Numerical Differentiation

Among other things, our goal is to show

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

Recall that for the Lagrange interpolating polynomial we proved the following theorem:

Theorem Suppose $x_1, \dots x_n$ are distinct numbers in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, for each $x \in [a, b]$ a number $c \in (a, b)$ exists with:

$$f(x) = P_{n-1}(x) + \frac{1}{n!} f^{(n)}(c) \prod_{i=1}^{n} (x - x_i),$$

$$P_{n-1}(x) = \sum_{k=1}^{n} f(x_k) L_{nk}(x),$$

$$L_{nk}(x) = \prod_{i=1, i \neq k}^{n} \frac{(x - x_i)}{(x_k - x_i)}.$$

If have $n + 1$ points $x_0, \dots x_n$ we can work with:

$$f(x) = P_n(x) + \frac{1}{(n+1)!} f^{(n+1)}(c) \prod_{i=0}^{n} (x - x_i), \qquad \text{(the } c \text{ in this equation is partly the problem)}$$

$$P_n(x) = \sum_{k=0}^{n} f(x_k) L_{nk}(x),$$

$$L_{nk}(x) = \prod_{i=0, i \neq k}^{n} \frac{(x - x_i)}{(x_k - x_i)}.$$

When deriving the point formulas for derivatives is is standard to use points starting at x_0, and use equally spaced points:

$$x_0, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h, \quad \dots \quad x_n = x_0 + nh.$$

The Error Term

- The difficulty in using the above expression for determining a derivative formula is partly the quantity c.
- Ultimately, we are going to be using these formulas to work in intervals $[a, b] = [x_0, x_0 + nh]$, and so the interval will depend on the value of h. This has an impact on c.
- The value of c actually depends on the interval we are in, and we should be thinking of $c = c(x) \in [x_0, x_0 + nh]$ since the value of c changes if we evaluate at different values of x.
- Before, everything was simply in the interval $[a, b]$ and that was all we needed, but let's be a bit more careful here and see what happens if we keep track of $c(x)$. What is important is that

$$\lim_{h \to 0} f^{(n+1)}(c) = f^{(n+1)}(x_0).$$

Starting from this expression for f, we can differentiate and then evaluate at $x = x_j$:

$$
\begin{aligned}
f(x) &= \sum_{k=0}^{n} f(x_k) L_{nk}(x) + \frac{1}{(n+1)!} f^{(n+1)}(c(x)) \prod_{i=0}^{n} (x - x_i), \\
f'(x) &= \sum_{k=0}^{n} f(x_k) L'_{nk}(x) + \frac{1}{(n+1)!} f^{(n+1)}(c(x)) \frac{d}{dx}\left[\prod_{i=0}^{n} (x - x_i)\right] + \frac{1}{(n+1)!} \frac{d}{dx}\left[f^{(n+1)}(c(x))\right] \prod_{i=0}^{n} (x - x_i), \\
f'(x_j) &= \sum_{k=0}^{n} f(x_k) L'_{nk}(x_j) + \frac{1}{(n+1)!} f^{(n+1)}(c(x_j)) \frac{d}{dx}\left[\prod_{i=0}^{n} (x - x_i)\right]_{x=x_j} + 0. \text{ (one of the factors is zero)}
\end{aligned}
$$

Notice that the choice to evaluate at x_j was important since it eliminates the need to compute $\frac{d}{dx}\left[f^{(n+1)}(c(x))\right]$ which would be difficult to do since we don't really know how $c(x)$ varies as function of x.

