Notes on September 5, 2019

MATH 4665/4875/7140/7300, Fall 2019, HKBU

Location for classes: LMC 514, HKBU

Time for classes: Wednesdays 15:30–16:20; Thursdays 13:30–15:20

Main text to use: Numerical Partial Differential Equations in Finance Explained by Karel in 't Hout, published by the Springer Nature, 2017

Lecture notes: They will be uploaded frequently to the Moodle system at HKBU

Assessment methods: homework and quizzes (20%); two numerical projects (probably for the weeks of 09/30–10/04 and 11/11–11/15; total 20%); final exam (60%)

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Approximations of Financial Derivatives via Finite Differences: the Fundamentals [3]

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Abstract: Finite differences have been widely used in mathematical theory as well as in scientific and engineering computations. These concepts are constantly mentioned in calculus. Most frequently-used difference formulas provide excellent approximations to various derivative functions, including those used in modelling important physical processes on uniform grids. However, our research reveals that difference approximations on uniform grids cannot be applied blindly on nonuniform grids, nor can difference formulas to form consistent approximations to second derivatives. At best, they may lose accuracy; at worst they are inconsistent. Detailed consistency and error analysis, together with some simulated examples, will be given.

1. Background. Different finite difference formulas have been constructed and utilized for approximating the rates of change of a function in applications. The function is given either as an analytical expression or as a set of numbers at discrete points in the region of interest. The mathematical models of most science and engineering problems require such an approximation if computer simulations are desirable.

In many discussions of one-dimensional finite differences, the aforementioned discrete points are uniformly distributed, that is, the distance between any two neighboring points is a positive constant h.

Let $f(t)$ be a differentiable function on (a, b). Recall the definition of the derivative at a fixed point $t \in (a, b)$:

$$f'(t) = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h}.$$

Thus, it is reasonable that the fraction

$$g(t, h) = \frac{f(t+h) - f(t)}{h}, \quad 0 < h \ll 1, \tag{1.1}$$

would provide an approximation of the derivative $f'(t)$ on the set $\mathcal{T} = \{t,\ t \pm h,\ t \pm 2h, \ldots\} \cap (a, b)$. In fact, it can be shown by Newton-Gregory interpolation formulas that $g(t, h)$ is indeed an approximation of $f'(t)$ [3]. Formula (1.1) is called a *first order forward difference* [2]. Based on it, a *second order forward difference* could be constructed:

$$\frac{g(t+h, h) - g(t, h)}{h} = \frac{f(t+2h) - 2f(t+h) + f(t)}{h^2}, \quad 0 < h \ll 1. \tag{1.2}$$

We will leave the discussion of (1.2) to Section IV.

This paper studies finite difference approximations on sets of discrete points, where distances between neighboring points vary. Many questions remain in the situation, such as:

1. How good can the formula (1.1) be in applications?
2. Are there different, or better, approximation formulas?
3. Can the formulas be used repeatedly for approximating higher derivatives?
4. How can we evaluate the errors in approximations?
5. Can we demonstrate our study through the use of computer simulations?

The preceding questions motivated our research in the subject. In this article, we will study some of the most popular finite differences for approximating the first and second order derivatives. Cases involving different types of grids over the intervals will be investigated. Section II will be for finite difference preliminaries. In Section III, we will concentrate on the first order differences. We will show that the same difference formula may possess different accuracies on different meshes. Then, we will show in Section IV that, although second order differences are in general acceptable on uniform meshes, naive applications of the formulas on nonuniform meshes will lead to incorrect results. Computer simulated numerical examples will be given to illustrate our conclusions in Section V. Our investigation will be summarized in Section VI.

2. Preliminaries. Let us consider an interval $[a, b]$, where $\infty > b > a > -\infty$, defined in $\mathbb{R}$. We will start with definitions of the uniform and nonuniform meshes, which are discrete sets of numbers used as domains for our finite differences. Meshes are also called grids in science and financial engineering computations [1, 3].

Definition 2.1. A *mesh* over the interval $[a, b]$ is defined as a set of $m + 2$ distinct numbers ($m \geq 0$) denoted as $\mathcal{T} = \{t_0, \ t_1, \ldots, t_{m+1}\}$, in which $t_{k+1} > t_k, \ k = 0, 1, \ldots, m$, and $t_0 = a, \ t_{m+1} = b$. The value t_k is called the *kth mesh point,* or *kth grid,* of $\mathcal{T}$. Moreover, we call the quantity

$$h_k = t_{k+1} - t_k, \quad m \geq k \geq 0,$$

the *kth step size* of the mesh. Step sizes are often less than one. $\mathcal{T}$ is called a *uniform mesh* if $h_k = h > 0, \ k = 0, 1, \ldots, m$, otherwise $\mathcal{T}$ is a *nonuniform mesh.*

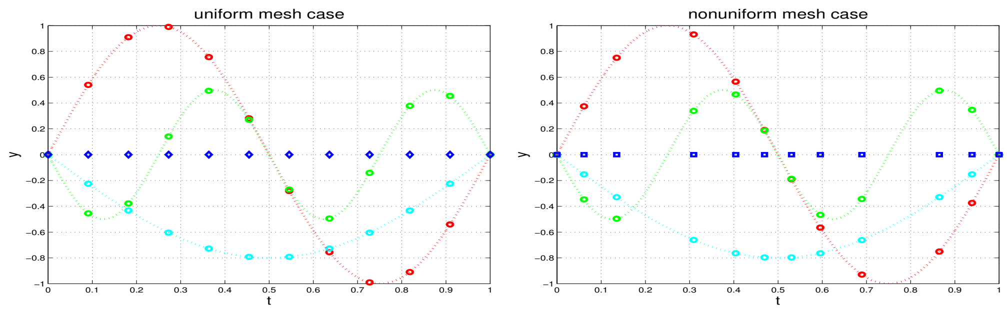

Figure 2.1. Plot of the trigonometric functions with different frequencies on the uniform mesh (LEFT) and the nonuniform mesh (RIGHT). Blue squares or diamonds on the t-axis indicate the mesh points used in each case. While dotted curves are the same between the left and right figures, locations of the plotted function values (large dots on the curves) corresponding to different meshes are significantly different.

