Extensions of the First and Second Complex-Step Derivative Approximations

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Abstract

A general framework for the first and second complex-step derivative approximation to compute numerical derivatives is presented. For first derivatives the complex-step approach does not suffer roundoff errors as in standard numerical finite-difference approaches. Therefore, since an arbitrarily small step size can be chosen, the complex-step approach can achieve near analytical accuracy. However, for second derivatives straight implementation of the complex-step approach does suffer from roundoff errors. Therefore, an arbitrarily small step size cannot be chosen. In this paper the standard complex-step approach is expanded by using general complex step sizes to provide a wider range of accuracy for both the first and second derivative approximations. Even higher accuracy formulations are obtained by repetitively applying Richardson extrapolations. The new extensions can allow the use of one step size to provide optimal accuracy for both derivative approximations.

Key words: Complex-Step, Jacobian, Hessian, Finite-Difference
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1 Introduction

Using complex numbers for computational purposes is often intentionally avoided because of the nonintuitive nature of this domain. However, this perception should not handicap our ability to seek better solutions to the problems associated with traditional (real-valued) finite-difference approaches. Many

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physical world phenomena actually have their roots in the complex domain (1). The complex-step derivative approximation can be used to determine first derivatives in a relatively easy way, while providing near analytic accuracy. Early work on obtaining derivatives via a complex-step approximation in order to improve overall accuracy is shown by Lyness and Moler (2), as well as Lyness (1). Various recent papers reintroduce the complex-step approach to the research community (3; 4; 5; 6; 7). The advantages of the complex-step approximation approach over a standard finite difference include: 1) the Jacobian approximation is not subject to roundoff errors, 2) it can be used on discontinuous functions, and 3) it is easy to implement in a black-box manner, thereby making it applicable to general nonlinear functions.

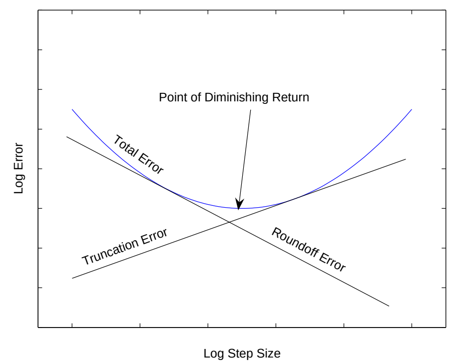


Fig. 1. Finite-Difference Error Versus Step Size

The complex-step approximation in the aforementioned papers is derived only for first derivatives. A second derivative approximation using the complex-step approach is straightforward to derive; however, this approach is subject to roundoff errors for small step sizes since difference errors arise, as shown by the classic plot in Figure 1. As the step size increases the accuracy decreases due to truncation errors associated with not adequately approximating the true slope at the point of interest. Decreasing the step size increases the accuracy, but only to an "optimum" point. Any further decrease results in a degradation of the accuracy due to roundoff errors. Hence, a tradeoff between truncation errors and roundoff exists.

The traditional first order complex-step derivative approximation is derived using a Taylor series expansion with an imaginary step size. In this paper, this will be replaced with a general complex step size. A general complex number is coupled with transcendental functions via Euler's relation; thus, in the context wherever appropriate, the Taylor series will be depicted in terms of an angle. A pair of Taylor series that are 180 deg apart is then used to derive both first and second order derivative approximations. As with the traditional complex-step first derivative, the new first derivative approximations do not suffer from roundoff errors, but provide better truncation error characteristics. The new second order derivative approximations offer better roundoff characteristics compared to the straightforward extension of the traditional complex-step approximation derivation. They also possess the benefit of better truncation characteristics from the complex-step phenomenon. The new approximations can be evaluated with step sizes at different magnitude. A weighted average is performed on them to achieve even better accuracy from further improvement of truncation errors. This technique is known as the Richardson extrapolation.

The organization of this paper proceeds as follows. First, the complex-step approximation for the first derivative of a scalar function is summarized, followed by the derivation of the second-derivative approximation. Then, the Jacobian and Hessian approximations for multi-variable functions are derived. Next, the generalized complex-step derivative approximations are derived. Finally, a numerical example is then shown that compares the accuracy of the new approximations to standard finite-difference approaches. A more thorough analysis could be found from Ref. (8).

2 Complex-Step Approximation to the Derivative

In this section the complex-step approximation is shown. First, the derivative approximation of a scalar variable is summarized, followed by an extension to the second derivative. Then, approximations for multi-variable functions are presented for the Jacobian and Hessian matrices.

2.1 Scalar Case

Numerical finite-difference approximations for any order derivative can be obtained by Cauchy's integral formula (9)

$$f^{(n)}(z) = \frac{n!}{2\pi i} \int_{\Gamma} \frac{f(\xi)}{(\xi - z)^{n+1}} d\xi \tag{1}$$

This function can be approximated by

$$f^{(n)}(z) \approx \frac{n!}{mh} \sum_{j=0}^{m-1} \frac{f\left(z + h\, e^{i\frac{2\pi j}{m}}\right)}{e^{i\frac{2\pi j n}{m}}} \tag{2}$$

where h is the step size and i is the imaginary unit, $\sqrt{-1}$. For example, when $n = 1$, $m = 2$

$$f^{'}(z) = \frac{1}{2\,h}\Big[f(z+h) - f(z-h)\Big] \tag{3}$$

We can see that this formula involves a subtraction that would introduce roundoff errors when the step size becomes too small.

2.1.1 *First Derivative*

The derivation of the complex-step derivative approximation is accomplished by approximating a nonlinear function with a complex variable using a Taylor's series expansion (7):

$$f(x+ih) = f(x) + ihf^{'}(x) - \frac{h^2}{2!}f^{''}(x) - i\frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots \tag{4}$$

Taking only the imaginary parts of both sides, dividing by h and rearranging gives

$$f^{'}(x) = \frac{\Im\Big\{f(x+ih)\Big\}}{h} + \underbrace{\frac{h^2}{3!}f^{(3)}(x) + \cdots}_{O(h^2)\approx 0} \tag{5}$$

Terms with order h^2 or higher can be ignored since the interval h can be chosen up to machine precision. Thus, to within first order the complex-step derivative approximation is given by

$$f^{'}(x) = \frac{\Im\Big\{f(x+ih)\Big\}}{h} \quad , \quad E_{\text{trunc}}(h) = \frac{h^2}{6}f^{(3)}(x) \tag{6}$$

where $E_{\text{trunc}}(h)$ denotes the truncation error. Note that this solution is not a function of differences, which ultimately provides better roundoff characteristics than a standard finite difference.

2.1.2 *Second Derivative*

In order to derive a second derivative approximation, the real components of Eq. (4) are taken, which gives

$$\Re\left\{\frac{h^2}{2!}f^{''}(x)\right\} = f(x) - \Re\Big\{f(x+ih)\Big\} + \frac{h^4}{4!}f^{(4)}(x) + \cdots \tag{7}$$

Analogous to the approach shown before, we solve for $f^{''}(x)$ and truncate up to the second-order approximation to obtain

$$f^{''}(x) = \frac{2}{h^2}\Big[f(x) - \Re\Big\{f(x+ih)\Big\}\Big] \quad , \quad E_{\text{trunc}}(h) = \frac{h^2}{12}f^{(4)}(x) \tag{8}$$

As with Cauchy's formula, this formula involves a subtraction that may introduce machine roundoff errors when the step size is too small.

2.2 Vector Case

The scalar case is now expanded to include vector functions. This case involves a vector $\mathbf{f}(\mathbf{x})$ of order m function equations and order n variables with $\mathbf{x} = [x_1, \ x_2, \ \cdots, \ x_n]^T$.

