Estimating Derivatives and Richardson Extrapolation

Suppose we want to approximate $f'(x)$ using values of f only. The natural approach would be to compute

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{for some small } h.$$

We can find the error in this approximation using Taylor's theorem:

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}h^2 f''(\xi)$$

or

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

or

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2}h f''(\xi).$$

This implies that the error is $O(h)$.

<derivative_and_difference_1.nb>

Can we improve on this situation?

Consider the Taylor series

$$f(x+h) = f(x) + h f'(x) + \frac{1}{2} h^2 f''(x) + \frac{1}{6} h^3 f'''(x) + \ldots$$

$$f(x-h) = f(x) - h f'(x) + \frac{1}{2} h^2 f''(x) - \frac{1}{6} h^3 f'''(x) + \ldots$$

If we subtract, we get

$$f(x+h) - f(x-h) = 2 h f'(x) + \frac{1}{3} h^3 f'''(x) + \ldots$$

So

$$f'(x) = \left[\frac{f(x+h) - f(x-h)}{2h} \right] - \frac{1}{6} h^2 f'''(x) + \ldots$$

This is clearly better, since the error is $O(h^2)$ rather than $O(h)$.

We can actually rewrite the error term as $-\frac{1}{6}h^2 f'''(\xi)$ for some ξ in the interval $[x-h, x+h]$.

<derivative_and_difference_2.nb>

As we can see, this works considerably better! Now here is a very clever idea. Observe that our previous subtraction

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

or

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + \ldots$$

since all of the odd power terms have cancelled each other out.

Now suppose we write

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

$$= f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \cdots$$

It is clear that as $h \to 0$, $\varphi(h) \to f'(x)$. But consider the relationship between $\varphi(h)$ and $\varphi(h/2)$.

$$\varphi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \cdots$$

$$\varphi(h/2) = f'(x) - a_2 \frac{h^2}{4} - a_4 \frac{h^4}{16} - a_6 \frac{h^6}{64} - \cdots$$

This means that

$$\varphi(h) - 4\varphi(h/2) = -3f'(x) - \frac{3}{4} a_4 h^4 - \frac{15}{16} a_6 h^6 \cdots$$

and so forth. Now we can ~~solve~~ get

$$-\frac{1}{3}\varphi(h) + \frac{4}{3}\varphi(h/2) = f'(x) + \frac{\cancel{3}1}{4} a_4 h^4 + \frac{\cancel{1}5}{16} a_6 h^6 + \cdots$$

$$\varphi(h/2) + \frac{1}{3}\left[\varphi\left(\frac{h}{2}\right) - \varphi(h)\right] =$$

We have now improved our error bound to $O(h^4)$ just by adding a correction term of $\frac{1}{3}[\varphi(\frac{h}{2})-\varphi(h)]$ to $\varphi(\frac{h}{2})$. This is shocking!

And we can play this game <u>again</u>:

Let

$$\Phi(h) = \frac{4}{3}\varphi(h/2) - \frac{1}{3}\varphi(h).$$

Then for some coefficients b_i,

$$\Phi(h) = f'(x) + b_4 h^4 + b_6 h^6 + \cdots$$

$$\Phi(\tfrac{h}{2}) = f'(x) + b_4 \frac{h^4}{16} + b_6 \frac{h^6}{64} + \cdots$$

so

$$\Phi(h) - 16\,\Phi(\tfrac{h}{2}) = -15\, f'(x) + \frac{3}{4} b_6 h^6 + \cdots$$

or

$$\Phi(\tfrac{h}{2}) + \frac{1}{15}\left[\Phi(\tfrac{h}{2}) - \Phi(h)\right] = f'(x) - \frac{1}{20} b_6 h^6 + \cdots$$

This procedure is called Richardson extrapolation.

<richardson_extrapolation.nb>

We can formalize the procedure inductively as follows. Suppose

$$\varphi(h) = L - \sum_{k=1}^{\infty} a_{2k} h^{2k}$$

and we want to compute L by computing $\varphi(h)$ at various h values.

For some given h, compute

$$D(n,0) = \varphi\left(\frac{h}{2^n}\right), \qquad n \geq 0$$

We know

$$D(n,0) = L + \sum_{k=1}^{\infty} A(k,0) \left(\frac{h}{2^n}\right)^{2k}$$

where the $A(i,j)$ are unknown coefficients.

We define

$$D(n,m) = \frac{4^m}{4^m - 1} D(n,m-1) - \frac{1}{4^m - 1} D(n-1,m-1).$$

Claim.

$$D(n,m) = L + \sum_{k=m+1}^{\infty} A(k,m) \left(\frac{h}{2^n}\right)^{2k}$$

We will now prove this by induction on m. For $m=0$, there's nothing to check, so assume this holds for $m-1$. Then

$$D(n,m) = \frac{4^m}{4^m - 1}\left[L + \sum_{k=m}^{\infty} A(k,m-1)\left(\frac{h}{2^n}\right)^{2k}\right]$$

$$- \frac{1}{4^m - 1}\left[L + \sum_{k=m}^{\infty} A(k,m-1)\left(\frac{h}{2^{n-1}}\right)^{2k}\right].$$

$$= L + \sum_{k=m}^{\infty} A(k,m-1)\,\frac{4^m - 2^{2k}}{4^m - 1}\left(\frac{h}{2^n}\right)^{2k}$$

So we can define

$$A(k,m) = A(k,m-1)\underbrace{\left(\frac{4^m - 4^k}{4^m - 1}\right)}_{\text{this is} < 1.}$$

Since

$$A(m,m) = 0,$$

we can write

$$D(n,m) = L + \sum_{k=m+1}^{\infty} A(k,m)\left(\frac{h}{2^n}\right)^{2k}. \qquad \square$$

We then compute

$$\begin{tikzcd}
D(0,0) & & \\
D(1,0) & D(1,1) \arrow[l] \arrow[ul] & \\
D(2,0) & D(2,1) \arrow[l] \arrow[ul] & D(2,2) \arrow[l] \arrow[ul]
\end{tikzcd}$$

To see what this looks like in practice we turn to

<richardson_extrapolation.nb>

The next general plan for computing derivatives is to fit a polynomial through some points near x and differentiate the polynomial instead.

Our previous pictures should convince you that this is dangerous!