1 Question 1:

1.1 Part (i):

The seven point Lagrangian polynomial approximation to $f(x)$ is (I have relabeled i here is $i = j - 4$ where j is the index in the textbook, I have dropped the dependence on n as it is not needed in this question, and I substitute in $x_i = x^* + ih$ where ever relevant)

$$f(x) \approx P(x) = \sum_{i=-3}^{3} f(x^* + ih) L_i(x) \tag{1.1}$$

with

$$L_i(x) = \prod_{\substack{j=-3 \\ j\neq i}}^{3} \left(\frac{x - x^* - jh}{(j-i)h} \right). \tag{1.2}$$

Differentiating the polynomial approximation and evaluating it at $x = x^*$ we have

$$f'(x) \approx P'(x^*) = \sum_{i=-3}^{3} f(x^* + ih) L_i'(x^*) \tag{1.3}$$

so we need to evaluate the "weights" $L_i'(x^*)$ for $i = -3, -2, -1, 0, 1, 2, 3$. Differentiating expression (1.2) using the product rule we have

$$L_i'(x) = \sum_{\substack{k=-3 \\ j\neq i}}^{3} \frac{1}{(k-i)h} \prod_{\substack{j=-3 \\ j\neq i \\ j\neq k}}^{3} \left(\frac{x - x^* - jh}{(j-i)h} \right) \tag{1.4}$$

$$\Rightarrow L_i'(x^*) = \sum_{\substack{k=-3 \\ j\neq i}}^{3} \frac{1}{(k-i)h} \prod_{\substack{j=-3 \\ j\neq i \\ j\neq k}}^{3} \left(\frac{-jh}{(j-i)h} \right). \tag{1.5}$$

First consider the weight $L_0'(x^*)$ using (1.5) we have

$$L_0'(x^*) = \sum_{\substack{k=-3 \\ j\neq 0}}^{3} \frac{1}{-kh} \prod_{\substack{j=-3 \\ j\neq 0 \\ j\neq k}}^{3} \left(\frac{-jh}{jh} \right). \tag{1.6}$$

$$= \frac{(-1)^6}{h} \sum_{\substack{k=-3 \\ j\neq 0}}^{3} \frac{1}{k} \tag{1.7}$$

$$= \frac{1}{h} \left(-\frac{1}{3} - \frac{1}{2} - \frac{1}{1} + \frac{1}{1} + \frac{1}{2} + \frac{1}{3} \right) \tag{1.8}$$

$$= 0 \tag{1.9}$$

Now consider the weights where $i \neq 0$ noting that the product in equation (1.5) is zero unless $k = 0$ we have

$$L_i'(x^*) = \frac{1}{-ih} \prod_{\substack{j=-3 \\ j\neq i \\ j\neq 0}}^{3} \left(\frac{-j}{(j-i)} \right) \qquad (i \neq 0) \tag{1.10}$$

$$= \frac{3^2.2^2.1^2}{i^2 h \prod_{\substack{j=-3 \\ j\neq i \\ j\neq 0}}^{3} (j-i)} \qquad (i \neq 0) \tag{1.11}$$

$$= \frac{36}{i^2 h \prod_{\substack{j=-3 \\ j\neq i \\ j\neq 0}}^{3} (j-i)} \qquad (i \neq 0). \tag{1.12}$$

thus evaluating the remaining weights we have

$$L_{-3}'(x^*) = \frac{1}{h} \frac{36}{9(-3-3)(-3-2)(-3-1)(-3+1)(-3+2)} = -\frac{1}{60h} \tag{1.13}$$

$$L_{-2}'(x^*) = \frac{1}{h} \frac{36}{4(-2-3)(-2-2)(-2-1)(-2+1)(-2+3)} = \frac{3}{20h} \tag{1.14}$$

$$L_{-1}'(x^*) = \frac{1}{h} \frac{36}{(-1-3)(-1-2)(-1-1)(-1+2)(1+3)} = -\frac{3}{4h} \tag{1.15}$$

$$L_{1}'(x^*) = -\frac{1}{h} \frac{36}{(-1-3)(-1-2)(-1-1)(-1+2)(1+3)} = \frac{3}{4h} \tag{1.16}$$

$$L_{2}'(x^*) = -\frac{1}{h} \frac{36}{4(-2-3)(-2-2)(-2-1)(-2+1)(-2+3)} = -\frac{3}{20h} \tag{1.17}$$

$$L_{3}'(x^*) = -\frac{1}{h} \frac{36}{9(-3-3)(-3-2)(-3-1)(-3+1)(-3+2)} = \frac{1}{60h}. \tag{1.18}$$

