NUMERICAL DIFFERENTIATION

There are two major reasons for considering numerically approximations of the differentiation process.

1. *Approximation of derivatives in ordinary differential equations and 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 function* $f(x)$ *which is known only as empirical data* $\{(x_i, y_i) \mid i = 1, \ldots, m\}$. The data generally is known only approximately, so that $y_i \approx f(x_i)$, $i = 1, \ldots, m$.

Recall the definition

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

This justifies using

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \equiv D_h f(x) \qquad (1)$$

for small values of h. The approximation $D_h f(x)$ is called a *numerical derivative* of $f(x)$ with stepsize h.

Example. Use $D_h f(x)$ to approximate the derivative of $f(x) = \cos(x)$ at $x = \pi/6$. In the table, the error is almost halved when h is halved.

h	$D_h f$	*Error*	*Ratio*
0.1	-0.54243	0.04243	
0.05	-0.52144	0.02144	1.98
0.025	-0.51077	0.01077	1.99
0.0125	-0.50540	0.00540	1.99
0.00625	-0.50270	0.00270	2.00
0.003125	-0.50135	0.00135	2.00

Error behaviour. Using Taylor's theorem,

$$f(x+h) = f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(c)$$

with c between x and $x+h$. Evaluating (1),

$$\begin{aligned} D_h f(x) &= \frac{1}{h}\left\{\left[f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(c)\right] - f(x)\right\} \\ &= f'(x) + \tfrac{1}{2}hf''(c) \end{aligned}$$

$$f'(x) - D_h f(x) = -\tfrac{1}{2}hf''(c) \tag{2}$$

Using a higher order Taylor expansion,

$$\begin{aligned} f'(x) - D_h f(x) &= -\tfrac{1}{2}hf''(x) - \tfrac{1}{6}h^2 f'''(c), \\ f'(x) - D_h f(x) &\approx -\tfrac{1}{2}hf''(x) \end{aligned} \tag{3}$$

for small values of h.

For $f(x) = \cos x$,

$$f'(x) - D_h f(x) = \tfrac{1}{2}h\cos c, \qquad c \in \left[\tfrac{\pi}{6}, \tfrac{\pi}{6} + h\right]$$

In the preceding table, check the accuracy of the approximation (3) with $x = \frac{\pi}{6}$.

The formula (1),

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

is called a *forward difference formula* for approximating $f'(x)$. In contrast, the approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}, \qquad h > 0 \tag{4}$$

is called a *backward difference formula* for approximating $f'(x)$. A similar derivation leads to

$$f'(x) - \frac{f(x) - f(x-h)}{h} = \frac{h}{2} f''(c) \tag{5}$$

for some c between x and $x - h$. The accuracy of the backward difference formula (4) is essentially the same as that of the forward difference formula (1).

The motivation for this formula is in applications to solving differential equations.

DIFFERENTIATION USING INTERPOLATION

Let $P_n(x)$ be the degree n polynomial that interpolates $f(x)$ at $n+1$ node points $x_0, x_1, \ldots, x_n$. To calculate $f'(x)$ at some point $x = t$, use

$$f'(t) \approx P_n'(t) \tag{6}$$

Many different formulas can be obtained by varying n and by varying the placement of the nodes $x_0, \ldots, x_n$ relative to the point t of interest.

Example. Take $n = 2$, and use evenly spaced nodes $x_0, x_1 = x_0 + h$, $x_2 = x_1 + h$. Then

$$\begin{aligned} P_2(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) \\ P_2'(x) &= f(x_0)L_0'(x) + f(x_1)L_1'(x) + f(x_2)L_2'(x) \end{aligned}$$

with

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$
$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$
$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

Forming the derivatives of these Lagrange basis functions and evaluating them at $x = x_1$

$$f'(x_1) \approx P_2'(x_1) = \frac{f(x_1+h) - f(x_1-h)}{2h} \equiv D_h f(x_1) \tag{7}$$

For the error,

$$f'(x_1) - \frac{f(x_1+h) - f(x_1-h)}{2h} = -\frac{h^2}{6} f'''(c_2) \tag{8}$$

with $x_1 - h \le c_2 \le x_1 + h$.

