5 Numerical Differentiation

5.1 Basic Concepts

This chapter deals with numerical approximations of derivatives. The first questions that comes up to mind is: why do we need to approximate derivatives at all? After all, we do know how to analytically differentiate every function. Nevertheless, there are several reasons as of why we still need to approximate derivatives:

- Even if there exists an underlying function that we need to differentiate, we might know its values only at a sampled data set without knowing the function itself.

- There are some cases where it may not be obvious that an underlying function exists and all that we have is a discrete data set. We may still be interested in studying changes in the data, which are related, of course, to derivatives.

- There are times in which exact formulas are available but they are very complicated to the point that an exact computation of the derivative requires a lot of function evaluations. It might be significantly simpler to approximate the derivative instead of computing its exact value.

- When approximating solutions to ordinary (or partial) differential equations, we typically represent the solution as a discrete approximation that is defined on a grid. Since we then have to evaluate derivatives at the grid points, we need to be able to come up with methods for approximating the derivatives at these points, and again, this will typically be done using only values that are defined on a lattice. The underlying function itself (which in this cased is the solution of the equation) is unknown.

A simple approximation of the first derivative is

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \tag{5.1}$$

where we assume that $h > 0$. What do we mean when we say that the expression on the right-hand-side of (5.1) is an approximation of the derivative? For linear functions (5.1) is actually an exact expression for the derivative. For almost all other functions, (5.1) is not the exact derivative.

Let's compute the approximation error. We write a Taylor expansion of $f(x+h)$ about x, i.e.,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi), \qquad \xi \in (x, x+h). \tag{5.2}$$

For such an expansion to be valid, we assume that $f(x)$ has two continuous derivatives. The Taylor expansion (5.2) means that we can now replace the approximation (5.1) with

an exact formula of the form

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\xi), \qquad \xi \in (x, x+h). \tag{5.3}$$

Since this approximation of the derivative at x is based on the values of the function at x and $x + h$, the approximation (5.1) is called a **forward differencing** or **one-sided differencing**. The approximation of the derivative at x that is based on the values of the function at $x - h$ and x, i.e.,

$$f'(x) \approx \frac{f(x) - f(x-h)}{h},$$

is called a **backward differencing** (which is obviously also a one-sided differencing formula).

The second term on the right-hand-side of (5.3) is the **error term**. Since the approximation (5.1) can be thought of as being obtained by truncating this term from the exact formula (5.3), this error is called the **truncation error**. The small parameter h denotes the distance between the two points x and $x + h$. As this distance tends to zero, i.e., $h \to 0$, the two points approach each other and we expect the approximation (5.1) to improve. This is indeed the case if the truncation error goes to zero, which in turn is the case if $f''(\xi)$ is well defined in the interval $(x, x+h)$. The "speed" in which the error goes to zero as $h \to 0$ is called the **rate of convergence**. When the truncation error is of the order of $O(h)$, we say that the method is **a first order method**. We refer to a methods as **a pth-order method** if the truncation error is of the order of $O(h^p)$.

It is possible to write more accurate formulas than (5.3) for the first derivative. For example, a more accurate approximation for the first derivative that is based on the values of the function at the points $f(x-h)$ and $f(x+h)$ is the **centered differencing** formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{5.4}$$

Let's verify that this is indeed a more accurate formula than (5.1). Taylor expansions of the terms on the right-hand-side of (5.4) are

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\xi_1),$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\xi_2).$$

Here $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-h, x)$. Hence

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12}[f'''(\xi_1) + f'''(\xi_2)],$$

which means that the truncation error in the approximation (5.4) is

$$-\frac{h^2}{12}[f'''(\xi_1) + f'''(\xi_2)].$$

If the third-order derivative $f'''(x)$ is a continuous function in the interval $[x - h, x + h]$, then the intermediate value theorem implies that there exists a point $\xi \in (x - h, x + h)$ such that

$$f'''(\xi) = \frac{1}{2}[f'''(\xi_1) + f'''(\xi_2)].$$

Hence

$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} - \frac{h^2}{6}f'''(\xi), \tag{5.5}$$

which means that the expression (5.4) is a second-order approximation of the first derivative.

