Solutions to exercise set 8

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1 Consider the function $f(x) = (x^2 + 1)e^x$.

a) Use central differences, i.e., the formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h},$$

with step sizes $h = 1$, $h = 1/2$, $h = 1/4$, $h = 1/8$, in order to approximate $f'(0)$.

b) Use Richardson extrapolation for obtaining a better approximation of $f'(0)$ from the values you have already computed.

Possible solution:

a) The approximations of $f'(0)$ for the different step sizes are:

$$\begin{aligned} h = 1 &: \quad 2.350402387287603, \\ h = \frac{1}{2} &: \quad 1.302738263734369, \\ h = \frac{1}{4} &: \quad 1.073602346434715, \\ h = \frac{1}{8} &: \quad 1.018271923834063. \end{aligned}$$

b)

- The first step in Richardson extrapolation uses the approximations of $f'(0)$ calculated above. These were:

$$\begin{aligned} D(0,0) &= 2.350402387287603, \\ D(1,0) &= 1.302738263734369, \\ D(2,0) &= 1.073602346434715, \\ D(3,0) &= 1.018271923834063. \end{aligned}$$

- In the next step, we compute the next "column" by the formula

$$D(k,1) = D(k,0) + \frac{1}{3}\big(D(k,0) - D(k-1,0)\big)$$

for $k \geq 1$. We obtain

$$\begin{aligned} D(1,1) &= 0.953516889216624, \\ D(2,1) &= 0.997223707334830, \\ D(3,1) &= 0.999828449633845. \end{aligned}$$

- Next we compute

$$D(k,2) = D(k,1) + \frac{1}{15}\big(D(k,1) - D(k-1,1)\big)$$

for $k \geq 2$, obtaining

$$D(2,2) = 1.000137495209377,$$
$$D(3,2) = 1.000002099120446.$$

- Finally, we have

$$D(3,3) = D(3,2) + \frac{1}{63}\big(D(3,2) - D(2,2)\big)$$

and thus

$$D(3,3) = 0.999999949976177.$$

(Note that the actual solution is $f'(0) = 1$. Thus the approximations indeed become significantly better.)

2 Derive an $\mathcal{O}(h^4)$ five point formula to approximate $f'(x_0)$ that uses $f(x_0-h)$, $f(x_0)$, $f(x_0+h)$, $f(x_0+2h)$ and $f(x_0+3h)$. Test the formula on $f(x) = \sin x$ at $x = 1$ and try to verify numerically that is has the stated order.

Hint: Consider the expression $Af(x_0-h)+Bf(x_0+h)+Cf(x_0+2h)+Df(x_0+3h)$. Expand in fourth Taylor polynomials, and choose A, B, C and D appropriately.

Possible solution:

We follow the hint and expand the terms in $Af(x_0-h)+Bf(x_0+h)+Cf(x_0+2h)+Df(x_0+3h)$ in fourth order Taylor polynomials and reorganize.

$$
\begin{aligned}
&Af(x_0-h)+Bf(x_0+h)+Cf(x_0+2h)+Df(x_0+3h)=\\
&=A\left[f(x_0)-hf'(x_0)+\frac{h^2}{2!}f''(x_0)-\frac{h^3}{3!}f^{(3)}(x_0)+\frac{h^4}{4!}f^{(4)}(x_0)-\frac{h^5}{5!}f^{(5)}(\xi_A)\right]\\
&+B\left[f(x_0)+hf'(x_0)+\frac{h^2}{2!}f''(x_0)+\frac{h^3}{3!}f^{(3)}(x_0)+\frac{h^4}{4!}f^{(4)}(x_0)+\frac{h^5}{5!}f^{(5)}(\xi_B)\right]\\
&+C\left[f(x_0)+2hf'(x_0)+\frac{(2h)^2}{2!}f''(x_0)+\frac{(2h)^3}{3!}f^{(3)}(x_0)+\frac{(2h)^4}{4!}f^{(4)}(x_0)+\frac{(2h)^5}{5!}f^{(5)}(\xi_C)\right]\\
&+D\left[f(x_0)+3hf'(x_0)+\frac{(3h)^2}{2!}f''(x_0)+\frac{(3h)^3}{3!}f^{(3)}(x_0)+\frac{(3h)^4}{4!}f^{(4)}(x_0)+\frac{(3h)^5}{5!}f^{(5)}(\xi_D)\right]\\
&=(A+B+C+D)f(x_0)+(-A+B+2C+3D)hf'(x_0)\\
&+(A+B+4C+9D)\frac{h^2}{2!}f''(x_0)+(-A+B+8C+27D)\frac{h^3}{3!}f^{(3)}(x_0)\\
&+(A+B+16C+81D)\frac{h^4}{4!}f^{(4)}(x_0)+(-A+B+32C+243D)4\frac{h^5}{5!}f^{(5)}(\xi)
\end{aligned}
$$

