Chapter 2

Discretization schemes

In this chapter:

- finite-difference formula by Taylor series
- finite-difference formula by Lagrange interpolation
- compact-difference formula by fictitious point method
- analysis of finite and compact difference schemes
- spectral methods

When solving partial differential equations on a computer, we have to replace spatial and temporal derivatives of continuous variables by their discrete representations. Space and time will be discretized by introducing a spatio-temporal grid on which we seek an approximation for the continuous solution of the partial differential equation. A wide range of representations on this grid are available, and we shall discover a few in this book. For the majority of our studies, we will concentrate on finite-difference approximations – and their variants – of continuous derivative operators.

2.1 Finite differences

We will represent a one-dimensional scalar function $f(x)$ on an ordered set of discrete points $\{x_j\}$ on the real line. Although many of the concepts introduced below generalize to an arbitrarily spaced set of points, we will often concentrate on regular grids, i.e., sets of ordered **equispaced** points $x_j = j\Delta x$ with $\Delta x > 0$ as the constant space step. With this definition we will approximate continuous functions $f(x)$ and their derivatives by **grid functions** $f_j = f(x_j)$; see figure 2.1.

The finite-difference (FD) method replaces continuous derivatives in the governing equations by finite-difference approximations. The underlying task then is to approximate the derivative $df/dx = f'(x)$ of the continuous function $f(x)$ evaluated

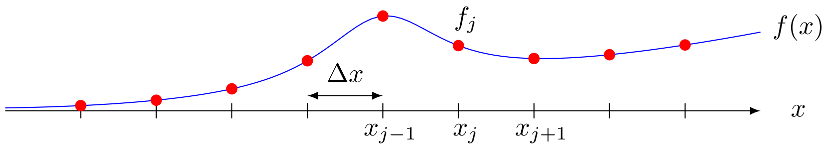


Fig. 2.1 Sketch of a one-dimensional equispaced grid and a discrete representation of a continuous function $f(x)$ on this grid.

at a specified grid point x_j by a linear combination of discrete function values f_j. For the case of a first derivative this may lead to

$$f'_j \approx \frac{f(x_j + \Delta x) - f(x_j)}{\Delta x} = \frac{f_{j+1} - f_j}{\Delta x}. \tag{2.1}$$

Of course, other choices are conceivable. In general we have to specify the number and location of discrete function values $\{f_j\}$ which are used in the approximation, as well as the location at which the derivative is to be evaluated. For example, taking into account three function values $\{f_{j-1},\ f_j,\ f_{j+1}\}$ and evaluating the first derivative at the central point x_j, we obtain the general setup

$$f'_j \approx af_{j-1} + bf_j + cf_{j+1} \tag{2.2}$$

with yet unknown coefficients a, b, and c.

Similar setups for higher derivatives, or for different locations of the involved function values, are imaginable. Once the unknown coefficients are determined, the derivatives in the governing equations can then be replaced by linear combinations of the function values, resulting in a linear or nonlinear system of equations for the function values $\{f_j\}$, which in turn has to be solved numerically.

Finite-difference formula via Taylor series expansions

To determine the weight coefficients a, b, and c in the above expression (2.2) for the first derivative, we use a Taylor series expansion of the function $f(x)$ about the point x_j where the derivative is sought. We obtain (assuming an equidistant grid)

$$\begin{aligned} f'_j \approx\ & a\left(f_j - f'_j \Delta x + \frac{1}{2} f''_j \Delta x^2 + \ldots\right) + \\ & b\ f_j + \\ & c\left(f_j + f'_j \Delta x + \frac{1}{2} f''_j \Delta x^2 + \ldots\right). \end{aligned} \tag{2.3}$$

Collecting terms on the right-hand side according to the order of the derivatives and matching them to the expression on the left-hand side, we are able to extract a set of three equations for the three unknown coefficients. We obtain

$$f_j \quad \rightarrow \qquad a + b + c = 0, \tag{2.4a}$$

$$f'_j \quad \rightarrow \qquad -a + c = 1/\Delta x, \tag{2.4b}$$

$$f''_j \quad \rightarrow \qquad a + c = 0. \tag{2.4c}$$

The solution of this system is easily determined as

$$a = -\frac{1}{2\Delta x}, \qquad b = 0, \qquad c = \frac{1}{2\Delta x}, \tag{2.5}$$

which produces the following approximation to the first derivative of $f(x)$ at the grid point x_j based on values of the function $f(x)$ evaluated at three locations in the neighborhood of x_j :

