Chapter 2
Numerical Differentiation

2.1 Introduction

This chapter is the first of two systematic introductions to the numerical treatment of differential equations. Differential equations and, thus, derivatives and integrals are of eminent importance in the modern formulation of natural sciences and in particular of physics. Very often the complexity of the expressions involved does not allow an analytical approach, although modern *symbolic* software can ease a physicists life significantly. Thus, in many cases a numerical treatment is unavoidable and one should be prepared.

We introduce here the notion of finite differences as a basic concept of numerical differentiation [1–3]. In contrast, the next chapter will deal with the concepts of numerical quadrature. Together, these two chapters will set the stage for a comprehensive discussion of algorithms designed to solve numerically differential equations. In particular, the solution of ordinary differential equations will always be based on an integration.

This chapter is composed of four sections. The first repeats some basic concepts of calculus and introduces formally finite differences. The second formulates approximates to derivatives based on finite differences, while the third section includes a more systematic approach based on an operator technique. It allows an arbitrarily close approximation of derivatives with the advantage that the expressions discussed in this section can immediately be applied to the problems at hand. The chapter is concluded with a discussion of some additional aspects.

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2.2 Finite Differences

Let us consider a smooth function $f(x)$ on the finite interval $[a, b] \subset \mathbb{R}$ of the real axis. The interval $[a, b]$ is divided into $N - 1 \in \mathbb{N}$ equally spaced sub-intervals of the form $[x_i, x_{i+1}]$ where $x_1 = a$, $x_N = b$. Obviously, x_i is then given by

$$x_i = a + (i - 1)\frac{b - a}{N - 1}, \quad i = 1, \ldots, N\,. \tag{2.1}$$

We introduce the distance h between two grid-points x_i by:

$$h = x_{i+1} - x_i = \frac{b - a}{N - 1}, \quad \forall i = 1, \ldots, N - 1\,. \tag{2.2}$$

For the sake of a more compact notation we restrict our discussion to equally spaced grid-points keeping in mind that the extension to arbitrarily spaced grid-points by replacing h by h_i is straight forward and leaves the discussion essentially unchanged.

Note that the number of grid-points and, thus, their distance h, has to be chosen in such a way that the function $f(x)$ can be sufficiently well approximated by its function values $f(x_i)$ as indicated in Fig. 2.1. We understand by *sufficiently well approximated* that some interpolation scheme in the interval $[x_i, x_{i+1}]$ will reproduce the function $f(x)$ within a required accuracy. In cases where the function is strongly varying within some sub-interval $[c, d] \subset [a, b]$ and is slowly varying within

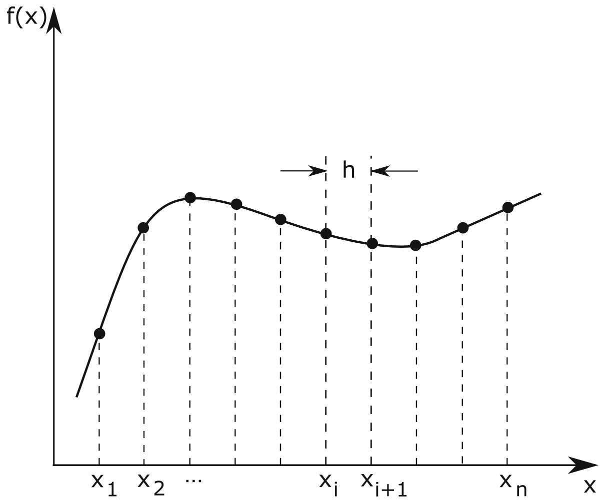

Fig. 2.1 We define equally spaced grid-points x_i on a finite interval on the real axis in such a way that the function $f(x)$ is sufficiently well approximated by its functional values $f(x_i)$ at these grid-points

$[a, b] \setminus [c, d]$ it might be advisable to use variable grid-spacing in order to reduce the computational cost of the procedure.

