Chapter 1

Finite differences

The scientific community agrees that finite-difference schemes were first used by Euler (1707-1783) to find approximate solutions of differential equations. The technique is known as *Euler method*. However, only after 1945 systematic research activity on the above topic has been strongly developed, when high-speed computers began to be available.

At present, finite-difference methods provide a powerful approach to solve differential equations and are widely used in any field of applied sciences. Equations with variable coefficients and even nonlinear problem can be treated by these techniques. Generally, the error of an approximating solution can be made arbitrary small. Rounding errors, which inevitably arise during the computational process, can be controlled by a preliminary analysis of the numerical stability of finite-difference schemes. Furthermore, numerical solutions can give suggestions to more general questions.

This chapter introduces to the most used finite-difference approximations of derivatives. In particular, the well-known forward, central and backward approximations are presented. The analysis systematically starts from Taylor's series expansion so that the truncation error can be immediately pointed out. Firstly, the approximation of first-order derivatives is dealt with, and, subsequently, the analysis is developed for higher-order derivatives. Exercises are proposed to give the Reader the opportunity to practice. Finally, we present some finite-difference operators, which are frequently found in literature. Their use can help to shorten long formulas in some cases.

1.1 Function discretization

Let us consider a function $u(x,t)$ depending on two variables $x \in [0, L]$ and $t \in [0, T]$. A discretization of function u is obtained by considering only the values $u_{i,j}$ on a finite number of points (x_i, t_j)

$$u_{i,j} = u(x_i, t_j) = u(i\Delta x, j\Delta t),\ i = 0, ..., m,\ j = 0, ..., n, \tag{1.1.1}$$

where $\Delta x = L/m$, $\Delta t = T/n$, fig. 1.1.1. Usually, instead of $u_{i,j}$, the notation u_i^j is also used.

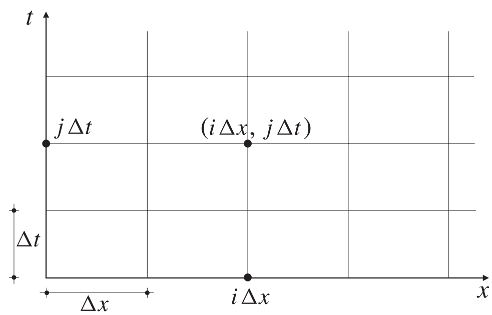

Fig. 1.1.1 Space-time grid

The formula for a function of one variable is immediately derived from (1.1.1). In addition, generalizing it in obvious way yields the case regarding a function of three or more variables.

A basic role to estimate the error involved in *finite-difference approximations* of function derivatives is played by the well-known Taylor's series expansion

$$f(x+\Delta x) = f(x) + \sum_{h=1}^{n-1} f^{(h)}(x)\frac{(\Delta x)^h}{h!} + f^{(n)}(x+\theta\Delta x)\frac{(\Delta x)^n}{n!}, \tag{1.1.2}$$

where $0 < \theta < 1$ and $f^{(h)}$ denotes the hth derivative of f. Noting that the last term is of order $(\Delta x)^n$, (1.1.2) can also be written as

$$f(x+\Delta x) = f(x) + \sum_{h=1}^{n-1} f^{(h)}(x)\frac{(\Delta x)^h}{h!} + O((\Delta x)^n), \tag{1.1.3}$$

where the symbol O (big o) has been used, defined as follows

$$g(y) = O(y^n),\ y \in \Omega \quad \Leftrightarrow \quad |g(y)| \le c y^n, \quad \forall y \in \Omega, \tag{1.1.4}$$

where c is a positive constant.

1.2 Finite-difference approximation of derivatives

Let us define the *forward approximation* for the partial derivative u_t. Applying Taylor's series expansion (1.1.3) to $u(x_i, t_j + \Delta t)$ gives

$$u(x_i, t_j + \Delta t) = u(x_i, t_j) + u_t(x_i, t_j)\Delta t + O((\Delta t)^2) \tag{1.2.1}$$

which, by using notation (1.1.1), is written as

$$u_{i,j+1} = u_{i,j} + (u_t)_{i,j}\Delta t + O((\Delta t)^2), \tag{1.2.2}$$

that is,

$$(u_t)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} + O(\Delta t). \tag{1.2.3}$$

Hence, it follows the approximation formula for the partial derivative of u with respect to t, called *forward approximation*,

$$(u_t)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t}. \tag{1.2.4}$$

Formula (1.2.4) evidently implies a leading error of order Δt. Similarly, from

$$(u_x)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{1.2.5}$$

it follows the forward approximation for u_x

$$(u_x)_{i,j} \approx \frac{u_{i+1,j} - u_{i,j}}{\Delta x}, \tag{1.2.6}$$

with a leading error of order Δx.