$$f'_j \approx \frac{f_{j+1} - f_{j-1}}{2\Delta x} \tag{2.6}$$

which we recognize as an application of the mean-value theorem. The coefficients were obtained by requiring a match between the Taylor-expanded right-hand side and the derivative term on the left-hand side. By our design, only three constants $\{a, b, c\}$ were available to make this match. As a consequence, an error term appears when higher-order derivative terms on the right-hand side do not cancel. The lowest of the non-cancelling terms is referred to as the **truncation error** e. In our case above we have

$$e = (c - a)\frac{f'''_j}{3!}\Delta x^3 = \frac{f'''_j}{3!}\Delta x^2 \sim \mathcal{O}(\Delta x^2) \tag{2.7}$$

which labels the finite-difference approximation of the first derivative second-order accurate. As the grid is refined, the truncation error decreases quadratically with the mesh width Δx. Representations of the first derivative to higher than second order require more function values f_j such that more coefficients can be used to eliminate even higher-order derivatives on the right-hand side.

Finite-difference formula via Lagrange interpolation

An alternative and arguably more elegant method to design finite-difference approximations to continuous derivatives is based on Lagrange interpolation. The idea is to reconstruct a local, approximate, but *continuous* representation of the function $f(x)$ by interpolating the discrete function values f_j using a polynomial of appropriate degree. This polynomial interpolant is then differentiated *exactly* and evaluated at the point of interest.

The concept thus relies on a three-step procedure:

(1) interpolation of the data points by a polynomial of appropriate degree,
(2) exact differentiation of the polynomial interpolant, and
(3) evaluation of the differentiated interpolant at the desired grid point.

This method is outlined graphically in figure 2.2 where, again, we choose three grid points $\{x_{j-1},\ x_j,\ x_{j+1}\}$ and function values $\{f_{j-1},\ f_j,\ f_{j+1}\}$ to derive an approximation to a first derivative f_j' at the middle grid point x_j.

