Chapter 1
Finite Difference Approximations

Let us begin by explaining the "finite difference" (FD) of the finite difference time domain (FDTD) methodology. We review the basic concepts and mathematical properties of different FD expressions, and introduce the basic concepts and the notation to be used throughout this book.

Topics:
- Elementary finite difference expressions
- Nonstandard finite difference expressions
- Computational molecules

1.1 Basic Finite Difference Expressions

There are three elementary FD expressions for the first derivative:

1. The forward FD (FFD) approximation,

$$\begin{aligned} f'(x) &\cong \frac{f(x+h)-f(x)}{h}, \\ &\cong \frac{d_x^{\mathrm{f}} f(x)}{h}, \end{aligned} \tag{1.1}$$

where

$$d_x^{\mathrm{f}} f(x) = f(x+h) - f(x). \tag{1.2}$$

Expanding $f(x+h)$ in a Taylor series, we find the error of the FFD approximation to be

$$\varepsilon_{\mathrm{FD}} = \frac{d_x^{\mathrm{f}} f(x)}{h} - f'(x)$$
$$= \frac{1}{2} h f''(x) + \frac{1}{6} h^2 f'''(x). \tag{1.3}$$

2. The backward FD (BFD) approximation,

$$f'(x) \cong \frac{f(x) - f(x-h)}{h}$$
$$\cong \frac{d_x^{\mathrm{b}} f(x)}{h}, \tag{1.4}$$

where

$$d_x^{\mathrm{b}} f(x) = f(x) - f(x-h). \tag{1.5}$$

Expanding $f(x + h)$, we find that the error of the BFD approximation is

$$\varepsilon_{\mathrm{BD}} = \frac{d_x^{\mathrm{b}} f(x)}{h} - f'(x)$$
$$= -\frac{1}{2} h f''(x) + \frac{1}{6} h^2 f'''(x) \cdots. \tag{1.6}$$

The forward- and backward-FD approximations are said to be first-order accurate or simply "first-order" because the error is proportional to the first power of h.

3. The central FD (CFD) approximation,

$$f'(x) \cong \frac{f(x + h/2) - f(x - h/2)}{h}$$
$$\cong \frac{d_x^{\mathrm{c}} f(x)}{h}, \tag{1.7}$$

where

$$d_x^{\mathrm{c}} f(x) = f(x + h/2) - f(x - h/2). \tag{1.8}$$

Expanding $f(x + h/2) - f(x - h/2)$, we find the error of the CFD approximation to be

$$\varepsilon_{\mathrm{CD}} = \frac{d_x^{\mathrm{c}} f(x)}{h} - f'(x)$$
$$= \frac{1}{24} h^2 f'''(x) + \cdots; \tag{1.9}$$

thus, the CFD approximation to f' is second-order accurate.

Comparing Eq. (1.3) with Eq. (1.9), one might suppose that $\varepsilon_{\rm CD} < \varepsilon_{\rm FD}$, but this is true only if $h^2 f'''(x)/24 + \cdots < hf''(x)/2 + \cdots$. For example, taking $f(x) = e^{\alpha x}$ with $\alpha > h$, the error of the FFD approximation is actually smaller than that of the CFD approximation.

Accuracy is not the only criterion for the choice of an FD expression in constructing an algorithm. It is essential that the algorithm be *numerically stable* as well as accurate. (See Section 2.4 for an example of how highly accurate FD algorithms can display perverse behavior.)

For future reference we derive the CFD approximation for $f''(x)$:

$$\begin{aligned} f''(x) &\cong \frac{d_x^{\rm c}}{h}\left[\frac{d_x^{\rm c}}{h} f(x)\right] \\ &= \frac{(d_x^{\rm c})^2}{h^2} f(x) \\ &= \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}, \end{aligned} \tag{1.10}$$

where $(d_x^{\rm c})^2 = d_x^{\rm c}\, d_x^{\rm c}$. It is straightforward to show that

$$(d_x^{\rm c})^2 f(x) = f(x+h) + f(x-h) - 2f(x). \tag{1.11}$$

Expanding Eq. (1.10) in a Taylor series about x, we find that

$$\frac{(d_x^{\rm c})^2}{h^2} f(x) = f''(x) + \frac{1}{12} h^2 f^{(4)}(x) + \cdots; \tag{1.12}$$

thus, the CFD approximation of f'' is second-order accurate.

We shall henceforth refer to the above FD expressions as standard finite difference (S-FD) expressions for reasons that will soon be apparent.

1.1.1 Higher-order finite difference approximations

Retaining only the first two terms of expansion of Eq. (A1.1.12) in Appendix 1, we obtain

$$\begin{aligned} \partial_x f(x) &\cong \frac{1}{h}\left[d_x^{\rm c} - \frac{1}{24}(d_x^{\rm c})^3\right] f(x) \\ &\cong \frac{1}{h}\left\{\frac{7}{8}[f(x+h/2) - f(x-h/2)] \right. \\ &\quad \left. - \frac{1}{24}[f(x+3h/2) - f(x-3h/2)]\right\}, \end{aligned} \tag{1.13}$$

where we have used Eq. (A1.2.25b) to expand $(d_x^{\rm c})^3 f(x)$. Expanding the right side in a Taylor series, we find that

$$\frac{1}{h}\left[d_x^{\mathrm{c}} - \frac{1}{24}(d_x^{\mathrm{c}})^3\right]f(x) = f'(x) - \frac{3}{640}h^4 f^{(5)}(x) + \cdots. \tag{1.14}$$

Thus, Eq. (1.14) is a fourth-order FD approximation to f'.

Similarly, the fourth-order approximation for the second derivative is found by retaining the first two terms of expansion Eq. (A1.13) and using Eq. (A1.2.25c) to expand $(d_x^{\mathrm{c}})^4 f(x)$ to obtain

$$\begin{aligned}\partial_x^2 f(x) &\cong \frac{1}{h^2}\left[(d_x^{\mathrm{c}})^2 - \frac{1}{12}(d_x^{\mathrm{c}})^4\right]f(x)\\ &\cong \frac{1}{h^2}\left\{\frac{4}{3}[f(x+h) + f(x-h)]\right.\\ &\qquad \left. - \frac{1}{12}[f(x+2h) + f(x-2h)] - \frac{5}{2}f(x)\right\}.\end{aligned} \tag{1.15}$$

Expanding the right side of Eq. (1.15) in a Taylor series, we find that

$$\frac{1}{h^2}\left[(d_x^{\mathrm{c}})^2 - \frac{1}{12}(d_x^{\mathrm{c}})^4\right]f(x) = f''(x) - \frac{h^4}{90}f^{(6)}(x) + \cdots; \tag{1.16}$$

hence, Eq. (1.16) is a fourth-order FD approximation to f''.

1.1.2 Computational molecules

The graphical representation of the difference operators yields useful insights. For example, the central difference operator for the first derivative, $d_x^{\mathrm{c}} f(x) = f(x + h/2) - f(x - h/2)$ in Eq. (1.8), can be represented by the graph in Fig. 1.1. The node position corresponds to the local function value, and its weight in the finite difference expression is indicated. Usually the function value is omitted.

The central difference operator for the second derivative, $(d_x^{\mathrm{c}})^2 f(x) = f(x+h) - 2f(x) + f(x-h)$ in Eq. (1.11), can be represented as shown in Fig. 1.2.

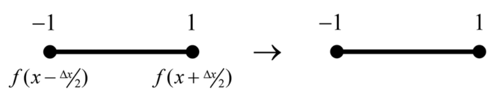

Figure 1.1 Computational molecule for d_x^{c}.

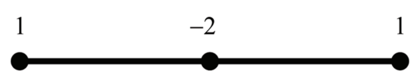

Figure 1.2 Computational molecule for $(d_x^{\mathrm{c}})^2$.

1.2 Nonstandard Finite Difference Expressions

Besides the forward-, backward-, and central-FD approximations, there is another more general class known as nonstandard finite difference (NS-FD) approximations, which were introduced by Mickens.[1] Using NS-FD expressions, it is sometimes possible to greatly reduce the error of an FD approximation and even to eliminate it.

