

NUMERICAL DIFFERENTIATION BY EXTRAPOLATION

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ABSTRACT

Presented in this paper is a simple extrapolation technique to obtain numerical derivative of an analytic function, complex or real. The function may be in tabular form or in functional form. A few numerical examples are added for the purpose of illustration.

1. DISCUSSION

The method of finding the temperature at which the volume of a gas becomes zero (a situation which cannot be reached in practice) by extrapolating the curve of relative volume versus temperature ($^{\circ}\text{C}$) to zero volume, prompted the idea of obtaining the numerical derivative of a function (that cannot be obtained numerically using the theoretical definition.

$$\text{Lt } \Delta x \rightarrow 0_{\pm} \frac{\Delta y}{\Delta x} = \frac{dy}{dx}$$

for any analytic function because of the precision limitation of any arbitrary computer used) by extrapolation.

Let us first consider a real function of a single real variable. The generalization to many variable functions and to complex functions then follows readily from it. Let Δx_1 , Δx_2 , Δx_3 be three small positive real numbers satisfying the inequality

$$\Delta x_1 > \Delta x_2 > \Delta x_3$$

and let x_0 be the point at which we want to obtain the derivative of $f(x)$. The problem is then posed as follows:

$$\Delta x_1 \rightarrow \frac{f(x_0 + [\Delta x_1/2]) - f(x_0 - [\Delta x_1/2])}{\Delta x_1}$$

$$\begin{aligned} \Delta x_2 &\longrightarrow \frac{f(x_0 + [\Delta x_2/2]) - f(x_0 - [\Delta x_2/2])}{\Delta x_2} \\ \Delta x_3 &\longrightarrow \frac{f(x_0 + [\Delta x_3/2]) - f(x_0 - [\Delta x_3/2])}{\Delta x_3} \\ 0 &\longrightarrow ? \end{aligned} \quad [1]$$

Evidently, the answer to the question mark (?) is the numerical derivative of the function at x_0 , and it can be obtained only by extrapolation since the quantities

$$\frac{f(x_0 + [0_+/2]) - f(x_0 - [0_+/2])}{0_+}$$

or

$$\frac{f(x_0 + [0_-/2]) - f(x_0 - [0_-/2])}{0_-}$$

cannot be obtained numerically due to obvious physical limitation. (0_+ indicates that $\Delta x \longrightarrow 0$ from the positive direction and 0_- indicates that $\Delta x \longrightarrow 0$ from the negative direction.)

2. EXTRAPOLATION METHOD

The aforesaid problem is one of quadratic extrapolation since r. h. s. informations are provided corresponding to three quantities Δx_1 , Δx_2 , Δx_3 only. One can as well pose the problem as cubic, biquadratic or any other extrapolation considering 4, 5 or more r.h.s. informations corresponding to 4, 5 or more quantities Δx_1 , Δx_2 , Δx_3 , Δx_4 , Δx_5 etc. It is, however, the fact that the use of biquadratic or higher-order extrapolation does not offer any significant advantage over quadratic or cubic extrapolation which is simpler and more economic¹. It is worth mentioning that the aforesaid situation is analogous to the fact that the Wilkes-Harvard and Newton-Raphson iterative division scheme with an order of convergence more than two or three are uneconomical for realization in computers¹. We therefore restrict ourselves to the discussion of quadratic and cubic extrapolation. The next problem is how to choose Δx_1 , Δx_2 , Δx_3 etc. Since we do not possess definite knowledge about what Δx 's should be so that the numerical derivative turns out to be the most accurate within the allowed precision of the computer, we devise the following iteration process.

We extrapolate the r.h.s. quantities to $x=0$, using Lagrange's interpolation formula of order 2 or 3. We choose for this purpose Δx_2 as $[\Delta x_1/2]$, Δx_3 as $[\Delta x_2/2]$, Δx_4 as $[\Delta x_3/2]$ and so on. We can, however, choose any other spacing of Δx 's, equidistant or non-equidistant. After

obtaining the numerical derivative of $f(x)$ by extrapolation, we reduce Δx_1 to half and pass through the identical procedure to obtain the second iteration value of numerical derivative. The process is repeated, halving the interval Δx_1 at each iteration till the continuously increasing or continuously decreasing numerical derivative attains a maximum or minimum value. The maximum or minimum value is the required numerical derivative. For greater accuracy, Δx_1 should be small (starting with, say, 1 or 2) but not too small.