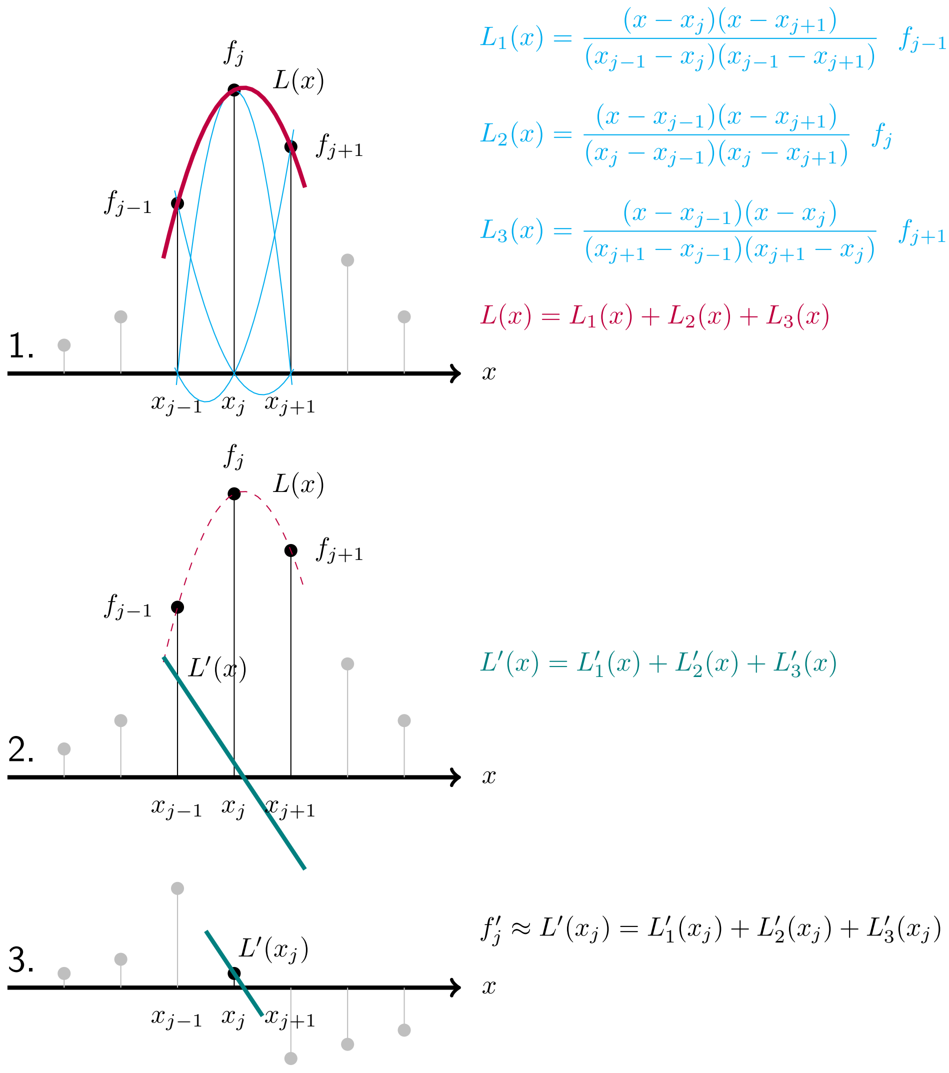


Fig. 2.2 Numerical differentiation based on polynomial interpolation. In a first step, a continuous representation of the discrete data points is determined using a polynomial Lagrange interpolant. This interpolant is then differentiated (second step) and evaluated at a prescribed point (third step).

The first step is best accomplished by forming the **Lagrange polynomial** for the data points under consideration. The second step is straightforward as well, and the last step only requires the choice of a reference point. We commence by constructing the (quadratic) Lagrange polynomial $L(x)$ through the points $(x_{j-1}, f_{j-1}), (x_j, f_j), (x_{j+1}, f_{j+1})$ as

$$\begin{aligned} L(x) = & \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f_{j-1} \\ & + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} f_j \\ & + \frac{(x - x_{j-1})(x - x_j)}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f_{j+1}. \end{aligned} \tag{2.8}$$

Following our procedure we differentiate the Lagrange polynomial with respect to x and obtain

$$\begin{aligned} L'(x) = & \frac{2x - (x_j + x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f_{j-1} \\ & + \frac{2x - (x_{j-1} + x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} f_j \\ & + \frac{2x - (x_{j-1} + x_j)}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f_{j+1}. \end{aligned} \tag{2.9}$$

Finally, evaluating the derivative $L'(x)$ of the polynomial at the reference point x_j and introducing the abbreviation $\Delta x_j = x_j - x_{j-1}$ we get

$$\begin{aligned} f'_j \approx L'(x_j) = & \left[-\frac{\Delta x_{j+1}}{\Delta x_j (\Delta x_j + \Delta x_{j+1})} \right] f_{j-1} + \\ & \left[\frac{\Delta x_{j+1} - \Delta x_j}{\Delta x_j \Delta x_{j+1}} \right] f_j + \\ & \left[\frac{\Delta x_j}{\Delta x_{j+1} (\Delta x_j + \Delta x_{j+1})} \right] f_{j+1} \end{aligned} \tag{2.10}$$

which gives the proper weights to assign to the function values f_{j-1}, f_j, f_{j+1} to obtain an approximation to the first derivative at the point x_j. For equispaced grids, i.e. $\Delta x_j = \Delta x_{j+1} \equiv \Delta x$, the above formula (2.10) simplifies to

$$f'_j \approx \left[\frac{1}{2\Delta x} \right] f_{j+1} - \left[\frac{1}{2\Delta x} \right] f_{j-1}. \tag{2.11}$$

which recovers the expression (2.6), derived via a Taylor series expansion about the reference point x_j.

In a similar fashion, we can determine the discrete approximation of the first derivative taking into account only function values at one side of the reference points. These approximations to derivatives of functions are known as **one-sided** formula and are of particular interest when derivatives have to be evaluated on the boundary of the computational domain, where function values are only available on one side of the reference point. In this case, we can evaluate the Lagrange polynomial, for example, at the point x_{j-1} which leads to

$$\begin{aligned} f'_{j-1} \approx \ & \left[-\frac{2\Delta x_j + \Delta x_{j+1}}{\Delta x_j(\Delta x_j + \Delta x_{j+1})}\right] f_{j-1} + \\ & \left[\frac{\Delta x_j + \Delta x_{j+1}}{\Delta x_j \Delta x_{j+1}}\right] f_j + \\ & \left[-\frac{\Delta x_j}{\Delta x_{j+1}(\Delta x_j + \Delta x_{j+1})}\right] f_{j+1} \end{aligned} \tag{2.12}$$

which, for equispaced grid points, reduces to

$$f'_{j-1} \approx \left[-\frac{3}{2\Delta x}\right] f_{j-1} + \left[\frac{2}{\Delta x}\right] f_j + \left[-\frac{1}{2\Delta x}\right] f_{j+1}. \tag{2.13}$$

n-th-order derivatives can be determined in the same way by differentiating the interpolating polynomial n times. This course of action then makes immediately clear that in order to determine the n-th derivative we need at least an n-th order polynomial which in turn requires $n + 1$ data points to be included in the finite-difference approximation; including even more points will increase the quality (or order of accuracy) of our approximation.