The most general NS-FD approximation is given by

$$f'(x)|_{x=y} \cong \frac{f(x+h) - a(h)f(x)}{s(h)}, \tag{1.17}$$

where a and s are functions. The central FD approximation is a special case of Eq. (1.17) with $y = x + h/2$, $a = 1$, and $s(h) = h$. For a NS-FD expression to be a valid approximation of the derivative, it must converge to $f'(x)$ in the limit $h \to 0$:

$$f'(x)|_{x=y} = \lim_{h\to 0}\frac{f(x+h) - a(h)f(x)}{s(h)}. \tag{1.18}$$

This constrains the forms of a and s. Nonstandard FD approximations can be used to improve the accuracy of FD algorithms, as we shall soon see.

A special case of the general NS-FD approximation that is used throughout much of this book is the central NS-FD approximation, given as

$$\begin{aligned} f'(x) &\cong \frac{d_x^c f(x)}{s(h)} \\ &= \frac{f(x+h/2) - f(x-h/2)}{s(h)}. \end{aligned} \tag{1.19}$$

1.2.1 Exact nonstandard finite difference expressions

With respect to certain sets of functions, it is possible to define exact NS-FD expressions for the derivative. For example, let $f(x) = e^{ikx}$ in Eq. (1.19). We find that $d_x^c e^{ikx} = 2i\sin(kh/2)$; thus, an exact central NS-FD expression for f' is

$$f'(x) = \frac{d_x^c f(x)}{s(h)}, \tag{1.20}$$

where

$$s(h) = \frac{2\sin(kh/2)}{k}, \tag{1.21}$$

and k is any complex number. Equation (1.20) together with Eq. (1.21) is an exact FD expression even when h is not infinitesimal. As $h \to 0$, $s(h) \to h$;

hence, Eq. (1.20) together with Eq. (1.21) constitutes a permissible FD expression for the derivative with respect to exponential functions.

Any differential equation with solutions of the form $\psi(x) = a_+e^{ikx} + a_-e^{-ikx}$ can be exactly modeled with central NS-FD expressions (and hence solved exactly with an FD algorithm).

Notice that in Eq. (1.21) s is independent of x. A NS-FD expression in which s depends on x is useless in a practical algorithm. For example, if $f(x) = x^n = e^{i[-in\ln(x)]}$, $n \neq 0$ and $x > 0$, an exact central NS-FD expression is

$$f'(x) = \frac{d_x^c f(x)}{s(x,h)}, \tag{1.22}$$

where

$$s(x,h) = \frac{2\sinh[n\ln(x)\,h/2]}{n\ln(x)}. \tag{1.23}$$

Although Eq. (1.23) does converge to $f'(x)$ in the limit $h \to 0$, the dependence of s on x and the restriction $x > 0$ render this NS-FD expression useless to model differential equations with solutions of the form

$$\psi(x) = \sum_n a_n x^n. \tag{1.24}$$

1.2.2 Terminology

Henceforth, we refer to the FD expressions introduced in Section 1.1 as standard (S) FD expressions to distinguish them from the nonstandard (NS) expressions introduced in this section.

Often, for the sake of notational simplicity, we drop the superscript "c" for the central difference operators so that $d^c \to d$.

1.3 Standard Finite Difference Expressions for the Laplacian

We now omit the superscript "c" for the central difference operators, and $d_u = d_u^c$ for any variable u unless otherwise specified. The Laplacian operator $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ has several different FD representations.

1.3.1 Two dimensions

In two dimensions, where $\nabla^2 = \partial_x^2 + \partial_y^2$, the most obvious FD approximation is

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}^2}{h^2} f(\mathbf{x}), \tag{1.25}$$

where $\mathbf{d}^2 = d_x^2 + d_y^2$; d_x and d_y are partial central difference operators of the form in Eq. (1.8). Expanding $\mathbf{d}^2 f(x)$ gives

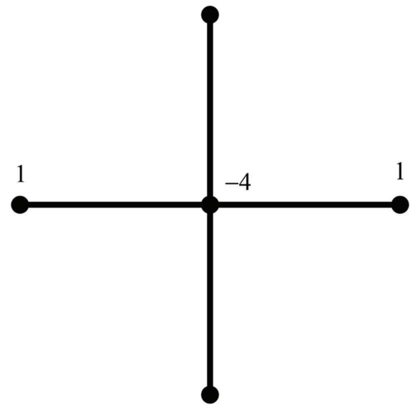

Figure 1.3 Computational molecule for $\mathbf{d}^2$.

$$\mathbf{d}^2 f(\mathbf{x}) = f(x+h,\ y) + f(x-h,\ y) + f(x,\ y+h) + f(x,\ y-h) - 4f(x,\ y), \tag{1.26}$$

and its computational molecule is depicted in Fig. 1.3; see Eq. (A1.1.17) for a deeper analysis of the significance of $\mathbf{d}^2$.

Using the points diagonally adjacent to $(x,\ y)$, we can construct another second-order S-FD approximation given by

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}'^2}{h^2} f(\mathbf{x}), \tag{1.27}$$

where

$$2\mathbf{d}'^2 f(\mathbf{x}) = f(x+h, y+h) + f(x+h, y-h) + f(x-h, y+h) + f(x-h, y-h) - 4f(x, y). \tag{1.28}$$

The factor of 2 in Eq. (1.28) takes into account the distance from $(x,\ y)$ to $(x \pm h,\ y \pm h)$, which is $h\sqrt{2}$. The computational molecule of $\mathbf{d}'^2$ is shown in Fig. 1.4.

Now let $0 \leq g \leq 1$ be a parameter; then a family of second-order FD approximations to ∇^2 is

$$\nabla^2 \cong \frac{g\mathbf{d}^2 + (1-g)\mathbf{d}'^2}{h^2}. \tag{1.29}$$

The computational molecule for $\mathbf{d}_g^2 = g\mathbf{d}^2 + (1-g)\mathbf{d}'^2$ is shown in Fig. 1.5. From the definition Eq. (1.11), we have the identity

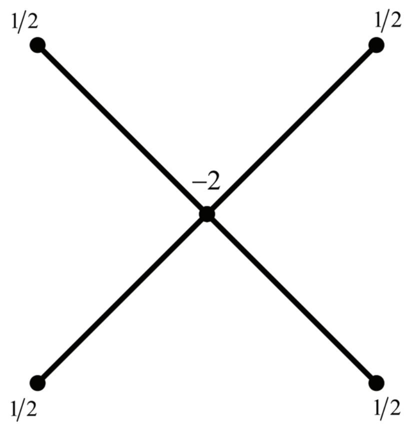

Figure 1.4 Computational molecule for $\mathbf{d}'^2$.

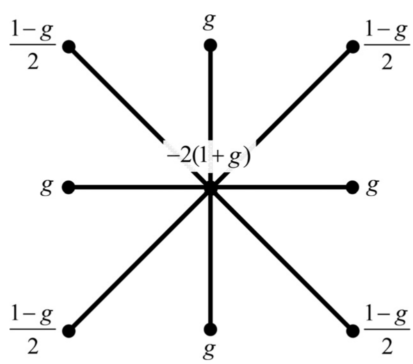

Figure 1.5 Computational molecule for $\mathbf{d}_g^2 = g\mathbf{d}^2 + (1-g)\mathbf{d}'^2$.

$$f(x+h) + f(x-h) = d_x^2 f(x) + 2f(x). \tag{1.30}$$

Applying Eq. (1.11) to $2\mathbf{d}'^2 f(\mathbf{x}) + 4f(\mathbf{x})$, we obtain

$$\begin{aligned}2\mathbf{d}'^2 f(\mathbf{x}) + 4f(\mathbf{x}) &= f(x+h, y+h) + f(x-h, y+h) + f(x+h, y-h) \\ &\quad + f(x-h, y-h) \\ &= d_x^2[f(x, y+h) + f(x, y-h)] + 2[f(x, y+h) + f(x, y-h)] \\ &= d_x^2[d_y^2 f(x,y) + 2f(x,y)] + 2[d_y^2 f(x,y) + 2f(x,y)] \\ &= d_x^2 d_y^2 f(x,y) + 2[d_x^2 + d_y^2] f(x,y) + 4f(x,y). \end{aligned} \tag{1.31}$$

