# Working with functions: differentiation + integration

## Numerical differentiation

We know from Calculus that $f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$.

To numerically approximate $f'(x)$ we could use $f'(x) \approx \frac{1}{h}[f(x+h)-f(x)]$ for small $h$.

In this section, we analyze this and other ways of numerically differentiating a function.

**Application.** These approximations are crucial for developing tools to numerically solve (partial) differential equations by discretizing them.

**Review.** We can express **Taylor's theorem** (Theorem 54) in the following manner:

$$f(x+h) = \underbrace{f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \ldots + \frac{1}{n!}f^{(n)}(x)h^n}_{\text{Taylor polynomial}} + \underbrace{\frac{1}{(n+1)!}f^{(n+1)}(\xi)h^{n+1}}_{\text{error}}$$

This form is particularly convenient for the kind of error analysis that we are doing here.

**Important notation.** When the exact form of the error is not so important, we simply write $O(h^{n+1})$ and say that the **error is of order** $n+1$.

**Definition 112.** We write $e(h) = O(h^n)$ if there is a constant $C$ such that $|e(h)| \leqslant Ch^n$ for all small enough $h$.

For our purposes, $e(h)$ is usually an error term and this notation allows us to talk about that error without being more precise than necessary.

If $e(h)$ is the error, then we often say that an approximation is of order $n$ if $e(h) = O(h^n)$.

**Caution.** This notion of order is different from the order of convergence that we discussed in the context of fixed-point iteration and Newton's method.

**Example 113.** Determine the order of the approximation $f'(x) \approx \frac{1}{h}[f(x+h)-f(x)]$.

**Comment.** This approximation of the derivative is called a **(first) forward difference** for $f'(x)$.

Likewise, $f'(x) \approx \frac{1}{h}[f(x)-f(x-h)]$ is a **(first) backward difference** for $f'(x)$.

**Solution.** By Taylor's theorem, $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + O(h^4)$. It follows that

$$\frac{1}{h}[f(x+h)-f(x)] = f'(x) + \boxed{\frac{h}{2}f''(x) + O(h^2)} = f'(x) + \boxed{O(h)}.$$

Hence, the $\boxed{\text{error}}$ is of order $1$.

**Comment.** The presence of the term $\frac{h}{2}f''(x)$ tells us that the order is exactly $1$ unless $f''(x) = 0$ (that is, the order cannot generally be improved to $\delta$ for some $\delta < 1$).

Armin Straub
straub@southalabama.edu

**Example 114.** Determine the order of the approximation $f'(x) \approx \frac{1}{2h}[f(x+h) - f(x-h)]$.

**Comment.** This approximation of the derivative is called a **(first) central difference** for $f'(x)$.

**Solution.** By Taylor's theorem (Theorem 54),

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O(h^5), \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O(h^5). \end{aligned} \tag{2}$$

(Note that the second formula just has $h$ replaced with $-h$.) Subtracting the second from the first, we obtain

$$\frac{1}{2h}[f(x+h) - f(x-h)] = f'(x) + \boxed{\frac{h^2}{6}f'''(x) + O(h^3)} = f'(x) + \boxed{O(h^2)}.$$

Hence, the $\boxed{\text{error}}$ is of order $2$.

**Example 115.** Use both forward and central differences to approximate $f'(x)$ for $f(x) = x^2$.

**Solution.** We get $\frac{1}{h}[f(x+h) - f(x)] = 2x + h$ and $\frac{1}{2h}[f(x+h) - f(x-h)] = 2x$.

**Comment.** In the forward difference case, the error is of order $1$ (also note that $\frac{h}{2}f''(x) = h$). In the central difference case, we find that we get $f'(x)$ without error. In hindsight, with the error formulas in mind, this is not a surprise and reflects the fact that $f'''(x) = 0$.

**Example 116.** Use both forward and central differences to approximate $f'(2)$ for $f(x) = 1/x$.

**Solution.** (Since $f'(x) = -1/x^2$, the exact value is $f'(2) = -1/4$.) In each case, we use $h = \frac{1}{10}$ and $h = \frac{1}{20}$.

