Numerical Differentiation

Hung Doan

May 28, 2018

Abstract

When calculating a derivative directly is not possible, or numerically cumbersome, it may be better to numerically approximate the derivative. We can do this by using a Taylor series to approximate the function. By rearranging the terms in the Taylor series, we are able to obtain a formula that approximates the error in the derivative of a function. In this case, we will be approximating $f(x) = \sin(x)$. After obtaining the error function, we can take the derivative of the function to find optimal solution of h, h_opt which minimizes the error in our approximation of the derivative. In this project, I will be using h values $h = 10^{-i}$ for $i = 1, 2, ..., 16$ to calculate the error in our approximation of the derivative. I will then compare the results to the optimal solution of h.

1 Introduction

In this project, we will be numerically approximating the derivative of the function $f(x) = \sin(x)$ at $x = a$ for $a = 0, 1$. The Taylor expansion is given by

$$f(a+h) = f(a) + f'(a)h + \frac{f''(c)}{2}h^2, \qquad c \in [a, a+h].$$

Using the definition of derivative, we can define D_h, to be

$$D_h = \frac{f(a+h) - f(a)}{h}. \qquad (*)$$

As $h \to 0$, $D_h \to f'(a)$. From the Taylor series, we can define D_h to be

$$D_h = f'(a) + \frac{f''(c)}{2}h. \qquad (**)$$

2 Error in the Approximation of the Derivative

By subtracting $f'(a)$ on both sides of $(**)$, and accounting for the machine error along with the magnification of the error created by the $\frac{1}{h}$ term in the D_h equation, we have our error equation given by

$$|D_h - f'(a)| \approx \frac{|f''(c)|}{2}h + \frac{2eps}{h}.$$

Next, we would like to find a bound M_2 such that $|f''(x)| \leq M_2$ for all $x \in [a, a+h]$. Since $|f''(x)| = |-\sin(x)|$ and $0 \leq |-\sin(x)| \leq 1$ for all x, we can choose $M_2 = 1$.
Now, define the error, $errD(h)$ as

$$errD(h) = M_2 \frac{h}{2} + \frac{2eps}{h}. \qquad (***)$$

Using $(***)$ with $h = 10^i$ for $i = 1, 2, ...16$, and $M_2 = 1$, we obtain Figure 1 and Table 1.

h	error (a=0)	error (a=1)
1.0000e-01	5.0000e-02	5.0000e-02
1.0000e-02	5.0000e-03	5.0000e-03
1.0000e-03	5.0000e-04	5.0000e-04
1.0000e-04	5.0000e-05	5.0000e-05
1.0000e-05	5.0000e-06	5.0000e-06
1.0000e-06	5.0044e-07	5.0044e-07
1.0000e-07	5.4441e-08	5.4441e-08
1.0000e-08	4.9409e-08	4.9409e-08
1.0000e-09	4.4459e-07	4.4459e-07
1.0000e-10	4.4409e-06	4.4409e-06
1.0000e-11	4.4409e-05	4.4409e-05
1.0000e-12	4.4409e-04	4.4409e-04
1.0000e-13	4.4409e-03	4.4409e-03
1.0000e-14	4.4409e-02	4.4409e-02
1.0000e-15	4.4409e-01	4.4409e-01
1.0000e-16	4.4409e+00	4.4409e+00

Table 1: Error in Approximation of the derivative when $a = 0$ and $a = 1$.

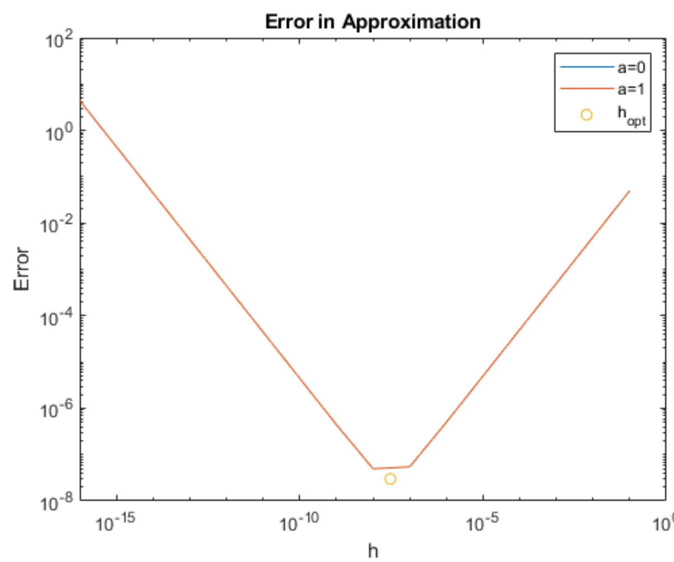

Figure 1: Error in Approximation of the derivative when $a = 0$ and $a = 1$.

We can see that error is as low as $4.9409 \cdot 10^{-8}$ at $h = 10^{-8}$ for both $a = 0$ and $a = 1$.

