

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 $Z_* \equiv Z(h = 0)$,
- ▶ $K = \text{const}$, and the exponent α is known.

Richardson extrapolation

Pick some $q \neq 1$, and

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

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,

$$\begin{aligned}Z_h &= \frac{f(x+h) - f(x-h)}{2h} \\&= f'(x) + K_2h^2 + K_4h^4 + \dots\end{aligned}$$

where K_s are h -independent.

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

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

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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:

$$\begin{array}{ccccccc}
 Z_h & & Z_{h/2} & & Z_{h/4} & & \dots \\
 & \swarrow & \uparrow & \swarrow & \uparrow & & \dots \\
 & & \frac{2^2 Z_{h/2} - Z_h}{2^2 - 1} & & \frac{2^2 Z_{h/4} - Z_{h/2}}{2^2 - 1} & & \dots \\
 & & & \swarrow & \uparrow & & \\
 & & & & \dots & &
 \end{array}$$

- ▶ 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 $h \rightarrow 0$
- ▶ 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 $z = x + i0$, 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

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