In a similar way we can approximate the values of higher-order derivatives. For example, it is easy to verify that the following is a second-order approximation of the second derivative

$$f''(x) \approx \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}. \tag{5.6}$$

To verify the consistency and the order of approximation of (5.6) we expand

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2}f''(x) \pm \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_\pm).$$

Here, $\xi_- \in (x - h, x)$ and $\xi_+ \in (x, x + h)$. Hence

$$\frac{f(x + h) - 2f(x) + f(x - h)}{h^2} = f''(x) + \frac{h^2}{24}\left(f^{(4)}(\xi_-) + f^{(4)}(\xi_+)\right) = f''(x) + \frac{h^2}{12}f^{(4)}(\xi),$$

where we assume that $\xi \in (x - h, x + h)$ and that $f(x)$ has four continuous derivatives in the interval. Hence, the approximation (5.6) is indeed a second-order approximation of the derivative, with a truncation error that is given by

$$-\frac{h^2}{12}f^{(4)}(\xi), \qquad \xi \in (x - h, x + h).$$

5.2 Differentiation Via Interpolation

In this section we demonstrate how to generate differentiation formulas by differentiating an interpolant. The idea is straightforward: the first stage is to construct an interpolating polynomial from the data. An approximation of the derivative at any point can be then obtained by a direct differentiation of the interpolant.

We follow this procedure and assume that $f(x_0), \ldots, f(x_n)$ are given. The Lagrange form of the interpolation polynomial through these points is

$$Q_n(x) = \sum_{j=0}^{n} f(x_j) l_j(x).$$

Here we simplify the notation and replace $l_i^n(x)$ which is the notation we used in Section **??** by $l_i(x)$. According to the error analysis of Section **??** we know that the interpolation error is

$$f(x) - Q_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_n) \prod_{j=0}^{n} (x - x_j),$$

where $\xi_n \in (\min(x, x_0, \ldots, x_n), \max(x, x_0, \ldots, x_n))$. Since here we are assuming that the points $x_0, \ldots, x_n$ are fixed, we would like to emphasize the dependence of ξ_n on x and hence replace the ξ_n notation by ξ_x. We that have:

$$f(x) = \sum_{j=0}^{n} f(x_j) l_j(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w(x), \tag{5.7}$$

where

$$w(x) = \prod_{i=0}^{n} (x - x_i).$$

Differentiating the interpolant (5.7):

$$f'(x) = \sum_{j=0}^{n} f(x_j) l_j'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) + \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x). \tag{5.8}$$

We now assume that x is one of the interpolation points, i.e., $x \in \{x_0, \ldots, x_n\}$, say x_k, so that

$$f'(x_k) = \sum_{j=0}^{n} f(x_j) l_j'(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_k}) w'(x_k). \tag{5.9}$$

Now,

$$w'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j) = \sum_{i=0}^{n} [(x - x_0) \cdot \ldots \cdot (x - x_{i-1})(x - x_{i+1}) \cdot \ldots \cdot (x - x_n)].$$

Hence, when $w'(x)$ is evaluated at an interpolation point x_k, there is only one term in $w'(x)$ that does not vanish, i.e.,

$$w'(x_k) = \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j).$$

The numerical differentiation formula, (5.9), then becomes

$$f'(x_k) = \sum_{j=0}^{n} f(x_j) l'_j(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_k}) \prod_{\substack{j=0 \\ j \neq k}} (x_k - x_j). \tag{5.10}$$

We refer to the formula (5.10) as a **differentiation by interpolation** algorithm.

Example 5.1

We demonstrate how to use the differentiation by integration formula (5.10) in the case where $n = 1$ and $k = 0$. This means that we use two interpolation points $(x_0, f(x_0))$ and $(x_1, f(x_1))$, and want to approximate $f'(x_0)$. The Lagrange interpolation polynomial in this case is

$$Q_1(x) = f(x_0) l_0(x) + f(x_1) l_1(x),$$

where

$$l_0(x) = \frac{x - x_1}{x_0 - x_1}, \qquad l_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

Hence

$$l'_0(x) = \frac{1}{x_0 - x_1}, \qquad l'_1(x) = \frac{1}{x_1 - x_0}.$$

We thus have

$$Q'_1(x_0) = \frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0} + \frac{1}{2} f''(\xi)(x_0 - x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} - \frac{1}{2} f''(\xi)(x_1 - x_0).$$

Here, we simplify the notation and assume that $\xi \in (x_0, x_1)$. If we now let $x_1 = x_0 + h$, then

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi),$$

which is the (first-order) forward differencing approximation of $f'(x_0)$, (5.3).

