Maths 3018/6111 - Numerical Methods

Worksheet 4 - Solutions

Theory

1. Convert the ODE
$$y''' + xy'' + 3y' + y = e^{-x}$$
into a first order system of ODEs.

Step by step we introduce

$$\begin{aligned} u &= y' \\ v &= u' \\ &= y''. \end{aligned}$$

We can therefore write the ODE into a system of ODEs. The first order ODEs for y and u are given by the definitions above. The ODE for v is given from the original equation, substituting in the definition of u where appropriate, to get

$$\begin{aligned} \begin{pmatrix} y \\ u \\ v \end{pmatrix}' &= \begin{pmatrix} u \\ v \\ e^{-x} - xy'' - 3y' - y \end{pmatrix} \\ &= \begin{pmatrix} u \\ v \\ e^{-x} - xv - 3u - y \end{pmatrix}. \end{aligned}$$

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2. Show by Taylor expansion that the backwards differencing estimate of $f'(x)$,
$$f'(x) \simeq \frac{f(x) - f(x-h)}{h}$$
is first order accurate.

We have the Taylor series expansion of $f(x-h)$ about x is

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) + \mathcal{O}(h^3).$$

Substituting this in to the backwards difference formula we find

$$\begin{aligned} \frac{f(x) - f(x-h)}{h} &= \frac{f(x) - f(x) + hf'(x) - \frac{h^2}{2!}f''(x) + \mathcal{O}(h^3)}{h} \\ &= f'(x) - \frac{h}{2!}f''(x) + \mathcal{O}(h^2). \end{aligned}$$

Therefore the difference between the exact derivative f' and the backwards difference estimate is $\propto h$ and hence the finite difference estimate is first order accurate.

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3. Use Taylor expansion to derive a symmetric or central difference estimate of $f^{(4)}(x)$ on a grid with spacing h.

For this we need the Taylor expansions

$$\begin{aligned}
f(x+h) &= f(x) + hf^{(1)}(x) + \frac{h^2}{2!}f^{(2)}(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) + \ldots \\
f(x-h) &= f(x) - hf^{(1)}(x) + \frac{h^2}{2!}f^{(2)}(x) - \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x) + \ldots \\
f(x+2h) &= f(x) + 2hf^{(1)}(x) + \frac{4h^2}{2!}f^{(2)}(x) + \frac{8h^3}{3!}f^{(3)}(x) + \frac{16h^4}{4!}f^{(4)}(x) + \frac{32h^5}{5!}f^{(5)}(x) + \ldots \\
f(x-2h) &= f(x) - 2hf^{(1)}(x) + \frac{4h^2}{2!}f^{(2)}(x) - \frac{8h^3}{3!}f^{(3)}(x) + \frac{16h^4}{4!}f^{(4)}(x) - \frac{32h^5}{5!}f^{(5)}(x) + \ldots
\end{aligned}$$

By a central or symmetric difference estimate we mean that the coefficient of $f(x \pm nh)$ should have the same magnitude. By comparison with central difference estimates for first and second derivatives we see that for odd order derivatives the coefficients should have opposite signs and for even order the same sign.

So we write our estimate as

$$f^{(4)}(x) \simeq Af(x) + B\left(f(x+h) + f(x-h)\right) + C\left(f(x+2h) + f(x-2h)\right)$$

and we then need to constrain the coefficients A, B, C. By looking at terms proportional to h^s we see

$$\begin{aligned}
h^0 &: & 0 &= A + 2B + 2C \\
h^1 &: & 0 &= 0 \\
h^2 &: & 0 &= B + 4C \\
h^3 &: & 0 &= 0 \\
h^4 &: & \frac{1}{h^4} &= \frac{B}{12} + \frac{16C}{12}.
\end{aligned}$$

This gives three constraints on our three unknowns so we cannot go to higher order. Solving the equations gives

$$A = \frac{6}{h^4}, \qquad B = -\frac{4}{h^4}, \qquad C = \frac{1}{h^4}.$$

Writing it out in obvious notation we have

$$f_1^{(4)} = \frac{1}{h^4}\left(6f_i - 4(f_{i+1} + f_{i-1}) + (f_{i+2} + f_{i-2})\right).$$

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4. State the convergence rate of Euler's method and the Euler predictor-corrector method.

Euler's method converges as h and the predictor-corrector method as h^2.

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5. Explain when multistage methods such as Runge-Kutta methods are useful.

Multistage methods require only one vector of initial data, which must be provided to completely specify the IVP; that is, the method is self-starting. It is also easy to adapt a multistage method to use variable step sizes; that is, to make the algorithm adaptive depending on local error estimates in order to keep the global error within some tolerance. Finally, it is relatively easy to theoretically show convergence. Combining this we see that multistage methods are useful as generic workhorse algorithms and in cases where the function defining the IVP may vary widely in behaviour, so that adaptive algorithms are required.

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6. [3018 only] Explain the power method for finding the largest eigenvalue of a matrix. In particular, explain why it is simpler to find the absolute value, and how to find the phase information.

The idea behind the power method is that most easily seen by writing out a generic vector $\mathbf{x}$ in terms of the eigenvectors of the matrix A whose eigenvalues we wish to find,

$$\mathbf{x} = \sum_{i=1}^{N} a_i \mathbf{e}_i,$$

where we assume that the eigenvectors are ordered such that the associated eigenvalues have the order $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_N|$. Note that we always assume that there is a unique eigenvalue λ_1 with largest magnitude.

We then note that multiplying this generic vector by the matrix A a number of times gives

$$A^k \mathbf{x} = \lambda_1^k \sum_{i=1}^{n} a_i \left(\frac{\lambda_i}{\lambda_1} \right)^k \mathbf{e}_i.$$

We then note that, for $i \neq 1$, the ratio of the eigenvalues $(\lambda_i / \lambda_1)^k$ must tend to zero as $k \to \infty$. Therefore in the limit we will "pick out" λ_1.

Of course, to actually get the eigenvalue itself we have to essentially divide two vectors. That is, we define a sequence $\mathbf{x}^{(k)}$ where the initial value $\mathbf{x}^{(0)}$ is arbitrary and at each step we multiply by A, so that

$$\mathbf{x}^{(k)} = A^k \mathbf{x}^{(0)}.$$

It follows that we can straightforwardly get λ_1 by looking at "the ratio of successive iterations". E.g.,

$$\lim_{k \to \infty} \frac{\|\mathbf{x}^{(k+1)}\|}{\|\mathbf{x}^{(k)}\|} = |\lambda_1|.$$

This only gives information about the magnitude as we have used the simplest way of getting from a vector to a real number, the absolute value. To retain information about the phase we need to replace the absolute value of the vectors with some linear functional such as the sum of the coefficients.