Where $f^{(5)}(\xi)=[f^{(5)}(\xi_A)+f^{(5)}(\xi_B)+f^{(5)}(\xi_C)+f^{(5)}(\xi_D)]/4$ for some $\xi\in(x_0-h,x_0+3h)$. To get a $\mathcal{O}(h^4)$ five point approximation for $f'(x_0)$ we require the coefficient in front of $f'(x_0)$ to equal 1 and the $\mathcal{O}(h^2)$-, $\mathcal{O}(h^3)$- and $\mathcal{O}(h^4)$-term to vanish. This yields the linear system of equations

$$
\begin{aligned}
h(-A+B+2C+3D)&=1,\\
A+B+4C+9D&=0,\\
-A+B+8C+27D&=0,\\
A+B+16C+81D&=0,
\end{aligned}
$$

which is easily solved for

$$A=-\frac{3}{12h},\quad B=\frac{18}{12h},\quad C=-\frac{6}{12h},\quad D=\frac{1}{12h}.$$

Inserting this into the expression and moving the term

$$(A+B+C+D)f(x_0)=\frac{10}{12h}f(x_0)$$

to the left hand side we get

$$
\begin{aligned}
&\frac{-3f(x_0-h)-10f(x_0)+18f(x_0+h)-6f(x_0+2h)+f(x_0+3h)}{12h}\\
&=f'(x_0)+2.4h^4f^{(5)}(\xi)=f'(x_0)+\mathcal{O}(h^4),
\end{aligned}
$$

so the expression on the left hand side is the desired five point formula.

To verify that this formula has indeed fourth order, we compute with it an approximation to the derivative of $f(x)=\sin x$ at $x=1$ for $h=1/2^i$ for $i=2,3,\ldots,9$, and plot the

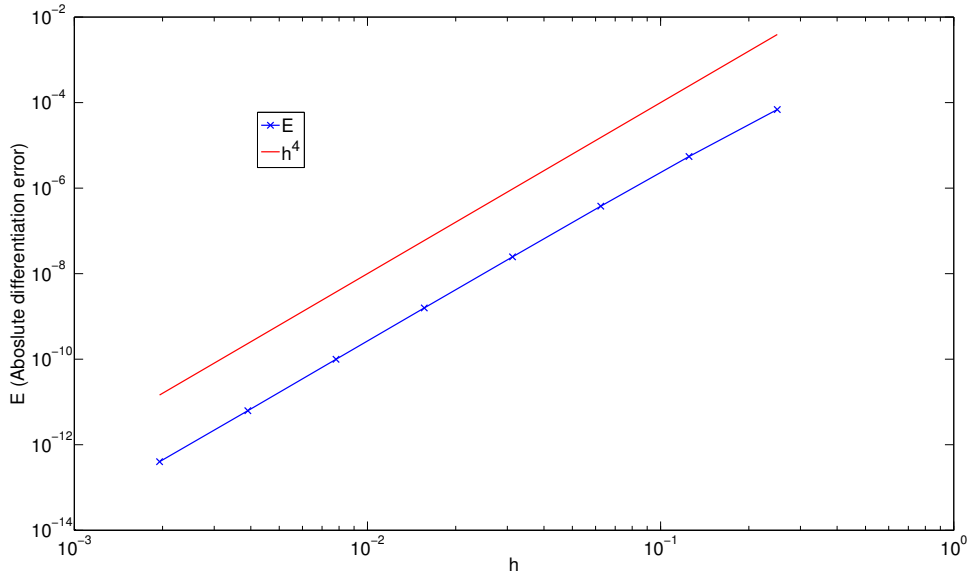

Figure 1:

absolute error, i.e. the abolute value of the difference between the computed value and $f'(1) = \cos 1$, against h with logarithmic axes in MATLAB, see Figure 1. We include a plot of the function h^4 (marked in red) for comparison.

If the formula is indeed fourth order, the absolute error should be $\mathcal{O}(h^4)$. This means that it behaves like the function ch^4 for some positive constant c and sufficiently small values of h. Denote this error by E. If $E \approx ch^4$ for small h then taking logarithms we see that $\log E \approx 4 \log h + \log c$. So if the formula is fourth order, our logarithmic error plot should be a straight line with the same slope as the plot of the function h^4. We observe precisely this. Note that reducing h further would cause the line to flatten out, since numerical rounding errors would then start to dominate.

