Chapter 2

Accuracy of finite-difference schemes

2.1 Standard finite-difference schemes

Let ϕ_j be the value of a function $\phi(x)$ at the discrete points x_j; moreover, let the grid size $h = x_{j+1} - x_j$ be constant. Given any finite-difference approximation of a derivative, its order of accuracy can be calculated by using Taylor series. Consider, for example, the following approximation:

$$\phi' \simeq \frac{\delta_c \phi_j}{\delta x} = \frac{\phi_{j+1} - \phi_{j-1}}{2h}, \tag{2.1}$$

where a prime denotes differentiation with respect to x, and $\delta_c \phi_j / \delta x$ denotes the central finite-difference approximation to the first derivative. To evaluate the accuracy of (2.1), expand ϕ_{j+1} and ϕ_{j-1} in Taylor series about point x_j:

$$\left\{ \begin{array}{lllllll} \phi_{j+1} & = & \phi_j & +\phi'_j h & +\phi''_j h^2/2! & +\phi'''_j h^3/3! & +o(h^4) \\ \phi_{j-1} & = & \phi_j & -\phi'_j h & +\phi''_j h^2/2! & -\phi'''_j h^3/3! & +o(h^4), \end{array} \right. \tag{2.2}$$

in which $o(h^4)$ represents terms of order h^4 and higher. Subtracting the second of (2.2) from the first yields

$$\frac{\delta_c \phi_j}{\delta x} = \frac{\phi_{j+1} - \phi_{j-1}}{2h} = \phi'_j + \phi'''_j \frac{h^2}{6} + o(h^3). \tag{2.3}$$

The second and third terms on the right-hand-side of (2.3) are the errors committed by replacing the analytical first derivative with the finite-difference approximation (2.1) (*truncation error*). Since the leading term of the truncation error is proportional to h^2, the approximation is said to be *second order accurate.*

Conversely, one can use Taylor series to construct a finite-difference scheme of any order of accuracy. For example, one can devise a second-order accurate forwards scheme (that is, one that uses only ϕ_j, ϕ_{j+1}, ϕ_{j+2} *etc.*) by multiplying the Taylor series expansion of ϕ_j by a parameter α, that of ϕ_{j+1} by β and that of ϕ_{j+2} by γ:

$$\left\{ \begin{array}{llllllll} \alpha\phi_j & = & \alpha\,[& \phi_j & & & &] \\ \beta\phi_{j+1} & = & \beta\,[& \phi_j & +\phi'_j h & +\phi''_j h^2/2! & +o(h^3) &] \\ \gamma\phi_{j+2} & = & \gamma\,[& \phi_j & +\phi'_j 2h & +\phi''_j 4h^2/2! & +o(h^3) &]. \end{array} \right. \tag{2.4}$$

Adding up the three expressions above and dividing through by h yields

$$(\alpha\phi_j + \beta\phi_{j+1} + \gamma\phi_{j+2})/h = (\alpha + \beta + \gamma)\phi_j/h + (\beta + 2\gamma)\phi'_j + (\beta + 4\gamma)\phi''_j h/2 + 0(h^2); \tag{2.5}$$

to determine the unknown constants α, β and γ, the coefficient of ϕ'_j must be set equal to one, and the zeroth- and first-order error terms must be required to vanish:

$$\begin{array}{rcc} \beta + 2\gamma = 1 & \Rightarrow & \beta = 1 - 2\gamma = 2 \\ \alpha + \beta + \gamma = 0 & \Rightarrow & \alpha = -\beta - \gamma = -3/2 \\ \beta + 4\gamma = 0 & \Rightarrow & \gamma = -1/2, \end{array}$$

which gives

$$\frac{\delta_+\phi_j}{\delta x} = \frac{1}{2h}(-3\phi_j + 4\phi_{j+1} - \phi_{j+2}) + o(h^2), \tag{2.6}$$

where $\delta_+\phi_j/\delta x$ denotes the forward finite-difference approximation to the first derivative. Commonly used finite-difference schemes are shown below.

