CME 108/MATH 114
Introduction to Scientific Computing
Summer 2017

Problem Set 1

Due: Thursday, July 6 at 9:30 AM

Total number of points: 100.

1. (20 points) A finite difference approximation of the first derivative $f'(x)$ at point x_j is given by the general formula

$$f'_j = a_0 f_j + a_1 f_{j+1} + a_2 f_{j+2} + a_3 f_{j+3}.$$

Assuming uniform grid spacing, use Taylor series expansion to find the unknown a_j coefficients that give the highest order of accuracy. *Note*: once you get a system of linear equations, $Ax = b$; use Matlab command $x = A\backslash b$, or use Wolfram/Alpha, to solve for the unknowns.

2. (20 points) Given the following function

$$f(x) = 5\cos(10x) + x^3 - 2x^2 - 6x + 10$$

(a) Find and plot the derivative $f'(x)$ for $x \in [0, 4]$. Use backward difference formula $f'_j = (f_j - f_{j-1})/h$ with $h = 0.1$. Use forward scheme for the left endpoint.

(b) Repeat the above calculations using Mablab function `diff`. *Note*: the results should be identical.

3. (25 points) Consider the following approximation to the first derivative

$$f'_j = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h}.$$

which was shown in class to be of order $O(h^4)$.

(a) Apply the formula to evaluate the derivative of the function $f(x) = \arctan(x)$ at $x = 0.5$ for step sizes of

$$h = 1, 0.5, 0.25, 0.125, 0.0625$$

and verify the order of accuracy of this scheme. Plot the decay of error with grid size on a log-log plot (as shown in the lecture). Use MATLAB for calculation and plotting.

(b) The truncation error is not directly dependent on h but on how h compares to a characteristic scale of the problem. To illustrate this point, we consider a function $f(x)$, make the transformation $\xi = Ax$ (where A is a constant) and apply the above scheme to evaluate the derivative with respect to ξ. How does the error term change with the transformation? Note that in the x coordinate, the step size h should also be scaled appropriately, i.e., $h_\xi = Ah$. Show (analytically) that the accuracy of the finite difference formula is not dependent on the choice of the independent variable (x or ξ). Verify this for the function $f(x) = \arctan(x)$ with $\xi = 100x$, at $x = 0.5$ and for the values of h used before. *Note*: To make a fair comparison between the errors in the ξ and x coordinates, you will need to define a relative error, which is:

$$\text{Relative Error} = \left| \frac{\text{Exact answer} - \text{Numerical answer}}{\text{Exact answer}} \right|.$$

4. (25 points) Consider the central finite difference operator, $\dfrac{\delta}{\delta x}$, defined as

$$\frac{\delta f_j}{\delta x} = \frac{f_{j+1} - f_{j-1}}{2h}.$$

(a) The product rule of differentiation in calculus gives

$$\frac{d(uv)}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}.$$

Does the following analogous finite difference expression hold in discrete form?

$$\frac{\delta(u_j v_j)}{\delta x} = u_j\frac{\delta v_j}{\delta x} + v_j\frac{\delta u_j}{\delta x}.$$

(b) Show that

$$\frac{\delta(u_j v_j)}{\delta x} = \bar{u}_j\frac{\delta v_j}{\delta x} + \bar{v}_j\frac{\delta u_j}{\delta x},$$

where an overbar indicates average over the nearest neighbors,

$$\bar{u}_j = \frac{u_{j+1} + u_{j-1}}{2}.$$

5. (10 points) (Bradie, 5.1.1, 5.1.4) Basic Lagrange interpolation.

(a) Let $x_0 = -1$, $x_1 = 1$, and $x_2 = 2$. Determine formulas for the Lagrange polynomials $L_{2,0}(x)$, $L_{2,1}(x)$, and $L_{2,2}(x)$ associated with the given interpolating points.

(b) Consider the function $f(x) = \ln(x)$. Construct the Lagrange form of the interpolating polynomial for f passing through $(1, \ln 1), (2, \ln 2), (3, \ln 3)$ and use it to estimate the values of $\ln 1.5$ and $\ln 2.4$. Finally, plot the polynomial you obtained and f on the same set of axes over the interval $[1/2, 7/2]$.