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A Paradoxical Consistency Between Dynamic and Conventional Derivatives on Hybrid Grids

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Abstract. It has been evident that the theory and methods of dynamic derivatives are playing an increasingly important rôle in hybrid modeling and computations. Being constructed on various kinds of hybrid grids, that is, time scales, dynamic derivatives offer superior accuracy and flexibility in approximating mathematically important natural processes with hard-to-predict singularities, such as the epidemic growth with unpredictable jump sizes and option market changes with high uncertainties, as compared with conventional derivatives. In this article, we shall review the novel new concepts, explore delicate relations between the most frequently used second-order dynamic derivatives and conventional derivatives. We shall investigate necessary conditions for guaranteeing the consistency between the two derivatives. We will show that such a consistency may never exist in general. This implies that the dynamic derivatives provide entirely different new tools for sensitive modeling and approximations on hybrid grids. Rigorous error analysis will be given via asymptotic expansions for further modeling and computational applications. Numerical experiments will also be given.

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Dedicated to Professor Yucheng Su on the Occasion of His 80th Birthday

1. Introduction

There has been a considerable amount of recent research activities in the study of different types of dynamic equations as well as their computational applications via hybrid grids [2,3,5,6,13]. The most important issues in the theory and methods include unifying existing continuous and discrete representation methodologies, bridging the discrepancies between traditional differential and difference equations, and promoting highly efficient hybrid tools for mathematical modeling and scientific computations. Many interesting results have been obtained in this rapidly developing field [1,6,8–10,13]. Latest research in

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the subject has been extended to partial and high-order dynamic equations with sophisticated applications [2, 6, 8–10].

A dynamic derivative is a special rate of change formula defined on a hybrid grid. Different dynamic derivatives are used as building blocks for dynamic equations on hybrid grids. Therefore, it is extremely important to understand precise connections between different dynamic derivatives and conventional derivatives so that correct mathematical formulations can be constructed for modeling and approximation purposes [5, 8, 9].

It is not always easy, however, to investigate such a sensitive problem since different concerns and criteria may apply in different dynamic derivatives in the literature. In this discussion, we shall restrict ourselves to the issue of the consistency between the derivatives via standard numerical analysis. Without loss of generality, we shall only consider hybrid grids which are sets of real numbers superimposed upon nonempty bounded intervals. This is a natural extension of the pioneer exploration in [7]. The hybrid grids defined in this way can be viewed as generalizations of many popular irregular grids in applications, such as the moving and adaptive grids in quenching and blow-up solution computations [4, 9–12].

Logically, we may expect a dynamic derivative defined on a hybrid set to be consistent with its conventional derivative counterpart on the interval, since both of the them are rate of change functions measuring variations of the targeted functions over the domains. We shall focus on the second-order Δ and ∇ dynamic derivatives and their crossed derivatives in this investigation [1–3, 6, 9]. Paradoxical relationships between the two derivatives over the hybrid grids will be discussed. We shall prove that the second-order dynamic derivatives are not consistent with conventional derivatives in general. However, interesting connections do exist between the two sides. Modifications of some dynamic derivative formulae may lead to good consistency. Proper incorporations of the underlying hybrid grid structures are often the keys to this success.

We would assume that the readers have a minimal working experience with the time scales theory and methods. Our approaches will be organized as follows. In Section 2, a brief introduction and a review of the dynamic derivatives as well as dynamic equations will be given. Concepts of approximations will also be established. Section 3 will be devoted to the study of the crossed second-order Δ, ∇ dynamic derivatives. We will then continue the exploration to non-crossed second-order dynamic derivatives in Section 4. The most paradoxical relations and numerical features from approximation point-of-view will be studied in these sections. Asymptotic expansions will be employed for deriving the local error estimates. A number of modified dynamic derivative formulae will be proposed on discrete hybrid grids. Finally, together with a number of straightforward numerical illustrations, our final conclusions and remarks will be delivered in Section 5.

2. Dynamic derivatives on hybrid grids

An *one-dimensional hybrid grid* $\mathscr{T}$ is defined as a nonempty closed subset of $\mathbb{R}$. Since $\mathscr{T}$ is bounded, we may set $a = \sup\mathscr{T}$, $b = \inf\mathscr{T}$ for the sake of convenience. In this case, a hybrid grid can be viewed as a closed set of real numbers superimposed over the interval $[a,\ b]$ from approximation point-of-view. We may define the *forward-jump* and *backward-jump functions* $\sigma,\ \rho$ for appropriate $t \in \mathscr{T}$ as

$$\sigma(t) = \inf\{s \in \mathscr{T} : s > t\}, \quad \rho(t) = \sup\{s \in \mathscr{T} : s < t\},$$

respectively. To simplify notations, we write $f^{\sigma}(t) = f(\sigma(t)),\ f^{\rho}(t) = f(\rho(t))$. We may also define the *forward-step* and *backward-step functions* $\mu,\ \eta$ as

$$\mu(t) = \sigma(t) - t, \quad \eta(t) = t - \rho(t),$$

respectively. We note that the jump operations on hybrid grids do not, in general, commute; that is,

$$\sigma(\rho(t)) \neq \rho(\sigma(t)), \quad \sigma(\rho(t)) \neq t \neq \rho(\sigma(t)), \quad t \in \mathscr{T}.$$

Let

$$\lambda(t) = \mu(t)/\eta(t)$$

if $\eta(t) \neq 0$. We further denote

$$\sigma^n(t) = \sigma(\sigma^{n-1}(t)),\ \rho^m(t) = \rho(\rho^{m-1}(t)), \quad n, m = 1, 2, \cdots,$$

under the agreement

$$\sigma^0(t) = \rho^0(t) = t.$$

Further, a point $t \in \mathscr{T}$ is called *left-scattered, right-scattered* if $\rho(t) < t,\ \sigma(t) > t$, respectively. A point $t \in \mathscr{T}$ is called *left-dense, right-dense* if $\rho(t) = t,\ \sigma(t) = t$, respectively. We define $\mathscr{T}^{\kappa} = \mathscr{T}$ if b is left-dense and $\mathscr{T}^{\kappa} = \mathscr{T} \setminus \{b\}$ if b is left-scattered. Similarly, we define $\mathscr{T}_{\kappa} = \mathscr{T}$ if a is right-dense and $\mathscr{T}_{\kappa} = \mathscr{T} \setminus \{a\}$ if a is right-scattered. We denote $\mathscr{T}^{\kappa} \cap \mathscr{T}_{\kappa} = \mathscr{T}_{\kappa}^{\kappa}$. By the same token, we can define extended hybrid grids $\mathscr{T}^{\kappa^m}$, $\mathscr{T}_{\kappa^n}$ and $\mathscr{T}_{\kappa^n}^{\kappa^m}$; $m, n = 0, 1, 2, \cdots$, under the notation $\mathscr{T}^{\kappa^0} = \mathscr{T}_{\kappa^0} = \mathscr{T}$. We say a hybrid grid $\mathscr{T}$ is *uniform* if for all $t \in \mathscr{T}_{\kappa}^{\kappa}$, $\mu(t) = \eta(t)$. A uniform hybrid grid is an interval if $\mu(t) = 0$, and is a uniform discrete grid if $\mu(t) > 0$. For the convenience of discussions, we may decompose $\mathscr{T}$ into the following sets [8,9]:

