Numerical Differentiation and Integration

Tutorial homework question: 12c.

H By Hand; **C** Computer; **T** Theory; **E** Extra; **A** Advanced.

Recommended: H1.b; H2.a; C3; T4; C6.a; H7.a; H8.a; H10.a; C12.b.

Differentition

H1. Use the most accurate three-point formula to determine $f'(x)$ and $f''(x)$ at each data point in the following tables:

a.

x	$f(x)$
0.9	7.91
1.0	9.91
1.1	12.35
1.2	15.33

b.

x	$f(x)$
4.3	−5.71
4.5	−6.33
4.7	−6.96
4.9	−7.59

c.

x	$f(x)$
2.5	3.939
2.75	3.351
3.0	2.608
3.25	1.708
3.5	1.216

H2. Use the five-point differentiation formulae to determine, as accurately as possible, approximations for $f'(x)$ at each data point in the following tables:

a.

x	$f(x)$
3.0	0.2902
3.25	0.6262
3.5	0.8808
3.75	1.0840
4.0	1.2530

b.

x	$f(x)$
−2.0	8.1333
−1.8	6.9987
−1.6	5.9458
−1.4	4.9748
−1.2	4.0858
−1.0	3.2789

C3. Estimate the first derivative of $f(x) = 1/(3 - 2x^2)$ at $x = 1$ using (i) the three-point centred-difference formula, the (ii) three-point forward difference formula, and (iii) the five-point centred difference formula, and the second derivative at $x = 1$ using (iv) the three-point fomulae and (v) the five-point centred formula. Use $h = 10^{-n}$ for $n = 0, 1, \ldots, 12$. Compute the errors in the approximations and verify the order of each method.

T4. Let ϵ denote a bound on the total error made in evaluating a function f, and M denotes a bound for the third derivative of f. Show that the total error in estimating $f'(x)$ using the three-point centred-difference formula is

$$e(h) = \frac{\epsilon}{h} + \frac{h^2}{6}M.$$

Which value of h should you choose to minimise the error?

A5. Show that if f is 5-times continuously differentiable, then

$$f'(x) = \frac{-3f(x-h) - 10f(x) + 18f(x+h) - 6f(x+2h) + f(x+3h)}{12h} - \frac{h^4}{20}f^{(5)}(\xi)$$

for some ξ between $x - h$ and $x + 3h$.

Show that if f is 6-times continuously differentiable, then

$$f''(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} - \frac{h^4}{90}f^{(6)}(\xi)$$

for some ξ between $x - 2h$ and $x + 2h$.

Use these formula to find better estimates to $f'(x)$ for the data entries next to the endpoints in Question 2, and to estimate the second derivatives.

Note: Other five-point second-derivative formulae are

$$f''(x) = \frac{11f(x-h) - 20f(x) + 6f(x+h) + 4f(x+2h) - f(x+3h)}{12h^2} - \frac{19}{360}\,h^4 f^{(6)}(\xi)$$
$$f''(x) = \frac{35f(x) - 104f(x+h) + 114f(x+2h) - 56f(x+3h) + 11f(x+4h)}{12h^2} - \frac{119}{90}\,h^4 f^{(6)}(\xi)$$

Integration

C6. Use Matlab's built-in `integral` command to evaluate the following integrals:

a. $\displaystyle\int_0^1 e^{-x^2/2}\,dx$ **b.** $\displaystyle\int_0^3 \frac{\sin x}{x}\,dx$

H7. Use (i) the midpoint rule, (ii) the trapezoidal rule and (iii) Simpson's rule with the indicated values of n, or the indicated h to approximate the following integrals.

a. $\displaystyle\int_1^3 x\log x\,dx, \quad n=4$ **b.** $\displaystyle\int_0^2 \frac{1}{x^2+9}\,dx, \quad h=\frac{1}{3}$

c. $\displaystyle\int_0^1 e^{-x^2/2}\,dx, \quad n=8$ **d.** $\displaystyle\int_0^3 \frac{\sin x}{x}\,dx \quad h=0.5$

Note: Take $\sin(0)/0 = \lim_{h\to 0}\sin(h)/h = 1$.

H8. Compute the Romburg integral $R_{3,3}$ approximating

a. $\displaystyle\int_1^3 x\log x\,dx$ **b.** $\displaystyle\int_0^2 e^{-x^2}\,dx$

Compare your answers with those obtained previously by using Simpson's rule, and explain any correspondences between your results.