3 Finding the Optimal h Value

Equation $(***)$ is given by

$$errD(h) = M_2 \frac{h}{2} + \frac{2eps}{h}.$$

The optimal h value is given when $errD(h)$ is 0. Then

$$\begin{aligned}
0 &= \frac{d}{dh}\left(M_2\frac{h}{2} + \frac{2eps}{h}\right) \\
0 &= \frac{M_2}{2} - \frac{2eps}{h^2} \\
\frac{M_2}{2} &= \frac{2eps}{h^2} \\
h^2 \cdot M_2 &= 4eps \\
h^2 &= \frac{4eps}{M_2} \\
h_{opt} &= 2\sqrt{\frac{eps}{M_2}}
\end{aligned}$$

We can now use this to find the optimal h value that minimizes the error in the derivative. Using our derived formula for h_{opt}, we have

$$h_{opt} = 2\sqrt{\frac{eps}{M_2}} = 2\sqrt{\frac{eps}{1}} = 2\sqrt{eps} = 2.9802 \cdot 10^{-8}.$$

This is in agreement to our observations in Figure 1.

4 Complex Step Differentiation (CSD)

Complex step differentiation is a method of numerically providing accurate approximations for the derivatives of functions. By slightly manipulating the definition of derivative, we obtain the scheme

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{6}f^{(3)}(x) + ...$$

We can subtract $f'(x)$ on both sides to obtain the error. Using the same methods as from above, we arrive at an error equation of

$$errD(h) = \frac{h^2}{6}M_2 + \frac{2eps}{h}$$

Setting the error to 0, we can obtain our h_opt.

$$
\begin{aligned}
0 &= \frac{d}{dh}\left(M_2\frac{h^2}{6} + \frac{2eps}{h}\right) \\
0 &= \frac{2M_2h}{6} - \frac{2eps}{h^2} \\
\frac{M_2h}{3} &= \frac{2eps}{h^2} \\
h^3 \cdot M_2 &= 6eps \\
h^3 &= \frac{6eps}{M_2} \\
h_{opt} &= \sqrt[3]{\frac{6eps}{M_2}}
\end{aligned}
$$

Again, I will be using h values $h = 10^{-i}$ for $i = 1, 2, ..., 16$ to calculate the error in our approximation of the derivative. I will then compare the results to the optimal solution of h.

h	error (a=0)	error (a=1)
1.0000e-01	1.6667e-03	1.6667e-03
1.0000e-02	1.6667e-05	1.6667e-05
1.0000e-03	1.6667e-07	1.6667e-07
1.0000e-04	1.6711e-09	1.6711e-09
1.0000e-05	6.1076e-11	6.1076e-11
1.0000e-06	4.4426e-10	4.4426e-10
1.0000e-07	4.4409e-09	4.4409e-09
1.0000e-08	4.4409e-08	4.4409e-08
1.0000e-09	4.4409e-07	4.4409e-07
1.0000e-10	4.4409e-06	4.4409e-06
1.0000e-11	4.4409e-05	4.4409e-05
1.0000e-12	4.4409e-04	4.4409e-04
1.0000e-13	4.4409e-03	4.4409e-03
1.0000e-14	4.4409e-02	4.4409e-02
1.0000e-15	4.4409e-01	4.4409e-01
1.0000e-16	4.4409e+00	4.4409e+00

Table 2: Error in Approximation of the derivative when $a = 0$ and $a = 1$.

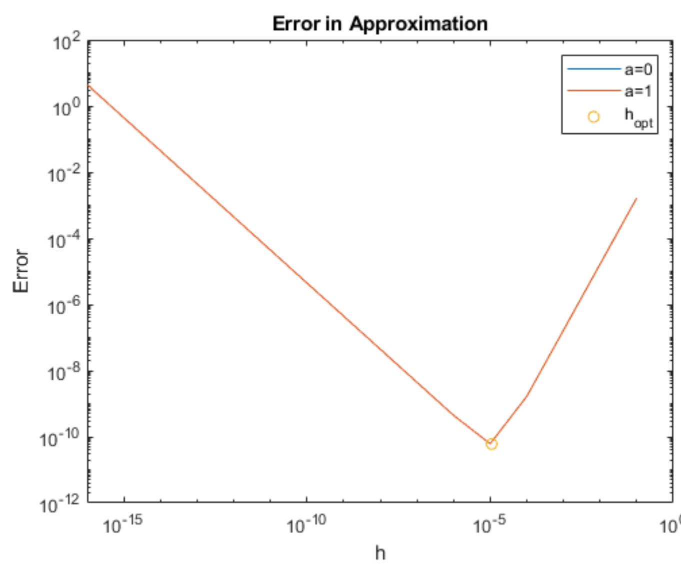

Figure 2: Error in Approximation of the derivative when $a = 0$ and $a = 1$.

This time, we can see that the error is a lot lower than with our previous methods. Here we have error as low as $6.1076 \cdot 10^{-11}$ and $h_{opt} = 1.1003 \cdot 10^{-5}$.