CHAPTER

14

Finite Difference Derivative Approximations

OUTLINE

Différance is the systematic play of differences, of the traces of differences, of the spacing by means of which elements are related to each other.

–Positions *by Jacques Derrida*

CHAPTER POINTS

- The definition of a derivative requires taking an infinitesimally small perturbation of a function.
- We cannot deal with infinitesimals on a compute so finite difference formulae are commonly used. These can be derived from the Taylor series polynomial of the function.
- The convergence of an approximate derivative can be inferred theoretically from the Taylor series and empirically from the error on a log-log plot.
- Using complex numbers allows the derivative to be approximated to a high degree of precision by obviating the need for taking differences of functions.

In introductory calculus, students are taught that the derivative of a function is defined via the limit

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

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On a computer we want to compute derivatives, but we cannot evaluate the derivative using an infinitesimally small value for h due to finite precision arithmetic. In this chapter we will derive formulas called finite difference derivatives because h will have a finite value rather than an infinitesimally small one. In one formula we will approximate the derivative in the same manners as the above equation using

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

The error we incur in doing so we also be discussed.

14.1 TAYLOR SERIES AND BIG-O NOTATION

We can approximate a function $f(x)$ near a point x using the Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \cdots + \frac{h^n}{n!}f^{(n)}(x) + \ldots.$$

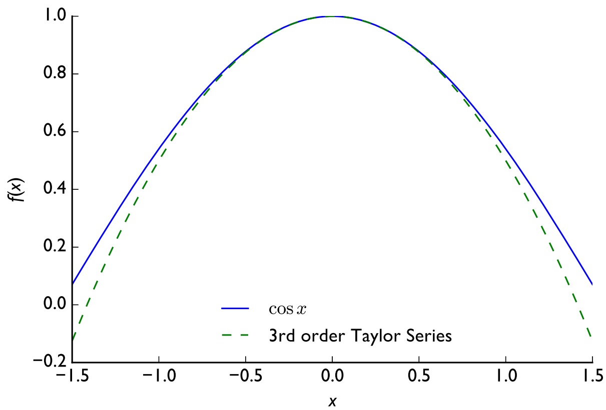
The Taylor series is an infinite sum. One way that this is commonly written is using a particular notation instead of the "$\ldots$":

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

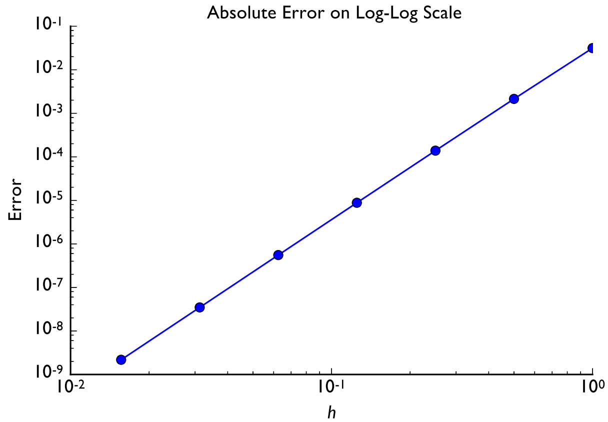
What the $O(h^4)$ means that the rest of the terms will be smaller than some constant times h^4 as $h \to 0$. We can see this through a simple example. Here we look at the approximation of

$$\cos h = \cos 0 - h \sin 0 - \frac{h^2}{2}\cos 0 + \frac{h^3}{6}\sin 0 + O(h^4).$$

Below we plot the both the function and its approximation.



The absolute difference between $\cos h$ and the third-order Taylor series as a function of h on a log-log scale is shown next. It appears to be a line with a slope that is approximately 4.



You might ask yourself, why is the slope 4? This can be answered by looking at the equation for the error:

$$f(x+h) - \left(f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x)\right) = Ch^4 + O(h^5),$$

in this equation we have used the fact that $O(h^4)$ means some constant, which here we call C, times h^4. The remaining terms we have written as $O(h^5)$.

