5. NUMERICAL DIFFERENTIATION

Numerical differentiation can be applied to engineering problems with functions whose derivatives cannot be computed analytically or when a set of values $(x_i, y_i),\ i = 0,1,2,...,n$ are given.

To approximate $f'(x_0),$ suppose that $x_0 \in (a,b),$ where $f \in C^2[a,b],$ and that $x_1 - x_0 = h,$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a,b].$ We express f in terms of the Lagrange polynomial with its error term:

$$f(x) = P_1(x) + \frac{f''(\xi(x))}{2!}(x - x_0)(x - x_1),$$

where

$$P_1(x) = f(x_0)L_0(x) + f(x_1)L_1(x)$$
$$L_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x - x_0 - h}{-h}$$
$$L_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x - x_0}{h}$$

i.e. $$P_1(x) = \frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h}$$

$$= \frac{f(x_0)(x - x_0)}{-h} + f(x_0) + \frac{f(x_0 + h)(x - x_0)}{h}$$
$$= \frac{[f(x_0 + h) - f(x_0)]}{h}(x - x_0) + f(x_0).$$

Thus,

$$f(x) = \frac{[f(x_0 + h) - f(x_0)]}{h}(x - x_0) + f(x_0) + \frac{f''(\xi(x))}{2!}(x - x_0)(x - x_0 - h)$$

$$\Rightarrow f'(x) = \frac{[f(x_0 + h) - f(x_0)]}{h} + \frac{2(x - x_0) - h}{2} f''(\xi(x)) + \frac{(x - x_0)(x - x_0 - h)}{2} \frac{\partial}{\partial x}\left(f''(\xi(x))\right)$$
$$\Rightarrow f'(x_0) = \frac{[f(x_0 + h) - f(x_0)]}{h} - \frac{h}{2} f''(\xi(x_0))$$

Therefore, for small values of $h,$

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}, \qquad \textbf{(5.1)}$$

with an error bounded by $\frac{|h|M}{2}$, where M is the upper bound of $|f''(\xi(x_0))|$ for $\xi(x_0)$ between x_0 and $x_0+h.$

Formula (5.1) is known as forward-difference formula if $h>0$ and backward-difference formula if $h<0.$

Example 5.1.1

A design engineer must make estimates of evaporation rates when the amount of needed water to meet irrigation demands is required. One input to frequently used formula for estimating evaporation rates is the slope of the saturation vapour pressure curve at air temperature $T.$ The table below shows values of saturation vapour pressure (e_s) in $mm\,Hg$ as a function of temperature T in ^oC:

$T\,(^oC)$	$e_s\,(mm\,Hg)$
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

Estimate evaporation rate at 22^oC using

(a) forward-difference formula (b) backward-difference formula

Solutions:

(a) Using forward-difference, we take $x_0=22$ and $x_1=23$ so that $h=x_1-x_0=1.$ Then

$$e_s'(x_0)\approx\frac{e_s(x_0+h)-e_s(x_0)}{h}\Rightarrow e_s'(22)\approx\frac{e_s(23)-e_s(22)}{1}=21.05-19.82=1.23\ mm\,Hg\,/^o\,C.$$

(b)) Using backward-difference, we take $x_0=22$ and $x_1=21$ so that $h=x_1-x_0=-1.$ Then

$$e_s'(x_0)\approx\frac{e_s(x_0+h)-e_s(x_0)}{h}\Rightarrow e_s'(22)\approx\frac{e_s(21)-e_s(22)}{-1}=\frac{18.65-19.82}{-1}=1.17\ mm\,Hg\,/^o\,C.$$

△

If $\{x_0, x_1, ..., x_n\}$ are $(n+1)$ distinct numbers in some interval I, then are $(n+1)-$point formula for approximating $f'(x_j)$ is

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'(x_j) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\prod_{\substack{k=0 \\ k\neq j}}^{n}(x_j - x_k).$$