We introduce the following notation: The function value of $f(x)$ at the grid-point x_i will be denoted by $f_i \equiv f(x_i)$ and its n-th derivative:

$$f_i^{(n)} \equiv f^{(n)}(x_i) = \left.\frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}\right|_{x=x_i} . \tag{2.3}$$

Furthermore, we define for arbitrary $\xi \in [x_i, x_{i+1})$

$$f_{i+\epsilon}^{(n)} = f^{(n)}(\xi) , \tag{2.4}$$

where $f_{i+\epsilon}^{(0)} \equiv f_{i+\epsilon}$ and ϵ is chosen to give:

$$\xi = x_i + \epsilon h , \qquad \epsilon \in [0, 1) . \tag{2.5}$$

Let us remember some basics from calculus: The first derivative, denoted $f'(x)$ of a function $f(x)$ which is smooth within the interval $[a, b]$, i.e. $f(x) \in \mathscr{C}^\infty[a, b]$ for arbitrary $x \in [a, b]$, is defined as

$$\begin{aligned} f'(x) &:= \lim_{h\to 0} \frac{f(x+h) - f(x)}{h} \\ &= \lim_{h\to 0} \frac{f(x) - f(x-h)}{h} \\ &= \lim_{h\to 0} \frac{f(x+h) - f(x-h)}{2h} . \end{aligned} \tag{2.6}$$

However, it is impossible to draw numerically the limit $h \to 0$ as discussed in Sect. 1.3, Eq. (1.22). This manifests itself in a non-negligible error due to subtractive cancellation.

This problem is circumvented by the use of TAYLOR's theorem. It states that if there is a function which is $(n+1)$-times continuously differentiable on the interval $[a, b]$ then $f(x)$ can be expressed in terms of a series expansion at point $x_0 \in [a, b]$:

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}[\zeta(x)]}{(n+1)!}(x - x_0)^{n+1}, \quad \forall x \in [a, b] . \tag{2.7}$$

Here, $\zeta(x)$ takes on a value between x and x_0.[1] The last term on the right hand side of Eq. (2.7) is commonly referred to as *truncation error*. (A more general definition of this error was given in Sect. 1.1.)

[1] Note that for $x_0 = 0$ the series expansion (2.7) is referred to as MCLAURIN series.

We introduce now the finite difference operators

$$\Delta_+ f_i = f_{i+1} - f_i \ , \tag{2.8a}$$

as the *forward difference*,

$$\Delta_- f_i = f_i - f_{i-1} \ , \tag{2.8b}$$

as the *backward difference*, and

$$\Delta_c f_i = f_{i+1} - f_{i-1} \ , \tag{2.8c}$$

as the *central difference*.[2] The derivative of $f(x)$ can be approximated with the help of TAYLOR's theorem (2.7). In a first step we consider (restricting to third order in h)

$$\begin{aligned} f_{i+1} &= f(x_i) + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \frac{h^3}{6} f'''[\zeta(x_i + h)] \\ &= f_i + hf_i' + \frac{h^2}{2} f_i'' + \frac{h^3}{6} f_{i+\epsilon_\zeta}''' \ , \end{aligned} \tag{2.9a}$$

with $f_{i+1} \equiv f(x_i + h)$. Here ϵ_ζ is the fractional part ϵ which has to be determined according to $\zeta(x_i + h)$. In analogue we find for f_{i-1}

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2} f_i'' - \frac{h^3}{6} f_{i+\epsilon_\zeta}''' \ . \tag{2.9b}$$

Solving Eqs. (2.9) for the derivative f_i' leads directly to the definition of finite difference derivatives.

2.3 Finite Difference Derivatives

We define the *finite difference derivative* or difference approximations

$$D_+ f_i = \frac{\Delta_+ f_i}{h} = \frac{f_{i+1} - f_i}{h} \ , \tag{2.10a}$$

as the *forward difference derivative*,

[2] Please note that the symbols Δ_+, Δ_-, and Δ_c in Eqs. (2.8) are linear operators acting on f_i. For a basic introduction to the theory of linear operators see for instance [4, 5].

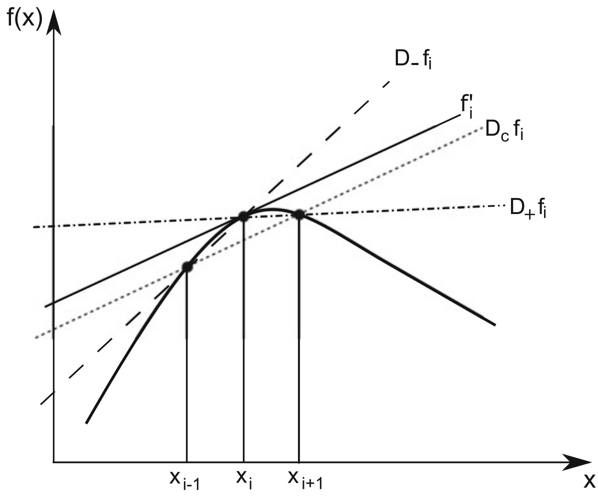

Fig. 2.2 Graphical illustration of different finite difference derivatives. The *solid line* labeled f_i' represents the real derivative for comparison

