Numerical Differentiation

We can use Taylor series expansions to derive formulas for numerical differentiation based on *finite divided differences*. For example, recall that

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2}h^2,$$

where $x_i \le \xi \le x_{i+1}$. Hence,

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi)}{2}h,$$

and an approximation for the first derivative is given by

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h).$$

Similarly, using the Taylor series expansion for $f'(x)$, we get

$$f'(x_{i+1}) = f'(x_i) + f''(x_i)h + \frac{f'''(\xi)}{2}h^2$$

or

$$f''(x_i) = \frac{f'(x_{i+1}) - f'(x_i)}{h} + O(h).$$

However, we also know that

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi_1)}{2}h,$$

for some $x_i \le \xi_1 \le x_{i+1}$, and

$$f'(x_{i+1}) = \frac{f(x_{i+2}) - f(x_{i+1})}{h} - \frac{f''(\xi_2)}{2}h,$$

for some $x_{i+1} \le \xi_2 \le x_{i+2}$. Putting these last three equations together, we get

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + \frac{f''(\xi_1) - f''(\xi_2)}{2} + O(h).$$

Now, since

$$f''(\xi_1) = f''(x_{i+1}) + f'''(x_{i+1})(\xi_1 - x_{i+1}) + O\left(h^2\right),$$

and

$$f''(\xi_2) = f''(x_{i+1}) + f'''(x_{i+1})(\xi_2 - x_{i+1}) + O\left(h^2\right),$$

it follows that

$$f''(\xi_1) - f''(\xi_2) = f'''(x_{i+1})(\xi_1 - \xi_2) + O\left(h^2\right) = O(h),$$

and we get

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h).$$

A similar approach can be used to get $O(h)$ approximations for derivatives of any order.

We can get improved approximations for derivatives by retaining more terms in the Taylor series expansion, and using the $O(h)$ approximations where necessary. For example, expanding again around x_i, we get

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + O(h^3)$$

or

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

Then using the $O(h)$ approximation for $f''(x_i)$, we get

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$
$$= \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2).$$

Similar finite-divided-difference formulas can be developed using so-called backward-differences and centered-differences, which we have not really talked about. A list of possible numerical differentiation formulas of this type is given in your book in Tables 23.1-23.3. It should be noted that the order of the truncation error for the centered-difference formulas is higher than the order for the forward-difference and backward-difference formulas, but that more data points are required for these formulas as well.

Example: Estimate the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using finite divided differences with a step size of $h = 0.25$. The true answer is $f'(0.5) = -0.9125$.

The data needed to complete this problem are:

$$
\begin{aligned}
x_{i-2} &= 0, & f(x_{i-2}) &= 1.2, \\
x_{i-1} &= 0.25, & f(x_{i-1}) &= 1.103516, \\
x_i &= 0.5, & f(x_i) &= 0.925, \\
x_{i+1} &= 0.75, & f(x_{i+1}) &= 0.6363281, \\
x_{i+2} &= 1, & f(x_{i+2}) &= 0.2.
\end{aligned}
$$

The answers based on the $O(h)$ and $O(h^2)$ forward-difference formulas in Table 23.1 are:

$$
\begin{aligned}
f'(0.5) &\approx \frac{f(x_{i+1}) - f(x_i)}{h} \\
&= \frac{f(0.75) - f(0.5)}{0.25} \\
&= -1.1546876, \quad \varepsilon_t = 26.5\%,
\end{aligned}
$$

$$
\begin{aligned}
f'(0.5) &\approx \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \\
&= \frac{-f(1) + 4f(0.75) - 3f(0.5)}{2(0.25)} \\
&= -0.859375, \quad \varepsilon_t = 5.82\%.
\end{aligned}
$$

The answers based on the $O(h)$ and $O(h^2)$ backward difference formulas are:

$$
\begin{aligned}
f'(0.5) &\approx \frac{f(x_i) - f(x_{i-1})}{h} \\
&= \frac{f(0.5) - f(0.25)}{0.25} \\
&= -0.714064, \quad \varepsilon_t = 21.7\%,
\end{aligned}
$$

$$
\begin{aligned}
f'(0.5) &\approx \frac{3f(x_i)-4f(x_{i-1})+f(x_{i-2})}{2h} \\
&= \frac{3f(0.5)-4f(0.25)+f(0)}{2(0.25)} \\
&= -0.878125, \quad \varepsilon_t = 3.77\%.
\end{aligned}
$$

The answers based on the $O(h^2)$ and $O(h^4)$ centered-difference formulas are:

$$
\begin{aligned}
f'(0.5) &\approx \frac{f(x_{i+1})-f(x_{i-1})}{2h} \\
&= \frac{f(0.75)-f(0.25)}{2(0.25)} \\
&= -0.934, \quad \varepsilon_t = 2.4\%,
\end{aligned}
$$

$$
\begin{aligned}
f'(0.5) &\approx \frac{-f(x_{i+2})+8f(x_{i+1})-8f(x_{i-1})+f(x_{i-2})}{12h} \\
&= \frac{-f(1)+8f(0.75)-8f(0.25)+f(0)}{12(0.25)} \\
&= -0.9125, \quad \varepsilon_t = 0\%.
\end{aligned}
$$

Notice that the answers based on the centered-difference formulas are the most accurate and that the answer based on the $O(h^4)$ centered-difference formula is exact. The $O(h^4)$ centered-difference formula will be exact whenever $f(x)$ is a fourth-degree polynomial.

Richardson's Extrapolation

Recall that we could improve the estimates of integrals based on successive applications of the trapezoidal rule using Richardson's extrapolation. In particular, if the samples of the function were evenly spaced, and $I(h_1)$ and $I(h_2)$ were two estimates of the integral with $h_2 = h_1/2$, then we could get a new estimate using the formula

$$I = \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1).$$

Further, this process could be repeated recursively using higher-order extrapolation formulas to give better and better estimates.

In a similar fashion, Richardson's extrapolation technique can be used to improve estimates of derivatives, and the formulas are the same. That is, if $D(h_1)$ and $D(h_2)$ are two estimates of a derivative with $h_2 = h_1/2$, then we can get a new estimate using the formula

$$D = \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1).$$

If the two original estimates were $O(h)$, then the new estimate is $O(h^2)$; if the two original estimates were $O(h^2)$, then the new estimate is $O(h^4)$; and so forth.

Derivatives of Unequally Spaced Data

If the function of interest is evaluated at unequally spaced points, the best approach to differentiation is probably to fit a low-order interpolating polynomial to the data and differentiate the resulting polynomial. For example, if we fit a second-order Lagrange interpolating polynomial to the three data points $\{x_0, x_1, x_2\}$, we get

$$
\begin{aligned}
f_2(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\
&\quad + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \\
&= \frac{x^2-(x_1+x_2)x+x_1x_2}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{x^2-(x_0+x_2)x+x_0x_2}{(x_1-x_0)(x_1-x_2)} f(x_1) \\
&\quad + \frac{x^2-(x_0+x_1)x+x_0x_1}{(x_2-x_0)(x_2-x_1)} f(x_2).
\end{aligned}
$$

Differentiating this formula gives the following approximation for the first derivative of the function

$$
\begin{aligned}
f'(x) &\approx f_2'(x) \\
&= \frac{2x-(x_1+x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{2x-(x_0+x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\
&\quad + \frac{2x-(x_0+x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2).
\end{aligned}
$$

Actually, since errors in the original data are often exaggerated by performing numerical differentiation, the approach of fitting a low-order polynomial to the data and differentiating to produce estimates of the derivative is a good general numerical differentiation technique in general.