On the extension of the complex-step derivative technique to pseudospectral algorithms

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1 Introduction

The complex-step derivative (CSD) technique is a convenient and highly-accurate strategy to perform a linearized "perturbation" analysis to determine a "directional derivative" via a minor modification of an existing nonlinear simulation code. The technique has previously been applied to nonlinear simulation codes (such as finite-element codes) which employ real arithmetic only. The present note examines the suitability of this technique for extension to efficient pseudospectral simulation codes which nominally use the fast Fourier transform (FFT) to convert back and forth between the physical and transformed representations of the system. It is found that, if used carefully, this extension retains the remarkable accuracy of the CSD approach. However, to perform this extension without sacrificing this accuracy, particular care must be exercised; specifically, the state (real) and perturbation (imaginary) components of the complexified system must be transformed separately and arranged in such a manner that they are kept distinct during the process of differentiation in the transformed space in order to avoid the linear combination of the large and small quantities in the analysis. It is shown that this is relatively straightforward to implement even in complicated nonlinear simulation codes, thus positioning the CSD approach as an attractive and relatively simple alternative to hand coding a perturbation (a.k.a. "tangent linear") code for determining the directional derivative even when pseudospectral algorithms are employed.

2 Background

The idea of using complex variables in order to differentiate a function was (apparently) first mentioned in [1] and [2]. The applicability of this old technique to differentiate a complicated function, such as that computed by an involved finite-element code, was recognized by [3]. Recently, the CSD technique has become popular in aerodynamic optimization [4–7]. This approach has proven to be very accurate and easy to apply to finite-element and finite-difference simulation codes but, to the best of our knowledge, has not yet been extended to pseudospectral simulation codes. The present note explores the suitability of this extension.

2.1 The Finite-Difference (FD) approximation

The directional derivative d of a continuous function $J(\phi)$ in the direction ϕ_1 is defined by

$$d \triangleq \frac{\mathcal{D}\mathcal{J}(\phi)}{\mathcal{D}\phi} \cdot \phi_1 = \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon} \left[\mathcal{J}(\phi + \varepsilon \phi_1) - \mathcal{J}(\phi) \right], \tag{1}$$

which is simply the amount $J(\phi)$ changes when ϕ is updated in the direction ϕ_1, scaled by the size of the update, in the limit that the size of the update approaches zero. There are a variety of ways to calculate numerically this seemingly simple quantity. The most straightforward method to compute d is to consider a Taylor series expansion of the function $\mathcal{J}(\phi + \varepsilon \phi_1)$ near ϕ, from which a first-order finite-difference (FD) formula for the directional derivative is easily obtained:

$$\mathcal{J}(\phi + \varepsilon \phi_1) = \mathcal{J}(\phi) + \varepsilon \frac{\mathcal{D}\mathcal{J}(\phi)}{\mathcal{D}\phi} \cdot \phi_1 + O(\varepsilon^2) \quad \Rightarrow \quad d = \frac{\mathcal{J}(\phi + \varepsilon \phi_1) - \mathcal{J}(\phi)}{\varepsilon} + O(\varepsilon).$$

Likewise, second- and higher-order finite-difference formulae for the directional derivative can be easily obtained. The drawback with these methods when using a finite-precision arithmetic computer is the difficulty in finding the most suitable value for the step size ε, since the accuracy of the numerical approximation of d is very sensitive to this value. When ε is large, the Taylor-series truncation is not valid, and when it is small, subtractive cancellation errors dominate.

To illustrate, the derivative of a scalar nonlinear function $f(x) = \frac{e^{-x}}{\sqrt{\tan x}}$ at $x = 1$ has been computed using FD approximations with both single- and double-precision arithmetic. Figure 1 shows that, for large ε, the error of these FD approximations scales with ε^n, where n is the order of truncation of the higher-order terms of the corresponding FD formulae. For small ε, the error of all three FD formula in Figure 1 is $O(1/\varepsilon)$ due to subtractive cancellation errors. In other words, when comparing two numbers which are almost the same using finite-precision arithmetic, the relative round-off error is proportional to the inverse of the difference between the two numbers. If the difference between the two numbers is decreased by an order of magnitude, the relative accuracy with which this difference may be calculated using finite precision arithmetic is also decreased by an order of magnitude.

2.2 The Complex-Step Derivative (CSD) approximation

The CSD approximation makes use of complex variables in order to compute the directional derivative. If the complex extension $\mathcal{J}(z)$ of a real-valued function $\mathcal{J}(\phi)$ is analytic, it can be expanded with a complex Taylor series. In particular, the expansion of $\mathcal{J}(\phi + i\varepsilon\phi_1)$, where $i = \sqrt{-1}$, may be written:

$$\mathcal{J}(\phi + i\varepsilon\phi_1) = \mathcal{J}(\phi) + i\varepsilon \frac{\mathcal{D}\mathcal{J}(\phi)}{\mathcal{D}\phi} \cdot \phi_1 - \varepsilon^2 E_1 - i\varepsilon^3 E_2 + O(\varepsilon^4), \tag{2}$$

