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,
- lacktriangle 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

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

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,

$$Z_h = \frac{f(x+h) - f(x-h)}{2h}$$

= $f'(x) + K_2h^2 + K_4h^4 + \cdots$

where K_s are h-independent.

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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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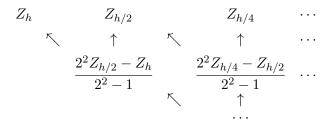
Likewise, the following extrapolant

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

has order $O(h^6)$.

Neville algorithm

Organization of computations: construct an upper triangular table:



- 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

- lacksquare 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

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

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Complex step differentiation

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