$$\begin{aligned}
\mathscr{A} &:= \{t \in \mathscr{T} : t \text{ is left-dense and right-scattered}\},\\
\mathscr{B} &:= \{t \in \mathscr{T} : t \text{ is left-scattered and right-dense}\},\\
\mathscr{C} &:= \{t \in \mathscr{T} : t \text{ is left-scattered and right-scattered}\},\\
\mathscr{D} &:= \{t \in \mathscr{T} : t \text{ is left-dense and right-dense}\}.
\end{aligned}$$

Without loss of generality, we may assume that $a \in \mathscr{A} \cup \mathscr{D}$ and $b \in \mathscr{B} \cup \mathscr{D}$.

Further, we say that a function f defined on $\mathscr{T}$ is Δ *differentiable on* $\mathscr{T}^{\kappa}$ if for all $\epsilon > 0$ there is a neighborhood U of $t \in \mathscr{T}^{\kappa}$ such that for some γ the inequality

$$|f^{\sigma}(t) - f(s) - \gamma(\sigma(t) - s)| < \epsilon|\sigma(t) - s|$$

is true for all $s \in U$, and in this case we write $f^{\Delta}(t) = \gamma$. Similarly, we say that a function f defined on $\mathscr{T}$ is ∇ *differentiable on* $\mathscr{T}_\kappa$ if for $\epsilon > 0$ there is a neighborhood V of t such that for some θ the inequality

$$|f^{\rho}(t) - f(s) - \theta(\rho(t) - s)| < \epsilon|\rho(t) - s|$$

is true for all $s \in V$, and in this case, we write $f^{\nabla}(t) = \theta$. Let $\mathscr{T}$ be uniform. Then the Δ, ∇ derivatives of f reduce to the conventional derivative f' if $\mu(t) = 0$ and f' exists, or to appropriate finite difference formulae if $\mu(t) > 0$. It is not difficult to show that the dynamic differential operators Δ and ∇ do not commute in general.

For second-order dynamic derivatives, we may define

$$f^{\Lambda_1\Lambda_2} = \left(f^{\Lambda_1}\right)^{\Lambda_2},$$

where Λ_1 and Λ_2 are any two dynamic differential operators from Δ and ∇. Higher order dynamic derivatives $f^{\Lambda_1\Lambda_2\cdots\Lambda_m}$, with dynamic differential operators $\Lambda_1,\ \Lambda_2, \cdots, \Lambda_m,\ m \geq 2$, can be defined in a similar way.

Finally, let functions f and g be defined on $\mathscr{T}$. If

$$|f(t) - g(t)| = \mathscr{O}\left(\max\{\mu^r(t), \eta^r(t)\}\right), \quad t \in \mathscr{T}, \tag{2.1}$$

where $0 \leq \mu,\ \eta < 1$, then we say that the two functions are *consistent on* $\mathscr{T}$ if $r > 0$. Let f and g be consistent. Then r is called the *order of accuracy* of g, should g be considered as an approximation of f on $\mathscr{T}$.

3. Crossed second-order dynamic derivatives

Under properly imbedded smoothness of the targeted function f over $[a,\ b]$, we state the following.

Lemma 3.1. *Let f be twice continuously differentiable in $[a,\ b]$, and μ be ∇ differentiable on $\mathscr{A}$. Then*

$$f^{\Delta\nabla}(t) = \begin{cases} \dfrac{\left(1 - \mu^{\nabla}(t)\right) f^{\Delta}(t) - f'(t)}{\mu(t)}, & t \in \mathscr{A} \cap \mathscr{T}_\kappa^\kappa, \\ \dfrac{f'(t) - f'(\rho(t))}{\eta(t)}, & t \in \mathscr{B} \cap \mathscr{T}_\kappa^\kappa, \\ \dfrac{\eta(t) f^{\sigma}(t) - (\eta(t) + \mu(t)) f(t) + \mu(t) f^{\rho}(t)}{\mu(t)\eta^2(t)}, & t \in \mathscr{C} \cap \mathscr{T}_\kappa^\kappa, \\ f''(t), & t \in \mathscr{D} \cap \mathscr{T}_\kappa^\kappa. \end{cases}$$

Proof. We only need to show the first two identities since the third identity has been addressed by [8] and the fourth one must hold according to definitions of the dynamic derivatives [1–4]. For $t \in \mathscr{A} \cap \mathcal{T}_\kappa^\kappa$, we observe that

$$\begin{aligned} f^{\Delta\nabla}(t) &= \left(f^{\Delta}(t)\right)^{\nabla} = \left(\frac{f(\sigma(t)) - f(t)}{\mu(t)}\right)^{\nabla} \\ &= \frac{\left(f(\sigma(t)) - f(t)\right)^{\nabla}\mu(t) - \left(f(\sigma(t)) - f(t)\right)\mu^{\nabla}(t)}{\mu(t)\mu(\rho(t))} \\ &= \frac{\left(f^{\nabla}(\sigma(t)) - f^{\nabla}(t)\right)\mu(t) - \left(f(\sigma(t)) - f(t)\right)\mu^{\nabla}(t)}{\mu^2(t)} \\ &= \frac{f^{\Delta}(t) - f'(t)}{\mu(t)} - \frac{f^{\Delta}(t)\mu^{\nabla}(t)}{\mu(t)} = \frac{1}{\mu(t)}\left(1 - \mu^{\nabla}(t)\right)f^{\Delta}(t) - \frac{f'(t)}{\mu(t)} \\ &= \frac{1}{\mu(t)}\left[\left(1 - \mu^{\nabla}(t)\right)f^{\Delta}(t) - f'(t)\right]. \end{aligned}$$

On the other hand, if $t \in \mathscr{B} \cap \mathcal{T}_\kappa^\kappa$, then

$$f^{\Delta\nabla}(t) = \left(f^{\Delta}(t)\right)^{\nabla} = \left(f'(t)\right)^{\nabla} = \frac{f'(t) - f'(\rho(t))}{\eta(t)}.$$

