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§4.3 Richardson Extrapolation (Continued)

Remember the setup: We have some function $\phi(h)$ which is a $\mathcal{O}\left(h^2\right)$ approximation for some quantity L:

$$\phi(h) = L + \sum_{k=1}^{\infty} a_{2k} h^{2k}.$$

We let

$$\begin{aligned} D(n,0) &= \phi\left(\frac{h}{2^n}\right), \\ D(n,m) &= \frac{4^m D(n,m-1) - D(n-1,m-1)}{4^m - 1}. \end{aligned}$$

We've seen how to compute $D(n,m)$ using a "triangular" construction.

We want to show that $D(n,n) = L + \mathcal{O}\left(h^{2(n+1)}\right)$, that is $D(n,n)$ is a $\mathcal{O}\left(h^{2(n+1)}\right)$ approximation to L. The following theorem gives this result:

Theorem 1 (Richardson Extrapolation). There are constants $a_{k,m}$ such that

$$D(n,m) = L + \sum_{k=m+1}^{\infty} a_{k,m} \left(\frac{h}{2^n}\right)^{2k} \qquad (0 \le m \le n).$$

Proof. Our proof is by induction. By definition of $D(n,0)$, and our assumptions on $\phi(h)$, the relation obviously holds for any n and with $m = 0$.

Now, given some n, m assume the relation to be proven holds for $D(n-1, m-1)$, and $D(n, m-1)$; we try to prove it for $D(n,m)$. This should be simple:

$$
\begin{aligned}
D(n,m) &= \frac{4^m D(n,m-1) - D(n-1,m-1)}{4^m - 1} \\
&= \frac{1}{4^m-1}\left[4^m L + 4^m \sum_{k=m}^{\infty} a_{k,m-1}\left(\frac{h}{2^n}\right)^{2k} - L - \sum_{k=m}^{\infty} a_{k,m-1}\left(\frac{h}{2^{n-1}}\right)^{2k}\right], \\
&= \frac{1}{4^m-1}\left[\left(4^m-1\right)L + 4^m a_{m,m-1}\left(\frac{h}{2^n}\right)^{2m} + 4^m \sum_{k=m+1}^{\infty} a_{k,m-1}\left(\frac{h}{2^n}\right)^{2k}\right. \\
&= \left. \qquad -a_{m,m-1}\left(\frac{h}{2^{n-1}}\right)^{2m} - \sum_{k=m+1}^{\infty} a_{k,m-1}\left(\frac{h}{2^{n-1}}\right)^{2k}\right], \\
&= L + \frac{1}{4^m-1}\left[4^m \sum_{k=m+1}^{\infty} a_{k,m-1}\left(\frac{h}{2^n}\right)^{2k} - \sum_{k=m+1}^{\infty} a_{k,m-1}\left(\frac{h}{2^{n-1}}\right)^{2k}\right], \\
&= L + \frac{1}{4^m-1}\left[\sum_{k=m+1}^{\infty} 4^m a_{k,m-1}\left(\frac{h}{2^n}\right)^{2k} - \sum_{k=m+1}^{\infty} a_{k,m-1}2^{2k}\left(\frac{h}{2^n}\right)^{2k}\right], \\
&= L + \sum_{k=m+1}^{\infty} \frac{4^m a_{k,m-1} - a_{k,m-1}2^{2k}}{4^m-1}\left(\frac{h}{2^n}\right)^{2k}, \\
D(n,m) &= L + \sum_{k=m+1}^{\infty} a_{k,m}\left(\frac{h}{2^n}\right)^{2k}.
\end{aligned}
$$

For the properly defined $a_{k,m}$. □

Using Richardson Extrapolation

We now try out the technique on an example or two.

Example 2. Approximate the derivative of $f(x) = \log x$ at $x = 1$.
The real answer is $f'(1) = 1/1 = 1$, but our computer doesn't know that. Define

$$\phi(h) = \frac{1}{2h}\left[f(1+h) - f(1-h)\right] = \frac{\log \frac{1+h}{1-h}}{2h}.$$

Let's use $h = 0.1$. We now try to find $D(2,2)$, which is supposed to be a $\mathcal{O}\left(h^6\right)$ approximation to $f'(1) = 1$:

$n \backslash m$	0	1	2
0	$\frac{\log \frac{1.1}{0.9}}{0.2} \approx 1.003353477$		
1	$\frac{\log \frac{1.05}{0.95}}{0.1} \approx 1.000834586$	≈ 0.999994954	
2	$\frac{\log \frac{1.025}{0.975}}{0.05} \approx 1.000208411$	≈ 0.999999686	≈ 1.000000002

This shows that the Richardson method is pretty good. However, notice that for this simple example, we have, already, that $\phi(0.00001) \approx 0.999999999$.

