# PHYS 410 - HOMEWORK 2

## QUESTION 1

The Lagrange interpolating polynomial of $f(x)$ using 7 points is

$$L(x) = \sum_{m=-3}^{3} f(x_m)\, l_m(x) , \qquad x_m = x_0 + mh,$$

where $l_m(x) = \prod_{k\neq m} \frac{x - x_k}{x_m - x_k}$. We want to evaluate $f'(x_0) \approx L'(x_0)$

The derivatives $l_m'(x)$ are a sum of many products, but only the term where $(x - x_0)$ was differentiated survives when evaluated at $x = x_0$. Therefore, we can write

$$f'(x_0) \simeq L'(x_0) = \sum_{m=-3}^{3} f(x_m)\, l_m'(x_0) , \quad \text{with}$$

$$\boxed{l_m'(x_0) = \frac{1}{x_m - x_0} \prod_{k\neq 0,m} \frac{x_0 - x_k}{x_m - x_k} = \frac{1}{mh} \prod_{k\neq 0,m} \frac{k}{k-m}} ,$$

which is straightforward to evaluate. The weights are thus

$$l_{\pm 3}'(x_0) = \pm 1/60h \; ; \; l_{\pm 2}'(x_0) = \mp 3/20h \; ; \; l_{\pm 1}'(x_0) = \pm 3/4h .$$

The case $m=0$ has to be considered separately, but it is easy to show that $l_0'(x_0) = 0$ using the $h \to -h$ symmetry about $x_0$.

To approximate the optimal value of $h$ by hand, we need to find an upper bound on the absolute error comprising both truncation and roundoff errors. Now, Taylor expanding the $f(x_0+mh)$ for $h$ small or, alternatively, taking the Lagrange remainder $R'(x_0) = \prod_{m\neq 0} (x_0 - x_m)\, f^{(7)}(\xi)/7!$, we have

$$f'(x_0) = L'(x_0) - \underbrace{\frac{f^{(7)}(\xi)\,h^6}{140}}_{\text{truncation error of 7-point centered difference}}, \quad \text{for some } \xi.$$

Using a line above a variable to denote its floating-point representation as calculated by a computer, we express the absolute error made by using $L'(x_0)$ as

$$E(h) = \max_{0 \le x \le 1} \left| f'(x) - \bar{L}'(x) \right|$$ (see Tutorial 5 if this is not clear to you)

$$= \max_{0 \le x \le 1} \left| L'(x) - \bar{L}'(x) - \frac{f^{(7)}(\xi)\,h^6}{140} \right|$$

$$\le \max_{0 \le x \le 1} \left[ \underbrace{\left| L'(x) - \bar{L}'(x) \right|}_{\text{roundoff error}} + \underbrace{\frac{|f^{(7)}(\xi)|\,h^6}{140}}_{\text{truncation error}} \right].$$

Roundoff error: Since it is the function evaluations themselves which suffer from roundoff errors, we write $\bar{f}(x) = f(x) + \varepsilon(x)$, such that $|\varepsilon(x)| \le \varepsilon = \text{M.P.} \ \forall x \in [0,1]$.
$(\varepsilon \approx 2.22 \times 10^{-16})$

Thus $\max_{0 \le x \le 1} \left| L'(x) - \bar{L}'(x) \right| \le \frac{11\varepsilon}{6h}$.

Truncation error: For $f(x) = \sin(x^2)$, one can show that

$$\max_{0 \le x \le 1} |f^{(7)}(x)| \le 2182.$$

Therefore, $\boxed{E(h) \le \frac{11\varepsilon}{6h} + \frac{2182\,h^6}{140}}$, and the optimal value of $h$ is such that $\frac{dE}{dh}(h^*) = 0 \Rightarrow \boxed{h^* \cong 4.28 \times 10^{-3}}$, which is very close to the value found numerically $h_{num} = 3.51 \times 10^{-3}$.