When we take the absolute value and the logarithm of each side we get

$$\log_{10}\left|f(x+h) - \left(f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x)\right)\right| \approx \log_{10}|C| + 4\log_{10} h,$$

which is a line with slope 4. The constant tells us what level the curve starts out at when $h = 1$. This formula is approximate because we have left out the h^5 and higher terms, which we assume to be small since h is small in our demonstration above.

BOX 14.1 NUMERICAL PRINCIPLE

When plotting the error of an approximation as a function of a parameter h on a log-log scale, the slope of the line is an approximation to how the error scales as h to some power. That is, if the slope in plot is m, then we can estimate that the error is

$$\text{error} = Ch^m = O(h^m).$$

The we have already seen the concept of Big-O notation when we discussed the scaling Gaussian Elimination, saying that it scaled as $O(n^3)$ where n was the number of equations in the linear system. One difference is that in the algorithm scaling discuss we were concerned about the scaling as $n \to \infty$, whereas here we are interested in $h \to 0$.

14.2 FORWARD AND BACKWARD DIFFERENCE FORMULAS

From the Taylor series at $x + h$,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4),$$

we notice that there is an $f'(x)$ term in the equation. If we "solve" for this derivative by subtracting $f(x)$ from both sides and then dividing by h we get

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

or in shorter form

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

Therefore the approximation

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

is an order h approximation because the error is proportional to h as h goes to 0. This is called a forward difference formula because the function is evaluated h forward of x to approximate the derivative.

We did this using $f(x+h)$ in our formula, but we could have also used $f(x-h)$ which has the Taylor series

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + O(h^4),$$

to get the formula

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

Therefore the approximation

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

is also an order h approximation because the error is proportional to h as h goes to 0. This formula is a backward difference formula because the function is evaluated h behind x.

BOX 14.2 NUMERICAL PRINCIPLE

The forward and backward finite difference formulas are first-order in h approximations to the derivative given by

Forward Difference

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h),$$

and

Backward Difference

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

14.3 HIGHER-ORDER APPROXIMATIONS

Both of these formulas for the derivative are first-order in h. These formulas are fine, but as we will see when we solve differential equations, first-order solutions typically have too much error for our purposes. We desire a way of getting higher-order approximations to the derivative.

Here we will derive a second-order approximation using both

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4),$$

and

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

Notice that if we subtract the $f(x-h)$ equation from the equation for $f(x+h)$ and then divide by $2h$ we get

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{6} f'''(x) + O(h^4),$$

or in shorter form

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

Therefore the approximation

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h},$$

is an order h^2 approximation because the error is proportional to h^2 as h goes to 0. This formula is called a central-difference formula because the function is evaluated around a center of x a value of h on either side. One thing to note is that the error terms in this approximation only have even powers of h because of the way the odd powers cancel when combining the two.

With a second-order approximation, if we cut h in half, the error goes down by a factor of 4, compared to a factor of 2 with a first-order method.

BOX 14.3 NUMERICAL PRINCIPLE

The central finite difference formula is a second-order in h approximation to the derivative given by

Central Difference

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

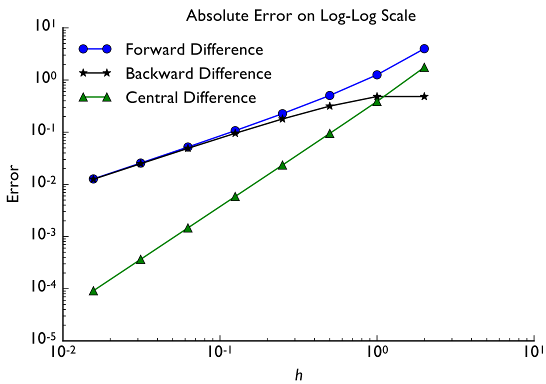
We could go through the process of obtaining even higher-order derivatives (third-order, fourth-order, etc.), but in practice this is generally not useful because the formulas become cumbersome and there are typically better ways of accomplishing higher-order accuracy. We will see one of these ways shortly.

