MAT360 Section Summary: 4.1b

More Numerical Differentiation

1. Summary Last time we looked at two- and three- point formulas. This time we want to go beyond those, to three and five point formulas.

2. **Definitions**

   - **Other three-point formulas:** Assume that $h > 0$.
     - **forward**:
$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3}f^{(3)}(\xi_f)$$
     - **backward**:
$$f'(x_0) = \frac{f(x_0-2h) - 4f(x_0-h) + 3f(x_0)}{2h} + \frac{h^2}{3}f^{(3)}(\xi_b)$$

     Recall that the centered-difference formula is a three-point formula, with the coefficient of the x_0 term equal to zero, and whose error term is of opposite sign and about twice as good (i.e., half as much):
$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - f^{(3)}(\xi_c)\frac{h^2}{6}$$
     This suggests that we might mix and match to create one of the following

   - **five-point formulas**
     - If we combine the backward and forward three-point formulas with four times the centered difference formula,
$$f'(x_0) \approx \frac{\text{forward} + 4\text{centered} + \text{backward}}{6}$$
       then we might hope that these errors will essentially cancel, and we end up with
$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi)$$
       Notice the exciting development: we went from an $O(h^2)$ method to an $O(h^4)$ method, dependent on the fifth derivative of f.
       Notice also that, although this is called a five-point method, only four points actually figure into the derivative calculations.
     - **forward**:
$$f'(x_0) = \begin{array}{c} \frac{1}{12h}[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) \\ +16f(x_0+3h) - 3f(x_0+4h)] \\ +\frac{h^4}{5}f^{(5)}(\xi) \end{array}$$
       This can be obtained using Taylor series and by carefully selecting the coefficients of the $f(x_0+ih)$, $i = 0, \ldots, 4$ so as to get cancellation up to the fifth derivative terms.

Then again, assuming continuity of the fifth derivative we can use the Intermediate Value Theorem to arrive at the error term.

$$\begin{bmatrix} \text{constant} & \text{first} & \text{second} & \text{third} & \text{fourth} & \text{fifth} \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 & 16 & 32 \\ 1 & 3 & 9 & 27 & 81 & 243 \\ 1 & 4 & 16 & 64 & 256 & 1024 \end{bmatrix}$$

We need a linear combination of these things that gives us

$$\begin{bmatrix} \text{constant} & \text{first} & \text{second} & \text{third} & \text{fourth} & \text{fifth} \\ 0 & 1 & 0 & 0 & 0 & \text{error} \end{bmatrix}$$

- Obviously there's a corresponding **backward** formula where we merely replace the formula above by the one obtained by setting h to $-h$.

These formulas are useful at the endpoints of data sets, where we don't have the neighboring points that we would need for a centered derivative approximation.

Each is an exercise in linear algebra, actually, and not so terribly complicated.

- **Higher order formulas**: Higher order terms can be arrived at via the Taylor series expansions, too: for example, the approximation

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi(x_0))$$

comes right of the Taylor series for

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(\xi_f(x_0))$$

and

$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(\xi_b(x_0))$$

3. Properties/Tricks/Hints/Etc.

One interesting observation is that if an error term is dependent on the n^{th} derivative term $f^{(n)}$, then the approximation will be exact for polynomial functions of degree $n-1$. So, if you knew that a certain phenomenon would theoretically be modelled by a cubic function, then we can get the derivatives exactly right using position data and the appropriate form of the approximation to the derivatives (e.g. a five-point scheme).