$$\begin{aligned}
\frac{\delta\phi_j}{\delta x} &= \frac{\phi_j - \phi_{j-1}}{h} + o(h) \qquad \text{(1st order backwards)} && (2.7)\\
&= \frac{\phi_{j+1} - \phi_j}{h} + o(h) \qquad \text{(1st order forwards)} && (2.8)\\
&= \frac{\phi_{j+1} - \phi_{j-1}}{2h} + o(h^2) \qquad \text{(2nd order central)} && (2.9)\\
&= \frac{3\phi_j - 4\phi_{j-1} + \phi_{j-2}}{2h} + o(h^2) \qquad \text{(2nd order backwards)} && (2.10)\\
&= \frac{-3\phi_j + 4\phi_{j+1} - \phi_{j+2}}{2h} + o(h^2) \qquad \text{(2nd order forwards)} && (2.11)\\
&= \frac{-\phi_{j+2} + 8\phi_{j+1} - 8\phi_{j-1} + \phi_{j-2}}{12h} + o(h^4) \qquad \text{(4th order central)} && (2.12)\\
\frac{\delta^2\phi_j}{\delta x^2} &= \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2} + o(h^2) \qquad \text{(2nd order central)} && (2.13)\\
&= \frac{\phi_j - 2\phi_{j-1} + \phi_{j-2}}{h^2} + o(h) \qquad \text{(1st order backwards)} && (2.14)\\
&= \frac{\phi_j - 2\phi_{j+1} + \phi_{j+2}}{h^2} + o(h) \qquad \text{(1st order forwards)} && (2.15)
\end{aligned}$$

The procedure described above shows that, if a stencil with n points is used to calculate a finite-difference approximation for a derivative, at most one can obtain an approximation of order h^{n-1}.

2.2 Padè approximants

More accurate (for a given stencil) approximations can be obtained by expanding both the function and its derivatives in Taylor series:

$$\left\{\begin{array}{lcllllllll}
\alpha_1\phi_{j+1} &=& \alpha_1\,[& \phi_j & +\phi_j'h & +\phi_j''h^2/2! & +\phi_j'''h^3/3! & +\phi_j^{iv}h^4/4! & +\phi_j^{v}h^5/5! & +o(h^6)\ ]\\
\alpha_2\phi_j &=& \alpha_2\,[& \phi_j & & & & & & \ ]\\
\alpha_3\phi_{j-1} &=& \alpha_3\,[& \phi_j & -\phi_j'h & +\phi_j''h^2/2! & -\phi_j'''h^3/3! & +\phi_j^{iv}h^4/4! & -\phi_j^{v}h^5/5! & +o(h^6)\ ]\\
\beta_1 h\phi_{j+1}' &=& \beta_1 h\,[& & \phi_j' & +\phi_j''h & +\phi_j'''h^2/2! & +\phi_j^{iv}h^3/3! & +\phi_j^{v}h^4/4! & +o(h^5)\ ]\\
\beta_3 h\phi_{j-1}' &=& \beta_3 h\,[& & \phi_j' & -\phi_j''h & +\phi_j'''h^2/2! & -\phi_j^{iv}h^3/3! & +\phi_j^{v}h^4/4! & +o(h^5)\ ].
\end{array}\right. \tag{2.16}$$

Adding up the expressions above yields

$$\begin{aligned}
\alpha_1\phi_{j+1} &+ \alpha_2\phi_j + \alpha_3\phi_{j-1} + \beta_1 h\phi_{j+1}' + \beta_3 h\phi_{j-1}' = (\alpha_1 + \alpha_2 + \alpha_3)\,\phi_j\\
&+ (\alpha_1 - \alpha_3 + \beta_1 + \beta_3)\,\phi_j'h + (\alpha_1 + \alpha_3 + 2\beta_1 - 2\beta_3)\,\phi_j''h^2/2!\\
&+ (\alpha_1 - \alpha_3 + 3\beta_1 + 3\beta_3)\,\phi_j'''h^3/3! + (\alpha_1 + \alpha_3 + 4\beta_1 - 4\beta_3)\,\phi_j^{iv}h^4/4!\\
&+ (\alpha_1 - \alpha_3 + 5\beta_1 + 5\beta_3)\,\phi_j^{v}h^5/5! + o(h^6).
\end{aligned} \tag{2.17}$$