The above equation completes the proof. □

Theorem 3.1. *Let f be four times continuously differentiable in $[a, b]$, and let μ be ∇ differentiable on $\mathscr{A}$. Then the $\Delta\nabla$ dynamic derivative of f*
(i) *is consistent with f'' at all right-dense points on $\mathcal{T}_\kappa^\kappa$;*
(ii) *is not consistent with f'' at any right-scattered point on $\mathcal{T}_\kappa^\kappa$ except when $\lambda(t) = 1$.*
Further,

$$f^{\Delta\nabla}(t) = \begin{cases} \frac{1}{2}\left(1 - \mu^{\nabla}(t)\right)f''(t) - \frac{\mu^{\nabla}(t)}{\mu(t)}f'(t) + \frac{\mu(t)}{6}\left(1 - \mu^{\nabla}(t)\right)f'''(\xi_1), & t \in \mathscr{A} \cap \mathcal{T}_\kappa^\kappa, \\ f''(t) - \frac{\eta(t)}{2}f'''(\xi_2), & t \in \mathscr{B} \cap \mathcal{T}_\kappa^\kappa, \\ \frac{1}{2}(1 + \lambda(t))f''(t) - \frac{\eta(t)}{6}\left(1 - \lambda^2(t)\right)f'''(t) & \\ \quad + \frac{\eta^2(t)}{12}\left(1 + \lambda^3(t)\right)f^{(4)}(\xi_3), & t \in \mathscr{C} \cap \mathcal{T}_\kappa^\kappa, \\ f''(t), & t \in \mathscr{D} \cap \mathcal{T}_\kappa^\kappa, \end{cases}$$

where $\xi_1, \xi_2, \xi_3 \in (a, b)$. The identities characterize asymptotically the approximation error involved, if $f^{\Delta\nabla}$ is considered as an approximation of f''.

Proof. We only need to show the first two identities in the theorem, since the third identity was investigated in [8] and the fourth one is studied in Lemma 3.1. Because of the imbedded smoothness of f, we are able to deduce that

$$f^{\sigma}(t) = f(t) + \mu(t)f'(t) + \frac{\mu^2(t)}{2!}f''(t) + \frac{\mu^3(t)}{3!}f'''(\xi_1), \quad \xi_1 \in (a, b). \tag{3.1}$$

Now, an application of (3.1) leads to the following:

$$\begin{aligned} f^{\Delta}(t) &= \frac{f(t)+\mu(t)f'(t)+\mu^2(t)f''(t)/2!+\mu^3(t)f'''(\xi_1)/3!-f(t)}{\mu(t)} \\ &= f'(t)+\frac{\mu(t)}{2!}f''(t)+\frac{\mu^2(t)}{3!}f'''(\xi_1), \quad \xi_1\in(a,\ b). \end{aligned}$$

Recall Lemma 3.1. We obtain subsequently that

$$\begin{aligned} f^{\Delta\nabla}(t) &= \frac{(1-\mu^{\nabla}(t))\left(f'(t)+\mu(t)f''(t)/2!+\mu^2(t)f'''(\xi_1)/3!\right)-f'(t)}{\mu(t)} \\ &= \frac{\left(1-\mu^{\nabla}(t)\right)f'(t)-f'(t)}{\mu(t)}+\frac{1-\mu^{\nabla}(t)}{2!}f''(t) \\ &\quad +\frac{\mu(t)\left(1-\mu^{\nabla}(t)\right)}{3!}f'''(\xi_1), \quad t\in\mathscr{A}\cap\mathscr{T}_{\kappa}^{\kappa}. \end{aligned}$$

Note that, on the other hand, we may claim that

$$f'(\rho(t))=f'(t)-\eta(t)f''(t)+\frac{\eta^2(t)}{2!}f'''(\xi_2), \quad \xi_2\in(a,\ b). \tag{3.2}$$

Thus, a direct substitution of (3.2) into the second identity in Lemma 3.1 yields

$$\begin{aligned} f^{\Delta\nabla}(t) &= \frac{f'(t)-f'(t)+\eta(t)f''(t)-\eta^2(t)f'''(\xi_2)/2}{\eta(t)} \\ &= f''(t)-\frac{\eta(t)}{2}f'''(\xi_2), \quad t\in\mathscr{B}\cap\mathscr{T}_{\kappa}^{\kappa}. \end{aligned}$$

Recall definition (2.1). Based on the relations obtained above, it becomes natural to conclude that for $t\in(\mathscr{B}\cup\mathscr{D})\cap\mathscr{T}_{\kappa}^{\kappa}$, the $\Delta\nabla$ dynamic derivative provides a first-order approximation to f''. On the other hand, however, for $t\in\mathscr{C}\cap\mathscr{T}_{\kappa}^{\kappa}$, the dynamic derivative is not consistent with f'' unless $\lambda(t)=1$, and in the latter special case the order of accuracy of the approximation raises to two. Finally, for $t\in\mathscr{A}\cap\mathscr{T}_{\kappa}^{\kappa}$, the dynamic derivative investigated may never be consistent with f'' due to the fact that $\mu^{\nabla}(t)\neq 0$. This completes the proof. □

Remark 3.1. Based on the discussions in Lemma 3.1 and Theorem 3.1, it is straightforward to verify that in the particular case if the hybrid grid $\mathscr{T}$ is discrete, then

$$\omega_{\Delta\nabla}(f)=\frac{2}{1+\lambda(t)}f^{\Delta\nabla}(t), \quad t\in\mathscr{T}_{\kappa}^{\kappa},$$

offers a first-order approximation to $f''(t)$, $t\in\mathscr{T}_{\kappa}^{\kappa}$, if $\lambda(t)\neq 1$; and a second-order approximation if $\lambda(t)=1$. The functional $\omega_{\Delta\nabla}(f)$ may be referred to as a *modified dynamic derivative formula*. In fact, it has already been used frequently in many adaptive finite difference and finite element computations [4,8,10].