It can be seen that we have used in [1] the central difference scheme and not forward or backward difference schemes for initial approximate derivatives. This is because central difference scheme produces a truncation error of the order of h^2 while forward or backward difference scheme produces an error of the order of h .

The suggested technique is also true for complex functions. The arithmetic employed here has to be complex. Functions of many variables do not pose any extra problem; in this case we obtain numerical partial derivatives.

If we use both the quadratic and cubic extrapolations, then the difference between the values of $f'(x_0)$, so obtained, provides us in the first place an idea of the accuracy and also an idea about the interval size to be chosen for the argument of the function. If the interval is big, so far as the nature of the variation of $\Delta f(x)/\Delta x$ is concerned, both quadratic and cubic fittings may produce results almost completely different, thereby indicating that the interval should be reduced.

A function $f(x)$ is said to be ill-conditioned with respect to its derivatives if $f(x)$ is violently fluctuating, i.e., a little change in x causes a very large change in $f(x)$. The degree of ill-conditioning² is dependent on the degree of fluctuation of $f(x)$. Such a function of $f(x)$, however, is a problem under any treatment. The basic fact is that the function $f(x)$ is a near approach to a discontinuous function.

If we denote $\Delta x_1, \Delta x_2, \Delta x_3$ by p_1, p_2, p_3 respectively and the corresponding right hand quantities in [I] by q_1, q_2, q_3 respectively, we then write, by Lagrange's interpolation formula, the extrapolated numerical derivative as

$$q(0) = \frac{p_2 p_3}{(p_1 - p_2)(p_1 - p_3)} q_1 + \frac{p_1 p_3}{(p_2 - p_1)(p_2 - p_3)} q_2 + \frac{p_1 p_2}{(p_3 - p_1)(p_3 - p_2)} q_3 \quad \text{[II]}$$

The formula in [II] is the result of quadratic fitting. Similarly we can obtain $f'(x)$ using cubic fitting.

3. NUMERICAL RESULTS

We have taken the Bessel functions $J_0(x)$, $J_1(x)$, $Y_0(x)$, $Y_1(x)$, $I_0(x)$, $I_1(x)$, $K_0(x)$ and $K_1(x)$ with real argument x as examples. The calculations are carried out in about 8 μ sec floating point arithmetic. The computer used is National Elliott 803 computer with fixed word-length of 40 bits. Numerical derivatives of the aforesaid functions at $x=2$, obtained by the present method are presented in Table 1. The starting value of Δx is 2 in each case. The calculation of the functions J_0 , J_1 , Y_0 , Y_1 , I_0 , I_1 , K_0 , K_1 are carried out using Chebyshev polynomial expansion².

TABLE I

Function $f(x_0)$	Quadratic Fittings		Cubic fitting	
	$f'(x_0)$	No. of iteration	$f'(x_0)$	No. of iteration
$J_0(2)$	-.57672439 (min)	5	-.57672486 (max)	3
$J_1(2)$	-.64470331x10 ⁻¹ (min)	7	-.64471851x10 ⁻¹ (max)	3
$Y_0(2)$.10703253 (min)	5	.10703247 (max)	3
$Y_1(2)$.56389175 (min)	5	.56389244 (max)	5
$I_0(2)$.15906365 x 10 (min)	4	.15906397 x 10 (max)	4
$I_1(2)$.14842662 x 10 (min)	5	.14842662 x 10 (max)	3
$K_0(2)$	-.13986553 (min)	5	-.13986603 (max)	3
$K_1(2)$	-.18382511 (min)	6	-.18382710 (max)	4

It is noted that in the quadratic fitting the derivative value decreases with iterations and after attaining a minimum value with 4 or 5 iterations starts increasing. The situation is just reverse in case of cubic fitting. In

In Table I the word 'min' within closed parenthesis under the heading 'quadratic fitting' indicates the minimum value attained by the derivative at the corresponding number of iterations mentioned alongside; this minimum value is our required numerical derivative. Similarly, in the case of cubic fitting, the maximum value of the derivative is the required derivative. The results are seen to be correct up to about 6 significant figures.

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5. REFERENCES

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