

PHY 210: Homework Set #1

1 Discrete Numerical Derivatives.

Use the various forms for the numerical first derivative for a uniform discrete mesh size h :

1. the 3-point formula

$$f' \approx \frac{1}{2h}(f_1 - f_{-1}), \quad (1)$$

2. the forward and backward 4-point formulas

$$f' \approx \pm \frac{1}{6h}(-2f_{\mp 1} - 3f_0 + 6f_{\pm 1} - f_{\pm 2}), \quad (2)$$

3. the 5-point formula

$$f' \approx \frac{1}{12h}(f_{-2} - 8f_{-1} + 8f_1 - f_2), \quad (3)$$

to evaluate the derivative

$$\frac{d}{dx}e^x|_{x=0} = 1.000000000000000000000000 \quad (4)$$

Use the quasi-logarithmic values for $h = 1., 0.3, 0.1, 0.03, 0.01, \dots 10^{-6}$. Use double precision and print out in scientific notation *the error* (i.e. subtract $1.d0$) with 14 significant figures shown (not that the last one or two will be significant). Print them out in a columnar table so the rates of convergence will be easy to see.

2 Seven Point Formula

We have discussed, and you have used, the 3-point and 5-point symmetric formulas for a derivative. This problem is: derive the corresponding 7-point formula.

Use the “seat of the pants” approach (which can be difficult to prove rigorously). Extrapolating from the 3-point and 5-point formulae, assume that, since $(f_3 - f_{-3})/6h$ gives some sort of approximation to the derivative, a 7-point form supposing

$$f' = A \frac{f_1 - f_{-1}}{2h} + B \frac{f_2 - f_{-2}}{4h} + C \frac{f_3 - f_{-3}}{6h} + \dots \quad (5)$$

with, of course, the Taylor expansion

$$f(x \pm h) = f(x) \pm h' + \frac{h^2}{2} f^{(2)} \pm \dots \quad (6)$$

allowing h to be replaced by $2h$ and $3h$ as may be useful. Use two of A, B, C to make the coefficients of h^3 and h^5 vanish, and solve for the other. Do $A + B + C$ sum to unity?

Plug this formula into your code from Problem 1 to check for improvement in numerical derivatives.