

Romberg integration applies **Richardson extrapolation** to the trapezoidal rule. First compute trapezoidal estimates $R(k, 0)$ with step sizes $h, h/2, h/4, \dots$ (the number of sub-intervals doubles each time, and the previous function values are reused):

$$R(k, 0) = \frac{1}{2} R(k-1, 0) + h_k \sum f(a + (2i-1)h_k), \quad h_k = (b-a)/2^k$$

Then improve them by extrapolation, eliminating the leading error terms $h^2, h^4, h^6, \dots$:

$$R(k, j) = [4^j \cdot R(k, j-1) - R(k-1, j-1)] / (4^j - 1), \quad j = 1, 2, \dots$$

The first extrapolated column ($j = 1$) is Simpson's 1/3 rule and the second column ($j = 2$) is Boole's rule. Stop when two successive diagonal entries agree to the required accuracy.

Example 3.4

Use Romberg integration to evaluate $\int_0^1 dx/(1+x^2)$ ($h = 1, 1/2, 1/4, 1/8$). Exact value: 0.785398.

Step	T ($j = 0$)	$j = 1$ (Simpson)	$j = 2$ (Boole)	$j = 3$
$h = 1$	0.750000			
$h = 1/2$	0.775000	0.783333		
$h = 1/4$	0.782794	0.785392	0.785529	
$h = 1/8$	0.784747	0.785398	0.785399	0.785396

Solution

$$R(0,0) = (1/2)[f(0) + f(1)] = (1/2)(1 + 0.5) = 0.750000$$

$$R(1,1) = [4R(1,0) - R(0,0)]/3 = [4(0.775000) - 0.750000]/3 = 0.783333$$

$$R(2,2) = [16R(2,1) - R(1,1)]/15 = 0.785529; R(3,3) = [64R(3,2) - R(2,2)]/63 = 0.785396$$

The best estimate is $R(3,3) = 0.785396$; exact $\pi/4 = 0.785398$, so the error is only 1.7×10^{-6} (5 correct decimals), compared with 651×10^{-6} for the plain trapezoidal value $R(3,0) = 0.784747$.

3.5 Numerical Double Integration

To evaluate $I = \iint f(x, y) dy dx$ over a rectangle $[a, b] \times [c, d]$, divide $[a, b]$ into n sub-intervals of width h and $[c, d]$ into m sub-intervals of width k , and apply a one-dimensional rule in each direction (an “iterated” rule). The result is a weighted sum of the function values on the grid:

$$I \approx \sum_i \sum_j w_i v_j f(x_i, y_j) \times (\text{scale factor})$$

- **Trapezoidal:** $I \approx (hk/4) \sum W_{ij} f_{ij}$, where the weight of a grid point is the product of the 1-D weights (1, 2, 2, ..., 2, 1): corner points get 1, edge points 2, interior points 4.
- **Simpson's 1/3:** $I \approx (hk/9) \sum W_{ij} f_{ij}$, with 1-D weights (1, 4, 2, 4, ..., 4, 1); for a 3×3 grid the weights are corners 1, edge mid-points 4, centre 16.

Example 3.5

Evaluate $I = \int_1^2 \int_1^2 dx dy / (x + y)$ by the trapezoidal and Simpson's 1/3 rules with $h = k = 0.5$, and compare with Simpson's rule using $h = k = 0.25$. The exact value is 0.339798.

$y \setminus x$	$x = 1.0$	$x = 1.5$	$x = 2.0$
$y = 1.0$	0.500000	0.400000	0.333333
$y = 1.5$	0.400000	0.333333	0.285714
$y = 2.0$	0.333333	0.285714	0.250000

Solution

Trapezoidal ($hk/4 = 0.0625$, weights 1-2-1 / 2-4-2 / 1-2-1): $I \approx 0.343304$

Simpson ($hk/9 = 0.027778$, weights 1-4-1 / 4-16-4 / 1-4-1): $I \approx 0.339881$

Simpson with $h = k = 0.25$ (5×5 grid): $I \approx 0.339804$

Exact value: $I = 0.339798$. The errors are 0.003505, 0.000083 and 0.00000560 respectively.

Note: The cost grows quickly with dimension (a 2-D grid with n intervals per direction needs $(n + 1)^2$ function values), so for higher dimensions Monte-Carlo methods are usually preferred.

Key Takeaways — Unit 3

- ✓ Numerical differentiation differentiates an interpolating polynomial; it is sensitive to data errors and to very small h .
- ✓ Forward and backward differences have error $O(h)$; the central difference $[f(x+h) - f(x-h)]/2h$ has error $O(h^2)$.
- ✓ Newton's formulas at a tabulated point: $y' = (1/h)[\Delta y_0 - \Delta^2 y_0/2 + \Delta^3 y_0/3 - \dots]$, $y'' = (1/h^2)[\Delta^2 y_0 - \Delta^3 y_0 + (11/12)\Delta^4 y_0 - \dots]$.
- ✓ Trapezoidal: $(h/2)[y_0 + 2\Sigma + y_n]$; Simpson 1/3 (n even): $(h/3)[y_0 + 4\Sigma_{\text{odd}} + 2\Sigma_{\text{even}} + y_n]$; Simpson 3/8 (n multiple of 3): $(3h/8)[\dots]$.
- ✓ Errors: trapezoidal $O(h^2)$; Simpson's rules $O(h^4)$.
- ✓ Romberg: $R(k, j) = [4^j R(k, j-1) - R(k-1, j-1)]/(4^j - 1)$ — extrapolation of trapezoidal results.
- ✓ Double integrals: apply the 1-D rule in both directions using product weights on the grid.

— End of Unit 3 —