$$D_- f_i = \frac{\Delta_- f_i}{h} = \frac{f_i - f_{i-1}}{h} \,, \tag{2.10b}$$

as the *backward difference derivative*, and

$$D_c f_i = \frac{\Delta_c f_i}{2h} = \frac{f_{i+1} - f_{i-1}}{2h} \,, \tag{2.10c}$$

as the *central difference derivative*.[3] A graphical interpretation of these expressions is straight forward and is presented in Fig. 2.2.

Using the above definitions (2.10) together with the expansions (2.9) we obtain

$$\begin{aligned} f_i' &= D_+ f_i - \frac{h}{2} f_i'' - \frac{h^2}{6} f_{i+\epsilon_\zeta}''' \\ &= D_- f_i + \frac{h}{2} f_i'' - \frac{h^2}{6} f_{i+\epsilon_\zeta}''' \\ &= D_c f_i - \frac{h^2}{6} f_{i+\epsilon_\zeta}''' \,. \end{aligned} \tag{2.11}$$

We observe that in the central difference approximation of f_i' the truncation error scales like h^2 while it scales like h in the other two approximations; thus the central

[3] The central difference derivative is related to the forward and backward difference derivatives via:

$$D_c = \frac{1}{2}(D_+ + D_-).$$

difference approximation should have the smallest methodological error. Note that the error is usually not dominated by the derivatives of $f(x)$ since we assumed that $f(x)$ is a smooth function and sufficiently well approximated on the grid within $[a, b]$. Furthermore we have to emphasize that the central difference approximation is essentially a *three point* approximation, including f_{i-1}, f_i and f_{i+1}, although f_i cancels. Thus, we can improve our approximation by taking even more grid-points into account. For instance, we could combine the above finite difference derivatives. Let us prepare this step by expanding Eqs. (2.9) to higher order derivatives. We then obtain for the forward difference derivative

$$D_+f_i = f_i' + \frac{h}{2}f_i'' + \frac{h^2}{6}f_i''' + \frac{h^3}{24}f_i^{IV} + \frac{h^4}{120}f_i^V + \dots\ , \tag{2.12}$$

for the backward difference derivative

$$D_-f_i = f_i' - \frac{h}{2}f_i'' + \frac{h^2}{6}f_i''' - \frac{h^3}{24}f_i^{IV} + \frac{h^4}{120}f_i^V \mp \dots\ , \tag{2.13}$$

and, finally, for the central difference derivative

$$D_cf_i = f_i' + \frac{h^2}{6}f_i''' + \frac{h^4}{120}f_i^V + \dots\ . \tag{2.14}$$

In order to improve the method we have to combine D_+f_i, D_-f_i and D_cf_i from different grid-points in such a way that at least the terms proportional to h^2 cancel. This can be achieved by observing that[4]

$$8D_cf_i - D_cf_{i-1} - D_cf_{i+1} = 6f_i' - \frac{h^4}{5}f_{i+\epsilon_\zeta}^V\ , \tag{2.15}$$

which gives

$$\begin{aligned} f_i' &= \frac{1}{6}\left(8D_cf_i - D_cf_{i+1} - D_cf_{i-1}\right) + \frac{h^4}{30}f_i^V \\ &= \frac{1}{12h}\left(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}\right) + \frac{h^4}{30}f_i^V\ . \end{aligned} \tag{2.16}$$

Note that this simple combination yields an improvement of two orders in h ! One can even improve the approximation in a similar fashion by simply calculating the derivative from even more points, for instance $f_{i\pm 3}$.

[4] Please note that the TAYLOR expansion of $(D_cf_{i-1} + D_cf_{i+1})/2 = (f_{i+2} - f_{i-2})/(4h)$ is equivalent to the expansion (2.14) of D_cf_i with h replaced by $2h$.