The coefficient of ϕ_j' can now be set equal to 1, to yield an equation relating the unknown constants α and β. Four more equations can be obtained by setting the coefficients of the zeroth- through fourth-order terms to zero. This gives

$$\alpha_1 = -\alpha_3 = 3/4; \qquad \alpha_2 = 0; \qquad \beta_1 = \beta_3 = -1/4. \tag{2.18}$$

Substituting (2.18) into (2.17) yields

$$\phi_{j-1}' + 4\phi_j' + \phi_{j+1}' = \frac{3}{h}\,(\phi_{j+1} - \phi_{j-1}) + o(h^4). \tag{2.19}$$

Equation (2.19) (known as *Padè's formula*) represents a system of linear algebraic equations for the unknown first derivative array $\boldsymbol{\phi}'$. Solving this system by a standard tridiagonal matrix inversion procedure yields a fourth-order accurate approximation of the first derivative. Even higher orders of accuracy can be obtained using the values of ϕ and ϕ' at additional points. One can write a generalized form of (2.19) in the following form:

$$\alpha\phi'_{j-1} + \phi'_j + \alpha\phi'_{j+1} = \frac{\mathrm{b}}{4h}\left(\phi_{j+2} - \phi_{j-2}\right) + \frac{\mathrm{a}}{2h}\left(\phi_{j+1} - \phi_{j-1}\right), \tag{2.20}$$

where

$$\mathrm{a} = 2(\alpha + 2)/3; \qquad \mathrm{b} = (4\alpha - 1)/3. \tag{2.21}$$

Padè's formula is recovered for $\alpha = 1/4$, while for $\alpha = 1/3$, the approximation given in (2.20) is sixth-order accurate [2].

Padè schemes can be obtained for the second derivatives as well. They can be written in the form

$$\alpha\phi''_{j-1} + \phi''_j + \alpha\phi''_{j+1} = \frac{\mathrm{b}}{4h^2}\left(\phi_{j+2} - 2\phi_j + \phi_{j-2}\right) + \frac{\mathrm{a}}{h^2}\left(\phi_{j+1} - 2\phi_j + \phi_{j-1}\right), \tag{2.22}$$

with

$$\mathrm{a} = 4(1 - \alpha)/3; \qquad \mathrm{b} = (-1 + 10\alpha)/3. \tag{2.23}$$

For $\alpha = 1/10$ the classical Padè scheme is recovered, while for $\alpha = 2/11$ a sixth-order accurate tridiagonal scheme is obtained.

While Padè schemes can significantly increase the accuracy of spatial differentiation, they also increase the cost of a computation, since they require additional operations due to the matrix inversions. Presently, they are often employed in explicit, time-accurate codes for the study of transitional or turbulent flows, in which the need to resolve accurately the small scales of motion makes high-order schemes attractive regardless of their cost.

2.3 Non-uniform grids

In most problems of technological interest the flow is not uniform: velocity gradients are larger in some regions of the flow (near a solid boundary, for instance) than elsewhere. In those cases, the use of a uniform mesh such as those examined so far is not ideal: if the grid size is fine enough to resolve the sharp gradients in the regions where they are significant, it will be excessively fine where the flow is smooth, leading to an excessive number of grid points, and unnecessarily increased cost of the calculation.

Non-uniform grids, in which the mesh spacing is smaller in regions in which gradients are expected to be larger, are commonly used in such cases. We will restrict ourselves to cases in which the mesh is refined near the left end of an interval $[0, L]$. Such arrangement is common for boundary-layer flows, and the considerations made here can easily be extended to cases in which the refinement occurs near the right end, or somewhere in the middle of the interval.