As an example, we will determine the finite-difference approximation for the second derivative using the same three data points above. For this purpose, we can reuse the above Lagrange polynomial and differentiate once more. We get

$$\begin{aligned} L''(x) = & \frac{2}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f_{i-1} \\ & + \frac{2}{(x_j - x_{j-1})(x_j - x_{j+1})} f_j \\ & + \frac{2}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f_{i+1}. \end{aligned} \tag{2.14}$$

The third step, evaluating the polynomial at the reference point, is trivial in this case, since any explicit x-dependence vanished with the second derivative. In terms of Δx_j and Δx_{j+1} we obtain the final expression

$$\begin{aligned} f''_j \approx \ & \left[\frac{2}{\Delta x_j(\Delta x_j + \Delta x_{j+1})}\right] f_{j-1} + \\ & \left[-\frac{2}{\Delta x_j \Delta x_{j+1}}\right] f_j + \\ & \left[\frac{2}{\Delta x_{j+1}(\Delta x_j + \Delta x_{j+1})}\right] f_{j+1} \end{aligned} \tag{2.15}$$

and its simplified version for equispaced grid points

$$f''_j \approx \left[\frac{1}{\Delta x^2}\right] f_{j-1} + \left[-\frac{2}{\Delta x^2}\right] f_j + \left[\frac{1}{\Delta x^2}\right] f_{j+1}. \tag{2.16}$$

A general algorithm

The Lagrange interpolation scheme illustrated above can be used to develop an algorithm for computing the finite-difference weights for a general stencil configuration and order of derivative. We recall that the Lagrange polynomial $L(x)$ of degree $N-1$ for N points $\{x_j\}$ satisfies

$$L(x_j) = f_j \qquad \text{for} \quad k = 1, \ldots, N. \tag{2.17}$$

The Lagrange form is given by a sum of individual $(N-1)$-degree polynomials that go through the point (x_j, f_j) and are zero at all other locations $x_k, k \neq j$. We have

$$L(x) = \sum_{j=1}^{N} w_j \ell_j(x) f_j \qquad \text{with} \qquad \ell_j(x) = \prod_{k \neq j} (x - x_k) \quad \text{and} \quad w_j = \frac{1}{\ell_j(x_j)}. \tag{2.18}$$

Using these definitions we have separated the numerator $\ell_j(x)$ from the denominator $\ell_j(x_j) = 1/w_j$ of the previous expression for $L(x)$ above; we confirm $L_j(x) = w_j \ell_j(x)$. We introduce the finite-difference weight $w_{j,m}$ for the j-th point (x_j, f_j) and the m-th derivative $f^{(m)}$ by considering the expression

$$f^{(m)}(0) \approx w_{1,m} f(x_1) + w_{2,m} f(x_2) + \cdots + w_{N,m} f(x_N). \tag{2.19}$$

Without loss of generality, we consider $x = 0$ as our reference point for the evaluation of the derivative. For the computation of the weights $w_{j,m}$ the grid spacing does not enter the above expression, since (2.19) is invariant under the transformations $x_j \to x_j \Delta x$ and $f^{(m)}(0) \to \Delta x^m f^{(m)}(0)$. It is easy to see that the finite-difference weights $w_{j,m}$ are equal to the coefficients of the polynomial $w_j \ell_j(x)$ multiplied by $m!$. A direct extraction of these coefficients, however, yields an inefficient and unstable numerical algorithm.

Instead, we rewrite the Lagrange polynomial in the form

$$L(x) = \underbrace{(x - x_1)(x - x_2) \cdots (x - x_N)}_{\ell^*(x)} \left[\frac{w_1}{x - x_1} f_1 + \frac{w_2}{x - x_2} f_2 + \cdots + \frac{w_N}{x - x_N} f_N \right]. \tag{2.20}$$

The idea is to compute the Lagrange weights w_j and the coefficients of the polynomial $\ell^*(x)$ ahead of time (since they only depend on the grid-point distribution but not on the derivative we seek) and then only account for the division by $(x - x_j)$ from the second factor (in square brackets).