14.4 COMPARISON OF THE APPROXIMATIONS

Consider the function

$$f(x) = \arctan(x)\cosh(x)$$

and look at approximations to $f'(x)$ at $x = 1$. The actual answer is $f'(1) = 1.694541176517952557683135$. In the following graph we show the error in the derivative estimate as a function of h for the three methods we have seen so far on a log-log scale.



The central difference result has a slope of about 2, between the forward and backward differences have a slope around 1 (1.01 and 0.989 between the last two points of each line for the forward and backward difference, respectively).

In this example we see that the errors decay as expected for the two first-order methods and the one second-order method. As we expect, as h gets smaller the second-order method wins out. Nevertheless, this does not mean that at a particular value of h the second-order method will have smaller error. The graph above shows that at $h = 2$, the backward difference approximation has the smallest error. This is due to the fact that order of the formula just says how the error changes with h and says nothing about the constant in front of the leading-order term. Eventually, the second-order method will win, but we cannot say anything about a particular point.

BOX 14.4 NUMERICAL PRINCIPLE

Just because a method has higher order accuracy than another does not mean that it will give a better approximation for a particular value of h. What higher order accuracy means is that the error will decrease faster as $h \to 0$.

14.5 SECOND DERIVATIVES

We may also want to compute the value of $f''(x)$. To do this we start with the Taylor series for $f(x+h)$ and $f(x-h)$:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O(h^4),$$

and

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

If we add these two equations together, notice that the h and h^3 terms cancel:

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

Now rearranging this formula to solve for the second-derivative we get

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

That is, we can get a second-order in h approximation to the second derivative by evaluating the function at $f(x)$ and $f(x \pm h)$.

BOX 14.5 NUMERICAL PRINCIPLE

A common formula for estimating a second-derivative with second-order accuracy is

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

Another derivative we may want to approximate in nuclear engineering is

$$\frac{d}{dx} D(x) \frac{d\phi}{dx}.$$

This term appears in the diffusion equation for neutrons or other particles. To approximate this, we first approximate $D(x + h/2)\phi'(x + h/2)$ using a central difference with $h/2$ as

$$D\left(x + \frac{h}{2}\right)\phi'\left(x + \frac{h}{2}\right) = D\left(x + \frac{h}{2}\right)\frac{\phi(x+h) - \phi(x)}{h} + O(h^2).$$

Doing the same with $D(x - h/2)\phi'(x - h/2)$ gives

$$D\left(x - \frac{h}{2}\right)\phi'\left(x - \frac{h}{2}\right) = D\left(x - \frac{h}{2}\right)\frac{\phi(x) - \phi(x-h)}{h} + O(h^2).$$

The final step involves writing

$$\frac{d}{dx} D(x) \frac{d\phi}{dx} = \frac{1}{h}\left(D\left(x + \frac{h}{2}\right)\phi'\left(x + \frac{h}{2}\right) - D\left(x - \frac{h}{2}\right)\phi'\left(x - \frac{h}{2}\right)\right) + O(h^2),$$

which is a central difference formula as well. Putting all of our results together gives

$$\frac{d}{dx} D(x) \frac{d\phi}{dx} = \frac{1}{h}\left(D\left(x + \frac{h}{2}\right)\frac{\phi(x+h) - \phi(x)}{h} - D\left(x - \frac{h}{2}\right)\frac{\phi(x) - \phi(x-h)}{h}\right).$$

With a constant value of $D(x)$ this formula becomes

$$\frac{d}{dx} D(x) \frac{d\phi}{dx} = \frac{D}{h^2}\left(\phi(x+h) - 2\phi(x) + \phi(x-h)\right).$$

One outstanding question is what order is this approximation. It is fairly obvious that it is second-order when D is constant. It is tedious, but straightforward, to show that the error is second-order in h even when D is changing.