Derivative formulas of any order of accuracy can be still obtained using the Taylor series method. Let $\phi = \phi_j$; $\phi_+ = \phi_{j+1}$; $\phi_- = \phi_{j-1}$, and $h_+ = x_{j+1} - x_j$, $h_- = x_j - x_{j-1}$. The approximation (2.9) in this case becomes

$$\frac{\delta\phi_j}{\delta x} = \frac{\phi_+ - \phi_-}{h_+ + h_-} = \phi'_j + \frac{h_+ - h_-}{2}\phi'' + o(h^2). \tag{2.24}$$

This expression is, apparently, only first-order accurate. However, if the grid is smooth, $h_+ \simeq h_-$ (in fact, one can construct a non-uniform grid such that $h_+ - h_- = o(h^2)$); the method then is effectively second-order accurate. A second-order accurate formula for the first derivative is

$$\frac{\delta\phi_j}{\delta x} = \frac{1}{h_+ + h_-}\left[\frac{h_-}{h_+}\phi_+ - \left(\frac{h_-}{h_+} - \frac{h_+}{h_-}\right)\phi - \frac{h_+}{h_-}\phi_-\right] = \phi'_j + o(h^2). \tag{2.25}$$

Commonly used transformation functions that cluster points around $x = 0$ are the hyperbolic tangent grid

$$x_j = L\left[1 + \frac{\tanh(\eta_j \tanh a)}{a}\right]; \qquad \eta_j = -1 + \frac{j-1}{N}; \qquad j = 1, \ldots, N+1; \tag{2.26}$$

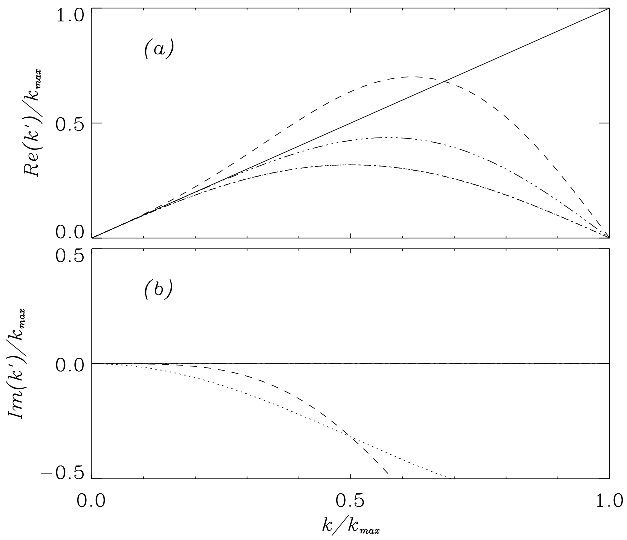

Figure 2.1: Modified wavenumber analysis for the approximation to the first derivative. ——— Exact; ········ first-order backwards (2.7); − − − second-order backwards (2.10); —·— second-order central (2.9); —···— fourth-order central (2.12). (a) Real part; (b) imaginary part.

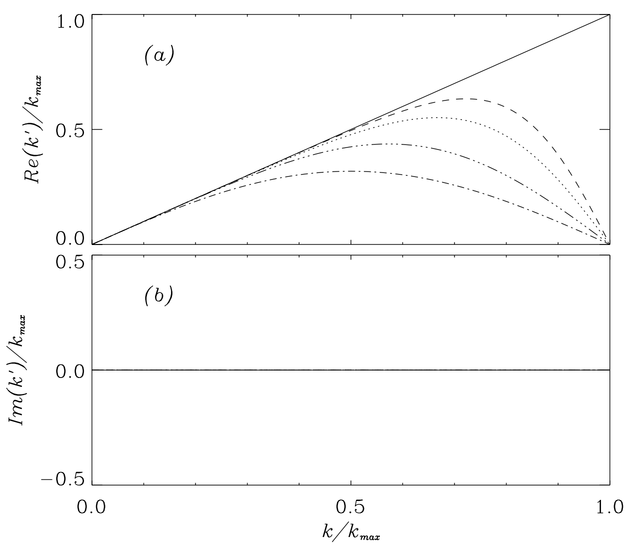

Figure 2.2: Modified wavenumber analysis for the approximation to the first derivative. ——— Exact; ········ fourth-order Padè; − − − sixth-order Padè; —·— second-order central (2.9); —···— fourth-order central (2.12). (a) Real part; (b) imaginary part.