Example 5.2

We repeat the previous example in the case $n = 2$ and $k = 0$. This time

$$Q_2(x) = f(x_0) l_0(x) + f(x_1) l_1(x) + f(x_2) l_2(x),$$

with

$$l_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}, \qquad l_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}, \qquad l_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}.$$

Hence

$$l_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}, \quad l_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}, \quad l_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}.$$

Evaluating $l_j'(x)$ for $j = 1, 2, 3$ at x_0 we have

$$l_0'(x_0) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}, \quad l_1'(x_0) = \frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}, \quad l_2'(x_0) = \frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Hence

$$Q_2'(x_0) = f(x_0)\frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \tag{5.11}$$
$$+ f(x_2)\frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{1}{6}f^{(3)}(\xi)(x_0 - x_1)(x_0 - x_2).$$

Here, we assume $\xi \in (x_0, x_2)$. For $x_i = x + ih$, $i = 0, 1, 2$, equation (5.11) becomes

$$Q_2'(x) = -f(x)\frac{3}{2h} + f(x + h)\frac{2}{h} + f(x + 2h)\left(-\frac{1}{2h}\right) + \frac{f'''(\xi)}{3}h^2$$
$$= \frac{-3f(x) + 4f(x + h) - f(x + 2h)}{2h} + \frac{f'''(\xi)}{3}h^2,$$

which is a one-sided, second-order approximation of the first derivative.

Remark. In a similar way, if we were to repeat the last example with $n = 2$ while approximating the derivative at x_1, the resulting formula would be the second-order centered approximation of the first-derivative (5.5)

$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} - \frac{1}{6}f'''(\xi)h^2.$$

5.3   The Method of Undetermined Coefficients

In this section we present the **method of undetermined coefficients**, which is a very practical way for generating approximations of derivatives (as well as other quantities as we shall see, e.g., when we discuss integration).

   Assume, for example, that we are interested in finding an approximation of the second derivative $f''(x)$ that is based on the values of the function at three equally spaced points, $f(x - h), f(x), f(x + h)$, i.e.,

$$f''(x) \approx Af(x + h) + B(x) + Cf(x - h). \tag{5.12}$$

The coefficients A, B, and C are to be determined in such a way that this linear combination is indeed an approximation of the second derivative. The Taylor expansions of the terms $f(x \pm h)$ are

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2}f''(x) \pm \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_\pm), \tag{5.13}$$

where (assuming that $h > 0$)

$$x - h \leqslant \xi_- \leqslant x \leqslant \xi_+ \leqslant x + h.$$

Using the expansions in (5.13) we can rewrite (5.12) as

$$f''(x) \approx Af(x+h) + Bf(x) + Cf(x-h) \tag{5.14}$$

$$= (A + B + C)f(x) + h(A - C)f'(x) + \frac{h^2}{2}(A + C)f''(x)$$

$$+ \frac{h^3}{6}(A - C)f^{(3)}(x) + \frac{h^4}{24}[Af^{(4)}(\xi_+) + Cf^{(4)}(\xi_-)].$$

Equating the coefficients of $f(x)$, $f'(x)$, and $f''(x)$ on both sides of (5.14) we obtain the linear system

$$\begin{cases} A + B + C = 0, \\ A - C = 0, \\ A + C = \dfrac{2}{h^2}. \end{cases} \tag{5.15}$$

The system (5.15) has the unique solution:

$$A = C = \frac{1}{h^2}, \quad B = -\frac{2}{h^2}.$$

In this particular case, since A and C are equal to each other, the coefficient of $f^{(3)}(x)$ on the right-hand-side of (5.14) also vanishes and we end up with

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{24}[f^{(4)}(\xi_+) + f^{(4)}(\xi_-)].$$

We note that the last two terms can be combined into one using an intermediate values theorem (assuming that $f(x)$ has four continuous derivatives), i.e.,

$$\frac{h^2}{24}[f^{(4)}(\xi_+) + f^{(4)}(\xi_-)] = \frac{h^2}{12}f^{(4)}(\xi), \qquad \xi \in (x - h, x + h).$$

Hence we obtain the familiar second-order approximation of the second derivative:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi).$$

In terms of an algorithm, the method of undetermined coefficients follows what was just demonstrated in the example:

1. Assume that the derivative can be written as a linear combination of the values of the function at certain points.

2. Write the Taylor expansions of the function at the approximation points.

3. Equate the coefficients of the function and its derivatives on both sides.

The only question that remains open is how many terms should we use in the Taylor expansion. This question has, unfortunately, no simple answer. In the example, we have already seen that even though we used data that is taken from three points, we could satisfy four equations. In other words, the coefficient of the third-derivative vanished as well. If we were to stop the Taylor expansions at the third derivative instead of at the fourth derivative, we would have missed on this cancellation, and would have mistakenly concluded that the approximation method is only first-order accurate. The number of terms in the Taylor expansion should be sufficient to rule out additional cancellations. In other words, one should truncate the Taylor series after the leading term in the error has been identified.

