Richardson Extrapolation

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$\mathcal{O}(h^k)$ and $o(h^k)$

We introduce a handy notation[1] used to discuss limiting behavior of a real valued function defined in a neighborhood of 0 on the real line.

For integer k and a functions f and g of this type we write

$$g \sim \mathcal{O}(h^k) \quad \text{and} \quad f \sim o(h^k)$$

(Pronounced: g is big "owe" of h^k and f is little "owe" of h^k)

when

$$\lim_{h\to 0} \frac{g(h)}{h^k} = C \quad \text{for some constant } C \quad \text{and} \quad \lim_{h\to 0} \frac{f(h)}{h^k} = 0.$$

If $k = 0$ this says $\lim_{h\to 0} g = C$ and $\lim_{h\to 0} f = 0$.

[1]Here we only care about limiting behavior as $h \to 0$, but the notation can be adapted to handle limiting behavior at any point, or $\pm\infty$

Examples

Consider $g(x) = \sin(x)$.

$$\lim_{x\to 0} \frac{g(x)}{x} = \lim_{x\to 0} \frac{sin(x)}{x} = \lim_{x\to 0} \frac{cos(x)}{1} = 1.$$

So $g \sim \mathcal{O}(h)$. $g(h)$ "goes to 0" at a similar rate to h.

And $\lim_{x\to 0} \frac{sin(x)}{1} = 0$ so $g \sim o(1)$.

Examples

Consider $f(x) = \cos(x) - 1 + x^2/2$.

$$\lim_{x\to 0} \frac{\cos(x) - 1 + x^2/2}{x^4} = \lim_{x\to 0} \frac{-\sin(x) + x}{4\,x^3} = \lim_{x\to 0} \frac{-\cos(x) + 1}{12\,x^2}$$
$$= \lim_{x\to 0} \frac{-\sin(x)}{24\,x} = \lim_{x\to 0} \frac{-\cos(x)}{24} = \frac{-1}{24}.$$

So $f \sim \mathcal{O}(h^4)$. $f(h)$ "goes to 0" at a similar rate to h^4.

But we can also see from the above that f is *not* $\mathcal{O}(h^5)$, nor is it even $o(h^4)$: h^5 goes to 0 faster than does $f(h)$.

The Rules for Manipulating the "O"s

The following rules are stated for Big O, but are also true with Big O replaced by Little o everywhere.

We presume $g \sim \mathcal{O}(h^k)$ and $f \sim \mathcal{O}(h^i)$ and M, N are real constants with $N \neq 0$.

(i) $Mf \sim \mathcal{O}(h^i)$.

(ii) $g + f \sim \mathcal{O}(h^{\min(\{k,i\})})$.

(iii) $gf \sim \mathcal{O}(h^{k+i})$.

(iv) $g/f \sim \mathcal{O}(h^{k-i})$ (for f nonzero in some neighborhood of 0.)

The Rules for Manipulating the "O"s

We use the notation $f = g + \mathcal{O}(h^i)$ to mean $f - g \sim \mathcal{O}(h^i)$.

And then we come to rule (v):

(v) $\frac{M+f}{N+g} = \frac{M}{N} + \mathcal{O}(h^{\min(\{k,i\})})$.

In addition to these ten facts (five for Big O and five for Little o) we have

(xi) When $j \geq k$ and $g \sim \mathcal{O}(h^k)$ and $f \sim o(h^j)$ then $f + g \sim \mathcal{O}(h^k)$

Approximation and Error

Suppose we are working with an approximation method A to estimate a number I and the accuracy of the approximation is dependent on a small number h with

$$\lim_{h\to 0} A(h) = I.$$

We could be talking about finding a **derivative of a function at some point**, or finding an **integral over an interval** using the trapezoid rule where h is the domain increment, or **finding the value of the solution to a DE at some time in the future**, where h is the step size in an Euler's method approximation to the solution there.

We define the error $E(h)$ of the approximation method by

$$I = A(h) + E(h).$$

We suppose here that $0 < k_1 < k_2$ and the error $E(h)$ is given by

$$E(h) = c_1\, h^{k_1} + c_2\, h^{k_2} + o(h^{k_2})$$

This kind of estimate can often be obtained when, for instance, the approximation method has something to do with a power series expansion of a function. Alternatively, k_1 can be guessed by applying the approximation technique to several standard situations with a variety of h choices.

The important thing to note here is that we have

$$I = A(h) + c_1\, h^{k_1} + c_2\, h^{k_2} + o(h^{k_2}) = A(h) + \mathcal{O}(h^{k_1}).$$

The approximation method $A(h)$ is said to be "good up to order k_1" by virtue of this representation of the error.

When h is small $c_2\, h^{k_2}$ is irrelevant with respect to h^{k_1}, and any remaining difference is small even in comparison to h^{k_2}.