Thus,

$$\mathbf{d}'^2 = d_x^2 + d_y^2 + \frac{1}{2} d_x^2 d_y^2$$
$$= \mathbf{d}^2 + \frac{1}{2} d_x^2 d_y^2. \tag{1.32}$$

See Eq. (A1.1.15) for a further analysis of the significance of $\mathbf{d}'^2$. Hence, the most general S-FD operator for the Laplacian is

$$\mathbf{d}_\gamma^2 = \mathbf{d}^2 + \gamma\, d_x^2 d_y^2, \tag{1.33}$$

where γ is a parameter, and the most general S-FD approximation to ∇^2 is

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}_\gamma^2}{h^2}. \tag{1.34}$$

The term $\mathbf{d}^2/h^2$ is a valid approximation of ∇^2 because $\lim_{h\to 0}[\mathbf{d}^2 f(\mathbf{x})/h^2] = \nabla^2 f(\mathbf{x})$. Since $d_x^2 d_y^2 f(\mathbf{x}) = h^4 \partial_x^2 \partial_y^2 f(\mathbf{x}) + \cdots$, $\lim_{h\to 0} d_x^2 d_y^2 f(\mathbf{x})/h^2 = \lim_{h\to 0}[h^2 \partial_x^2 \partial_y^2 f(\mathbf{x})] = 0$; thus, $\lim_{h\to 0}[\mathbf{d}_\gamma^2 f(\mathbf{x})/h^2] = \nabla^2 f(\mathbf{x})$. This is true regardless of the value of γ, so γ is a free parameter.

As we shall later see, when h is not infinitesimal, the value of γ can be chosen such that the error of the finite difference expression is minimized with respect to certain classes of functions.

1.3.2 Three dimensions

In three dimensions, $\mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2$ and

$$\mathbf{d}^2 f(\mathbf{x}) = f(x+h, y, z) + f(x-h, y, z) + f(x, y+h, z) + f(x, y-h, z)$$
$$+ f(x, y, z+h) + f(x, y, z-h) - 6f(x, y, z). \tag{1.35}$$

Now there are two additional FD operators, $\mathbf{d}'^2$ and $\mathbf{d}''^2$, given by

$$4\mathbf{d}'^2 f(\mathbf{x}) = f(x, y+h, z+h) + f(x, y-h, z+h)$$
$$+ f(x, y+h, z-h) + f(x, y-h, z-h)$$
$$+ f(x+h, y, z+h) + f(x-h, y, z+h)$$
$$+ f(x+h, y, z-h) + f(x-h, y, z-h)$$
$$+ f(x+h, y+h, z) + f(x-h, y+h, z)$$
$$+ f(x+h, y-h, z) + f(x-h, y-h, z) - 12f(x, y, z), \tag{1.36}$$

and

$$\begin{aligned}4\mathbf{d}''^2 f(\mathbf{x}) = {} & f(x+h, y+h, z+h) + f(x-h, y-h, z-h) \\ & + f(x+h, y-h, z+h) + f(x-h, y+h, z-h) \\ & + f(x-h, y+h, z+h) + f(x+h, y-h, z-h) \\ & + f(x-h, y-h, z+h) + f(x+h, y+h, z-h) - 8f(x, y, z). \end{aligned} \tag{1.37}$$

Thus,

$$\nabla^2 \cong \frac{\mathbf{d}'^2}{h^2}, \tag{1.38}$$

$$\nabla^2 \cong \frac{\mathbf{d}''^2}{h^2}. \tag{1.39}$$

Again using identity Eq. (1.30), it can be shown that

$$\mathbf{d}'^2 = \mathbf{d}^2 + \frac{1}{4}(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2), \tag{1.40}$$

$$\mathbf{d}''^2 = \mathbf{d}^2 + \frac{1}{2}(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{4} d_x^2 d_y^2 d_z^2, \tag{1.41}$$

and the most general second-order FD operator for ∇^2 in three dimensions is

$$\mathbf{d}_\gamma^2 = \mathbf{d}^2 + \gamma_1(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2, \tag{1.42}$$

where $\gamma = (\gamma_1, \gamma_2)$ is arbitrary. The most general S-FD expression is thus

$$\nabla^2 \cong \frac{\mathbf{d}_\gamma^2}{h^2}. \tag{1.43}$$

1.4 Nonstandard Finite Difference Expressions for the Laplacian

Since solutions of the wave equation and Maxwell's equations can be expressed in terms of Fourier components, it is of great interest to find FD expressions for ∇^2 that are accurate with respect to $e^{i\mathbf{k}\bullet\mathbf{x}}$, where $\mathbf{k} = (k_x, k_y, k_z)$.

In Section 1.2.1 it was shown that

$$d_x e^{ikx}/e^{ikx} = 2i\sin(kh/2) \Rightarrow d_x^2 e^{ikx}/e^{ikx} = -4\sin^2(kh/2)$$

and thus $d_x^2/s(h)^2 = \partial_x^2 e^{ikx}$, exactly, where $s(h) = 2\sin(kh/2)/k$.

Evaluating $\mathbf{d}^2 e^{i\mathbf{k}\bullet\mathbf{x}}$, we find that

$$\frac{\mathbf{d}^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} = -4[\sin^2(k_x h/2) + \sin^2(k_y h/2) + \sin^2(k_z h/2)]; \tag{1.44}$$

thus,

$$\frac{\mathbf{d}^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{s(h,\mathbf{k})^2} = \nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}, \tag{1.45}$$

exactly, where

$$s(h,\mathbf{k})^2 = \frac{4[\sin^2(k_x h/2) + \sin^2(k_y h/2) + \sin^2(k_z h/2)]}{k^2}, \tag{1.46}$$

and $k^2 = |\mathbf{k}|^2 = k_x^2 + k_y^2 + k_z^2$.

Although Eq. (1.45) is an exact NS-FD expression, it is unsatisfactory because it is exact only for one direction of $\mathbf{k}$. We would like an expression that is exact for all $\mathbf{k}$ directions. Unfortunately, this is impossible, but it is possible to find an NS-FD expression that is much more accurate than the S-FD expression of Eq. (1.25).

1.4.1 Two dimensions

Using the general S-FD operator $\mathbf{d}_\gamma^2$ given by Eq. (1.33), let us seek a value of γ such that $\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}} = -4\sin^2(kh/2)\, e^{i\mathbf{k}\bullet\mathbf{x}}$, independently of the direction of $\mathbf{k}$. That is, we want

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = \frac{(d_x^2 + d_y^2 + \gamma d_x^2 d_y^2) e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2)$$
$$= 0 \tag{1.47}$$

for some value of γ. Evaluating the right side of Eq. (1.47), we obtain

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = 4[\sin^2(kh/2) - \sin^2(k_x h/2)$$
$$- \sin^2(k_y h/2)] + 16\gamma \sin^2(k_x h/2)\sin^2(k_y h/2), \tag{1.48}$$

where $(k_x, k_y) = k(\cos\theta, \sin\theta)$. The right side of Eq. (1.48) can be made to vanish with the choice $\gamma = \gamma(k_x, k_y)$, where

$$\gamma(k_x, k_y) = \frac{\sin^2(k_x h/2) + \sin^2(k_y h/2) - \sin^2(kh/2)}{4\sin^2(k_x h/2)\sin^2(k_y h/2)}. \tag{1.49}$$

Expanding Eq. (1.49) in a Taylor series about $kh = 0$, we find that

$$\gamma = \frac{1}{6} + \frac{(kh)^2}{180} + \frac{(kh)^4}{16}\left[\frac{19}{7560} + \frac{\cos(4\theta)}{1512}\right] + \cdots. \tag{1.50}$$

Although γ is not independent of the $\mathbf{k}$ direction, its dependence is weak, and thus for practical discretizations ($0 < kh < 1$), the fourth-order terms in kh, $O(kh)^4$, and higher orders, can be dropped, leaving

$$\gamma = \frac{1}{6} + \frac{(kh)^2}{180}. \tag{1.51}$$

Now inserting $\gamma = 1/6$ into Eq. (1.48) and expanding the right side in a Taylor series about $kh = 0$, we find that

$$\frac{\mathbf{d}^2_{1/6} e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = \frac{(kh)^6}{1440}[1 - \cos(4\theta)] + \cdots. \tag{1.52}$$