What about higher derivatives? As we did in the diffusion operator, we can just apply the same formula over and over until we get a derivative of any degree we like. We will not go further into the higher-degree derivative formulas here because the formulae are usually for specialized problems and can be generated easily. One thing to note, as we saw when we went from first to second derivatives (two points to three points), the number of points you need to evaluate the function at grows with the derivative degree.

14.6 RICHARDSON EXTRAPOLATION

If we want high-order approximations to derivatives (or many other quantities), we can use Richardson extrapolation. This idea goes back to Lewis Fry Richardson, one of the first people to solve problems using computers. Though in his case in the early 1900s the computers were adolescent boys doing calculations on slide rules. This also is where the notion of an expensive algorithm might come from because Richardson paid the "computeers" by the operation.

In any case, Richardson extrapolation combines two approximations to get a more accurate answer. To see how this works, we can look at a central difference approximation to the first derivative using h and $h/2$:

$$\frac{f(x+h)-f(x-h)}{2h} = f'(x) + \frac{h^2}{6} f'''(x) + O(h^4),$$

and

$$\frac{f(x+h/2)-f(x-h/2)}{h} = f'(x) + \frac{h^2}{24} f'''(x) + O(h^4).$$

For simplicity we define

$$\hat{f}'_h \equiv \frac{f(x+h)-f(x-h)}{2h},$$

and

$$\hat{f}'_{h/2} \equiv \frac{f(x+h/2)-f(x-h/2)}{h}.$$

Notice that if we take the combination

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

This is a fourth-order approximation to the derivative as the error term scales as h^4 as h is decreased. In this case we obtained two extra orders of accuracy by combining two second-order approximations because the central difference approximation only has even powers of h in its error term.

The same type of extrapolation can be done with the forward or backward difference scheme. For the forward difference method we have

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

and

$$\frac{f(x+h/2)-f(x)}{h/2} = f'(x) + \frac{h}{4} f''(x) + \frac{h^2}{24} f'''(x) + O(h^3).$$

Now we can write

$$2\hat{f}'_{h/2} - \hat{f}'_h = f'(x) + O(h^2),$$

where the $\hat{f}'$s are now the forward difference estimates. Notice there that we only improved the order of accuracy by one order this time. This is the most common case with Richardson extrapolation.

We can generalize what we did to get a general Richardson extrapolation formula. Call R_{k+1} the Richardson extrapolated quantity of order $k+1$, and $\hat{g}_h$ a quantity estimated using h and $\hat{g}_{h/n}$ a quantity estimated with the same method using h/n. If the original method is order k accurate, then the Richardson extrapolated estimate is

$$R_{k+1} = \frac{n^k \hat{g}_{h/n} - \hat{g}_h}{n^k - 1} = g + O(h^{k+1}).$$

In the example above using central differences, $n = 2$ and $k = 2$, that is why the 4 appeared in the numerator and a 3 appeared in the denominator. In that example we had

$$R_3 = \frac{4\hat{f}'_{h/2} - \hat{f}'_h}{3}.$$

We call this R_3 even though we obtained fourth-order accuracy in this case because there are no odd-order powers of h in the error term.

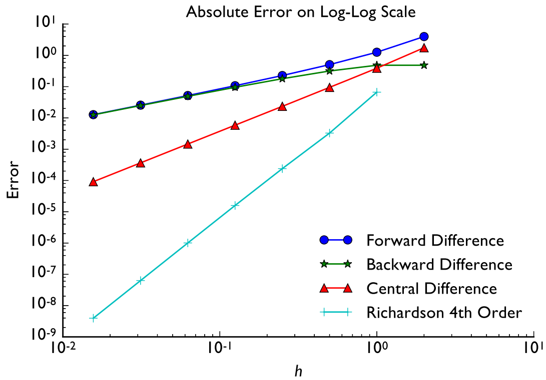
BOX 14.6 NUMERICAL PRINCIPLE

Richardson extrapolation applies a numerical approximation with several values of h and uses the knowledge for how the error scales in h to cancel leading-order error terms. To boot, you can apply Richardson extrapolation repeatedly to get more and more accurate approximations.

