MC3010: Differential Equations & Numerical Methods

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NUMERICAL COMPUTATION

Lecture – 04: Numerical Differentiation

Introduction

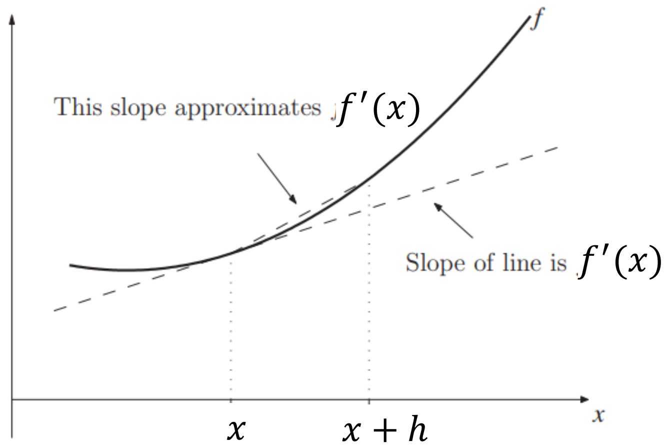
Many engineering applications involve rates of change of quantities with respect to variables such as time. For example, linear damping force is directly proportional to velocity, which is the rate of change of displacement with respect to time. Other applications may involve definite integrals. For example, the voltage across a capacitor at any specified time is proportional to the integral of the current taken from an initial time to that specified time.

Numerical Differentiation

Numerical differentiation is desirable in various situations. Sometimes the analytical expression of the function to be differentiated is known but **analytical differentiation proves to be either very difficult or even impossible**. In that case, the function is discretized to generate several points (values), which are subsequently used by a numerical method to approximate the derivative of the function at any of the generated points.

Finite Difference Formula

A simple approximation of the first derivative is



$$f'(x) \approx \frac{f(x+h) - f(x)}{h},$$ where we assume that $h > 0$.

For linear functions, it is actually an exact expression for the derivative. For almost all other functions, it is not the exact derivative.

Let's compute the approximation error. We write a Taylor expansion of $f(x + h)$ about x, i.e.,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi), \qquad \xi \in (x, x+h).$$

For such an expansion to be valid, we assume that $f(x)$ has two continuous derivatives

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi), \qquad \xi \in (x, x+h).$$

Truncation error denotes as $\boldsymbol{O}(h)$

Since this approximation of the derivative at x is based on the values of the function at x and $x + h$, the approximation is called a **forward differencing or one-sided differencing**.

Finite Difference Formula

The approximation of the derivative at x that is based on the values of the function at $x - h$ and x, i.e.,

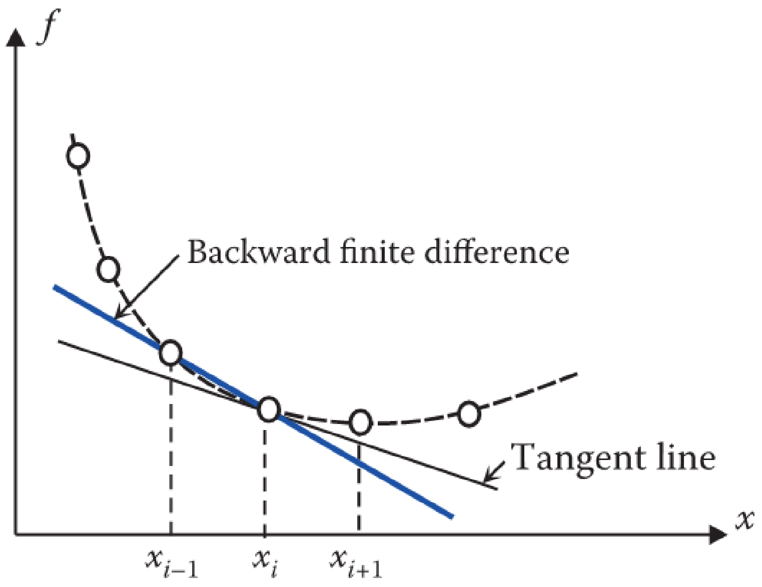
$$f'(x) \approx \frac{f(x) - f(x-h)}{h},$$