2.4 A Systematic Approach: The Operator Technique

We would like to obtain a general expression which will allow to calculate the finite difference derivatives of arbitrary order up to arbitrary order of h in the truncation error. We achieve this goal by introducing the shift operator T and its inverse operator T^{-1} as[5]

$$Tf_i = f_{i+1} \ , \tag{2.18}$$

and

$$T^{-1}f_i = f_{i-1} \ , \tag{2.19}$$

where $TT^{-1} = \mathbb{1}$ is the unity operator. We can write these operators in terms of the forward and backward difference operators Δ_+ and Δ_- of Eqs. (2.8), in particular

$$T = \mathbb{1} + \Delta_+ \ , \tag{2.20}$$

and

$$T^{-1} = \mathbb{1} - \Delta_- \ . \tag{2.21}$$

Moreover, if $D \equiv \mathrm{d}/\mathrm{d}x$ denotes the derivative operator and if the n-th power of this operator D is understood as the n-th successive application of it, we can rewrite the TAYLOR expansions (2.9) as

$$\begin{aligned} f_{i+1} &= \left[\mathbb{1} + hD + \frac{1}{2}h^2D^2 + \frac{1}{3!}h^3D^3 + \dots\right] f_i \\ &\equiv \exp(hD) f_i \ , \end{aligned} \tag{2.22}$$

[5] We note in passing that the shift operators form the discrete translational group, a very important group in theoretical physics. Let $T(n) = T^n$ denote the shift by $n \in \mathbb{N}$ grid-points. We then have

$$T(n)T(m) = T(n+m) \ , \tag{2.17a}$$

$$T(0) = \mathbb{1} \ , \tag{2.17b}$$

and

$$T(n)^{-1} = T(-n) \ , \tag{2.17c}$$

which are the properties required to form a group. Here $\mathbb{1}$ denotes unity. Moreover, we have

$$T(n)T(m) = T(m)T(n) \ , \tag{2.17d}$$

i.e. it is an Abelian group. The group of discrete translations is usually denoted by $\mathbb{T}^d$ [6].

and

$$f_{i-1} = \left[\mathbb{1} - hD + \frac{1}{2}h^2D^2 - \frac{1}{3!}h^3D^3 \pm \ldots\right] f_i$$
$$\equiv \exp(-hD) f_i \ , \tag{2.23}$$

Hence, we find that [7][6]

$$T = \mathbb{1} + \Delta_+ \equiv \exp(hD) \ , \tag{2.24}$$

and, accordingly, that

$$T^{-1} = \mathbb{1} - \Delta_- \equiv \exp(-hD) \ . \tag{2.25}$$

Finally, we obtain the central difference operator:

$$\Delta_c = T - T^{-1} = \exp(hD) - \exp(-hD) \equiv 2\sinh(hD) \ . \tag{2.26}$$

Equations (2.24), (2.25) and (2.26) can be inverted for hD:

$$hD = \begin{cases} \ln(\mathbb{1} + \Delta_+) = \Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3 \mp \ldots \ , \\ -\ln(\mathbb{1} - \Delta_-) = \Delta_- + \frac{1}{2}\Delta_-^2 + \frac{1}{3}\Delta_-^3 + \ldots \ , \\ \sinh^{-1}\left(\frac{\Delta_c}{2}\right) = \frac{\Delta_c}{2} - \frac{1}{3!}\left(\frac{\Delta_c}{2}\right)^3 + \frac{3^2}{5!}\left(\frac{\Delta_c}{2}\right)^5 \mp \ldots \ . \end{cases} \tag{2.27}$$

Again, the n-th power of an operator K (with $K = \Delta_+, \Delta_-, \Delta_c$) $K^n f_i$ is understood as the n-th successive action of the operator K on f_i, i.e. $K^{n-1}(Kf_i)$. Expression (2.27) allows to approximate the derivatives up to arbitrary order using finite differences. Furthermore, we can take the k-th power of Eq. (2.27) in order to get an approximate k-th derivative, $(hD)^k$ [7].

