5.4 Numerical Differentiation

- There are two major reasons for considering numerical differentiation.

1. Approximation of derivatives in (ODEs) ordinary differential equations and (PDEs) partial differential equations: this is done in order to reduce the differential equation to a form that can be solved more easily than the original differential equation.
2. Forming the derivative of a discontinuous function $f(x)$ which is known only as the given data $\{(x_i, y_i) \mid i = 1, \cdots, m\}$: y_i is given approximately, i.e., $y_i \approx f(x_i)$ for $i = 1, 2, \cdots, m$.

- Recall the definition of derivative

$$f'(x) = \frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \lim_{x \to a} \frac{f(x) - f(a)}{x - a},$$

where f is a smooth function. Then the numerical derivative of $f(x)$ is given by

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

Example1

Find $D_h f(x)$ for the function $f(x) = \cos x$ at $x = \pi/6$. We can see that the errors are nearly proportional to h. See the table in the next page. This can be proved using the Taylor's theorem.

h	$D_h f$	Error	Ratio
$1/10$	-0.54243	0.04243	
$1/20$	-0.52144	0.02144	1.98
$1/40$	-0.51077	0.01077	1.99
$1/80$	-0.50540	0.00540	1.99
$1/160$	-0.50270	0.00270	2.00
$1/320$	-0.50135	0.00135	2.00

- Two types of the numerical derivative

1. The forward difference formula:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \quad \text{for } h > 0.$$

2. The backward difference formula

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}, \quad \text{for } h > 0.$$

- For two cases we have the error formula

$$\left|f'(x) - D_h f(x)\right| = \frac{h}{2}\left|f''(c)\right|,$$

where $c \in (x, x+h)$ or $c \in (x-h, h)$.

- Using the interpolating polynomial $P_2(x)$, we can derive the central difference formula

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

which is more accurate than the forwarded difference formula.

Theorem

Assume that $f \in C^{n+2}[a, b]$. Let $x_0, x_1, x_2, \cdots, x_n \in [a, b]$ be $n+1$ distinct interpolation nodes and $t \in [a, b]$ be an arbitrary given point. Then we have

$$f'(t) - P_n'(t) = \Psi_n(t) \frac{f^{(n+1)}(c_1)}{(n+2)!} + \Psi_n'(t) \frac{f^{(n+1)}(c_2)}{(n+1)!},$$

where

$$\Psi_n(t) = (t - x_0)(t - x_1) \cdots (t - x_n).$$

- Using the previous theorem, we can derive the error formula for the central difference formula:

$$\left| f'(x) - \frac{f(x+h) - f(x-h)}{2h} \right| = \frac{h^2}{6} \left| f'''(c_2) \right|$$

with $x - h \leq c_2 \leq x + h$.

- **The method of undetermined coefficients**

To derive an approximation for $f''(x)$ at $x = t$, we write

$$f''(t) \approx D_h^{(2)} f(t) = A f(t+h) + B f(t) + C f(t-h),$$

where A, B, and C are unknown coefficients. Then using the Taylor polynomial approximation and assuming that $f \in C^4[a, b]$, we can get

$$D_h^{(2)} f(t) = \frac{f(t+h) - 2f(t) + f(t-h)}{h^2}. \tag{1}$$

The error formulas is

$$\left| f''(t) - D_h^{(2)} f(t) \right| \approx \frac{h^2}{12} \left| f^{(4)}(t) \right|. \tag{2}$$

- **Effects of Error in Function Values**

Recall that

$$D_h^{(2)} f(x_1) = \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2} \approx f''(x_1),$$

where $h > 0$ is the size of subintervals. Let $\widehat{f_0}, \widehat{f_1}, \widehat{f_2}$ be the actual values used in the computation at $x = x_0 = x_1 - h$, $x = x_1$ and $x = x_2 = x_1 + h$, respectively. Then the errors are given by

$$f(x_i) - \widehat{f_i} = \varepsilon_i, \quad \text{for } i = 0, 1, 2.$$

Also the actual value $\widehat{D}_h^{(2)} f(x_1)$ is defined by

$$\widehat{D}_h^{(2)} f(x_1) = \frac{\widehat{f_2} - 2\widehat{f_1} + \widehat{f_0}}{h^2}.$$

Thus we can derive the error formula

$$\left| f''(x_1) - \widehat{D}_h^{(2)} f(x_1) \right| \le \frac{h^2}{12} \left| f^{(4)}(x_i) \right| + \frac{|\varepsilon_2 - 2\varepsilon_1 + \varepsilon_0|}{h^2}.$$

- The errors ε_i with $i = 1,2,3$ in the interval $[-\delta, \delta]$. Then the error formula becomes

$$\left|f''(x_1) - \widehat{D}_h^{(2)} f(x_1)\right| \le \frac{h^2}{12}\left|f^{(4)}(x_i)\right| + \frac{4\delta}{h^2}.$$

Example2

Calculate $\widehat{D}_h^{(2)} f(x_1)$ for $f(x) = \cos(x)$ at $x_1 = \pi/3$. To show the effect of rounding errors, the actual values $\widehat{f}_i$ are obtained by rounding $f(x_i)$ to six digits and the errors satisfy

$$|\varepsilon_i| \le 5.0 \times 10^{-7} = \delta, \quad i = 0,1,2.$$

Calculation of $\widehat{D}_h^{(2)} f(x_i)$

h	$\widehat{D}_h^{(2)} f(x_i)$	Error
0.5	-0.848128	0.017987
0.25	-0.861504	0.004521
0.125	-0.864832	0.001193
0.0625	-0.865536	0.000489