The *backward approximation* is inferred in analogous way. Applying Taylor's expansion (1.1.3) to $u(x_i, t_j - \Delta t)$ and $u(x_i - \Delta x, t_j)$ implies, respectively, the following

$$(u_t)_{i,j} \approx \frac{u_{i,j} - u_{i,j-1}}{\Delta t}, \tag{1.2.7}$$

$$(u_x)_{i,j} \approx \frac{u_{i,j} - u_{i-1,j}}{\Delta x}, \tag{1.2.8}$$

which give the *backward approximations* for the first partial derivatives, with the same leading error of the last case.

Let us define the *central approximation*. Applying Taylor's expansion (1.1.3) with $n = 4$ yields

$$u_{i,j+1} = u_{i,j} + (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}\frac{(\Delta t)^2}{2!} + (u_{ttt})_{i,j}\frac{(\Delta t)^3}{3!} + O((\Delta t)^4), \quad (1.2.9)$$

$$u_{i,j-1} = u_{i,j} - (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}\frac{(\Delta t)^2}{2!} - (u_{ttt})_{i,j}\frac{(\Delta t)^3}{3!} + O((\Delta t)^4). \quad (1.2.10)$$

Subtracting the second expression from the first gives

$$u_{i,j+1} - u_{i,j-1} = 2(u_t)_{i,j}\Delta t + O((\Delta t)^3), \quad (1.2.11)$$

that is,

$$(u_t)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t} + O((\Delta t)^2). \quad (1.2.12)$$

Hence, we obtain the *central approximation* for u_t

$$(u_t)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t}, \quad (1.2.13)$$

with a leading error of order $(\Delta t)^2$. Similarly, it follows

$$(u_x)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O((\Delta x)^2). \quad (1.2.14)$$

Hence,

$$(u_x)_{i,j} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}, \quad (1.2.15)$$

which gives the central approximation for u_x with the same error.

The preceding finite-difference approximations consider the values of a function on two points of the xt grid and are the most used. However, formulas involving three or more grid points can also be deduced with a smaller error, in general. Firstly, let us discuss the *three-point forward approximation* for u_t. Using again Taylor's expansion (1.1.3) gives

$$u_{i,j+1} - u_{i,j} = (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}(\Delta t)^2/2 + O((\Delta t)^3), \quad (1.2.16)$$

$$u_{i,j+2} - u_{i,j} = (u_t)_{i,j}2\Delta t + (u_{tt})_{i,j}2(\Delta t)^2 + O((\Delta t)^3), \quad (1.2.17)$$

which imply

$$(u_t)_{i,j} = \frac{4u_{i,j+1} - 3u_{i,j} - u_{i,j+2}}{2\Delta t} + O((\Delta t)^2). \tag{1.2.18}$$

Hence it follows the *three-point forward approximation*

$$(u_t)_{i,j} \approx \frac{4u_{i,j+1} - 3u_{i,j} - u_{i,j+2}}{2\Delta t}, \tag{1.2.19}$$

with a leading error of order $(\Delta t)^2$. Similarly, the three-point forward approximation for u_x can be obtained

$$(u_x)_{i,j} \approx \frac{4u_{i+1,j} - 3u_{i,j} - u_{i+2,j}}{2\Delta x}. \tag{1.2.20}$$

Exercise 1.2.1 Show the following three-point backward approximations

$$(u_t)_{i,j} \approx \frac{-4u_{i,j-1} + 3u_{i,j} + u_{i,j-2}}{2\Delta t}, \tag{1.2.21}$$

$$(u_x)_{i,j} \approx \frac{-4u_{i-1,j} + 3u_{i,j} + u_{i-2,j}}{2\Delta x}. \tag{1.2.22}$$

Exercise 1.2.2 Deduce the following four-point forward and backward approximations

$$(u_t)_{i,j} \approx \frac{-u_{i,j+2} + 6u_{i,j+1} - 3u_{i,j} - 2u_{i,j-1}}{6\Delta t}, \tag{1.2.23}$$

$$(u_t)_{i,j} \approx \frac{u_{i,j-2} - 6u_{i,j-1} + 3u_{i,j} + 2u_{i,j+1}}{6\Delta t}, \tag{1.2.24}$$

and verify that the leading error is of order $(\Delta t)^3$. Write similar formulas for the partial derivative u_x.