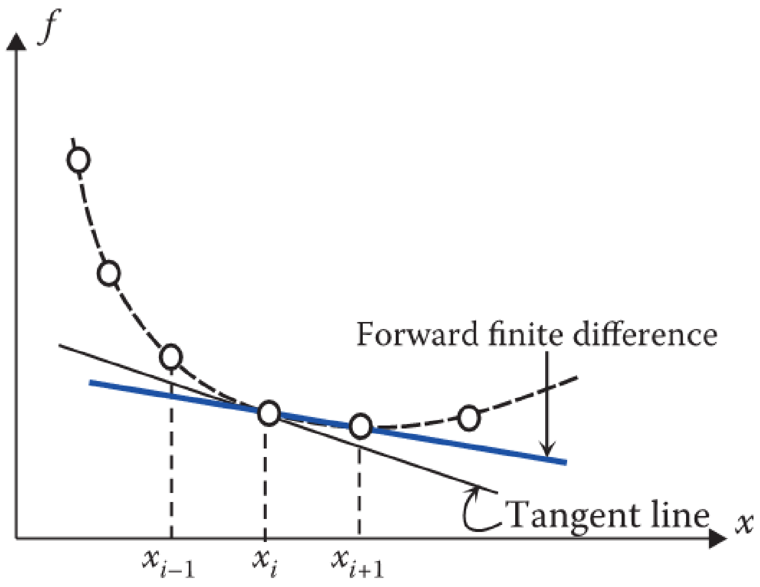
is called a **backward differencing** (which is obviously also a one-sided differencing formula).

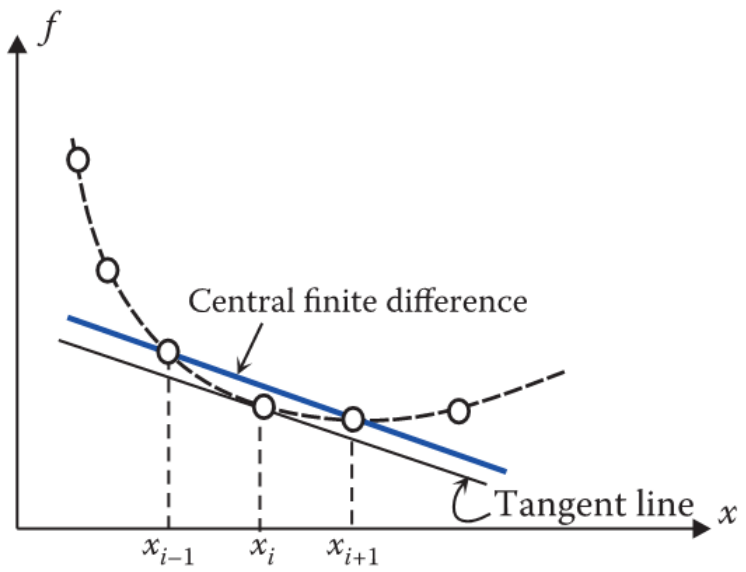
A more accurate approximation for the first derivative that is based on the values of the function at the points $f(x-h)$ and $f(x+h)$ is the **centered differencing formula**

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

Backward, Forward and Central finite difference







$$f'(x) \approx \frac{f(x) - f(x-h)}{h},$$

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

The Central-difference Formula of Order $\boldsymbol{O}(h^2)$

Theorem **(Centered Formula of Order $O(h^2)$).** Assume that $f \in C^3[a, b]$ and that $x - h, x, x + h \in [a, b]$. Then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

Formula 01

Furthermore, there exists a number $c = c(x) \in [a_1 b]$ such that

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} + E_{\text{trunc}}(f, h),$$

where

$$E_{\text{trunc}}(f, h) = -\frac{h^2 f^{(3)}(c)}{6} = O(h^2).$$

The term $E(f, h)$ is called the ***truncation error***.

The Central-difference Formula of Order $\boldsymbol{O}(h^4)$

Theorem (Centered Formula of Order $O(h^4)$). Assume that $f \in C^5[a, b]$ and that $x - 2h, x - h, x, x + h, x + 2h \in [a, b]$. Then

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}$$

Formula 02

Furthermore, there exists a number $c = c(x) \in [a, b]$ such that

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{\text{trunc}}(f, h),$$

where

$$E_{\text{trunc}}(f, h) = \frac{h^4 f^{(5)}(c)}{30} = O(h^4).$$

Example : 1

Let $f(x) = \cos(x)$

a) Use formulas 1 and 2 with step sizes $h = 0.1, 0.01, 0.001$ *and* 0.0001 and calculate approximations for $f'(0.8) = -\sin(0.8)$. Carry nine decimal places in all the calculations.

b) Compare with the true value $f'(0.8) = -\sin(0.8)$.