Then putting weights (1.9) and (1.13-1.18) into (1.3) we get the approximation for the derivative

$$f'(x) \approx \frac{1}{60h} \Big[f(x+3h) - 9f(x+2h) + 45f(x+h) - 45f(x+h) + 9f(x+2h) - f(x+3h) \Big] \tag{1.19}$$

1.2 Part (ii)

First we will calculate an upper bound on the error due to the Lagrangian interpolation then we will calculate an upper bound on the error due to rounding.

1.2.1 Error due to interpolation

The remainder theorem for Lagragian polynomials gives us

$$f(x) = P(x) + R(x) \tag{1.20}$$

$$\Rightarrow \; f'(x^*) = P'(x^*) + R'(x^*) \tag{1.21}$$

where

$$R(x) = \frac{f^{(7)}(x)}{7!} \prod_{i=-3}^{3} (x - x^* - ih) \tag{1.22}$$

so

$$|R'(x)| \leq \frac{|f^{(7)}(\xi)|}{7!} \sum_{j=-3}^{3} \left| \prod_{\substack{i=-3 \\ \neq j}}^{3} (-ih) \right| \tag{1.23}$$

where ξ is the value $x^* - 3h < \xi < x^* + 3h$ such that $|f^8(\xi)|$ is maximised. Only the $j = 0$ term above is non zero so we have

$$|R'(x)| \leq \frac{|f^{(7)}(\xi)|}{7!} \left| \prod_{\substack{i=-3 \\ \neq j}}^{3} (-ih) \right| \tag{1.24}$$

$$= \frac{|f^{(7)}(\xi)|}{140} h^6. \tag{1.25}$$

1.2.2 Error due to rounding:

The error due to rounding r when evaluating the right hand side of the expression (1.19) is bound by

$$|\text{round off error}| \leq r = \frac{1}{60h} \Big[\epsilon + 9\epsilon + 45\epsilon + 45\epsilon + 9\epsilon + \epsilon \Big] \tag{1.26}$$

$$= \frac{11}{6h} \epsilon. \tag{1.27}$$

where ϵ is the precision of a single operation (in MatLab $\epsilon = 1 \times 10^{-16}$).

1.2.3 Minimising total error.

The total error is therefore bound by $B(h)$,

$$|\text{total error}| \leq B(h) \equiv \frac{|f^{(7)}(\xi)|}{140} h^6 + \frac{11}{6h} \epsilon. \tag{1.28}$$

Differentiating and setting to zere to minimise we have

$$B'(h_{\mathrm{m}}) = 0 \tag{1.29}$$

$$\Rightarrow \quad 0 = \frac{3|f^{(7)}(\xi)|}{70} h_{\mathrm{m}}^5 - \frac{11}{6h_{\mathrm{m}}^2} \epsilon \tag{1.30}$$

$$\Rightarrow \quad h_{\mathrm{m}} = \left(\frac{385\epsilon}{9|f^{(7)}(\xi)|} \right)^{\frac{1}{7}} \approx 1.71014 \left(\frac{\epsilon}{|f^{(7)}(\xi)|} \right)^{\frac{1}{7}} \tag{1.31}$$

at which point the error bound is

$$B(h_{\mathrm{m}}) = 1.25071 |f^{(7)}(\xi)|^{\frac{1}{7}} \epsilon^{\frac{6}{7}} \tag{1.32}$$

Numerically we expect $\frac{|f^{(7)}(\xi)|}{7!} \sim 1$ or $|f^{(7)}(\xi)| \sim 7!$ in which case (using $\epsilon \sim 10^{-16}$ and only keeping one significant figure)

$$h_{\mathrm{m}} \sim 0.003 \tag{1.33}$$

$$B(h_{\mathrm{m}}) \sim 8 \times 10^{-14} \tag{1.34}$$

(if one uses instead $|f^{(7)}(\xi)| \sim 1$ one gets $h_{\mathrm{m}} \sim 0.008$).