1.3 Approximation for higher-order derivatives

Let us introduce the *forward approximation* for the second derivative u_{tt}. Multiply (1.2.16) by 2 and subtract the result to (1.2.17)

$$(u_{tt})_{i,j} = \frac{u_{i,j+2} - 2u_{i,j+1} + u_{i,j}}{(\Delta t)^2} + O(\Delta t). \tag{1.3.1}$$

Hence, it follows the quoted approximation

$$(u_{tt})_{i,j} \approx \frac{u_{i,j+2} - 2u_{i,j+1} + u_{i,j}}{(\Delta t)^2} \tag{1.3.2}$$

with a leading error of order Δt. A similar result holds for the second derivative u_{xx}

$$(u_{xx})_{i,j} \approx \frac{u_{i+2,j} - 2u_{i+1,j} + u_{i,j}}{(\Delta x)^2}. \tag{1.3.3}$$

By analogous arguments the *backward approximations* of the same derivatives can be inferred

$$(u_{tt})_{i,j} \approx \frac{u_{i,j-2} - 2u_{i,j-1} + u_{i,j}}{(\Delta t)^2}, \tag{1.3.4}$$

$$(u_{xx})_{i,j} \approx \frac{u_{i-2,j} - 2u_{i-1,j} + u_{i,j}}{(\Delta x)^2}, \tag{1.3.5}$$

with a leading error of order Δt and Δx, respectively.

Summing (1.2.9), (1.2.10)

$$u_{i,j+1} + u_{i,j-1} = 2u_{i,j} + (u_{tt})_{i,j}(\Delta t)^2 + O((\Delta t)^4) \tag{1.3.6}$$

and solving with respect to $(u_{tt})_{i,j}$ gives the *central approximation*

$$(u_{tt})_{i,j} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta t)^2}. \tag{1.3.7}$$

Formula (1.3.7) is more accurate than (1.3.2), (1.3.4), because its leading error is of order $(\Delta t)^2$. A similar result holds for u_{xx}

$$(u_{xx})_{i,j} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}. \tag{1.3.8}$$

When functions of two or more variables are considered, the mixed derivatives must also be discussed. Let us start with the *forward approximation* to u_{xt}. Applying (1.2.3) to the derivative u_x yields

$$(u_{xt})_{i,j} = \frac{(u_x)_{i,j+1} - (u_x)_{i,j}}{\Delta t} + O(\Delta t). \tag{1.3.9}$$

Hence, considering (1.2.5) implies

$$(u_{xt})_{i,j} = \frac{u_{i+1,j+1} - u_{i,j+1} - u_{i+1,j} + u_{i,j}}{\Delta x \Delta t} + O(\Delta x) + O(\Delta t), \tag{1.3.10}$$

and, therefore, with a leading error of order $O(\Delta x) + O(\Delta t)$,

$$(u_{xt})_{i,j} \approx \frac{u_{i+1,j+1} - u_{i,j+1} - u_{i+1,j} + u_{i,j}}{\Delta x \Delta t}. \tag{1.3.11}$$

The same formula is found by applying (1.2.5) to u_t and using (1.2.3), as it is easily verified.

Similarly, the *backward approximation*

$$(u_{xt})_{i,j} \approx \frac{u_{i-1,j-1} - u_{i,j-1} - u_{i-1,j} + u_{i,j}}{\Delta x \Delta t}, \tag{1.3.12}$$

and the *central approximation*

$$(u_{xt})_{i,j} \approx \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4\Delta x \Delta t}, \tag{1.3.13}$$

can be derived with a leading error of order $O(\Delta x)+O(\Delta t)$ and $O((\Delta x)^2)+O((\Delta t)^2)$, respectively.

Higher order derivatives can be evaluated by analogous arguments.

Exercise 1.3.1 Mix suitably the first derivative approximations and derive the other (six) finite-difference formulas for u_{xt}.

1.4 Finite-difference operators

Sometimes finite-difference formulas can become very long. Using finite-difference operators can be convenient in these situations. With reference to an arbitrary function $f(x)$, frequently used operators are the following

$$\Delta f_i = f_{i+1} - f_i, \quad \text{(forward)}, \tag{1.4.1}$$

$$\nabla f_i = f_i - f_{i-1}, \quad \text{(backward)}, \tag{1.4.2}$$

$$\delta f_i = f_{i+1/2} - f_{i-1/2}, \quad \text{central)}, \tag{1.4.3}$$

$$\mu f_i = (f_{i+1/2} + f_{i-1/2})/2, \quad \text{(average)}, \tag{1.4.4}$$

$$E f_i = f_{i+1}, \quad \text{(shift)}. \tag{1.4.5}$$

When functions $u = u(x,t)$ depending on two or more variables are considered, the variable which the operator is applied to must be specified;

for example

$$\Delta_t u_{i,j} = u_{i,j+1} - u_{i,j}, \tag{1.4.6}$$

$$\nabla_x u_{i,j} = u_{i,j} - u_{i-1,j}. \tag{1.4.7}$$

Exercise 1.4.1 Verify that

$$\delta\mu f_i = (f_{i+1} - f_{i-1})/2, \tag{1.4.8}$$

$$\delta^2 f_i = \delta\delta f_i = f_{i+1} - 2f_i + f_{i-1}. \tag{1.4.9}$$

Further Reading: [Ames (1992)], [Collatz (1966)], [Lapidus and Pinter (1982)], [Mitchell and Griffiths (1995)], [Morton and Mayers (2002)], [Necati Ozisik (1994)], [Smith (1985)], [Thomas (1995)].