Example 2.1. Consider meshes with twelve points over the interval $[0, 1]$. A uniform mesh is $\mathcal{T}_1 = \{t_k = k \times h\}_{k=0}^{11}$ with $h = 1/11$ (blue diamonds in Figure 2.1), while a nonuniform mesh can be $\mathcal{T}_2 = \{t_0 = 0, \ t_{k+1} = t_k + h_k, \ k = 0, 1, \ldots, 10\}$, where $h_k, \ k = 0, 1, \ldots, 10$, are calculated based on an equi-arclength formula for $y = \sin(2\pi t)$; that is, $h_k, \ k = 1, 2, \ldots, 11$, are obtained by evenly dividing the arc of the curve of the function over $[0, 1]$, and then vertically projecting the resulting arc pieces with equal arclength to the t-axis (the mesh steps are separated by blue squares in Figure 2.1). A composite trapezoidal rule is employed to evaluate the arclength. Let $y_1 = \sin(2\pi t), \ y_2 = -0.5\sin(4\pi t)$, and $y_3 = -0.8\sin(\pi t)$ be three trigonometric functions with distinct frequencies. Their graphs over $\mathcal{T}_1$ (LEFT) and $\mathcal{T}_2$ (RIGHT) are given in Figure 2.1 as red, green and cyan dots, respectively. The true functions (continuous curves) are shown for comparisons.

Definition 2.2. Let function $y = f(t)$ be defined on the interval $[a, b]$ in addition to $n \geq 1$. We say that f is *n times continuously differentiable on* $[a, b]$ if in additional to the continuity of the nth derivative $f^{(n)}(t), \ t \in (a, b)$, both directional derivatives, $f^{(n)}(a^+), \ f^{(n)}(b^-)$, exist. We further say that f is *sufficiently smooth on* $[a, b]$ if n can be as large as we wish.

Definition 2.3. Let functions $y = f(t)$ and $y = g(t)$ be defined on the mesh $\mathcal{T}$, where g is considered as an approximation of f. If

$$|f(t) - g(t)| = O\left(h^p\right), \quad t \in \mathcal{T},$$

where $h = \max_{0 \leq k \leq m} h_k$, then we say that the approximation at t is *accurate to the order p* with respect to the step sizes. From the approximation point of view, an approximation g is *consistent* if and only if $p > 0$.

Definition 2.4. Let $f = \{f_0,\ f_1, \ldots, f_{m+1}\},\ g = \{g_0,\ g_1, \ldots, g_{m+1}\}$ be two functions defined on the mesh $\mathcal{T}$, where g is considered as an approximation of f. We define the *scaled local difference* between the two functions at t_k as

$$\mathrm{sld}(f,g)_k = \frac{f_k - g_k}{a}, \quad k = 0,\ 1, \ldots, m+1,$$

where $a = \max_{0 \le k \le m+1} |f_k| > 0$. The *scaled global error indicator* is defined as

$$\mathrm{sgei}(f,g) = \max_{0 \le k \le m+1} |\mathrm{sld}(f,g)_k| .$$

Note that the above definitions are different from standard definitions of local and global relative errors, where signs are rarely considered. The value of $\mathrm{sld}(f,g)_k$ offers not only scaled relative error information, but also the *direction of the error,* that is, whether g_k is greater or less than f_k. The latter is particularly useful if approximations of oscillatory problems are investigated. The function $\mathrm{sgei}(f,g)$ provides a scaled overall error estimate and is easy to use for its simplicity in structure. Both definitions can be used when some of the f_k values are zero.

3. First order differences.

We assume that the function $y = f(t)$ is n times continuously differentiable on $[a,b]$. Let $\mathcal{T}$ be a mesh over $[a,b]$. Similar to that in [2], we define the forward, backward, and central difference operations as follows:

$$D_+ f(t_k) = \frac{f(t_{k+1}) - f(t_k)}{t_{k+1} - t_k}, \quad k = 0, 1, \ldots, m, \tag{3.1}$$

$$D_- f(t_k) = \frac{f(t_k) - f(t_{k-1})}{t_k - t_{k-1}}, \quad k = 1, 2, \ldots, m+1, \tag{3.2}$$

$$\delta f(t_k) = \frac{f(t_{k+1}) - f(t_{k-1})}{t_{k+1} - t_{k-1}}, \quad k = 1, 2, \ldots, m. \tag{3.3}$$

Theorem 3.1. *Let $\mathcal{T}$ be nonuniform and f be twice continuously differentiable. Then the forward, backward, and central differences are first order approximations of the derivative function f' on $\mathcal{T}$. Further,*

$$D_+ f(t_k) - f'(t_k) = \frac{h_k}{2} f''(\xi_1), \tag{3.4}$$

$$D_- f(t_k) - f'(t_k) = -\frac{h_{k-1}}{2} f''(\zeta_1), \tag{3.5}$$

$$\delta f(t_k) - f'(t_k) = \frac{1}{2(h_k + h_{k-1})} \left[h_k^2 f''(\xi_2) - h_{k-1}^2 f''(\zeta_2) \right], \tag{3.6}$$

where $t_{k+1} > \xi_\ell > t_k,\ t_k > \zeta_\ell > t_{k-1},\ \ell = 1, 2.$

Proof. Here let us only need to show the cases involving forward and central differences. First, according to the Maclaurin series expansion, we have

$$f(t_{k+1}) = f(t_k) + h_k f'(t_k) + \frac{h_k^2}{2} f''(t_k) + \cdots + \frac{h_k^n}{n!} f^{(n)}(\xi), \tag{3.7}$$

$$f(t_{k-1}) = f(t_k) - h_{k-1} f'(t_k) + \frac{h_{k-1}^2}{2} f''(t_k) - \cdots + (-1)^n \frac{h_{k-1}^n}{n!} f^{(n)}(\zeta). \tag{3.8}$$

Therefore, letting $n = 2$,

$$f(t_{k+1}) - f(t_k) = h_k f'(t_k) + \frac{h_k^2}{2} f''(\xi),$$

$$f(t_{k+1}) - f(t_{k-1}) = (h_k + h_{k-1}) f'(t_k) + \frac{1}{2} \left[h_k^2 f''(\xi) - h_{k-1}^2 f''(\zeta) \right].$$

Equations (3.4) and (3.6) become obvious. Since $h_k/(h_k+h_{k-1}) < 1$ and $h_{k-1}/(h_k+h_{k-1}) < 1$, according to Definition 2.3, the differences involved are indeed first order approximations. □

