Chapter 3
Numerical Differentiation

For more complex problems analytical derivatives are not always available and have to be approximated by numerical methods. Numerical differentiation is also very important for the discretization of differential equations (Sect. 12.2). The simplest approximation uses a forward difference quotient (Fig. 3.1) and is not very accurate. A symmetric difference quotient improves the quality. Even higher precision is obtained with the extrapolation method. Approximations to higher order derivatives can be obtained systematically with the help of polynomial interpolation.

3.1 One-Sided Difference Quotient

The simplest approximation of a derivative is the ordinary difference quotient which can be taken forward

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) \approx \frac{\Delta f}{\Delta x} = \frac{f(x+h) - f(x)}{h} \tag{3.1}$$

or backward

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) \approx \frac{\Delta f}{\Delta x} = \frac{f(x) - f(x-h)}{h}. \tag{3.2}$$

Its truncation error can be estimated from the Taylor series expansion

$$\frac{f(x+h) - f(x)}{h} = \frac{f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \cdots - f(x)}{h}$$
$$= f'(x) + \frac{h}{2}f''(x) + \cdots . \tag{3.3}$$

The error order is $O(h)$. The step width should not be too small to avoid rounding errors. Error analysis gives

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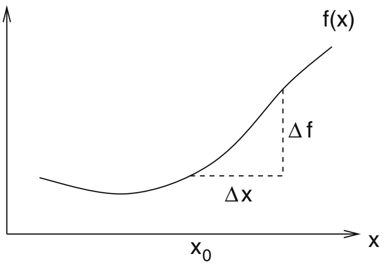


Fig. 3.1 (Numerical differentiation) Numerical differentiation approximates the differential quotient by a difference quotient $\frac{\mathrm{d}f}{\mathrm{d}x} \approx \frac{\Delta f}{\Delta x}$. However, approximation by a simple forward difference $\frac{\mathrm{d}f}{\mathrm{d}x}(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$, is not very accurate

$$\begin{aligned}\widetilde{\Delta f} &= fl_-\left(f(x+h)(1+\varepsilon_1), f(x)(1+\varepsilon_2)\right)\\ &= (\Delta f + f(x+h)\varepsilon_1 - f(x)\varepsilon_2)(1+\varepsilon_3)\\ &= \Delta f + \Delta f\varepsilon_3 + f(x+h)\varepsilon_1 - f(x)\varepsilon_2 + \cdots\end{aligned} \tag{3.4}$$

$$\begin{aligned}fl_\div(\widetilde{\Delta f}, h(1+\varepsilon_4)) &= \frac{\Delta f + \Delta f\varepsilon_3 + f(x+h)\varepsilon_1 - f(x)\varepsilon_2}{h(1+\varepsilon_4)}(1+\varepsilon_5)\\ &= \frac{\Delta f}{h}(1+\varepsilon_5-\varepsilon_4+\varepsilon_3) + \frac{f(x+h)}{h}\varepsilon_1 - \frac{f(x)}{h}\varepsilon_2.\end{aligned} \tag{3.5}$$

The errors are uncorrelated and the relative error of the result can be estimated by

$$\frac{\left|\frac{\widetilde{\Delta f}}{\Delta x} - \frac{\Delta f}{\Delta x}\right|}{\frac{\Delta f}{\Delta x}} \le 3\varepsilon_M + \left|\frac{f(x)}{\frac{\Delta f}{\Delta x}}\right| 2\frac{\varepsilon_M}{h}. \tag{3.6}$$

Numerical extinction produces large relative errors for small step width h. The optimal value of h gives comparable errors from rounding and truncation. It can be found from

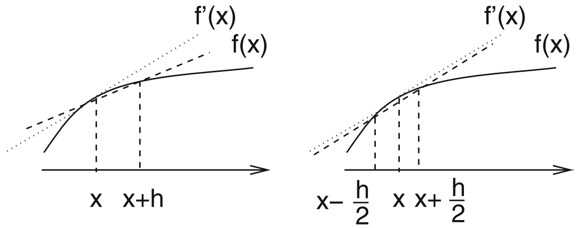
$$\frac{h}{2}|f''(x)| = |f(x)|\frac{2\varepsilon_M}{h}. \tag{3.7}$$

Assuming that the magnitude of the function and the derivative are comparable, we have the rule of thumb

$$h_o = \sqrt{\varepsilon_M} \approx 10^{-8}$$

(double precision). The corresponding relative error is of the same order.