2.2.1 First Derivative

The Jacobian of a vector function is a simple extension of the scalar case. This Jacobian and its complex-step approximation are defined by

$$F_x \triangleq \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \frac{\partial f_1(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_p} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \frac{\partial f_2(\mathbf{x})}{\partial x_1} & \frac{\partial f_2(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial f_2(\mathbf{x})}{\partial x_p} & \dots & \frac{\partial f_2(\mathbf{x})}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_q(\mathbf{x})}{\partial x_1} & \frac{\partial f_q(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial f_q(\mathbf{x})}{\partial x_p} & \dots & \frac{\partial f_q(\mathbf{x})}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \frac{\partial f_m(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_p} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix} \tag{9a}$$

$$\equiv \frac{1}{h} \Im \begin{bmatrix} f_1(\mathbf{x}+ih\mathbf{e}_1) & f_1(\mathbf{x}+ih\mathbf{e}_2) & \cdots & f_1(\mathbf{x}+ih\mathbf{e}_p) & \dots & f_1(\mathbf{x}+ih\mathbf{e}_n) \\ f_2(\mathbf{x}+ih\mathbf{e}_1) & f_2(\mathbf{x}+ih\mathbf{e}_2) & \cdots & f_2(\mathbf{x}+ih\mathbf{e}_p) & \dots & f_2(\mathbf{x}+ih\mathbf{e}_n) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ f_q(\mathbf{x}+ih\mathbf{e}_1) & f_q(\mathbf{x}+ih\mathbf{e}_2) & \cdots & f_q(\mathbf{x}+ih\mathbf{e}_p) & \dots & f_q(\mathbf{x}+ih\mathbf{e}_n) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ f_m(\mathbf{x}+ih\mathbf{e}_1) & f_m(\mathbf{x}+ih\mathbf{e}_2) & \cdots & f_m(\mathbf{x}+ih\mathbf{e}_p) & \dots & f_m(\mathbf{x}+ih\mathbf{e}_n) \end{bmatrix} \tag{9b}$$

where $\mathbf{e}_p$ is the p^{th} column of an n^{th}-order identity matrix and f_q is the q^{th} equation of $\mathbf{f}(\mathbf{x})$.

2.2.2 Second Derivative

The procedure to obtain the Hessian matrix is more involved than the Jacobian case. The Hessian matrix for the q^{th} equation of $\mathbf{f}(\mathbf{x})$ and its complex-step appriximation are defined by

$$F_{xx}^q \triangleq \begin{bmatrix} \frac{\partial^2 f_q(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_1 \partial x_p} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f_q(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_2^2} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_2 \partial x_p} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 f_q(\mathbf{x})}{\partial x_n \partial x_1} & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_n \partial x_p} & \cdots & \frac{\partial^2 f_q(\mathbf{x})}{\partial x_n^2} \end{bmatrix} \tag{10a}$$

$$\equiv \begin{bmatrix} F_{xx}^q(1,1) & F_{xx}^q(1,2) & \cdots & F_{xx}^q(1,p) & \cdots & F_{xx}^q(1,n) \\ F_{xx}^q(2,1) & F_{xx}^q(2,2) & \cdots & F_{xx}^q(2,p) & \cdots & F_{xx}^q(2,n) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ F_{xx}^q(n,1) & F_{xx}^q(n,2) & \cdots & F_{xx}^q(n,p) & \cdots & F_{xx}^q(n,n) \end{bmatrix} \tag{10b}$$

where $F_{xx}^q(i,j)$ is obtained by using Eq. (8). The easiest way to describe this procedure is by showing pseudocode, given by

$F_{xx} = \mathbf{0}_{n \times n \times m}$
for $\xi = 1$ **to** m
  $\texttt{out1} = \mathbf{f}(\mathbf{x})$
  for $\kappa = 1$ **to** n
    $\mathbf{small} = \mathbf{0}_{n \times 1}$
    $\mathbf{small}(\kappa) = 1$
    $\texttt{out2} = \mathbf{f}(\mathbf{x} + i * h * \mathbf{small})$
    $F_{xx}(\kappa, \kappa, \xi) = \frac{2}{h^2}\Big[\texttt{out1}(\xi) - \Re\Big\{\texttt{out2}(\xi)\Big\}\Big]$
  end
  $\lambda = 1$
  $\kappa = n - 1$
  while $\kappa > 0$
    for $\phi = 1$ **to** κ
      $\mathbf{img\_vec} = \mathbf{0}_{n \times 1}$
      $\mathbf{img\_vec}(\phi \ldots \phi + \lambda, 1) = 1$
      $\texttt{out2} = \mathbf{f}(\mathbf{x} + i * h * \mathbf{img\_vec})$
      $F_{xx}(\phi, \phi + \lambda, \xi) = \left[\frac{2}{h^2}\Big[\texttt{out1}(\xi) - \Re\Big\{\texttt{out2}(\xi)\Big\}\Big] - \sum_{\alpha=\phi}^{\phi+\lambda}\sum_{\beta=\phi}^{\phi+\lambda} F_{xx}(\alpha, \beta, \xi)\right]/2$
      $F_{xx}(\phi + \lambda, \phi, \xi) = F_{xx}(\phi, \phi + \lambda, \xi)$
    end
    $\kappa = \kappa - 1$

$\lambda = \lambda + 1$
end
end

where $\Re\{\cdot\}$ denotes the real value operator. The first part of this code computes the diagonal elements and the second part computes the off-diagonal elements. The Hessian matrix is a symmetric matrix, so only the upper or lower triangular elements need to be computed.

3 Generalized Complex-Step Derivative Approximation

It can easily be seen from Eq. (4) that deriving second-derivative approximations without some sort of difference is difficult, if not intractable. With any complex number I that has $|I| = 1$, it's impossible for $I^2 \perp 1$ and $I^2 \perp I$. But, it may be possible to obtain better approximations than Eq. (8).

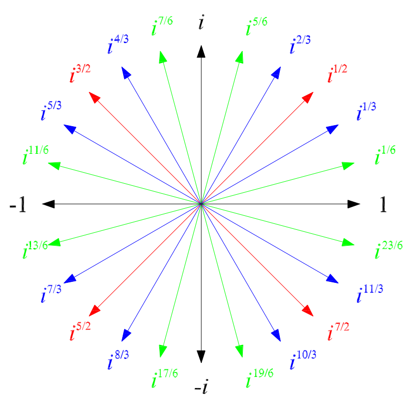
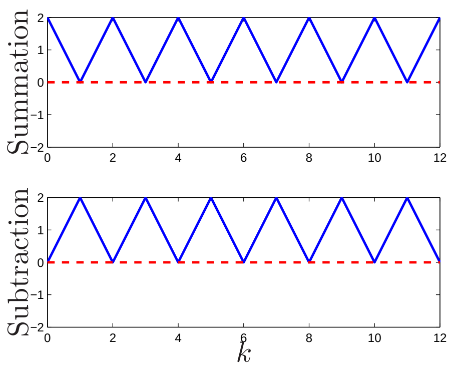


Fig. 2. Various Complex Numbers

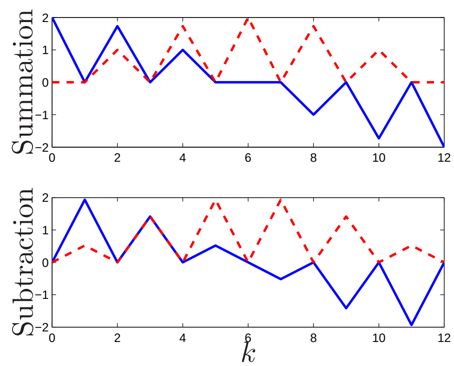
Figure 2 shows the unity magnitude complex number raised to various rational number powers with common denominator of 6, i.e. multiple of 15°. It is convenient to represent the complex number in another way. With help from trigonometry identities, these can be derived using $i^{p/q} = e^{i\theta}$ with phase angle $\theta = \frac{p}{q}90^\circ = \frac{p}{2q}\pi$ rad. The Taylor series expansion pair with complex step sizes can then be written as

$$f(x + e^{i\theta}h) = f(x) + \sum_{n=1}^{\infty} e^{ni\theta}\frac{h^n}{n!}f^{(n)}(x) \tag{11a}$$

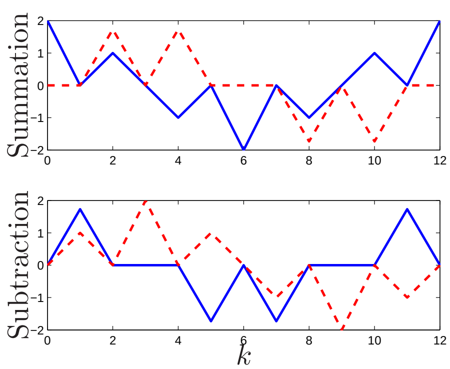
$$f(x + e^{i(\theta+\pi)}h) = f(x) + \sum_{n=1}^{\infty} e^{ni(\theta+\pi)}\frac{h^n}{n!}f^{(n)}(x) \tag{11b}$$