Theorem 3.2. *Let $\mathcal{T}$ be uniform. Then the central difference becomes a second order approximation of the derivative function f' if f is three times continuously differentiable while the forward and backward differences remain as first order approximations of f' if f is at least twice continuously differentiable. Further,*

$$D_+f(t_k) - f'(t_k) = \frac{h}{2}f''(\xi_1), \tag{3.9}$$

$$D_-f(t_k) - f'(t_k) = -\frac{h}{2}f''(\zeta_1), \tag{3.10}$$

$$\delta f(t_k) - f'(t_k) = \frac{h^2}{6}\left[f'''(\xi_2) + f'''(\zeta_2)\right], \tag{3.11}$$

where $t_{k+1} > \xi_\ell > t_k,\ t_k > \zeta_\ell > t_{k-1},\ \ell = 1, 2.$

Proof. The corollary is a direct extension of the Theorem 3.1 due to $h_k = h_{k-1} = h$, Definition 2.3, and (3.7), (3.8). □

Remark 3.1. Though $D_+f(t_k) = D_-f(t_{k+1})$ for $k = 0, 1, \ldots, m$, on any mesh considered, the central difference is not a simple combination of the forward and backward differences on a nonuniform mesh. The central difference can be viewed as an arithmetic average of the forward and backward differences only on any uniform mesh. Interestingly, this average improves the accuracy of the approximation significantly.

Remark 3.2. The right-hand-side of (3.4)-(3.6) and (3.9)-(3.11) can be viewed as errors of the respective approximations.

4. Second order differences.

Let function $y = f(t)$ be n times continuously differentiable on $[a, b]$, where n is sufficiently large. We will investigate if we can approximate the second order derivative function by applying the forward, backward and central differences repeatedly.

Theorem 4.1. *Let $\mathcal{T}$ be nonuniform. Then*

$$P(Qf(t_k)) \neq Q(Pf(t_k)) \quad \textit{for any applicable } t_k \in \mathcal{T},$$

where P and Q are any two different difference operations denoted by D_+, D_- or δ.

Proof. We only need to show the cases involving $D_+(D_-f(t_k))$ and $D_+(\delta f(t_k))$. According to (3.1) and (3.2), we have

$$\begin{aligned} D_+(D_-f(t_k)) &= \frac{D_-f(t_{k+1}) - D_-f(t_k)}{h_k} = \left[\frac{f(t_{k+1}) - f(t_k)}{h_k} - \frac{f(t_k) - f(t_{k-1})}{h_{k-1}}\right]/h_k \\ &= \frac{h_{k-1}f(t_{k+1}) - (h_k + h_{k-1})f(t_k) + h_kf(t_{k-1})}{h_k^2h_{k-1}}. \end{aligned} \tag{4.1}$$

By the same token,

$$\begin{aligned} D_-(D_+f(t_k)) &= \frac{D_+f(t_k) - D_+f(t_{k-1})}{h_{k-1}} = \left[\frac{f(t_{k+1}) - f(t_k)}{h_k} - \frac{f(t_k) - f(t_{k-1})}{h_{k-1}}\right]/h_{k-1} \\ &= \frac{h_{k-1}f(t_{k+1}) - (h_k + h_{k-1})f(t_k) + h_kf(t_{k-1})}{h_kh_{k-1}^2}. \end{aligned} \tag{4.2}$$

Recalling that $h_k \neq h_{k-1}$, we have

$$D_+(D_-f(t_k)) \neq D_-(D_+f(t_k)).$$

Further,

$$\begin{aligned} D_+(\delta f(t_k)) &= \frac{\delta f(t_{k+1}) - \delta f(t_k)}{h_k} = \left[\frac{f(t_{k+2}) - f(t_k)}{h_{k+1} + h_k} - \frac{f(t_{k+1}) - f(t_{k-1})}{h_k + h_{k-1}}\right] / h_k \\ &= \frac{(h_k + h_{k-1})(f(t_{k+2}) - f(t_k)) - (h_{k+1} + h_k)(f(t_{k+1}) - f(t_{k-1}))}{(h_{k+1} + h_k)h_k(h_k + h_{k-1})}. \qquad (4.3) \\ \delta(D_+f(t_k)) &= \frac{D_+f(t_{k+1}) - D_+f(t_{k-1})}{h_k + h_{k-1}} \\ &= \left[\frac{f(t_{k+2}) - f(t_{k+1})}{h_{k+1}} - \frac{f(t_k) - f(t_{k-1})}{h_{k-1}}\right] / (h_k + h_{k-1}) \\ &= \frac{h_{k-1}(f(t_{k+2}) - f(t_{k+1})) - h_{k+1}(f(t_k) - f(t_{k-1}))}{h_{k+1}(h_{k-1} + h_k)h_{k-1}}. \qquad (4.4) \end{aligned}$$

Therefore

$$\delta(D_+f(t_k)) \neq D_+(\delta f(t_k))$$

unless $h_{k-1} = h_k = h_{k+1}$. □

Corollary 4.1. *Let $\mathcal{T}$ be uniform. Then we have*

$$P(Qf(t_k)) = Q(Pf(t_k)) \quad \text{for all applicable } t_k \in \mathcal{T},$$

where P and Q are any two different difference operations denoted by D_+, D_- or δ.

The proof of the corollary follows from (4.1)-(4.4). To explore interesting features of the proposed formulas on different meshes, we require exceptionally high orders of the derivative functions in the following theorem. The requirements can be conveniently eased when the types of the meshes are fixed.

Theorem 4.2. *Let $\mathcal{T}$ be nonuniform. Then none of the second order differences $P(Qf(t_k))$, where P and Q are any two difference operations denoted by D_+, D_-*

or δ, is a consistent approximation of $f''(t_k)$. Further, if f is sufficiently smooth,