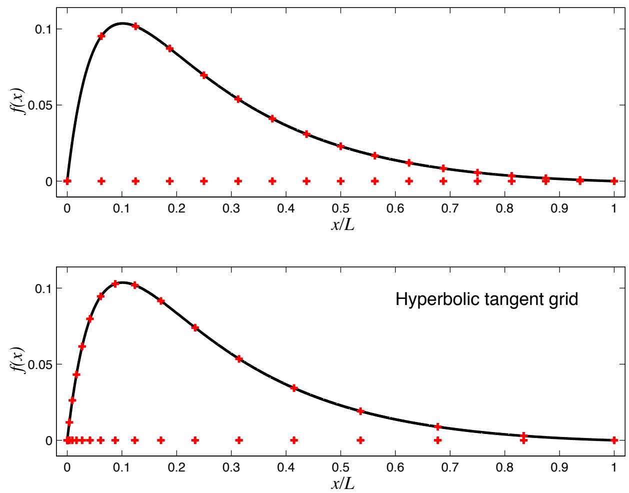

Figure 2.3: Uniform and non-uniform-grid representations of the function $f(x) = \sin x/(x+1)^4$.

the cosine grid

$$x_j = L\left(-1 + \cos\theta_j\right); \qquad \theta_j = \frac{j-1}{N}\frac{\pi}{2}; \qquad j = 1, \ldots, N+1; \tag{2.27}$$

and the exponential grid

$$x_j = x_{j-1} + \Delta x_{j-1}; \qquad \Delta x_j = \Delta x_o \alpha^j; \qquad j = 1, \ldots, N+1. \tag{2.28}$$

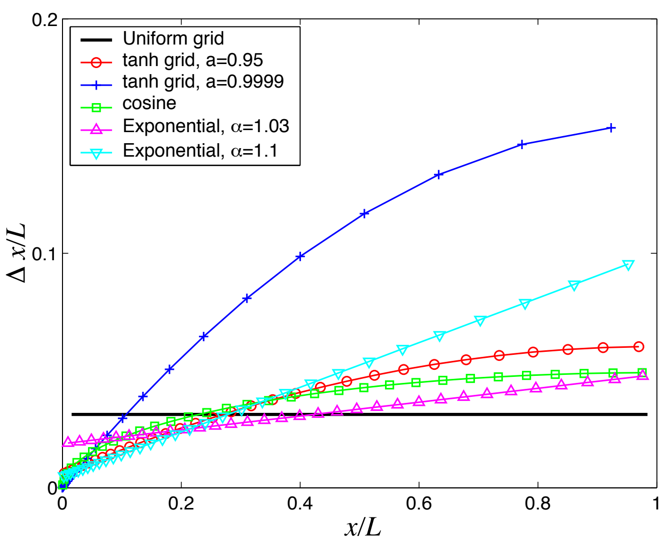

Figure 2.4: Grid spacing obtained using various grid transformations.

The grid spacing obtained with the above transformations is shown in Fig. 2.4.

Figure 2.5 compares the derivative of the function $\sin x/(x+1)^4$ for $0 \le x \le 2\pi$, evaluated on different uniform and non-uniform grids. The better approximation of the derivative obtained with non-uniform meshes is evident. The error associated with each methods is shown in Fig. 2.6. The error is defined as

$$\epsilon_2 = \left[\frac{1}{L}\sum_{j=2}^{N}\left(\frac{\delta f}{\delta x} - \frac{df}{dx}\right)^2\right]^{1/2} \tag{2.29}$$

Note that the hyperbolic-tangent grid gives 2nd-order accuracy, whereas with the exponentially stretched mesh the error flattens out. This is due to the fact that, as the number of points is doubled, the maximum grid spacing is not halved; the maximum error, therefore, remains nearly constant and results in the behavior in the figure.