where E_1 and E_2 are real and are related to the higher-order derivatives of $\mathcal{J}$. Taking the imaginary part and dividing by ε gives a formula for the directional derivative:

$$d = \Im\{\frac{\mathcal{J}(\phi + i\varepsilon\phi_1)}{\varepsilon}\} + O(\varepsilon^2); \tag{3}$$

note that the error in this formula is $O(\varepsilon^2)$ because the leading-order error of (2) is real. This method has the advantage that it does not face the problem of the subtractive cancellation error; that is, d is computed simply by taking the imaginary part of the complex number $\mathcal{J}(\phi + i\varepsilon\phi_1)$. As seen in Figure 1, for small ε, the relative error of the CSD approximation reaches an asymptotic value given by the machine precision. Thus, when the CSD method is applied to this test problem, *any* choice of the step-size (providing it is sufficiently small) gives a very accurate result. Similar results are also seen when the CSD approach is applied to much more complicated functions, such as the calculation of the drag of a wing using an involved finite-element code [6,7]. As the CSD technique is both highly accurate and quite easy to apply to an existing nonlinear simulation code (simply convert all real variables in the code to complex and perturb the imaginary component of the control variable), it has become a popular technique for computing the directional derivative.

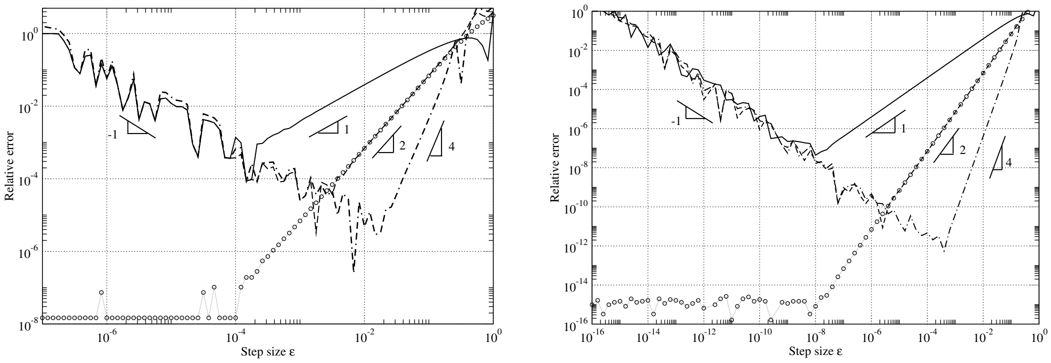

Fig. 1. Relative error of the directional derivative of $f(x) = \frac{e^{-x}}{\sqrt{\tan x}}$ at $x = 1$ given by (solid) first-order, (dashed) second-order, and (dot-dashed) fourth-order FD approaches and (circles+dots) the CSD approach using single-precision arithmetic (left) and double-precision arithmetic (right). Note that both plots have essentially the same shape.

3 Extension of the CSD approach to Fourier-based pseudospectral codes

Many codes in both fundamental turbulence research and numerical weather prediction are pseudospectral. In such codes, products are computed in physical space, spatial derivatives are computed in some “transformed” space, and the conversion between these two representations is made efficiently with a fast transform technique, usually some variant of the fast Fourier transform (FFT). Pseudospectral techniques are essential for the accurate computation of spatial derivatives in multiscale fluid systems when marginal resolution is employed.

The most common and, perhaps, simplest pseudospectral approach is that in which the transformed system is represented as a Fourier series. Unfortunately, as Fourier-based pseudospectral codes already employ complex arithmetic, direct application of the standard complex-step derivative method, as discussed above, is not possible. However, as the FFT is simply a linear manipulation of an otherwise real problem, the idea behind the CSD method is still valid. In order to implement the CSD method in an existing Fourier-based pseudospectral code, it is necessary to convert all formerly real arrays into complex arrays, double the size of all formerly complex arrays [1], and modify the FFT calls appropriately; we consider here two possible strategies:

A. Simply replace the real→complex FFTs with complex→complex FFTs.
B. Transform the state (real) and perturbation (imaginary) components with separate real→complex transforms, storing the results of these two transforms in the original (complex) data array (now doubled in size) in such a manner that performing spatial differentiation in the transformed space does not combine the state and perturbation components of the analysis. For example, in the Fourier-based case with transforms applied in the x direction only, defining $f = f_r + f_i$ where f_r is real and f_i is pure imaginary, it follows that $\hat{f}_r(k_x) = \hat{f}_r^*(-k_x)$ and $\hat{f}_i(k_x) = -\hat{f}_i^*(-k_x)$. Thus, for example, one may define the result of the physical→Fourier transform of the quantity f as:

$$\hat{f}(k_x) \triangleq \begin{cases} \hat{f}_r(k_x) & \text{for } k_x \geq 0, \\ \hat{f}_i(k_x) & \text{for } k_x < 0, \\ \hat{f}_i(0) & \text{for } k_x = NX/2 \text{ (the so-called ``oddball'' wavenumber).} \end{cases}$$

Spatial derivatives may then be computed using the original simulation code (however complicated) without further modification. Further, this representation provides enough information to recover both f_r and f_i upon separate complex→real inverse transforms while insuring that the state and perturbation components of the analysis are not combined during either the (forward and inverse) transforms or when applying the differentiation operations at each wavenumber.