$$
\begin{aligned}
D_+(D_+f(t_k)) &= \frac{h_{k+1}+h_k}{2h_k}f''(t_k)+\frac{(h_{k+1}+h_k)(h_{k+1}+2h_k)}{6h_k}f'''(t_k) \\
&\quad +\frac{h_{k+1}+h_k}{24h_kh_{k+1}}\left[(h_{k+1}+h_k)^3f^{(4)}(\tilde{\xi})-h_k^3f^{(4)}(\xi)\right], \qquad (4.5)\\
D_-(D_-f(t_k)) &= \frac{h_{k-1}+h_{k-2}}{2h_{k-1}}f''(t_k)-\frac{(h_{k-1}+h_{k-2})(2h_{k-1}+h_{k-2})}{6h_{k-1}}f'''(t_k) \\
&\quad +\frac{h_{k-1}+h_{k-2}}{24h_{k-1}h_{k-2}}\left[-h_{k-1}^3f^{(4)}(\zeta)+(h_{k-1}+h_{k-2})^3f^{(4)}(\tilde{\zeta})\right], \qquad (4.6)\\
\delta(\delta f(t_k)) &= \frac{h_{k+1}+h_k+h_{k-1}+h_{k-2}}{2(h_k+h_{k-1})}f''(t_k) \\
&\quad +\frac{(h_{k+1}+h_k)^2-(h_{k-1}+h_{k-2})^2}{6(h_k+h_{k-1})}f'''(t_k) \\
&\quad +\frac{(h_k+h_{k+1})^3+(h_{k-1}+h_{k-2})^3}{24(h_k+h_{k-1})}f^{(4)}(t_k) \\
&\quad +\frac{(h_{k+1}+h_k)^4f^{(5)}(\tilde{\xi})-(h_{k-1}+h_{k-2})^4f^{(5)}(\tilde{\zeta})}{120(h_k+h_{k-1})}, \qquad (4.7)\\
D_+(D_-f(t_k)) &= \frac{h_k+h_{k-1}}{2h_k}f''(t_k)+\frac{h_k^2-h_{k-1}^2}{6h_k}f'''(t_k)+\frac{h_k^3+h_{k-1}^3}{24h_k}f^{(4)}(t_k) \\
&\quad +\frac{1}{120h_k}\left[h_k^4f^{(5)}(\xi)-h_{k-1}^4f^{(5)}(\zeta)\right], \qquad (4.8)\\
D_-(D_+f(t_k)) &= \frac{h_k+h_{k-1}}{2h_{k-1}}f''(t_k)+\frac{h_k^2-h_{k-1}^2}{6h_{k-1}}f'''(t_k)+\frac{h_k^3+h_{k-1}^3}{24h_{k-1}}f^{(4)}(t_k) \\
&\qquad +\frac{1}{120h_{k-1}}\left[h_k^4f^{(5)}(\xi)-h_{k-1}^4f^{(5)}(\zeta)\right], \qquad (4.9)\\
D_+(\delta f(t_k)) &= \frac{h_{k+1}+h_{k-1}}{2h_k}f''(t_k)+\frac{(h_{k+1}+h_k)^2-h_k^2+h_kh_{k-1}-h_{k-1}^2}{6h_k}f'''(t_k) \\
&\quad +\frac{1}{24h_k(h_k+h_{k-1})}\left[(h_k+h_{k-1})(h_{k+1}+h_k)^3f^{(4)}(\tilde{\xi})\right. \\
&\qquad \left.-h_k^4f^{(4)}(\xi)-h_{k-1}^4f^{(4)}(\zeta)\right], \qquad (4.10)\\
\delta(D_+f(t_k)) &= \frac{h_{k+1}+2h_k+h_{k-1}}{2(h_k+h_{k-1})}f''(t_k)+\frac{(h_k+h_{k+1})^3-h_k^3-h_{k+1}h_{k-1}^2}{6h_{k+1}(h_k+h_{k-1})}f'''(t_k)
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{24h_{k+1}(h_k+h_{k-1})}\left[(h_{k+1}+h_k)^4f^{(4)}(\tilde{\xi})-h_k^4f^{(4)}(\xi)\right. \\
&\left. h_{k-1}^3h_{k+1}f^{(4)}(\zeta)\right], \qquad (4.11)
\end{aligned}
$$

$$
\begin{aligned}
D_-(\delta f(t_k)) &= \frac{h_k+h_{k-2}}{2h_{k-1}} f''(t_k) + \frac{h_k^3+h_{k-1}^3-(h_k+h_{k-1})(h_{k-1}+h_{k-2})^2}{6(h_k+h_{k-1})h_{k-1}} f'''(t_k) \\
&\quad + \frac{1}{24(h_k+h_{k-1})h_{k-1}} \Big[h_k^4 f^{(4)}(\xi) + (h_{k-1}+h_{k-2})^4 f^{(4)}(\zeta) \\
&\quad + (h_k+h_{k-1})(h_{k-1}+h_{k-2})^3 f^{(4)}(\tilde{\zeta}) \Big], \qquad (4.12) \\
\delta(D_- f(t_k)) &= \frac{h_k+2h_{k-1}+h_{k-2}}{2(h_k+h_{k-1})} f''(t_k) + \frac{h_{k-2}h_k^2+h_{k-1}^3-(h_{k-1}+h_{k-2})^3}{6h_{k-2}(h_k+h_{k-1})} f'''(t_k) \\
&\quad + \frac{1}{24(h_k+h_{k-1})h_{k-2}} \Big[h_{k-2}h_k^3 f^{(4)}(\xi) - h_{k-1}^4 f^{(4)}(\zeta) \\
&\quad + (h_{k-1}+h_{k-2})^4 f^{(4)}(\tilde{\zeta}) \Big], \qquad (4.13)
\end{aligned}
$$

where $\tilde{\xi},\ \xi,\ \tilde{\zeta}$ *and* ζ *are different numbers and* $t_{k+2} > \tilde{\xi} > t_k,\ t_{k+1} > \xi > t_k,\ t_k > \zeta > t_{k-1},\ t_k > \tilde{\zeta} > t_{k-2}$.

Proof. Due to their similarities, here we only present proof of the case involving $D_+(D_+ f(t_k))$. We have the Maclaurin series

$$
\begin{aligned}
f(t_{k+2}) &= f(t_k) + (h_{k+1}+h_k) f'(t_k) + \frac{(h_{k+1}+h_k)^2}{2} f''(t_k) \\
&\quad + \frac{(h_{k+1}+h_k)^3}{6} f'''(t_k) + \cdots + \frac{(h_{k+1}+h_k)^n}{n!} f^{(n)}(\tilde{\xi}), \qquad (4.14) \\
f(t_{k-2}) &= f(t_k) - (h_{k-1}+h_{k-2}) f'(t_k) + \frac{(h_{k-1}+h_{k-2})^2}{2} f''(t_k) \\
&\quad - \frac{(h_{k-1}+h_{k-2})^3}{6} f'''(t_k) + \cdots + (-1)^n \frac{(h_{k-1}+h_{k-2})^n}{n!} f^{(n)}(\tilde{\zeta}). \qquad (4.15)
\end{aligned}
$$