Fig. 3.2 (Difference quotient) The central difference quotient (***Right side***) approximates the derivative (*dotted*) much more accurately than the one-sided difference quotient (***Left side***)



3.2 Central Difference Quotient

Accuracy is much higher if a symmetric central difference quotient is used (Fig. 3.2):

$$\frac{\Delta f}{\Delta x} = \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h}$$
$$= \frac{f(x) + \frac{h}{2}f'(x) + \frac{h^2}{8}f''(x) + \cdots - \left(f(x) - \frac{h}{2}f'(x) + \frac{h^2}{8}f''(x) + \cdots\right)}{h}$$
$$= f'(x) + \frac{h^2}{24}f'''(x) + \cdots . \quad (3.8)$$

The error order is $O(h^2)$. The optimal step width is estimated from

$$\frac{h^2}{24}|f'''(x)| = |f(x)|\frac{2\varepsilon_M}{h} \quad (3.9)$$

again with the assumption that function and derivatives are of similar magnitude as

$$h_0 =^3 \sqrt{48\varepsilon_M} \approx 10^{-5}. \quad (3.10)$$

The relative error has to be expected in the order of $\frac{h_0^2}{24} \approx 10^{-11}$.

3.3 Extrapolation Methods

The Taylor series of the symmetric difference quotient contains only even powers of h:

$$D(h) = \frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{3!}f'''(x) + \frac{h^4}{5!}f^{(5)}(x) + \cdots . \quad (3.11)$$

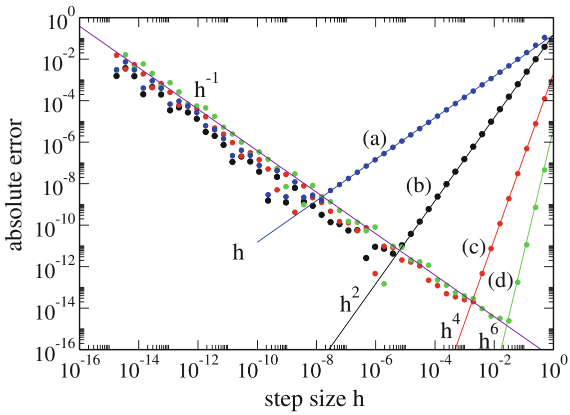


Fig. 3.3 (Numerical differentiation) The derivative $\frac{d}{dx}\sin(x)$ is calculated numerically using algorithms with increasing error order (3.1, 3.8, 3.14, 3.18). For very small step sizes the error increases as h^{-1} due to rounding errors (Problem 3.1)

The Extrapolation method [16] uses a series of step widths, e.g.

$$h_{i+1} = \frac{h_i}{2} \tag{3.12}$$

and calculates an estimate of $D(0)$ by polynomial interpolation (Fig. 3.3). Consider $D_0 = D(h_0)$ and $D_1 = D(\frac{h_0}{2})$. The polynomial of degree 1 (with respect to h^2) $p(h) = a + bh^2$ can be found by the Lagrange method

$$p(h) = D_0 \frac{h^2 - \frac{h_0^2}{4}}{h_0^2 - \frac{h_0^2}{4}} + D_1 \frac{h^2 - h_0^2}{\frac{h_0^2}{4} - h_0^2}. \tag{3.13}$$

Extrapolation for h = 0 gives

$$p(0) = -\frac{1}{3} D_0 + \frac{4}{3} D_1. \tag{3.14}$$

Taylor series expansion shows

$$p(0) = -\frac{1}{3}\left(f'(x) + \frac{h_0^2}{3!} f'''(x) + \frac{h_0^4}{5!} f^{(5)}(x) + \cdots\right) +$$

$$+ \frac{4}{3}\left(f'(x) + \frac{h_0^2}{4 \cdot 3!} f'''(x) + \frac{h_0^4}{16 \cdot 5!} f^{(5)}(x) + \cdots\right) \tag{3.15}$$

$$= f'(x) - \frac{1}{4}\frac{h_0^4}{5!} f^{(5)}(x) + \cdots \tag{3.16}$$

that the error order is $O(h_0^4)$. For 3 step widths $h_0 = 2h_1 = 4h_2$ we obtain the polynomial of second order (in h^2)