Using **Formula 01** with $h = 0.01$

Theorem (Centered Formula of Order $O(h^2)$). Assume that $f \in C^3[a, b]$ and that $x - h, x, x + h \in [a, b]$. Then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

$$f'(0.8) \approx \frac{f(0.81) - f(0.79)}{0.02} \approx \frac{0.689498433 - 0.703845316}{0.02} \approx -0.717344150.$$

Using **Formula 02** with $h = 0.01$

Theorem (Centered Formula of Order $O(h^4)$). Assume that $f \in C^5[a, b]$ and that $x - 2h, x - h, x, x + h, x + 2h \in [a, b]$. Then

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

$$\begin{aligned} f'(0.8) &\approx \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{0.12} \\ &\approx \frac{-0.682221207 + 8(0.689498433) - 8(0.703845316) + 0.710913538}{0.12} \\ &\approx -0.717356108. \end{aligned}$$

Table Numerical Differentiation Using Formulas 1 and 2

Step size	Approximation by Formula 01	Error using Formula 01	Approximation by Formula 02	Error using Formula 02
0.1	−0.716161095	−0.001194996	−0.717353703	−0.000002389
0.01	−0.717344150	−0.000011941	−0.717356108	0.000000017
0.001	−0.717356000	−0.000000091	−0.717356167	0.000000076
0.0001	−0.717360000	−0.000003909	−0.717360833	0.000004742

(b) The error in approximation for formulas 1 and 2 turns out to be −0.000011941 and 0.000000017, respectively. In this example, formula 2 gives a better approximation to $f'(0.8)$ than formula 1 when $h = 0.01$. The error analysis will illuminate this example and show why this happened . The other calculations are summarized in Table

Finite Difference Formulas for First Derivatives

Difference Formula	First Derivative	Truncation error
Two-point backward	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Two-point forward	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Two-point central	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
Three-point backward	$f'(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
Three-point forward	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Four-point central	$f'(x_i) = \dfrac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

Finite Difference Formulas for Second Derivatives

Difference Formula	Second Derivative	Truncation Error
Three-point backward	$f''(x_i) = \dfrac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Three-point forward	$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
Three-point central	$f''(x_i) = \dfrac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
Four-point backward	$f''(x_i) = \dfrac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Four-point forward	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Five-point central	$f''(x_i) = \dfrac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

Finite Difference Formulas for Third Derivatives

Difference Formula	Third Derivative	Truncation Error
Four-point backward	$f'''(x_i) = \dfrac{-f(x_{i-3}) + 3f(x_{i-2}) - 3f(x_{i-1}) + f(x_i)}{h^3}$	$O(h)$
Four-point forward	$f'''(x_i) = \dfrac{-f(x_i) + 3f(x_{i+1}) - 3f(x_{i+2}) + f(x_{i+3})}{h^3}$	$O(h)$
Four-point central	$f'''(x_i) = \dfrac{-f(x_{i-2}) + 2f(x_{i-1}) - 2f(x_{i+1}) + f(x_{i+2})}{2h^3}$	$O(h^2)$
Five-point backward	$f'''(x_i) = \dfrac{3f(x_{i-4}) - 14f(x_{i-3}) + 24f(x_{i-2}) - 18f(x_{i-1}) + 5f(x_i)}{2h^3}$	$O(h^2)$
Five-point forward	$f'''(x_i) = \dfrac{-5f(x_i) + 18f(x_{i+1}) - 24f(x_{i+2}) + 14f(x_{i+3}) - 3f(x_{i+4})}{2h^3}$	$O(h^2)$
Six-point central	$f'''(x_i) = \dfrac{f(x_{i-3}) - 8f(x_{i-2}) + 13f(x_{i-1}) - 13f(x_{i+1}) + 8f(x_{i+2}) - f(x_{i+3})}{8h^3}$	$O(h^4)$

