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 113. 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 114. 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 δ for some $\delta < 1$).

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Example 115. 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),

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

(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 116. 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 117. 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 118. 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 119. 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:

$$\begin{array}{r|lll}
 & f[\cdot] & f[\cdot,\cdot] & f[\cdot,\cdot,\cdot] \\ \hline
x & f(x) & & \\
 & & \frac{f(x+h)-f(x)}{h} =: c_1 & \\
x+h & f(x+h) & & \frac{f(x+2h)-2f(x+h)+f(x)}{2h^2} =: c_2 \\
 & & \frac{f(x+2h)-f(x+h)}{h} & \\
x+2h & f(x+2h) & &
\end{array}$$

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 120. (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:

$$\begin{array}{r|lll}
 & f[\cdot] & f[\cdot,\cdot] & f[\cdot,\cdot,\cdot] \\ \hline
x-2h & f(x-2h) & & \\
 & & \dfrac{f(x)-f(x-2h)}{2h} =: c_1 & \\
x & f(x) & & \dfrac{2f(x+3h)-5f(x)+3f(x-2h)}{30h^2} =: c_2 \\
 & & \dfrac{f(x+3h)-f(x)}{3h} & \\
x+3h & f(x+3h) & &
\end{array}$$

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

  $$\begin{aligned} p'(x) &= c_1 + 2hc_2 = \frac{f(x)-f(x-2h)}{2h} + \frac{2f(x+3h)-5f(x)+3f(x-2h)}{15h} \\ &= \frac{4f(x+3h)+5f(x)-9f(x-2h)}{30h}. \end{aligned}$$

  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 $p''(x) = 2c_2 = \dfrac{2f(x+3h)-5f(x)+3f(x-2h)}{15h^2}$.

  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.