PH3105 Problem Set 3

Q 1) Write a program that calculates the numerical derivative of the function $\ln x$ at $x = 1$ by the forward difference method :

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

for a series of values of h ranging from $h = 0.1$ to $h = 10^{-6}$ and prints out both the derivative and the error E , which is the difference (absolute value) between this result and the exact value $f'(1) = 1$, to an output file. Plot $\ln E$ versus $\ln h$ using gnuplot. Fit a straight line to this plot using gnuplot's fit command and check that the slope of this curve is almost 1 (since $E \propto h$, we expect $\ln E \sim c + \ln h$).

Modify the program again, this time to make h go down all the way to 10^{-20}. Plot the graph of $\ln E$ versus $\ln h$ again - can you explain this behavior?

Q 2) Repeat the problem, but this time for the central difference algorithm

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

Note that the slope of the $\ln E$ versus $\ln h$ graph will give you the order of the approximation, but only if you fit a suitable range of h.

Q 3) The 5-point stencil formula for estimating the first derivative of a function is given by

$$f'(x) \approx \frac{8(f(x+h) - f(x-h)) - (f(x+2h) - f(x-2h))}{12h}$$

Write a program that will print out the estimated derivatives and corresponding errors for the function

$$f(x) = e^{-x} \sin x$$

at $x = 1$. Estimate the order of h in the error.

Q 4) Repeat Q3 - but this time for the estimate of the second derivative by the 7-point stencil formula

$$f''(x) \approx \frac{1}{h^2}\left[\frac{1}{90}(f_{+3} + f_{-3}) - \frac{3}{20}(f_{+2} + f_{-2}) + \frac{3}{2}(f_{+1} + f_{-1}) - \frac{49}{18} f_0\right]$$

where f_i is shorthand for $f(x + ih)$. For this problem, choose equally spaced h from .01 to 0.1 in steps of 0.01. Estimate the order of h in the error for this algorithm.

Q 5) The trapezoidal formula for estimating the definite integral is given by

$$\int_a^b f(x)\,dx \approx h\left[\frac{f(a) + f(b)}{2} + f(a+h) + f(a+2h) + f(a+3h) + \ldots f\left(a + \overline{N-1}h\right)\right]$$

where $h=\frac{b-a}{N}$. Write a program trapezoid.py that estimates the integral

$$\int_0^1 \sin^2 x dx$$

by the trapezoid method for $N=1,10,100,\ldots 10^6$. Try to find an estimate for the order of error in the estimate as a power of h.

Q 6) Write a program that uses the Simpson-1/3 rule

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(a)+f(b)+4\left(f_1+f_3+\ldots+f_{2N-1}\right)+2\left(f_2+f_4+\ldots+f_{2N-2}\right)\right]$$

where $h=\dfrac{b-a}{2N}$ and $f_i \equiv f(a+ih)$ to estimate the integral

$$\int_0^1 \frac{dx}{1+x^2}$$

Take the number of intervals, $2N$, to be $10,20,40,80,\ldots 10240$. Try to find an estimate for the order of error in the estimate as a power of h.

Q 7) The single-step Boole's formula for estimating an integral is given by

$$\int_a^b f(x)\,dx \approx \frac{b-a}{90}\left[7f_0+32f_1+12f_2+32f_3+7f_4\right]$$

Use this formula to estimate the value of

$$\int_0^h e^x dx$$

for the values $h=2,1,\frac{1}{2},\frac{1}{2^2},\frac{1}{2^3},\ldots\frac{1}{2^{10}}$. Use your results to estimate the order of error in Boole's rule as a power of h.

Q 8) Gauss quadrature estimates an integral by the formula

$$\int_{-1}^1 f(x)\,dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

where the Npoints $x_i \in (-1,1)$ and the N weights w_i are chosen in such a way that the estimate is exact for all polynomial function $f(x)$ up to degree $2N-1$. A few roots and weights for different values of N are given in the table below:

Number of points, N	Points, x_i	Weights, w_i
2	$\pm\sqrt{\frac{1}{3}}$	1
3	0	$\frac{8}{9}$
	$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
4	$\pm\sqrt{\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}}}$	$\frac{18+\sqrt{30}}{36}$
	$\pm\sqrt{\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}}$	$\frac{18-\sqrt{30}}{36}$

Write a program that will ask the user for a value of N out of $2, 3$ and 4, values of a and b and use N-point Gauss quadrature to estimate the value of

$$\int_a^b \sin^2 x dx$$

Note that to use the Gauss quadrature formula for arbitrary iontervals, you have to carry out a change of variables

$$x = \frac{b-a}{2} t + \frac{b+a}{2}$$