Lemma 3.2. *Let f be twice continuously differentiable in $[a,\ b]$, and η be Δ differentiable on B. Then*

$$f^{\nabla\Delta}(t)=\begin{cases}\dfrac{f'(\sigma(t))-f'(t)}{\mu(t)}, & t\in\mathscr{A}\cap\mathscr{T}_\kappa^\kappa,\\ \dfrac{f'(t)-\left(1+\eta^\Delta(t)\right)f^\nabla(t)}{\eta(t)}, & t\in\mathscr{B}\cap\mathscr{T}_\kappa^\kappa,\\ \dfrac{\eta(t)f^\sigma(t)-(\eta(t)+\mu(t))f(t)+\mu(t)f^\rho(t)}{\mu^2(t)\eta(t)}, & t\in\mathscr{C}\cap\mathscr{T}_\kappa^\kappa,\\ f''(t), & t\in\mathscr{D}\cap\mathscr{T}_\kappa^\kappa.\end{cases}$$

Proof. Again, we only need to show the first two identities since the rest of the proof is similar. To start, we may notice that due to definitions of the Δ, ∇ dynamic derivatives [1-4], for $t\in\mathscr{A}\cap\mathscr{T}_\kappa^\kappa$,

$$\begin{aligned}f^{\nabla\Delta}(t)&=\left(f^\nabla(t)\right)^\Delta=\left(f'(t)\right)^\Delta\\&=\frac{f'(\sigma(t))-f'(t)}{\mu(t)}.\end{aligned}$$

Further, by the same token, for $t\in\mathscr{B}\cap\mathscr{T}_\kappa^\kappa$ we acquire that

$$\begin{aligned}f^{\nabla\Delta}(t)&=\left(f^\nabla(t)\right)^\Delta=\left(\frac{f(t)-f(\rho(t))}{\eta(t)}\right)^\Delta\\&=\frac{\left(f(t)-f(\rho(t))\right)^\Delta\eta(t)-\left(f(t)-f(\rho(t))\right)\eta^\Delta}{\eta(t)\eta(\sigma(t))}\\&=\frac{\left(f^\Delta(t)-f^\Delta(\rho(t))\right)\eta(t)-\left(f(t)-f(\rho(t))\right)\eta^\Delta}{\eta^2(t)}\\&=\frac{f'(t)-f^\nabla(t)}{\eta(t)}-\frac{f^\nabla(t)\eta^\Delta(t)}{\eta(t)}\\&=\frac{1}{\eta(t)}\left[f'(t)-\left(1+\eta^\Delta(t)\right)f^\nabla(t)\right].\end{aligned}$$

The above completes successfully our arguments. □

Theorem 3.2. *Let f be four times continuously differentiable in $[a,\ b]$, and η be Δ differentiable on $\mathscr{B}$. Then the $\nabla\Delta$ dynamic derivative of f*

(i) *is consistent with f'' at all left-dense points on $\mathscr{T}_\kappa^\kappa$;*

(ii) *is not consistent with f'' at any left-scattered point on $\mathscr{T}_\kappa^\kappa$ except in the case that $\lambda(t)=1$.*

Further,

$$f^{\nabla\Delta}(t)=$$
$$\begin{cases} f''(t)+\dfrac{\mu(t)}{2}f'''(\zeta_1), & t\in\mathscr{A}\cap\mathscr{T}_\kappa^\kappa,\\ \dfrac{1}{2}\left(1+\eta^\Delta(t)\right)f''(t)-\dfrac{\eta^\Delta(t)}{\eta(t)}f'(t)+\dfrac{\eta(t)}{6}\left(1+\eta^\Delta(t)\right)f'''(\zeta_2), & t\in\mathscr{B}\cap\mathscr{T}_\kappa^\kappa,\\ \dfrac{1}{2}\left(1+\dfrac{1}{\lambda(t)}\right)f''(t)+\dfrac{\mu(t)}{6}\left(1-\dfrac{1}{\lambda^2(t)}\right)f'''(t) & \\ \qquad+\dfrac{\mu^2(t)}{12}\left(1+\dfrac{1}{\lambda^3(t)}\right)f^{(4)}(\zeta_3), & t\in\mathscr{C}\cap\mathscr{T}_\kappa^\kappa,\\ f''(t), & t\in\mathscr{D}\cap\mathscr{T}_\kappa^\kappa, \end{cases}$$

where $\zeta_1,\ \zeta_2,\ \zeta_3\in(a,\ b)$. *The identities characterize asymptotically the approximation error involved.*

Proof. It is clear that we only need to show the first two identities since proofs of the rest are similar to those in [7,8]. For this purpose, based on the embedded smoothness conditions, we may claim that

$$f'(\sigma(t))=f'(t)+\mu(t)f''(t)+\frac{\mu^2(t)}{2!}f'''(\zeta_1),\quad \zeta_1\in(a,\ b), \tag{3.3}$$

$$f^\rho(t)=f(t)-\eta(t)f'(t)+\frac{\eta^2(t)}{2!}f''(t)-\frac{\eta^3(t)}{3!}f'''(\zeta_2),\quad \zeta_2\in(a,\ b). \tag{3.4}$$

It follows immediately that substitutions of (3.3) and (3.4) directly into the first two identities given by Lemma 3.2, respectively, yield readily the two identities we expect. Next, based on the identities obtained, we realize immediately that for all $t\in(\mathscr{A}\cup\mathscr{D})\cap\mathscr{T}_\kappa^\kappa$, that is, t are left-dense, the $\nabla\Delta$ dynamic derivative offers a first-order approximation to f''. On the other hand, however, for any $t\in\mathscr{C}\cap\mathscr{T}_\kappa^\kappa$ the dynamic derivative cannot be consistent with f'' because the coefficient term involving f'' in the expansions cannot be one unless $\lambda(t)=1$. In the latter particular case the dynamic derivative reduces to a second-order finite difference approximation. Finally, for $t\in\mathscr{B}\cap\mathscr{T}_\kappa^\kappa$, the dynamic derivative can never be consistent with f'' due to the fact that $\eta^\Delta(t)$ is nontrivial. Hence the theorem is proved. □

Remark 3.2. Based on the discussions in Lemma 3.2 and Theorem 3.2, it is not difficult to observe that in the particular case if the hybrid grid $\mathscr{T}$ is discrete, then

$$\omega_{\nabla\Delta}(f)=\frac{2\lambda(t)}{1+\lambda(t)}f^{\nabla\Delta}(t),\quad t\in\mathscr{T}_\kappa^\kappa,$$

provides a first-order approximation to $f''(t),\ t\in\mathscr{T}_\kappa^\kappa$, if $\lambda(t)\neq 1$; and a second-order approximation if $\lambda(t)=1$. In fact, the above *modified dynamic derivative formula* for the $\nabla\Delta$ dynamic derivative has already been adopted in various kinds of adaptive finite difference and finite element schemes [4,8,9].

