Estimating derivatives

We saw in chapter 3 that we could sample a known function $f(x)$ at several points and then construct an interpolating polynomial $p(x)$ that passes through those points. By computing $p(x)$ at some x of our choosing we could develop an estimate for $f(x)$.

We can use a similar procedure to estimate the value of $f'(x)$ at some point: all we have to do is to evaluate $p'(x)$ instead.

Here is an even more systematic way to estimate $f'(x)$:

1. Sample $f(x)$ at the points $[x\text{-}h,x,x+h]$ and construct an interpolating polynomial $p(x)$.
2. Compute $p'(x)$ as an estimate for $f'(x)$.

In fact, we can do this in the abstract by computing the interpolating polynomial that passes through the points $(x\text{-}h,f(x\text{-}h))$, $(x,f(x))$, and $(x+h,f(x+h))$:

$$p(t,h) = f(x\text{-}h) + \frac{f(x) - f(x\text{-}h)}{h}(t - x + h) + \frac{\frac{f(x+h) - f(x)}{h} - \frac{f(x)\text{-}f(x\text{-}h)}{h}}{2h}(t - x + h)(t\text{-}x)$$

and then evaluating the derivative of this interpolating polynomial at $t = x$:

$$p'(x,h) = \frac{f(x) - f(x\text{-}h)}{h} + \left(2\,x - 2x + h\right)\left(\frac{\frac{f(x+h) - f(x)}{h} - \frac{f(x)\text{-}f(x\text{-}h)}{h}}{2h}\right) = \frac{f(x+h) - f(x\text{-}h)}{2\,h}$$

This results in what is formally known as the *three point centered difference formula*.

Other variations are possible. For example, using the sample points $[x,x+h,x+2h]$ gives the estimate

$$p'(x,h) = -\frac{3\,f(x)}{2\,h} + \frac{2\,f(x+h)}{h} - \frac{f(x+2\,h)}{2h}$$

We can also use more sample points. For example, using the grid of sample points $[x\text{-}2h,x\text{-}h,x,x+h,x+2h]$ produces a five point centered estimate:

$$p'(x,h) = \frac{f(x\text{-}2h)}{12\,h} - \frac{2\,f(x\text{-}h)}{3\,h} + \frac{2\,f(x+h)}{3h} - \frac{f(x+2h)}{12\,h}$$

Error estimates for derivative formulas

The derivative formulas developed in section 4.1 are all based on constructing a Lagrange interpolating polynomial $P(x)$ for a function $f(x)$ in the neighborhood of a point x_0 and then differentiating $P(x)$ to get an approximation for the derivative of $f(x)$ at x_0. The key to getting an error estimate for this process is to start with the theorem from chapter 3 that gives error bounds for Lagrange interpolating polynomials:

Theorem If the function $f(x)$ has n+1 continuous derivatives on some interval $[a,b]$ and the polynomial $P(x)$ is the

Lagrange interpolating polynomial constructed to interpolate a set of points $(x_0, f(x_0))$, $(x_1, f(x_1))$, ... , $(x_n, f(x_n))$ with $x_k \in [a,b]$ for all k then for each x in $[a,b]$ there is a $\xi(x)$ such that

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,(x - x_0)(x - x_1)\cdots(x - x_n)$$

We can develop an error estimate for our differentiation trick by simply differentiating the error formula from the theorem:

$$f'(x) = P'(x) + \left(\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,(x - x_0)(x - x_1)\cdots(x - x_n)\right)'$$