However, it turns out that the expansion (2.27) in terms of the central difference Δ_c does not optimally use the grid because it contains only odd powers of Δ_c. For instance, the third power $\Delta_c^3 f_i$ includes the function values $f_{i\pm3}$ and $f_{i\pm1}$ at 'odd' grid-points but ignores the function values f_i and $f_{i\pm2}$ at 'even' grid-points. Since this is true for all odd powers of Δ_c we observe that the expansion (2.27) uses only half of the grid. On the other hand, if one computes the square $(hD)^2$ of (2.27) only 'even' grid-points are used, while the 'odd' grid-points are ignored. This reduces the accuracy of the method and an improvement is required. The easiest remedy

[6]This representation of the shift operator T explains why the derivative operator D is frequently referred to as the *infinitesimal generator of translations* [6].

is to formally introduce function values $T^{\pm\frac{1}{2}} f_i \stackrel{!}{=} f_{i\pm 1/2}$ at *intermediate* grid-points[7] $x_{i\pm 1/2} = x_i \pm h/2$. This definition allows to introduce the central difference operator δ_c of intermediate grid-points,

$$\delta_c = T^{\frac{1}{2}} - T^{-\frac{1}{2}} = 2\sinh\left(\frac{hD}{2}\right), \tag{2.28}$$

and the average operator:

$$\mu = \frac{1}{2}\left(T^{\frac{1}{2}} + T^{-\frac{1}{2}}\right) = \cosh\left(\frac{hD}{2}\right). \tag{2.29}$$

The central difference operator Δ_c on the grid is connected to the central difference operator δ_c of intermediate grid-points by:

$$\Delta_c = 2\mu\delta_c. \tag{2.30}$$

To avoid the problem of Eq. (2.27) that only odd or even grid-points are accounted for we replace all shift operators $\Delta_c/2$ by δ_c and then multiply the right hand side of Eq. (2.27) by μ. This ensures that function values at intermediate grid-points will not appear in the final expression. Hence, we obtain for the first order derivative operator:

$$D = \frac{1}{h}\begin{cases} \Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3 \mp \ldots, \\ \Delta_- + \frac{1}{2}\Delta_-^2 + \frac{1}{3}\Delta_-^3 + \ldots, \\ \mu\delta_c - \frac{1}{3!}\mu\delta_c^3 + \frac{3^2}{5!}\mu\delta_c^5 \mp \ldots \end{cases} \tag{2.31}$$

When higher order derivatives are calculated, we replace, again, $\Delta_c/2$ by δ_c and multiply odd powers of δ_c by μ. This procedure results, for instance, in the second order derivative operator:

$$D^2 = \frac{1}{h^2}\begin{cases} \Delta_+^2 - \Delta_+^3 + \frac{11}{12}\Delta_+^4 \mp \ldots, \\ \Delta_-^2 + \Delta_-^3 + \frac{11}{12}\Delta_-^4 + \ldots, \\ \delta_c^2 - \frac{1}{3}\delta_c^4 + \frac{8}{45}\delta_c^6 \mp \ldots. \end{cases} \tag{2.32}$$

[7] These intermediate grid-points are virtual, auxiliary grid-points which will be eliminated in due course.

In particular, we obtain for the central difference derivative

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + \mathscr{O}(h^2) , \tag{2.33}$$

and

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \mathscr{O}(h^2) . \tag{2.34}$$

Here, $\mathscr{O}(h^2)$ indicates that this term is of the order of h^2 and we get the important result that the truncation error is of the order $\mathscr{O}(h^2)$.[8]

2.5 Concluding Discussion

First of all, although Eq. (2.27) allows to approximate a derivative of any order k arbitrarily close, it is still an infinite series which leaves us with the decision at which order to truncate. This choice will highly depend on the choice of h which in turn depends on the function we would like to differentiate. Consider, for instance, the periodic function

$$f(x) = \exp(i\omega x) , \tag{2.35}$$

where $\omega, x \in \mathbb{R}$ and i is the imaginary unit with $i^2 = -1$. Its first derivative is

$$f'(x) = i\omega \exp(i\omega x) . \tag{2.36}$$

We now introduce grid-points by

$$x_k = x_0 + kh , \tag{2.37}$$

where h is the grid-spacing and x_0 is some finite starting point on the real axis. Accordingly,

$$f_k = \exp[i\omega(x_0 + kh)] , \tag{2.38}$$

[8] The leading order of the truncation error can be determined by inserting the dominant contribution of Eqs. (2.28) and (2.29) into the remainder of Eqs. (2.31) and (2.32), respectively. For instance, it follows from Eq. (2.29) that $\mu \sim \mathscr{O}(1)$ and from Eq. (2.28) that $\delta_c \sim \mathscr{O}(h)$ and, hence, we find with the help of Eq. (2.31) that $\mu\delta_c^3/h \sim \mathscr{O}(h^2)$. In analogue, we obtain from Eq. (2.32) that $\delta_c^4/h^2 \sim \mathscr{O}(h^2)$.