4. Non-crossed second-order dynamic derivatives

Under the required smoothness conditions, we may state

Lemma 4.1. *Let f be twice continuously differentiable in $[a,\ b]$. Then*

$$f^{\Delta\Delta}(t)=\begin{cases}\dfrac{f'(\sigma(t))-f^{\Delta}(t)}{\mu(t)}, & t\in(\mathscr{A}\cup\mathscr{C})\cap\mathscr{T}^{\kappa^2},\ \sigma(t)\in\mathscr{B},\\[2ex] \dfrac{\mu(t)f^{\sigma^2}(t)-(\mu(t)+\mu^{\sigma}(t))f^{\sigma}(t)+\mu^{\sigma}(t)f(t)}{\mu^2(t)\mu^{\sigma}(t)}, & t\in(\mathscr{A}\cup\mathscr{C})\cap\mathscr{T}^{\kappa^2},\ \sigma(t)\in\mathscr{C},\\[2ex] f''(t), & t\in(\mathscr{B}\cup\mathscr{D})\cap\mathscr{T}^{\kappa^2},\end{cases}$$

$$f^{\nabla\nabla}(t)=\begin{cases}\dfrac{f^{\nabla}(t)-f'(\rho(t))}{\eta(t)}, & t\in(\mathscr{B}\cup\mathscr{C})\cap\mathscr{T}_{\kappa^2},\ \rho(t)\in\mathscr{A},\\[2ex] \dfrac{\eta^{\rho}(t)f(t)-(\eta^{\rho}(t)+\eta(t))f^{\rho}(t)+\eta(t)f^{\rho^2}(t)}{\eta^2(t)\eta^{\rho}(t)}, & t\in(\mathscr{B}\cup\mathscr{C})\cap\mathscr{T}_{\kappa^2},\ \rho(t)\in\mathscr{C},\\[2ex] f''(t), & t\in(\mathscr{A}\cup\mathscr{D})\cap\mathscr{T}_{\kappa^2}.\end{cases}$$

Proof. We only need to show the first identity in each set of the identities for the $\Delta\Delta$ and $\nabla\nabla$ dynamic derivatives, since proofs of the two second identities can be viewed as natural extensions of the results obtained in [8], and the last two identities can be generated readily according to definitions of the corresponding dynamic derivatives. Now, according to [1–4] we obtain that

$$\begin{aligned}f^{\Delta\Delta}(t) &= \left(f^{\Delta}(t)\right)^{\Delta} = \left(\frac{f(\sigma(t))-f(t)}{\mu(t)}\right)^{\Delta}\\ &= \frac{1}{\mu(t)}\left(\lim_{s\to 0^+}\frac{f(\sigma(t)+s)-f(\sigma(t))}{s}-\frac{f(\sigma(t))-f(t)}{\mu(t)}\right)\\ &= \frac{f'(\sigma(t))-f^{\Delta}(t)}{\mu(t)},\quad t\in(\mathscr{A}\cup\mathscr{C})\cap\mathscr{T}^{\kappa^2},\ \sigma(t)\in\mathscr{B}.\end{aligned}$$

Similarly,

$$\begin{aligned}f^{\nabla\nabla}(t) &= \left(f^{\nabla}(t)\right)^{\nabla} = \left(\frac{f(t)-f(\rho(t))}{\eta(t)}\right)^{\nabla}\\ &= \frac{1}{\eta(t)}\left(\frac{f(t)-f(\rho(t))}{\eta(t)}-\lim_{s\to 0^+}\frac{f(\rho(t))-f(\rho(t)-s)}{s}\right)\\ &= \frac{f^{\nabla}(t)-f'(\rho(t))}{\eta(t)},\quad t\in(\mathscr{B}\cup\mathscr{C})\cap\mathscr{T}_{\kappa^2},\ \rho(t)\in\mathscr{A}.\end{aligned}$$

Therefore the proof of the theorem is completed. ☐

Theorem 4.1. *Let f be four times continuously differentiable in $[a,\ b]$. Then the $\Delta\Delta$ dynamic derivative of f*

(i) *is consistent with f'' at all right-dense points on $\mathscr{T}^{\kappa^2}$;*

(ii) *is not consistent with f'' at any right-scattered point on $\mathscr{T}^{\kappa^2}$ except in the case that $\lambda^\sigma(t) = 1$.*

Further,

$$f^{\Delta\Delta}(t) = \begin{cases} \dfrac{1}{2} f''(t) + \dfrac{\mu(t)}{6}\left(3f'''(\xi_4) - f'''(\zeta_4)\right), & t \in (\mathscr{A} \cup \mathscr{C}) \cap \mathscr{T}^{\kappa^2},\ \sigma(t) \in \mathscr{B}, \\ \dfrac{1}{2}(1 + \lambda^\sigma(t))\left(f''(t) + \mu(t)\phi_1(\mu, f)\right), & t \in (\mathscr{A} \cup \mathscr{C}) \cap \mathscr{T}^{\kappa^2},\ \sigma(t) \in \mathscr{C}, \\ f''(t), & t \in (\mathscr{B} \cup \mathscr{D}) \cap \mathscr{T}^{\kappa^2} \end{cases}$$

where

$$\phi_1(\mu, f) = \frac{2 + \lambda^\sigma(t)}{3} f'''(t) + \frac{\mu^\sigma(t)}{12}\left[\left(1 + \frac{1}{\lambda^\sigma(t)}\right)^3 f^{(4)}(\xi_6) - \frac{1}{(\lambda^\sigma(t))^3} f^{(4)}(\zeta_6)\right]$$

and $\xi_4,\ \xi_6,\ \zeta_4,\ \zeta_6 \in (a,\ b)$. The identities characterize asymptotically the approximation error involved.

Proof. Due to their interesting similarities, we delay this proof till that for the next theorem. ☐

Theorem 4.2. *Let f be four times continuously differentiable in $[a,\ b]$. Then the $\nabla\nabla$ dynamic derivative of f*

(iii) *is consistent with f'' at all left-dense points on $\mathscr{T}_{\kappa^2}$;*

(iv) *is not consistent with f'' at any left-scattered point on $\mathscr{T}_{\kappa^2}$ except when $\lambda^\rho(t) = 1$.*

Further,

$$f^{\nabla\nabla}(t) = \begin{cases} \dfrac{1}{2} f''(t) + \dfrac{\eta(t)}{6}\left(f'''(\xi_5) - 3f'''(\zeta_5)\right), & t \in (\mathscr{B} \cup \mathscr{C}) \cap \mathscr{T}_{\kappa^2},\ \rho(t) \in \mathscr{A}, \\ \dfrac{1}{2}\left(1 + \dfrac{1}{\lambda^\rho(t)}\right)\left(f''(t) + \eta(t)\psi_1(\eta, f)\right) & t \in (\mathscr{B} \cup \mathscr{C}) \cap \mathscr{T}_{\kappa^2},\ \rho(t) \in \mathscr{C}, \\ f''(t), & t \in (\mathscr{A} \cup \mathscr{D}) \cap \mathscr{T}_{\kappa_2}, \end{cases}$$

where

$$\psi_1(\eta, f) = -\frac{1 + 2\lambda^\rho(t)}{3\lambda^\rho(t)} f'''(t) + \frac{\eta^\rho(t)}{12}\left[\frac{(1 + \lambda^\rho(t))^3}{\lambda^\rho(t)} f^{(4)}(\xi_7) - (\lambda^\rho(t))^2 f^{(4)}(\zeta_7)\right]$$

and $\xi_5,\ \xi_7,\ \zeta_5,\ \zeta_7 \in (a,\ b)$. Again, the identities characterize asymptotically the approximation error involved.

