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008

USING COMPLEX VARIABLES TO ESTIMATE DERIVATIVES OF REAL FUNCTIONS*

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Abstract. A method to approximate derivatives of real functions using complex variables which avoids the subtractive cancellation errors inherent in the classical derivative approximations is described. Numerical examples illustrating the power of the approximation are presented.

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1. Overview. A standard method to approximate the derivative of a real valued function $F(x)$ at the point x_0 is to use the central difference formula

$$F'(x_0) \sim (F(x_0 + h) - F(x_0 - h))/2h. \tag{1}$$

The truncation error is $O(h^2)$. With most derivative approximations one is faced with the dilemma of using a small h to minimize the truncation error vs. avoiding a small h because of the subtractive cancellation error. Work has been done to improve the answer obtained using equation 1 by analyzing its monotonic behavior as h goes to zero. It turns out that when the roundoff error becomes significant, the estimate from equation (1) oscillates around the correct answer, and this behavior can be used to select an optimal h; see [1, 5]. This approach provides only marginal improvement, whereas allowing h to take on a complex value results in an entirely different approximation with unexpected properties.

Using complex variables to develop differentiation formulas originated with Lyness and Moler [2] and Lyness [3]. Since most current numerical analysis textbooks do not normally cover complex variables, we thought a sample of this work with representative computations would be of interest.

In equation (1) we replace h with ih ($i = \mathrm{sqrt}(-1)$). If F is analytic then, letting $Im(F)$ represent the imaginary part of the function F, the approximation in (1) can be rewritten

$$F'(x_0) \sim Im(F(x_0 + ih)/h. \tag{2}$$

Formula (2) involves the evaluation of the function at a complex argument, but it eliminates the subtractive cancellation error. One way to understand the approximation in (2) is to recast the problem in terms of functions of a complex variable. Let $F(z)$ be an analytic function of the complex variable z; also assume that F is real on the real axis. F may be expanded in a Taylor series about the real point x_0 as follows:

$$F(x_0 + ih) = F(x_0) + ihF'(x_0) - h^2F''(x_0)/2! - ih^3F^{(3)}(x_0)/3! + \cdots. \tag{3}$$

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TABLE 1
$F(x) = x^{9/2}$.

h	Equation 1	Equation 2
0.1D-01	0.18602018344501897D+02	0.18599607128036329D+02
0.1D-02	0.18600824790342307D+02	0.18600800678177631D+02
0.1D-03	0.18600812854818738D+02	0.18600812613698936D+02
0.1D-04	0.18600812735480865D+02	0.18600812733054151D+02
0.1D-05	0.18600812734248517D+02	0.18600812734247702D+02
0.1D-06	0.18600812735081185D+02	0.18600812734259637D+02
0.1D-07	0.18600812723423843D+02	0.18600812734259757D+02
0.1D-08	0.18600812723423843D+02	0.18600812734259759D+02
0.1D-09	0.18600814222224926D+02	0.18600812734259759D+02
0.1D-10	0.18600815332447951D+02	0.18600812734259759D+02
0.1D-11	0.18600898599174798D+02	0.18600812734259759D+02
0.1D-12	0.18601231666082185D+02	0.18600812734259759D+02
0.1D-13	0.18585133432225120D+02	0.18600812734259759D+02
0.1D-14	0.18596235662471372D+02	0.18600812734259759D+02
0.1D-15	0.20539125955565396D+02	0.18600812734259759D+02
0.1D-16	0.00000000000000000D+00	0.18600812734259759D+02
0.1D-17	0.00000000000000000D+00	0.18600812734259759D+02
0.1D-18	0.00000000000000000D+00	0.18600812734259759D+02
0.1D-19	0.00000000000000000D+00	0.18600812734259759D+02

Taking the imaginary parts of both sides of equation (3) and dividing both sides by h yields

$$Im[F(x_0 + ih)]/h = F'(x_0) - h^2 F^{(3)}(x_0)/3! + \cdots . \tag{4}$$

The left-hand side of (4) is an approximation to $F'(x_0)$ with approximation error $O(h^2)$. $Im[F(x_0 + ih)]/h$ is real although it involves a complex argument, and, importantly, it is not subject to subtractive cancellation.

2. Numerical examples. We present two examples which illustrate the power of this approach. The output comes from a FORTRAN program run on a Digital Equipment Corporation VAX 6000-620, using standard FORTRAN complex variable features. The first example is in double precision, and the second is in single precision. Both examples show that equation (2) yields an accurate derivative approximation for any realistic value of h whereas equation 1 quickly succumbs to subtractive cancellation as h decreases.

Example 1. Let $F(x) = x^{9/2}$ and $x_0 = 1.5$; then to seventeen places $F'(1.5) = 18.600812734259759$. Table 1 shows the approximation obtained from equations (1) and (2) for h ranging from 0.01 to 10^{-19}. Equation (1) approximation improves for a while then deteriorates quickly, finally becoming 0.0 because of subtractive cancellation. Equation (2) approximation experiences no such problems.

Example 2. Lyness and Sande [4] used the function $F(x) = e^x/(\sin(x)^3 + \cos(x)^3)$ to illustrate a similar type of calculation. Again let $x_0 = 1.5$; the value of the derivative is 3.62203. The output is shown in Table 2; here single precision is used. The table has the same behavior as shown in Table 1.

3. Summary. In this note we have shown that unexpected results are obtained by using a complex variable approach to estimating derivatives of real valued functions.

TABLE 2
$F(x) = e^x/(\sin(x)^3 + \cos(x)^3)$.

h	Equation 1	Equation 2
0.100000E-01	0.362298E+01	0.362109E+01
0.100000E-02	0.362229E+01	0.362202E+01
0.100000E-03	0.362158E+01	0.362203E+01
0.100000E-04	0.360012E+01	0.362203E+01
0.100000E-05	0.357628E+01	0.362203E+01
0.100000E-06	0.476837E+01	0.362203E+01
0.100000E-07	0.000000E+00	0.362203E+01
0.100000E-08	0.000000E+00	0.362203E+01
0.100000E-09	0.000000E+00	0.362203E+01
0.100000E-10	0.000000E+00	0.362203E+01

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