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 52) 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 110. 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 111. 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 112. 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 52),

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

(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 113. 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 114. 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 115. 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 116. 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:

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

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 117. (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:

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

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.

Example 118. Python Let us see how the forward and central difference compare in practice.

```
>>> def forward_difference(f, x, h):
        return (f(x+h)-f(x))/h
```

```
>>> def central_difference(f, x, h):
        return (f(x+h)-f(x-h))/(2*h)
```

We apply these to $f(x) = 2^x$ at $x = 1$. In that case, the exact derivative is $f'(1) = 2\ln(2) \approx 1.386$.

```
>>> def f(x):
        return 2**x
```

```
>>> [forward_difference(f, 1, 10**-n) for n in range(5)]
```

```
[2.0, 1.4354692507258626, 1.3911100113437769, 1.3867749251610384, 1.3863424075299946]
```

```
>>> [central_difference(f, 1, 10**-n) for n in range(5)]
```

```
[1.5, 1.3874047099948572, 1.3863054619682957, 1.3862944721280135, 1.3862943622289237]
```

It is probably easier to see what happens to the error if we subtract the true value from these approximations:

```
>>> from math import log
```

```
>>> [forward_difference(f, 1, 10**-n) - 2*log(2) for n in range(12)]
```

```
[0.6137056388801094, 0.04917488960597205, 0.004815650223886303, 0.00048056404114782403,
4.80464101040301e-05, 4.804564444071957e-06, 4.80467807983942e-07, 4.703673917028084e-
08, 7.068710283775204e-09, 2.7352223619381277e-07, 1.161700655893938e-06,
1.8925269049896443e-05]
```

```
>>> [central_difference(f, 1, 10**-n) - 2*log(2) for n in range(12)]
```

```
[0.11370563888010943, 0.001110348874966638, 1.1100848405165564e-05,
1.1100812291608975e-07, 1.1090330875873633e-09, 1.879385536085465e-11,
7.43052286367174e-11, -7.028508886008922e-10, 7.068710283775204e-09,
1.6249993373129712e-07, 1.161700655893938e-06, 7.823038803644877e-06]
```

For the forward difference, we can see how the error decreases roughly by $1/10$ initially, as expected. Likewise, for the central difference, the error decreases roughly by $1/10^2$ (order 2) initially. However, in both cases, the errors end up increasing after a while before getting close to machine precision. We discuss this in the next section.

Note how, for the forward difference, our best approximation has error $7.07 \cdot 10^{-9}$ while, for the central difference, our best approximation has error $1.88 \cdot 10^{-11}$. While the latter is an improvement, either is worryingly large.