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

  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:**

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

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.

constant	first	second	third	fourth	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

We need a linear combination of these things that gives us

constant	first	second	third	fourth	fifth
0	1	0	0	0	error

- 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(x0) = f(x0)

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

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).