Next, taking $\gamma = 1/6 + (kh)^2/180$ in Eq. (1.48), we find that

$$\frac{\mathbf{d}^2_{\gamma} e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = -\frac{(kh)^8}{2^8}\left[\frac{127}{30240} - \frac{11}{2520}\cos(4\theta) + \frac{1}{6048}\cos(8\theta)\right] + \cdots. \tag{1.53}$$

A simple calculation shows that the maximum deviation of $\mathbf{d}^2_{\gamma} e^{i\mathbf{k}\bullet\mathbf{x}}/e^{i\mathbf{k}\bullet\mathbf{x}}$ from $-4\sin^2(kh/2)$ is

$$\max\left|\frac{\mathbf{d}^2_{\gamma} e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2)\right| = \frac{11}{322560}(kh)^8. \tag{1.54}$$

We have shown[2] that for $\gamma = \gamma'$, where $\gamma' = \gamma(k'_x, k'_y)$ and $(k'_x, k'_y) = k(2^{-1/4}, \sqrt{1 - 2^{-1/2}})$, the deviation from $4\sin^2(kh/2)$ is even further reduced; however, in practical calculations, it is sufficient to take the value of γ given by Eq. (1.51), and often it is sufficient to use $\gamma = 1/6$.

For practical purposes, $\mathbf{d}^2_{\gamma} e^{i\mathbf{k}\bullet\mathbf{x}}/e^{i\mathbf{k}\bullet\mathbf{x}} = 4\sin^2(kh/2)$ is an excellent approximation; thus, a nearly exact NS-FD approximation with respect to $e^{i\mathbf{k}\bullet\mathbf{x}}$ is

$$\nabla^2 \cong \frac{\mathbf{d}^2_{\gamma}}{s(h)^2}, \tag{1.55}$$

where $s(h) = 2\sin(kh/2)/k$, as in the one-dimensional (1D) case. Defining the relative error of the NS-FD approximation for ∇^2 with respect to $e^{i\mathbf{k}\bullet\mathbf{x}}$ as

$$\varepsilon_{NS}(\gamma) = \frac{1}{\nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}}\left[\frac{\mathbf{d}_\gamma^2}{s(h)^2} - \nabla^2\right]e^{i\mathbf{k}\bullet\mathbf{x}}$$
$$= -\frac{\left[4\sin^2(kh/2) + \mathbf{d}_\gamma^2\right]e^{i\mathbf{k}\bullet\mathbf{x}}}{4\sin^2(kh/2)e^{i\mathbf{k}\bullet\mathbf{x}}}, \tag{1.56}$$

and expanding ε_{NS} in a Taylor series about $kh = 0$, we find that

$$\varepsilon_{NS}(1/6) = \frac{(kh)^4}{1440}[1 - \cos(4\theta)] + \cdots, \tag{1.57}$$

$$\varepsilon_{NS}(1/6 + (kh)^2/180) = \frac{(kh)^6}{256}\left[\frac{11}{2520} - \frac{\cos(4\theta)}{270} - \frac{\cos(8\theta)}{1512}\right] + \cdots. \tag{1.58}$$

A simple calculation shows that the maximum error of the NS-FD Laplacian expression is

$$\max|\varepsilon_{NS}[1/6 + (kh)^2/180]| = \frac{1}{34560}(kh)^6. \tag{1.59}$$

On the other hand, the error of the S-FD expression is

$$\varepsilon_S = \frac{1}{\nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}}\left(\frac{\mathbf{d}^2}{h^2} - \nabla^2\right)e^{i\mathbf{k}\bullet\mathbf{x}}$$
$$= -\left[\frac{((kh)^2 + \mathbf{d}^2)e^{i\mathbf{k}\bullet\mathbf{x}}}{(kh)^2 e^{i\mathbf{k}\bullet\mathbf{x}}}\right]$$
$$= -\frac{(kh)^2}{16}\left[1 + \frac{\cos(4\theta)}{3}\right] + \cdots. \tag{1.60}$$

In conclusion, by cleverly combining second-order FD operators, we can construct NS-FD expressions for $\nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}$ with up to sixth-order accuracy.

1.4.2 Three dimensions

The above developments in two dimensions can be extended to three. In spherical coordinates (θ and φ) $\mathbf{k} = k(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. The deviation of $\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}/e^{i\mathbf{k}\bullet\mathbf{x}}$ from $-4\sin^2(kh/2)$ is

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2)$$
$$= \frac{\left[d_x^2 + d_y^2 + d_z^2 + \gamma_1(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2\right] e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2), \tag{1.61}$$

where $\gamma = (\gamma_1, \gamma_2)$. Expanding Eq. (1.61) in a Taylor series about $kh = 0$, we find that

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = -\frac{(kh)^4}{48}(6\gamma_1 - 1)\sin^2(\theta)$$
$$\times \left[\frac{\sin^2(2\varphi + \theta)}{2} + \frac{\sin^2(2\varphi - \theta)}{2} - \sin^2(2\varphi) + 7\sin^2(\theta) - 8\right]$$
$$+ O(kh)^6 + \cdots. \tag{1.62}$$

Thus, setting $\gamma_1 = 1/6$ causes the $(kh)^4$ term to vanish, regardless of the value of γ_2. Now taking $\gamma = [1/6 + \alpha(kh/2]^2, \gamma_2)$ in Eq. (1.62), we seek α and γ_2 such that the $(kh)^6$ term vanishes. Carrying out expansion in Eq. (1.62) to the sixth order in kh, we see that $-9\alpha + \gamma_2 + 1/6 = 0$, which implies that $\gamma_2 = 9\alpha - 1/6$ so that the constant (non-angular dependent) part of the $(kh)^6$ term vanishes. Setting $\gamma = (1/6 + \alpha(kh/2)^2, 9\alpha - 1/6)$ in Eq. (1.62), we find that

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = \left(\alpha - \frac{1}{45}\right)\frac{(kh)^6}{64}$$
$$\times [\sin^4\theta\sin^2(2\varphi)(1 - 36\cos^2\theta) + \sin^2(2\theta)] + \cdots. \tag{1.63}$$

Thus, taking $\alpha = 1/45$ eliminates the $(kh)^6$ term, leaving only higher-order terms. Taking

$$\gamma_1 = \frac{1}{6} + \frac{(kh)^2}{180}, \tag{1.64a}$$

$$\gamma_2 = \frac{1}{30}, \tag{1.64b}$$

we obtain

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}}{e^{i\mathbf{k}\bullet\mathbf{x}}} + 4\sin^2(kh/2) = O(kh/2)^8. \tag{1.65}$$

We find that

$$\varepsilon_{\mathrm{NS}}[1/6+(kh)^2/180, 1/30] = (kh/2)^6 \times [\text{complicated expressions in}\,\theta\,\text{and}\,\varphi]. \tag{1.66}$$

On the other hand, the S-FD error is

$$\varepsilon_{\mathrm{S}} = (kh/2)^2 \times [\text{complicated expressions in}\,\theta\,\text{and}\,\varphi]. \tag{1.67}$$

Thus motivated, we now define the NS Laplacian operator to be

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6}+\frac{(kh)^2}{180}\right]\left(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2\right) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \tag{1.68}$$

In two dimensions, where $d_z^2 = 0$, this definition reduces to

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6}+\frac{(kh)^2}{180}\right] d_x^2 d_y^2. \tag{1.69}$$

As we have seen, $\mathbf{d}_\gamma^2 e^{i\mathbf{k}\bullet\mathbf{x}}/e^{i\mathbf{k}\bullet\mathbf{x}} = 4\sin^2(kh/2)$ almost exactly for any practical discretization when $0 < kh < 1$; hence,

$$\frac{\tilde{\mathbf{d}}^2}{s(h)^2} e^{i\mathbf{k}\bullet\mathbf{x}} = \nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}. \tag{1.70}$$

almost exactly, where $s(h) = 2\sin(kh/2)/k$, and the error is $O(kh)/2^8$.

