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Chapter 6

NUMERICAL DIFFERENTIATION

6.1 Introduction

Suppose we wish to estimate the derivative of a function $f(x)$ at some point x, given only discrete data points $(x_i, f(x_i))$. One approach would be to determine an interpolating or fitting polynomial, and then differentiate that polynomial analytically. However, it is also possible to estimate the derivative using a direct numerical method.

6.2 First derivative

Consider the Taylor expansions

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \cdots \tag{6.1}$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots \tag{6.2}$$

Subtracting (6.1) from (6.2) yields

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!}f'''(x) + \cdots \tag{6.3}$$

and we truncate the infinite series on the right of the equality to give the approximation

$$f(x+h) - f(x-h) \approx 2hf'(x)$$

which we can rewrite as

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{6.4}$$

This is the *finite-difference* representation of the first derivative of $f(x)$ at x.

Note: The truncated terms $\frac{h^3}{3!}f'''(x) + \cdots$ from (6.3) constitute the approximation error, i.e.

$$\left| f'(x) - \frac{f(x+h) - f(x-h)}{2h} \right| = \left| \frac{2h^2}{3!}f'''(x) + \cdots \right|$$

The error would tend toward zero as $h \to 0$ and (6.4) would become exact. Since we are working with Taylor expansions, we may replace the error by the Lagrange estimate of the error

$$\left| \frac{2h^2}{3!}f'''(x) + \frac{2h^4}{5!}f^{(5)}(x) + \cdots \right| \leq \left| \frac{2h^2}{3!}f'''(\xi) \right|$$

where $x < \xi < x + h$. Due to the function being unknown, we cannot determine its higher-order derivatives analytically and it would be difficult to determine an upper bound on the Lagrange estimate of the error and therefore we analyse the behaviour of h as it is changed. If $0 < h < 1$, then $\left|a_0h^2 + a_1h^4 + a_2h^6 + \cdots\right| \leq M\left|h^2\right|$ for some positive constant $M \in \mathbb{R}$. We introduce the notation $O(\cdot)$ to indicate this boundedness; the approximation error above can then be rewritten as

$$\left|\frac{2h^2}{3!}f'''(x) + \frac{2h^4}{5!}f^{(5)}(x) + \cdots\right| \in O(h^2).$$

The behaviour of the error pending changes in the step size can then be illustrated by the following example. Suppose that the approximation error is given by $e(h) = 10h^2$ and thus $e(h) \in O(h^2)$ by the previous statements. If $h = 0.1$, then $e\,(0.1) = 0.1$. If the step size were to be halved $h^* = h/2 = 0.05$, then the error becomes $e(0.05) = 0.025$; halving the error further yields $e(0.025) = 0.00625$. Therefore, as the step size is decreased the error will also decrease proportional to h^2. Since the error in (6.4) is of order h^2, we require that h be reasonably small in order for (6.4) to be reasonably accurate.

6.3 Second derivative

If we add (6.1) and (6.2) we obtain

$$f(x-h) + f(x+h) = 2f(x) + h^2f''(x) + O(h^4)$$

which yields

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \tag{6.5}$$

with an error of $O(h^2)$. This is the *finite-difference* representation of the second derivative of $f(x)$ at x. Since the error is $O(h^2)$ we would expect that, if h is small enough for (6.4) to be accurate, then (6.5) will also be accurate. Both (6.4) and (6.5) are known as *central-difference formulae*.

Note: If we use the notation $x_{i-1} = x - h$, $x_i = x$, $x_{i+1} = x + h$ we have

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}. \tag{6.6}$$

Using the subscripted notation we have

$$f''(x_i) = 4\left(\frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{(x_{i+1} - x_{i-1})^2}\right). \tag{6.7}$$

We can simplify the notation in (6.6) and (6.7) more by letting $y_i = f(x_i)$, $y_{i+1} = f(x_{i+1})$, $y_{i-1} = f(x_{i-1})$, etc. Then (6.6) becomes

$$y_i' = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{2h}$$

and (6.7) becomes

$$y_i'' = \frac{y_{i+1} + y_{i-1} - 2y_i}{h^2}.$$

Note: The approximation formula for $f'(x_i)$ is dependent on the values of $f(x)$ at the neighbouring points x_{i-1} and x_{i+1} and that the approximation formula for $f''(x_i)$ is dependent on the values of $f(x)$ at x_{i-1}, x_i and x_{i+1}. Since the approximation error is proportional to h^2, we see that as h is reduced so the error is reduced. The converse is also true: if h is large then the error will be large. Numerical differentiation must thus be used with caution, particularly if h is large (the discrete data points are far apart).

6.4 Higher-order derivatives

There are higher-order expressions that may be derived. We will not go into the details of their derivation (the principles are the same as for the expressions above), but we will state them for completeness.

