LECTURE 4: *Constructing Finite Difference Formulas*

1.7 *Application: Interpolants for Finite Difference Formulas*

The most obvious use of interpolants is to construct polynomial models of more complicated functions. However, numerical analysts rely on interpolants for many other numerical chores. For example, in a few weeks we shall see that common techniques for approximating definite integrals amount to exactly integrating a polynomial interpolant. Here we turn to a different application: the use of interpolating polynomials to derive finite difference formulas that approximate derivatives, the to use those formulas to construct approximations of differential equation boundary value problems.

1.7.1 *Derivatives of Interpolants*

Theorem 1.3 from the last lecture showed how well the interpolant $p_n \in \mathcal{P}_n$ approximates f. Here we seek deeper connections between p_n and f.

$$\boxed{\text{How well do derivatives of } p_n \text{ approximate derivatives of } f\,?}$$

Let $p \in \mathcal{P}_n$ denote the degree-n polynomial that interpolates f at the distinct points $x_0, \ldots, x_n$. We want to derive a bound on the error $f'(x) - p'(x)$. Let us take the proof of Theorem 1.3 as a template, and adapt it to analyze the error in the derivative.

For simplicity, assume that $\widehat{x} \in \{x_0, \ldots, x_n\}$, i.e., assume that $\widehat{x}$ is one of the interpolation points. Suppose we extend $p(x)$ by one degree so that the derivative of the resulting polynomial at $\widehat{x}$ matches $f'(\widehat{x})$. To do so, use the Newton form of the interpolant, writing the new polynomial as

$$p(x) + \lambda w(x),$$

again with

$$w(x) := \prod_{j=0}^{n} (x - x_j).$$

The derivative interpolation condition at $\widehat{x}$ is

$$f'(\widehat{x}) = p'(\widehat{x}) + \lambda w'(\widehat{x}), \tag{1.8}$$

and since $w(x_j) = 0$ for $j = 0, \ldots, n$, the new polynomial maintains the standard interpolation at the $n+1$ interpolation points:

$$f(x_j) = p(x_j) + \lambda w(x_j), \qquad j = 0, \ldots, n. \tag{1.9}$$

Here we must tweak the proof of Theorem 1.3 slightly. As in that proof, define the error function

$$\phi(x) := f(x) - \big(p(x) + \lambda w(x)\big).$$

Because of the standard interpolation conditions (1.9) at $x_0, \ldots, x_n$, ϕ must have $n+1$ zeros. Now Rolle's theorem implies that ϕ' has (at least) n zeros, each of which occurs strictly between every two consecutive interpolation points. But in addition to these points, ϕ' must have another root at $\widehat{x}$ (which we have required to be one of the interpolation points, and thus distinct from the other n roots). Thus, ϕ' has $n+1$ distinct zeros on $[a,b]$.

Now, repeatedly apply Rolle's theorem to see that ϕ'' has n distinct zeros, ϕ''' has $n-1$ distinct zeros, etc., to conclude that $\phi^{(n+1)}$ has a zero: call it ξ. That is,

$$0 = \phi^{(n+1)}(\xi) = f^{(n+1)}(\xi) - \big(p^{(n+1)}(\xi) + \lambda w^{(n+1)}(\xi)\big). \tag{1.10}$$

We must analyze

$$\phi^{(n+1)}(x) = f^{(n+1)}(x) - \big(p^{(n+1)}(x) + \lambda w^{(n+1)}(x)\big).$$

Just as in the proof of Theorem 1.3, note that $p^{(n+1)} = 0$ since $p \in \mathcal{P}_n$ and $w^{(n+1)}(x) = (n+1)!$. Thus from (1.10) conclude

$$\lambda = \frac{f^{(n+1)}(\xi)}{(n+1)!}.$$

From (1.8) we arrive at

$$f'(\widehat{x}) - p'(\widehat{x}) = \lambda w'(\widehat{x}) = \frac{f^{(n+1)}(\xi)}{(n+1)!} w'(\widehat{x}).$$

To arrive at a concrete estimate, perhaps we should say something more specific about $w'(\widehat{x})$. Expanding w and computing w' explicitly will take us far into the weeds; it suffices to invoke an interesting result from 1889.

Lemma 1.1 was proved by Andrey Markov in 1889, generalizing a result for $n = 2$ that was obtained by the famous chemist Mendeleev in his research on specific gravity. Markov's younger brother Vladimir extended it to higher derivatives (with a more complicated right-hand side) in 1892. The interesting history of this inequality (and further extensions into the complex plane) is recounted in a paper by Ralph Boas, Jr. on 'Inequalities for the derivatives of polynomials,' *Math. Magazine* 42 (4) 1969, 165–174. The result is called the 'Markov brothers' inequality' to distinguish it from the more famous 'Markov's inequality' in probability theory (named, like 'Markov chains,' for Andrey; Vladimir died of tuberculosis at the age of 25 in 1897).

