Numerical differentiation for AMSC 460

Prof. Jacob Bedrossian
University of Maryland, College Park

In these notes we discuss the problem of numerical differentiation. Recall that from Taylor's theorem the formula:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h) \tag{1}$$

Formulas of this type are called *finite difference formulas*. This specific formula is called the *first order forward difference*. The "first order" refers to the 1 in $O(h^1)$, and hence specifies the accuracy. The "forward" refers to the fact that the formula for $f'(x)$ only uses values of f at points to the right of y. The *first order backward difference* is

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

The *second order central difference* is

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

For all three formulas, one can verify the accuracy by just Taylor expanding everything around x and cancelling terms. However, if one wants to derive higher order finite difference formulas, you can imagine that this gets quickly a mess. It is useful to think about the geometric interpretation of these formulas. The formula (1) is the slope of the line that goes through the points $(x, f(x))$, $(x+h, f(x+h))$ whereas (2) is the slope of the secant line that goes through the points $(x, f(x))$, $(x-h, f(x-h))$, and (3) is the slope of the secant line that goes through the points$(x-h, f(x-h))$, $(x+h, f(x+h))$. This gives us one good idea for deriving further schemes. Suppose c_j are given for $1 \leq j \leq \nu$ and we are interested in finding a finite difference formula of the form:

$$\frac{1}{h}\sum_{j=1}^{\nu} a_j f(hc_j) = f'(0) + O(h^p), \tag{4}$$

for some $p \geq 1$. Notice that it suffices to only care about $x = 0$, this would give us the following formula by translation:

$$\frac{1}{h}\sum_{j=1}^{\nu} a_j f(x + hc_j) = f'(x) + O(h^p), \tag{5}$$

A natural guess is to define the $\nu - 1$ degree polynomial which goes through the points $(x+hc_j, f(x+hc_j))$, call it $Q_{\nu-1}$, and find a_j such that

$$Q'(0) = \frac{1}{h}\sum_{j=1}^{\nu} a_j f(hc_j). \tag{6}$$

Recall that we can write down the Lagrange form of Q "explicitly":

$$Q(x) = \sum_{j=1}^{\nu} f(hc_j)\frac{\Pi_{i=1, i\neq j}^{n}(x - hc_i)}{\Pi_{i=1, i\neq j}^{n}(x_j - hc_i)}. \tag{7}$$

Hence, we have

$$Q'(x) = \sum_{j=1}^{\nu} f(hc_j) \frac{d}{dx} \left(\frac{\Pi_{i=1,i\neq j}^{n}(x - hc_i)}{\Pi_{i=1,i\neq j}^{n}(hc_j - hc_i)} \right). \tag{8}$$

Therefore we have a candidate formula for how to pick the a_j's:

$$a_j = h \frac{d}{dx} \left(\frac{\Pi_{i=1,i\neq j}^{\nu}(x - hc_i)}{\Pi_{i=1,i\neq j}^{\nu}(hc_j - hc_i)} \right) |_{x=0}. \tag{9}$$

If you think about it for a bit, you'll see that a_j is *independent of* h. To see this, expand the polynomial for some coefficients p_j independent of h such that:

$$\Pi_{i=1,i\neq j}^{\nu}(x - hc_i) = \sum_{k=0}^{\nu-1} p_k h^{\nu-k-1} x^k. \tag{10}$$

Hence,

$$a_j = \frac{p_1}{\Pi_{i=1,i\neq j}^{\nu}(c_j - c_i)}. \tag{11}$$

Note if we choose a_j like this, we will get the difference formula:

$$\frac{1}{h} \sum_{j=1}^{\nu} a_j f(hc_j) = f'(0) + O(h^p), \tag{12}$$

hopefully for some $p \geq 1$. Now, of course this is not a pretty or very explicit formula (you can compute p_1 explicitly in terms of the c_j's but its still ugly), The above gives us an algorithm for determining the coefficients of a finite difference formula regardless of how we choose c_j, though in the vast majority of cases, finite difference formulas are used where $c_j's$ are integers (positive or negative). However, one can be more general, for example, if one needs to adapt the accuracy of your formula to x, you might want to use different h's at different x's. This will lead to more complicated formulas (that you can compute with some effort, or in many cases, program your computer to compute). Now, if I give you a higher order difference scheme, for example,

$$f'(x) = \frac{-\frac{1}{12}f(x+2h) + \frac{2}{3}f(x+h) - \frac{2}{3}f(x-h) + \frac{1}{12}f(x-2h)}{h} + O(h^4), \tag{13}$$

you could in theory at least, expand every term out to 5th order using Taylor's theorem and match up terms until you verified that the formula is indeed 4-th order accurate. However, there's a more direct method, which is the following theorem.

