

How to develop, analyse and test a numerical algorithm

The aim of this section is give one example of how to develop an algorithm, how to analyse it and how to perform and present the result of an numerical experiment. Numerical differentiation is chosen as an example here. Roughly the steps are:

- Given a problem, or rather a class of problems.
- Suggest an algorithm for finding a numerical approximation to the solution of the problem.
- Do some analysis of the algorithm, usually an error/convergence analysis.
- Choose carefully some test problems, and use those to confirm that the algorithm behaves as expected.
- Present the result.

So let us see how this applies to the example of numerical differentiation.

Problem: Given an $f \in C^1(a, b)$ and some arbitrary $x_0 \in (a, b)$, find a numerical approximation to $f'(x_0)$.

Algorithm: In this case, we can simply use the definition of the derivative:

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}.$$

So our algorithm is: Given $h > 0$ (and we assume h to be small) the approximation is

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}. \quad (1)$$

This particular approximation is called *the forward difference approximation*.

Error analysis: The error is

$$e(h; f, x_0) = f'(x_0) - \frac{f(x_0+h) - f(x_0)}{h}.$$

So the error depends on the method parameter h , which we can control, and of the problem, in this case the function f and the point x_0 . In the following, we will for short use $e(h)$ unless we want to emphasise the dependence on f and/or x_0 . The sign of the error does usually not matter.

To get an expression for the error, make a taylor expansion of $f(x_0+h)$:

$$e(h) = f'(x_0) + \frac{f(x_0) + hf'(x_0) + \frac{1}{2}h^2 f''(\xi)}{h} - \frac{f(x_0) + hf'(x_0) + \frac{1}{2}h^2 f''(\xi)}{h} = \frac{1}{2}hf''(\xi), \quad \xi \in (x_0, x_0+h). \quad (2)$$

This is in fact an exact expression for the error, but ξ is unknown, and in practice we do not know $f''(x)$ (after all, we want an approximation for $f'(x)$). We may however add the assumption that $f''(x)$ exists and is bounded on the open interval (a, b) , that is there exist a constant $M > 0$ such that

$$|f''(x)| \leq M, \quad \text{for all } x \in (a, b). \quad (3)$$

which again leads to the *error bound*

$$|e(h)| \leq \frac{1}{2}Mh \tag{4}$$

Now to complete the argument: Since (a, b) is an open interval, $x_0 \in (a, b)$ then also $x_0 + h \in (a, b)$ for sufficiently small h . From (4) we can then conclude that the approximation (1) converges to $f'(x_0)$, in the sense that

$$|e(h)| \xrightarrow{h \rightarrow 0} 0.$$

Numerical verification: The next step is now to verify the theory by some numerical experiments. Choose a test problem that

- satisfies all conditions of the theory,
- for which an exact solution is known (if possible),
- is not too trivial¹.

In our case, let us choose the test problem

$$f(x) = \sin(x), \quad x_0 = 0.5. \tag{5}$$

with exact solution $f'(x) = \cos(x)$. Since $f \in C^\infty(\mathbb{R})$ and $|f^{(p)}| \leq 1$, the conditions of the theory is satisfied with $M = 1$. Let us now justify the error expression (2). We will pretend that f'' is unknown. If f'' is continuous around x_0 , then for small values of h , we have $f''(\xi) \approx f''(x_0)$ so that $|e(h)| \approx Ch$, and $|e(h/2)| \approx |e(h)|/2$. And this is something that we can measure. The results the of experiment is given in Table 1.

h	$ e(h) $	$ e(h)/e(h/2) $
0.1	$2.54 \cdot 10^{-2}$	2.06
0.05	$1.23 \cdot 10^{-2}$	2.03
0.025	$6.08 \cdot 10^{-3}$	2.02
0.0125	$3.02 \cdot 10^{-3}$	

So, the result of this experiment complies with the error expression (2).

Convergence plots In this course, we will several time be in the situation that the error of our methods is given by

$$|e(h)| \approx Ch^p \tag{6}$$

where C is some unknown constant, and h is some method dependent parameter. In this case the method is said to be *of order p*. Assume that we have measured $e(h)$ for different values of h . The results can of course be presented in a table, as above, but it may be even more illustrative using a graph, in particular if several methods are compared. Now, taking the logarithm on both sides of (6), we get

$$\log |e(h)| \approx p \log h + \log C,$$

¹Well: in the process of implementing the algorithm, it is often a good idea to use examples with trivial solutions, just to rule out coding bugs.

which is a straight line with slope p . For this reason, the correct way to display the error as a function of h is to use a loglog plot. An example of this is given in Figure 1. In this plot, also a reference line ($y(h) = h^1$) is included, making it easy to see that this method really is of order 1.

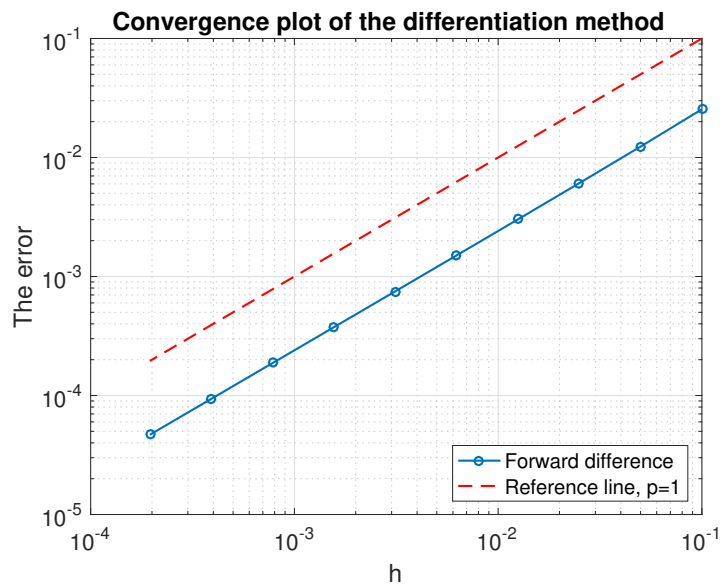


Figure 1: Errors of the forward difference approximation to $f'(x_0)$ with $f(x) = \sin x$ and $x_0 = 0.5$.