As before, we aim to derive a formula for

$$\left. \frac{d^m L(x)}{dx^m} \right|_{x=0} = m! \sum_{j=1}^{N} c_{j,m} w_j f_j \tag{2.21}$$

from which we can determine the finite-difference weights as $w_{j,m} = m!\ w_j\ c_{j,m}$. We start by computing $\ell^*(x)$ according to

$$\ell^*(x) = \prod_{j=1}^{N} (x - x_j) \tag{2.22}$$

and convert this polynomial from a root-representation (with roots x_j) to coefficient-form, i.e.,

$$\ell^*(x) = \sum_{j=0}^{N} C_j x^j. \tag{2.23}$$

This is best accomplished in a recursive manner: the multiplication of a polynomial in coefficient form $a_0 + a_1 x + a_2 x^2 + \cdots$ by a root-factor $(x - \alpha)$ yields a polynomial $b_0 + b_1 x + b_2 x^2 + \cdots$ with

$$b_0 = -\alpha a_0, \tag{2.24a}$$

$$b_j = -\alpha a_j + a_{j-1} \qquad \text{for} \quad j \geq 1 \tag{2.24b}$$

which we will use to efficiently compute the coefficients C_j in (2.23). The same recursive formula can be reverted to equally efficiently deal with the division by $(x - \alpha)$ which is needed to account for the influence of the terms in the square bracket of (2.20). We have

$$a_0 = -b_0/\alpha \tag{2.25a}$$

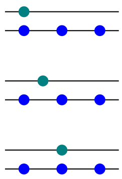
$$a_j = (a_{j-1} - b_j)/\alpha \qquad \text{for} \quad j \geq 1. \tag{2.25b}$$

This then provides all ingredient for an efficient and robust algorithm for computing the finite-difference weights of the m-th derivative on a set of grid points $\{x_j\}_{j=1,\ldots,N}$. The MATLAB$^{\text{TM}}$ function **FDweights.m** implements the above procedure: first computing the Lagrange weights w_j and the coefficients C_j of the polynomial $\ell^*(x)$ for a given set of points $\{x_j\}$, before dividing by factors $w_j/(x - x_j)$ to finally obtain the finite-difference weights $c_{j,m}$.

Finite-difference approximations to first and second derivatives

The general algorithm (implemented in **FDweights.m**) has been applied to determine a variety of common finite-difference stencils for both collocated and staggered grid configurations. Figures 2.3, 2.4 and 2.5 present the weight coefficients for finite-difference approximations to a first derivative using three, four or five evaluation points, respectively, for one-sided, staggered, and centered configurations. The order of accuracy is also listed, using the notation $\mathcal{O}(\Delta x^p) = \mathcal{O}(p)$.

Figures 2.6, 2.7 and 2.8 repeat the same exercise for the second derivative, again using various stencil widths and evaluation points.

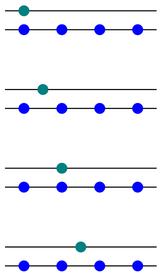


1 $$f'_{-1} = -\frac{3}{2}f_{-1} + 2f_0 - \frac{1}{2}f_1 + \mathcal{O}(2)$$

2 $$f'_{-1/2} = -f_{-1} + f_0 + \mathcal{O}(2)$$

3 $$f'_0 = -\frac{1}{2}f_{-1} + \frac{1}{2}f_1 + \mathcal{O}(2)$$

Fig. 2.3 Three-point stencil finite-d1ifference schemes for the first derivative.



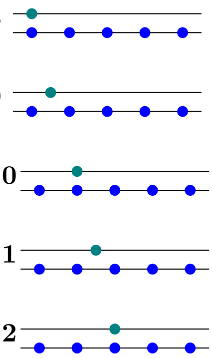
4 $$f'_{-1} = -\frac{11}{6}f_{-1} + 3f_0 - \frac{3}{2}f_1 + \frac{1}{3}f_2 + \mathcal{O}(3)$$

5 $$f'_{-1/2} = -\frac{23}{24}f_{-1} + \frac{7}{8}f_0 + \frac{1}{8}f_1 - \frac{1}{24}f_2 + \mathcal{O}(3)$$

6 $$f'_0 = -\frac{1}{3}f_{-1} - \frac{1}{2}f_0 + f_1 - \frac{1}{6}f_2 + \mathcal{O}(3)$$

7 $$f'_{1/2} = \frac{1}{24}f_{-1} - \frac{9}{8}f_0 + \frac{9}{8}f_1 - \frac{1}{24}f_2 + \mathcal{O}(4)$$

Fig. 2.4 Four-point stencil finite-difference schemes for the first derivative.



