Richardson extrapolation

Consider some quantity $Z(h)$ which depends on h with some exponent α:

$$Z(h) = Z_* + Kh^\alpha$$

Suppose that

- can only compute $Z(h)$ at various values of $h > 0$,
- are interested in the limiting value $Z_* \equiv Z(h = 0)$,
- $K = \mathrm{const}$, and the exponent α is known.

Richardson extrapolation

Pick some $q \neq 1$, and

$$\begin{cases} Z(h) = Z_* + K\, h^\alpha \\ Z\left(\dfrac{h}{q}\right) = Z_* + K\left(\dfrac{h}{q}\right)^\alpha \end{cases}$$

Then,

$$\frac{q^\alpha Z\left(\frac{h}{q}\right) - Z(h)}{q^\alpha - 1} = Z_*$$

Richardson extrapolation: 2nd order central difference

Consider a second order central finite difference scheme,

$$\begin{aligned} Z_h &= \frac{f(x+h) - f(x-h)}{2\,h} \\ &= f'(x) + K_2 h^2 + K_4 h^4 + \cdots \end{aligned}$$

where K_s are h-independent.

Richardson extrapolation: 2nd order central difference

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where K_s are h-independent.

Z_h has order $O(h^2)$. The Richardson extrapolant

$$
Z_h^{(2)} = \frac{q^2 Z_{h/q} - Z_h}{q^2 - 1}
$$

has order $O(h^4)$.

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Likewise, the following extrapolant

$$Z_h^{(4)} = \frac{q^4 Z_{h/q}^{(2)} - Z_h^{(2)}}{q^4 - 1}$$

has order $O(h^6)$.

Neville algorithm

Organization of computations: construct an upper triangular table:

$$
\begin{array}{cccccc}
Z_h & & Z_{h/2} & & Z_{h/4} & \cdots \\
 & \nwarrow & \uparrow & \nwarrow & \uparrow & \cdots \\
 & & \dfrac{2^2 Z_{h/2} - Z_h}{2^2 - 1} & & \dfrac{2^2 Z_{h/4} - Z_{h/2}}{2^2 - 1} & \cdots \\
 & & & \nwarrow & \uparrow & \\
 & & & & \cdots &
\end{array}
$$

- Start in the upper left corner and proceed column by column.
- In each column, evaluate $f(x)$ only once. All other elements of the table are computed as linear combinations.
- Each row contains approximations of $f'(x)$ at progressively smaller steps. Discrepancies estimate the error.

Finite differences

Two (competing) sources of errors:

- Truncation error, $\epsilon_t \sim h^a$ as $h \to 0$
- Roundoff error, $\epsilon_r \sim 1/h$

Complex step differentiation

Suppose that

- $f(x)$ can be analytically continued into the complex plane
- the resulting complex-valued function, $f(z) = u(x, y) + iv(x, y)$, is an analytic function of the complex variable $z = x + iy$.

Complex step differentiation

Since by assumption $f(z)$ is an analytic function in the vicinity of $z = x + i\,0$, expand it into a Taylor series

$$f(x+ih) = f(x) + f'(x)\,ih + \frac{f''(x)}{2}\,(-h^2) + \frac{f'''(x)}{6}\,(-ih^3) + \dots$$

Separating the imaginary part, we have

$$f'(x) = \frac{\operatorname{Im} f(x+ih)}{h} + O(h^2)$$

Complex step differentiation

$$f'(x) = \frac{\operatorname{Im} f(x+ih)}{h} + O(h^2)$$