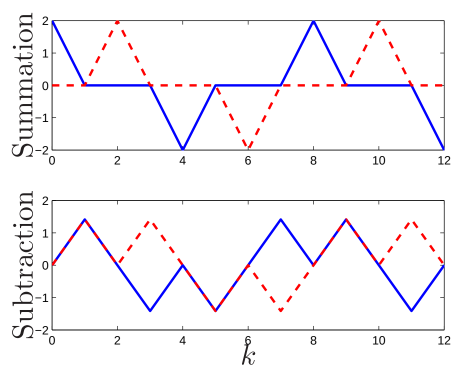
(a) $i^{0/6}$ or $\theta = 0°$



(b) $i^{1/6}$ or $\theta = 15°$



(c) $i^{2/6}$ or $\theta = 30°$



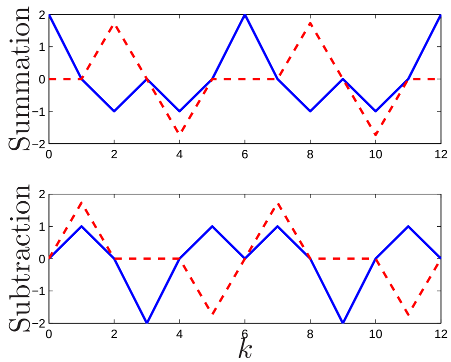
(d) $i^{3/6}$ or $\theta = 45°$

Fig. 3. Summation and Subtraction for θ from 0° to 45° (Solid Lines = Real, Dotted Lines = Imaginary)

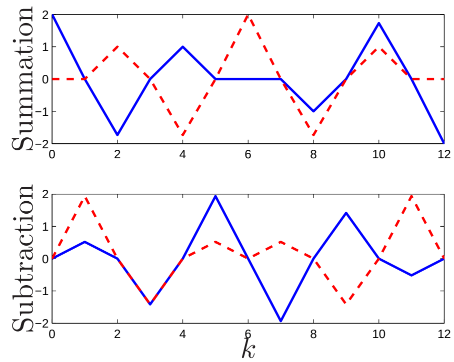
Note that $e^{i(\theta \pm \pi)} = -e^{i\theta}$. Instead of representing the complex step with powered i or in exponential form, we can also represent it by using trigonometry with Euler's relation, $e^{i\theta} = \cos\theta + i\sin\theta$, which bridges the field of algebra with geometry. From Eqs. (11) the summation and subtraction pairs are given by

$$f(x + e^{i\theta}h) + f(x + e^{i(\theta+\pi)}h) = 2f(x) + 2\sum_{n=1}^{\infty}\Big[\cos 2n\theta + i\sin 2n\theta\Big]\frac{h^{2n}}{(2n)!}f^{(2n)}(x) \quad (12a)$$

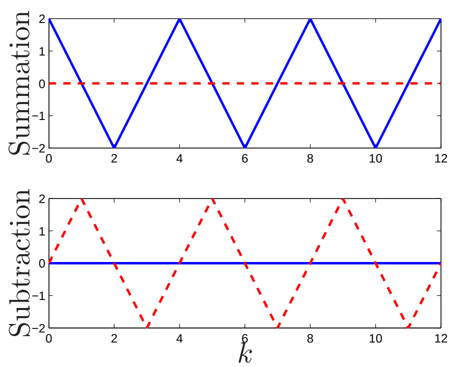
$$f(x + e^{i\theta}h) - f(x + e^{i(\theta+\pi)}h) = 2\sum_{n=1}^{\infty}\Big[\cos[(2n-1)\theta] + i\sin[(2n-1)\theta]\Big]\frac{h^{2n-1}}{(2n-1)!}f^{(2n-1)}(x) \quad (12b)$$



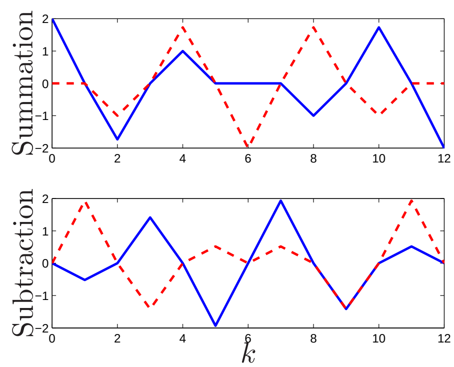
(a) $i^{4/6}$ or $\theta = 60°$



(b) $i^{5/6}$ or $\theta = 75°$



(c) $i^{6/6}$ or $\theta = 90°$



(d) $i^{7/6}$ or $\theta = 105°$

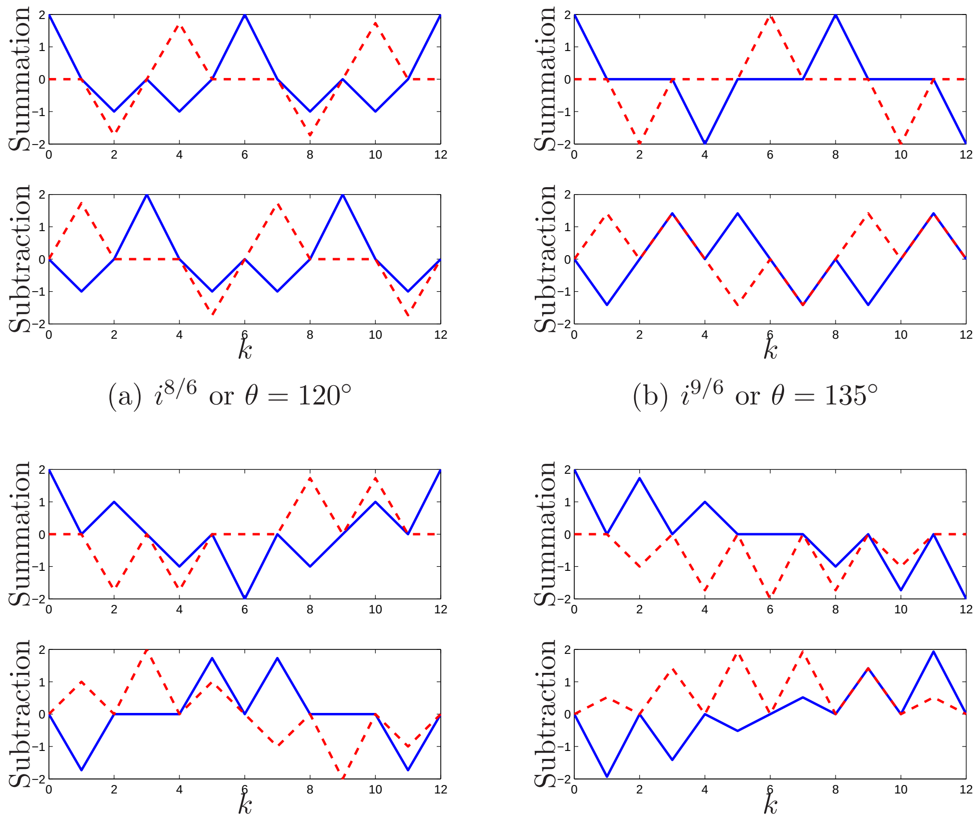
Fig. 4. Summation and Subtraction for θ from 60° to 105° (Solid Lines = Real, Dotted Lines = Imaginary)

Finally solving for $f''(x)$ and $f'(x)$ yields

$$\begin{aligned} f''(x) = &\frac{f(x+e^{i\theta}h) - 2f(x) + f(x+e^{i(\theta+\pi)}h)}{[\cos 2\theta + i\sin 2\theta]h^2} \\ &- 2\sum_{n=2}^{\infty}\left[\cos[(2n-2)\theta] + i\sin[(2n-2)\theta]\right]\frac{h^{2n-2}}{(2n)!}f^{(2n)}(x) \qquad \text{(13a)} \\ f'(x) = &\frac{f(x+e^{i\theta}h) - f(x+e^{i(\theta+\pi)}h)}{2[\cos\theta + i\sin\theta]h} \\ &- \sum_{n=2}^{\infty}\left[\cos[(2n-2)\theta] + i\sin[(2n-2)\theta]\right]\frac{h^{2n-2}}{(2n-1)!}f^{(2n-1)}(x) \qquad \text{(13b)} \end{aligned}$$

