

IIIT Vadodara
WINTER 2020-21
MA202 Numerical Techniques
LAB#5 Numerical Differentiation¹

1. Difference approximations of the first derivative of a function: For a function $f(x)$ of a variable x , its first derivative is defined as,

$$f^{(1)}(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \quad (1)$$

However, this gives our computers a headache, since they do not know how to consider the limit. Any input number given to computers must be a definite number and can be neither too small nor too large to be understood by the computer. The ‘theoretically’ infinitesimal number h involved in this equation is a problem. A simple approximation for computational implementation is the forward difference approximation

$$D_{f1}(x, h) = \frac{f(x+h) - f(x)}{h}, \quad (2)$$

where h is a finite step size. How far equation (2) approximation from the true value of (1)? In order to do the error analysis, we take the Taylor series expansion of $f(x+h)$ about x as

$$f(x+h) = f(x) + hf^{(1)}(x) + \frac{h^2}{2!}f^{(2)}(x) + \frac{h^3}{3!}f^{(3)}(x) + \dots \quad (3)$$

where $f^{(n)}(x)$ is the differentiation of $f(x)$ at n^{th} order. Now, let us approximate first order derivative of $f(x)$, i.e., $f^{(1)}(x)$. Subtracting $f(x)$ from both sides and dividing both sides by the step size h yields

$$f^{(1)}(x, h) \approx \frac{f(x+h) - f(x)}{h}, \quad (4)$$

where h is a finite step size.

$$D_{f1}(x, h) = f^{(1)}(x) + \mathcal{O}(h), \quad (5)$$

where $\mathcal{O}(g(h))$ denotes a truncation error term proportional to $g(h)$ for $|h| \prec 1$. This means that the error of the forward difference approximation (2) of the first derivative is proportional to the step size h , or, equivalently, in the order of h .

Now, in order to derive another approximation formula for the first derivative having a smaller error, let's remove the first-order term with respect to h from Eq. (4) by substituting $2h$ for h , and subtracting this result from two times the equation. Then, we get

$$D_{f2}(x, h) = f^{(1)}(x) + \mathcal{O}(h^2), \quad (6)$$

which can be regarded as an improvement over Eq. (4), since it has the truncation error of $\mathcal{O}(h^2)$ for $|h| \prec 1$.

The backward difference approximation $D_{b1}(x, h) = D_{f1}(x, -h)$ also has an error of $\mathcal{O}(h)$ and can be processed to yield an improved version having a truncation error of $\mathcal{O}(h^2)$.

In order to derive another approximation formula for the first derivative, we take the Taylor series expansion of $f(x+h)$ and $f(x-h)$ up to the fifth order in equation (3) and divide the

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difference between these two equations by $2h$ to get the central difference approximation for the first derivative as

$$D_{c2}(x, h) = f^{(1)}(x) + \mathcal{O}(h^2), \quad (7)$$

which has an error of $\mathcal{O}(h^2)$ similarly to Eqs.(5) and (6). This can also be processed to yield an improved version having a truncation error of $\mathcal{O}(h^4)$.

$$2^2 D_{c2}(x, h) - D_{c2}(x, 2h) = f'(x) + \mathcal{O}(h^4). \quad (8)$$

Furthermore, this procedure can be formularized into a general formula, called ‘Richardson’s extrapolation’, for improving the difference approximation of the derivatives.

Difference approximation for the second derivative using central difference method

For a function $f(x)$ of a variable x , its second derivative is defined as,

$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2). \quad (9)$$

where h is the step size.

- Q. 1: (a) Write a MATLAB script to calculate numerical derivative of $\tan^{-1}(x)$ at $x = 1$.
 (b) Find the error using forward difference, backward difference, and central difference methods. Comment on order of accuracy.
 (c) Plot the error using log-log scale for the step size $h = 1e - 04$.
 (d) Use step sizes ranging from 10^{-1} to 10^{-8} . Plot the error using log-log scale for each of your step sizes.(Note: Use array operations not a for loop).
 (e) Comment on trade-off between truncation error and roundoff error, i.e., look at the minima of different methods in the graphs.

- Q. 2: Write a MATLAB script to calculate first order as well as second order numerical derivative of $2 - x + \ln(x)$ at $x = 1$.
 Repeat the steps (b), (c), (d), and (e) of Q.1

- Q. 3: (a) Write a MATLAB script to calculate partial derivative of

$$f(x) = \sin(x_1)\exp(-x_2) \quad (10)$$

at $x_1 = 0.5$ and $x_2 = 1$.

- (b) Find the error using central difference method.
 (c) Plot the error using log-log scale for the step size $h = 1e - 06$.