Central-difference, $O(h^2)$

$$
\begin{aligned}
y_i' &= \frac{y_{i+1} - y_{i-1}}{2h} \\
y_i'' &= \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \\
y_i''' &= \frac{y_{i+2} - 2y_{i+1} + 2y_{i-1} - y_{i-2}}{2h^3} \\
y_i^{(4)} &= \frac{y_{i+2} - 4y_{i+1} + 6y_i - 4y_{i-1} + y_{i-2}}{h^4}
\end{aligned}
$$

Central-difference, $O(h^4)$

$$
\begin{aligned}
y_i' &= \frac{-y_{i+2} + 8y_{i+1} - 8y_{i-1} + y_{i-2}}{12h} \\
y_i'' &= \frac{-y_{i+2} + 16y_{i+1} - 30y_i + 16y_{i-1} - y_{i-2}}{12h^2} \\
y_i''' &= \frac{-y_{i+3} + 8y_{i+2} - 13y_{i+1} + 13y_{i-1} - 8y_{i-2} + y_{i-3}}{8h^3} \\
y_i^{(4)} &= \frac{-y_{i+3} + 12y_{i+2} - 39y_{i+1} + 56y_i - 39y_{i-1} + 12y_{i-2} - y_{i-3}}{6h^4}
\end{aligned}
$$

Forward-difference, $O(h)$

$$
\begin{aligned}
y_i' &= \frac{y_{i+1} - y_i}{h} \\
y_i'' &= \frac{y_{i+2} - 2y_{i+1} + y_i}{h^2} \\
y_i''' &= \frac{y_{i+3} - 3y_{i+2} + 3y_{i+1} - y_i}{h^3} \\
y_i^{(4)} &= \frac{y_{i+4} - 4y_{i+3} + 6y_{i+2} - 4y_{i+1} + y_i}{h^4}
\end{aligned}
$$

Forward-difference, $O(h^2)$

$$
\begin{aligned}
y_i' &= \frac{-y_{i+2} + 4y_{i+1} - 3y_i}{2h} \\
y_i'' &= \frac{-y_{i+3} + 4y_{i+2} - 5y_{i+1} + 2y_i}{h^2} \\
y_i''' &= \frac{-3y_{i+4} + 14y_{i+3} - 24y_{i+2} + 18y_{i+1} - 5y_i}{2h^3} \\
y_i^{(4)} &= \frac{-2y_{i+5} + 11y_{i+4} - 24y_{i+3} + 26y_{i+2} - 14y_{i+1} + 3y_i}{h^4}
\end{aligned}
$$

Backward-difference, $O(h)$

$$
\begin{aligned}
y_i' &= \frac{-y_{i-1} + y_i}{h} \\
y_i'' &= \frac{y_{i-2} - 2y_{i-1} + y_i}{h^2} \\
y_i''' &= \frac{-y_{i-3} + 3y_{i-2} - 3y_{i-1} + y_i}{h^3} \\
y_i^{(4)} &= \frac{y_{i-4} - 4y_{i-3} + 6y_{i-2} - 4y_{i-1} + y_i}{h^4}
\end{aligned}
$$

Backward-difference, $O(h^2)$

$$
\begin{aligned}
y_i' &= \frac{y_{i-2} - 4y_{i-1} + 3y_i}{2h} \\
y_i'' &= \frac{-y_{i-3} + 4y_{i-2} - 5y_{i-1} + 2y_i}{h^2} \\
y_i''' &= \frac{3y_{i-4} - 14y_{i-3} + 24y_{i-2} - 18y_{i-1} + 5y_i}{2h^3} \\
y_i^{(4)} &= \frac{-2y_{i-5} + 11y_{i-4} - 24y_{i-3} + 26y_{i-2} - 14y_{i-1} + 3y_i}{h^4}
\end{aligned}
$$

The forward-difference and backward-difference formulae should only be used when data points to the left or right of x_i are not available. The central-difference expressions generally give better results.

Example 6.1. The following table shows discrete data points corresponding to the function $\sin x$ on the interval $[0, \frac{\pi}{2}]$. We have used $h = \frac{\pi}{20}$.

$\boldsymbol{i}$	$\boldsymbol{x_i}$	$\mathbf{sin}\, \boldsymbol{x_i}$
1	0	0
2	0.15707	0.15643
3	0.31415	0.30901
4	0.47123	0.45399
5	0.62831	0.58778
6	0.78539	0.70710
7	0.94247	0.80901
8	1.09955	0.89100
9	1.25663	0.98768
10	1.41371	0.98768
11	1.57079	1

In the following table we show the various derivatives calculated using the various expressions given above, at the point $x = \frac{\pi}{4}$.

	$y'\left(\frac{\pi}{4}\right)$	$y''\left(\frac{\pi}{4}\right)$	$y'''\left(\frac{\pi}{4}\right)$	$y^{(4)}\left(\frac{\pi}{4}\right)$
Exact	0.70710	−0.70710	−0.70710	0.70710
CD $O(h^2)$	0.70420	−0.70565	−0.70275	0.70420
CD $O(h^4)$	0.70709	−0.70710	−0.70708	0.70709
FD $O(h)$	0.64878	−0.80735	−0.52088	0.88734
FD $O(h^2)$	0.71219	−0.72553	−0.72996	0.76774
BD $O(h)$	0.75962	−0.58657	−0.85001	0.45212
BD $O(h^2)$	0.71355	−0.72009	−0.74348	0.74088

The central-difference expressions give better results, and the $O(h^4)$ results have an error of better than 10^{-4}. Also, the results for the $O(h^2)$ forward-difference and backward difference expressions are considerably better than those for the corresponding $O(h)$ expressions.