Note 1.1

Consider a medium in which the refractive index is piecewise constant, ranging from $n = 1$ (the ambient medium) to n_s (in a "scatterer"), The local wavenumber thus lies between k_0 and $n_s k_0$. In many practical FDTD calculations, it is sufficient to take

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6}+\frac{(k_0 h)^2}{180}\right]\left(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2\right) + \frac{1}{30} d_x^2 d_y^2 d_z^2, \tag{1.71}$$

so that $\tilde{\mathbf{d}}^2$ is not a function of position. In fact, for sufficiently small $k_0 h$, we can simply take

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \frac{1}{6}\left(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2\right) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \tag{1.72}$$

The last term of Eq. (1.72), although small, is needed to ensure the stability of NS-FDTD.

1.5 Factoring the Nonstandard Finite Difference Laplacian

To construct an NS-FD algorithm to solve Maxwell's equations, we would like to find a NS-difference operator $\mathbf{d}'$, such that $\mathbf{d}' \bullet \mathbf{d}' = \tilde{\mathbf{d}}^2$. Unfortunately, this is impossible. Although $\mathbf{d} \bullet \mathbf{d} = \mathbf{d}^2$, $\mathbf{d}'$ does not exist, but we can find $\tilde{\mathbf{d}}$ such that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$ (but $\tilde{\mathbf{d}} \bullet \tilde{\mathbf{d}} \neq \tilde{\mathbf{d}}^2$).

1.5.1 Two dimensions

As we have seen, for function $f(x, y)$, $\partial_x f \cong d_x f/h$. There is another FD approximation given by $\partial_x f \cong d'_x f/h$, where

$$2d'_x f(x, y) = f(x + h/2, y + h) + f(x + h/2, y - h) - [f(x - h/2, y + h) + f(x - h/2, y - h)]. \tag{1.73}$$

Similarly, $\partial_y f \cong d'_x f/h$, where

$$2d'_y f(x, y) = f(x + h, y + h/2) + f(x - h, y + h/2) - [f(x + h, y - h/2) + f(x - h, y - h/2)]. \tag{1.74}$$

Using identity Eq. (1.30), it is easy to show that

$$d'_x = d_x\left(1 + \frac{1}{2}d_y^2\right), \tag{1.75a}$$

$$d'_y = d_y\left(1 + \frac{1}{2}d_x^2\right). \tag{1.75b}$$

Forming the vector difference operator $\mathbf{d}' = (d'_x, d'_y)$ and defining $\tilde{\mathbf{d}} = (\tilde{d}_x, \tilde{d}_y)$, we postulate the form $\tilde{\mathbf{d}} = \mathbf{d} + \alpha(d_x d_y^2, d_y d_x^2)$, or

$$\tilde{d}_x = d_x + \alpha d_y^2, \tag{1.76a}$$

$$\tilde{d}_y = d_y + \alpha d_x^2. \tag{1.76b}$$

Requiring that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$, we find that

$$\alpha = \frac{1}{12} + \frac{(kh)^2}{360}. \tag{1.77}$$

1.5.2 Three dimensions

In three dimensions, besides $\partial_x f \cong d_x f/h$, there are two additional FD expressions, $\partial_x f \cong d'_x f/h$ and $\partial_x f \cong d''_x f/h$, where

$$\begin{aligned} 4d'_x f(x,y,z) = {} & f(x+h/2, y+h, z+h) + f(x+h/2, y+h, z-h) \\ & + f(x+h/2, y-h, z+h) + f(x+h/2, y-h, z-h) \\ & - f(x-h/2, y+h, z+h) - f(x-h/2, y+h, z-h) \\ & - f(x-h/2, y-h, z+h) - f(x-h/2, y-h, z-h), \end{aligned} \tag{1.78}$$

$$\begin{aligned} 4d''_x f(x,y,z) = {} & f(x+h/2, y+h, z) + f(x+h/2, y-h, z) \\ & + f(x+h/2, y, z+h) + f(x+h/2, y, z-h) \\ & - f(x-h/2, y+h, z) - f(x-h/2, y-h, z) \\ & - f(x-h/2, y, z+h) - f(x-h/2, y, z-h). \end{aligned} \tag{1.79}$$

The corresponding difference operators for ∂_y and ∂_z can be found by analogy with ∂_x. Using Eq. (1.30), it can be straightforwardly shown that

$$d'_x = d_x\left(1 + \frac{d_y^2 + d_z^2}{2} + \frac{d_y^2 d_z^2}{4}\right), \tag{1.80a}$$

$$d'_y = d_y\left(1 + \frac{d_x^2 + d_z^2}{2} + \frac{d_x^2 d_z^2}{4}\right), \tag{1.80b}$$

$$d'_z = d_z\left(1 + \frac{d_x^2 + d_y^2}{2} + \frac{d_x^2 d_y^2}{4}\right), \tag{1.80c}$$

and

$$d''_x = d_x\left(1 + \frac{d_y^2 + d_z^2}{4}\right), \tag{1.81a}$$

$$d''_y = d_y\left(1 + \frac{d_x^2 + d_z^2}{4}\right), \tag{1.81b}$$

$$d''_z = d_z\left(1 + \frac{d_x^2 + d_y^2}{4}\right). \tag{1.81c}$$

Since we want the 3D form of $\tilde{\mathbf{d}}$ to reduce the 2D form for $d_z = 0$, we postulate that

$$\tilde{d}_x = d_x\left[1 + \alpha(d_y^2 + d_z^2) + \beta d_y^2 d_z^2\right], \tag{1.82a}$$

$$\tilde{d}_y = d_y\left[1 + \alpha(d_x^2 + d_z^2) + \beta d_x^2 d_z^2\right], \tag{1.82b}$$

$$\tilde{d}_z = d_z\left[1 + \alpha(d_x^2 + d_y^2) + \beta d_y^2 d_z^2\right], \tag{1.82c}$$

where α is given by Eq. (1.77). Again requiring that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$, we find that $\beta = 1/90$. Thus,

$$\tilde{\mathbf{d}} = \mathbf{d} + \left(\frac{1}{12} + \frac{(kh)^2}{360}\right)\begin{bmatrix} d_x(d_y^2 + d_z^2) \\ d_y(d_x^2 + d_z^2) \\ d_z(d_x^2 + d_y^2) \end{bmatrix} + \frac{1}{90}\begin{bmatrix} d_x(d_y^2 d_z^2) \\ d_y(d_x^2 d_z^2) \\ d_z(d_x^2 d_y^2) \end{bmatrix}, \tag{1.83}$$

where the column matrices represent vector difference operators. The 2D form of $\tilde{\mathbf{d}}$ is obtained by setting $d_z = 0$ in Eq. (1.83).

This formulation will be used in Chapter 10.

Important Points of Chapter 1

- We introduce the notation to be used throughout this book:
  Central partial difference operator:

  $$d_x f(x, y) = f(x + h/2, y) - f(x - h/2, y).$$

  Second partial difference operator:

  $$d_x d_x = d_x^2, \quad d_x^2 f(x, y) = f(x + h, y) + f(x - h, y) - 2f(x, y).$$

  Gradient difference operator:

  $$\text{standard: } \mathbf{d} = (d_x, d_y, d_z); \text{nonstandard: } \tilde{\mathbf{d}} = (\tilde{d}_x, \tilde{d}_y, \tilde{d}_z).$$

  Laplacian difference operator:

  $$\text{standard: } \mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2; \text{nonstandard: } \tilde{\mathbf{d}}^2 = \mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d}.$$

- Useful expressions:

  $$d_x e^{ikx} = 2i\sin(k\Delta x/2)\frac{k^2}{4\sin^2(kh/2)}\tilde{\mathbf{d}}^2 e^{i\mathbf{k}\bullet\mathbf{x}}$$
  $$= \nabla^2 e^{i\mathbf{k}\bullet\mathbf{x}}, \text{ almost exactly.}$$

- There exist exact finite difference expressions for the derivatives of the single-variable exponential functions.
- All finite difference expressions are equal (as $h \to 0$), but some finite difference expressions are more equal than others (for non-infinitesimal h).

Appendix 1.1 Mathematical Properties of Finite Difference Operators

We can gain useful insights by more closely examining the relationship between derivatives and finite difference expressions; this relationship also yields some useful expressions.

