UNIVERSITY OF SUSSEX
Scientific Computing
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Problem Sheet 6 (Both problems will be assessed)

1. The Fourier law of heat conduction states that the unit time rate of heat transfer through a material is proportional to the negative gradient in the temperature. In its simplest form, it can be expressed as:

$$Q_x = -k\frac{dT}{dx}, \tag{1}$$

where x is the distance (in m) along the path of heat flow, T is the temperature (in degrees), k is the thermal conductivity and Q_x is the heat flux (W/m^2).

Given the following table:

x	0	0.1	0.2	0.3
T	15	10	5	3

compute k as precisely as you can if Q_x at $x = 0$ is $40\,W/m^2$. What order approximation did you use? [20]

Solution: In order to calculate k, given the value of Q_x at $x = 0$, we have to evaluate the derivative dT/dx at the same point.

The table data provided gives the value of the function $T(x)$ at $x = 0$ and then 3 more forward values, equally spaced, with $h = 0.1$. In order to evaluate the required derivative, we start from the Taylor expansions at these three points:

$$f(x{+}h) = f(x){+}hf'(x){+}\frac{h^2}{2}f''(x){+}\frac{h^3}{6}f'''(x){+}O(h^4)f(x{+}2h) = f(x){+}2hf'(x){+}\frac{4h^2}{2}f''(x){+}\frac{8h}{6}$$

We then use pairs of above 3 equations (e.g. 1 and 2, then 1 and 3) to eliminate the $f'''(x)$ terms, finding:

$$8f(x{+}h){-}f(x{+}2h) = 7f(x){+}6hf'(x){+}2h^2f''(x){+}O(h^4)27f(x{+}h){-}f(x{+}3h) = 26f(x){+}24hf'$$

Finally, we eliminate the second derivatives and solve for $f'(x)$, finding:

$$f'(x) = \frac{2f(x+3h) - 9f(x+2h) + 18f(x+h) - 11f(x)}{6h} + O(h^3)$$

This is the best approximation for our derivative based on the given data - it is third order, forward finite difference. Plugging the table numbers in the derived expression for the derivative, we find:

$$\frac{dT}{dx}(0) = f'(0) = \frac{2 \times 3 - 9 \times 5 + 18 \times 10 - 11 \times 15}{6 \times 0.1} = -40\,K/m$$

thus,

$$k = \frac{Q_x}{-dT/dx} = 1\,\frac{W}{K \cdot m}$$

2. (a) Derive central difference approximations for $f'(x)$ accurate to $O(h^4)$ by applying the Richardson extrapolation, starting with the central difference approximation of $O(h^2)$ (given in the lecture notes).

   (b) Use the approximations in (a) to estimate the derivative of $f(x) = x + e^x$ at $x = 1$ using $h = 0.5$. What are the errors for each of the two approximations? Do they behave as expected? [20]

Solution: [(a)] We start from the central finite-difference approximation to $f'(x)$ given in the lecture notes:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

We apply Richardson's extrapolation formula for $h_2 = h$ and $h_1 = 2h$, finding

$$f''(x) = \frac{2^2 g(h) - g(2h)}{2^2 - 1},$$

where $g(h)$ is given by the second-order approximation above.

Expanded, this gives

$$f'(x) = \frac{1}{3}\left[4\frac{f(x+h) - 2f(x-h)}{2h} - \frac{f(x+2h) - f(x-2h)}{4h}\right] + O(h^4)$$

or

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4)$$

Which is a fourth-order central finite-difference approximation to the first derivative.

(b) The numerical estimate required could be done either by hand, or using Python, e.g. as follows:

```
import numpy as np

def f(x):
    f=np.exp(x)+x
    return f

def df(x):
    df=np.exp(x)+1
    return df

h=0.5
x=1.

dfdx2=(f(x+h)-f(x-h))/2./h
dfdx4=(8.*f(x+h)-8.*f(x-h)-f(x+2.*h)+f(x-2.*h))/12./h

error2=df(x)-dfdx2
error4=df(x)-dfdx4

print 'values= ',dfdx2,dfdx4,'exact=',df(x)
print 'errors=',error2,error4
print 'error ratio=',error2/error4
```

i.e. we first set up the function to be differentiated and its derivative (for checking the results), and then directly evaluatethe expression derived in (a). Once the approximation is obtained we find the (absolute) errors by comparing to the exact result.

This results in:

```
values=  3.83296779964 3.71244771636 exact= 3.71828182846
errors= -0.114685971179 0.00583411209691
error ratio= -19.6578278363
```

Clearly, the fourth order finite-difference approximation is much more precise than the second-order one (in fact more precise than generally expected - should have been a factor of approximately $1/h^2 = 4$ better).