For example, if $n=2$, we get the $3-$point formulas as follows:

$$x_1 - x_0 = h,\ x_2 - x_1 = h \Rightarrow x_2 = x_0 + h + h = x_0 + 2h$$

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \Rightarrow L_0'(x) = \frac{2x - x_1 - x_2}{2h^2}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \Rightarrow L_1'(x) = \frac{2x - x_0 - x_2}{-h^2}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \Rightarrow L_2'(x) = \frac{2x - x_0 - x_1}{2h^2}$$

$$\begin{aligned} f'(x_j) &= f(x_0)L_0'(x_j) + f(x_1)L_1'(x_j) + f(x_2)L_2'(x_j) + \frac{f^{(3)}(\xi(x_j))}{3!}\prod_{\substack{k=0 \\ k\neq j}}^{2}(x_j - x_k) \\ &= f(x_0)\left[\frac{2x_j - x_1 - x_2}{2h^2}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{-h^2}\right] + f(x_2)\left[\frac{2x_j - x_0 - x_1}{2h^2}\right] \\ &\quad + \frac{f^{(3)}(\xi(x_j))}{6}\prod_{\substack{k=0 \\ k\neq j}}^{2}(x_j - x_k) \end{aligned}$$

$$\begin{aligned} \therefore\ f'(x_0) &= f(x_0)\left[\frac{2x_0 - 2x_0 - 3h}{2h^2}\right] - f(x_1)\left[\frac{2x_0 - 2x_0 - 2h}{h^2}\right] + f(x_2)\left[\frac{2x_0 - 2x_0 - h}{2h^2}\right] + \frac{h^2}{3}f'''(\xi(x_0)) \\ &= \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f'''(\xi(x_0)) \\ &= \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_0)) \qquad (5.2) \end{aligned}$$

Doing the same for $x_j = x_1 = x_0 + h$ and $x_j = x_2 = x_0 + 2h$, we get

$$f'(x_1) = f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f'''(\xi(x_1)) \qquad (5.3)$$

$$f'(x_2) = f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_2)) \qquad (5.4)$$

Substituting x_0 for $x_0 + h$ in (5.3), we get

$$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f((x_0+h)-h) + \frac{1}{2}f((x_0+h)+h)\right] - \frac{h^2}{6}f'''(\xi(x_1))$$

$$\Rightarrow f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6}f'''(\xi(x_1))$$

and substituting x_0 for $x_0 + 2h$ in (5.4), we get

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f((x_0+2h)-2h) - 2f((x_0+2h)-h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_2))$$

$$\Rightarrow f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3}f'''(\xi(x_2))$$

Note that equation (5.4) can be obtained from (5.2) by replacing h with $-h$. Thus, we have only two formulas:

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_0)), \qquad \textbf{(5.5)}$$

where $\xi(x_0)$ lies between x_0 and $x_0 + h$ and

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f'''(\xi(x_1)) \qquad \textbf{(5.6)}$$

where $\xi(x_1)$ lies between $x_0 - h$ and $x_0 + h$.

Formula (5.5) is known as three-point endpoint formula and (5.6) is known as three-point midpoint formula. Thus,

$$f'(x_0) \approx \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right]$$

$$f'(x_0) \approx \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right]$$

We can use the same approach to get the following five-point formulas:

$5-$<u>point endpoint formula</u>:

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5}f^{(5)}(\xi)$$

where ξ lies between x_0 and $x_0 + 4h$

$$\Rightarrow f'(x_0) \approx \frac{1}{12h}\left[-25f(x_0)+48f(x_0+h)-36f(x_0+2h)+16f(x_0+3h)-3f(x_0+4h)\right]$$

$5-$ point Midpoint formula:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\right]+\frac{h^4}{30}f^{(5)}(\xi)$$

where ξ lies between x_0-2h and x_0+2h

$$\Rightarrow f'(x_0) \approx \frac{1}{12h}\left[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\right]$$

NOTE: (1) Midpoint formula gives more accurate values than endpoint formula.

(2) Using more evaluation points produces greater accuracy.