1.3 Part (iii):results for $f(x) = \sin(x^2)$:

The MatLab script `Hwk2Q1sol.m` tests the seven point differentiation formula (1.19) whith the function $f(x) = \sin(x^2)$ on the range $0 \leq x \leq 1$. This function has the exact derivative $f'(x) = 2x\cos(x^2)$. The approximation (1.19) with the value h_{m} from (1.19) for h along with the exact derivative in figure 1.1 and we see the two curves lie on top of on and other. The difference between the exact derivative and the approximation (1.19) with $h = h_{\mathrm{m}}$ is plotted in figure 1.2 and we see that the absolute error is always less than the error bound 8×10^{-14} derived in part (ii). Finally we vary h and calculated the mean squared error across our plotting points the results are plotted in figure 1.3 from which can confirm h_m is the optimum value for h.

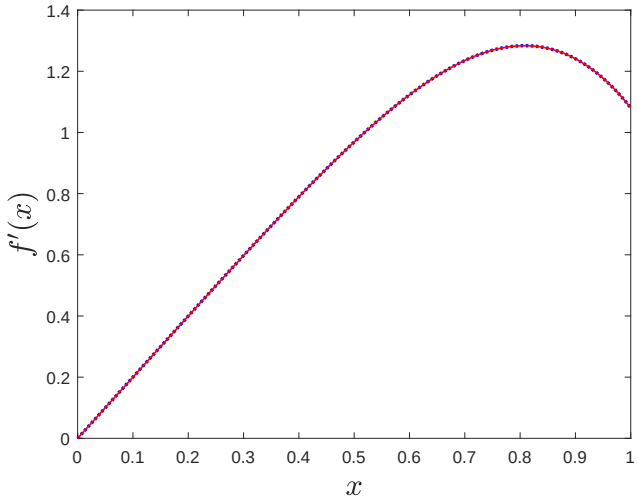

Figure 1.1: The approximation (1.19) (dotted line) and the exact derivitive $f'(x)$ (thin solid line).

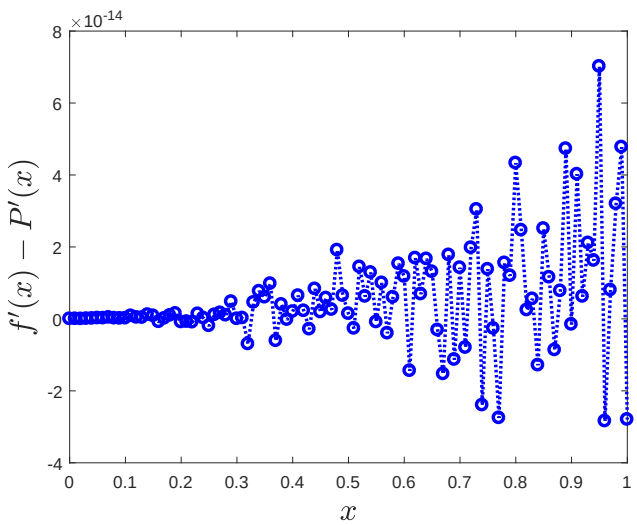

Figure 1.2: The error of the approximation (1.19) to derivitive $f'(x)$.

2 Question 2:

2.1 Method

Let $T_{m,0}$ be the trapezoid rule approximation to to the integral $\int_a^b \mathrm{d}x f(x)$ with 2^m regions

$$T_{m,0} = \frac{(b-a)}{2^m}\left[\sum_{n=0}^{2^m} f\left(a + n\frac{b-a}{2^m}\right) - \tfrac{1}{2}(f(a)+f(b))\right]. \tag{2.1}$$

This has a error of $\mathcal{O}(h^2)$ where $h = \frac{b-a}{2^m}$ and the error only depends on even powers of h. We can use the Richardson extrapolation formula to build higher order approximations to the integral,

$$T_{m+k,k} = \frac{2^{2k}T_{m+k,k-1} - T_{m+k-1,k-1}}{2^{2k}-1} \tag{2.2}$$

the result has an error of $\mathcal{O}(h^{2+2k})$. To complete the calculation of $T_{m+k,k}$ for a given k one needs to first calculate the values $\{T_{m,0}, T_{m+1,0}, \ldots, T_{m+k,0}\}$ on can do this efficiently using the following formula from the textbook (there