To illustrate the difference in accuracy between the FD method and the two variants of the CSD method described above when applied to a pseudospectral simulation code, both methods have been implemented on an artificial optimization problem in which the dynamical system is governed by the nonlinear viscous Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

[1] Note that, when computing the FFT of a real function f (in one-dimensional, two-dimensional and three-dimensional problems), it is only necessary to store half of the Fourier coefficients, since the other half may be recovered by the identity $\hat{f}(\mathbf{k}) = \hat{f}^*(-\mathbf{k})$. This identity no longer holds if f is complex.

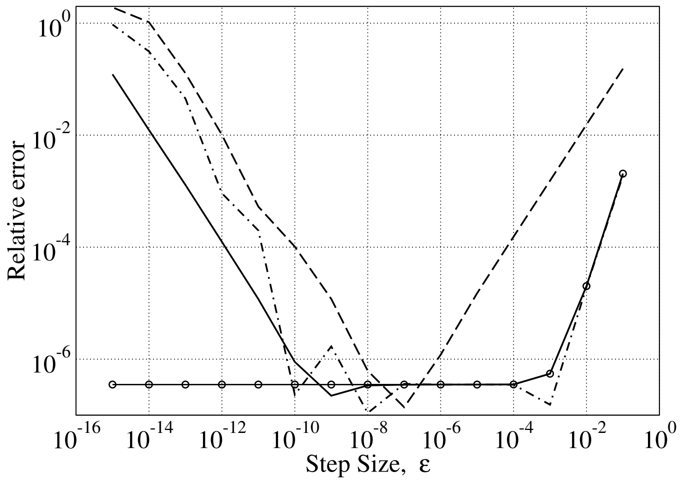

Fig. 2. Relative error of (dashed) first-order and (dot-dashed) second-order FD approaches and the CSD approach using (solid) strategy A and (solid-circle) strategy B.

in the periodic domain $x \in [0, 2\pi]$. A pseudospectral technique (FFT) is used to compute the spatial derivatives. The system is advanced in time from 0 to T, and the values $\nu = 0.067$ and $T = 6$ were used in the numerical simulation. The initial condition is given by $u(0) = 1 + 0.2\sin(x) + 0.02\sin^2(x-1) + \phi\sin(x-1)$, where ϕ is the "control parameter". The function of interest is defined as $\mathcal{J}(\phi) = \int_0^T \int_{4.5}^{5.0} |u(x,t)|^2\,dx\,dt$. The relative errors of both the FD and CSD approximations of $d\mathcal{J}/d\phi$ at $\phi = 0$ are shown in Figure 2. The exact value is obtained with a "direct" method, formed by writing a separate numerical code (sometimes called a "tangent linear" code) which explicitly calculates the perturbation equation (for further discussion, see, e.g., [8]). As seen in Figure 2, for large ε, the errors of both the FD and CSD approximations are seen to scale with ε in a manner which is similar to the case evaluated in Figure 1.

The CSD approach using strategy B (in which the real and imaginary parts are transformed separately) achieves an asymptotic value of the error for small ε in the same manner as it did in Figure 1. The selection of ε thus has no effect on the accuracy of the calculation, as long as it is chosen to be sufficiently small.

However when using strategy A (in which the real and imaginary parts are transformed simultaneously using a complex→complex transform), the error of the CSD method does not approach an asymptotic value. Instead, it scales like $O(1/\varepsilon)$ for small ε. This is due to the fact that complex→complex Fourier transforms combine the real and imaginary parts of the analysis. Thus, the large (real) and small (imaginary) numbers in the analysis are combined by the FFTs, leading to numerical inaccuracies which are found to be comparable to the subtractive cancellation errors of the second-order FD approach.

4 Discussion and extension to other pseudospectral methods

The present analysis extends directly to other efficient pseudospectral methods based on fast transforms, such as those based on Chebyshev transforms, sine/cosine transforms, etc. Note that, at their core, most such methods make use of FFTs and therefore face issues quite similar to those explored above. More precisely, if the CSD calculation anywhere involves a linear combination of the state and perturbation components of the analysis, the CSD method will fail to provide an asymptotic (small) error as ε is made small.

However, via a minor modification of the wrappers on the forward and inverse transformation algorithms, it appears always to be possible to transform the state and perturbation components of the analysis separately and to keep these two components isolated during the process of spatial differentiation in the transformed representation, thereby retaining the remarkable accuracy of the CSD approach for computing the directional derivative over a broad range of the perturbation magnitude via a minor modification of the original simulation code. The CSD method for computing the directional derivative has thus been found to extend to pseudospectral simulation codes in a favorable manner, providing an attractive and simple alternative to writing a separate "tangent linear" code from scratch for the computation of the directional derivative.

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