8 $$f'_{-2} = -\frac{25}{12}f_{-2} + 4f_{-1} - 3f_0 + \frac{4}{3}f_1 - \frac{1}{4}f_2 + \mathcal{O}(4)$$

9 $$f'_{-3/2} = -\frac{11}{12}f_{-2} + \frac{17}{24}f_{-1} + \frac{3}{8}f_0 - \frac{5}{24}f_1 + \frac{1}{24}f_2 + \mathcal{O}(4)$$

10 $$f'_{-1} = -\frac{1}{4}f_{-2} - \frac{5}{6}f_{-1} + \frac{3}{2}f_0 - \frac{1}{2}f_1 + \frac{1}{12}f_2 + \mathcal{O}(4)$$

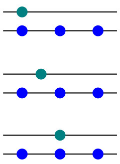
11 $$f'_{-1/2} = \frac{1}{24}f_{-2} - \frac{9}{8}f_{-1} + \frac{9}{8}f_0 - \frac{1}{24}f_1 + \mathcal{O}(4)$$

12 $$f'_0 = \frac{1}{12}f_{-2} - \frac{2}{3}f_{-1} + \frac{2}{3}f_1 - \frac{1}{12}f_2 + \mathcal{O}(4)$$

Fig. 2.5 Five-point stencil finite-difference schemes for the first derivative.

2.2 Compact differences

When higher-order accurate schemes are necessary, the stencil widths of finite-difference schemes become increasingly large. Wide stencils, however, are problematic for various reasons. Near boundaries they have to be modified to result in non-central schemes, even though throughout the computational domain they are central. More importantly, the polynomial interpolation through equispaced points can suffer from the Runge phenomenon which results in oscillations of the inter-

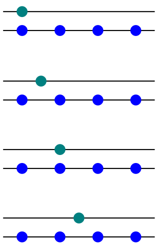


13 $$f''_{-1} = f_{-1} - 2f_0 + f_1 + \mathcal{O}(1)$$

14 $$f''_{-1/2} = f_{-1} - 2f_0 + f_1 + \mathcal{O}(1)$$

15 $$f''_0 = f_{-1} - 2f_0 + f_1 + \mathcal{O}(2)$$

Fig. 2.6 Three-point stencil finite-difference schemes for the second derivative.



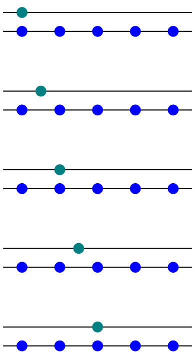
16 $$f''_{-1} = 2f_{-1} - 5f_0 + 4f_1 - f_2 + \mathcal{O}(2)$$

17 $$f''_{-1/2} = \frac{3}{2}f_{-1} - \frac{7}{2}f_0 + \frac{5}{2}f_1 - \frac{1}{2}f_2 + \mathcal{O}(2)$$

18 $$f''_0 = f_{-1} - 2f_0 + f_1 + \mathcal{O}(2)$$

19 $$f''_{1/2} = \frac{1}{2}f_{-1} - \frac{1}{2}f_0 - \frac{1}{2}f_1 + \frac{1}{2}f_2 + \mathcal{O}(2)$$

Fig. 2.7 Four-point stencil finite-difference schemes for the second derivative.



20 $$f''_{-2} = \frac{35}{12}f_{-2} - \frac{26}{3}f_{-1} + \frac{19}{2}f_0 - \frac{14}{3}f_1 + \frac{11}{12}f_2 + \mathcal{O}(3)$$

21 $$f''_{-3/2} = \frac{43}{24}f_{-2} - \frac{14}{3}f_{-1} + \frac{17}{4}f_0 - \frac{5}{3}f_1 + \frac{7}{24}f_2 + \mathcal{O}(3)$$

22 $$f''_{-1} = \frac{11}{12}f_{-2} - \frac{5}{3}f_{-1} + \frac{1}{2}f_0 + \frac{1}{3}f_1 - \frac{1}{12}f_2 + \mathcal{O}(3)$$

23 $$f''_{-1/2} = \frac{7}{24}f_{-2} + \frac{1}{3}f_{-1} - \frac{7}{4}f_0 + \frac{4}{3}f_1 - \frac{5}{24}f_1 + \mathcal{O}(3)$$

24 $$f''_0 = -\frac{1}{12}f_{-2} + \frac{4}{3}f_{-1} - \frac{5}{2}f_0 + \frac{4}{3}f_1 - \frac{1}{12}f_2 + \mathcal{O}(4)$$

Fig. 2.8 Five-point stencil finite-difference schemes for the second derivative.

polant in-between grid points. While the Lagrangre polynomial still reproduces the function values at the grid points, the derivative(s) at the grid points become inaccurate.

An alternative method yielding higher-order accuracte results while maintaining a narrow stencil involves **compact differences** or **implicit schemes**. In this method, we work with two interpolants: one for the function values at the grid points, and another for its derivative at the same or different grid points.