H9. The following data (x, y) are arise from the function $y = f(x)$.

x	1.4	1.6	1.8	2.0	2.2	2.4	2.6
y	2.2575	2.8773	3.1409	3.0833	3.0592	3.0391	3.3111

Approximate $\int_{1.4}^{2.6} f(x)\,dx$ as accurately as possible using (i) the midpoint rule, (ii) the trapezoidal rule and (iii) Simpson's rule.

H10. Use (i) the midpoint rule, (ii) the trapezoidal rule, and (iii) Simpson's rule to approximate the integrals

a. $\displaystyle\int_2^3 x^3\,dx$ **b.** $\displaystyle\int_1^3 x\log x\,dx$

Use $n=1$, $n=2$ and $n=4$ for the midpoint and trapezoidal rules, and $n=2$ and $n=4$ for Simpson's rule. Compare your results with the exact values (a) $65/4$ and (b) $\frac{9}{2}\log 3 - 2$.

How do your results correspond to what you would expect given the order of the methods?

A11. Use the error formula to find a bound for the error for each integral in Question 10, and compare the bound to the actual error.

H12. For each of the data in Question 1, use your finite-difference estimates of $f'(x_i)$ and the trapezoid rule to estimate $\int_{x_0}^{x_m} \sqrt{1+f'(x)^2}\,dx$, where x_0 is the first data point and x_m the last.

C13. Write Matlab functions to approximate $\int_a^b f(x)\,dx$ using (i) the midpoint rule, (ii) the trapezoidal rule, (iii) Simpson's rule and (iv) Romburg integration with a given value of n. Test your code by computing the following integrals with the given values of n.

a. $\displaystyle\int_0^3 \frac{\sin x}{x}\,dx, \quad n = 8, 16$ **b.** $\displaystyle\int_0^1 e^{-x^2/2}\,dx, \quad n = 8, 16$ **c.** $\displaystyle\int_4^5 \frac{1}{\sqrt{x^2-9}}\,dx, \quad n = 8, 16$

Compare and comment on the number of function evaluations needed for the various methods to obtain a given accuracy.

A14. For the following integrals, compute the trapezoid rule approximations $T(f; [a, b])$, $T(f; [a, \frac{a+b}{2}])$ and $T(f; \frac{a+b}{2}, b])$, and verify the estimate given in the adaptive trapezoid error estimate.

a. $\displaystyle\int_0^{\sqrt{\pi/2}} x\sin(x^2)\,dx.$ **b.** $\displaystyle\int_{1/3\pi}^{1/\pi} \sin(1/x)\,dx.$

Use the adaptive trapezoid rule to find approximations to within 10^{-2} for the integrals.

A15. Write a Matlab function to estimate $\int_a^b f(x)\,dx$ with accuracy ϵ using an adaptive version of the composite trapezoid rule. Test your code by estimating the integrals below to accuracy 10^{-4}.

a. $\displaystyle\int_0^{\sqrt{3\pi}} x\sin(x^2)\,dx$ **b.** $\displaystyle\int_{1/3\pi}^{4/\pi} \sin(1/x)\,dx.$

For **a**, the exact answer is 1. What is the minimum value of n for which the trapezoid rule yields an approximation to within 10^{-4}? How does this compare with the number of nodes required for the adaptive trapezoid rule?

E16. In a multivariable calculus and in statistics courses, it is shown that

$$\int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}\,dx = 1$$

for any positive σ. The function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}$$

is the *normal density function* with *mean* $\mu = 0$ and *standard deviation* σ. The probability that a randomly chosen value described by this distribution lies in $[a, b]$ is given by $\int_a^b f(x)dx$. Approximate to within 10^{-5} the probability that a randomly chosen value described by this distribution will lie in $[-k\sigma, k\sigma]$ for $k = 1, \ldots, 5$.

E17. The study of light diffraction at a rectangular aperture involves the Fresnel integrals

$$c(t) = \int_0^t \cos(\tfrac{\pi}{2}w^2)\,dw \quad \text{and} \quad s(t) = \int_0^t \sin(\tfrac{\pi}{2}w^2)\,dw\,.$$

Construct a table of values for $c(t)$ and $s(t)$ that is accurate to within 10^{-4} for values of $t = 0.1, 0.2, \ldots, 1.0$.