A proof of this begins with the interpolation error formula

$$\begin{aligned} f(x) - P_2(x) &= \Psi_2(x) f[x_0, x_1, x_2, x] \\ \Psi_2(x) &= (x - x_0)(x - x_1)(x - x_2) \end{aligned}$$

Differentiate to get

$$\begin{aligned} f'(x) - P_2'(x) &= \Psi_2(x) \frac{d}{dx} f[x_0, x_1, x_2, x] \\ &\quad + \Psi_2'(x) f[x_0, x_1, x_2, x] \end{aligned}$$

$$
\begin{aligned}
f'(x) - P_2'(x) &= \Psi_2(x) \frac{d}{dx} f[x_0, x_1, x_2, x] \\
&\qquad + \Psi_2'(x) f[x_0, x_1, x_2, x]
\end{aligned}
$$

With properties of the divided difference, we can show

$$
f'(x) - P_2'(x) = \tfrac{1}{24} \Psi_2(x) f^{(4)}\left(c_{1,x}\right) + \tfrac{1}{6} \Psi_2'(x) f^{(3)}\left(c_{2,x}\right)
$$

with $c_{1,x}$ and $c_{2,x}$ between the smallest and largest of the values $\{x_0, x_1, x_2, x\}$. Letting $x = x_1$ and noting that $\Psi_2(x_1) = 0$, we obtain (8).

Example. Take $f(x) = \cos(x)$ and $x_1 = \frac{1}{6}\pi$. Then (7) is illustrated as follows.

h	$D_h f$	*Error*	*Ratio*
0.1	-0.49916708	-0.0008329	
0.05	-0.49979169	-0.0002083	4.00
0.025	-0.49994792	-0.00005208	4.00
0.0125	-0.49998698	-0.00001302	4.00
0.00625	-0.49999674	-0.000003255	4.00

Note the smaller errors and faster convergence as compared to the forward difference formula (1).

UNDETERMINED COEFFICIENTS

Derive an approximation for $f''(x)$ at $x = t$. Write

$$\begin{aligned} f''(t) \approx D_h^{(2)} f(t) \equiv {} & Af(t+h) \\ & + Bf(t) + Cf(t-h) \end{aligned} \tag{9}$$

with A, B, and C unspecified constants. Use Taylor polynomial approximations

$$\begin{aligned} f(t-h) &\approx f(t) - hf'(t) + \frac{h^2}{2} f''(t) \\ &\quad - \frac{h^3}{6} f'''(t) + \frac{h^4}{24} f^{(4)}(t) \\ f(t+h) &\approx f(t) + hf'(t) + \frac{h^2}{2} f''(t) \\ &\quad + \frac{h^3}{6} f'''(t) + \frac{h^4}{24} f^{(4)}(t) \end{aligned} \tag{10}$$

Substitute into (9) and rearrange:

$$
\begin{aligned}
D_h^{(2)} f(t) \approx{} & (A+B+C) f(t) \\
& + h(A-C) f'(t) + \frac{h^2}{2}(A+C) f''(t) \\
& + \frac{h^3}{6}(A-C) f'''(t) + \frac{h^4}{24}(A+C) f^{(4)}(t)
\end{aligned}
\tag{11}
$$

To have

$$
D_h^{(2)} f(t) \approx f''(t) \tag{12}
$$

for arbitrary functions $f(x)$, require

$$
\begin{aligned}
A+B+C = 0: &\quad \text{coefficient of } f(t) \\
h(A-C) = 0: &\quad \text{coefficient of } f'(t) \\
\frac{h^2}{2}(A+C) = 1: &\quad \text{coefficient of } f''(t)
\end{aligned}
$$

Solution:

$$
A = C = \frac{1}{h^2}, \qquad B = -\frac{2}{h^2} \tag{13}
$$

This determines

$$D_h^{(2)} f(t) = \frac{f(t+h) - 2f(t) + f(t-h)}{h^2} \tag{14}$$

For the error, substitute (13) into (11):

$$D_h^{(2)} f(t) \approx f''(t) + \frac{h^2}{12} f^{(4)}(t)$$

Thus

$$f''(t) - \frac{f(t+h) - 2f(t) + f(t-h)}{h^2} \approx \frac{-h^2}{12} f^{(4)}(t) \tag{15}$$

Example. Let $f(x) = \cos(x)$, $t = \frac{1}{6}\pi$; use (14) to calculate $f''(t) = -\cos\left(\frac{1}{6}\pi\right)$.

h	$D_h^{(2)} f$	*Error*	*Ratio*
0.5	-0.84813289	$-1.789\text{E}-2$	
0.25	-0.86152424	$-4.501\text{E}-3$	3.97
0.125	-0.86489835	$-1.127\text{E}-3$	3.99
0.0625	-0.86574353	$-2.819\text{E}-4$	4.00
0.03125	-0.86595493	$-7.048\text{E}-5$	4.00