We start with an example: we wish to derive a high-order approximation to a first derivative using the five equispaced points $\{x_{j-2},\ x_{j-1},\ x_j,\ x_{j+1},\ x_{j+2}\}$ to represent the function values and the three points $\{x_{j-1},\ x_j,\ x_{j+1}\}$ to capture the first-derivative values. Exploiting the symmetry of the proposed stencil, we use a symmetric form to express the first derivative of a function $f(x)$ in terms of neighboring function values. We propose

$$\alpha \left(f'_{j+1} + f'_{j-1} \right) + f'_j \approx a \, \frac{f_{j+1} - f_{j-1}}{2\Delta x} + b \, \frac{f_{j+2} - f_{j-2}}{4\Delta x}. \tag{2.26}$$

Similar to the case of finite-difference approximations, the coefficients for compact schemes can be obtained by a Taylor series expansion of both sides and subsequent matching of the expansion coefficients. For the above scheme we have (using $x = x_j$ as our expansion point)

$$\begin{aligned} \alpha \left(2f'_j + \Delta x^2 f'''_j + \cdots \right) + f'_j = \; & \frac{a}{2\Delta x} \left(2\Delta x f'_j + \frac{1}{3}\Delta x^3 f'''_j + \cdots \right) + \\ & \frac{b}{4\Delta x} \left(4\Delta x f'_j + \frac{1}{3} 8\Delta x^3 f'''_j + \cdots \right). \end{aligned} \tag{2.27}$$

Matching derivatives $f'_j, f'''_j, f^{(\mathrm{v})}_j$ on either side, we obtain a system of equations for the three unknown coefficients a, b and α as follows

$$f'_j \quad \rightarrow \quad a + b - 2\alpha = 1, \tag{2.28a}$$

$$f'''_j \quad \rightarrow \quad \frac{1}{6}a + \frac{2}{3}b - \alpha = 0, \tag{2.28b}$$

$$f^{(\mathrm{v})}_j \quad \rightarrow \quad \frac{1}{120}a + \frac{2}{15}b - \frac{1}{12}\alpha = 0, \tag{2.28c}$$

which results in

$$a = \frac{14}{9}, \qquad b = \frac{1}{9}, \qquad \alpha = \frac{1}{3}. \tag{2.29}$$

The compact-difference stencil for the first derivative, based on the above stencils for the function and its derivative, thus reads

$$f'_{j+1} + 3f'_j + f'_{j-1} \approx \frac{7}{3\Delta x} \, \left(f_{j+1} - f_{j-1} \right) + \frac{1}{12\Delta x} \, \left(f_{j+2} - f_{j-2} \right). \tag{2.30}$$

It should be self-evident that the above scheme — and compact-difference schemes in general —, by their design, cannot be solved for first derivative. Rather, the coupling of the derivatives at different grid points on the left-hand side requires the formulation of the differentiation operation in matrix form and the inversion of a banded matrix. The banded nature of the matrix to invert allows for very efficient algorithms to determine the derivative values at all grid points, given the function values at all grid points. Special care has to be taken at the boundary points of the computational domain, where one-sided compact differences have to be employed.

Although the above procedure for determining the coefficient of compact difference schemes based on Taylor series expansions is often employed, a more efficient algorithm, based on the finite-difference algorithm above, is preferred. We

scheme	f''_{j-1}	f''_j	f''_{j+1}	$=$	f_{j-1}	f_j	f_{j+1}	f_{j+2}	f_{j+3}
20	1	0	0		$\frac{35}{12}$	$-\frac{26}{3}$	$\frac{19}{2}$	$-\frac{14}{3}$	$\frac{11}{12}$
22	0	1	0		$\frac{11}{12}$	$-\frac{5}{3}$	$\frac{1}{2}$	$\frac{1}{3}$	$-\frac{1}{12}$
24	0	0	1		$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$

will demonstrate this technique by considering the compact formula for the second derivative that uses the three collocation points $\{x_{j-1},\ x_j,\ x_{j+1}\}$ for both the function and its derivative, i.e.,

$$\alpha f''_{j-1} + \beta f''_j + \gamma f''_{j+1} \approx a f_{j-1} + b f_j + c f_{j+1} \tag{2.31}$$

As usual, our expansion point is $x = x_j$.