The obvious difficulty here comes in understanding what happens when we differentiate that rather cumbersome error term. Before we tackle that question, it may be useful to be a bit more specific about the sample points we are using. Recall that the methods in section 4.1 typically select the point of interest x_0 as one of the sample points and then use a set of evenly spaced sample points centered at that point. For example, to develop a five point formula we would use sample points $x_0 - 2\,h$, $x_0 - h$, x_0, $x_0 + h$, and $x_0 + 2\,h$. Constructing the error term for these specific points then gives an error estimate

$$\left(\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,(x - x_0 + 2\,h)(x - x_0 + h)(x - x_0)(x - x_0 - h)(x - x_0 - 2\,h)\right)'$$

$$= \frac{f^{(n+2)}(\xi(x))}{(n+1)!}\,\xi'(x)\,(x - x_0 + 2\,h)(x - x_0 + h)(x - x_0)(x - x_0 - h)(x - x_0 - 2\,h)$$

$$+ \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,((x - x_0 + h)(x - x_0)(x - x_0 - h)(x - x_0 - 2\,h) + (x - x_0 + 2\,h)(x - x_0)(x - x_0 - h)(x - x_0 - 2\,h) + (x - x_0 + 2\,h)(x - x_0 + h)(x - x_0 - h)(x - x_0 - 2\,h) + (x - x_0 + 2\,h)(x - x_0 + h)(x - x_0)(x - x_0 - 2\,h) + (x - x_0 + 2\,h)(x - x_0 + h)(x - x_0)(x - x_0 - h))$$

This is a mess, but it quickly simplifies when we realize that what we are really interested in is what happens when we set $x = x_0$. As soon as we do that, many terms vanish and the error estimate reduces to

$$\frac{f^{(n+1)}(\xi(x_0))}{(n+1)!}\,\big((x_0 - x_0 + 2\,h)(x_0 - x_0 + h)(x_0 - x_0 - h)(x_0 - x_0 - 2\,h)\big)$$

$$= \frac{f^{(n+1)}(\xi(x_0))}{(n+1)!}\,4\,h^4 = O(h^4)$$

Thus we see that the five point centered formula has an error term of order $O(h^4)$. By similar reasoning we can show that the three point centered formula has an error term of order $O(h^2)$.

The Richardson extrapolation

We can summarize what we learned about the five point formula above as

$$f'(x_0) = P'(x_0) + O(h^4)$$

Another way to state this is to say that there is a function $N_1(x,h)$ and constants K_4, K_5, … such that

$$f'(x_0) = N_1(x,h) + K_4\, h^4 + K_5\, h^5 + \cdots$$

Note that our interpolating polynomial $P'(x) = N_1(x,h)$ truly is a function of both x and h, because the spacing h determines where we place the sample points used to construct the interpolating polynomial.

The Richardson extrapolation is a cheesy trick designed to produce formulas with better error terms from existing formulas and their error terms. The trick is to write down two versions of the formula for different values of h and then use simple algebra to eliminate the highest order error terms. For example, if we write down a version of our formula with h replaced with $2\,h$ we get

$$f'(x_0) = N_1(x,2\,h) + K_4\,(2\,h)^4 + K_5\,(2\,h)^5 + \cdots$$

Note that this equation has a first error term of $K_4\,(2\,h)^4 = 16\,K_4\,h^4$. Another way to generate a formula with that exact same error term is to take the original formula and multiply both sides by 16:

$$16\,f'(x_0) = 16\,N_1(x,h) + 16\,K_4\,h^4 + 16\,K_5\,h^5 + \cdots$$

Subtracting these two equations produces

$$15\,f'(x_0) = 16\,N_1(x,h) - N_1(x,2\,h) + (2^5 - 16)\,K_5\,h^5 + \cdots$$

or

$$f'(x_0) = \frac{16\,N_1(x,h) - N_1(x,2\,h)}{15} + \frac{(2^5 - 16)}{15}\,K_5\,h^5 + \cdots$$

This is an $O(h^5)$ formula for estimating $f'(x_0)$. Provided that we have a simple and convenient formula for $N_1(x,h)$ that makes it easy to compute

$$\frac{16\,N_1(x,h) - N_1(x,2\,h)}{15}$$

this is a cheap and easy way to extrapolate an $O(h^4)$ formula into an $O(h^5)$ formula. In practice, we get even more fortunate in that often the resulting formula will be even better than the $O(h^5)$ suggested here. Often the result is $O(h^6)$ because K_5 happens to be 0.

For example, applying the Richardson extrapolation to the three point centered difference formula above produces a method that is identical to the five point centered difference formula above, and does it with much less algebra.