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

$$f(x + h) = f(x) + hf'(x) + \frac{h^2 f''(\xi)}{2!}$$

where $\xi$ is some number between $x$ 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 $\frac{f(x + h) - f(x)}{h}$ is said to be a “first-order” approximation.

If $h > 0$, say $h = \Delta x$ where $\Delta x$ 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

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(\xi_1)}{3!}, \quad \xi_1 \in (x, x + \Delta x)$$

$$f(x - \Delta x) = f(x) - \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(\xi_2)}{3!}, \quad \xi_2 \in (x - \Delta x, x)$$

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

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

Hence $\frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}$ is an approximation of $f'(x)$ whose error is proportional to $\Delta x^2$. 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

\[
\begin{align*}
f(x + \Delta x) &= f(x) + \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(x)}{4!} + \Delta x^5 \frac{f^{(5)}(\xi)}{5!}
f(x - \Delta x) &= f(x) - \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(x)}{4!} - \Delta x^5 \frac{f^{(5)}(\xi_2)}{5!}
f(x + 2\Delta x) &= f(x) + 2\Delta x f'(x) + 4\Delta x^2 \frac{f''(x)}{2!} + 8\Delta x^3 \frac{f'''(x)}{3!} + 16\Delta x^4 \frac{f^{(4)}(x)}{4!} + 32\Delta x^5 \frac{f^{(5)}(\xi_3)}{5!}
f(x - 2\Delta x) &= f(x) - 2\Delta x f'(x) + 4\Delta x^2 \frac{f''(x)}{2!} - 8\Delta x^3 \frac{f'''(x)}{3!} + 16\Delta x^4 \frac{f^{(4)}(x)}{4!} - 32\Delta x^5 \frac{f^{(5)}(\xi_4)}{5!}
\end{align*}
\]

Taking \(8 \times (\text{first expansion} - \text{second expansion}) - (\text{third expansion} - \text{fourth expansion})\) cancels out the \(\Delta x^2\) and \(\Delta x^3\) 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

\[
\begin{align*}
f(x + \Delta x) &= f(x) + \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} + \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(\xi_1)}{4!} \ldots 
f(x - \Delta x) &= f(x) - \Delta x f'(x) + \Delta x^2 \frac{f''(x)}{2!} - \Delta x^3 \frac{f'''(x)}{3!} + \Delta x^4 \frac{f^{(4)}(\xi_2)}{4!} \ldots 
\end{align*}
\]

gives

\[
\frac{f(x + \Delta x) + f(x - \Delta x)}{2\Delta x} = 2f(x) + \Delta x^2 f''(x) + \Delta x^4 \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{24}, \text{ so that}
\]

\[
\frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} = f''(x) = \Delta x^2 \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{24}
\]

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:

\[
\begin{align*}
f'(x) &\colon \left\{ f(x + \Delta x) - f(x - \Delta x) \right\} / (2\Delta x) 
f''(x) &\colon \left\{ f(x + \Delta x) - 2f(x) + f(x - \Delta x) \right\} / \Delta x^2 
\end{align*}
\]

\(O(\Delta x^2)\) forward difference approximations:

\[
\begin{align*}
f'(x) &\colon \left\{ -3f(x) + 4f(x + \Delta x) - f(x + 2\Delta x) \right\} / (2\Delta x) 
f''(x) &\colon \left\{ 2f(x) - 5f(x + \Delta x) + 4f(x + 2\Delta x) - f(x + 3\Delta x) \right\} / \Delta x^3
\end{align*}
\]

\(O(\Delta x^2)\) backward difference approximations:

\[
\begin{align*}
f'(x) &\colon \left\{ 3f(x) - 4f(x - \Delta x) + f(x - 2\Delta x) \right\} / (2\Delta x) 
f''(x) &\colon \left\{ 2f(x) - 5f(x - \Delta x) + 4f(x - 2\Delta x) - f(x - 3\Delta x) \right\} / \Delta x^3
\end{align*}
\]

\(O(\Delta x^4)\) centered difference approximations:

\[
\begin{align*}
f'(x) &\colon \left\{ -f(x + 2\Delta x) + 8f(x + \Delta x) - 8f(x - \Delta x) + f(x - 2\Delta x) \right\} / (12\Delta x) 
f''(x) &\colon \left\{ -f(x + 2\Delta x) + 16f(x + \Delta x) - 30f(t) + 16f(x - \Delta x) - f(x - 2\Delta x) \right\} / (12\Delta x^2)
\end{align*}
\]

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.