We can continue that to even higher order by applying Richardson extrapolation multiple times. As a test we will use our example function from above. The first thing we will do is define a Richardson extrapolation function:

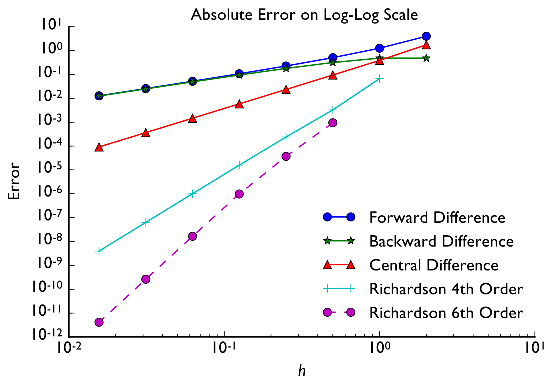
```
In [1]: def RichardsonExtrapolation(fh, fhn, n, k):
            """Compute the Richardson extrapolation based on
            two approximations of order k
            where the finite difference parameter h is used in fh and h/n in fhn.
            Inputs:
            fh:  Approximation using h
            fhn: Approximation using h/n
            n:   divisor of h
            k:   original order of approximation

            Returns:
            Richardson estimate of order k+1"""

            numerator = n**k * fhn - fh
            denominator = n**k - 1
            return numerator/denominator
```

Using this function we can approximate the derivate using Richardson extrapolation. In the following figure, the slope between the last two points in the Richardson extrapolation estimate is 3.998:

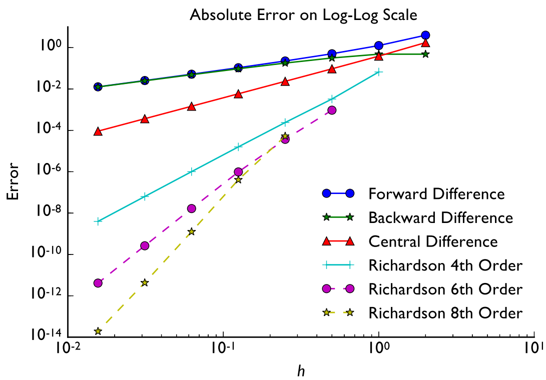


Notice that there is one fewer point in the Richardson line relative to the other lines because it takes two estimates to apply Richardson extrapolation.

We can apply Richardson extrapolation again to get a sixth-order approximation (note that we skip 5 just as we skipped 3). That is we apply the Richardson extrapolation function to the estimate we computed using Richardson extrapolation on the central-difference estimate. The results from this double-extrapolation yield a slope of about 6, as expected:



We can apply Richardson extrapolation again to get an eighth-order approximation:



In this case the slope between the last two points is 7.807. This is because floating point precision is starting to affect the estimate.

The overall results are pretty compelling: the 8th-order approximation is about 10 orders of magnitude better than the original central difference approximation at the finest level of h. The only trade-off is that the original central difference needs two points to approximate the derivative and the eighth-order extrapolated value needs several central difference approximations to get the accurate answer it does.

Richardson extrapolation is a powerful tool to have in your numerical toolkit. All you need to know is an estimate of the order of accuracy for your base method and the level by which you refined h. Knowing this and computing several approximations, you can combine them with Richardson extrapolation to get a better answer.

14.7 COMPLEX STEP APPROXIMATIONS

For functions that are real-valued for a real argument *and* can be evaluated for a complex number, we can use complex arithmetic to get an estimate of the derivative without taking a difference. Consider the Taylor series approximation of a function at $f(x+ih)$:

$$f(x+ih) = f(x) + ihf'(x) - \frac{h^2}{2}f''(x) - \frac{ih^3}{6}f'''(x) + O(h^4). \tag{14.1}$$

