Problem Set No: 1

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1. The difference between, different derivative methods:

   The derivative of a function in a point x_i with the use of function values at two points, is defined in different manners. Consider these three methods, so called, "*forward difference*" (Δ^+), "*backward difference*" (Δ^-) and the "*centered difference*" (δ), as follows

$$
\begin{aligned}
\Delta^+ f(x_i) &= \frac{f(x_{i+1}) - f(x_i)}{\Delta} \\
\Delta^- f(x_i) &= \frac{f(x_i) - f(x_{i-1})}{\Delta} \\
\delta f(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta}
\end{aligned}
$$

   Question: What is the accuracy of each method?

   (a) Use the Taylor expansion of the r.h.s. functions.

   (b) Assume $f(x_i) = \hat{g}\exp(ikx_i)$ then, compare the exact derivative with these approximations.

2. How to construct the derivative of the order n

   We can construct a derivative of the order n by using the linear combination of p arbitrary points ($p \geqslant n+1$).

$$
\left(\frac{d^n f(x)}{dx^n}\right)_{x_i} = \underbrace{A_1 f(x_{i+\alpha}) + A_2 f(x_{i-\beta}) + \ldots + A_p f(x_i)}_{\text{p point}}
$$

   For this purpose, expand the r.h.s functions, put the coefficients of first $n-1$ terms equal to zero, the nth term equal one and the rest from $n+1$ to p equal to zero. By this method you will find the derivatives with the accuracy which, at least, is of the order of Δ^{n-1}. You can find your error by looking at the coefficient of the first nonzero term after the pth one.

   Question: What is the discrete form of the second order derivative?

(a) Use the points $f(x_i)$, $f(x_{i+1})$ and $f(x_{i-1})$. What is the order of errors?

(b) Use the points $f(x_i)$, $f(x_{i+1})$, $f(x_{i-1})$, $f(x_{i+2})$ and $f(x_{i-2})$. What is the error in this new form?

3. The competition betwean error of discretization method and the round off error:

   The error of numerical schemes become small when the size of space mesh attain to zero. But, the round off error in computers with decreasing of space mesh size will increase. We represent the sum of these two error as the total error:

$$\varepsilon_{\text{tot}} = \underbrace{A\Delta^{\alpha}}_{\text{Numerical scheme error}} + \underbrace{B\Delta^{-\beta}}_{\text{Round off error}} \tag{1}$$

   Therefor here a Δ_m exist for which the total error is minimum. The constants A, α, B and β depend on the computer and the kind of numerical scheme.

   Question: What is the order of Δ_m for the following problem?

4. First derivative of $\sin(x)$ at $x = \pi/8$.

5. Plot the total error as a function of Δ.