Numerical Analysis

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with thanks to Endre Süli

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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

$$T = T_h + K_1 h + K_2 h^2 + \cdots + \mathcal{O}(h^n) \quad (16.1)$$

$$\text{then } T = T_k + K_1 k + K_2 k^2 + \cdots + \mathcal{O}(k^n) \quad (16.2)$$

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for some other value, k, of the small parameter.

In this case subtracting (16.1) from (16.2) 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:

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

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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 + K_6^{(2)} h^6 + \cdots + \mathcal{O}(h^{2n}) \\
\text{and } T &= T_{\frac{h}{2}}^{(2)} + K_4^{(2)} \frac{h^4}{16} + K_6^{(2)} \frac{h^6}{64} + \cdots + \mathcal{O}(h^{2n}) \\
\text{so } T &= \underbrace{\frac{16 T_{\frac{h}{2}}^{(2)} - T_h^{(2)}}{15}}_{T_h^{(3)}} + K_6^{(3)} h^6 + \cdots + \mathcal{O}(h^{2n})
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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

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

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

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

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

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So[1] $c_4 = 2.8284$, $c_8 = 3.0615$, $c_{16} = 3.1214$.

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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 $h = (b-a)/2^n$.

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$$\int_a^b f(x)\,\mathrm{d}x - T_h = K_2h^2 + K_4h^4 + \cdots$$

we could apply Richardson Extrapolation as above to yield

$$T - \frac{4T_{\frac{h}{2}} - T_h}{3} = K_4h^4 + \cdots .$$

There is such as series: the Euler–Maclaurin formula

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

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

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

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

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

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

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

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Extrapolate

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

This builds a triangular table:

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

Theorem: C. Trapezium C. Simpson ... ... Romberg

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 $j = 0, 1, \ldots, 2n-1$, and then

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

compared to

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

for nonperiodic functions!

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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 semiaxes 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 $B = \frac{1}{4}$,

$$\begin{aligned} T_8 &= 4.2533, \\ T_{16} &= 4.2878, \\ T_{32} &= 4.2892 = T_{64} = \cdots \qquad \text{(to 4 decimal places).} \end{aligned}$$