The imaginary part of this series is

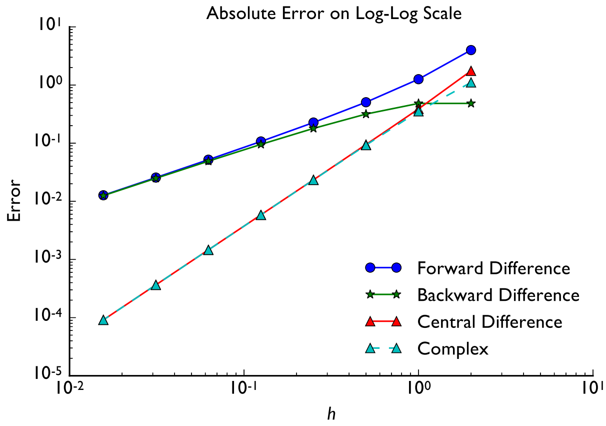
$$\mathrm{Im}\{f(x+ih)\} = hf'(x) - \frac{h^3}{6}f'''(x) + O(h^5),$$

which leads to

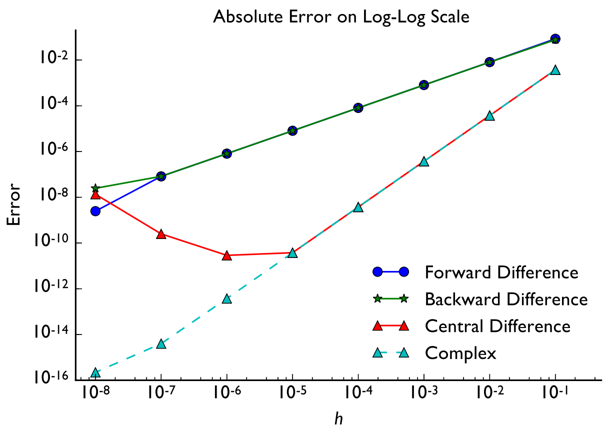
$$f'(x) = \frac{\mathrm{Im}\{f(x+ih)\}}{h} + O(h^2).$$

This is the complex step approximation and it can estimate the derivative by evaluating the function at a complex value and dividing by h. This will be a second-order in h approximation to the derivative. At first, this may seem like it is no better than the central difference formula, and worse than our high-order Richardson extrapolation estimates.

Indeed, if we apply the complex approximation to the derivative on the function from before and the same values of h, we see that it does not perform noticeably different.



Nevertheless, if we let h get even smaller, the central difference approximation reaches a minimum error value before rising. This is due to the fact that the error in finite precision arithmetic starts to dominate the difference between the function values in the central difference formula. In the complex step method there are no differences, and the error in the approximation can go much lower:



Though we have not shown it here, the Richardson extrapolation estimates based on the central difference formula do not reach a lower error than the central difference approximations.

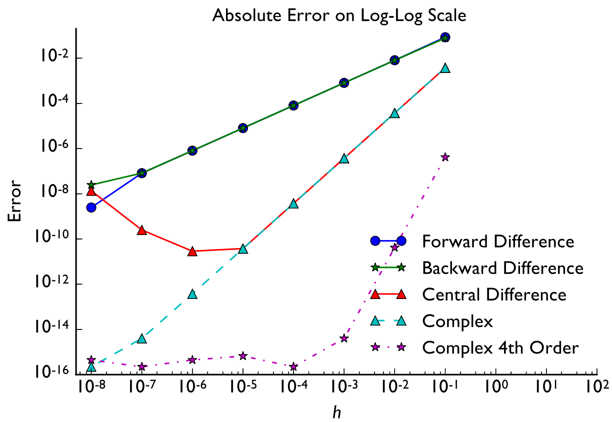
Finally, we will show that it is possible to get a fourth-order complex step approximation. To do this we will combine Eq. (14.1) with the equation for a step of size $h/2$:

$$f\left(x + \frac{ih}{2}\right) = f(x) + \frac{ih}{2} f'(x) - \frac{h^2}{8} f''(x) - \frac{ih^3}{24} f'''(x) + O(h^4). \tag{14.2}$$

Inspecting these two equations, we can get an approximation for $f'(x)$ without the $f'''(x)$ term by adding $-1/8$ times Eq. (14.1) to Eq. (14.2) and multiplying the sum by $8/3$ to get

$$f'(x) = \frac{8}{3h}\text{Im}\left\{f\left(x + \frac{ih}{2}\right) - \frac{1}{8}f\left(x + ih\right)\right\} + O(h^4).$$

This approximation requires two evaluations of the function, but as we can see it reaches the minimum error with a relatively large value of h:



The complex step method is a useful approximation to the derivative when one has a function that can be evaluated with a complex argument. As we have seen, it can be much more accurate than real finite differences, including Richardson extrapolations of those approximations.