A1.1.1 Forward finite difference operator

Letting n be a positive integer, we express the definition of the derivative in the form

$$\frac{d}{dx}f(x) = \lim_{n\to\infty}\frac{f(x+h/n)-f(x)}{h/n}. \quad \text{(A1.1.1)}$$

For large n,

$$f(x+h/n) \cong \left(1+\frac{h}{n}\partial_x\right)f(x), \quad \text{(A1.1.2)}$$

where $\partial_x = d/dx$.

Readers who are familiar with Lie group theory will recognize ∂_x to be the generator of translations. Iterating Eq. (A1.1.2), we find that

$$\begin{aligned} f(x+2h/n) &\cong \left(1+\frac{h}{n}\partial_x\right)f(x+h/n) \\ &= \left(1+\frac{h}{n}\partial_x\right)^2 f(x). \end{aligned} \quad \text{(A1.1.3)}$$

By induction, we obtain

$$f(x+h) \cong \left(1+\frac{h}{n}\partial_x\right)^n f(x), \quad \text{(A1.1.4)}$$

and in the limit $n \to \infty$,

$$f(x+h) = e^{h\partial_x}f(x). \quad \text{(A1.1.5)}$$

Equation (A1.1.5) is the Taylor series expansion of $f(x + h)$ about x, and $e^{h\partial_x}$ is the Lie group element that produces the translation $x \to x + h$.

Thus, the forward difference $d_x^{\mathrm{f}}f(x) = f(x+h) - f(x)$ is given by

$$d_x^{\mathrm{f}}f(x) = (e^{h\partial_x} - 1)f(x); \quad \text{(A1.1.6)}$$

hence,

$$\begin{aligned} d_x^{\mathrm{f}} &= e^{h\partial_x} - 1 \\ &= h\partial_x + \frac{1}{2!}h^2\partial_x^2 + \frac{1}{3!}h^3\partial_x^3 + \cdots. \end{aligned} \quad \text{(A1.1.7)}$$

Solving for ∂_x in terms of FD operators, we obtain

$$\begin{aligned}\partial_x &= \frac{\ln(1+d_x^{\mathrm{f}})}{h} \\ &= \frac{1}{h}\left[d_x^{\mathrm{f}} - \frac{(d_x^{\mathrm{f}})^2}{2} + \frac{(d_x^{\mathrm{f}})^3}{3} \mp \cdots\right].\end{aligned} \tag{A1.1.8}$$

Thus, the differential equation $\partial_x f(x) = g(x)$ is equivalent to the difference equation $\left[d_x^{\mathrm{f}} - (d_x^{\mathrm{f}})^2/2 \pm \cdots\right] f(x) = hg(x)$; likewise, the difference equation $d_x^{\mathrm{f}} f(x) = hg(x)$ is equivalent to the differential equation $[\,\partial_x + h\,\partial_x^2/2 + \cdots\,] f(x) = g(x)$. It is therefore not surprising that the solution of a differential equation generally differs from that of its difference equation model.

A1.1.2 Central finite difference operator

We can derive similar expressions for the central FD operators. Using the results above, we find that

$$\begin{aligned}d_x^{\mathrm{c}} &= [e^{(h/2)\partial_x} - e^{-(h/2)\partial_x}] f(x) \\ &= 2\sinh[(h/2)\partial_x] f(x).\end{aligned} \tag{A1.1.9}$$

Hence, the central FD operator can be expressed in terms of derivatives as

$$\begin{aligned}d_x^{\mathrm{c}} &= 2\sinh[(h/2)\partial_x] \\ &= h\partial_x + \frac{1}{24}h^3\partial_x^3 + \frac{1}{1920}h^5\partial_x^5.\end{aligned} \tag{A1.1.10}$$

It is easily seen from the above that

$$\begin{aligned}(d_x^{\mathrm{c}})^2 &= 4\sinh^2[(h/2)\partial_x] \\ &= h^2\partial_x^2 + \frac{1}{12}h^4\partial_x^4 + \frac{1}{360}h^6\partial_x^6 + \cdots.\end{aligned} \tag{A1.1.11}$$

Solving Eq. (A1.1.11) for ∂_x, the expansion of the derivative in terms of central FD operators is

$$\begin{aligned}\partial_x &= \frac{1}{h}2\sinh^{-1}(d_x^{\mathrm{c}}/2) \\ &= \frac{1}{h}\left[d_x^{\mathrm{c}} - \frac{1}{24}(d_x^{\mathrm{c}})^3 + \frac{3}{640}(d_x^{\mathrm{c}})^5 \mp \cdots\right].\end{aligned} \tag{A1.1.12}$$

From Eq. (A1.1.12), we find that

$$\begin{aligned}\partial_x^2 &= \frac{1}{h^2}4[\sinh^{-1}(d_x^{\mathrm{c}}/2)]^2\\ &= \frac{1}{h^2}\left[(d_x^{\mathrm{c}})^2 - \frac{1}{12}(d_x^{\mathrm{c}})^4 + \frac{1}{90}(d_x^{\mathrm{c}})^6 \mp \cdots\right]. \qquad \text{(A1.1.13)}\end{aligned}$$

A1.1.3 Multiple variables

Equation (A1.1.5) can be generalized to the case of several variables:

$$f(x+h_x, y+h_y+z+h_z) = e^{h_x\partial_x + h_y\partial_y + h_z\partial_z} f(x, y, x). \qquad \text{(A1.1.14)}$$

For example, $2\mathbf{d}'^2 f(x)$ in Eq. (1.28),

$$\begin{aligned}2\mathbf{d}'^2 f(\mathbf{x}) =& f(x+h, y+h) + f(x+h, y-h)\\ &+ f(x-h, y+h) + f(x-h, y-h) - 4f(x, y),\end{aligned}$$

is equivalent to

$$\begin{aligned}2\mathbf{d}'^2 f(\mathbf{x}) &= [e^{h\partial_x + h\partial_y} + e^{-(h\partial_x + h\partial_y)} + e^{h\partial_x - h\partial_y} + e^{-(h\partial_x - h\partial_y)} - 4] f(x, y)\\ &= 2[\cosh(h\partial_x + h\partial_y) + \cosh(h\partial_x - h\partial_y) - 2] f(x, y)\\ &= \left\{h^2\left(\partial_x^2 + \partial_y^2\right) + h^4\left[\frac{1}{12}(\partial_x^4 + \partial_y^4) + \frac{1}{2}\partial_x^2\partial_y^2\right] + \cdots\right\} f(x, y).\end{aligned}$$

(A1.1.15)

On the other hand,

$$\begin{aligned}\mathbf{d}^2 f(\mathbf{x}) =& f(x+h, y) + f(x-h, y) + f(x, y+h)\\ &+ f(x, y-h) - 4f(x, y) \qquad \text{(A1.1.16)}\end{aligned}$$

is equivalent to

$$\begin{aligned}\mathbf{d}^2 f(\mathbf{x}) &= [e^{h\partial_x} + e^{-h\partial_x} + e^{h\partial_y} + e^{-h\partial_y} - 4] f(x, y)\\ &= 2[\cosh(h\partial_x) + \cosh(h\partial_y) - 2] f(x, y)\\ &= \left\{h^2\left(\partial_x^2 + \partial_y^2\right) + \frac{1}{12}h^4\left(\partial_x^4 + \partial_y^4\right) + \cdots\right\} f(x, y). \qquad \text{(A1.1.17)}\end{aligned}$$

Appendix 1.2 Noninteger-Order Sums and Differences

Except for Note A1.2.1, this Appendix 1.2 is not directly relevant to the main text. We include it as a reference for those interested in modeling phenomena outside the scope of this book. Certain physical phenomena (such as quantum entanglement) appear to be nonlocal, and it is interesting to note that noninteger-order differences and sums are also nonlocal.

Sums and differences can be extended to noninteger-order and are useful in modeling stochastic processes such as Brownian motion. Interesting insight can be gained by examining these generalizations.

Note that in this appendix, d denotes the forward finite difference.

