Numerical Analysis Hilary Term 2018
Lecture 16: Richardson Extrapolation

Extrapolation is based on the general idea that if T_h is an approximation to T, computed by a numerical approximation with (small!) parameter h, and if there is an error formula of the form

$$\begin{aligned} T &= T_h + K_1 h + K_2 h^2 + \cdots + O(h^n) \quad (1) \\ \text{then } T &= T_k + K_1 k + K_2 k^2 + \cdots + O(k^n) \quad (2) \end{aligned}$$

for some other value, k, of the small parameter. In this case subtracting (1) from (2) gives

$$(k-h)T = kT_h - hT_k + K_2(kh^2 - hk^2) + \cdots$$

i.e., the linear combination

$$\underbrace{\frac{kT_h - hT_k}{k-h}}_{\text{“extrapolated formula”}} = T + \underbrace{K_2 kh}_{\text{2nd order error}} + \cdots$$

In particular if only *even* terms arise:

$$\begin{aligned} T &= T_h + K_2 h^2 + K_4 h^4 + \cdots + O(h^{2n}) \\ \text{and } k = \tfrac{1}{2}h : T &= T_{\frac{h}{2}} + K_2 \frac{h^2}{4} + K_4 \frac{h^4}{16} + \cdots + O(\frac{h^{2n}}{2^{2n}}) \\ \text{then } T &= \frac{4T_{\frac{h}{2}} - T_h}{3} - \frac{K_4}{4} h^4 + \cdots + O(h^{2n}). \end{aligned}$$

This is the first step of **Richardson extrapolation**. Call this new, more accurate formula

$$T_h^{(2)} := \frac{4T_{\frac{h}{2}} - T_h}{3},$$

where $T_h^{(1)} := T_h$. Then the idea can be applied again:

$$\begin{aligned} T &= T_h^{(2)} + K_4^{(2)} h^4 + \cdots + O(h^{2n}) \\ \text{and } T &= T_{\frac{h}{2}}^{(2)} + K_4^{(2)} \frac{h^4}{16} + \cdots + O(h^{2n}) \\ \text{so } T &= \underbrace{\frac{16T_{\frac{h}{2}}^{(2)} - T_h^{(2)}}{15}}_{T_h^{(3)}} + K_6^{(3)} h^6 + \cdots + O(h^{2n}) \end{aligned}$$

is a more accurate formula again. Inductively we can define

$$T_h^{(j)} := \frac{1}{4^{j-1}-1}\left[4^{j-1} T_{\frac{h}{2}}^{(j-1)} - T_h^{(j-1)}\right]$$

for which

$$T = T_h^{(j)} + O(h^{2j})$$

so long as there are high enough order terms in the error series.

Example: approximation of π by inscribed polygons in unit circle. For a regular n-gon, the circumference $= 2n\sin(\pi/n) \le 2\pi$, so let $c_n = n\sin(\pi/n) \le \pi$, or if we put $h = 1/n$,

$$c_n = \frac{1}{h}\sin(\pi h) = \pi - \frac{\pi^3 h^2}{6} + \frac{\pi^5 h^4}{120} + \cdots$$

so that we can use Richardson extrapolation. Indeed $c_2 = 2$ and

$$\begin{aligned} c_{2n} = &\ 2n\sin(\pi/2n) = 2n\sqrt{\tfrac{1}{2}(1-\cos(\pi/n))} \\ = &\ 2n\sqrt{\tfrac{1}{2}(1-\sqrt{1-\sin^2(\pi/n)})} = 2n\sqrt{\tfrac{1}{2}(1-\sqrt{1-(c_n/n)^2})}\ . \end{aligned}$$

So[1] $c_4 = 2.8284$, $c_8 = 3.0615$, $c_{16} = 3.1214$. Extrapolating between c_4 and c_8 we get $c_4^{(2)} = 3.1391$ and similarly from c_8 and c_{16} we get $c_8^{(2)} = 3.1214$. Extrapolating again between $c_4^{(2)}$ and $c_8^{(2)}$, we get $c_4^{(3)} = 3.141590\ldots$.

Example 2: Romberg Integration. Consider the Composite Trapezium Rule for integrating $T = \int_a^b f(x)\,\mathrm{d}x$:

$$T_h = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{2^n-1} f(x_j)\right]$$

with $x_0 = a$, $x_j = a + jh$ and $h = (b-a)/2^n$. Recall from Lecture 3 that the error is $(b-a)\frac{h^2}{12}f''(\xi)$ for some $\xi \in (a,b)$. If there were an (asymptotic) error series of the form

$$\int_a^b f(x)\,\mathrm{d}x - T_h = K_2 h^2 + K_4 h^4 + \cdots$$

we could apply Richardson extrapolation as above to yield

$$T - \frac{4T_{\frac{h}{2}} - T_h}{3} = K_4 h^4 + \cdots$$

There is such as series: the Euler–Maclaurin formula

$$\begin{aligned} \int_a^b f(x)\,\mathrm{d}x - T_h = &\ -\sum_{k=1}^{r}\frac{B_{2k}}{(2k)!}h^{2k}[f^{(2k-1)}(b) - f^{(2k-1)}(a)] \\ &+(b-a)\frac{h^{2r+1}B_{2r+2}}{(2r+2)!}f^{(2r+2)}(\xi) \end{aligned}$$

where $\xi \in (a,b)$ and B_{2k} are called the Bernoulli numbers, defined by

$$\frac{x}{e^x - 1} = \sum_{\ell=0}^{\infty} B_l \frac{x^\ell}{\ell!}$$

[1] This expression is sensitive to roundoff errors, so we rewrite it as $c_{2n} = c_n/\sqrt{\frac{1}{2}+\frac{1}{2}\sqrt{1-(c_n/n)^2}}$.

so that $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$, etc.