CODA

The flip side of numerical differentiation is numerical integration. This will be covered in the next chapter. Whereas, in numerical differentiation the answers got better as the distance between points became smaller, in numerical integration we will break a domain into a finite number of subdivisions and the error will go to zero as the width of those subdivisions goes to zero. The principle of order of accuracy and Richardson extrapolation will be useful in our discussion there as well.

FURTHER READING

The complex step method dates back to the 1960s, but it has only found widespread application in the past few decades [19]. There are also other methods of approximating derivatives called differential quadrature methods [20] that are the derivative versions of the integral quadrature methods that we will encounter in the next chapter.

PROBLEMS

Short Exercises

Compute using $h = 2^{-1}, 2^{-2}, \ldots 2^{-5}$ and the forward, backward, and centered difference, as well as the two complex step approximations the following derivatives.

14.1. $f(x) = \sqrt{x}$ at $x = 0.5$. The answer is $f'(0.5) = 2^{-1/2} \approx 0.70710678118$.
14.2. $f(x) = \arctan(x^2 - 0.9x + 2)$ at $x = 0.5$. The answer is $f'(0.5) = \frac{5}{212}$.
14.3. $f(x) = J_0(x)$, at $x = 1$, where $J_0(x)$ is a Bessel function of the first kind given by

$$J_\alpha(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\,\Gamma(m+\alpha+1)} \left(\frac{x}{2}\right)^{2m+\alpha}.$$

The answer is $f'(1) \approx -0.4400505857449335$. Repeat the calculation using the second-order complex step approximation to get a Richardson extrapolated fourth-order estimate. Compare this to the fourth-order complex step approximation.

Programming Projects

1. Comparison of Methods

Consider the function

$$f(x) = e^{-\frac{x^2}{\sigma^2}}.$$

We will use finite differences to estimate derivatives of this function when $\sigma = 0.1$.

- Using forward, backward, and centered differences, and the two complex step approximations evaluate the error in the approximate derivative of the function at 1000 points between $x = -1$ and $x = 1$ (`np.linspace` will be useful) using the following values of h:

  $$h = 2^0, 2^{-1}, 2^{-2}, \ldots, 2^{-7}.$$

  For each set of approximations compute the average absolute error over the one thousand points

  $$\text{Average Absolute Error} = \frac{1}{N} \sum_{i=1}^{N} |f'(x_i) - f'_{\text{approx}}(x_i)|,$$

  where $f'_{\text{approx}}(x_i)$ is the value of an approximate derivative at x_i and N is the number of points the function derivative is evaluated at. You will need to find the exact value of the derivative to complete this estimate.
  Plot the value of the average absolute error from each approximation on the same figure on a log-log scale. Discuss what you see. Is the highest-order method always the most accurate? Compute the order of accuracy you observe by computing the slope on the log-log plot.

Next, compute the maximum absolute error for each value of h as

$$\text{Maximum Absolute Error} = \max_i |f'(x_i) - f'_{\text{approx}}(x_i)|.$$

Plot the value of the maximum absolute error from each approximation on the same figure on a log-log scale. Discuss what you see. Is the highest-order method always the most accurate?

- Repeat the previous part using the second-order version of the second-derivative approximation discussed above. You will only have one formula in this case.
- Now derive a formula for the fourth derivative and predict its order of accuracy. Then repeat the calculation and graphing of the average and maximum absolute errors and verify the order of accuracy.