Example 5.1.2

The table below shows values for $f(x) = xe^x$. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Solutions:

With $x_0 = 2.0$ and $h = 0.1$, we can use $3-$ point endpoint formula so that

$x_0 + h = 2.1$ and $x_0 + h = 2.2$ to get

$$f'(x_0) \approx \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right] \Rightarrow f'(2.0) \approx \frac{1}{2(0.1)}\left[-3f(2.0)+4f(2.1)-f(2.2)\right]$$

$$= \frac{1}{0.2}[-3(14.778112)+4(17,148957)-19.855030] = 22.032310.$$

With $h = -0.1$, the $3-$ point endpoint formula becomes

$$f'(2.0) \approx \frac{1}{-2(0.1)}\left[-3f(2.0)+4f(1.9)-f(1.8)\right]$$

$$= \frac{1}{-0.2}[-3(14.778112)+4(12.703199)-10.889365] = 22.054525.$$

With $h = 0.1,$ the $3-$point midpoint formula gives

$$f'(2.0) \approx \frac{1}{2(0.1)}[f(2.1)-f(1.9)] = \frac{1}{0.2}[17.148957-12.703199] = 22.22879.$$

With $h = 0.2,$ the $3-$point midpoint formula becomes

$$f'(2.0) \approx \frac{1}{2(0.2)}[f(2.2)-f(1.8)] = 22.4141625.$$

(The $3-$point midpoint formula gives the same values when $h = -0.1$ or $h = -0.2$)

To use the $5-$point endpoint formula with $h = 0.1,$ we need

$$x_0 = 2.0,\ x_0 + h = 2.1,\ x_0 + 2h = 2.2,\ x_0 + 3h = 2.3 \text{ and } x_0 + 4h = 2.4.$$

To use the $5-$point midpoint formula with $h = 0.1,$ we need

$$x_0 - 2h = 1.8,\ x_0 - h = 1.9,\ x_0 + h = 2.1 \text{ and } x_0 + 2h = 2.2.$$

Therefore, based on the data given in the table, only the $5-$point midpoint formula can be used.

$$\begin{aligned}
\therefore\ f'(x_0) &\approx \frac{1}{12h}\left[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)\right]\\
&= \frac{1}{12(0.1)}[f(1.8)-8f(1.9)+8f(2.1)-f(2.2)]\\
&= \frac{1}{1.2}[10.889365-8(12.703199)+8(17.148957)-19.855030]\\
&= 22.166999.
\end{aligned}$$

Note that the true value is $f'(2) = (2+1)e^2 = 22.167168$ showing that the $5-$point formula gives a more accurate approximate than other formulas.

△

We can derive formulas for higher order derivatives. For example, it can be shown that the second derivative midpoint formula is

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi(x)), \qquad \textbf{(5.7)}$$

where $x_0 - h < \xi(x) < x_0 + h,$ so that

$$f''(x_0) \approx \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)]$$

Example 5.1.3

Approximate $f''(2.0)$ from Example 5.1.2.

Solutions:

With $h = 0.1$(or $h = -0.1$), we get

$$f''(x_0) \approx \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] \Rightarrow f''(2.0) \approx \frac{1}{(0.1)^2}[f(1.9) - 2f(2.0) + f(2.1)]$$

$$= \frac{1}{0.01}[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.5932.$$

With $h = 0.2,$

$$f''(2.0) \approx \frac{1}{(0.2)^2}[f(1.8) - 2f(2.0) + f(2.2)] = \frac{1}{0.004}[12.703199 - 2(14.778112) + 19.855030]$$

$$= 29.704275.$$

△

5. 1 RICHARDSON'S EXTRAPOLATION

Extrapolation can be applied whenever it is known that an approximation technique has an error that depends on the step size $h.$ Suppose that for $h \neq 0,$ a formula $N_1(h)$ approximates an unknown constant M and that the truncation error has the form

$$M - N_1(h) = k_1 h + k_2 h^2 + k_3 h^3 + ...$$

for some collection of unknown constants $k_1, k_2, k_3, ...$ The truncation error is $O(h)$ and

