East Asian Journal on Applied Mathematics Vol. **7**, No. 4, pp. 810-826
doi: 10.4208/eajam.161016.300517a November 2017

Linear Regression to Minimize the Total Error of the Numerical Differentiation

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Received 16 October 2016; Accepted (in revised version) 30 May 2017.

Abstract. It is well known that numerical derivative contains two types of errors. One is truncation error and the other is rounding error. By evaluating variables with rounding error, together with step size and the unknown coefficient of the truncation error, the total error can be determined. We also know that the step size affects the truncation error very much, especially when the step size is large. On the other hand, rounding error will dominate numerical error when the step size is too small. Thus, to choose a suitable step size is an important task in computing the numerical differentiation. If we want to reach an accuracy result of the numerical difference, we had better estimate the best step size. We can use Taylor Expression to analyze the order of truncation error, which is usually expressed by the big O notation, that is, $E(h) = Ch^k$. Since the leading coefficient C contains the factor $f^{(k)}(\xi)$ for high order k and unknown ξ, the truncation error is often estimated by a roughly upper bound. If we try to estimate the high order difference $f^{(k)}(\xi)$, this term usually contains larger error. Hence, the uncertainty of ξ and the rounding errors hinder a possible accurate numerical derivative.
We will introduce the statistical process into the traditional numerical difference. The new method estimates truncation error and rounding error at the same time for a given step size. When we estimate these two types of error successfully, we can reach much better modified results. We also propose a genetic approach to reach a confident numerical derivative.

AMS subject classifications: 65M10, 78A48

Key words: Truncation error, leading coefficient, asymptotic constant, rounding error.

1. Introduction

In numerical computation, the total numerical error comes from two types of errors. The first one is rounding error due to the limitation of hardware so as not to represent the real number. The second one is truncation error as a result of the approximation ability of specific numerical method. It is important to control errors of numerical computation for many applications. To get the best numerical derivative, we must select the best step size

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to balance rounding error and truncation error. However, there are some unknown factors in truncation error analysis, so that we could not decide the best step size.

We first give some definitions that will be used in this paper.

Definition 1.1. Let $f \in C^{\infty}(R)$, the k-th order numerical derivative of function f at x_0 that is computed by the step size h is denoted by $D^{(k)}(f, x_0, h)$.

For example, $D^{(1)}(f,x,h) = (f(x+h) - f(x))/h$ is the forward difference to approximate $f'(x)$ and $D^{(2)}(f,x,h) = (f(x+h) - 2f(x) + f(x-h))/h^2$ is the central difference to approximate $f''(x)$. Because there are three types of approximation methods (forward, backward and central) and every approximation method has its specific truncation error, we use the notation $D^{(k)}_{F,n}(f,x,h)$ to indicate the numerical derivative is forward method with n-th order truncation error. Similarly, $D^{(k)}_{C,n}(f,x,h)$ indicates the central method with n-th order truncation error and $D^{(k)}_{B,n}(f,x,h)$ indicates the backward method with n-th order truncation error.

To know the error of approximation $(f(x+h) - f(x))/h \approx f'(x)$, we use Taylor expression

$$f(x+h) = f(x) + f'(x)h + \frac{f''(\xi)}{2}h^2, \tag{1.1}$$

where $\xi \in (x, x+h)$. Hence, we have $D^{(1)}_{F,1}(f,x,h) - f'(x) = f''(\xi)h/2 = O(h)$. The error term $f''(\xi)h/2$ contains two unknowns. One is the function $f''(x)$ and the other is ξ. We call this term $f''(\xi)h/2$ is the truncation error. To analyse the truncation error, we have $|D^{(1)}_{F,1}(f,x,h) - f'(x)| \le Kh$, where $K = \max_{\xi \in (x,x+h)} |f''(\xi)/2|$. In practice, we will assume that h is small and $f''(x)$ is a continuous function, then the value of $f''(x)$ is closed to $f''(\xi)$. To see the error of central difference to approximate $f''(x)$, we express $f(x+h)$ and $f(x-h)$ by

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f^{(3)}(x)}{6}h^3 + \frac{f^{(4)}(\xi_1)}{24}h^4 \tag{1.2}$$

and

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f^{(3)}(x)}{6}h^3 + \frac{f^{(4)}(\xi_2)}{24}h^4, \tag{1.3}$$

where $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-h, x)$. We have

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{f^{(4)}(\xi)}{12}h^2, \tag{1.4}$$

for some $\xi \in (x-h, x+h)$. Thus, we use $D^{(2)}_{C,2}(f,x,h)$ to denote $(f(x+h) - 2f(x) + f(x-h))/h^2$.

The total error of $D^{(1)}_{F,1}(f,x,h)$ is also related to the rounding error. We assume that the machine epsilon is ϵ. Evaluate $f(x+h)$ and $f(x)$ will include the rounding errors, so-called e_1 and e_2, and the rounding error will be proportional to the value of f. That is