Example 3. Consider the ugly function:

$$f(x) = \arctan(x).$$

Attempt to find $f'(\sqrt{2})$. Recall that $f'(x) = \frac{1}{1+x^2}$, so the value that we are seeking is $\frac{1}{3}$. Let's use $h = 0.01$. We now try to find $D(2, 2)$, which is supposed to be a $\mathcal{O}\left(h^6\right)$ approximation to $\frac{1}{3}$:

$n \backslash m$	0	1	2
0.333339506181068			
0.333334876543723	0.333333333331274		
0.33333371913582	0.333333333333186	0.333333333333313	
0.333333429783966	0.333333333333348	0.333333333333359	0.33333333333336

Note that we have some motiviation to use Richardson's method in this case: If we let

$$\phi(h) = \frac{1}{2h}\left[f(\sqrt{2}+h) - f(\sqrt{2}-h)\right],$$

then making h small gives a good approximation to $f'\left(\sqrt{2}\right)$ *until subtractive cancelling takes over*. The following table illustrates this:

h	$\phi(h)$
1.0	0.392699081698724
0.1	0.333950696774319
0.01	0.333339506181068
0.001	0.333333395061697
0.0001	0.333333333950581
1×10^{-5}	0.333333333341068
1×10^{-6}	0.333333333324415
1×10^{-7}	0.333333333157881
1×10^{-8}	0.333333327606766
1×10^{-9}	0.333333360913457
1×10^{-15}	0.333066907387547
1×10^{-16}	0.0

Notice that $\phi(h)$ gives at most 10 decimal places of accuracy, then begins to deteriorate; We get 13 decimal places from $D(2, 2)$.

A Big Question

Many of the techniques we have looked at in the past few classes have relied on some pretty broad assumptions about the function $f(x)$: we have assumed continuity and boundedness of derivatives. In class on Monday, Aaron asked whether there is any way of testing some arbitrary black box function for these properties. I flailed about trying to answer the question.

The sad fact is that there is *no* way of testing existence of derivatives of a function $f(x)$, or of the continuity or boundedness of those derivatives. Here's why:

Imagine some subroutine that took a black box function $f(x)$, tested it's value at a finite number of values, say $x_0, x_1, \ldots, x_n$, then declares that $f(x)$ has k continuous derivatives, and it's k^{th} derivative is bounded by some constant M_k.

I claim, however, there is some function $g(x)$ which happens to interpolate $f(x)$ at $x_0, x_1, \ldots, x_n$, and which is not continuous, and thus has no derivatives. To construct $g(x)$, let $p(x)$ be the unique polynomial of degree $\leq n$ that interpolates $f(x)$ at these nodes. Then let

$$g(x) = \begin{cases} p(x) & \text{if } x \text{ is a node } x_i, \text{ or } x \text{ is rational} \\ p(x)+1 & \text{otherwise} \end{cases}$$

Our subroutine could not discern between some black box function $f(x)$ which has continuous derivatives, and the ugly function $g(x)$ which is not continuous. We have to conclude that such a subroutine does not exist.

Approximating the Second Derivative

Suppose we want to approximate the second derivative of some blackbox function $f(x)$. Again, start with Taylor's Theorem:

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(x)}{4!}h^4 + \ldots \\ f(x-h) &= f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(x)}{4!}h^4 - \ldots \end{aligned}$$

Now *add* the two series to get

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + 2\frac{f^{(4)}(x)}{4!}h^4 + 2\frac{f^{(6)}(x)}{6!}h^6 + \ldots$$

Then let

$$\begin{aligned} \psi(h) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} &= f''(x) + 2\frac{f^{(4)}(x)}{4!}h^2 + 2\frac{f^{(6)}(x)}{6!}h^4 + \ldots, \\ &= f''(x) + \sum_{k=1}^{\infty} b_{2k} h^{2k}. \end{aligned}$$

Thus we can use Richardson Extrapolation on $\psi(h)$ to get higher order approximations.