$$p(h) = D_0 \frac{(h^2 - \frac{h_0^2}{4})(h^2 - \frac{h_0^2}{16})}{(h_0^2 - \frac{h_0^2}{4})(h_0^2 - \frac{h_0^2}{16})} + D_1 \frac{(h^2 - h_0^2)(h^2 - \frac{h_0^2}{16})}{(\frac{h_0^2}{4} - h_0^2)(\frac{h_0^2}{4} - \frac{h_0^2}{16})} + D_2 \frac{(h^2 - h_0^2)(h^2 - \frac{h_0^2}{4})}{(\frac{h_0^2}{16} - h_0^2)(\frac{h_0^2}{16} - \frac{h_0^2}{4})} \tag{3.17}$$

and the improved expression

$$p(0) = D_0 \frac{\frac{1}{64}}{\frac{3}{4} \cdot \frac{15}{16}} + D_1 \frac{\frac{1}{16}}{\frac{-3}{4} \cdot \frac{3}{16}} + D_2 \frac{\frac{1}{4}}{\frac{-15}{16} \cdot \frac{-3}{16}} =$$

$$= \frac{1}{45} D_0 - \frac{4}{9} D_1 + \frac{64}{45} D_2 = f'(x) + O(h_0^6). \tag{3.18}$$

Often used is the following series of step widths:

$$h_i^2 = \frac{h_0^2}{2^i}. \tag{3.19}$$

The Neville method

$$P_{i \cdots k}(h^2) = \frac{(h^2 - \frac{h_0^2}{2^i}) P_{i+1 \cdots k}(h^2) - (h^2 - \frac{h_0^2}{2^k}) P_{i \cdots k-1}(h^2)}{\frac{h_0^2}{2^k} - \frac{h_0^2}{2^i}} \tag{3.20}$$

gives for h=0

$$P_{i \cdots k} = \frac{P_{i \cdots k-1} - 2^{k-i} P_{i+1 \cdots k}}{1 - 2^{k-i}} \tag{3.21}$$

which can be written as

$$P_{i \cdots k} = P_{i+1 \cdots k} + \frac{P_{i \cdots k-1} - P_{i+1 \cdots k}}{1 - 2^{k-i}} \tag{3.22}$$

and can be calculated according to the following scheme:

$$\begin{matrix} P_0 = D(h^2) & P_{01} & P_{012} & P_{0123} \\ P_1 = D(\frac{h^2}{2}) & P_{12} & P_{123} & \\ P_2 = D(\frac{h^2}{4} & P_{23} & & \\ \vdots & \vdots & \vdots & \ddots \end{matrix} \tag{3.23}$$

Here the values of the polynomials are arranged in matrix form

$$P_{i \cdots k} = T_{i,k-i} = T_{i,j} \tag{3.24}$$

with the recursion formula

$$T_{i,j} = T_{i+1,j-1} + \frac{T_{i,j-1} - T_{i+1,j}}{1 - 2^j}. \tag{3.25}$$

3.4 Higher Derivatives

Difference quotients for higher derivatives can be obtained systematically using polynomial interpolation. Consider equidistant points

$$x_n = x_0 + nh = \cdots x_0 - 2h, x_0 - h, x_0, x_0 + h, x_0 + 2h, \cdots . \tag{3.26}$$

From the second order polynomial

$$\begin{aligned}
p(x) &= y_{-1}\frac{(x-x_0)(x-x_1)}{(x_{-1}-x_0)(x_{-1}-x_1)} + y_0\frac{(x-x_{-1})(x-x_1)}{(x_0-x_{-1})(x_0-x_1)} \\
&+ y_1\frac{(x-x_{-1})(x-x_0)}{(x_1-x_{-1})(x_1-x_0)} = \\
&= y_{-1}\frac{(x-x_0)(x-x_1)}{2h^2} + y_0\frac{(x-x_{-1})(x-x_1)}{-h^2} \\
&+ y_1\frac{(x-x_{-1})(x-x_0)}{2h^2}
\end{aligned} \tag{3.27}$$

we calculate the derivatives

$$p'(x) = y_{-1}\frac{2x - x_0 - x_1}{2h^2} + y_0\frac{2x - x_{-1} - x_1}{-h^2} + y_1\frac{2x - x_{-1} - x_0}{2h^2} \tag{3.28}$$

$$p''(x) = \frac{y_{-1}}{h^2} - 2\frac{y_0}{h^2} + \frac{y_1}{h^2} \tag{3.29}$$

which are evaluated at x_0:

$$f'(x_0) \approx p'(x_0) = -\frac{1}{2h}y_{-1} + \frac{1}{2h}y_1 = \frac{f(x_0+h) - f(x_0-h)}{2h} \tag{3.30}$$

$$f''(x_0) \approx p''(x_0) = \frac{f(x_0-h) - 2f(x_0) + f(x_0+h)}{h^2}. \tag{3.31}$$