$$M - N_1(h) \approx k_1 h,$$

$$\text{i.e. } M - N_1(h) = k_1 h + O(h).$$

If we replace h by $\frac{h}{2}$ and eliminate k_1 we get

$$\begin{array}{l|l} M - N_1(h) = k_1 h + k_2 h^2 + k_3 h^3 + \ldots & -1 \\ M - N_1\left(\frac{h}{2}\right) = k_1\left(\frac{h}{2}\right) + k_2\left(\frac{h}{2}\right)^2 + k_3\left(\frac{h}{2}\right)^3 + \ldots & 2 \end{array}$$

$$M + N_1(h) - 2N_1\left(\frac{h}{2}\right) = \left(-k_2 h^2 + k_2\frac{2h^2}{2^2}\right) + \left(-k_3 h^3 + k_3\frac{2h^3}{2^3}\right) + \ldots$$

$$\Rightarrow M - \left(2N_1\left(\frac{h}{2}\right) - N_1(h)\right) = -k_2\left(\frac{h^2}{2}\right) - k_3\left(\frac{3h^3}{4}\right) - \ldots.$$

Defining $N_2(h)$ as $N_2(h) = 2N_1\left(\frac{h}{2}\right) - N_1(h),$ we have that

$$M - N_2(h) = -\frac{h^2}{2}k_2 + O(h^2).$$

Note that combining $N_1(h)$ formulas produce $N_2(h)$ with truncation error $O(h^2)$. We can combine $N_2(h)$ formulas to get $N_3(h)$ with truncation error $O(h^3)$ and so on. Many formulas used for extrapolation have truncation errors that contain only even powers of h, that is, have the form

$$M = N_1(h) + k_1 h^2 + k_2 h^4 + k_3 h^6 + \ldots. \qquad \textbf{(5.8)}$$

As done before, replacing h with $\frac{h}{2}$ gives the $O(h^2)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + k_1\left(\frac{h^2}{4}\right) + k_2\left(\frac{h^4}{16}\right) + k_3\left(\frac{h^6}{64}\right) + \ldots. \qquad \textbf{(5.9)}$$

Combining (5.8) and (5.9) and eliminating k_1 gives

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] - k_2\left(\frac{h^4}{4}\right) - k_3\left(\frac{5h^6}{16}\right) - \ldots.$$

Defining $N_2(h)$ as $N_2(h)=\dfrac{4N_1\left(\frac{h}{2}\right)-N_1(h)}{3}$, we get

$$M-N_2(h)=-k_2\left(\frac{h^4}{4}\right)+O(h^6)$$

with truncation error $O(h^6)$. Continuing this procedure, we get the recursive formula

$$N_j(h)=\frac{4^{j-1}N_{j-1}\left(\frac{h}{2}\right)-N_{j-1}(h)}{4^{j-1}-1},\quad j=2,3,4,...$$

with truncation error $O(h^{2j})$. Thus, we have the following extrapolation table showing the order in which the approximations are generated:

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1. $N_1(h)$			
2. $N_1\left(\frac{h}{2}\right)$	3. $N_2(h)$		
4. $N_1\left(\frac{h}{4}\right)$	5. $N_2\left(\frac{h}{2}\right)$	6. $N_3(h)$	
7. $N_1\left(\frac{h}{8}\right)$	8. $N_2\left(\frac{h}{4}\right)$	9. $N_3\left(\frac{h}{2}\right)$	10. $N_4(h)$

Example 5.1.4

1. Taylor's theorem can be used to express the $3-$point midpoint formula as

$$f'(x_0)=\frac{1}{2h}[f(x_0+h)-f(x_0-h)]-\frac{h^2}{6}f'''(x_0)-\frac{h^4}{120}f^{(5)}(x_0)-...$$

   Find approximations of order $O(h^2)$, $O(h^4)$, $O(h^6)$ and $O(h^8)$ for $f'(2.0)$ when $f(x)=xe^x$ and $h=0.2.$

2. Using the formula

$$f''(x_0)=\frac{1}{h^2}[f(x_0-h)-2f(x_0)+f(x_0+h)]-\frac{h^2}{12}f^{(4)}(x_0),$$

find an approximation of order $O(h^4)$ for $f''(2.0)$ with $h = 0.1$.