Lemma 1.1 (Markov brothers' inequality for first derivatives).
For any polynomial $q \in \mathcal{P}_n$,

$$\max_{x\in[a,b]} |q'(x)| \le \frac{2n^2}{b-a} \max_{x\in[a,b]} |q(x)|.$$

We can thus summarize our discussion as the following theorem, an analogue of Theorem 1.3.

Theorem 1.6 (Bound on the derivative of an interpolant)**.**
Suppose $f \in C^{(n+1)}[a,b]$ and let $p_n \in \mathcal{P}_n$ denote the polynomial that interpolates $\{(x_j, f(x_j))\}_{j=0}^n$ at distinct points $x_j \in [a,b]$, $j = 0,\ldots,n$. Then for every $x_k \in \{x_0,\ldots,x_n\}$, there exists some $\xi \in [a,b]$ such that

$$f'(x_k) - p_n'(x_k) = \frac{f^{(n+1)}(\xi)}{(n+1)!} w'(x_k),$$

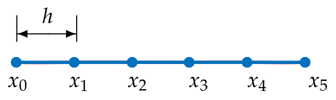
where $w(x) = \prod_{j=0}^n (x - x_j)$. From this formula follows the bound

$$(1.11)\quad |f'(x_k) - p_n'(x_k)| \le \frac{2n^2}{b-a}\left(\max_{\xi\in[a,b]} \frac{|f^{(n+1)}(\xi)|}{(n+1)!}\right)\left(\max_{x\in[a,b]} \prod_{j=0}^n |x - x_j|\right).$$

Contrast the bound (1.11) with (1.7) from Theorem 1.3: the bounds are the same, aside from the leading constant $2n^2/(b-a)$ inherited from Lemma 1.1.

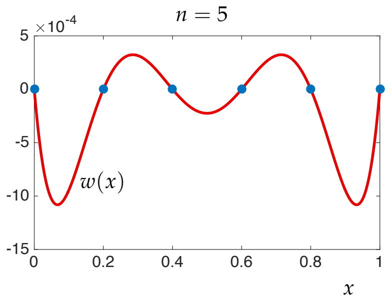
For our later discussion it will help to get a rough bound for he case where the interpolation points are uniformly distributed, i.e.,

$$x_j = a + j/h, \qquad j = 0,\ldots,n$$



with spacing equal to $h := (b-a)/n$. We seek to bound

$$\max_{x\in[a,b]} \prod_{j=0}^n |x - x_j|,$$



i.e., maximize the product of the distances of x from each of the interpolation points. Consider the sketch in the margin. Think about how you would place $x \in [x_0, x_n]$ so as to make $\prod_{j=0}^n |x - x_j|$ as large as possible. Putting x somewhere toward the ends, but not too near one of the interpolation points, will maximize product. Convince yourself that, regardless of where x is placed within $[x_0, x_n]$:

- at least one interpolation point is no more than $h/2$ away from x;
- a different interpolation point is no more than h away from x;
- a different interpolation point is no more than $2h$ away from x;

  $\vdots$
- the last remaining (farthest) interpolation point is no more than $nh = b - a$ away from x.

This reasoning gives the bound

$$(1.12)\qquad \max_{x\in[a,b]} \prod_{j=0}^n |x - x_j| \le \frac{h}{2}\cdot h \cdot 2h \cdots nh = \frac{h^{n+1} n!}{2}.$$

Substituting this into (1.11) gives the following result.

Corollary 1.1 (The derivative of an interpolant at equispaced points)**.** Suppose $f \in C^{(n+1)}[a,b]$ and let $p_n \in \mathcal{P}_n$ denote the polynomial that interpolates $\{(x_j, f(x_j))\}_{j=0}^n$ at equispaced points $x_j = a + jh$ for $h = (b-a)/n$. Then for every $x_k \in \{x_0, \ldots, x_n\}$,

$$|f'(x_k) - p_n'(x_k)| \le \frac{nh^{n+1}}{n+1}\left(\max_{\xi\in[a,b]} |f^{(n+1)}(\xi)|\right). \tag{1.13}$$

1.7.2 *Finite difference formulas*

The preceding analysis was toward a very specific purpose: to use interpolating polynomials to develop formulas that approximate derivatives of f from the value of f at a few points.

Example 1.3 (First derivative)**.** We begin with the simplest case: formulas for the first derivative $f'(x)$. Pick some value for x_0 and some spacing parameter $h > 0$.