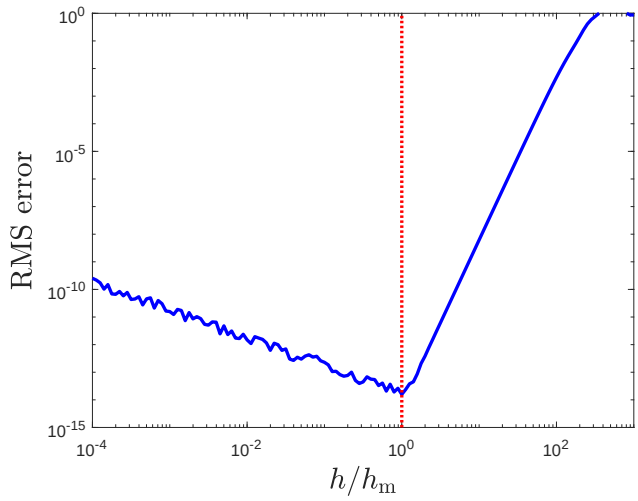

Figure 1.3: The root mean squared (RMS) error of the approximation (1.19) (solid line) to derivitive $f'(x)$ ploted as a function of h . The verticle dotted lined shows the value h_{m}.

i is my $(2n-1)$ which runs over all odd numbers upto 2^m- as specified in the textbook)

$$T_{m+j,0} = \tfrac{1}{2}T_{m+j-1,0} + \frac{b-a}{2^{m+j}} \sum_{n=1}^{2^{m+j-1}} f\left(a + (2n-1)\frac{b-a}{2^{m+j}}\right). \tag{2.3}$$

2.2 Results:

The MatLab script `Hwk2Q2sol.m` gives the results in this section. We calculate numerical approximations to the integral

$$\mathfrak{I} = \int_0^1 \mathrm{d}x \sin x = 1 - \cos 1 \tag{2.4}$$

if we use $m = 1$ and $k = 3$ so the error will be $\mathcal{O}(h^8)$ (I also accepted solutions where the order was $\mathcal{O}(h^6)$ without penalty) in the above we find the following values for $\mathcal{I}$

$$\text{Romberg } \mathfrak{I} = 0.459697694227842 \tag{2.5}$$

$$1 - \cos 1 = 0.459697694131860 \tag{2.6}$$

the absolute value of the error is already $\sim 4 \times 10^{-12}$ with $h = 1/2$. We investigate how the error changes with h. We have plotted the error in figure 2.1 and we see that the error does in fact go like h^8 right down to numerical precision.

Notes:

I have a couple of notes about the "comparison" parts of the marking scheme:

- In question one you are asked to asses the accuracy of the numerical derivative to the function $f(x)$ on the range $1 \geq x \geq 0$ so when you compare the results of the approximation you should compare a large number of points on this range. The easiest way to do this way to do do this is with a graph like figure 1.1 in this document which shows that the exact result and approximation are indistinguishable by eye. But it does not tell us how big the difference was so full marks were not awarded for a figure like 1.1. In order to get full marks one needed to plot the error like in figure 1.2 or to calculate a measure of error involving a large number of points (like the RMS error) as well as something like figure 1.1.
- In question two we cannot asses how good the approximation is unless we have both the result and the error. Showing two long decimal numbers like in equations (2.5-2.6) is not enough as it is hard to read.

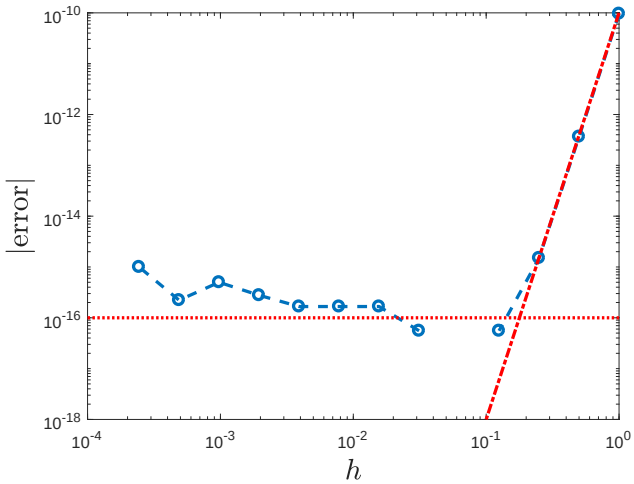

Figure 2.1: The scaling of the error of the Romberg method with h. The absolute value of the error (○'s joined by a dashed line) is shown along with the curve $10^{-10}h^8$ (red dash-dotted line) and the numerical precision of 10^{-16} (horizontal red doted line).