Theorem 1. *Let a_j and c_j be such that for all polynomials of degree $\leq m$, there holds*

$$\sum_{j=1}^{\nu} a_j p(c_j) = p'(0). \tag{14}$$

Then,

$$\frac{1}{h} \sum_{j=1}^{\nu} a_j f(hc_j) = f'(0) + O(h^m). \tag{15}$$

Proof. By Taylor's theorem,

$$f'(hc_j) = \sum_{k=0}^{m} \frac{f^{(k)}(0)}{k!}(hc_j)^k + O(h^{m+1}). \tag{16}$$

Define the m-degree polynomial:

$$p(x) = \frac{1}{h}\sum_{k=0}^{m} \frac{f^{(k)}(0)}{k!}(hx)^k, \tag{17}$$

which implies

$$\frac{1}{h}\sum_{j=1}^{\nu} a_j f(hc_j) = \sum_{j=1}^{\nu} a_j p(c_j) + O(h^m). \tag{18}$$

Then *by the assumption* (14),

$$\sum_{j=1}^{\nu} a_j p(c_j) = p'(0). \tag{19}$$

Finally, we observe,

$$p'(x) = \frac{1}{h}\sum_{k=1}^{m} \frac{f^{(k)}(0)k}{k!}h^k x^{k-1} = \sum_{k=1}^{m} \frac{f^{(k)}(0)}{(k-1)!}h^{k-1}x^{k-1} = f'(0) + \sum_{k=2}^{m} \frac{f^{(k)}(0)}{(k-1)!}h^{k-1}x^{k-1}. \tag{20}$$

Hence,

$$p'(0) = f'(0). \tag{21}$$

The result then follows from (18). □

Using Theorem 1, we can deduce the following.

Theorem 2. *The finite difference formula* (12) *is satisfied for* $p \geq \nu - 1$.

Proof. By construction, if p is at most a $\nu - 1$ degree polynomial, then the interpolating polynomial $Q = p$. □

There are three general classes which come up often. Forward one-sided differences:

$$f'(x) = \frac{1}{h}\sum_{j=1}^{\nu} a_j f(x + hj) + O(h^{\nu-1}), \tag{22}$$

backward one-sided differences:

$$f'(x) = \frac{1}{h}\sum_{j=1}^{\nu} a_j f(x - hj) + O(h^{\nu-1}), \tag{23}$$

and central differences: for even $\nu \geq 2$,

$$f'(x) = \frac{1}{h}\sum_{j=1}^{\nu/2} a_j \left(f(x + hj) - f(x - hj)\right) + O(h^{\nu}). \tag{24}$$

Let us see why the accuracy is $O(h^\nu)$ as opposed to $O(h^{\nu-1})$ as one might expect. First observe that for all *even* polynomials p of *any* degree:

$$0 = p'(0) = \sum_{j=1}^{\nu/2} a_j \left(p(j) - p(-j)\right). \tag{25}$$

Now, we choose a_j so that (14) holds for as many odd polynomials as possible. For $p(x) = x$, this gives the constraint:

$$1 = \sum_{j=1}^{\nu/2} 2ja_j. \tag{26}$$

For $p(x) = x^{2p+1}$ with $p \geq 0$, (14) gives

$$\sum_{j=1}^{\nu/2} 2j^{2p+1}a_j = \begin{cases} 1 & p = 0 \\ 0 & p \geq 1. \end{cases} \tag{27}$$

We have $\nu/2$ unknowns and therefore we can form a square linear system for the a_j's by requiring they satisfy (27) for $p \leq \nu/2-1$. The linear system has a unique solution by the arguments we made when we studied interpolation, so we can uniquely choose a_j so that (27) holds for $p \leq \nu/2 - 1$. Therefore,

$$p'(0) = \sum_{j=1}^{\nu/2} a_j \left(p(j) - p(-j)\right), \tag{28}$$

holds for all odd polynomials of degree $\leq \nu - 1$. However, we have already seen that the formula is automatically exact for all even polynomials and hence (28) holds for all polynomials of degree less than or equal to ν and Theorem 1 implies the error estimate stated in (24).

