Math 450
Section 4.1: Numerical Differentiation

Main Idea: To derive formulas for numerical differentiation, we start with a Lagrange interpolating polynomial such that $f(x) = \sum_{n=0}^{n} f(x_j)L_j(x) + \frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(z(x))$. We differentiate this expression, and observe what happens when we evaluate $f(x)$ when $x = x_k$ (one of the values our interpolating polynomial is based upon). This gives us both an approximation formula for the derivative $f'(x_k)$ and an expression for the error in this approximation in terms of $f^{(n+1)}(z(x_k))$.

The two point approximation formula:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(z_0)$$

Three point approximation formulas:

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] - \frac{h^2}{3} f'''(z_0)$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f'''(z_1)$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f'''(z_2)$$

Some five point approximation formulas:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30} f^{(5)}(z)$$

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5} f^{(5)}(z)$$

Example: Suppose that we have the following data:

x	0.78	0.79	0.80	0.81	0.82
$f(x) = \tan x$	0.9892615369	1.009246288	1.029638557	1.050455142	1.071713723

We wish to approximate $f'(0.80)$. Notice that in this table, $h = 0.01$. Also, if we wish to compute upper bounds on the error in our approximations, we will need to compute several derivatives of $f(x) = \tan x$.

$f'(x) = \sec^2 x$. $f''(x) = 2\sec^2(x)\tan(x)$. $f'''(x) = 4\sec^2(x)\tan^2(x) + 2\sec^4(x)$
$f^{(4)}(x) = 8\sec^2(x)\tan^3(x) + 16\sec^4(x)\tan(x)$,
and $f^{(5)}(x) = 16\sec^2(x)\tan^4(x) + 88\sec^4(x)\tan^2(x) + 16\sec^6(x)$

Recall that both $\tan x$ and $\sec x$ are positive and increasing on the interval $\left[0, \frac{\pi}{2}\right)$. Therefore, the maxima of the derivatives of $f(x)$ will occur at the right hand endpoint of the interval in question (assuming h is sufficiently small).

One Point Approximations:

- A Backwards Estimate: $f'(x_0) \approx \dfrac{f(0.79) - f(.80)}{-0.01} = \dfrac{1.009246288 - 1.029638557}{-.01} \approx 2.0392269$
- *Error Bound:* $\frac{h}{2} f''(z_0) \leq \frac{0.01}{2} f''(.80) \approx 0.02121215597$
- A Forward Estimate: $f'(x_0) \approx \dfrac{f(0.81) - f(0.80)}{0.01} = \dfrac{1.050455142 - 1.029638557}{.01} \approx 2.0816585$
- *Error Bound:* $\frac{h}{2} f''(z_0) \leq \frac{0.01}{2} f''(.81) \approx 0.02209586179$

Three Point Approximations:

- A Forward Estimate: $f'(x_0) \approx \dfrac{1}{2(.01)}\left[-3f(.80)+4f(.81)-f(.82)\right]$

$= \dfrac{1}{.02}\left[-3(1.029638557)+4(1.050455142)-(1.071713723)\right] \approx 2.05955865$

- *Error Bound:* $\frac{h^2}{3}f'''(z_0) \leq \frac{(.01)^2}{3}f''(.82) \approx 0.0006367948289$

- A "Middle" Estimate: $f'(x_0) \approx \dfrac{1}{2(0.01)}\left[-f(.79)+f(.81)\right]$

$= \dfrac{1}{.02}\left[-(1.009246288)+(1.050455142)\right] \approx 2.06044270$

- *Error Bound:* $\frac{h^2}{6}f'''(z_0) \leq \frac{(.01)^2}{6}f'''(.81) \approx 0.0003022223166$

- A Backwards Estimate: $f'(x_0) \approx \dfrac{1}{2(.01)}\left[f(.78)-4f(.79)+3f(.80)\right]$

$= \dfrac{1}{.02}\left[(0.9892615369)-4(1.009246288)+3(1.029638557)\right] \approx 2.0596028$

- *Error Bound:* $\frac{h^2}{3}f'''(z_0) \leq \frac{(.01)^2}{3}f'''(.80) \approx 0.0005741607773$

A Five Point Approximation:

- A "Middle" Estimate: $f'(x_0) \approx \dfrac{1}{12(.01)}\left[f(.78)-8f(.79)+8f(.81)-f(.82)\right]$

$= \dfrac{1}{.12}\left[(0.9892615369)-8(1.009246288)+8(1.050455142)-(1.071713723)\right] \approx 2.060155379$

- *Error Bound:* $\frac{h^4}{30}f^{(5)}(z_0) \leq \frac{(.01)^4}{30}f^{(5)}(.82) \approx 2.235473421 \times 10^{-7}$

Notice that we do not have all of the data values needed to use the other 5 point estimate at $x = 0.80$.