5.4 Richardson's Extrapolation

Richardson's extrapolation can be viewed as a general procedure for improving the accuracy of approximations when the structure of the error is known. While we study it here in the context of numerical differentiation, it is by no means limited only to differentiation and we will get back to it later on when we study methods for numerical integration.

We start with an example in which we show how to turn a second-order approximation of the first derivative into a fourth order approximation of the same quantity. We already know that we can write a second-order approximation of $f'(x)$ given its values in $f(x \pm h)$. In order to improve this approximation we will need some more insight on the internal structure of the error. We therefore start with the Taylor expansions of $f(x \pm h)$ about the point x, i.e.,

$$
\begin{aligned}
f(x + h) &= \sum_{k=0}^{\infty} \frac{f^{(k)}(x)}{k!} h^k, \\
f(x - h) &= \sum_{k=0}^{\infty} \frac{(-1)^k f^{(k)}(x)}{k!} h^k.
\end{aligned}
$$

Hence

$$
f'(x) = \frac{f(x + h) - f(x - h)}{2h} - \left[\frac{h^2}{3!} f^{(3)}(x) + \frac{h^4}{5!} f^{(5)}(x) + \ldots \right]. \tag{5.16}
$$

We rewrite (5.16) as

$$
L = D(h) + e_2 h^2 + e_4 h^4 + \ldots, \tag{5.17}
$$

where L denotes the quantity that we are interested in approximating, i.e.,

$$L = f'(x),$$

and $D(h)$ is the approximation, which in this case is

$$D(h) = \frac{f(x+h) - f(x-h)}{2h}.$$

The error is

$$E = e_2 h^2 + e_4 h^4 + \ldots$$

where e_i denotes the coefficient of h^i in (5.16). The important property of the coefficients e_i's is that they do not depend on h. We note that the formula

$$L \approx D(h),$$

is a second-order approximation of the first-derivative which is based on the values of $f(x)$ at $x \pm h$. We assume here that in general $e_i \neq 0$. In order to improve the approximation of L our strategy will be to eliminate the term $e_2 h^2$ from the error. How can this be done? one possibility is to write another approximation that is based on the values of the function at different points. For example, we can write

$$L = D(2h) + e_2 (2h)^2 + e_4 (2h)^4 + \ldots. \tag{5.18}$$

This, of course, is still a second-order approximation of the derivative. However, the idea is to combine (5.17) with (5.18) such that the h^2 term in the error vanishes. Indeed, subtracting the following equations from each other

$$\begin{aligned}
4L &= 4D(h) + 4e_2 h^2 + 4e_4 h^4 + \ldots, \\
L &= D(2h) + 4e_2 h^2 + 16 e_4 h^4 + \ldots,
\end{aligned}$$

we have

$$L = \frac{4D(h) - D(2h)}{3} - 4e_4 h^4 + \ldots$$

In other words, a fourth-order approximation of the derivative is

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4). \tag{5.19}$$

Note that (5.19) improves the accuracy of the approximation (5.16) by using more points.

This process can be repeated over and over as long as the structure of the error is known. For example, we can write (5.19) as

$$L = S(h) + a_4 h^4 + a_6 h^6 + \ldots \tag{5.20}$$

where

$$S(h) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

Equation (5.20) can be turned into a sixth-order approximation of the derivative by eliminating the term $a_4 h^4$. We carry out such a procedure by writing

$$L = S(2h) + a_4 (2h)^4 + a_6 (2h)^6 + \ldots \tag{5.21}$$

Combining (5.21) with (5.20) we end up with a sixth-order approximation of the derivative:

$$L = \frac{16 S(h) - S(2h)}{15} + O(h^6).$$

Remarks.

1. In (5.18), instead of using $D(2h)$, it is possible to use other approximations, e.g., $D(h/2)$. If this is what is done, instead of (5.19) we would get a fourth-order approximation of the derivative that is based on the values of f at $x - h, x - h/2, x + h/2, x + h$.

2. Once again we would like to emphasize that Richardson's extrapolation is a general procedure for improving the accuracy of numerical approximations that can be used when the structure of the error is known. It is not specific for numerical differentiation.