Finite Difference Methods

We turn to the problem of computing derivatives.

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

$$\lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

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 definition is used to approximate the derivative.

If we take just the first two terms ($n = 1$), then the Taylor polynomial is

$$f(x+h) \approx f(x) + f'(x)(x+h-x))$$

$$f(x+h) - f(x) \approx f'(x)(h)$$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

So the error is $\frac{f''(c)}{2}(x+h-x)^2 = \frac{h}{2}f''(c) \approx \mathcal{O}(h)$.

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 $\frac{h}{2}f''(c)$?

The question is referencing the fact that we probably can't compute the constant of proportionality, other than for test problems where we already know the correct solutions. But it's still useful to know how the error scales with h, and that's the most important part of the formula. Higher order formulas should improve faster for the same improvements of h.

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

If you cut h in half, you should also (roughly) cut the error in half.

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 $f(x) = 2x^2$.

For $h = 1$, $f'(2) \approx \frac{f(3)-f(2)}{1} = 18 - 8 = 10$.

For $h = 0.5$, $f'(2) \approx \frac{f(2.5)-f(2)}{0.5} = 2(2(\frac{25}{4}) - 8) = 25 - 16 = 9$.

For $h = 0.1$, $f'(2) \approx \frac{f(2.1)-f(2)}{0.1} = 10(2(4.41) - 8) = 10(0.82) = 8.2$.

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

Definition 8. The *two-point backward-difference formula* is

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

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

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?

Consider the formulas with an extra term, going out to the third derivative. Then

$$f'(x)+f'(x) = \frac{f(x+h) - f(x)}{h} + \frac{f(x) - f(x-h)}{h} - \frac{h}{2}f''(x) + \frac{h}{2}f''(x) - \frac{f'''(c_1)}{6}h^2 - \frac{f'''(c_2)}{6}h^2$$

so we have

$$f'(x) = \frac{1}{2}(\frac{f(x+h) - f(x+h)}{h} - \frac{f'''(c_1)}{6}h^2 - \frac{f'''(c_2)}{6}h^2).$$

The new formula, without error term, is then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

The formula appears to be second order, instead of first.

Theorem 9 (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 $2f'''(c) = f'''(c_1) + f'''(c_2)$. So we can properly write that the error term is $\frac{h^2}{6}f'''(c)$.

Definition 10. 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 $h = 0.1$.

$f'(2) \approx \frac{f(2.1)-f(1.9)}{0.2} = 5(2)(4.41 - 3.61) = 8$

We got exactly the correct answer, because $f'''(x) = 0$ for all x.

Second Derivative

Question 11. Return to the Taylor formulas for $f(x+h)$ and $f(x-h)$. Can you derive a formula for $f''(x)$?

Instead of subtracting so that the second derivative cancels, we should add. Since the third derivatives will also cancel, we should take the formulas out to the fourth derivative.

$$\begin{aligned} f(x+h) + f(x-h) &= (f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_1)) \\ &\quad + (f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_2)) \\ &= 2f(x) + h^2 f''(x) + \frac{h^4}{24}f^{(4)}(c_3) \end{aligned}$$

Solving for the second derivative,

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

for c between $x - h$ and $x + h$.

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

$f''(0) = \frac{cos(h)-2+cos(-h)}{h^2}$

h	$f''(0)$
0.1	-0.9991669
0.01	-0.9999917
0.001	-0.999999167

Numerical Stability

Example 5. Approximate the derivative of e^x at $x = 0$. Experiment with different powers of 10 for h.

h	2PFD	$\lvert error \rvert$	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 12. Why did the error start going back up? What previously discussed numerical problems are present in all of these formulas?

There are two of the huge numerical warning flags in all of these formulas: the denominator is division by tiny numbers, which amplifies errors, and the numerator is subtraction of nearly identical numbers which results in loss of significance. Numerical differentiation is an inherently unstable process.

Question 13. How do we know what h we should use?

It depends on the formula, but for the three-point centered-difference formula it should be about the cubed root of machine epsilon. Here's the derivation. Let $\hat{f}$ denote the computed value (thus the value in double precision).

$$\begin{aligned}
f'(x) - \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h} &= f'(x) - \frac{f(x+h) + \epsilon_1 - f(x-h) + \epsilon_2}{2h} \\
&= \left(f'(x) - \frac{f(x+h) - f(x-h)}{2h} \right) + \frac{\epsilon_1 - \epsilon_2}{2h} \\
&= (f'(x)_{\text{correct}} - f'(x)_{\text{formula}}) + \text{error}_{\text{rounding}}
\end{aligned}$$

We assume that $f(x)$ is of order 1 so that the computed values are off by at most machine epsilon. Then the rounding error term is bounded by

$$\left|\frac{\epsilon_1 - \epsilon_2}{2h}\right| \le \frac{2\epsilon_{\text{mach}}}{2h} = \frac{\epsilon_{\text{mach}}}{h}.$$

Then the total error, with both the formula and the rounding error, is at most

$$\frac{h^2}{6}f'''(c) + \frac{\epsilon_{\text{mach}}}{h}$$

where c is between $x - h$ and $x + h$. Assume $|f'''(c)| \leq M$ for c near x. Then the minimum value occurs when

$$\frac{M}{3}h - \frac{\epsilon_{\text{mach}}}{h^2} = 0$$

and solving for h gives

$$h = \left(\frac{3\epsilon_{\text{mach}}}{M}\right)^{\frac{1}{3}}.$$

Thus for the previous function, $f(x) = e^x$, we want h right about the cubed root of machine epsilon, or 10^{-5}. This is consistent with the errors in the table.

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

Order 1:

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

Order 3:

$$Q - F(\frac{h}{2}) \approx \frac{1}{2^3}(Q - F(h))$$

So in general we expect:

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

Solving for Q:

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

Definition 15. The *Richardson extrapolation* or *extrapolation* formula for $F(h)$ is

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

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

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

The 3PCD formula is an order 2 formula. So the new formula is

$$\begin{aligned} F(x) &= \frac{2^2 F_2(\frac{h}{2}) - F_2(h)}{2^2 - 1} \\ &= \frac{(4\frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h} - \frac{f(x+h) - f(x-h)}{2h})}{3} \\ &= \frac{f(x-h) - 8f(x-\frac{h}{2}) + 8f(x+\frac{h}{2}) - f(x+h)}{6h} \end{aligned}$$

Applying extrapolation should get the order to go up at least one. In fact, here it goes up two. Note that $F(h) = F(-h)$, so the error must be the same for h as for $-h$. Therefore the error terms can be even powers of h only. (Or you can return to the Taylor formulas and observe the same cancellation)

Example 7. Apply extrapolation to the second derivative formula.

$$\begin{aligned} F(x) &= \frac{2^2 F_2(\frac{h}{2}) - F_2(h)}{2^2 - 1} \\ &= \frac{4\frac{f(x+\frac{h}{2}) - 2f(x) + f(x-\frac{h}{2})}{\frac{h^2}{4}} - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}{3} \\ &= \frac{16(f(x+\frac{h}{2}) - 2f(x) + f(x-\frac{h}{2})) - (f(x+h) - 2f(x) + f(x-h))}{3h^2} \\ &= \frac{-f(x-h) + 16f(x-\frac{h}{2}) - 30f(x) + 16f(x+\frac{h}{2}) - f(x+h)}{3h^2} \end{aligned}$$

For the same reason as the previous example, this must be a 4th order formula.