Finite Difference Formulas for Fourth Derivatives

Difference Formula	Fourth Derivative	Truncation error
Five-point backward	$f^{(4)}(x_i)=\dfrac{f(x_{i-4})-4f(x_{i-3})+6f(x_{i-2})-4f(x_{i-1})+f(x_i)}{h^4}$	$O(h)$
Five-point forward	$f^{(4)}(x_i)=\dfrac{f(x_i)-4f(x_{i+1})+6f(x_{i+2})-4f(x_{i+3})+f(x_{i+4})}{h^4}$	$O(h)$
Five-point central	$f^{(4)}(x_i)=\dfrac{f(x_{i-2})-4f(x_{i-1})+6f(x_i)-4f(x_{i+1})+f(x_{i+2})}{h^4}$	$O(h^2)$
Six-point backward	$f^{(4)}(x_i)=\dfrac{-2f(x_{i-5})+11f(x_{i-4})-24f(x_{i-3})+26f(x_{i-2})-14f(x_{i-1})+3f(x_i)}{h^4}$	$O(h^2)$
Six-point forward	$f^{(4)}(x_i)=\dfrac{3f(x_i)-14f(x_{i+1})+26f(x_{i+2})-24f(x_{i+3})+11f(x_{i+4})-2f(x_{i+5})}{h^4}$	$O(h^2)$
Seven-point central	$f^{(4)}(x_i)=\dfrac{f(x_{i-3})+12f(x_{i-2})-39f(x_{i-1})+56f(x_i)+39f(x_{i+1})+12f(x_{i+2})-f(x_{i+3})}{6h^4}$	$O(h^4)$

Example : 2

Use a **forward difference**, and the values of h shown, to approximate the derivative of $\cos(a)$ $at\ a = \pi/3$. Work to 8 decimal places throughout.

a) h = 0.1
b) h = 0.01
c) h = 0.001
d) h = 0.0001

Solution

(a) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.41104381-0.5}{0.1} = -0.88956192$

(b) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49131489-0.5}{0.01} = -0.86851095$

(c) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49913372-0.5}{0.001} = -0.86627526$

(d) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49991339-0.5}{0.0001} = -0.86605040$

One advantage of doing a simple example first is that we can compare these approximations with the 'exact' value which is

$$f'(a) = -\sin(\pi/3) = -\frac{\sqrt{3}}{2} = -0.86602540 \quad \text{to 8 d.p.}$$

Note that the accuracy levels of the four approximations

(a) 1 d.p. (b) 2 d.p. (c) 3 d.p. (d) 3 d.p. (almost 4 d.p.)

The errors to 6 d.p. are:

(a) 0.023537 (b) 0.002486 (c) 0.000250 (d) 0.000025

Notice that the errors reduce by about a factor of 10 each time.

Example : 3

Use a **central difference**, and the values of h shown, to approximate the derivative of $\cos(a)\ at\ a\ =\ \pi/3$. Work to 8 decimal places throughout.

a) h = 0.1
b) h = 0.01
c) h = 0.001
d) h = 0.0001

Solution

(a) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a-h)}{2h} = \dfrac{0.41104381 - 0.58396036}{0.2} = -0.86458275$

(b) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a-h)}{2h} = \dfrac{0.49131489 - 0.50863511}{0.02} = -0.86601097$

(c) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a-h)}{2h} = \dfrac{0.49913372 - 0.50086578}{0.002} = -0.86602526$

(d) $f'(a) \approx \dfrac{\cos(a+h)-\cos(a-h)}{2h} = \dfrac{0.49991339 - 0.50008660}{0.0002} = -0.86602540$

Example : 4

The distance x of a runner from a fixed point is measured (in meters) at intervals of half a second. The data obtained are

t	0.0	0.5	1.0	1.5	2.0
x	0.00	3.65	6.80	9.90	12.15

Use central differences to approximate the runner's velocity at times t = 0.5 s and t = 1.25 s.

Solution

Our aim here is to approximate $x'(t)$. The choice of h is dictated by the available data given in the table.

Using data with $t = 0.5$ s at its centre we obtain

$$x'(0.5) \approx \frac{x(1.0) - x(0.0)}{2 \times 0.5} = 6.80 \text{ m s}^{-1}.$$

Data centred at $t = 1.25$ s gives us the approximation

$$x'(1.25) \approx \frac{x(1.5) - x(1.0)}{2 \times 0.25} = 6.20 \text{ m s}^{-1}.$$

Note the value of h used.

Theorem (**Centered Formula of Order $O(h^2)$**). Assume that $f \in C^3[a, b]$ and that $x - h, x, x + h \in [a, b]$. Then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

END OF
NUMERICAL DIFFERENCIATION

Thank You