A1.2.1 Noninteger-order summation

Let $x = \chi h$ and $f_\chi = f(\chi h)$, and define the summation operator by

$$Sf|_0^\chi = \sum_{i=0}^{\chi-1} f_i \tag{A1.2.1}$$

in the limit

$$\lim_{h\to 0} h\ Sf|_0^\chi = \int_0^x dt f(t), \tag{A1.2.2}$$

defining the double summation

$$S^2 f|_0^\chi = \sum_{i=0}^{\chi-1}\sum_{j=0}^{i} f_j, \tag{A1.2.3}$$

where $\chi \geq 2$. Notice that in the second sum, j runs from 0 to i, not to $i - 1$. In the limit

$$\lim_{h\to 0} h^2 S^2 f|_0^\chi = \int_0^x dt \int_0^t dt' f(t'), \tag{A1.2.4}$$

by definition,

$$\begin{aligned}
&\sum_{j=0}^{0} f_j = f_0,\\
&\sum_{j=0}^{1} f_j = f_0 + f_1,\\
&\sum_{j=0}^{2} f_j = f_0 + f_1 + f_2;\\
&\qquad\vdots
\end{aligned} \tag{A1.2.5}$$

thus,

$$\sum_{i=0}^{\chi-1}\sum_{j=0}^{i} f_j = \chi f_0 + (\chi-1) f_1 + (\chi-2) f_2 + \cdots + f_{\chi-1}, \tag{A1.2.6}$$

and hence,

$$S^2 f|_0^\chi = \sum_{i=0}^{\chi-1} (\chi - i) f_i. \tag{A1.2.7}$$

Notice the similarity of Eq. (A1.2.7) to the two-fold integral $I^2 f|_0^x = \int_0^x dt\,(x-t)\,f(t)$ given by Eq. (A2.2.3).

Evaluating the triple summation

$$S^3 f|_0^\chi = \sum_{i=0}^{\chi-1} \sum_{j=0}^{i} \sum_{k=0}^{j} f_k, \tag{A1.2.8}$$

we find that

$$\begin{aligned}\sum_{j=0}^{i}\sum_{k=0}^{j} f_k = f_0 & \\ & + f_0 + f_1 \\ & + f_0 + f_1 + f_2 \\ & + \\ & \vdots \\ & + f_0 + f_1 + \cdots + f_i \\ &= (i+1) f_0 + i f_1 + (i-1) f_2 + \cdots + f_1 \\ &= \sum_{j=0}^{i} (i+1-j) f_j. \end{aligned} \tag{A1.2.9}$$

Thus,

$$\begin{aligned}\sum_{i=0}^{\chi-1}\sum_{j=0}^{i}\sum_{k=0}^{j} f_k = f_0 & \\ & + 2f_0 + f_1 \\ & + 3f_0 + 2f_1 + f_2 \\ & \vdots \\ & + \chi f_0 + (\chi-1) f_1 + (\chi-2) f_2 + \cdots + f_{\chi-1} \\ &= f_0 \frac{(\chi+1)\chi}{2} + f_1 \frac{\chi(\chi-1)}{2} + f_2 \frac{(\chi-1)(\chi-2)}{2} + \cdots + f_{\chi-1} \\ &= \frac{1}{2}\sum_{i=0}^{\chi-1} (\chi+1-i)(\chi-i) f_i. \end{aligned} \tag{A1.2.10}$$

Therefore,

$$S^3 f|_0^\chi = \frac{1}{2}\sum_{i=0}^{\chi-1}\frac{(\chi+1-i)!}{(\chi-1-i)!}f_i. \tag{A1.2.11}$$

By induction, we obtain

$$S^n f|_0^\chi = \frac{1}{(n-1)!}\sum_{i=0}^{\chi-1}\frac{(\chi+n-2-i)!}{(\chi-i-1)!}f_i. \tag{A1.2.12}$$

Substituting Γ functions in place of the factorial functions, and using $\Gamma(n) = (n-1)!$, noninteger-order summation for $n \geq 0$ is defined by

$$S^n f|_0^\chi = \frac{1}{\Gamma(n)}\sum_{i=0}^{\chi-1}\frac{\Gamma(\chi+n-1-i)}{\Gamma(\chi-i)}f_i. \tag{A1.2.13}$$

Note A1.2.1

The Γ function[3] is defined by

$$\Gamma(x) = \int_0^\infty dt e^{-t} t^{x-1.} \tag{A1.2.14}$$

This definition is valid for noninteger arguments. When $n > 1$ is an integer, $\Gamma(n) = (n-1)!$ The Taylor expansion of $1/\Gamma(x)$ about $n = 0$ is

$$\frac{1}{\Gamma(x)} = x + \cdots; \tag{A1.2.15}$$

hence,

$$\lim_{x\to 0}\frac{1}{\Gamma(x)} = 0. \tag{A1.2.16}$$

From Eq. (A1.2.13), we have

$$S^0 f|_0^\chi = \frac{1}{\Gamma(0)}\left[\frac{\Gamma(N-1)}{\Gamma(N)}f_0 + \frac{\Gamma(N-2)}{\Gamma(N-1)}f_1 + \frac{\Gamma(N-3)}{\Gamma(N-2)}f_1 + \cdots \frac{\Gamma(0)}{\Gamma(1)}\right], \tag{A1.2.17}$$

and using Eq. (A1.2.16), we find that

$$S^0 f|_0^\chi = f_{\chi-1}. \tag{A1.2.18}$$

One might have hoped that $S^0 f|_0^\chi$ would be f_χ so that S^0 would be the identity operator **1**. However, $\lim_{h\to 0} f(\chi h - h) = f(\chi h) \Rightarrow \lim_{h\to 0} f_{\chi-1} = f_\chi$; thus, $\lim_{h\to 0} S^0 f|_0^\chi = f_\chi$ and, hence,

$$\lim_{h\to 0} S^0 = \mathbf{1}. \tag{A1.2.19}$$

If the upper limit of the summation in Eq. (A1.2.1) were to taken to be χ instead of $\chi - 1$, we would have $S^0 f|_0^\chi = f_\chi$, but this would give (see Section A1.2.2) $dS^0 f|_0^\chi = f_{\chi+1}$ instead of f_χ (where $df_\chi = f_{\chi+1} - f_\chi$); thus, d would not be the inverse of S.

Example 1

Letting $f(x) = x$, $Sf|_0^\chi = h\sum_{i=0}^{\chi-1} i$ is the summation of an arithmetic series. $S^{1/2} f|_0^\chi$ is given by

$$S^{1/2} f|_0^\chi = \frac{h}{\Gamma(1/2)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi - i - 1/2)}{\Gamma(\chi - i)} i$$
$$= h \sum_{i=0}^{\chi-1} \frac{i}{(\chi - i - 1)!} \frac{1}{2^{\chi-i-1}} \prod_{j=0}^{\chi-i} |2j - 1|, \qquad \text{(A1.2.20)}$$

where

$$\frac{\Gamma(n - 1/2)}{\Gamma(1/2)} = \frac{1}{2^{n-1}} \prod_{m=0}^{n-1} |2m - 1|. \qquad \text{(A1.2.21)}$$

Taking $\chi = 5$ and $h = 1$, we obtain the weighted sum,

$$S^{1/2} f|_0^5 = \frac{3 \cdot 5 \cdot 7}{2^3 3!} \cdot 1 + \frac{3 \cdot 5}{2^2 2!} \cdot 2 + \frac{3}{2^1 1!} \cdot 3 + 4,$$
$$= \frac{35}{16} \cdot 1 + \frac{15}{8} \cdot 2 + \frac{3}{2} \cdot 3 + 1 \cdot 4. \qquad \text{(A1.2.22)}$$

Example 2

Taking $f(x) = \sin(\pi x/2.1)/e^{x/6}\sqrt{x+1} - (1 - e^{-x/30})\sqrt{x}$, $\chi = 10$, and $h = 1$, we plot $S^n f|_0^{10}$ versus n in Fig. A1.2.1. Here, n is real (not necessarily an integer); obviously, the noninteger sum is a smooth generalization from integer-order summation to noninteger-order summation.