Instead of raising i to a number, Eqs. (13) clearly has the advantage of separating the real and imaginary components. If the separation is not necessary, they can be expressed in a simpler form

$$f''(x) = \frac{f(x+e^{i\theta}h) - 2f(x) + f(x-e^{i\theta}h)}{(e^{i\theta}h)^2} - 2\sum_{n=2}^{\infty}\frac{(e^{i\theta}h)^{2n-2}}{(2n)!}f^{(2n)}(x) \qquad \text{(14a)}$$



(a) $i^{8/6}$ or $\theta = 120^\circ$

(b) $i^{9/6}$ or $\theta = 135^\circ$

(c) $i^{10/6}$ or $\theta = 150^\circ$

(d) $i^{11/6}$ or $\theta = 165^\circ$

Fig. 5. Summation and Subtraction for θ from 120° to 165° (Solid Lines = Real, Dotted Lines = Imaginary)

$$f'(x) = \frac{f(x + e^{i\theta}h) - f(x - e^{i\theta}h)}{2e^{i\theta}h} - \sum_{n=2}^{\infty} \frac{(e^{i\theta}h)^{2n-2}}{(2n-1)!} f^{(2n-1)}(x) \tag{14b}$$

This generalization also works for pure real-valued finite differences by simply using $\theta = 0$. The extension of all the aforementioned approximations to multi-variables for the Jacobian and Hessian matrices is straightforward, which follow along similar lines as the previous section.

The first and second order complex-step derivative approximations (CSDAs) have so far been generalized for any angle of the complex step. However, a suitable angle θ is needed to unlock the full potential of the CSDA. Figures 3, 4 and 5 show the real and imaginary of the summation (for finding second derivative) and subtraction (for finding first derivative) pairs of the Taylor series expansion with complex step sizes that are 180° apart, i.e. from Eqs. (12). The x-axis represents the derivative of the function. Notice that $k \neq n$, in fact, $k = 2n$ for the summation (second derivative) cases and $k = 2n - 1$ for the subtraction (first derivative) cases. These figures are generated with $i^{k\frac{p}{q}} \pm i^{k\frac{2q+p}{q}}$. These figures give some intuitive perception into the CSDAs.

There are several *interesting* cases where certain elements (real or imaginary component) of the series annihilate, shown as “flat lines” in the plots. With reference to Eqs. (12) and (14), these correspond to when sine or cosine evaluates to zero. This phenomenon is desirable and to be taken advantage to increase the convergence rate of the Taylor series approximation towards the original nonlinear function. In fact, this is the main goal of evaluating functions with a complex step size. With a carefully chosen “angle,” we can eliminate terms that we do no wish to evaluate.

In most applications, the more terms in the Taylor series that do no need to be evaluated, the higher order the approximation, which leads to better accuracy. Thus, more “flat lines” lead to higher accuracy. Most cases have few or no flat lines where annihilation occurs. A flat line or annihilation occurs when the transcendental function sine or cosine evaluates to zero. This obviously has to occur at 90° or 270° for cosine and 0° or 180° for sine. From Euler’s relation, cosine is coupled to the real component and sine to the imaginary component. Therefore, the CSDA angle needs to be related to these four angles to produce the greatest numbers of flat lines. Thus, it is not surprising to see that 45° produces the greatest number of flat lines for the summation cases and 60° produces the most flat lines for the subtraction cases. In addition, it is desired to have more flat lines at the lower k number, since k links to the order of derivative, and canceling of these terms enhances the derivative approximation accuracy with higher-order truncation error.

3.1 Richardson Extrapolation

Richardson’s extrapolation is now summarized (10). Assuming D as the derivative approximation, let the first column of a to-be-determined matrix be

$$D_{\alpha,1} = D(h/q^{\alpha-1}) \quad \text{for } \alpha = 1, \ldots, n \tag{15}$$

and other elements as

$$D_{\alpha,\beta} = \frac{q^{k_{\beta-1}} D_{\alpha,\beta-1} - D_{\alpha-1,\beta-1}}{q^{k_{\beta-1}} - 1} \quad \text{for } \beta = 2, \ldots, n \tag{16}$$

Then we can find higher precision approximation by filling up a lower triangle matrix

$$
\begin{array}{lllll}
D_{1,1} & & & & \\
D_{2,1} & D_{2,2}=\frac{q^{k_1}D_{2,1}-D_{1,1}}{q^{k_1}-1} & & & \\
D_{3,1} & D_{3,2}=\frac{q^{k_1}D_{3,1}-D_{2,1}}{q^{k_1}-1} & D_{3,3}=\frac{q^{k_2}D_{3,2}-D_{2,2}}{q^{k_2}-1} & & \\
\vdots & \vdots & \vdots & \ddots & \\
D_{n,1} & D_{n,2}=\frac{q^{k_1}D_{n,1}-D_{n-1,1}}{q^{k_1}-1} & D_{n,3}=\frac{q^{k_2}D_{n,2}-D_{n-1,2}}{q^{k_2}-1} & \cdots & D_{n,n}=\frac{q^{k_{n-1}}D_{n,n-1}-D_{n-1,n-1}}{q^{k_{n-1}}-1}
\end{array}
$$

where the last element, $D_{n,n}$ is the most accurate approximation with error $O(h^{k_n})$.

3.2 Useful Cases

This section studies the two cases with the most flat lines (i.e. highest accuracy or convergence rate) at $\theta = 45°$ and $\theta = 60°$. There is a tradeoff between first-derivative accuracy and second-derivative accuracy. For example 45° may work best for second-order accuracy but offers no CSDA benefit for the first derivative. On the other hand, 60° offers better first-order derivative accuracy at the expense of accuracy in the second-order derivative.

3.2.1 $\theta = 45°$

From Eq. (14a) with $\theta = 45°$ and taking only the imaginary components gives

$$f''(x) = \frac{\Im\left\{f(x+i^{1/2}h) + f(x+i^{5/2}h)\right\}}{h^2} \quad , \quad E_{\text{trunc}}(h) = \frac{h^4}{360} f^{(6)}(x) \quad (17)$$

Note that when $n = 2$, the imaginary component $\sin 2n\theta = 0$, thus the first non-zero value occurs when $n = 3$ corresponds to $O(h^4)$, which is the main goal of the complex-step derivative approximation. This approximation is still subject to difference errors, but the truncation error associated with this approximation is $h^4 f^{(6)}(x)/360$ whereas the error associated with Eq. (8) is $h^2 f^{(4)}(x)/12$. It will also be shown through simulation that Eq. (17) is less sensitive to roundoff errors than Eq. (8).

Unfortunately, to obtain the first and second derivatives using Eqs. (6) and (17) requires function evaluations of $f(x+ih)$, $f(x+i^{1/2}h)$ and $f(x+i^{5/2}h)$. To obtain a first-derivative expression that involves $f(x+i^{1/2}h)$ and $f(x+i^{5/2}h)$, we substitute $\theta = 45^\circ$ into Eq. (14b) and again take the imaginary components:

$$f^{'}(x) = \frac{f(x + i^{1/2}h) - f(x + i^{5/2}h)}{\sqrt{2}\,(i+1)\,h} \tag{18}$$

Actually either the imaginary or real parts of Eq. (18) can be taken to determine $f^{'}(x)$; however, it's better to use the imaginary parts since no differences exist (they are actually *additions* of imaginary numbers) since $f(x + i^{1/2}h) - f(x + i^{5/2}h) = f(x + i^{1/2}h) - f(x - i^{1/2}h)$. This yields

$$f^{'}(x) = \frac{\Im\left\{f(x + i^{1/2}h) - f(x + i^{5/2}h)\right\}}{h\sqrt{2}} \quad , \quad E_{\mathrm{trunc}}(h) = -\frac{h^2}{6} f^{(3)}(x) \tag{19}$$

The approximation in Eq. (19) has errors equal to Eq. (6). Hence, both forms yield identical answers; however, Eq. (19) uses the same function evaluations as Eq. (17).