Proof. We begin with proofs of the asymptotic expansion based identities first. Since the last identity in each set of the identities in the theorem can be viewed as consequences of definitions of the corresponding dynamic derivatives [1,2,9], we only need to focus on proofs of the other identities discussed. For this purpose, we recall (3.1), (3.4) and observe that

$$f^{\Delta}(t)=f'(t)+\frac{\mu(t)}{2}f''(t)+\frac{\mu^2(t)}{3!}f'''(\xi_4),\quad \xi_4\in(a,\ b), \tag{4.1}$$

$$f^{\nabla}(t)=f'(t)-\frac{\eta(t)}{2}f''(t)+\frac{\eta^2(t)}{3!}f'''(\xi_6),\quad \xi_6\in(a,\ b). \tag{4.2}$$

Next, with the help of the expansion (3.3), we may realize that the following must be true:

$$\begin{aligned}&\frac{f'(\sigma(t))-f^{\Delta}(t)}{\mu(t)}\\ =&\frac{f'(t)+\mu(t)f''(t)+\mu^2(t)f'''(\xi_4)/2-f'(t)-\mu(t)f''(t)/2-\mu^2(t)f'''(\zeta_4)/6}{\mu(t)}\\ =&\frac{f''(t)}{2}+\frac{\mu(t)}{6}\left(3f'''(\xi_4)-f'''(\zeta_4)\right),\quad t\in(\mathscr{A}\cup\mathscr{C})\cap\mathscr{T}^{\kappa^2},\ \sigma(t)\in\mathscr{B}.\end{aligned}$$

Now, according to (3.2) we may claim that

$$\begin{aligned}&\frac{f^{\nabla}(t)-f'(\rho(t))}{\eta(t)}\\ =&\frac{f'(t)-\eta(t)f''(t)/2+\eta^2(t)f'''(\xi_5)/6-f'(t)+\eta(t)f''(t)-\eta^2(t)f'''(\zeta_5)/2}{\eta(t)}\\ =&\frac{f''(t)}{2}+\frac{\eta(t)}{6}\left(f'''(\xi_5)-3f'''(\zeta_5)\right),\quad t\in(\mathscr{B}\cup\mathscr{C})\cap\mathscr{T}_{\kappa^2},\ \rho(t)\in\mathscr{A}.\end{aligned}$$

Needless to say, the relations we just obtained have secured the two first identities we want for cases of $\Delta\Delta$ and $\nabla\nabla$ dynamic derivative approximations. To continue our pursuit, we replace $\mu^{\sigma}(t)/\mu(t),\ \eta(t)/\eta^{\rho}(t)$ in the equations by notations $\lambda^{\sigma}(t),\ \lambda^{\rho}(t)$, respectively. Thus, by restructuring and simplifying the new equations acquired, the rest of identities in the theorem becomes obvious immediately.

To explore further properties of the aforementioned approximations, we consider situations involving the $\Delta\Delta$ dynamic derivative first. Based on previous identities, for the case of $t\in(\mathscr{B}\cup\mathscr{D})\cap\mathscr{T}^{\kappa^2}$, the dynamic derivative is equivalent to f''. Therefore it is a consistent approximation. However, in the case when $t\in(\mathscr{A}\cup\mathscr{C})\cap\mathscr{T}^{\kappa^2}$, that is, t is right-scattered, the dynamic derivative is not a consistent approximation to f'' unless $\lambda^{\sigma}(t)=1$, which means that $\sigma(t)$ must be a uniformly discrete point on the hybrid grid. Furthermore, with $\sigma(t)\in\mathscr{B}\cap\mathscr{T}^{\kappa^2}$, the dynamic derivative can never be an approximation to f'' because of the existence of the non-unity coefficient for the f'' term. Now, consider the cases for the $\nabla\nabla$ dynamic derivative. Based on definitions of the ∇ derivative, it can be shown that for all $t\in(\mathscr{A}\cup\mathscr{D})\cap\mathscr{T}_{\kappa^2}$, that is, t is left-dense, the dynamic derivative is equivalent to f''.

Thus it is a consistent approximation in the situation. However, when $t \in (\mathscr{B} \cup \mathscr{C}) \cap \mathscr{T}_{\kappa^2}$, that is, t is left-scattered, the dynamic derivative is not a consistent approximation to f'' unless $\lambda^\rho(t) = 1$, which indicates that $\rho(t)$ must be a uniformly discrete point on the hybrid grid. As for the last case when $\rho(t) \in \mathscr{A} \cap \mathscr{T}_{\kappa^2}$, the dynamic derivative can never be consistent with f'' due to the existence of the non-unity coefficient for the f'' term in the expansion. This completes our verification successfully. □

Remark 4.1. It is interesting to observe that the strict smoothness constraints on μ, η may not be necessary in Lemma 4.1, Theorem 4.1 and Theorem 4.2. This effectively improves the applicability of the dynamic derivative approximations, since derivatives of the step functions do not exist in general [5, 8, 10]. Let the hybrid grid $\mathscr{T}$ be discrete. It is not difficult to verify that the following *modified dynamic derivative formula* holds:

$$\omega_{\Delta\Delta}(f) = \frac{2}{1+\lambda^\sigma(t)} f^{\Delta\Delta}(t), \quad t \in \mathscr{T}^{\kappa^2},$$
$$\omega_{\nabla\nabla}(f) = \frac{2\lambda^\rho(t)}{1+\lambda^\rho(t)} f^{\nabla\nabla}(t), \quad t \in \mathscr{T}_{\kappa^2}.$$

However, both formulae can only offer first-order approximations to $f''(t)$, $t \in \mathscr{T}_\kappa^\kappa$, no matter whether $\lambda^\rho(t) = 1$ or $\lambda^\sigma(t) = 1$. These modified formulae are particularly similar to those used in upwind or downwind type finite difference schemes for attacking nonlinear differential equations possessing strong singularities such as boundary layers and shock waves [11, 12, 14].