Similar to (4.1) and (4.2), we have

$$
D_+(D_+ f(t_k)) = \frac{h_k f(t_{k+2}) - (h_{k+1}+h_k) f(t_{k+1}) + h_{k+1} f(t_k)}{h_{k+1} h_k^2}. \qquad (4.16)
$$

Now, according to (3.7), (4.14),

$$
\begin{aligned}
& h_k f(t_{k+2}) - (h_{k+1}+h_k) f(t_{k+1}) + h_{k+1} f(t_k) \\
&= h_k \left(f(t_k) + (h_{k+1}+h_k) f'(t_k) + \frac{(h_{k+1}+h_k)^2}{2} f''(t_k) + \cdots + \frac{(h_{k+1}+h_k)^n}{n!} f^{(n)}(\tilde{\xi}) \right) \\
&\quad - (h_{k+1}+h_k) \left(f(t_k) + h_k f'(t_k) + \frac{h_k^2}{2} f''(t_k) + \cdots + \frac{h_k^n}{n!} f^{(n)}(\xi) \right) + h_{k+1} f(t_k) \\
&= \frac{h_k h_{k+1}(h_{k+1}+h_k)}{2} f''(t_k) + \frac{h_k (h_{k+1}+h_k) \left[(h_{k+1}+h_k)^2 - h_k^2 \right]}{3!} f'''(t_k) + \cdots \\
&\quad + \frac{h_k (h_{k+1}+h_k)}{n!} \left[(h_{k+1}+h_k)^{n-1} f^{(n)}(\tilde{\xi}) - h_k^{n-1} f^{(n)}(\xi) \right] \\
&= \frac{h_k h_{k+1}(h_{k+1}+h_k)}{2} f''(t_k) + \frac{h_k h_{k+1} (h_{k+1}+h_k)(h_{k+1}+2h_k)}{3!} f'''(t_k) + \cdots \\
&\quad + \frac{h_k (h_{k+1}+h_k)}{n!} \left[(h_{k+1}+h_k)^{n-1} f^{(n)}(\tilde{\xi}) - h_k^{n-1} f^{(n)}(\xi) \right].
\end{aligned}
$$

Substituting the above into (4.16) and letting $n = 4$, we obtain (4.5) which indicates that the difference is not a consistent approximation of $f''(t_k)$ unless $h_{k+1} = h_k$. □

Corollary 4.2. *Let $\mathcal{T}$ be any mesh. Then*

$$D_+(D_-f(t_k)) = \frac{h_{k-1}}{h_k} D_-(D_+f(t_k)), \quad t_k \in \mathcal{T}.$$

Corollary 4.3. *Let α be a positive constant, and let $h_{\ell+1} = \alpha h_\ell$ for all possible ℓ on a nonuniform mesh $\mathcal{T}$. Then a necessary and sufficient condition for any aforementioned finite difference formula to be a consistent approximation of f'' is*

$$\alpha \equiv 1.$$

Proof. Because the proofs of different cases are similar, we will show only one of them. Consider $\delta(D_-f(t_k))$. To have a consistent approximation, we must require the coefficient of $f''(t_k)$ in (4.13) to be one, that is,

$$\frac{h_k + 2h_{k-1} + h_{k-2}}{2(h_k + h_{k-1})} = \frac{\alpha^2 h_{k-2} + 2\alpha h_{k-2} + h_{k-2}}{2(\alpha^2 h_{k-2} + \alpha h_{k-2})} = \frac{\alpha^2 + 2\alpha + 1}{2(\alpha^2 + \alpha)} = 1.$$

Solving the above equation, we acquire $\alpha^2 + 2\alpha + 1 = 2\alpha^2 + 2\alpha$ which implies that $\alpha^2 = 1$. Since α is positive, therefore $\alpha \equiv 1$ is our only solution. $\square$

Theorem 4.3. *Let $\mathcal{T}$ be uniform. Then for any valid index k, $\delta(\delta f(t_k))$, $D_+(D_-f(t_k))$ and $D_-(D_+f(t_k))$ are second order approximations of $f''(t_k)$ if f is four times continuously differentiable, and all other second order differences are first order approximations of $f''(t_k)$ if f is three times continuously differentiable. Further,*

$$\begin{aligned}
\delta(\delta f(t_k)) - f''(t_k) &= \frac{h^2}{6}\left[f^{(4)}(\tilde{\xi}) + f^{(4)}(\tilde{\zeta})\right], \\
D_+(D_-f(t_k)) - f''(t_k) &= \frac{h^2}{24}\left[f^{(4)}(\xi) + f^{(4)}(\zeta)\right], \\
D_-(D_+f(t_k)) - f''(t_k) &= D_+(D_-f(t_k)) - f''(t_k), \\
D_+(D_+f(t_k)) - f''(t_k) &= \frac{h}{3}\left[4f'''(\tilde{\xi}) - f'''(\xi)\right], \\
D_-(D_-f(t_k)) - f''(t_k) &= \frac{h}{3}\left[f'''(\tilde{\zeta}) - 4f'''(\zeta)\right], \\
D_+(\delta f(t_k)) - f''(t_k) &= \frac{h}{12}\left[8f'''(\tilde{\xi}) - f'''(\xi) - f'''(\zeta)\right], \\
\delta(D_+f(t_k)) - f''(t_k) &= D_+(\delta f(t_k)) - f''(t_k), \\
D_-(\delta f(t_k)) - f''(t_k) &= \frac{h}{12}\left[f'''(\xi) + f'''(\zeta) - 8f'''(\tilde{\zeta})\right], \\
\delta(D_-f(t_k)) - f''(t_k) &= D_-(\delta f(t_k)) - f''(t_k),
\end{aligned}$$

where $\tilde{\xi}$, ξ, $\tilde{\zeta}$ and ζ are constants for which $t_{k+2} > \tilde{\xi} > t_k$, $t_{k+1} > \xi > t_k$, $t_k > \zeta > t_{k-1}$, $t_k > \tilde{\zeta} > t_{k-2}$.

Proof. We only need to show the nine equations listed. This can be implemented by letting $h_{k+1} = h_k = h_{k-1} = h_{k-2} = h$ in (4.5)-(4.13) and choosing proper values of n in the Maclaurin series (3.7), (3.8), (4.14) and (4.15). $\square$

Remark 4.1. The difference formula (1.2) is a consistent first order approximation of $f''(t)$ on a uniform mesh.

