Second Semester 2008
MATH2200 Scientific Computing   Assignment 3 Numerical Differentiation and Integration

Weighting: 10%
Due Date: 4.00pm on 5 Sept 2008, in the course Assignment Box in the Priestley Building (67).

Please hand in a hard-copy of the assignment (assignments on disk, CD, etc. will not be accepted). Interpreting your results and commenting your code extensively will help to understand your work. Uncommented code will lose marks.

1. (*1 point*)
Derive the two points formula for numerical differentiation:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h). \tag{1}$$

What is the meaning of $O(h)$?

2. (*1 point*)
Derive the same formula as 1 with three points formula

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

3. (*1 point*)
The discretization error in Eq. 1 is defined as

$$E_2(h) = |f'(x) - \frac{f(x+h) - f(x)}{h}| \tag{3}$$

In the same way, the discretization error in Eq. 2 is defined as

$$E_3(h) = |f'(x) - \frac{f(x+h) - f(x-h)}{h^2}| \tag{4}$$

Prove that the discretization error for f'(1), where $f(x) = \exp(x)$ is given by

$$E_2(h) = e|1 - \frac{e^h - 1}{h}| = e\frac{h}{2} + O(h^2) \tag{5}$$

$$E_3(h) = e|1 - \frac{e^h - e^{-h}}{2h}| = e\frac{h^2}{6} + O(h^3) \tag{6}$$

4. (*2 points*) Use Matlab to calculate numerically $f'(1)$, with $f(x) = exp(x)$, taking values of h between 10^{-12} and 10^{-1}. Use the Matlab *loglog* function to plot the numerical error in the calculation of the derivative versus h and compare the results with the formula 5 and 6. Discuss the behavior of the numerical error for small values of h.

5. (*3 points*) Use the rectangle, trapezoid, and Simpson's rule to approximate the integral of $x\cos(x)$ from 0 to π. Rather than using predefined functions from Matlab, develop your own code to calculate the integrals. Compare the discretization error of these three methods taking different step sizes. Finally, use the Matlab-function *quad* to calculate the integral. Compare and discuss the efficiency of the function *quad* with your implementation.

6. (*2 points*) Determine the harmonic approximation for the Lennard-Jones Potential:

$$V(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{7}$$

where ϵ and σ are parameters of the potential. Use Symbolic tools in Matlab (e.g. *symb*, *subs* and *diff*) to demonstrate that the point of equilibrium ($V(r_0) = 0$) is given by $r_0 = 2^{\frac{1}{6}}\sigma$. Then show that the harmonic approximation around the equilibrium point $V(r) \approx \frac{1}{2}V''(r_0)(r - r_0)^2$ is

$$V(r) = \frac{1}{2}k(r - r_0)^2 \tag{8}$$

where $k = c\epsilon/\sigma^2$. What is the exact value of c?.