Note on Numerical Differentiation

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1 Introduction

We review method of numerical differentiation. Naturally, our problem is the following:

Problem 1
We want to obtain numerically the derivative of a function $f(x)$ at x_0.

2 One-Sided and Two-Sided Differentiation

The definition of the derivative is the following:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

Therefore, natural way to numerically obtain the derivative is to use the following formula:

$$f'(x_0) \simeq \frac{f(x_0 + h) - f(x_0)}{h}$$

with small h.
There is another way to derive numerical derivative as follows:

$$f'(x_0) \simeq \frac{f(x_0 + h) - f(x_0 - h)}{2h}$$

with a small h
Actually, it can be shown that the two-sided numerical derivative has a smaller error than the one-sided counterpart. Why?
Use Taylor expansion of order 3 around x_0 and we can obtain:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \frac{1}{6} f'''(x_0)(x - x_0)^3 + R_3(x)$$

At $x = x_0 + h$, this expression gives:

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2} f''(x_0)h^2 + \frac{1}{6} f'''(x_0)h^3 + R_3(x_0 + h)$$

We can easily solve the equation for the one sided formula as follows:

$$\frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + \frac{1}{2} f''(x_0)h + \frac{1}{6} f'''(x_0)h^2 + \frac{R_3(x_0 + h)}{h}$$

In order to derive a similar formula for two-sided formula, evaluate Taylor expansion formula at $x = x_0 - h$:

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + R_3(x_0 - h)$$

Combine the expression for $x = x_0 + h$ and $x = x_0 - h$, we can obtain:

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} = f'(x_0) + \frac{1}{6}f'''(x_0)h^2 + \frac{R_3(x_0 + h) - R_3(x_0 - h)}{2h}$$

Notice that the approximation error for one-sided formula is:

$$\frac{1}{2}f''(x_0)h + \frac{1}{6}f'''(x_0)h^2 + \frac{R_3(x_0 + h)}{h}$$

while the approximation error for the two-sided formula is:

$$\frac{1}{6}f'''(x_0)h^2 + \frac{R_3(x_0 + h) - R_3(x_0 - h)}{2h}$$

As long as the approximation error is small enough, the error associated with the two-sided formula is smaller, because the one-sided formula has an additional term $\frac{1}{2}f''(x_0)h$.

3 Computational Issue

Generally the approximation is more precise if we use smaller h. However, computer is not good at handling precise small number. Usually, if you are using double precision in fortran, you cannot trust a real which is smaller than 10^{-16} in general. So, if you are computing a numerical derivative using two-sided formula, use the following formula with a small h:

$$f'(x_0) \simeq \frac{f(x_0 + h) - f(x_0 - h)}{(x_0 + h) - (x_0 - h)}$$

Notice that the denominator might not be precisely $2h$. That's why this formula helps to avoid trouble associated with a small number h.