Week 11: Monday, Apr 9

Maximizing an interpolating quadratic

Suppose that a function f is evaluated on a reasonably fine, uniform mesh $\{x_i\}_{i=0}^n$ with spacing $h = x_{i+1} - x_i$. How can we find any local maxima inside the mesh interval (x_0, x_n)?

A natural first approximation is to simply find local maxima in the discrete sequence $\{f(x_i)\}_{i=0}^n$. I would usually do that by looking for a place where differences between adjacent points change from positive to negative (the discrete analog of looking for a critical point where the derivative changes from positive to negative):

```
% [idx] = find_local_max(fi)
%
% Based on samples fi of a function on a uniform mesh over
% an interval, find the indices of mesh points where there
% are discrete local maxima.

function [idx] = find_local_max(fi)

  d_fi = fi(2:end)-fi(1:end-1);
  idx  = find( d_fi:end-1) > 0 & d_fi(2:end) <= 0 );
  idx  = idx+1;
```

Unfortunately, unless we use a rather fine mesh, this method is unlikely to give us more than a couple digits of accuracy. A simple method of improving the accuracy of the result is to fit a polynomial interpolant to the data near the discrete local maximum, and use a maximum of the interpolating polynomial as an estimate for the local maximum of f. The simplest variant of this is to fit a quadratic; let's look in a little detail at how this works.

Suppose x_j is an interior mesh point where f has a discrete local maximum. We would like to find a corrected estimate of the local maximum, $x_* = x_j + z$, by maximizing a quadratic interpolant through x_{j-1}, x_j, and

x_{j+1}. In terms of the correction z, the interpolation conditions are

$$\begin{aligned} p(0) &= f(x_j + 0) = f(x_j) \\ p(h) &= f(x_j + h) = f(x_{j+1}) \\ p(-h) &= f(x_j - h) = f(x_{j-1}) \end{aligned}$$

In a homework exercise, we saw how to differentiate a polynomial interpolant written in the Newton basis. For variety, let's now write things in terms of the Lagrange polynomials for $\{0, h, -h\}$:

$$\begin{aligned} p(z) &= \frac{p(0)}{h^2}(h^2 - z^2) + \frac{p(h)}{2h^2} z(z+h) + \frac{p(-h)}{2h^2} z(z-h) \\ &= p(0) + \left(\frac{p(h) - p(-h)}{2h} \right) z + \frac{1}{2} \left(\frac{p(h) - 2p(0) + p(-h)}{h^2} \right) z^2. \end{aligned}$$

Note that this last expression is just $p(z)$ expressed in Taylor series form:

$$p(z) = p(0) + p'(0)z + \frac{1}{2} p''(0) z^2.$$

where

$$\begin{aligned} p'(0) &= p[h, -h] = \frac{p(h) - p(-h)}{2h}, \\ p''(0) &= 2p[h, 0, -h] = \frac{p(h) - 2p(0) + p(-h)}{h^2}. \end{aligned}$$

Therefore, the maximum z_* for p satisfies

$$z_* = -\frac{p'(0)}{p''(0)}, \qquad p(z_*) = p(0) - \frac{p'(0)^2}{2p''(0)}.$$

It's worth comparing this maximization to what we would do if we took x_j as an initial guess at the maximum and did one step of Newton iteration to improve our guess:

$$x^{\text{new}} = x_j - \frac{f'(x_j)}{f''(x_j)}$$

The correction z_* looks just like what we would compute in one Newton step, but with the approximations $f'(x_j) \approx p'(0)$ and $f''(x_j) \approx p''(0)$!

Two ways to numerical differentiation

One way to approximate derivatives is by *interpolation*. If we can use interpolation to estimate function values, why not use it to estimate derivatives as well? The basic procedure here is:

- Interpolate f at some nodes $x_0, \ldots, x_n$.
- Differentiate the interpolating polynomial in order to approximate derivatives of f. Usually, one is interested in the derivative at one of the node points.

In general, if the interpolation points $x_0, \ldots, x_n$ all lie within an interval of length h, and if f has enough continuous derivatives in that interval, we have

$$p^{(k)}(x_j) = O(h^{n+1-k}).$$

The error analysis is relatively straightforward, and is in the book; but I did not drag you through the algebra in class, and do not intend to do so here.

This, therefore, is one way of thinking about numerical differentiation. Another way to get to the same end is to manipulate Taylor series. For example, in the previous section we derived the *centered difference* approximations by differentiating a quadratic interpolant:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}, \quad f''(x) \approx \frac{f(x+h) - 2f(0) + f(x-h)}{h^2}.$$

We could have also said "we have $f(x)$, $f(x+h)$, and $f(x-h)$; what linear combination of these values best approximates $f'(x)$ (or $f''(x)$)?" That is, we somehow want to choose coefficients a_+, a_0, a_- so that we get a good approximation of $f'(x)$ of the form

$$f'(x) \approx \hat{f}'(x) \equiv a_0 f(x) + a_+ f(x+h) + a_- f(x-h).$$

Note that we can Taylor expand the terms in $\hat{f}'(x)$ about x to get

$$\begin{aligned}
\hat{f}'(x) = &(a_0 + a_+ + a_-) f(x) \\
&+ h(a_+ - a_-) f'(x) \\
&+ \frac{h^2}{2}(a_+ + a_-) f''(x) \\
&+ \frac{h^3}{6}(a_+ - a_-) f'''(x) \\
&+ O(h^4)
\end{aligned}$$

We can adjust the three coefficients to match the first three terms in this series with the the (trivial) Taylor series for $f'(x)$ by solving the linear system

$$\begin{aligned}(a_0 + a_+ + a_-) &= 0 \\ h(a_+ - a_-) &= 1 \\ \frac{h^2}{2}(a_+ + a_-) &= 0.\end{aligned}$$

This gives us

$$a_0 = 0, \quad a_\pm = \pm\frac{1}{2h}$$

or

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

Let's walk through the same exercise for computing the second derivative. We want a formula of the form

$$\hat{f}''(x) = b_0 f(x) + b_+ f(x+h) + b_- f(x-h),$$

and Taylor expanding each term in the right hand side about zero gives

$$\begin{aligned}\hat{f}'(x) = &(b_0 + b_+ + b_-)f(x) \\ &+ h(b_+ - b_-)f'(x) \\ &+ \frac{h^2}{2}(b_+ + b_-)f''(x) \\ &+ \frac{h^3}{6}(b_+ - b_-)f'''(x) \\ &+ O(h^4)\end{aligned}$$

Setting the first three terms in this series to match $f''(x)$, we get the equations

$$\begin{aligned}(b_0 + b_+ + b_-) &= 0 \\ h(b_+ - b_-) &= 0 \\ \frac{h^2}{2}(b_+ + b_-) &= 1,\end{aligned}$$

which has the solution

$$b_0 = -\frac{2}{h^2}, \quad b_\pm = \frac{1}{h^2}.$$

Notice that because $b_+ - b_-$, we also automatically get that

$$\frac{h^3}{6}(b_+ - b_-)f''(x) = 0,$$

and so

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

which is one better order of accuracy than we might have expected from looking too uncautiously at the bound based on the derivation via polynomial interpolation.