Now, a Richardson extrapolation is applied for further refinement. From Eq. (16) with $q = 2$ and $k_1 = 4$,

$$\begin{aligned} f^{''}(x) &= \frac{2^4 \frac{\Im\left\{f\left(x+i^{1/2}\frac{h}{2}\right)+f\left(x+i^{5/2}\frac{h}{2}\right)\right\}}{h^2/4} - \frac{\Im\left\{f(x+i^{1/2}h)+f(x+i^{5/2}h)\right\}}{h^2}}{2^4 - 1} \\ &= \Im\left\{64\left[f\left(x + i^{1/2}\frac{h}{2}\right) + f\left(x + i^{5/2}\frac{h}{2}\right)\right]\right. \\ &\qquad \left. - \left[f\left(x + i^{1/2}h\right) + f\left(x + i^{5/2}h\right)\right]\right\} / \left(15h^2\right) \quad , \\ &\qquad E_{\mathrm{trunc}}(h) = -\frac{h^8}{1,814,400} f^{(10)}(x) \end{aligned} \tag{20}$$

This approach can be continued *ad nauseam* using the next value of k. However, the next highest-order derivative-difference past $O(h^8)$ that has imaginary parts is $O(h^{12})$. This error is given by $\frac{h^{12}}{4.35891456\times10^{10}} f^{(14)}(x)$. Hence, it seems unlikely that the accuracy will improve much by using more terms. The same approach can be applied to the first derivative as well. Applying the Richardson extrapolation with $q = 2$, $k_1 = 2$, to Eq. (19) yields

$$\begin{aligned} f^{'}(x) &= \Im\left\{8\left[f\left(x + i^{1/2}\frac{h}{2}\right) - f\left(x + i^{5/2}\frac{h}{2}\right)\right]\right. \\ &\qquad \left. - \left[f\left(x + i^{1/2}h\right) - f\left(x + i^{5/2}h\right)\right]\right\} / (3\sqrt{2}\,h) \quad , \\ &\qquad E_{\mathrm{trunc}}(h) = \frac{h^4}{120} f^{(5)}(x) \end{aligned} \tag{21}$$

Performing the Richardson extrapolation again would cancel fifth-order derivative errors, which leads to the following approximation:

$$f^{'}(x) = \Im\Bigg\{4096\left[f\left(x + i^{1/2}\frac{h}{4}\right) - f\left(x + i^{5/2}\frac{h}{4}\right)\right] - 640\left[f\left(x + i^{1/2}\frac{h}{2}\right) - f\left(x + i^{5/2}\frac{h}{2}\right)\right] + 16\Big[f(x + i^{1/2}h) - f(x + i^{5/2}h)\Big]\Bigg\}/(720\sqrt{2}\,h) \quad ,$$

$$E_{\text{trunc}}(h) = \frac{h^6}{5040} f^{(7)}(x) \qquad (22)$$

As with Eq. (19), the approximations in Eq. (21) and Eq. (22) are not subject to roundoff error, so an arbitrarily small value of h can be chosen up to the roundoff error.

3.2.2 $\underline{\theta = 60^\circ}$

From Eq. (14) with $\theta = 60^\circ$ and taking only the imaginary components gives

$$f^{'}(x) = \frac{\Im\Big\{f(x + i^{2/3}h) - f(x + i^{8/3}h)\Big\}}{\sqrt{3}h} \quad , \quad E_{\text{trunc}}(h) = \frac{h^4}{120} f^{(5)}(x) \quad (23a)$$

$$f^{''}(x) = \frac{\Im\Big\{f(x + i^{2/3}h) + f(x + i^{8/3}h)\Big\}}{\sqrt{3}h} \quad , \quad E_{\text{trunc}}(h) = \frac{h^2}{24} f^{(4)}(x) \quad (23b)$$

Performing a Richardson extrapolation once on each of these equations yields

$$f^{'}(x) = \Im\Bigg\{32\left[f\left(x + i^{2/3}\frac{h}{2}\right) - f\left(x + i^{8/3}\frac{h}{2}\right)\right] - \Big[f(x + i^{2/3}h) - f(x + i^{8/3}h)\Big]\Bigg\}/\left(15\sqrt{3}\,h\right) \quad ,$$

$$E_{\text{trunc}}(h) = -\frac{h^6}{5040} f^{(7)}(x) \qquad (24a)$$

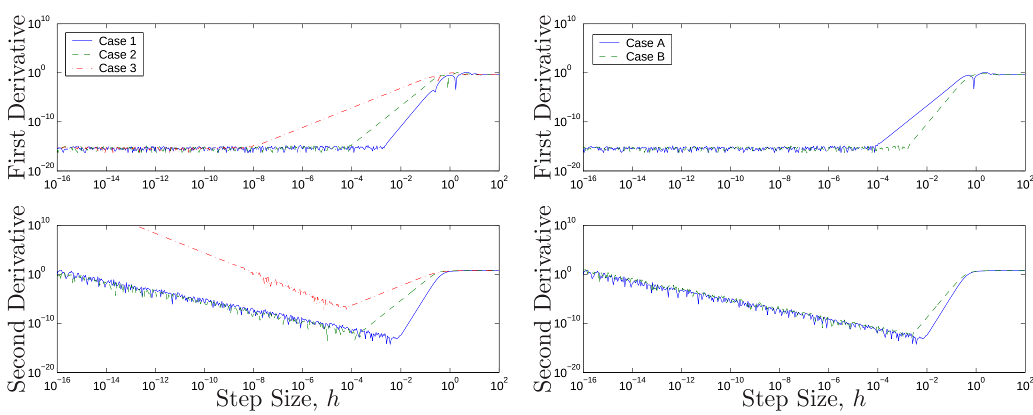
$$f^{''}(x) = 2\Im\Bigg\{\Big[f(x + i^{2/3}h) + f(x + i^{8/3}h)\Big] - 16\Big[f(x + i^{2/3}\frac{h}{2}) + f(x + i^{8/3}\frac{h}{2})\Big]\Bigg\}/\left(3\sqrt{3}\,h^2\right) \quad ,$$

$$E_{\text{trunc}}(h) = -\frac{h^6}{40320} f^{(8)}(x) \quad (24b)$$

These solutions have the same order of accuracy as Eq. (22), but involves less function evaluations. Using $i^{2/3}$ instead of $i^{1/2}$ for the second-derivative approximation yields worse results than Eq. (20) since the approximation has errors on the order of $h^6\, f^{(8)}(x)$ instead of $h^8\, f^{(10)}(x)$. Hence, a tradeoff between the first-derivative and second-derivative accuracy will always exist if using the same function evaluations for both is desired. Higher-order versions of Eq. (24) are given by

$$\begin{aligned} f'(x) = \Im\Big\{ & 3072\left[f(x+i^{2/3}\tfrac{h}{4}) - f(x+i^{8/3}\tfrac{h}{4})\right] \\ & - 256\left[f(x+i^{2/3}\tfrac{h}{2}) - f(x+i^{8/3}\tfrac{h}{2})\right] \\ & + 5\left[f(x+i^{2/3}h) - f(x+i^{8/3}h)\right]\Big\}/(645\sqrt{3}\,h) \quad , \\ & E_{\text{trunc}}(h) = \frac{h^{10}}{39916800} f^{(11)}(x) \end{aligned} \tag{25a}$$

$$\begin{aligned} f''(x) = 2\,\Im\Big\{ & 15\left[f(x+i^{2/3}h) + f(x+i^{8/3}h)\right] \\ & + 16\left[f(x+i^{2/3}\tfrac{h}{2}) + f(x+i^{8/3}\tfrac{h}{2})\right] \\ & - 4096\left[f(x+i^{2/3}\tfrac{h}{4}) + f(x+i^{8/3}\tfrac{h}{4})\right]\Big\}/(237\sqrt{3}\,h^2) \quad , \\ & E_{\text{trunc}}(h) = \frac{h^{8}}{3628800} f^{(10)}(x) \end{aligned} \tag{25b}$$



(a) First and Second Derivative Errors (b) First and Second Derivative Errors

Fig. 6. Comparisons of the Various Complex-Derivative Approaches

3.3 Simple Examples

Consider the following highly nonlinear function:

$$f(x) = \frac{e^x}{\sqrt{\sin^3(x) + \cos^3(x)}} \tag{26}$$

evaluated at $x = -0.5$. Error results for the first and second derivative approximations are shown in Figure 6(a). Case 1 shows results using Eqs. (22) and (20) for the first and second order derivatives, respectively. Case 2 shows results using Eqs. (21) and (17) for the first and second order derivatives, respectively. Case 3 shows results using Eqs. (6) and (8) for the first and second order derivatives, respectively. We again note that using Eq. (19) produces the same results as using Eq. (6). Using Eqs. (22) and (20) for the approximations allows one to use only one step size for all function evaluations. For this example, setting $h = 0.024750$ gives a first derivative error on the order of 10^{-16} and a second derivative error on the order of 10^{-15}. Figure 6(b) shows results using Eqs. (21) and (20), Case A, versus results using Eqs. (24a) and (24b), Case B, for the first and second derivatives, respectively. For this example using Eqs. (24a) and (24b) provides the best overall accuracy with the least amount of function evaluations for both derivatives.