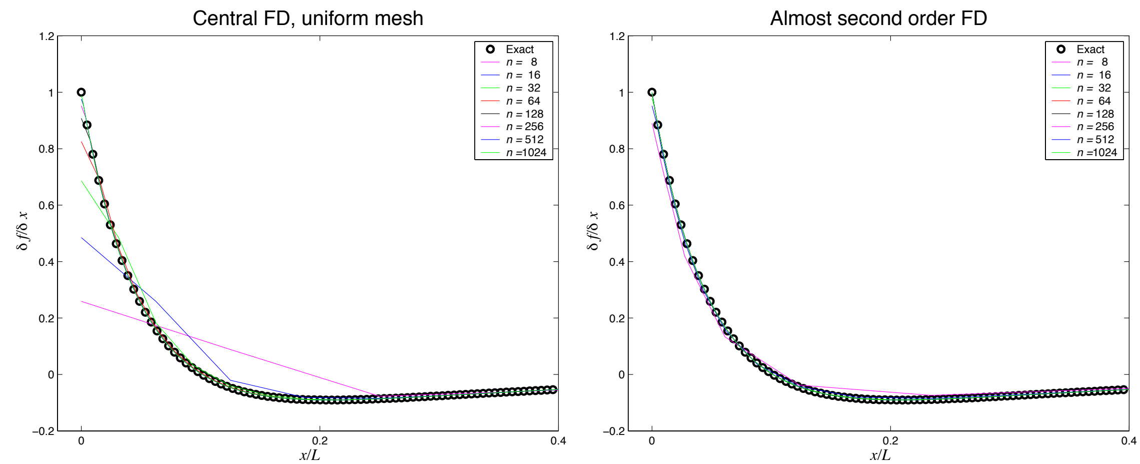

Figure 2.5: Uniform and non-uniform-grid representations of the derivative of $f(x) = \sin x/((x+1)^4$.

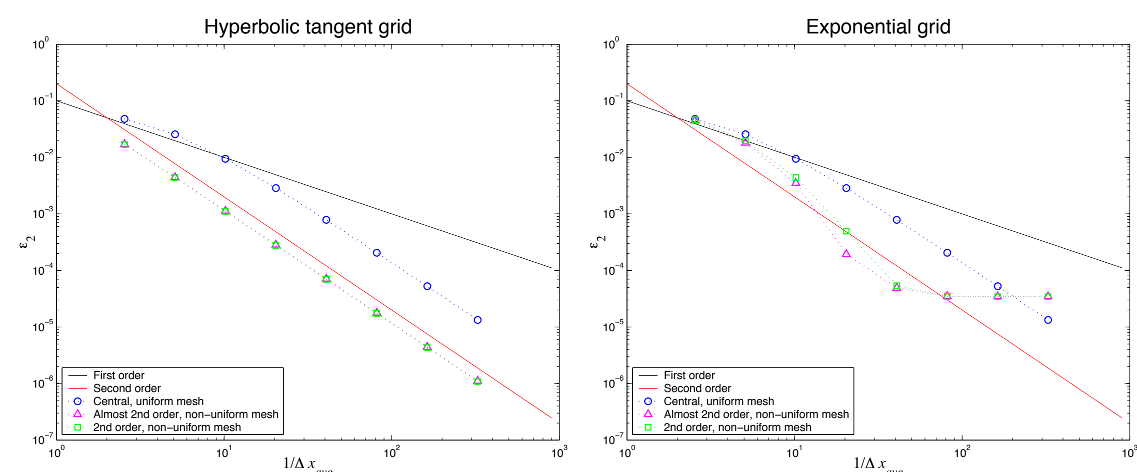

Figure 2.6: Uniform and non-uniform-grid representations of the function $f(x) = \sin x/(x+1)^4$.

Bibliography

[1] J. Ferziger and M. Perić. “Computational Methods for Fluid Dynamics.” Springer-Verlag, 1996.

[2] S. K. Lele. Compact finite difference schemes with spectral-like resolution. *J. Comput. Phys.*, **103** 1642, 1992.