We can use implicit differentiation to work out the derivative we still need: $\frac{d}{dx}\left[\prod_{i=0}^{n} (x - x_i)\right]_{x=x_j}$:

$$
\begin{aligned}
y &= \prod_{i=0}^{n} (x - x_i), \\
\ln y &= \sum_{i=0}^{n} \ln(x - x_i), \\
\frac{y'}{y} &= \sum_{i=0}^{n} \frac{1}{x - x_i}, \\
y' &= \left(\prod_{i=0}^{n} (x - x_i)\right)\left(\sum_{i=0}^{n} \frac{1}{x - x_i}\right), \\
y'\Big|_{x=x_j} &= \left(\prod_{i=0}^{n} (x_j - x_i)\right)\left(\sum_{i=0}^{n} \frac{1}{x_j - x_i}\right), \\
&= ((x_j - x_0)\cdots(x_j - x_{j-1})(x_j - x_j)(x_j - x_{j+1})\cdots(x_j - x_n)) \\
&\qquad \times \left(\frac{1}{(x_j - x_0)} + \cdots + \frac{1}{(x_j - x_j)} + \cdots + \frac{1}{(x_j - x_n)}\right), \\
&= (x_j - x_0)\cdots(x_j - x_{j-1})(x_j - x_{j+1})\cdots(x_j - x_n), \\
&= \prod_{i=0, i\neq j}^{n} (x_j - x_i). \qquad \text{(all other have an } x_j - x_k \text{ in numerator, and are zero)}
\end{aligned}
$$

So we have created an $n+1$-point formula to approximate $f'(x_j)$:

$$
f'(x_j) = \sum_{k=0}^{n} f(x_k) L'_{nk}(x_j) + \frac{1}{(n+1)!} f^{(n+1)}(c_j) \prod_{i=0, i\neq j}^{n} (x_j - x_i),
$$

where $c(x_j) = c_j \in [x_0, x_n]$.

2-point formulas: $n = 1$

$$f'(x_j) = \sum_{k=0}^{1} f(x_k) L'_{1k}(x_j) + \frac{1}{(2)!} f^{(2)}(c_j) \prod_{i=0, i\neq j}^{1} (x_j - x_i).$$

Choose nodes $x_0, x_1 = x_0 + h$:

$$f'(x_j) = f(x_0) L'_{10}(x_j) + f(x_1) L'_{11}(x_j) + \frac{1}{2!} f^{(2)}(c_j) \prod_{i=0, i\neq j}^{1} (x_j - x_i),$$

$$L_{10}(x) = \frac{x - x_1}{x_0 - x_1} \qquad \Rightarrow \qquad L'_{10}(x) = \frac{1}{x_0 - x_1} = -\frac{1}{h},$$

$$L_{11}(x) = \frac{x - x_0}{x_1 - x_0} \qquad \Rightarrow \qquad L'_{10}(x) = \frac{1}{x_1 - x_0} = +\frac{1}{h}.$$

Choose $x_j = x_0$ we get (where $x_0 \le c_0 \le x_1$):

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} + \frac{1}{2!} f^{(2)}(c_0)(x_0 - x_1),$$

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f^{(2)}(c_0),$$

Let $x = x_0$: $f'(x) = \dfrac{f(x+h) - f(x)}{h} - \dfrac{h}{2} f^{(2)}(c_0).$ (forward-difference formula if $h > 0$)

Choose $x_j = x_1$ we get (where $x_0 \le c_1 \le x_1$):

$$f'(x_1) = \frac{f(x_1) - f(x_0)}{h} + \frac{1}{2!} f^{(2)}(c_1)(x_1 - x_0),$$

$$f'(x_1) = \frac{f(x_1) - f(x_1 - h)}{h} + \frac{h}{2} f^{(2)}(c_1),$$ (since $x_0 = x_1 - h$)

Let $x = x_1$: $f'(x) = \dfrac{f(x) - f(x-h)}{h} + \dfrac{h}{2} f^{(2)}(c_0).$ (backward-difference formula if $h > 0$)

We can easily generate more $n+1$-point formulas for derivatives using *Mathematica* to do the algebra for us.