5. Numerical examples and conclusions

As an example used frequently in wave computations, let us consider a highly oscillatory exponential function,

$$f(x,y) = a\exp\{-iW(x+y)\}, \quad 0 \le x,\ y \le 1, \tag{5.1}$$

where $a > 0$ is a constant, $i = \sqrt{-1}$ and $W \gg 1$ is the wave parameter. It is obvious that

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial y^2} = -aW^2\exp\{-iW(x+y)\}.$$

Without loss of generality, we may consider only the partial derivative in x-direction. Fix $y = \hat{y}$. We adopt a monotonically decreasing nonuniform finite set,

$$\mathscr{T}_n = \left\{x_k\ :\ x_0 = 0,\ x_k = x_{k-1} + r^k,\ k = 1, 2, \cdots, n\right\}, \quad 0 < r < 1.$$

Let $a = 1$, $W = \pi$. Evidently, when n is sufficiently large, $\mathscr{T}_n$ can be viewed as a hybrid grid from the computational point-of-view, since the grid points are dense near the right-end of the set. First, let us select $r = 0.8$ and $n = 80$. In Figs. 1-4 we plot the real parts of

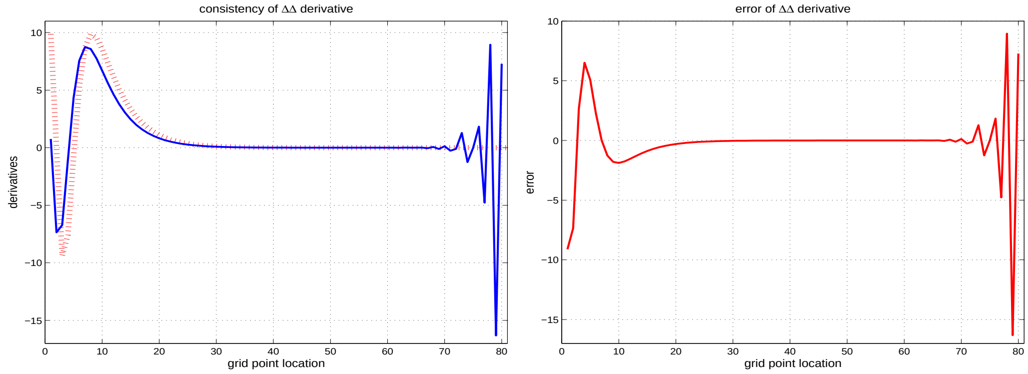

Figure 1: LEFT: Real parts of dynamic derivative $f_{xx}^{\Delta\Delta}(x,\hat{y})$ (solid curve) and conventional derivative $f_{xx}(x,\hat{y})$ (dotted curve) in the first 80 grid points. Inconsistencies near left and right ends are obvious. RIGHT: The difference (error) between the two derivatives.

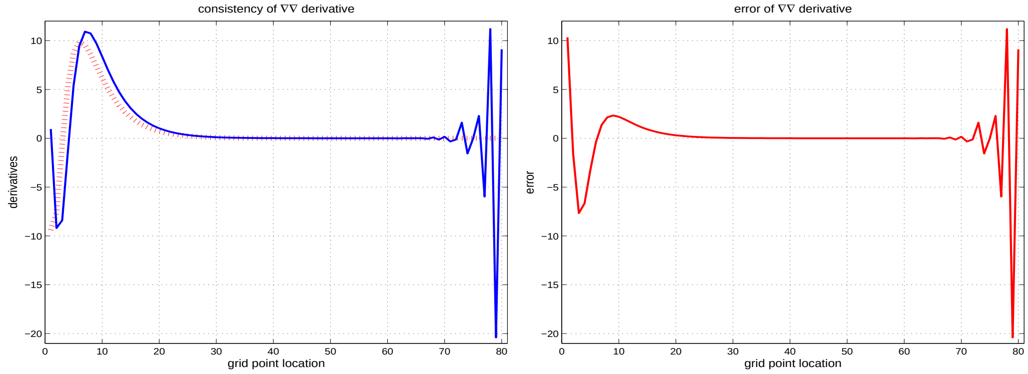

Figure 2: LEFT: Real parts of dynamic derivative $f_{xx}^{\nabla\nabla}(x,\hat{y})$ (solid curve) and conventional derivative $f_{xx}(x,\hat{y})$ (dotted curve) in the first 80 grid points. Inconsistencies near left and right ends are obvious. RIGHT: The difference (error) between the two derivatives.

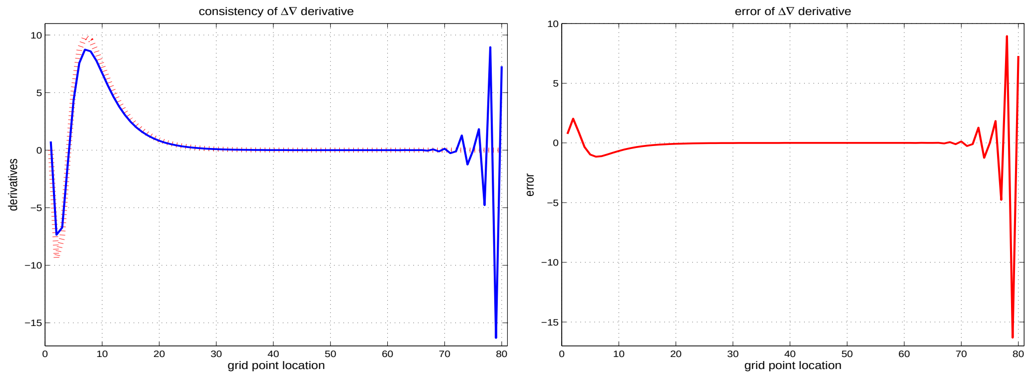

Figure 3: LEFT: Real parts of dynamic derivative $f_{xx}^{\Delta\nabla}(x,\hat{y})$ (solid curve) and conventional derivative $f_{xx}(x,\hat{y})$ (dotted curve) in the first 80 grid points. Inconsistencies near left and right ends are obvious. RIGHT: The difference (error) between the two derivatives.

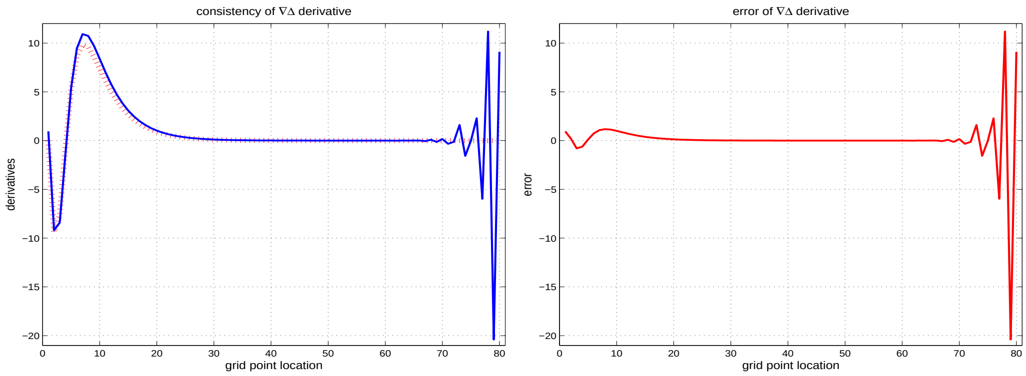

Figure 4: LEFT: Real parts of dynamic derivative $f_{xx}^{\nabla\Delta}(x,\hat{y})$ (solid curve) and conventional derivative $f_{xx}(x,\hat{y})$ (dotted curve) in the first 80 grid points. Inconsistencies near left and right ends are obvious. RIGHT: The difference (error) between the two derivatives.

