Maths 3018/6111 - Numerical Methods

Worksheet 3 - Solutions

Theory

1. Apply Simpson's rule to compute
$$\int_0^{\pi/2} \cos(x)\, dx$$
using 3 points (so $h = \pi/4$) and 5 points (so $h = \pi/8$).

The exact solution is, of course, 1.

Simpson's rule (composite version) is

$$I = \frac{h}{3}\left[f(a) + f(b) + 2\sum_{j=1}^{N/2-1} f(x_{2j}) + 4\sum_{j=1}^{N/2} f(x_{2j-1} \right]$$

where we are using $N+1$ points with $x_0 = a$, $x_N = b$, equally spaced with grid spacing $h = (b-a)/N$.

With 3 points we have $N = 2$ and $h = (\pi/2)/2 = \pi/4$, and so we have nodes and samples given by

i	x_i	$f(x_i)$
0	0	1
1	$\pi/4$	$\frac{1}{\sqrt{2}}$
2	$\pi/2$	0

Using Simpsons rule we then get

$$\begin{aligned} I &= \frac{h}{3}\left[f_0 + f_2 + 4f_1\right] \\ &= \frac{\pi}{12}\left(1 + 2\sqrt{2}\right) \\ &\approx 1.0023. \end{aligned}$$

With 5 points we have $N = 4$ and $h = (\pi/2)/4 = \pi/8$, and so we have nodes and samples given by

i	x_i	$f(x_i)$
0	0	1
1	$\pi/8$	$\cos(\pi/8) \approx 0.9239$
2	$\pi/4$	$\frac{1}{\sqrt{2}}$
3	$3\pi/8$	$\cos(3\pi/8) \approx 0.3827$
4	$\pi/2$	0

Using Simpsons rule we then get

$$\begin{aligned} I &= \frac{h}{3}\left[f_0 + f_4 + 4(f_1 + f_3) + 2f_2\right] \\ &= \frac{\pi}{24}\left(1 + 4(\cos(\pi/8) + \cos(3\pi/8)) + \sqrt{2}\right) \\ &\approx 1.00013. \end{aligned}$$

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2. Apply Richardson extrapolation to the result above; does the answer improve?

Simpson's rule has order of accuracy 4. We note that we have just computed the result using 3 ($N = 2$) and 5 ($N = 4$) points. Richardson extrapolation gives the result

$$\begin{aligned} R_4 &= \frac{2^4 I_4 - I_2}{2^4 - 1} \\ &\approx 0.999992. \end{aligned}$$

We note that the error has gone from 2.3×10^{-3} for I_2 to 1.3×10^{-4} for I_4 and now to 8.4×10^{-6} for the Richardson extrapolation R_4, a good improvement.

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3. State the rate of convergence of the trapezoidal rule and Simpson's rule, and sketch (or explain in words) the proof.

For the trapezoidal rule the error converges as h^2. For Simpson's rule the error converges as h^4.

In both cases the proof takes a similar path. Consider the quadrature over a single subinterval. Taylor series expand the quadrature rule about a suitable point x_j (left edge for trapezoidal rule, centre for Simpson's rule) to get an expression for the quadrature of the interval in terms of h and the function f and its derivatives as evaluated at x_j.

Next write down the anti-derivative $F(t)$ of f for the interval as a function of the width of the interval t. This, when evaluated at $t = h$, is the exact solution for the quadrature of the subinterval. Taylor series expand F about $t = 0$ to get an expression for the exact result in terms of h and the function f and its derivatives as evaluated at x_j.

By comparing the two expressions we have a bound on the error in terms of h and derivatives of f. By summing over all intervals (note that at this stage we lose a power of h as we have N subintervals with $N \propto h^{-1}$) we can bound the global error in terms of h and the maximum value of a derivative of f.

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4. Explain in words adaptive and Gaussian quadrature, in particular the aims of each and the times when one or the other is more useful.

Adaptive quadrature uses any standard quadrature method and some error estimator, such as Richardson extrapolation, to place additional nodes wherever required to ensure that the error is less than some desired tolerance. Each subinterval is tested to ensure that its (appropriately weighted) contribution to the total error is sufficiently small. If it is not, the subinterval is further subdivided by introducing more nodes in a fashion appropriate for the quadrature method used. This is a straightforward way of getting high accuracy for low computational cost using standard quadrature algorithms.

Gaussian quadrature aims to get the best result for a *generic* function by allowing both the choice of nodes and weights to vary. The location of the nodes and the value of the weights is given by ensuring that the quadrature is exact for as many polynomials as possible; i.e., if we have N nodes (and hence N weights) we should be able to exactly integrate x^s for $0 \le s \le 2N - 1$. By introduing a weighting function we can also deal with integrands that are (mildly) singular at the boundaries of the domain, or unbounded domains. Provided the function can be evaluated anywhere this is an effective way of getting high accuracy with few function evaluations for most functions.

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5. [3018 only] Show how the speed of convergence of a nonlinear root finding method depends and the derivatives of the map $g(x)$ near the fixed point s.

We assume we are constructing an iterative sequence x_n where $x_{n+1} = g(x_n)$, and that the error at step n is $e_n = x_n - s$. Then if we assume that the step x_{n+1} is sufficiently close to the root s then we can write

$$\begin{aligned} e_{n+1} &= x_{n+1} - s \\ &= g(x_n) - g(s) \end{aligned}$$

using the definition of the sequence and the fixed point

$$= g'(s)(x_n - s) + \frac{g''(s)}{2!}(x_n - s)^2 + \mathcal{O}\left((x_n - s)^3\right)$$

by Taylor expanding

$$= g'(s)e_n + \frac{g''(s)}{2!}e_n^2 + \mathcal{O}\left(e_n^3\right).$$

Hence if $g'(s) \neq 0$ we have that the error reduces by a constant amount proportional to the derivative at each step. If the derivative does vanish the error at each iteration is proportional to the square of the previous error which leads to faster convergence.

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6. [3018 only] Use Newton's method to find the root in $[0, 1]$ of

$$f(x) = \sin(x) - e^x + 0.9 + x.$$

Start from $x_0 = 1/2$ and retain 3 significant figures. Take 3 steps.

For Newton's method we have

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

So first we compute the derivative,

$$f'(x) = \cos(x) - e^x + 1.$$

It follows that the iterative scheme is give by

$$x_{n+1} = x_n - \frac{\sin(x_n) - e^{x_n} + 0.9 + x_n}{\cos(x_n) - e^{x_n} + 1}.$$

We start from $x_0 = 1/2$ and compute with full precision but only retain 3 significant figures for the values of the x_n:

$$\begin{aligned} x_1 &= x_0 - \frac{\sin(x_0) - e^{x_0} + 0.9 + x_0}{\cos(x_0) - e^{x_0} + 1} \\ &\approx -0.508; \end{aligned}$$

retaining 3 s.f. we set $x_1 = -0.508$, and find

$$\begin{aligned} x_2 &= x_1 - \frac{\sin(x_1) - e^{x_1} + 0.9 + x_1}{\cos(x_1) - e^{x_1} + 1} \\ &\approx 0.0393; \end{aligned}$$

retaining 3 s.f. we set $x_2 = 0.0393$, and find

$$\begin{aligned} x_3 &= x_2 - \frac{\sin(x_2) - e^{x_2} + 0.9 + x_2}{\cos(x_2) - e^{x_2} + 1} \\ &\approx 0.103. \end{aligned}$$

After 5 steps you would see, to 3 s.f., that it has converged to 0.106, so after 3 steps it does quite well; a better approximation to the solution is $0.106022965\ldots$.