Example 43: Let $y(x) = a\ln(x) + b\cos(x)$

Write down the normal equations.

Assume nodes x_i and values y_i given for $i=0,\dots,n$.

Then, error in l_2-norm:

$$E_2(a,b) = \sum_{i=0}^{n} \left(y(x_i) - y_i \right)^2$$
$$= \sum_{i=0}^{n} \left(a\ln(x_i) + b\cos(x_i) - y_i \right)^2$$

Necessary condition for min: $\frac{\partial E_2}{\partial a} = 0 = \frac{\partial E_2}{\partial b}$

The second derivative test is not needed, because the function is convex in a and b. Thus, only a minimum exists.

Now: $\frac{\partial E_2}{\partial a} = \sum_i 2\left(a\ln(x_i) + b\cos(x_i) - y_i \right)\ln(x_i)$

and $\frac{\partial E_2}{\partial a} = 0 \Leftrightarrow a\sum_i (\ln(x_i))^2 + b\sum_i \cos(x_i)\ln(x_i) = \sum_i y_i\ln(x_i)$

analog: $\frac{\partial E_2}{\partial b} = 0$

$$\Leftrightarrow a\sum_i \ln(x_i)\cos(x_i) + b\sum_i (\cos(x_i))^2 = \sum_i y_i\cos(x_i)$$

This linear system of equations can be formulated as $\phi\,\phi^t\binom{a}{b} = \phi\,\vec{y}$,

where

$$\phi = \begin{bmatrix} \ln(x_0) & \cdots & \ln(x_n) \\ & & \\ \cos(x_0) & \cdots & \cos(x_n) \end{bmatrix}$$

that is again the collocation matrix

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5 Differentiation and Integration

5.1 Difference quotients

When analytical computations of derivatives are not feasible, approximations need to be taken into account

From calculus: $\lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = f'(x)$

So, for h small enough we may approximate

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{forward differencing}$$

How large is the error?

Taylor series expansion:

$$\boxed{f(x+h) = f(x) + h \cdot f'(x) + \frac{h^2}{2} f''(\xi)}, \ \xi \in (x, x+h)$$

$$\Leftrightarrow \ f'(x) = \frac{f(x+h) - f(x)}{h} + \underbrace{\frac{h}{2} f''(\xi)}_{\text{error}}$$

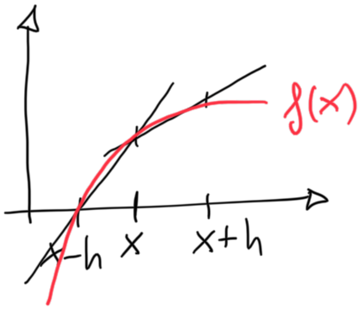
asymptotically $\mathcal{O}(h)$

exact error is $\frac{h}{2} f''(\xi)$

What happens if we do the following approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

backward differencing



Error?

$$\boxed{f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(\xi)} \quad \xi \in (x-h, x)$$

$$\Leftrightarrow \ f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2} f''(\xi)$$

of same error as forward $\overbrace{\text{differencing}}^{\mathcal{O}(h)}$.

Now take the two Taylor series expansions and subtract them:

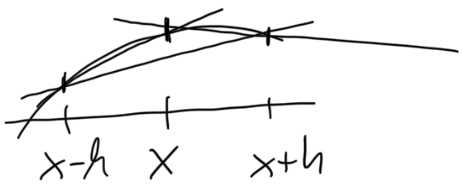
$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(\xi_1)$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(\xi_2)$$

$$\overline{f(x+h) - f(x-h)} = 2h f'(x) + \frac{h^3}{3!}\left[f'''(\xi_1) + f'''(\xi_2)\right]$$

$$\Leftrightarrow \quad f'(x) = \frac{f(x+h) - f(x-h)}{2h} \underbrace{- \frac{h^2}{12}\left[f'''(\xi_1) + f'''(\xi_2)\right]}_{\text{error}}$$

<u>central differencing</u> error asymptotically $\mathcal{O}(h^2)$



5.2 Richardson extrapolation:

Approach for producing higher order approximations from lower order approximations:

Suppose we have a low order approximation $\varphi(h)$ of derivative, e.g.

$$f'(x) = \varphi(h) + a_2 h^2 + a_3 h^3 + \ldots$$

e.g. first order forward difference, i.e. $\varphi(h) = \dfrac{f(x+h) - f(x)}{h}$

For φ = central differencing, i.e. $\varphi(h) = \dfrac{f(x+h) - f(x-h)}{2h}$

(T) $\boxed{f'(x) = \varphi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots}$

I $\quad \boxed{f'(x) = \varphi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots}$

<u>Trick</u>: Evaluate this approximation for $h = \frac{h}{2}$

then
$$f'(x) = \varphi\left(\frac{h}{2}\right) + a_2\left(\frac{h}{2}\right)^2 + a_4\left(\frac{h}{2}\right)^4 + a_6\left(\frac{h}{2}\right)^6 + \dots$$

II $\quad \boxed{= \varphi\left(\frac{h}{2}\right) + \frac{a_2}{4} h^2 + \frac{a_4}{16} h^4 + \frac{a_6}{64} h^6 + \dots}$

<u>Idea</u>: Combine I and II such that the low order error terms cancel out.

I $- 4\,$II:

$$f'(x) - 4 f'(x) = \varphi(h) - 4\varphi\left(\frac{h}{2}\right) + a_4\left(1 - \frac{4}{16}\right)^4 + a_6\left(1 - \frac{4}{64}\right) h^6 + \dots$$

$$\Leftrightarrow \; -3 f'(x) = \varphi(h) - 4\varphi\left(\frac{h}{2}\right) + a_4 \frac{3}{4} h^4 + a_6 \frac{15}{16} h^6 + \dots$$

$$\Leftrightarrow \; f'(x) = \frac{4\varphi\left(\frac{h}{2}\right) - \varphi(h)}{3} \underbrace{- a_4/4\, h^4 - a_6 \frac{5}{16} h^6 - \dots}_{\text{asymptotically } \mathcal{O}(h^4)}$$

In particular, when φ = central differencing:

$$f'(x) \approx \frac{f(x-h) - 8f\left(x-\frac{h}{2}\right) + 8f\left(x+\frac{h}{2}\right) - f(x+h)}{6h}$$

The process of halving the step size and cancelling out terms of the error can be repeated:
We get better approximations at the price of more lower order terms in the approximation.

5.3 Higher order derivatives

Again, Taylor series helps:

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f''''(\xi_1)$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f''''(\xi_2)$$

where $\xi_1 \in (x, x+h)$

add both equations: $\xi_2 \in (x-h, x)$

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{1}{4!} h^4 \left[f''''(\xi_1) + f''''(\xi_2) \right]$$

$$\Leftrightarrow \quad f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \underbrace{\frac{1}{4!} h^2 \left[f''''(\xi_1) + f''''(\xi_2) \right]}_{O(h^2)}$$

<u>3 point stencil</u> $[1, -2, 1]$

Again, Richardson extrapolation can be used to get better approximation.