and the exact value of the first derivative is

$$f'_k = i\omega \exp\left[i\omega(x_0 + kh)\right] = i\omega f_k \ . \tag{2.39}$$

We calculate the forward, backward, and central difference derivatives according to Eqs. (2.10) and obtain

$$D_+ f_k = i\omega f_k \exp\left(\frac{ih\omega}{2}\right) \operatorname{sinc}\left(\frac{h\omega}{2}\right) \ , \tag{2.40a}$$

with $\operatorname{sinc}(x) = \sin(x)/x$ and

$$D_- f_k = i\omega f_k \exp\left(-\frac{ih\omega}{2}\right) \operatorname{sinc}\left(\frac{h\omega}{2}\right) \ , \tag{2.40b}$$

and

$$D_c f_k = i\omega f_k \operatorname{sinc}(h\omega) \ . \tag{2.40c}$$

We divide the approximate derivatives by the true value (2.39) and take the modulus. We get

$$\left|\frac{D_+ f_k}{f'_k}\right| = \left|\frac{D_- f_k}{f'_k}\right| = \operatorname{sinc}\left(\frac{h\omega}{2}\right), \tag{2.41}$$

and

$$\left|\frac{D_c f_k}{f'_k}\right| = \operatorname{sinc}(h\omega) \ . \tag{2.42}$$

Since $|\sin(x)| \leq |x|$, $\forall x \in \mathbb{R}$ we obtain that in all three cases this ratio is less than one independent of h, unless $\omega = 0$. (Please keep in mind that $\operatorname{sinc}(x) \to 1$ as $x \to 0$.) Hence, the first order finite difference approximations underestimate the true value of the derivative. The reason is easily found: $f(x)$ oscillates with frequency ω while the finite difference derivatives applied here approximate the derivative linearly. Higher order corrections will, of course, improve the approximation significantly. Furthermore, we observe that the one-sided finite difference derivatives (2.40a) and (2.40b) are exactly zero if $h\omega = 2n\pi$, $n \in \mathbb{N}$, i.e. if the grid-spacing h matches a multiple of the frequency $2\pi\omega$ of the function $f(x)$. The same occurs when central derivatives (2.40c) are used, but now for $h\omega = \pi n$. This is not really a problem in our example because we choose the grid-spacing $h \ll 2\pi/\omega$ in order to approximate the function $f(x)$ sufficiently well. However, in many cases the analytic form of the function is unknown and we only have its representation on the grid. In this case one has to check carefully by changing h whether the function is periodic or not.

We discuss, finally, how to approximate partial derivatives of functions which depend on more than one variable. Basically this can be achieved by independently discretisizing the function of interest in each particular variable and then by defining the corresponding finite difference derivatives. We will briefly discuss the case of two variables and the extension to even more variables is straight forward. We regard a function $g(x, y)$ where $(x, y) \in [a, b] \times [c, d]$. We denote the grid-spacing in x-direction by h_x and in y-direction by h_y. The evaluation of derivatives of the form $\frac{\partial^n}{\partial x^n} g(x, y)$ or $\frac{\partial^n}{\partial y^n} g(x, y)$ for arbitrary n are approximated with the help of the schemes discussed above, only the respective grid-spacing has to be accounted for. We will now briefly discuss mixed partial derivatives, in particular the derivative $\frac{\partial^2}{\partial x \partial y} g(x, y)$. Higher orders can be easily obtained in the same fashion. Here, we will restrict to the case of the central difference derivative. Again, the extension to the other two forms of derivatives is straight forward. We would like to approximate the derivative at the point $(a + ih_x, c + jh_y)$, which will be abbreviated by (i, j). Hence, we compute

$$\begin{aligned}
\frac{\partial}{\partial y} \frac{\partial}{\partial x} g(x, y)\bigg|_{(i,j)} &= \frac{1}{2h_x}\left[\frac{\partial}{\partial y} g(x, y)\bigg|_{(i+1,j)} - \frac{\partial}{\partial y} g(x, y)\bigg|_{(i-1,j)}\right] + \mathcal{O}(h_x^2) \\
&= \frac{1}{2h_x}\left[\frac{g_{i+1,j+1} - g_{i+1,j-1}}{2h_y} + \mathcal{O}(h_y^2)\bigg|_{(i+1,j)}\right. \\
&\qquad \left. - \frac{g_{i-1,j+1} - g_{i-1,j-1}}{2h_y} - \mathcal{O}(h_y^2)\bigg|_{(i-1,j)}\right] + \mathcal{O}(h_x^2) , \qquad (2.43)
\end{aligned}$$

