Problem set 1

Problem 1

(a) Starting with the Taylor expansions for the four points surrounding x:

$$f(x+\delta) = f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) + \frac{\delta^3}{6} f'''(x) + \frac{\delta^4}{24} f^{(vi)}(x) + \frac{\delta^5}{120} f^{(v)}(\zeta_1)$$

$$f(x-\delta) = f(x) - \delta f'(x) + \frac{\delta^2}{2} f''(x) - \frac{\delta^3}{6} f'''(x) + \frac{\delta^4}{24} f^{(iv)}(x) - \frac{\delta^5}{120} f^{(v)}(\zeta_2)$$

$$f(x+2\delta) = f(x) + 2\delta f'(x) + 2\delta^2 f''(x) + \frac{4\delta^3}{3} f'''(x) + \frac{2\delta^4}{3} f^{(iv)}(x) + \frac{4\delta^5}{15} f^{(v)}(\zeta_3)$$

$$f(x-2\delta) = f(x) - 2\delta f'(x) + 2\delta^2 f''(x) - \frac{4\delta^3}{3} f'''(x) + \frac{2\delta^4}{3} f^{(iv)}(x) - \frac{4\delta^5}{15} f^{(v)}(\zeta_4)$$

We can then combine the the derivative approximations algebraically to get an approximation for $f'(x)$:

$$[f(x+\delta) - f(x-\delta)] = 2\delta f'(x) + \frac{\delta^3}{3} f'''(x) + \frac{\delta^5}{120}\left[f^{(v)}(\zeta_1) + f^{(v)}(\zeta_2)\right]$$

$$[f(x+2\delta) - f(x-2\delta)] = 4\delta f'(x) + \frac{8\delta^3}{3} f'''(x) + \frac{4\delta^5}{15}\left[f^{(v)}(\zeta_3) + f^{(v)}(\zeta_4)\right]$$

$$8[f(x+\delta) - f(x-\delta)] - [f(x+2\delta) - f(x-2\delta)] = 12\delta f'(x) + \frac{\delta^5}{15}[f^{(v)}(\zeta_1) + f^{(v)}(\zeta_2) - 4f^{(v)}(\zeta_3) - 4f^{(v)}(\zeta_4)]$$

$$\frac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta} = f'(x) + \frac{\delta^4}{180}[f^{(v)}(\zeta_1) + f^{(v)}(\zeta_2) - 4f^{(v)}(\zeta_3) - 4f^{(v)}(\zeta_4)]$$

So we see that the approximation for the first derivative is:

$$\boxed{f'(x) \approx \frac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta}}$$

With an absolute truncation error of:

$$\boxed{\frac{\delta^4}{180}[f^{(v)}(\zeta_1) + f^{(v)}(\zeta_2) + 4f^{(v)}(\zeta_3) + 4f^{(v)}(\zeta_4)]}$$

With a leading expansion error of $\delta^4 f^{(v)}$.

(b) In order to understand the best value for in order to minimize the total error we have to also think about the round-off error in addition to the truncation error. The round-off error is going to be:

$$\frac{8\epsilon_{i+1} - 8\epsilon_{i+1} - \epsilon_{i+2} + \epsilon_{i-2}}{12\delta}$$

Where:

$$f(x+\delta) = \overline{f(x+\delta)} - \epsilon_{i+1}$$

For the rounded value of $\overline{f(x+\delta)}$. The total error is then going to be:

$$\frac{8\epsilon_{i+1} - 8\epsilon_{i+1} - \epsilon_{i+2} + \epsilon_{i-2}}{12\delta} + \frac{\delta^4 f^{(v)}(\zeta)}{18}$$

To minimize the total error we can take the derivative with respect to δ and set it equal to zero:

$$\frac{8\epsilon_{i+1} - 8\epsilon_{i+1} - \epsilon_{i+2} + \epsilon_{i-2}}{12\delta^2} = \frac{2\delta^3 f^{(v)}(\zeta)}{9}$$

So δ should be on the order of:

$$\delta \sim \left(\frac{\epsilon}{f^{(v)}}\right)^{1/5}$$

For double precision, the smallest value ϵ can be is 2^{-52}. Checking this approximation for the function $f(x) = e^x$ (see code) we can see our error on the derivative is of the order 10^{-14}. I note that while I tried the same value of δ for the function $f(x) = e^{0.1x}$ I did not get what seemed to be an appropriate error so there could be a mistake for the estimate of the optimal δ.

Problem 2

See code. dx was approximated in a similar way to above with the difference that there were only two points used to approximate the derivative. When using a known function like $f(x) = e^x$ it's simple to calculate the fractional error of the derivative since we know the true derivative. However, it would be good to generalize this to take any function and calculate the error without previously knowing its derivative. In order to do this I took a similar approach as the previous problem with the total error approximated by the truncation and round-off error. The total error will then be on the order of:

$$\sim \frac{f\epsilon}{dx} + f''' dx^2$$

Since the third order of the Taylor expansion is now the leading term of the truncation error since we are only using two points in the centered derivative, unlike in problem 1. In coding the error I was having trouble with the f''' term so I believe that my error is slightly under- representative of what the true error is by a factor of 10.

Problem 3

See code. For the error approximation on the interpolation I did the bootstrapping-like approach of randomly choosing 80% of the points creating the interpolation function based on those points. The remaining 20% of the points I used to check against the solution that the interpolation function produced. Since we have the true y value of each point it was possible to get the interpolated y value and true value of these test points and subtract them to get the errors. This entire process was repeated 25 times to get a sample of 625 errors which I can then average and get the standard deviation of.

Problem 4

See code.