So for any fixed positive constant t we have

$$\begin{aligned} E(th) - t^{k_1} E(h) &= c_1\, t^{k_1} h^{k_1} + c_2\, t^{k_2} h^{k_2} - t^{k_1}\, c_1\, h^{k_1} - t^{k_1}\, c_2\, h^{k_2} + o(h^{k_2}) \\ &= c_2\, (t^{k_2} - t^{k_1})\, h^{k_2} + o(h^{k_2}) \sim \mathcal{O}(h^{k_2}). \end{aligned}$$

Therefore we have a relationship between errors:

$$E(th) = t^{k_1} E(h) + \mathcal{O}(h^{k_2}).$$

This gives

$$I - A(th) - t^{k_1}(I - A(h)) = E(th) - t^{k_1} E(h) \sim \mathcal{O}(h^{k_2}).$$

Then

$$I(1 - t^{k_1}) - A(th) + t^{k_1} A(h) \sim \mathcal{O}(h^{k_2}) \Longrightarrow I = \frac{A(th) - t^{k_1} A(h)}{1 - t^{k_1}} + \mathcal{O}(h^{k_2}).$$

This is the Richardson technique for enhancing the accuracy of an approximation method and is valid for *any* positive t *whenever* the error can be describes as indicated above.

Note: k_1 is needed to apply the technique. k_1 can be guessed by applying the original approximation to a standard situation for a variety of h values. k_2 will, subsequently, be *revealed* by this same means applied to the Richardson improvement!

For instance, in the case $t = 1/2$ and $k_1 = 2$ we have

$$I = \frac{A\left(\frac{h}{2}\right) - \frac{A(h)}{4}}{1 - \frac{1}{4}} + \mathcal{O}(h^{k_2}) = \frac{4\,A\left(\frac{h}{2}\right) - A(h)}{3} + \mathcal{O}(h^{k_2}).$$

Or when $t = 5/9$ and $k_1 = 4$ we have

$$I = \frac{A\left(\frac{5h}{9}\right) - \frac{625\,A(h)}{6561}}{1 - \frac{625}{6561}} + \mathcal{O}(h^{k_2}) = \frac{6561\,A\left(\frac{5h}{9}\right) - 625\,A(h)}{5936} + \mathcal{O}(h^{k_2}).$$

A Puzzle

Here is a puzzle I found in Chapra *"Applied Numerical Methods for Engineers and Scientists 4th Ed."* (2018) in Ch. 20.

There Chapra claims that the Richardson technique applied to the trapezoid rule for integration should improve the error term from $\mathcal{O}(h^2)$ to $\mathcal{O}(h^4)$.

This is a gigantic, almost unbelievably good, improvement. How can this be?

Chapra references Ralston and Rabinowitz *"A First Course in Numerical Analysis 2nd Ed."* (1978) and I got that book (Amazon is Amazing) but found their discussion opaque. So (following their hints) I created my own opaque discussion.

Suppose

$$f(x) = \sum_{k=0}^{\infty} a_k\, x^k$$

and this series is absolutely convergent on an interval $[-h,\, h]$.

It will be important to note that $a_k = \frac{f^{(k)}(0)}{k!}$ and we will be interested in the maximum magnitude of fractions of this form where the derivative is evaluated not just at 0 but on a specific interval $[a, b]$.

We will let M_k denote $\max\left\{\left|\frac{f^{(k)}(x)}{k!}\right| \mid x \in [a, b]\right\}$.

(Each M_k can actually be realized as $\left|\frac{f^{(k)}(\zeta_k)}{k!}\right|$ for some $\zeta_k \in [a, b]$.)

We will let A denote the 1-step trapezoid approximation to

$$I = \int_{-h}^{h} f(x)\, dx$$

and B the more accurate 2-step approximation and C the 1-step 1/3 Simpson's rule approximation to the integral on this interval.

$$A = \frac{f(-h) + f(h)}{2}\, 2h \quad \text{and} \quad B = \frac{f(-h) + f(0)}{2}\, h + \frac{f(0) + f(h)}{2}\, h$$

$$\text{and} \quad C = \frac{h}{3}\left(f(-h) + 4f(0) + f(h)\right).$$

Somewhat surprisingly, the $t = \frac{1}{2}$ Richardson improvement to the trapezoid rule, which is $\frac{4}{3}B - \frac{1}{3}A$, expands to

$$\frac{4}{6}f(-h)\,h + \frac{4}{6}f(0)\,h + \frac{4}{6}f(0)\,h + \frac{4}{6}f(h)\,h - \frac{1}{3}f(-h)\,h - \frac{1}{3}f(h)\,h$$
$$= \frac{1}{3}f(-h)\,h + \frac{4}{3}f(0)\,h + \frac{1}{3}f(h)\,h$$
$$= C. \quad \text{(!!!)}$$

In words, the Richardson improvement with this t ***is the 1/3 Simpson rule approximation!***

An integral on general $[a, b]$ may be broken up[2] into $\frac{b-a}{2h}$ integrals of length $2h$. After you break the integral into pieces slide each piece in turn along the x axis so the left edge is at $-h$.

This translation does not alter the integral of the piece or the form of the trapezoid or Simpson's rule approximation to it. Then add up these numbers to form the composite estimate.