where we made use of the notation $g_{i,j} \equiv g(x_i, y_j)$. Neglecting higher order contributions yields

$$\frac{\partial}{\partial y} \frac{\partial}{\partial x} g(x, y)\bigg|_{(i,j)} \approx \frac{1}{2h_x} \frac{g_{i+1,j+1} - g_{i+1,j-1} - g_{i-1,j+1} + g_{i-1,j-1}}{2h_y} . \qquad (2.44)$$

This simple approximation is easily improved with the help of methods developed in the previous sections.

It should be noted that there are also other methods to approximate derivatives. One of the most powerful methods, is the method of *finite elements* [8]. The conceptual difference to the method of finite differences is that one divides the domain in finite sub-domains (elements) rather than by replacing these by sets of discrete grid-points. The function of interest, say $g(x, y)$, is then replaced within each element by an interpolating polynomial. However, this method is quite complex and definitely beyond the scope of this book. Another interesting method, which is particularly useful for the solution of hyperbolic differential equations, is the method of *finite volumes*. The interested reader is referred to the book by R. J. LeVeque [9].

Summary

In a first step the notion of finite differences was introduced: All functions are approximated only by their functional values at discrete grid-points and by interpolation schemes between these points. This served as a basis for the definition of finite difference derivatives. Three different types were discussed: the forward, the backward, and the central difference derivative. A more systematic approach to finite difference derivatives was then offered by the operator technique. It provided ready to use equations which allowed to approximate a particular derivative of arbitrary order to arbitrary order of grid-spacing. The two methodological errors introduced by this method, namely the subtractive cancellation error due to too dense a grid and the truncation error due to too coarse a grid were discussed in detail.

Problems

1. Derive Eq. (2.32).
2. Calculate numerically the derivative of the function

$$f(x) = \cos(\omega_1 x) + \exp(-x^2/2)\sin(\omega_2 x),$$

   with $\omega_2 = 0.5$ and $\omega_2 = 10\omega_1$. Use a non-uniform grid. Calculate locally the relative error of your approximation.
3. Extend your code of the previous example to arbitrary $\omega_1 \leq 10\omega_2$ and $\omega_2 = 0.5$ by implementing an adaptive grid-spacing. In particular, write a routine which recursively finds a suitable grid-spacing.
4. Consider the finite interval $I = [-5, 5]$ on the real axis. Define N equally spaced grid-points $x_i = x_1 + (i-1)h$, $i = 1, \ldots, N$. Investigate the functions

$$g(x) = \exp\left(-x^2\right) \quad \text{and} \quad h(x) = \sin(x).$$

   a. Plot these functions within the interval I by defining these functions on the grid-points x_i.
   b. Plot the first derivative of these functions by analytical differentiation.
   c. Calculate and plot the first derivatives of these functions by employing the first order backward, forward, and central difference derivatives. For the central difference derivative use an algorithm which is based on the grid-points x_{i-1} and x_{i+1} rather than the method based on intermediate grid-points $x_{i\pm\frac{1}{2}}$.
   d. Calculate and plot the first central difference derivatives of these functions by employing second order corrections. These corrections can be obtained by applying the sum representation of the derivative operator defined in Sect. 2.4, last line of Eq. (2.31), i.e. take the term proportional to δ_c^3 into account!

e. Calculate the absolute and the relative error of the above methods. Note that the exact values are known analytically.
f. Repeat the above steps for the second derivative of the function $h(x)$. For the second order correction of the central difference derivative take the term proportional to δ_c^4 in Eq. (2.32) into account.
g. Try different values of N.

5. Consider the function:

$$f(x, y) = \cos(x)\exp(-y^2).$$

a. Calculate numerically its gradient $\nabla f(x, y)$ and compare with the analytical result.
b. Demonstrate numerically that gradient fields are curl-free, i.e. $\nabla \times \nabla f(x, y) = 0$ for all x and y.

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