Another example is given by using Halley's method for root finding. The iteration function is given by

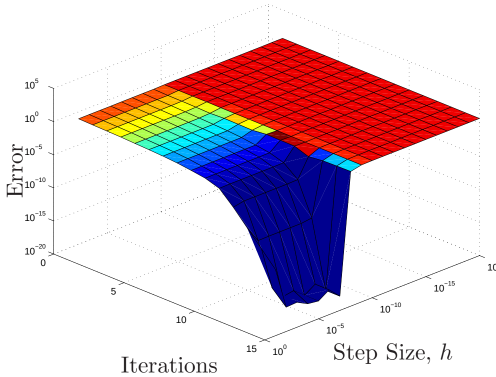
$$x_{n+1} = x_n - \frac{2\, f(x_n)\, f'(x_n)}{2\,[f'(x_n)]^2 - f(x_n)\, f''(x_n)} \tag{27}$$

The following function is tested:

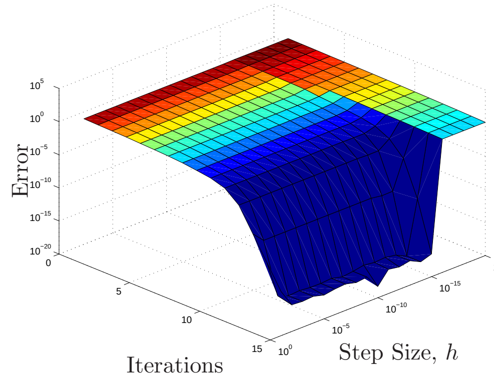
$$f(x) = \frac{(1 - e^x)\, e^{3x}}{\sqrt{\sin^4(x) + \cos^4(x)}} \tag{28}$$

which has a root at $x = 0$. Equation (27) is used to determine the root with a starting value of $x_0 = 5$. Equations (21) and (20) are used for the complex-step approximations. For comparison purposes the derivatives are also determined using a symmetric 4-point approximation for the first derivative and a 5-point approximation for the second derivative:

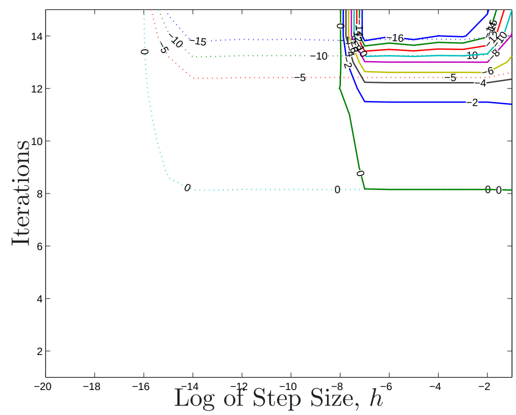
$$f'(x) = \frac{f(x - 2\,h) - 8\,f(x - h) + 8\,f(x + h) - f(x + 2\,h)}{12h}\,, \quad E_{\text{trunc}}(h) = \frac{h^4}{30} f^{(5)}(x) \tag{29a}$$



(a) Finite-Difference



(b) Complex-Step



(c) Error Contour Plot (in Log Scale), Solid Lines = Finite-Difference, Dotted Lines = Complex-Step

Fig. 7. Error Plots for Root Finding Problem by using the Halley's Method

$$f''(x) = \frac{-f(x-2\,h) + 16\,f(x-h) - 30\,f(x) + 16\,f(x+h) - f(x+2\,h)}{12\,h^2}\quad ,$$

$$E_{\text{trunc}}(h) = \frac{h^6}{90} f^{(6)}(x) \quad (29b)$$

MATLAB® is used to perform the numerical computations. Various values of h are tested in decreasing magnitude (by one order each time), starting at $h = 1$ and going down to $h = 1 \times 10^{-20}$ and results shown in Fig. 7. Referring to Fig. 7(c), values of $h = 0.1$ to $h = 1 \times 10^{-7}$ both methods converge, but the complex-step approach convergence is faster or (at worst) equal to the standard finite-difference approach. For values less than 1×10^{-7}, e.g. when $h = 1 \times 10^{-8}$, the finite-difference approach becomes severally degraded. For h values from 1×10^{-8} down to 1×10^{-15}, the complex-step approach always converges in less than 15 iterations. When $h = 1 \times 10^{-16}$ the finite-difference approach produces a zero-valued correction for all iterations, while the complex-step approach converges in about 40 iterations (not shown in figure).

3.4 Multi-Variable Numerical Example

A multi-variable example is now shown to assess the performance of the complex-step approximations. The infinity norm[‖] is used to access the accuracy of the numerical finite-difference and complex-step approximation solutions. The relationship between the magnitude of the various solutions and step size is also discussed. The function to be tested is given by two equations with four variables:

$$\mathbf{f} \triangleq \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} x_1^2 x_2 x_3 x_4^2 + x_2^2 x_3^3 x_4 \\ x_1^2 x_2 x_3^2 x_4 + x_1 x_2^3 x_4^2 \end{bmatrix} \tag{30}$$

These functions will be evaluated nominally at $\mathbf{x} = [5,\ \ 3,\ \ 6,\ \ 4]^T$.

Numerical Solutions

The step size for the Jacobian and Hessian calculations (both for complex-step approximation and numerical finite-difference) is 1×10^{-4}. The absolute Jacobian error between the true and complex-step solutions, and true and numerical finite-difference solutions, respectively, are

$$|\Delta^c F_x| = \begin{bmatrix} 0.0000\ 0.0000\ 0.3600\ 0.0000 \\ 0.0000\ 0.8000\ 0.0000\ 0.0000 \end{bmatrix} \times 10^{-8} \tag{31a}$$

$$|\Delta^n F_x| = \begin{bmatrix} 0.2414\ 0.3348\ 0.0485\ 0.1074 \\ 0.1051\ 0.4460\ 0.0327\ 0.0298 \end{bmatrix} \times 10^{-7} \tag{31b}$$

The infinity norms of Eq. (31) are 8.0008×10^{-9} and 7.3217×10^{-8}, respectively, which means that the complex-step solution is more accurate than the finite-difference one. The absolute Hessian error between the true solutions and the complex-step and numerical finite-difference solutions, respectively, are

$$|\Delta^c F_{xx}^1| = \begin{bmatrix} 0.0000\ 0.0011\ 0.0040\ 0.0016 \\ 0.0011\ 0.0010\ 0.0011\ 0.0009 \\ 0.0040\ 0.0011\ 0.0019\ 0.0021 \\ 0.0016\ 0.0009\ 0.0021\ 0.0004 \end{bmatrix} \tag{32a}$$

[‖] The largest row sum of a matrix A, $|A|_\infty = \max\{\sum |A^T|\}$.

$$|\Delta^n F^1_{xx}| = \begin{bmatrix} 0.0002 & 0.0010 & 0.0041 & 0.0017 \\ 0.0010 & 0.0009 & 0.0011 & 0.0011 \\ 0.0041 & 0.0011 & 0.0021 & 0.0019 \\ 0.0017 & 0.0011 & 0.0019 & 0.0003 \end{bmatrix} \tag{32b}$$

and

$$|\Delta^c F^2_{xx}| = \begin{bmatrix} 0.0018 & 0.0007 & 0.0030 & 0.0064 \\ 0.0007 & 0.0016 & 0.0010 & 0.0018 \\ 0.0030 & 0.0010 & 0.0018 & 0.0004 \\ 0.0064 & 0.0018 & 0.0004 & 0.0029 \end{bmatrix} \tag{33a}$$