Romberg Integration *is* composite Trapezium for $n = 0, 1, 2, 3, ...$, and the repeated application of Richardson extrapolation. Changing notation ($T_h \to T_n$, h = stepsize, 2^n = number of composite steps), we have

$$\begin{aligned} T_0 = &\ \frac{b-a}{2}[f(a)+f(b)] = R_{0,0} \\ T_1 = &\ \frac{b-a}{4}[f(a)+f(b)+2f(a+\tfrac{1}{2}(b-a))] \\ = &\ \tfrac{1}{2}[R_{0,0}+(b-a)f(a+\tfrac{1}{2}(b-a))] = R_{1,0}. \end{aligned}$$

Extrapolation then gives

$$R_{1,1} = \frac{4R_{1,0} - R_{0,0}}{3}.$$

with error $O(h^4)$. Also

$$\begin{aligned} T_2 = &\ \frac{b-a}{8}[f(a)+f(b)+2f(a+\tfrac{1}{2}(b-a)) \\ &\ \quad + 2f(a+\tfrac{1}{4}(b-a)) + 2f(a+\tfrac{3}{4}(b-a))] \\ = &\ \frac{1}{2}\left[R_{1,0} + \frac{b-a}{2}[f(a+\tfrac{1}{4}(b-a)) + f(a+\tfrac{3}{4}(b-a))\right] = R_{2,0}. \end{aligned}$$

Extrapolation gives

$$R_{2,1} = \frac{4R_{2,0} - R_{1,0}}{3}$$

with error $O(h^4)$. Extrapolation again gives

$$R_{2,2} = \frac{16R_{2,1} - R_{1,1}}{15}$$

now with error $O(h^6)$. At the ith stage

$$T_i = R_{i,0} = \frac{1}{2}\left[R_{i-1,0} + \frac{b-a}{2^{i-1}} \underbrace{\sum_{j=1}^{2^{i-1}} f\left(a + \left(j - \frac{1}{2}\right)\frac{b-a}{2^{i-1}}\right)}_{\text{evaluations at new interlacing points}}\right].$$

Extrapolate

$$R_{i,j} = \frac{4^j R_{i,j-1} - R_{i-1,j-1}}{4^j - 1} \quad \text{for} \quad j = 1, 2, \ldots$$

This builds a triangular table:

$$\begin{array}{lllll} R_{0,0} & & & & \\ R_{1,0} & R_{1,1} & & & \\ R_{2,0} & R_{2,1} & R_{2,2} & & \\ \vdots & \vdots & \vdots & \ddots & \\ R_{i,0} & R_{i,1} & R_{i,2} & \ldots & R_{i,i} \end{array}$$

Theorem: Composite Trapezium ($R_{i,0}$); Composite Simpson ($R_{i,1}$)

Notes 1. The integrand must have enough derivatives for the Euler–Maclaurin series to exist (the whole procedure is based on this!).

2. $R_{n,n} \to \int_a^b f(x)\,\mathrm{d}x$ in general much faster than $R_{n,0} \to \int_a^b f(x)\,\mathrm{d}x$.

A final observation: because of the Euler–Maclaurin series, if $f \in \mathrm{C}^{2n+2}[a,b]$ and is *periodic* of period $b-a$, then $f^{(j)}(a) = f^{(j)}(b)$ for $j = 0, 1, \ldots, 2n-1$, so

$$\int_a^b f(x)\,\mathrm{d}x - T_h = (b-a)\frac{h^{2n+1}B_{2n+2}}{(2n+2)!}f^{(2n+2)}(\xi)$$

c.f.,

$$\int_a^b f(x)\,\mathrm{d}x - T_h = (b-a)\frac{h^2}{12}f''(\xi)$$

for nonperiodic functions! That is, the Composite Trapezium Rule is extremely accurate for the integration of periodic functions. If $f \in \mathrm{C}^\infty[a,b]$, then $T_h \to \int_a^b f(x)\,\mathrm{d}x$ faster than any power of h.

Example: the circumference of an ellipse with semi-axes A and B is

$$\int_0^{2\pi} \sqrt{A^2 \sin^2\phi + B^2 \cos^2\phi}\;\mathrm{d}\phi.$$

For $A = 1$ and $B = \frac{1}{4}$, $T_8 = 4.2533$, $T_{16} = 4.2878$, $T_{32} = 4.2892 = T_{64} = \cdots$.