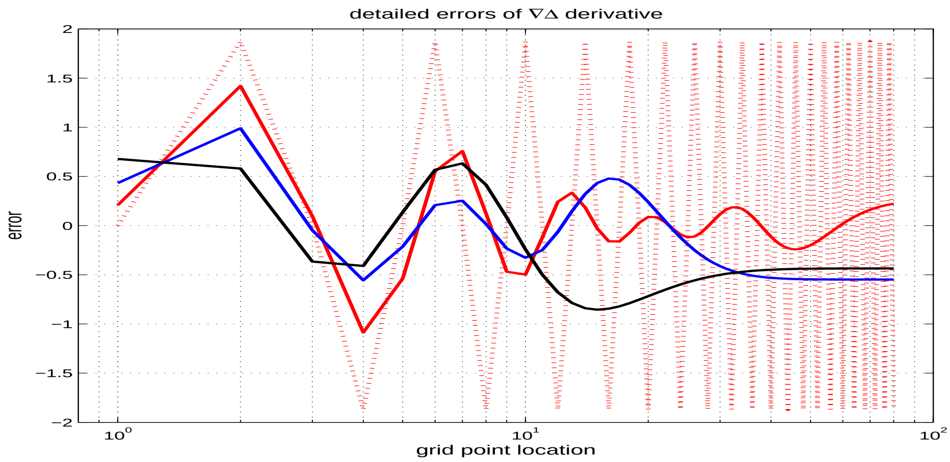

Figure 5: Difference (error) between the real parts of dynamic derivative $f_{xx}^{\nabla\Delta}(x,\hat{y})$ and conventional derivative $f_{xx}(x,\hat{y})$ in the first 80 grid points.

$f_{xx}(x,\hat{y})$ and $f_{xx}^{\Delta\Delta}(x,\hat{y})$, $f_{xx}^{\nabla\nabla}(x,\hat{y})$, $f_{xx}^{\Delta\nabla}(x,\hat{y})$, $f_{xx}^{\nabla\Delta}(x,\hat{y})$, respectively with $\hat{y}=1$. To see more clearly the consistency of the dynamic derivatives, we use the number of grids rather than x values in the x-direction. We may observe that the differences between the dynamic derivatives and conventional derivative are relatively large in the beginning. This is because that the practical step sizes, r^k, are relatively large as k being small. The consistency is improved continuously till near the end of computation, where the numerical error increases dramatically and nonphysical oscillations appear, ignore the fact that the final steps, say, $r^{80}\approx 8.8342\times 10^{-9}$, used are extremely small on a highly accurate computer platform. This indicates that the convergence of the dynamic derivatives to f_{xx} is highly impossible. Careful readers may notice that the approximations given by the $f_{xx}^{\Delta\nabla}(x,\hat{y})$ and $f_{xx}^{\nabla\Delta}(x,\hat{y})$ derivatives are slightly better than the other dynamic derivatives. This are shown in our analysis, since that the two dynamic derivatives are in fact extensions of the central differences if $\mathscr{T}$ is a discrete set.

Table 1: Profiles of the real parts of dynamic derivative $f_{xx}^{\nabla\Delta}(x, \hat{y})$ and conventional derivative $f_{xx}(x, \hat{y})$.

r	x_{80}	$x_{80} - x_{79}$	$f_{xx}^{\Delta\nabla}(x_{80}, \hat{y})$	$f_{xx}(x_{80}, \hat{y})$	$\max\left\lvert f_{xx}^{\Delta\nabla} - f_{xx}\right\rvert$
0.80	2.500000	8.834235e-009	9.104421	1.369583	20.393899
0.85	3.333325	1.128454e-006	-5.371646	-4.935004	0.854487
0.90	4.998907	1.092372e-004	-10.417853	-9.869546	0.989253
0.95	9.834846	0.008257	8.793424	8.570686	1.420024
1.0	40.0	0.50	8.0	9.869604	1.869604

As an illustration, in Fig. 5, we show the differences between the real parts of $f_{xx}(x, \hat{y})$ and $f_{xx}^{\nabla\Delta}(x, \hat{y}),\ \hat{y} = 1$, while different r values are employed. A logarithmic scale is used. The dotted curve is for the case when $r = 1$, for which a uniform grid is presented. The difference tends to be stable and matches the known theory of finite difference approximations. The second curve (red, or the second curve at the first peak location) is for the case of $r = 0.95$. The third curve (blue, or the third curve at the first peak location) is for the case of $r = 0.9$, while the last curve is for the case of $r = 0.85$. Table 1 gives the terminal step sizes and x locations for each of the cases. We may notice that the consistency is improved as r is reduced within the range. However, this will not be the case as $n \to \infty$ due to the inconsistency demonstrated in Figs. 1-4. The use of smaller ratio r may lead to earlier nonphysical oscillations so that the dynamic derivatives may collapse in computations.

Let $\mathscr{T}$ be a set of real numbers superimposed on $[a,\ b]$, $\mathscr{T}$ is nonempty, and $f(t)$ is sufficiently smooth on $[a,\ b]$. Then the second-order dynamic derivatives, including the Δ, ∇ dynamic derivatives and their combinations, are not consistent with the conventional derivative f'' in general. However, the dynamic derivatives can be consistent approximations of f'' in certain special cases, in particular when discrete hybrid grids are employed. In many cases, the second-order dynamic derivatives can be reformulated to yield consistent approximations to f'' too. The key for achieving so includes a proper incorporation of the particular hybrid grid structures into the underlying dynamic derivative formulae. However, the order of a modified dynamic derivative formula is usually low, and the new formula generated may be complicated and might be lacking certain useful features such as the iterative property. These create unexpected difficulties in further generalizations of the formulae, in particularly in the study of higher order dynamic derivatives in approximations. The inconsistency, on the other hand, offers tremendous amount of freedom in formulating sensitive approximations of many important natural phenomena possessing unpredictable singularities [1, 5, 6, 8–10, 13]. We will leave these temporarily for the readers to explore.

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