Richardson Extrapolation

There is another technique for deriving the central difference schemes which has its uses in other branches of numerical analysis (including, for example, numerical integration). This is called *Richardson extrapolation*. It is easiest to just explain the basic idea with an example. By Taylor's theorem, we have the following (which is less annoying to derive than it looks):

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \left[\frac{f^{(3)}h^2}{3!} + \frac{f^{(5)}h^4}{5!}\right] + O(h^6). \tag{29}$$

Of course, then also means that:

$$f'(x) = \frac{f(x+2h) - f(x-2h)}{4h} + \left[\frac{f^{(3)}(2h)^2}{3!} + \frac{f^{(5)}(2h)^4}{5!}\right] + O(h^6). \tag{30}$$

However, this means we can cleverly combine the formulas to *cancel* the leading order term in the error:

$$f'(x) = \frac{4}{3}\left(\frac{f(x+h) - f(x-h)}{2h}\right) - \frac{1}{3}\left(\frac{f(x+2h) - f(x-2h)}{4h}\right) + O(h^4). \tag{31}$$

This therefore gives an alternative derivation of (13). If one is intrepid and motivated, its clear that one can continue this procedure to recover all of the central difference formulas. This is also a general idea that is useful in many settings: if you know the leading order expansion of the error term, then you can combine discretizations at different choices of h in a clever way to cancel it out and obtain higher order accuracy. The general concept is called *Richardson extrapolation*. One of the advantages is that you don't really need to explicitly compute (13), you really just need to combine the answers from your second order approximations as in (31). This isn't staggeringly useful in this example but it can be convenient in certain settings.

Higher order derivatives

The ideas put forward for first derivatives are easily extended (at least with a little technical calculation), to higher order derivatives. In particular, we have the theorem:

Theorem 3. *Suppose that the following formula holds for all polynomials of degree* $\leq m+q-1$*:*

$$\sum_{j=1}^{\nu} a_j p(c_j) = p^{(q)}(0). \tag{32}$$

Then,

$$\frac{1}{h^q}\sum_{j=1}^{\nu} a_j f(hc_j) = f^{(q)}(0) + O(h^m). \tag{33}$$

Proof. The proof is similar, but lets do it so we can see how the q turns up where it does:

$$\frac{1}{h^q}\sum_{j=1}^{\nu} a_j f(hc_j) = \frac{1}{h^q}\sum_{j=1}^{\nu} a_j \sum_{k=0}^{m+q-1} \frac{f^{(k)}(0)}{k!}(hc_j)^k + O(h^m). \tag{34}$$

Then set

$$p(x) = \frac{1}{h^q}\sum_{k=0}^{m+q-1} \frac{f^{(k)}(0)}{k!}(hx)^k. \tag{35}$$

Computing the q-th derivative efficiently will require some thought if you haven't seen it before, but if you work it through, you'll get

$$p^{(q)}(x) = \frac{1}{h^q}\sum_{k=q}^{m+q-1} \frac{f^{(k)}(0)}{k!} h^k k(k-1)...(k-q+1)h^k x^{k-q} = \sum_{k=q}^{m+q-1} \frac{f^{(k)}(0)}{(k-q)!}(hx)^{k-q}. \tag{36}$$

Hence,

$$p^{(q)}(0) = f^{(q)}(0). \tag{37}$$

□

The above theorem suggests we might need a lot more points to get decent approximations. For this, central differences are even more useful. The standard way of computing second derivatives is

$$f'(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2). \tag{38}$$

By Richardson extrapolation or by considering even and odd polynomials again, you can derive the 4-th order approximation:

$$f'(x) = \frac{1}{h^2}\left(-\frac{1}{12}f(x-2h) + \frac{4}{3}f(x-h) - \frac{5}{2}f(x) + \frac{4}{3}f(x+h) - \frac{1}{12}f(x+2h)\right) + O(h^4). \tag{39}$$