Solutions:

1. Letting $M = f'(2.0)$ and $N_1(h) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right]$, we have the constants $k_1 = -\frac{h^2}{6} f'''(x_0)$ and $k_2 = -\frac{h^4}{120} f^{(5)}(x_0) - \ldots$ exist.

   Thus, the $O(h^2)$ approximation is

   $$f'(2.0) = M \approx N_1(h) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] = \frac{1}{2(0.2)}\left[f(2.2) - f(1.8)\right] = 22.414160.$$

   $$N_1\left(\frac{0.2}{2}\right) = N_1(0.1) = \frac{1}{2(0.1)}\left[f(2.1) - f(1.9)\right] = 22.228786$$

   Thus, the $O(h^4)$ approximation is

   $$\begin{aligned} f'(2.0) \approx N_2(0.2) = \frac{4N_1\left(\frac{0.2}{2}\right) - N_1(0.2)}{4-1} &= \frac{4N_1(0.1) - N_1(0.2)}{3} \\ &= \frac{4(22.228786) - 22.414160}{3} \\ &= 22.1669950. \end{aligned}$$

   $$\begin{aligned} N_2\left(\frac{0.2}{2}\right) = \frac{4N_1\left(\frac{\frac{0.2}{2}}{2}\right) - N_1\left(\frac{0.2}{2}\right)}{4-1} &= \frac{4\left[\frac{1}{2(0.05)}\left[f(2.05) - f(1.95)\right]\right] - 22.228786}{3} \\ &= \frac{4(22.182564) - 22.228786}{3} \\ &= 22.167157 \end{aligned}$$

   $\therefore$ the $O(h^6)$ approximation is

   $$\begin{aligned} f'(2.0) \approx N_3(0.2) = \frac{4^2 N_2\left(\frac{0.2}{2}\right) - N_2(0.2)}{4^2 - 1} &= \frac{16(22.167157) - 22.166995}{15} \\ &= 22.167168. \end{aligned}$$

$$N_3\left(\frac{0.2}{2}\right)=\frac{4^2 N_2\left(\frac{0.2}{4}\right)-N_2\left(\frac{0.2}{2}\right)}{4^2-1}=\frac{16N_2\left(0.05\right)-N_2\left(0.1\right)}{15}$$

$$=\frac{16\left[\frac{4N_1\left(\frac{0.05}{2}\right)-N_1(0.05)}{3}\right]-N_1(0.1)}{15}$$

$$=\frac{\frac{64\left[\frac{1}{2(0.025)}\left[f(2.025)-f(1.975)\right]\right]-16(22.182564)}{3}-22.167157}{15}$$

$$=\frac{64(22.17102)-16(22.182564)-22.167157}{15}$$

$$=22.167173.$$

$\therefore$ the $O(h^8)$ approximation is

$$f'(2.0)\approx N_4(0.2)=\frac{4^3 N_3\left(0.1\right)-N_3(0.2)}{4^3-1}=\frac{64(22.167157)-22.167168}{63}=22.167173.$$

2. Taking $N_1(h)=\frac{1}{h^2}[f(x_0-h)-2f(x_0)+f(x_0+h)]$, we get $O(h^2)$ approximation

$$f''(2.0)=M\approx N_1(0.1)=\frac{1}{(0.1)^2}[f(1.9)-2f(2.0)+f(2.1)]=29.5932.$$

$$N_1\left(\frac{0.1}{2}\right)=N_1\left(0.05\right)=\frac{1}{(0.05)^2}[f(1.95)-2f(2.0)+f(2.05)]$$

$$=400(13.705941)-2(14.778112)+15.924197$$

$$=29.5656.$$

Thus, the $O(h^4)$ approximation is

$$f''(2.0)\approx N_2(0.1)=\frac{4N_1\left(\frac{0.1}{2}\right)-N_1(0.1)}{4-1}=\frac{4N_1\left(0.05\right)-N_1(0.1)}{3}$$

$$=\frac{4(29.5656)-29.5632}{3}$$

$$=29.5564.$$

△

<u>THE END!</u>