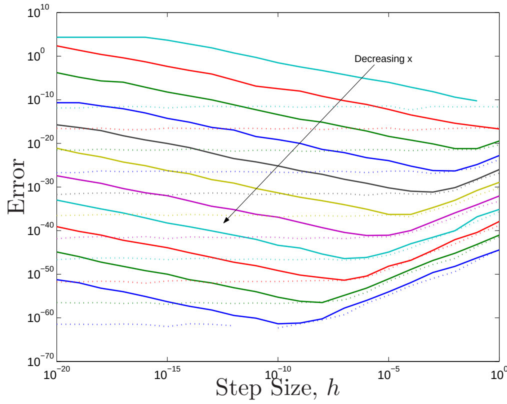
$$|\Delta^n F^2_{xx}| = \begin{bmatrix} 0.0018 & 0.0007 & 0.0031 & 0.0065 \\ 0.0007 & 0.0015 & 0.0008 & 0.0021 \\ 0.0031 & 0.0008 & 0.0018 & 0.0006 \\ 0.0065 & 0.0021 & 0.0006 & 0.0025 \end{bmatrix} \tag{33b}$$

The infinity norms of Eq. (32) are 9.0738×10^{-3} and 9.1858×10^{-3}, respectively, and the infinity norms of Eq. (33) are 1.1865×10^{-3} and 1.2103×10^{-3}, respectively. As with the Jacobian, the complex-step Hessian approximation solutions are more accurate than the finite-difference solutions.

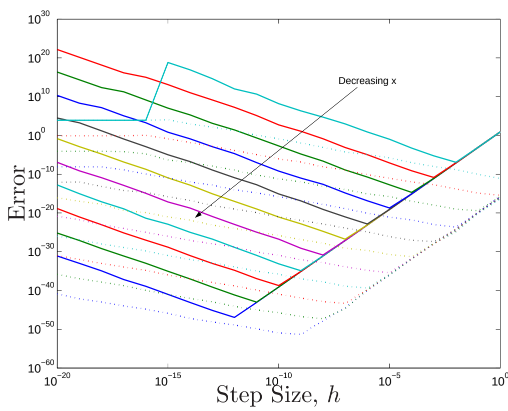
Performance Evaluation

The performance of the complex-step approach in comparison to the numerical finite-difference approach is examined further here using the same function. Tables 1 and 2 shows the infinity norm of the error between the true and the approximated solutions. The difference between the finite-difference solution and the complex-step solution is also included in the last three rows, where positive values indicate the complex-step solution is more accurate. In most cases, the complex-step approach performs either comparable or better than the finite-difference approach. The complex-step approach provides accurate solutions for h values from 0.1 down to 1×10^{-9}. However, the range of accurate solutions for the finite-difference approach is significantly smaller than that of complex-step approach. Clearly, the complex-step approach is much more robust than the numerical finite-difference approach.

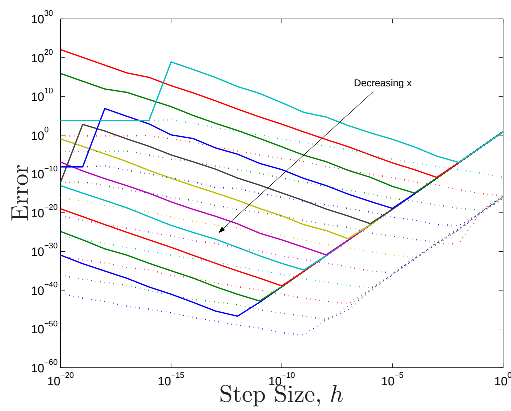
Figure 8 shows plots of the infinity norm of the Jacobian and Hessian errors obtained using a numerical finite-difference and the complex-step approximation. The function is evaluated at different magnitudes by multiplying the



(a) Jacobian

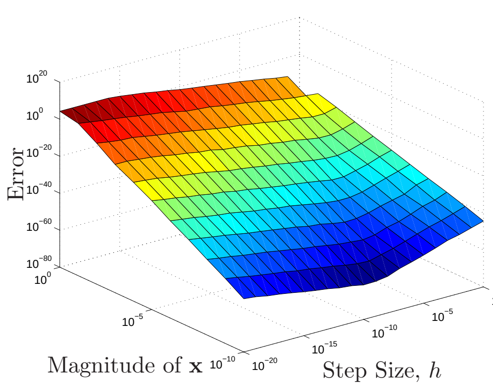


(b) Hessian 1

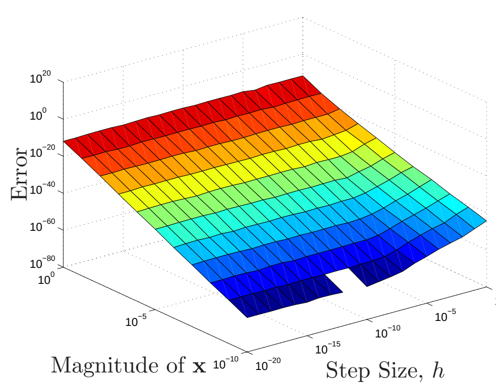


(c) Hessian 2

Fig. 8. Infinity Norm of the Error Matrix for Different Magnitudes (Solid Lines = Finite-Difference, Dotted Lines = Complex-Step)



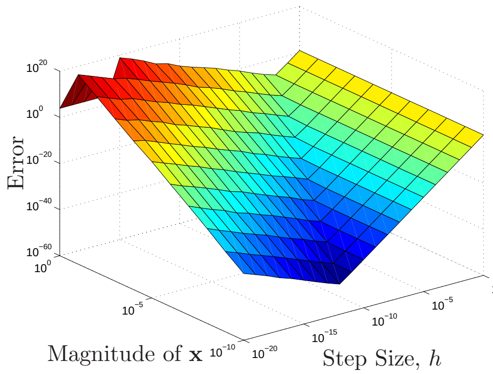
(a) Jacobian - Finite-Difference



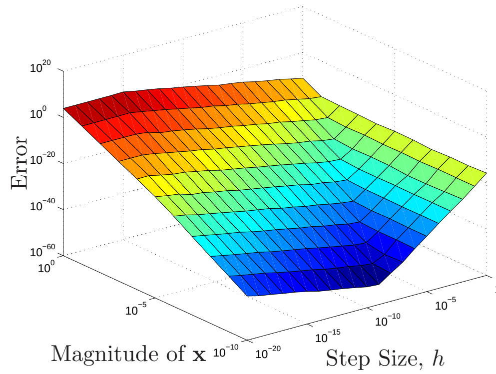
(b) Jacobian - Complex-Step

Fig. 9. Infinity Norm of the Jacobian Error Matrix for Different Magnitudes and Step Sizes

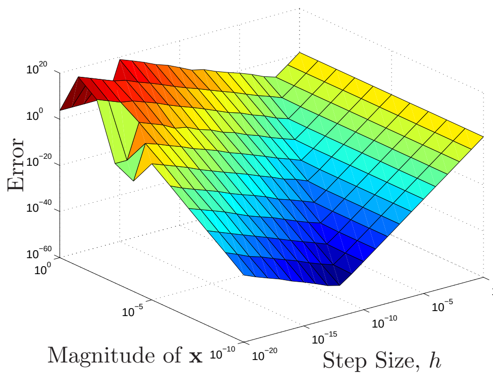
nominal values with a scale factor from 1 down to 1×10^{-10}. The direction of the arrow shows the solutions for decreasing $\mathbf{x}$. The solutions for the complex-



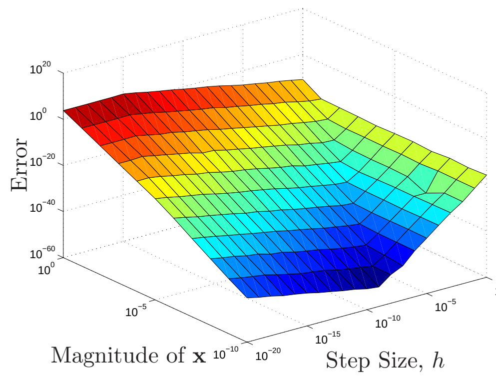
(a) Hessian 1 - Finite-Difference



(b) Hessian 1 - Complex-Step



(c) Hessian 2 - Finite-Difference



(d) Hessian 2 - Complex-Step

Fig. 10. Infinity Norm of the Hessian Error Matrix for Different Magnitudes and Step Sizes

step and finite-difference approximation using the same $\mathbf{x}$ value are plotted with the same color within a plot.