Higher order polynomials can be evaluated with an algebra program. For five sample points

$$x_0 - 2h, x_0 - h, x_0, x_0 + h, x_0 + 2h$$

we find

$$f'(x_0) \approx \frac{f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)}{12h} \tag{3.32}$$

$$f''(x_0) \approx \frac{-f(x_0-2h) + 16f(x_0-h) - 30f(x_0) + 16f(x_0+h) - f(x_0+2h)}{12h^2} \tag{3.33}$$

$$f'''(x_0) \approx \frac{-f(x_0-2h) + 2f(x_0-h) - 2f(x_0+h) + f(x_0+2h)}{2h^3} \tag{3.34}$$

$$f^{(4)}(x_0) \approx \frac{f(x_0-2h) - 4f(x_0-h) + 6f(x_0+h) - 4f(x_0+h) + f(x_0+2h)}{h^4}.$$

3.5 Partial Derivatives of Multivariate Functions

Consider polynomials of more than one variable. In two dimensions we use the Lagrange polynomials

$$L_{i,j}(x,y) = \prod_{k \neq i} \frac{(x-x_k)}{(x_i-x_k)} \prod_{j \neq l} \frac{(y-y_l)}{(y_j-y_l)}. \tag{3.35}$$

The interpolating polynomial is

$$p(x,y) = \sum_{i,j} f_{i,j} L_{i,j}(x,y). \tag{3.36}$$

For the nine sample points

$$\begin{matrix} (x_{-1},y_1) & (x_0,y_1) & (x_1,y_1) \\ (x_{-1},y_0) & (x_0,y_0) & (x_1,y_0) \\ (x_{-1},y_{-1}) & (x_0,y_{-1}) & (x_1,y_{-1}) \end{matrix} \tag{3.37}$$

we obtain the polynomial

$$p(x,y) = f_{-1,-1} \frac{(x-x_0)(x-x_1)(y-y_0)(y-y_1)}{(x_{-1}-x_0)(x_{-1}-x_1)(y_{-1}-y_0)(y_{-1})-y_1)} + \cdots \tag{3.38}$$

which gives an approximation to the gradient

$$\operatorname{grad} f(x_0 y_0) \approx \operatorname{grad} p(x_0 y_0) = \begin{pmatrix} \frac{f(x_0+h,y_0)-f(x_0-h,y_0)}{2h} \\ \frac{f(x_0,y_0+h)-f(x_0,y_0-h)}{2h} \end{pmatrix}, \tag{3.39}$$

the Laplace operator

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)f(x_0,y_0)\approx\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)p(x_0,y_0)$$
$$=\frac{1}{h^2}\left(f(x_0,y_0+h)+f(x_0,y_0-h)+f(x_0,y_0+h)+f(x_0,y_0-h)-4f(x_0,y_0)\right) \tag{3.40}$$

and the mixed second derivative

$$\frac{\partial^2}{\partial x\partial y}f(x_0,y_0)\approx\frac{\partial^2}{\partial x\partial y}p(x_0,y_0)$$
$$=\frac{1}{4h^2}\left(f(x_0+h,y_0+h)+f(x_0-h,y_0-h)-f(x_0-h,y_0+h)-f(x_0+h,y_0-h)\right). \tag{3.41}$$

Problems

Problem 3.1 Numerical Differentiation

In this computer experiment we calculate the derivative of $f(x)=\sin(x)$ numerically with

- the single sided difference quotient

$$\frac{df}{dx}\approx\frac{f(x+h)-f(x)}{h}, \tag{3.42}$$

- the symmetrical difference quotient

$$\frac{df}{dx}\approx D_h f(x)=\frac{f(x+h)-f(x-h)}{2h}, \tag{3.43}$$

- higher order approximations which can be derived using the extrapolation method

$$-\frac{1}{3}D_h f(x)+\frac{4}{3}D_{h/2}f(x) \tag{3.44}$$

$$\frac{1}{45}D_h f(x)-\frac{4}{9}D_{h/2}f(x)+\frac{64}{45}D_{h/4}f(x). \tag{3.45}$$

The error of the numerical approximation is shown on a log-log plot as a function of the step width h.