In determining the unknown coefficients $\{\alpha,\ \beta,\ \gamma\}$ and $\{a,\ b,\ c\}$ we proceed by introducing two fictitious points at which the function $f(x)$ will be evaluated. These points will be taken arbitrarily as x_{j+2} and x_{j+3}; the final result (i.e., the value of the six coefficients) is independent of this choice. We then compute the *finite-difference* weights for each of the grid points of the derivative for this extended stencil on the function side. We obtain

$$f''_{j-1} \approx \frac{35}{12} f_{j-1} - \frac{26}{3} f_j + \frac{19}{2} f_{j+1} - \frac{14}{3} f_{j+2} + \frac{11}{12} f_{j+3}, \tag{2.32a}$$
$$f''_j \approx \frac{11}{12} f_{j-1} - \frac{5}{3} f_j + \frac{1}{2} f_{j+1} + \frac{1}{3} f_{j+2} - \frac{1}{12} f_{j+3}, \tag{2.32b}$$
$$f''_{j+1} \approx -\frac{1}{12} f_{j-1} + \frac{4}{3} f_j - \frac{5}{2} f_{j+1} + \frac{4}{3} f_{j+2} - \frac{1}{12} f_{j+3}. \tag{2.32c}$$

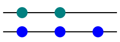
The three stencils are also displayed in table **??**.
A linear combination of these three finite-difference stencils is then formed such that the weights for the two ficticious points, x_{j+2} and x_{j+3}, are zero. In our case, this leads to the compact stencil

$$f''_{j-1} + 10 f''_j + f''_{j+1} \approx 12 f_{j-1} - 24 f_j + 12 f_{j+1}. \tag{2.33}$$

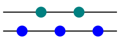
This technique of ficticious points has been implemented in the MATLAB™ function **CDweights.m**.

Compact difference approximations to first and second derivatives

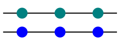
Figures 2.9 and 2.10 display the weight coefficients for compact-difference stencils to a first derivative using three and four evaluation points for the function values $\{f_j\}$, respectively. The stencil weights for the second derivative are listed in figures 2.11 and 2.12, again for three and four evaluation points for the function values.

25 

$$f'_{-1} + 2f'_0 = -\frac{5}{2}f_{-1} + 2f_0 + \frac{1}{2}f_1 + \mathcal{O}(3)$$

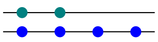
26 

$$f'_{-1/2} - f'_{1/2} = -f_{-1} + 2f_0 - f_1 + \mathcal{O}(3)$$

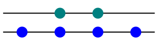
27 

$$f'_{-1} + 4f'_0 + f'_1 = -3f_{-1} + 3f_1 + \mathcal{O}(4)$$

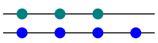
Fig. 2.9 Three-point stencil compact-difference schemes for the first derivative.

28 

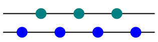
$$f'_{-1} + 3f'_0 = -\frac{17}{6}f_{-1} + \frac{3}{2}f_0 + \frac{3}{2}f_1 - \frac{1}{6}f_2 + \mathcal{O}(4)$$

29 

$$f'_0 + f'_1 = -\frac{1}{6}f_{-1} - \frac{3}{2}f_0 + \frac{3}{2}f_1 + \frac{1}{6}f_2 + \mathcal{O}(4)$$

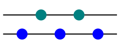
30 

$$f'_{-1} + 6f'_0 + 3f'_1 = -\frac{10}{3}f_{-1} - 3f_0 + 6f_1 + \frac{1}{3}f_2 + \mathcal{O}(5)$$

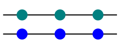
31 

$$f'_{-1/2} + \tfrac{62}{9}f'_{1/2} + f'_{3/2} = -\tfrac{17}{27}f_{-1} - 7f_0 + 7f_1 + \tfrac{17}{27}f_2 + \mathcal{O}(6)$$

Fig. 2.10 Four-point stencil compact-difference schemes for the first derivative.

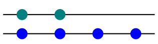
32 

$$f''_{-1/2} + f''_{1/2} = 2f_{-1} - 4f_0 + 2f_1 + \mathcal{O}(2)$$

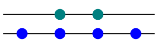
33 

$$f''_{-1} + 10f''_0 + f''_1 = 12f_{-1} - 24f_0 + 12f_1 + \mathcal{O}(4)$$

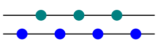
Fig. 2.11 Three-point stencil compact-difference schemes for the second derivative.

34 

$$f''_{-1} + 11f''_0 = 13f_{-1} - 27f_0 + 15f_1 - f_2 + \mathcal{O}(3)$$

35 

$$f''_0 - f''_1 = f_{-1} - 3f_0 + 3f_1 - f_2 + \mathcal{O}(3)$$

36 

$$f''_{-1/2} + \tfrac{14}{5}f''_{1/2} + f''_{3/2} = \tfrac{12}{5}f_{-1} - \tfrac{12}{5}f_0 - \tfrac{12}{5}f_1 + \tfrac{12}{5}f_2 + \mathcal{O}(4)$$

Fig. 2.12 Four-point stencil compact-difference schemes for the second derivative.