For the case of the finite-difference Jacobian, shown in Figure 8(a), at some certain point of decreasing step size, as mentioned before, the roundoff error becomes dominant which decreases the accuracy. The complex-step solution does not exhibit this phenomenon and the accuracy continues to increase with decreasing step size up to machine precision. As a higher-order complex-step approximation is used, Eq. (24a) instead of Eq. (6), the truncation errors for the complex-step Jacobian at larger step sizes are also greatly reduced to the extent that the truncation errors are almost unnoticeable, even at large $\mathbf{x}$ values. The complex-step approximation for the Hessian case also benefits from the higher-order approximation, as shown in Figures 8(b) and 8(c). The complex-step Hessian approximation used to generate these results is given by Eq. (24b). One observation is that there is always only one (global) optimum of specific step size with respect to the error.

Figures 9 and 10 represent the same information in more intuitive looking

Table 1
Infinity Norm of the Difference from Truth for Larger Step Sizes, h

h	1×10^{0}	1×10^{-1}	1×10^{-2}
$\|\Delta^n F_x\|$	8.0004×10^{-9}	8.0554×10^{-9}	8.2664×10^{-9}
$\|\Delta^c F_x\|$	8.0026×10^{-9}	8.0004×10^{-9}	8.0013×10^{-9}
$\|\Delta^n F^1_{xx}\|$	8.0000	9.1000×10^{-3}	9.1000×10^{-3}
$\|\Delta^c F^1_{xx}\|$	9.1000×10^{-3}	9.1000×10^{-3}	9.1000×10^{-3}
$\|\Delta^n F^2_{xx}\|$	7.9990	1.1100×10^{-2}	1.1900×10^{-2}
$\|\Delta^c F^2_{xx}\|$	1.1900×10^{-2}	1.1900×10^{-2}	1.1900×10^{-2}
$\|\Delta^n F_x\| - \|\Delta^c F_x\|$	-2.2737×10^{-12}	5.5024×10^{-11}	2.6512×10^{-10}
$\|\Delta^n F^1_{xx}\| - \|\Delta^c F^1_{xx}\|$	7.9909	-5.0477×10^{-11}	3.5698×10^{-10}
$\|\Delta^n F^2_{xx}\| - \|\Delta^c F^2_{xx}\|$	7.9871	-8.0000×10^{-4}	-6.5184×10^{-8}

h	1×10^{-3}	1×10^{-4}
$\|\Delta^n F_x\|$	9.6984×10^{-9}	7.3218×10^{-8}
$\|\Delta^c F_x\|$	8.0026×10^{-9}	8.0008×10^{-9}
$\|\Delta^n F^1_{xx}\|$	9.1000×10^{-3}	9.2000×10^{-3}
$\|\Delta^c F^1_{xx}\|$	9.1000×10^{-3}	9.1000×10^{-3}
$\|\Delta^n F^2_{xx}\|$	1.1900×10^{-2}	1.2100×10^{-2}
$\|\Delta^c F^2_{xx}\|$	1.1900×10^{-2}	1.1900×10^{-2}
$\|\Delta^n F_x\| - \|\Delta^c F_x\|$	1.6958×10^{-9}	6.5217×10^{-8}
$\|\Delta^n F^1_{xx}\| - \|\Delta^c F^1_{xx}\|$	1.5272×10^{-6}	1.1200×10^{-4}
$\|\Delta^n F^2_{xx}\| - \|\Delta^c F^2_{xx}\|$	-5.3940×10^{-8}	2.3823×10^{-4}

three-dimensional plots. The “depth” of the error in log scale is represented as a color scale with dark red being the highest and dark blue being the lowest. A groove is clearly seen in most of the plots (except the complex-step Jacobian), which corresponds to the optimum step size. The “empty surface” in Figure 9 corresponds to when the difference between the complex-step solution and the truth is below machine precision. This is shown as “missing line” in Figure 8(a). Clearly, the complex-step approximation solutions are comparable or more accurate than the finite-difference solutions.

Table 2
Infinity Norm of the Difference from Truth for Smaller Step Sizes, h

h	1×10^{-5}	1×10^{-6}	1×10^{-7}
$\lvert\Delta^n F_x\rvert$	1.0133×10^{-6}	6.4648×10^{-6}	5.8634×10^{-5}
$\lvert\Delta^c F_x\rvert$	8.0026×10^{-9}	8.0004×10^{-9}	8.0026×10^{-9}
$\lvert\Delta^n F^1_{xx}\rvert$	1.0160×10^{-1}	7.6989	9.5627×10^{2}
$\lvert\Delta^c F^1_{xx}\rvert$	9.1000×10^{-3}	9.1000×10^{-3}	9.1000×10^{-3}
$\lvert\Delta^n F^2_{xx}\rvert$	7.3500×10^{-2}	4.2094	3.1084×10^{2}
$\lvert\Delta^c F^2_{xx}\rvert$	1.1900×10^{-2}	1.1900×10^{-2}	1.1700×10^{-2}
$\lvert\Delta^n F_x\rvert - \lvert\Delta^c F_x\rvert$	1.0053×10^{-6}	6.4568×10^{-6}	5.8626×10^{-5}
$\lvert\Delta^n F^1_{xx}\rvert - \lvert\Delta^c F^1_{xx}\rvert$	9.2500×10^{-2}	7.6898	9.5626×10^{2}
$\lvert\Delta^n F^2_{xx}\rvert - \lvert\Delta^c F^2_{xx}\rvert$	6.1600×10^{-2}	4.1976	3.1082×10^{2}

h	1×10^{-8}	1×10^{-9}	1×10^{-10}
$\lvert\Delta^n F_x\rvert$	5.0732×10^{-4}	3.5000×10^{-3}	3.1200×-2
$\lvert\Delta^c F_x\rvert$	8.0013×10^{-9}	7.9995×10^{-9}	7.9999×-9
$\lvert\Delta^n F^1_{xx}\rvert$	5.2882×10^{4}	2.2007×10^{6}	1.5916×8
$\lvert\Delta^c F^1_{xx}\rvert$	9.1000×10^{-3}	1.4800×10^{-2}	1.2730×-1
$\lvert\Delta^n F^2_{xx}\rvert$	4.9658×10^{4}	7.6182×10^{5}	2.4253×8
$\lvert\Delta^c F^2_{xx}\rvert$	1.3500×10^{-2}	8.8000×10^{-3}	9.9700×-2
$\lvert\Delta^n F_x\rvert - \lvert\Delta^c F_x\rvert$	5.0731×10^{-4}	3.5000×10^{-3}	3.1200×-2
$\lvert\Delta^n F^1_{xx}\rvert - \lvert\Delta^c F^1_{xx}\rvert$	5.2882×10^{4}	2.2007×10^{6}	1.5916×8
$\lvert\Delta^n F^2_{xx}\rvert - \lvert\Delta^c F^2_{xx}\rvert$	4.9658×10^{4}	7.6182×10^{5}	2.4253×8

4 Conclusion

This paper demonstrated the ability of numerically obtaining derivative information via complex-step approximations. For the Jacobian case, unlike standard derivative approaches, more control in the accuracy of the standard complex-step approximation is provided since it does not succumb to roundoff errors for small step sizes. For the Hessian case, however, an arbitrarily small step size cannot be chosen due to roundoff errors. Also, using the standard complex-step approach to approximate second derivatives was found to be less accurate than the numerical finite-difference obtained one. The generalized complex-step derivative approximations were derived for first and second derivatives and their truncation errors were decreased by evaluating the function with complex step at various angles. These new approximations offer a wider range of accuracy for larger step sizes in both the Jacobian and Hessian approximations by using the same function evaluations and step sizes for both. These new expressions allow a designer to choose one step size in order to provide very accurate approximations, which minimizes the required number of function evaluations. Another main advantage is that a "black box" can be employed to obtain the Jacobian or Hessian matrices for any vector function. Further increase in accuracy can be achieved with Richardson extrapolations.

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