Remark 4.2. The right-hand sides of the nine equations in Theorem 4.3 can be viewed as errors of the respective approximations on uniform meshes.

Remark 4.3. Although none of the standard second order differences discussed in this paper may approximate f'' on a nonuniform mesh, specially formulated finite difference formulas may work. An example is

$$\mathcal{D}_2 f(t_k) = \frac{D_+ f(t_k) - D_- f(t_k)}{(h_{k-1} + h_k)/2}, \quad t_k \in \mathcal{T}. \tag{4.17}$$

It can be shown by using Maclaurin series that (4.17) provides a first order approximation of $f''(t_k)$ on any nonuniform mesh.

5. Numerical examples.

It has been known that trigonometric functions $y = \sin(at)$, $y = \cos(bt)$ possess excellent smoothness for applications. The functions are infinitely differentiable. To illustrate our results, we choose the function

$$y = -\sin(4\pi t), \quad 0 \le t \le 1. \tag{5.1}$$

The corresponding derivatives are

$$y' = -4\pi \cos(4\pi t), \; y'' = (4\pi)^2 \sin(4\pi t), \quad 0 \le t \le 1. \tag{5.2}$$

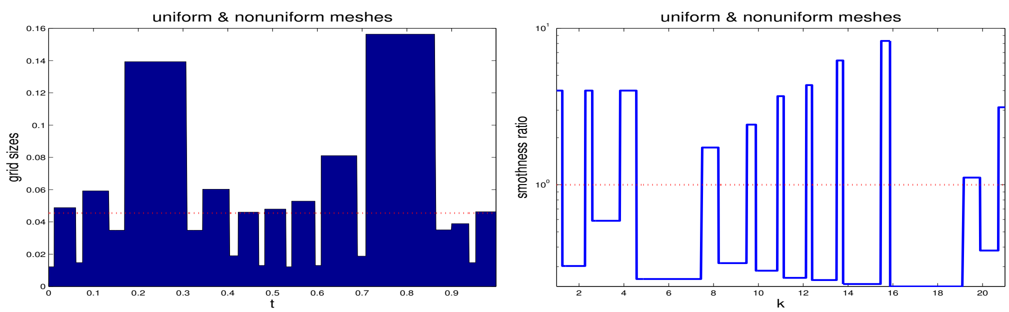

Figure 5.1. Plot of grid step sizes (red dotted line is for the uniform mesh and blue solid curve and area are for the nonuniform mesh, LEFT). In this figure, $[0, 1]$ is divided into 22 subregions proportional to the 22 steps used. Height of each of the bars located in the subregion is the actual size of the corresponding step size; The second figure is for smoothness ratio for the uniform mesh (red dotted line) and the nonuniform mesh (blue curve). In the case, $[0, 1]$ is divided into 21 subregions proportional to the first 21 steps used. Height of each bar is for the corresponding ratio.

To achieve better simulation resolution, we add eleven additional external points into the uniform and nonuniform meshes introduced in Example 2.1, respectively. The new points are separated by the original points. The new points in the nonuniform mesh are particularly set to be closer to their right-side points, as plotted in Figure 5.1 (LEFT). In the second frame of Figure 5.1, we show the ratio h_{k+1}/h_k, $k = 1, 2, \ldots, 21$, (the red line is for the uniform mesh and the blue curve is for the nonuniform mesh). A logarithmic scale in the Y-direction is used to show more precisely the ratio, which is often called the *smoothness ratio* in engineering computations and is chosen between 0 and 10.

Numerical computations will be carried out for a number of the differences. In our experiments, a numerical solution g is acceptable if $\mathrm{sgei}(f, g) < k \ll 1$, and it is unacceptable if $\mathrm{sgei}(f, g) \ge 1$. MATLAB® will be used throughout the experiments.

Example 5.1. Consider the first difference δf. The true first derivative in (5.2), and the central difference are plotted in Figure 5.2. Though the approximations in both cases are consistent, we may observe that the approximation in the uniform case is much better than that in the nonuniform case, since in the former situation the approximation is second order.

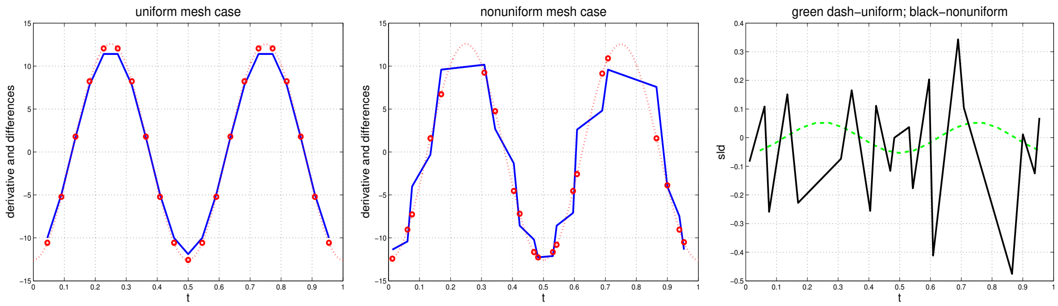

Figure 5.2. Plot of true solution (red dotted curves) and approximations (blue curves) on the uniform mesh (LEFT) and the nonuniform mesh (MIDDLE). Corresponding scaled local difference curves are given (RIGHT: green for the uniform mesh case and black for the nonuniform case). We may observe from the first two pictures that, even though approximations on both meshes are consistent, the approximation on the uniform mesh is much "nicer" than that on the nonuniform mesh. The third picture confirms this by showing the scaled difference values over the domain (the black curve acts more violently with a relatively large amplitude).

These are further confirmed by the third frame in Figure 5.2 in which relative errors are given. While the scaled global error indicator in the uniform mesh case sgei $\approx$ 0.0535, in the nonuniform case, it reaches 0.4759 which is about 9 times the uniform mesh case! The irregular smoothness ratios shown in Figure 5.1 may explain why the error in the nonuniform grid case is oscillatory.

Example 5.2. Consider the second difference $D_+(D_+f)$. We plot the true second derivative given in (5.2) and the difference in Figure 5.3. It can be observed that while the difference approximates the derivative function reasonably over the uniform mesh (global error indicator value sgei $\approx$ 0.5559 because relatively large steps are used), it produces an unacceptable results on the nonuniform mesh with an indicator value sgei $\approx$ 2.5487. The irregular oscillations of the finite difference on nonuniform mesh is also unacceptable.