EFFECTS OF ERROR IN FUNCTION VALUES

Recall

$$D_h^{(2)} f(x_1) = \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2} \approx f''(x_1)$$

with $x_2 = x_1 + h$, $x_0 = x_1 - h$. Assume the actual function values used in the computation contain data error, and denote these values by $\widehat{f}_0$, $\widehat{f}_1$, and $\widehat{f}_2$. Introduce the data errors:

$$\epsilon_i = f(x_i) - \widehat{f}_i, \qquad i = 0, 1, 2 \tag{16}$$

The actual quantity calculated is

$$\widehat{D}_h^{(2)} f(x_1) = \frac{\widehat{f}_2 - 2\widehat{f}_1 + \widehat{f}_2}{h^2} \tag{17}$$

For the error in this quantity, replace $\widehat{f}_j$ by $f(x_j) - \epsilon_j$, $j = 0, 1, 2$, to obtain the following:

$$
\begin{aligned}
f''(x_1) - \widehat{D}_h^{(2)} f(x_1) &= f''(x_1) \\
&\quad - \frac{[f(x_2) - \epsilon_2] - 2[f(x_1) - \epsilon_1] + [f(x_0) - \epsilon_0]}{h^2} \\
&= \left[f''(x_1) - \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2} \right] \\
&\qquad + \frac{\epsilon_2 - 2\epsilon_1 + \epsilon_0}{h^2} \\
&\approx -\tfrac{1}{12} h^2 f^{(4)}(x_1) + \frac{\epsilon_2 - 2\epsilon_1 + \epsilon_0}{h^2}
\end{aligned}
\tag{18}
$$

The last line uses (15).

The errors $\{\epsilon_0, \epsilon_1, \epsilon_2\}$ are generally random in some interval $[-\delta, \delta]$. If $\left\{\widehat{f}_0, \widehat{f}_1, \widehat{f}_2\right\}$ are experimental data, then δ is a bound on the experimental error. If $\left\{\widehat{f}_j\right\}$ are obtained from computing $f(x)$ in a computer, then the errors ϵ_j are the combination of rounding or chopping errors and δ is a bound on these errors.

In either case, (18) yields the approximate inequality

$$\left|f''(x_1) - \widehat{D}_h^{(2)} f(x_1)\right| \le \frac{h^2}{12}\left|f^{(4)}(x_1)\right| + \frac{4\delta}{h^2} \quad (19)$$

This suggests that as $h \to 0$, the error will eventually increase, because of the final term $\frac{4\delta}{h^2}$.

Example. Calculate $\widehat{D}_h^{(2)}(x_1)$ for $f(x) = \cos(x)$ at $x_1 = \frac{1}{6}\pi$. To show the effect of rounding errors, the values $\widehat{f}_i$ are obtained by rounding $f(x_i)$ to six significant digits; and the errors satisfy

$$|\epsilon_i| \le 5.0 \times 10^{-7} = \delta, \qquad i = 0, 1, 2$$

Other than these rounding errors, the formula $\widehat{D}_h^{(2)} f(x_1)$ is calculated exactly. In this example, the bound (19) becomes

$$\begin{aligned}\left|f''(x_1) - \widehat{D}_h^{(2)} f(x_1)\right| &\le \tfrac{1}{12} h^2 \cos\left(\tfrac{1}{6}\pi\right) \\ &\quad + \left(\tfrac{4}{h^2}\right)\left(5 \times 10^{-7}\right) \\ &\doteq 0.0722 h^2 + \tfrac{2\times 10^{-6}}{h^2} \equiv E(h)\end{aligned}$$

For $h = 0.125$, the bound $E(h) \doteq 0.00126$, which is not too far off from the actual error given in the table.

h	$\widehat{D}_h^{(2)} f(x_1)$	*Error*
0.5	-0.848128	-0.017897
0.25	-0.861504	-0.004521
0.125	-0.864832	-0.001193
0.0625	-0.865536	-0.000489
0.03125	-0.865280	-0.000745
0.015625	-0.860160	-0.005865
0.0078125	-0.851968	-0.014057
0.00390625	-0.786432	-0.079593

The bound $E(h)$ indicates that there is a smallest value of h, call it h_*, below which the error bound will begin to increase. To find it, let $E'(h) = 0$, with its root being h_*. This leads to $h_* \doteq 0.0726$, which is consistent with the behavior of the errors in the table.