First we are going to examine the power series for the error terms $I - A$ and then $I - C$ on one piece of the integral, calculating I by integrating the power series term-by-term, and expressing C and A as series by evaluating the series for f at $-h$, 0 and h.

In each case we'll get a clear look at the form of the error term. Then we add 'em up to estimate the total error.

[2] Choose h so that $(b - a)/h$ is an even integer.

$$\int_{-h}^{h} f(x)\,dx = \int_{-h}^{h}\left(\sum_{k=0}^{\infty} a_k\,x^k\right)dx = \sum_{k=0}^{\infty} \frac{a_k\,[\,h^{k+1} - (-h)^{k+1}\,]}{k+1}.$$

$$A = \frac{f(-h) + f(h)}{2}\,2\,h = h\sum_{k=0}^{\infty} a_k\,[\,h^k + (-h)^k\,]$$
$$= \sum_{k=0}^{\infty} a_k\,[\,1 + (-1)^k\,]\,h^{k+1}.$$

Bringing it all together for the one-step trapezoid rule we have

$$I - A = \sum_{k=0}^{\infty} \frac{a_k\,[\,h^{k+1} - (-h)^{k+1}\,]}{k+1} - \sum_{k=0}^{\infty} a_k\,[\,1 + (-1)^k\,]\,h^{k+1}$$
$$= \sum_{k=0}^{\infty} a_k\left(\frac{1 + (-1)^k}{k+1} - [1 + (-1)^k]\right)h^{k+1}$$

These coefficients are obviously all zero for odd k, and also for $k = 0$.

And when $k = 2$ we have coefficient $-4a_2/3$ on h^3 and when $k = 4$ we have coefficient $-8a_4/5$ on h^5.

So the trapezoid rule error term for this interval of length $2h$ is of the form

$$\frac{-4}{3}a_2 h^3 + \frac{-8}{5}a_4 h^5 + h^7 \sum_{k=6}^{\infty} a_k \left(\frac{1+(-1)^k}{k+1} - [1+(-1)^k] \right) h^{k-6}.$$

For an interval of length $b-a$ we would have roughly $\frac{b-a}{2h}$ pieces each contributing an error of this type, so the **magnitude** of the error of the *composite* trapezoid rule can be no larger than

$$E_T(h) = \frac{2M_2(b-a)}{3}h^2 + \frac{4M_4(b-a)}{5}h^4 + \mathcal{O}(h^6).$$

(Recall that $M_k = \max\left\{ \left| f^{(k)}(x)/k! \right| \;\middle|\; x \in [a,b] \right\}$.)

Here is the error analysis for the 1/3 Simpson rule.

$$\text{Let} \quad C = \frac{h}{3}\left(f(-h) + 4f(0) + f(h) \right)$$
$$= \frac{h}{3}\left(4a_0 + \sum_{k=0}^{\infty} a_k [1+(-1)^k] h^k \right).$$

$$I - C = \sum_{k=0}^{\infty} \frac{a_k [h^{k+1} - (-h)^{k+1}]}{k+1} - \frac{4a_0 h}{3} - \frac{h}{3}\sum_{k=0}^{\infty} a_k [1+(-1)^k] h^k$$
$$= -\frac{4a_0 h}{3} + \sum_{k=0}^{\infty} a_k \left(\frac{1+(-1)^k}{k+1} - \frac{1+(-1)^k}{3} \right) h^{k+1}$$

As with the trapezoid rule, the coefficients are zero for odd k.

Here though the nonzero even-k terms start with $k=4$. The coefficient there, corresponding to the h^5 term, is $\frac{-4}{15}a_4$ and the h^7 term, $k=6$, has coefficient, is $\frac{-8}{21}a_6$.

The Simpson's rule error term for this interval of length $2h$ is therefor of the form

$$\frac{-4}{15}a_4 h^5 + \frac{-8}{21}a_6 h^7 + h^9 \sum_{k=6}^{\infty} a_k \left(\frac{1+(-1)^k}{k+1} - [1+(-1)^k] \right) h^{k-6}.$$

For an interval of length $b-a$ we would have roughly $\frac{b-a}{2h}$ pieces each contributing an error of this type, so the **magnitude** of the error of the *composite* 1/3 Simpson's rule is of the form

$$E_S(h) = \frac{2M_4(b-a)}{15}h^4 + \frac{4M_6(b-a)}{21}h^6 + \mathcal{O}(h^8).$$

So the composite Richardson-trapezoid rule error term (which is identical to the 1/3 Simpson rule) has 4th order error

$$E_S(h) = \frac{2M_4(b-a)}{15}h^4 + o(h^4).$$

And on each segment of length $2h$ there are 3 function calls (two of which are "new") versus 2 function calls (one of which is "new") for the Trapezoid rule.

Doubling the (new) function calls per segment and using Richardson-trapezoid *increases the order of the error by two full powers.* Using the trapezoid rule alone and cutting h in half (which also doubles the function calls) will *decrease the error only by a factor of four.*