Available online at www.sciencedirect.com
ScienceDirect
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
Journal of Computational and Applied Mathematics 219 (2008) 276–293
www.elsevier.com/locate/cam

Extensions of the first and second complex-step derivative approximations

K.-L. Lai*, J.L. Crassidis

State University of New York at Buffalo, Department of Mechanical & Aerospace Engineering, Buffalo, NY 14260, USA

Received 3 November 2006; received in revised form 2 July 2007

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.
© 2007 Elsevier B.V. All rights reserved.

Keywords: Complex step; Jacobian; Hessian; Finite-difference

1. Introduction

Using complex numbers for computational purposes are 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 physical world phenomena actually have their roots in the complex domain [4]. The complex-step derivative approximation (CSDA) 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 in [5], as well as in [4]. Various recent papers reintroduce the complex-step approach to the research community [1,2,7,8,10]. 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.

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 Fig. 1. As the

* Corresponding author.
E-mail addresses: klai_ny@hotmail.com (K.-L. Lai), johnc@eng.buffalo.edu (J.L. Crassidis).

0377-0427/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2007.07.026

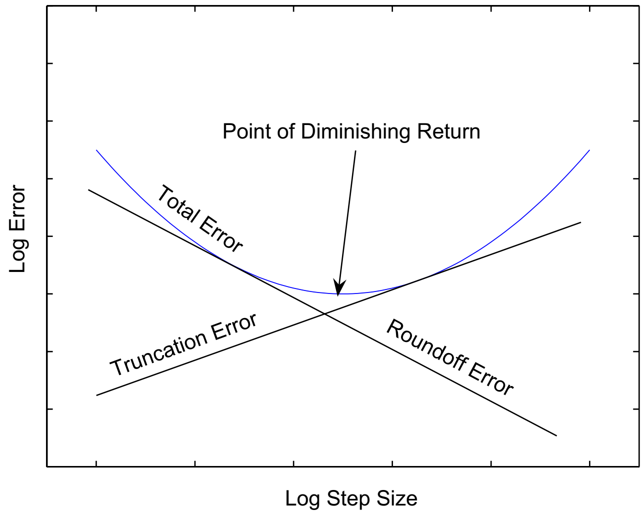

Fig. 1. Finite-difference error versus step size.

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 CSDA 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° 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 CSDAS 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. [3].

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 [6]

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

Download English Version:

https://daneshyari.com/en/article/4641626

Download Persian Version:

https://daneshyari.com/article/4641626

Daneshyari.com