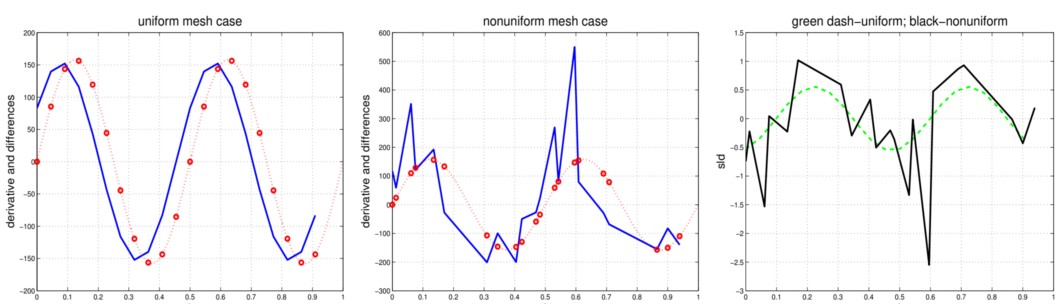

Figure 5.3. Plot of true solution (red dotted curves) and approximations (blue curves) on the uniform mesh (LEFT) and the nonuniform mesh (MIDDLE). Corresponding scaled local difference curves are given (RIGHT: green for the uniform mesh case and black for the nonuniform case). We may observe from the first two pictures that, while the approximation on the uniform mesh is still reasonable, the approximation on the nonuniform mesh becomes unacceptable. The third picture confirms these by showing the scaled difference values over the domain (the black curve acts violently with a significantly large amplitude).

Example 5.3. Consider the second difference $\delta(D_- f)$. The intention of using the central difference is to improve the numerical result. It is found in Figure 5.4 that

$$\begin{aligned} \text{sgei} &\approx 0.2817 \quad \text{when } \mathcal{T} \text{ is uniform} \\ \text{sgei} &\approx 0.7829 \quad \text{when } \mathcal{T} \text{ is nonuniform} \end{aligned}$$

In addition to a larger global relative error, in Figure 5.4, we may also observe that if a nonuniform mesh is used, there is a great irregularity in errors. If the difference is used as an approximation, very incorrect answers will probably result.

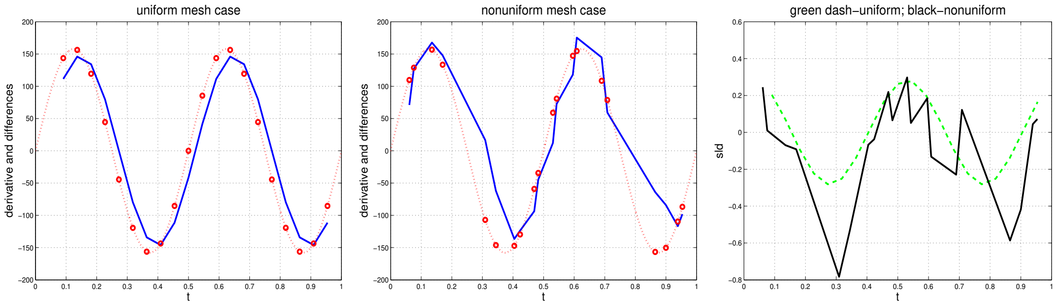

Figure 5.4. Plot of true solution (red dotted curves) and approximations (blue curves) on the uniform mesh (LEFT) and the nonuniform mesh (MIDDLE). Corresponding scaled local difference curves are given (RIGHT: green for the uniform mesh case and black for the nonuniform case). We may observe from the first two pictures that, while the approximation on the uniform mesh looks good, the approximation on the nonuniform mesh becomes unacceptable. The third picture again confirms these by showing the scaled difference values over the domain (the black curve oscillates violently with a large amplitude).

Example 5.4. Consider the second difference $\delta(\delta f)$. Although the use of central differences continues to improve the numerical result, it still cannot change the basic features of the approximations. In this case, we have

$$\begin{aligned} \text{sgei} &\approx 0.1031 \quad \text{when } \mathcal{T} \text{ is uniform} \\ \text{sgei} &\approx 0.5080 \quad \text{when } \mathcal{T} \text{ is nonuniform} \end{aligned}$$

The strong irregularity in the nonuniform mesh case shown in Figure 5.5 is not surprising.

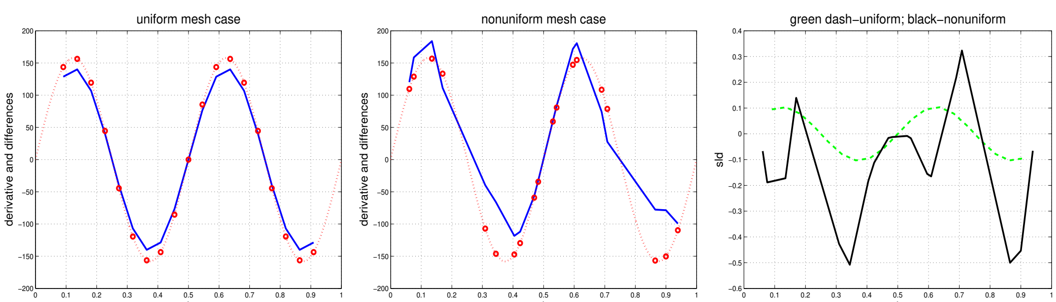

Figure 5.5. Plot of true solution (red dotted curves) and approximations (blue curves) on the uniform mesh (LEFT) and the nonuniform mesh (MIDDLE). Corresponding scaled local difference curves are given (RIGHT: green for the uniform mesh case and black for the nonuniform case). We may observe from the first two pictures that, while the approximation on the uniform mesh is improved due to the use of central difference, the inconsistency of the formula on the nonuniform mesh remains the same. These are again confirmed by the third picture through the scaled difference values over the domain (the black curve oscillates successively with a large amplitude).

Example 5.5. Let us consider the simple harmonic oscillator problem where neither a driving force nor friction is assumed [3]. If $\phi(t)$ is the displacement of the system at time t, then the second derivative $\phi''(t)$ is its acceleration. Based on Hooke's Law and Newton's Second Law, we obtain the following second order differential equation,

$$\phi''(t) = -\kappa\phi(t), \quad t > t_0, \tag{5.3}$$

together with the initial conditions

$$\phi(t_0) = 1, \quad \phi'(t_0) = -1, \tag{5.4}$$

where κ is a positive constant.