A1.2.2 Noninteger-order differences

The forward finite difference operator d acting on f is defined by

$$df_\chi = f_{\chi+1} - f_\chi. \qquad \text{(A1.2.23)}$$

Iterating Eq. (A1.2.23) n fold, it is easy to show that

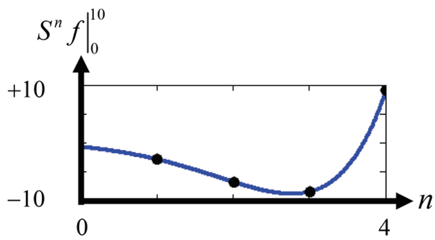

Figure A1.2.1 The integer and noninteger-order sums of Example 1.2. Dots denote integer-order sums, and lines denote noninteger-order sums.

$$d^n f_\chi = \sum_{\ell=0}^{n} \frac{(-1)^\ell n!}{(n-\ell)!\ell!} f_{\chi+n-\ell}, \tag{A1.2.24}$$

where $n \geq 0$ is an integer.

Note A1.2.2

The substitution $f(x) \to f(x - nh/2) \Rightarrow f_{\chi+n-\ell} \to f_{\chi+(n/2)-\ell}$ in Eq. (A1.2.24) yields the n^{th} central difference. $d^c f_\chi = f_{\chi+1/2} - f_{\chi-1/2}$, and

$$(d^c)^2 f_\chi = f_{\chi+1} - 2f_\chi + f_{\chi+1}, \tag{A1.2.25a}$$

$$(d^c)^3 f_\chi = f_{\chi+3/2} - 3f_{\chi+1/2} + 3f_{\chi-1/2} - f_{\chi-3/2}, \tag{A1.2.25b}$$

$$(d^c)^4 f_\chi = f_{\chi+2} - 4f_{\chi+1} + 6f_\chi - 4f_{\chi-1} + f_{\chi-2}, \tag{A1.2.25c}$$

etc.

Evaluating Eq. (A1.2.24) for $n = 0$ gives $d^0 f_\chi = f_\chi$; hence,

$$d^0 = \mathbf{1}. \tag{A1.2.26}$$

It is easy to show that $dSf|_0^\chi = f_\chi \Rightarrow dS = \mathbf{1}$. Thus, d is the left inverse of S:

$$d = S_{\text{left}}^{-1}. \tag{A1.2.27}$$

However, $Sd \neq dS$, thus, $Sd \neq \mathbf{1}$; instead,

$$Sdf|_0^\chi = \sum_{\tau=0}^{\chi-1} [f_{\tau+1} - f_\tau]$$
$$= f_\chi - f_0. \tag{A1.2.28}$$

Note A1.2.3

If the upper limit of the summation in Eq. (A1.2.1) had been taken to be χ instead of $\chi - 1$, then we would have had $dSf|_0^\chi = f_{\chi+1}$, and d would not be the left inverse of S.

We now proceed to extend the difference operation defined in Eq. (A1.2.24) to noninteger values. Simply replacing the factorial terms with Γ functions does not yield a useful definition. Instead, we make use of noninteger-order summation. Taking $0 \leq \nu < 1$, we define

$$d^{\nu} = dd^{\nu-1} = dd^{-(1-\nu)} = dS^{1-\nu}, \qquad \text{(A1.2.29)}$$

where $d^{-(1-\nu)} = S^{1-\nu}$ because d is the left inverse of S. Thus, from Eq. (A1.2.13),

$$\begin{aligned} d^{\nu} f_{\chi} &= \frac{1}{\Gamma(1-\nu)} d \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi-\nu-i)}{\Gamma(\chi-i)} f_i \\ &= f_{\chi} - \frac{\nu}{\Gamma(1-\nu)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi-\nu-i)}{\Gamma(\chi+1-i)} f_i. \end{aligned} \qquad \text{(A1.2.30)}$$

Setting $\nu = 0$ in Eq. (A1.2.30), we find that $d^0 f_{\chi} = f_{\chi} \Rightarrow d^0 = \mathbf{1}$, in accordance with Eq. (A1.2.26).

Next, using Eq. (A1.2.29), let us evaluate $d^1 f_{\chi} = \lim_{\nu \to 1} dS^{1-\nu} f|_0^{\chi}$, using $S^0 f|_0^{\chi} = f_{\chi-1} = f_{\chi-1}$ from Eq. (A1.2.18). This yields

$$df_{\chi} = f_{\chi} - f_{\chi-1}, \qquad \text{(A1.2.31)}$$

which contradicts the definition in Eq. (A1.2.23). The definition of a noninteger (ν^{th})-order difference [Eq. (A1.2.28)] is thus inconsistent with the definition of the integer-order difference in the limit $\nu = n \to 1$. However, since

$$\lim_{h \to 0} \frac{f_{\chi} - f_{\chi-1}}{h} = \lim_{h \to 0} \frac{f_{\chi+1} - f_{\chi}}{h} = f'(x), \qquad \text{(A1.2.32)}$$

d^{ν}, as defined by Eq. (A1.2.29), does converge to d in the double limits $h \to 0$ and $\nu \to 1$; that is,

$$\lim_{h \to 0} (\lim_{\nu \to 1} d^{\nu}) = d. \qquad \text{(A1.2.33)}$$

One could try to redefine the sum and difference operators to make $\lim_{\nu \to 1} d^{\nu} = d$ even when h is not infinitesimal, but this approach leads to much more complicated expressions that are not intuitively obvious.

For noninteger $n + \nu$, where $n \geq 0$ is an integer and $0 < \nu < 1$ is real, we define $d^{\nu+n}$ in two steps by

$$g_{\chi} = d^n f_{\chi}, \qquad \text{(A1.2.34a)}$$

$$d^{n+\nu} f_{\chi} = d^{\nu} g_{\chi}, \qquad \text{(A1.2.34b)}$$

where $d^n f_\chi$ is computed using Eq. (A1.2.24), and $d^\nu g_\chi$ is computed using Eq. (A1.2.30).

While for integer n, $d^n f_\chi$ depends only on the values of $f_{\chi+1}$ in the range $0 \le i \le n$, $d^{n+\nu} f_\chi$ depends on all the values of f_i in the range $0 \le i \le \chi + n$.

Example 3

Let $\chi = 5$, $h = 1$, and $f(x) = x^2$; then, $df_\chi = 2\chi h + h^2$. Using Eqs. (A1.2.29) and (A1.2.30) together with Eq. (A1.2.21), we find that

$$d^{1/2} f_\chi = \chi^2 - \frac{1}{2\,\Gamma(1/2)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi - i - 1/2)}{(\chi - i)!} i^2$$

$$= \chi^2 - \sum_{i=0}^{\chi-1} \frac{1}{(\chi - i)!} \frac{i^2}{2^{\chi-i}} \prod_{j=0}^{\chi-i} |2j - 1| \qquad \text{(A1.2.35)}$$

Example 4

Let $f(x) = 10e^{-x/16}\sin(\pi x/8)$ and $1 \le \chi \le 32$, and plot $d^n f_\chi$ versus χ for different values of n. Figure A1.2.2 shows that as $0 < \varepsilon \to 0$, $\lim_{\varepsilon \to 0} d^{n+\varepsilon} f_\chi = d^n f_\chi$, but $\lim_{\varepsilon \to 0} \partial^{n-\varepsilon} f_\chi \ne d^2 f_\chi$. For example, $d^{2.01} f_\chi \cong d^2 f_\chi$, but $d^{1.99} f_\chi \ncong d^2 f_\chi$.

Further details on noninteger sums and differences can be found in Ref. 4.

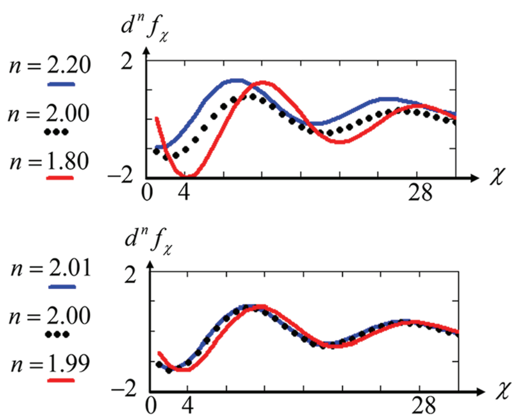

Figure A1.2.2 Integer and noninteger-order differences.

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