A 3-point formula: $n = 2, j = 0$, then set $x = x_0$

$$f'(x) = \frac{1}{2h}\Big(-3f(x) + 4f(x+h) - f(x+2h)\Big) + \frac{h^2}{3} f^{(3)}(c), \quad x \le c \le x + 2h.$$

A 3-point formula: $n = 2, j = 1$, then set $x = x_0 + h$ (Eq. 5.7 in the text)

$$f'(x) = \frac{1}{2h}\Big(f(x+h) - f(x-h)\Big) - \frac{h^2}{6} f^{(3)}(c), \quad x - h \le c \le x + h.$$

A 5-point formula: $n = 4, j = 2$, then set $x = x_0 - 2h$

$$f'(x) = \frac{1}{12h}\Big(f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)\Big) + \frac{h^4}{30} f^{(5)}(c), \quad x - 2h \le c \le x + 2h.$$

This last equation is Eq. 5.16 in the text (with $h \to 2h$) which was arrived at via Richardson's extrapolation. The process we have used to derive this expression already contains the fact that it is $O(h^4)$.

Higher Derivative Point Formulas

You can create higher derivative point formulas by starting from the Taylor series and combining formulas in a manner that eliminates all derivatives except the one you are looking for. We also need to make sure to define c appropriately along the way. To do that we need a theorem.

Generalized Intermediate Value Theorem Let f be a continuous function on the interval $[a, b]$. Let $x_0, \dots, x_n$ be points in $[a, b]$ and $a_0, \dots, a_n > 0$. Then there exists a number c between a and b such that

$$a_1 f(x_1) + \cdots + a_n f(x_n) = (a_1 + \cdots + a_n) f(c).$$

Proof is in the text (it is pretty straightforward, relying of course on the Intermediate Value Theorem).

Example

Start with Taylor Series:

$$f(x) = f(x_0) + f^{(1)}(x_0)(x - x_0) + \frac{1}{2} f^{(2)}(x_0)(x - x_0)^2 + \frac{1}{6} f^{(3)}(x_0)(x - x_0)^3 + \frac{1}{24} f^{(4)}(c)(x - x_0)^4,$$

where c is between x and x_0.

Now evaluate at $x = x_0 + h$ and $x = x_0 - h$, where $h > 0$

$$f(x_0 + h) = f(x_0) + f^{(1)}(x_0)h + \frac{1}{2} f^{(2)}(x_0)h^2 + \frac{1}{6} f^{(3)}(x_0)h^3 + \frac{1}{24} f^{(4)}(c_1)h^4, \qquad \text{where } c_1 \in [x_0, x_0 + h]$$
$$f(x_0 - h) = f(x_0) - f^{(1)}(x_0)h + \frac{1}{2} f^{(2)}(x_0)h^2 - \frac{1}{6} f^{(3)}(x_0)h^3 + \frac{1}{24} f^{(4)}(c_2)h^4, \qquad \text{where } c_2 \in [x_0 - h, x_0]$$

and adding the above equations and solving for $f^{(2)}(x_0)$ yields

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + f^{(2)}(x_0)h^2 + \frac{h^4}{24}\left(f^{(4)}(c_1) + f^{(4)}(c_2)\right),$$
$$f^{(2)}(x_0) = \frac{1}{h^2}\Big(f(x_0 - h) - 2f(x_0) + f(x_0 + h)\Big) - \frac{h^2}{24}\left(f^{(4)}(c_1) + f^{(4)}(c_2)\right).$$

Using the Generalized Intermediate Value Theorem, we have

$$f^{(4)}(c_1) + f^{(4)}(c_2), = 2f^{(4)}(c), \qquad \text{where } c \in [x_0 - h, x_0 + h].$$

So we have constructed a 3-point second derivative formula (Eq. 5.8 in the text):

$$f^{(2)}(x_0) = \frac{1}{h^2}\Big(f(x_0 - h) - 2f(x_0) + f(x_0 + h)\Big) - h^2 \frac{f^{(4)}(c)}{12}, \qquad \text{where } c \in [x_0 - h, x_0 + h]$$
$$f^{(2)}(x_0) = \frac{1}{h^2}\Big(f(x_0 - h) - 2f(x_0) + f(x_0 + h)\Big) + O(h^2).$$

Note: You can use $n + 1$-point formulas on given functions $f(x)$ or data sets (x_i, y_i).

If you use them on data sets you may have to use different formulas on the endpoints of the region.