- $h = \frac{1}{10}$: $\frac{1}{h}[f(x+h) - f(x)] = -\frac{5}{21} \approx -0.2381$, error $0.0119$
  $h = \frac{1}{20}$: $\frac{1}{h}[f(x+h) - f(x)] = -\frac{10}{41} \approx -0.2439$, error $0.0061$ (reduced by about $\frac{1}{2}$)
- $h = \frac{1}{10}$: $\frac{1}{2h}[f(x+h) - f(x-h)] = -\frac{100}{399} \approx -0.25063$, error $-0.00063$
  $h = \frac{1}{20}$: $\frac{1}{2h}[f(x+h) - f(x-h)] = -\frac{400}{1599} \approx -0.25016$, error $-0.00016$ (reduced by about $\frac{1}{4}$)

**Important comment.** The forward difference has an error of order $1$. In other words, for small $h$, it should behave like $Ch$. In particular, if we replace $h$ by $h/2$, then the error should be about $1/2$ (as we saw above). On the other hand, the central difference has an error of order $2$ and so should behave like $Ch^2$. In particular, if we replace $h$ by $h/2$, then the error should be about $1/2^2 = 1/4$ (and, again, this is what we saw above).

**Example 117.** Find a central difference for $f''(x)$ and determine the order of the error.

**Solution.** Adding the two expansions in (2) to kill the $f'(x)$ terms, and subtracting $2f(x)$, we find that

$$\frac{1}{h^2}[f(x+h) - 2f(x) + f(x-h)] = f''(x) + \boxed{\frac{h^2}{12}f^{(4)}(x) + O(h^3)} = f''(x) + \boxed{O(h^2)}.$$

The $\boxed{\text{error}}$ is of order $2$.

**Alternatively.** If we iterate the approximation $f'(x) \approx \frac{1}{2h}[f(x+h) - f(x-h)]$ (in the second step, we apply it with $x$ replaced by $x \pm h$), we obtain

$$f''(x) \approx \frac{1}{2h}[f'(x+h) - f'(x-h)] \approx \frac{1}{4h^2}[f(x+2h) - 2f(x) + f(x-2h)],$$

which is the same as what we found above, just with $h$ replaced by $2h$.

**Example 118.** Obtain approximations for $f'(x)$ and $f''(x)$ using the values $f(x)$, $f(x+h)$, $f(x+2h)$ as follows: determine the polynomial interpolation corresponding to these values and then use its derivatives to approximate those of $f$. In each case, determine the order of the approximation and the leading term of the error.

**Solution.** We first compute the polynomial $p(t)$ that interpolates the three points $(x, f(x))$, $(x+h, f(x+h))$, $(x+2h, f(x+2h))$ using Newton's divided differences:

| | $f[\cdot]$ | $f[\cdot,\cdot]$ | $f[\cdot,\cdot,\cdot]$ |
|---|---|---|---|
| $x$ | $f(x)$ | | |
| | | $\frac{f(x+h)-f(x)}{h} =: c_1$ | |
| $x+h$ | $f(x+h)$ | | $\frac{f(x+2h)-2f(x+h)+f(x)}{2h^2} =: c_2$ |
| | | $\frac{f(x+2h)-f(x+h)}{h}$ | |
| $x+2h$ | $f(x+2h)$ | | |

Hence, reading the coefficients from the top edge of the triangle, the interpolating polynomial is

$$p(t) = f(x) + c_1(t-x) + c_2(t-x)(t-x-h).$$

- **(approximating $f'(x)$)** Since $p'(t) = c_1 + c_2(2t-2x-h)$, we have

$$\begin{aligned} p'(x) &= c_1 - hc_2 = \frac{f(x+h)-f(x)}{h} - \frac{f(x+2h)-2f(x+h)+f(x)}{2h} \\ &= \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}. \end{aligned}$$

  This is our approximation for $f'(x)$. To determine the order and the error, we combine

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{f'''(x)}{6}h^3 + O(h^4), \\ f(x+2h) &= f(x) + 2f'(x)h + 2f''(x)h^2 + \frac{4f'''(x)}{3}h^3 + O(h^4) \end{aligned}$$

  (note that the latter is just the former with $h$ replaced by $2h$) to find

$$-f(x+2h)+4f(x+h)-3f(x) = 2f'(x)h - \frac{2f'''(x)}{3}h^3 + O(h^4).$$

  Hence, dividing by $2h$, we conclude that

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h} = f'(x) - \frac{f'''(x)}{3}h^2 + O(h^3).$$

  Consequently, the approximation is of order $2$.

