Finite Difference Methods

We turn to the problem of computing derivatives.

Question 1. Let $y = f(x)$. What is the definition of the derivative $\frac{dy}{dx}$?

Theorem 2 (Taylor's Formula). *If $f(x)$ has derivatives of all orders throughout an open interval I containing a, then for each natural number n and for each $x \in I$,*

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \frac{f^{(n+1)}(c)}{n!}(x-a)^{n+1}$$

for some c between a and x.

The last term, $\frac{f^{(n+1)}(c)}{n!}(x-a)^{n+1}$, is called the error term, while the equation without it is called the Taylor polynomial.

Question 3. Use Taylor's Formula to find the error when the fraction from the derivative definition is used to approximate the derivative.

Definition 4. The *two-point forward-difference formula* is

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(c)$$

where c is between x and $x + h$.

For any of our formulas, if the error is $\mathcal{O}(h^k)$, we say that the formula an *order k approximation*. However, do note that since c depends on h, then as we bring h closer to 0, the constant of proportionality changes. But as long as f'' is continuous, then $f''(c)$ goes to $f''(x)$ so we can legitimately say the two-point forward-difference formula is first order.

Question 5. Given that we are approximating $f'(x)$, what good is the error formula $\frac{h}{2}f''(c)$?

Question 6. If you cut h in half, how much more accurate should the answer get when using the two-point forward difference formula?

Example 1. Use the two-point forward-difference formula to approximate $f'(2)$ with $h = 1, h = 0.5$, and $h = 0.1$ for the function $f(x) = 2x^2$.

Question 7. What formula would be called the two-point backward-difference formula? Include an error term.

Example 2. Combine the two-point forward-difference and backward difference formulas to get a new approximation for $f'(x)$. What order is the formula?

Theorem 8 (Generalized Intermediate Value Theorem)**.** *Let f be a continuous function on the interval $[a, b]$. Let $x_1, \ldots, x_n$ be points in $[a, b]$ and $a_1, \ldots, a_n > 0$. Then there exists a number c between a and b such that $(a_1 + \ldots + a_n)f(c) = a_1 f(x_1) + \ldots + a_n f(x_n)$.*

The Generalized Intermediate Value Theorem tells us there exists a c in $[x - h, x + h]$ where $f''(c) = f''(c_1) + f''(c_2)$. So we can properly write that the error term is $\frac{h^2}{6} f''(c)$.

Definition 9. The *three-point centered-difference formula* is

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f''(c)$$

where c satisfies $x - h < c < x + h$.

Example 3. Use the three-point centered-difference formula to compute $f'(2)$ for $f(x) = 2x^2$ using $h = 0.1$.

Second Derivative

Question 10. Return to the Taylor formulas for $f(x+h)$ and $f(x-h)$. Can you derive a formula for $f''(x)$?

Example 4. Approximate the second derivative of $f(x) = \cos(x)$ at 0 using $h = 0.1, 0.01$, and 0.001.

Numerical Stability

Example 5. Approximate the derivative of e^x at $x = 0$. Experiment with different powers of 10 for h to see the effects on the forward error.

h	2PFD	$\|error\|$	3PCD	error
10^{-1}	1.051709180756477	0.05	1.001667500198441	0.002
10^{-2}	1.005016708416795	0.005	1.000016666749992	0.00002
10^{-3}	1.000500166708385	0.0005	1.000000166666681	0.0000002
10^{-4}	1.000050001667141	0.00005	1.000000001666890	0.000000002
10^{-5}	1.000005000006965	0.000005	1.000000000012102	0.00000000001
10^{-6}	1.000000499962184	0.0000005	0.999999999973245	0.00000000003
10^{-7}	1.000000049433680	0.00000005	0.999999999473644	0.0000000005
10^{-8}	0.999999993922529	0.000000006	0.999999993922529	0.000000006
10^{-9}	1.000000082740371	0.00000008	1.000000027229220	0.00000003

Question 11. Why did the error start going back up? What previously discussed numerical problems are present in all of these formulas?

Question 12. How do we know what h we should use?

Extrapolation

Suppose that generally you have an order n formula $F(h)$ for approximating a quantity Q. Then the order means that

$$Q \approx F(h) + Ch^n$$

where C is roughly constant over the range of h we are considering. The error can then be written as (by rearranging terms)

$$Q - F(h) \approx Ch^n.$$

Then if the formula is order 2, we expect an input of $\frac{h}{2}$ to do:

$$Q \approx F(\frac{h}{2}) + C(\frac{h}{2})^2$$

$$Q - F(\frac{h}{2}) \approx \frac{1}{2^2}Ch^2$$

$$Q - F(\frac{h}{2}) \approx \frac{1}{2^2}(Q - F(h))$$

Question 13. Express $Q - F(\frac{h}{2})$ in terms of $Q - F(h)$ for an order 1 and an order 3 formula.

Definition 14. The *Richardson extrapolation* or *extrapolation* formula for $F(h)$.

Essentially, extrapolation is a method to derive higher-order approximation formulas.

Example 6. Apply extrapolation to the three-point centered-difference formula.

Example 7. Apply extrapolation to the second derivative formula.