It is not difficult to verify [3] that the solution of (5.3), (5.4) is

$$\phi(t) = -\frac{1}{\sqrt{\kappa}} \sin \sqrt{\kappa} t + \cos \sqrt{\kappa} t, \quad t \geq t_0. \tag{5.5}$$

On the other hand, replacing the second derivative in (5.3) by the backward-forward difference, we acquire

$$D_-(D_+ w) = -\kappa w(t), \quad t \in \mathcal{T}, \tag{5.6}$$

where $\mathcal{T}$ is a mesh over the interval $[t_0, b]$. We wish the solution of (5.6), (5.4) to be an approximation of the solution of (5.3), (5.4).

First, we let $\mathcal{T}_1$ be a nonuniform mesh over the interval $[t_0, b]$ with decreasing steps $h_k = rh_{k-1}, \ k = 1, \ 2, \ldots, \ m$, for $h_0 = 1/10, \ r = 50/59$ and $m = 200$. Second, we let $\mathcal{T}_2$ be an uniform mesh with $h = (b - t_0)/10$.

Let $\kappa = 4\pi^2, \ t_0 = 0$ and $b = \sum_{k=0}^{m} h_k \approx 59/90$. In Figure 5.6 (LEFT), we plot the numerical solutions of (5.6), (5.4) on $\mathcal{T}_1$ (blue dashed curve), exact solution of the initial value problem (5.3), (5.4) (red dotted curve) together with a numerical solution of (5.6), (5.4) on $\mathcal{T}_2$ (green curve). A forward difference is used to approximate the first derivative in (5.4). Although errors defined for the numerical solution of initial value problems are slightly different from those used for function approximations, to illustrate the inconsistency of second order derivative approximations on nonuniform meshes, let us continue to use the measurements introduced by Definition 2.4. Scaled local differences of the numerical solutions on $\mathcal{T}_1$ (blue dashed curve) and on $\mathcal{T}_2$ (green curve) are given in Figure 5.6 (RIGHT).

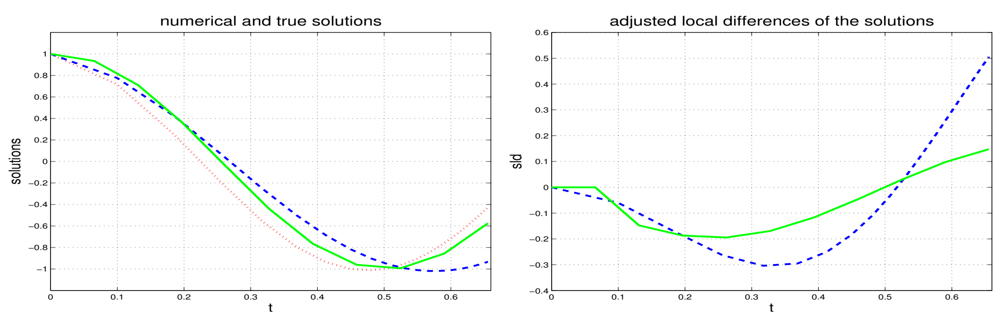

Figure 5.6. Plots of the solutions of the difference equation problem (5.6), (5.4) and the true solution (LEFT); and the scaled local difference values of the numerical solutions (RIGHT) on the nonuniform mesh and uniform mesh, respectively. While the numerical solution and related sld values on the nonuniform mesh $\mathcal{T}_1$ are given by blue dashed curves, the numerical solution and related sld values on the uniform mesh $\mathcal{T}_2$ are represented by solid green curves. We may observe in the first picture that, while the numerical solution on the uniform mesh maintains a good match to the true solution, which is indicated by the red dotted curve, the numerical solution on the nonuniform mesh swings away as t increases. The phenomena are confirmed by the second picture through the scaled difference values over the domain used (the blue curve oscillates and its amplitude increases rapidly as $t \to b$).

It is interesting to observe that while the numerical solution obtained on the uniform mesh keeps a steady error level from the true solution, although relatively large step is being used ($h = 59/900 \approx 0.0656$), the numerical solution obtained on the nonuniform mesh runs away rapidly from the true solution, despite of the fact that finer steps are employed ($h_k < 0.001$ for $k \geq 14$).

The global error indicator values for the two cases are also significantly different. It is found that sgei ≈ 0.5055 on $\mathcal{T}_1$ and occurs at $x = b$ while sgei ≈ 0.1945 on $\mathcal{T}_2$ and occurs at $x \approx 0.2622$.

Since the sizes of h and h_k do not play a major role in the aforementioned error phenomena, what can be the main cause for the unsatisfactory approximation on $\mathcal{T}_1$?

To see the answer, we may notice that

$$\frac{h_k + h_{k-1}}{2h_{k-1}} = \frac{r+1}{2} \neq 1.$$

Therefore, according to (4.9) in Theorem 4.2, difference equation (5.6) actually approximates

$$\frac{1+r}{2}\psi''(t) = -\kappa\psi(t), \quad t > t_0,$$

instead of (5.3)! Thus the numerical solution cannot be satisfactory. Of course, there are several factors, such as stability, that may affect the numerical solution. Needless to say, however, consistency is the most fundamental factor.

Conversely, it is not hard to verify that the improved $\mathcal{D}_2$ difference given in (4.17) offers a good approximation. The reader may wish to experiment with the interesting computations!

6. Conclusions. From the foregoing discussions and numerical experiments, we may conclude that:

1. The key issue for any finite difference formula is its consistency. Only consistent formulas can be used for approximating derivatives. The effectiveness of an approximation can be measured by its order of accuracy. For instance, (1.1) is an order one formula according to Theorems 3.1 and 3.2.

2. Consistent finite difference approximations can be derived on uniform or nonuniform grids. Generally speaking, the higher the order of accuracy is, the more accurate the finite difference formula can be.

3. Difference approximations on uniform meshes cannot be applied blindly on nonuniform meshes, nor can difference formulas be composed to form consistent approximations to second derivatives. At best, they may lose accuracy; at worst they are not consistent.

4. Assuming that the functions involved are sufficiently smooth, errors of approximations can be estimated by using Maclaurin series. Errors in numerical experiments can also be computed via local and global error formulas.

5. The consistency and accuracy of different approximations can be demonstrated through the use of computer simulations. Since simulations are based on particular examples, they are not as rigorous as mathematical proofs.

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