- **(approximating $f''(x)$)** Since $p''(t) = 2c_2$, we have $p''(x) = 2c_2 = \frac{f(x+2h)-2f(x+h)+f(x)}{h^2}$.
  This is our approximation for $f''(x)$. To determine the order and the error, we proceed as before to find

$$f(x+2h) - 2f(x+h) + f(x) = f''(x)h^2 + f'''(x)h^3 + O(h^4).$$

  Hence, dividing by $h^2$, we conclude that

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

  Consequently, the approximation is of order $1$.

**Comment.** Alternatively, can you derive these approximations by combining $f(x)$ with the Taylor expansions of $f(x+h)$ and $f(x+2h)$? As a third way of producing such approximations, we will soon see that the present order $2$ approximation of $f'(x)$ can be obtained by applying Richardson extrapolation to $f'(x) \approx \frac{1}{h}[f(x+h)-f(x)]$.

**Example 119. (homework)** Obtain approximations for $f'(x)$ and $f''(x)$ using the values $f(x-2h)$, $f(x)$, $f(x+3h)$ as follows: determine the polynomial interpolation corresponding to these values and then use its derivatives to approximate those of $f$. In each case, determine the order of the approximation and the leading term of the error.

**Solution.** We first compute the polynomial $p(t)$ that interpolates the three points $(x-2h, f(x-2h))$, $(x, f(x))$, $(x+3h, f(x+3h))$ using Newton's divided differences:

| | $f[\cdot]$ | $f[\cdot,\cdot]$ | $f[\cdot,\cdot,\cdot]$ |
|---|---|---|---|
| $x-2h$ | $f(x-2h)$ | | |
| | | $\frac{f(x)-f(x-2h)}{2h} =: c_1$ | |
| $x$ | $f(x)$ | | $\frac{2f(x+3h)-5f(x)+3f(x-2h)}{30h^2} =: c_2$ |
| | | $\frac{f(x+3h)-f(x)}{3h}$ | |
| $x+3h$ | $f(x+3h)$ | | |

Hence, reading the coefficients from the top edge of the triangle, the interpolating polynomial is

$$p(t) = f(x-2h) + c_1(t-x+2h) + c_2(t-x+2h)(t-x).$$

- **(approximating $f'(x)$)** Since $p'(t) = c_1 + c_2(2t-2x+2h)$, we have

$$\begin{aligned} p'(x) &= c_1 + 2h\,c_2 = \frac{f(x)-f(x-2h)}{2h} + \frac{2f(x+3h)-5f(x)+3f(x-2h)}{15h} \\ &= \frac{4f(x+3h)+5f(x)-9f(x-2h)}{30h}. \end{aligned}$$

  This is our approximation for $f'(x)$. To determine the order and the error, we combine

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{f'''(x)}{6}h^3 + O(h^4), \\ f(x-2h) &= f(x) - 2f'(x)h + 2f''(x)h^2 - \frac{4f'''(x)}{3}h^3 + O(h^4), \\ f(x+3h) &= f(x) + 3f'(x)h + \frac{9}{2}f''(x)h^2 + \frac{9f'''(x)}{2}h^3 + O(h^4) \end{aligned}$$

  to find

$$4f(x+3h) + 5f(x) - 9f(x-2h) = 30f'(x)h + 30f'''(x)h^3 + O(h^4).$$

  Hence, dividing by $30h$, we conclude that

$$\frac{4f(x+3h)+5f(x)-9f(x-2h)}{30h} = f'(x) + f'''(x)h^2 + O(h^3).$$

  Consequently, the approximation is of order $2$.

- **(approximating $f''(x)$)** Since $p''(t) = 2c_2$, we have $p''(x) = 2c_2 = \frac{2f(x+3h)-5f(x)+3f(x-2h)}{15h^2}$.
  This is our approximation for $f''(x)$. To determine the order and the error, we proceed as before to find

$$2f(x+3h) - 5f(x) + 3f(x-2h) = 15f''(x)h^2 + 5f'''(x)h^3 + O(h^4).$$

  Hence, dividing by $15h^2$, we conclude that

$$\frac{2f(x+3h)-5f(x)+3f(x-2h)}{15h^2} = f''(x) + \frac{1}{3}f'''(x)h + O(h^2).$$

  Consequently, the approximation is of order $1$.