Numerical differentiation: finite differences

The derivative of a function f at the point x is defined as the limit of a difference quotient:

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

In other words, the difference quotient $\dfrac{f(x+h) - f(x)}{h}$ is an approximation of the derivative $f'(x)$, and this approximation gets better as h gets smaller.
How does the error of the approximation depend on h?
Taylor's theorem with remainder gives the Taylor series expansion

$$f(x+h) = f(x) + hf'(x) + h^2 \frac{f''(\xi)}{2!} \quad \text{where } \xi \text{ is some number between } x \text{ and } x+h.$$

Rearranging gives

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

which tells us that the error is proportional to h to the power 1, so $\dfrac{f(x+h) - f(x)}{h}$ is said to be a "first-order" approximation.
If $h > 0$, say $h = \Delta x$ where Δx is a finite (as opposed to infinitesimal) positive number, then

$$\frac{f(x+\Delta x) - f(x)}{\Delta x}$$

is called the first-order or $O(\Delta x)$ *forward difference* approximation of $f'(x)$.
If $h < 0$, say $h = -\Delta x$ where $\Delta x > 0$, then

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

is called the first-order or $O(\Delta x)$ *backward difference* approximation of $f'(x)$.

By combining different Taylor series expansions, we can obtain approximations of $f'(x)$ of various orders. For instance, subtracting the two expansions

$$\begin{aligned} f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(\xi_1)}{3!}, \qquad && \xi_1 \in (x,\ x+\Delta x) \\ f(x-\Delta x) &= f(x) - \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(\xi_2)}{3!}, \qquad && \xi_2 \in (x-\Delta x,\ x) \end{aligned}$$

gives $f(x+\Delta x) - f(x-\Delta x) = 2\Delta x\, f'(x) + \Delta x^3 \dfrac{\big(f'''(\xi_1) + f'''(\xi_2)\big)}{6}$, so that

$$\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} - f'(x) = \Delta x^2 \frac{\big(f'''(\xi_1) + f'''(\xi_2)\big)}{12}$$

Hence $\dfrac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$ is an approximation of $f'(x)$ whose error is proportional to Δx^2. It is called the second-order or $O(\Delta x^2)$ *centered difference* approximation of $f'(x)$.

If we use expansions with more terms, higher-order approximations can be derived, e.g. consider

$$
\begin{aligned}
f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(x)}{4!} + \Delta x^5 \frac{f^{(5)}(\xi_1)}{5!} \\
f(x-\Delta x) &= f(x) - \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(x)}{4!} - \Delta x^5 \frac{f^{(5)}(\xi_2)}{5!} \\
f(x+2\Delta x) &= f(x) + 2\Delta x\, f'(x) + 4\Delta x^2 \frac{f''(x)}{2!} + 8\Delta x^3 \frac{f'''(x)}{3!} + 16\Delta x^4 \frac{f^{(4)}(x)}{4!} + 32\Delta x^5 \frac{f^{(5)}(\xi_3)}{5!} \\
f(x-2\Delta x) &= f(x) - 2\Delta x\, f'(x) + 4\Delta x^2 \frac{f''(x)}{2!} - 8\Delta x^3 \frac{f'''(x)}{3!} + 16\Delta x^4 \frac{f^{(4)}(x)}{4!} - 32\Delta x^5 \frac{f^{(5)}(\xi_4)}{5!}
\end{aligned}
$$

Taking $8 \times$ (first expansion $-$ second expansion) $-$ (third expansion $-$ fourth expansion) cancels out the Δx^2 and Δx^3 terms; rearranging then yields a fourth-order centered difference approximation of $f'(x)$.

Approximations of higher derivatives $f''(x), f'''(x), f^{(4)}(x)$ etc. can be obtained in a similar manner. For example, adding

$$
\begin{aligned}
f(x+\Delta x) &= f(x) + \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(\xi_1)}{4!} \cdots \\
f(x-\Delta x) &= f(x) - \Delta x\, f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(\xi_2)}{4!} \cdots
\end{aligned}
$$

gives $f(x+\Delta x) + f(x-\Delta x) = 2f(x) + \Delta x^2 f''(x) + \Delta x^4 \frac{\left(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right)}{24}$, so that

$$
\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} - f''(x) = \Delta x^2 \frac{\left(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right)}{24}
$$

Hence $\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2}$ is a second-order centered difference approximation of the second derivative $f''(x)$.

Here are some commonly used second- and fourth-order "finite difference" formulas for approximating first and second derivatives:

$O(\Delta x^2)$ centered difference approximations:
- $f'(x)$: $\{f(x+\Delta x) - f(x-\Delta x)\}/(2\Delta x)$
- $f''(x)$: $\{f(x+\Delta x) - 2f(x) + f(x-\Delta x)\}/\Delta x^2$

$O(\Delta x^2)$ forward difference approximations:
- $f'(x)$: $\{-3f(x) + 4f(x+\Delta x) - f(x+2\Delta x)\}/(2\Delta x)$
- $f''(x)$: $\{2f(x) - 5f(x+\Delta x) + 4f(x+2\Delta x) - f(x+3\Delta x)\}/\Delta x^3$

$O(\Delta x^2)$ backward difference approximations:
- $f'(x)$: $\{3f(x) - 4f(x-\Delta x) + f(x-2\Delta x)\}/(2\Delta x)$
- $f''(x)$: $\{2f(x) - 5f(x-\Delta x) + 4f(x-2\Delta x) - f(x-3\Delta x)\}/\Delta x^3$

$O(\Delta x^4)$ centered difference approximations:
- $f'(x)$: $\{-f(x+2\Delta x) + 8f(x+\Delta x) - 8f(x-\Delta x) + f(x-2\Delta x)\}/(12\Delta x)$
- $f''(x)$: $\{-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(t) + 16f(x-\Delta x) - f(x-2\Delta x)\}/(12\Delta x^2)$

In science and engineering applications it is often the case that an exact formula for $f(x)$ is not known. We may only have a set of data points (x_1, y_1), $(x_2, y_2), \ldots, (x_n, y_n)$ available to describe the functional dependence $y = f(x)$. If we need to estimate the rate of change of y with respect to x in such a situation, we can use finite difference formulas to compute approximations of $f'(x)$. It is appropriate to use a forward difference at the left endpoint $x = x_1$, a backward difference at the right endpoint $x = x_n$, and centered difference formulas for the interior points.