3 Cf. Cheney and Kincaid, Exercises 4.1.16–17

Assume that the function φ has the form

$$\varphi(h) = L - c_1 h - c_2 h^2 - c_3 h^3 - c_4 h^4 - \dots$$

a) Combine the values $\varphi(h)$ and $\varphi(h/2)$ in order to obtain a higher order approximation of L.

b) Try to generalize the idea of Richardson extrapolation to the function φ.

Possible solution:

a) We have

$$\begin{aligned}\varphi(h) =& L - c_1 h - c_2 h^2 - c_3 h^3 - c_4 h^4 - \dots,\\ \varphi(h/2) =& L - c_1 \frac{h}{2} - c_2 \frac{h^2}{4} - c_3 \frac{h^3}{8} - c_4 \frac{h^4}{16} - \dots\end{aligned}$$

Consequently,

$$2\varphi(h/2) - \varphi(h) = L + c_2 \frac{h^2}{2} + c_3 \frac{3h^3}{4} + c_4 \frac{7h^4}{8} + \dots,$$

which is an approximation of L of order $\mathcal{O}(h^2)$.

b) Assume now that

$$\psi(h) = L - a_m h^m - a_{m+1} h^{m+1} - a_{m+2} h^{m+2} - \dots$$

is an order $\mathcal{O}(h^m)$ approximation of L. Then

$$\psi(h/2) = L - a_m \frac{h^m}{2^m} - a_{m+1} \frac{h^{m+1}}{2^{m+1}} - a_{m+2} \frac{h^{m+2}}{2^{m+2}} - \dots,$$

and therefore

$$2^m \psi(h/2) - \psi(h) = (2^m - 1)L + a_{m+1} \frac{h^{m+1}}{2} + a_{m+1} \frac{3h^{m+2}}{4} + \dots$$

Thus

$$\psi(h/2) + \frac{1}{2^m - 1}\big(\psi(h/2) - \psi(h)\big) = L + d_{m+1} h^{m+1} + d_{m+1} h^{m+2} + \dots$$

is an order $\mathcal{O}(h^{m+1})$ approximation of L. Thus is makes sense to compute approximations of L by:

- Compute approximations

  $$D(k, 0) := \phi(2^{-k} h).$$

  (This is the same as for the usual Richardson extrapolation.)
- Compute recursively

  $$D(k, m) := D(k, m-1) + \frac{1}{2^m - 1}\big(D(k, m-1) - D(k-1, m-1)\big).$$

  (This is almost the same as the usual Richardson extrapolation, but the factor $1/(4^m - 1)$ is replaced by $1/(2^m - 1)$.)

4 Compute numerical approximations of the definite integral

$$\int_0^1 \sin(x^2)\, dx$$

using the composite trapezoid rule with $h = 1$, $h = 1/2$, and $h = 1/4$. In addition, provide estimates for the approximation error.

Possible solution:

The trapezoid rule yields the following approximations of the integral:

$$T(f,0,1) = \Big(\frac{1}{2}\sin(0) + \frac{1}{2}\sin(1)\Big) \approx 0.4207,$$

$$T(f,0,1,1/2) = \frac{1}{2}\Big(\frac{1}{2}\sin(0) + \sin(1/4) + \frac{1}{2}\sin(1)\Big) \approx 0.3341,$$

$$T(f,0,1,1/4) = \frac{1}{4}\Big(\frac{1}{2}\sin(0) + \sin(1/16) + \sin(1/4) + \sin(9/16) + \frac{1}{2}\sin(1)\Big) \approx 0.3160.$$

For the approximation error we use the estimate

$$|T(f,a,b,h) - \int_0^1 f(x)\,dx| \le \frac{b-a}{12}h^2 \sup_{x\in[a,b]} |f''(x)|.$$

In our case,

$$f''(x) = 2\cos(x^2) - 4x^2\sin(x^2),$$

and thus (since cos and sin are both bounded by 1)

$$\sup_{x\in[0,1]} |f''(x)| \le 6.$$

Hence we obtain

$$|T(f,a,b,h) - \int_0^1 f(x)\,dx| \le \frac{h^2}{2}.$$

For $h = 1$, $h = 1/2$, and $h = 1/4$ the respective error bounds are therefore $1/2$, $1/8$, and $1/32$.

Note: In this case better estimates can be obtained quite easily: The function f'' is decreasing on the interval $[0,1]$ because both $\cos(x^2)$ and $-x^2\sin(x^2)$ are. Thus we can estimate

$$\sup_{x\in[0,1]} |f''(x)| \le \max\{|f''(0)|, |f''(1)|\} \approx 2.285.$$

From this we would obtain the estimate

$$|T(f,a,b,h) - \int_0^1 f(x)\,dx| \le \frac{2.285}{12}h^2$$

and hence the error estimates 0.1904, 0.0476, and 0.0119.