First construct the linear interpolant to f at x_0 and $x_1 = x_0 + h$. Using the Newton form, we have

$$\begin{aligned} p_1(x) &= f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) \\ &= f(x_0) + \frac{f(x_1) - f(x_0)}{h}(x - x_0). \end{aligned}$$

Take a derivative of the interpolant:

$$p_1'(x) = \frac{f(x_1) - f(x_0)}{h}, \tag{1.14}$$

which is precisely the conventional definition of the derivative, if we take the limit $h \to 0$. But how accurate an approximation is it? Appealing to Corollary 1.1 with $n = 1$ and $[a,b] = [x_0, x_1] = x_0 + [0,h]$, we have

$$|f'(x_k) - p_1'(x_k)| \le \left(\frac{1}{2}\max_{\xi\in[x_0,x_1]} |f''(\xi)|\right) h \tag{1.15}$$

Does the bound (1.15) improve if we use a quadratic interpolant to f through x_0, $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$? Again using the Newton form, write

$$p_2(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) + \frac{f(x_2) - f(x_0) - \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}(x - x_0)(x - x_1)$$

$$= f(x_0) + \frac{f(x_1) - f(x_0)}{h}(x - x_0) + \frac{f(x_0) - 2f(x_1) + f(x_2)}{2h^2}(x - x_0)(x - x_1). \tag{1.16}$$

Taking a derivative of this interpolant with respect to x gives

$$p_2'(x) = \frac{f(x_1) - f(x_0)}{h} + \frac{f(x_0) - 2f(x_1) + f(x_2)}{2h^2}(2x - x_0 - x_1).$$

Evaluate this at $x = x_0$, $x = x_1$, and $x = x_2$ and simplify as much as possible to get:

$$p_2'(x_0) = \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h} \tag{1.17}$$

$$p_2'(x_1) = \frac{f(x_2) - f(x_0)}{2h} \tag{1.18}$$

$$p_2'(x_2) = \frac{f(x_0) - 4f(x_1) + 3f(x_2)}{2h}. \tag{1.19}$$

These beautiful formulas are *right-looking*, *central*, and *left-looking* approximations to f'. Though we used an interpolating polynomial to derive these formulas, those polynomials are now nowhere in sight: they are merely the scaffolding that lead to these formulas. How accurate are these formulas? Corollary 1.1 with $n = 2$ and $[a, b] = [x_0, x_2] = x_0 + [0, 2h]$ gives

These formulas are often derived by strategically combining Taylor expansions for $f(x + h)$ and $f(x - h)$. That is an easier route to the simple formulas like (1.18), but becomes harder when more sophisticated approximations like (1.17) and (1.19) (and beyond) are needed.

$$|f'(x_k) - p_2'(x_k)| \le \left(\frac{2}{3} \max_{\xi \in [x_0, x_2]} |f'''(\xi)|\right) h^2. \tag{1.20}$$

Notice that these approximations indeed scale with h^2, rather than h, and so the quadratic interpolant leads to a much better approximation to f', at the cost of evaluating f at three points (for $f'(x_0)$ and $f'(x_2)$), rather than two.

Example 1.4 (Second derivative)**.** While we have only proved a bound for the error in the first derivative, $f'(x) - p'(x)$, you can see that similar bounds should hold when higher derivatives of p are used to approximate corresponding derivatives of f. Here we illustrate with the second derivative.

Since p_1 is linear, $p_1''(x) = 0$ for all x, and the linear interpolant will not lead to any meaningful bound on $f''(x)$. Thus, we focus on the quadratic interpolant to f at the three uniformly spaced points x_0, x_1, and x_2. Take two derivatives of the formula (1.16) for $p_2(x)$ to obtain

$$p_2''(x) = \frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2}, \tag{1.21}$$

which is a famous approximation to the second derivative that is often used in the finite difference discretization of differential equations. One can show that, like the approximations $p_2'(x_k)$, this formula is accurate to order h^2.

Example 1.5 (*Mathematica* code for computing difference formulas)**.** *Code to follow. . . .*

1.7.3 *Application: Boundary Value Problems*

Example 1.6 (Dirichlet boundary conditions)**.** Suppose we want to solve the differential equation

$$-u''(x) = g(x), \qquad x \in [0,1]$$

for the unknown function u, subject to the *Dirichlet* boundary conditions

$$u(0) = u(1) = 0.$$

One common approach to such problems is to approximate the solution u on a uniform grid of points

$$0 = x_0 < x_1 < \cdots < x_n = 1$$

with $x_j = j/N$.

We seek to approximate the solution $u(x)$ at each of the grid points $x_0, \dots, x_n$. The Dirichlet boundary conditions give the end values immediately:

$$u(x_0) = 0, \qquad u(x_n) = 0.$$

At each of the interior grid points, we require a local approximation of the equation

$$-u''(x_j) = g(x_j), \qquad j = 1, \dots, n-1.$$

For each, we will (implicitly) construct the quadratic interpolant $p_{2,j}$ to $u(x)$ at the points x_{j-1}, x_j, and x_{j+1}, and then approximate

$$-p''_{2,j}(x_j) \approx -u''(x_j) = g(x_j).$$

Aside from some index shifting, we have already constructed $p''_{2,j}$ in equation (1.21):

$$p''_{2,j}(x) = \frac{u(x_{j-1}) - 2u(x_j) + u(x_{j+1})}{h^2}.$$

Just one small caveat remains: we cannot construct $p''_{2,j}(x)$, *because we do not know the values of* $u(x_{j-1})$*,* $u(x_j)$*, and* $u(x_{j+1})$: finding those values is the point of our entire endeavor. Thus we define approximate values

$$u_j \approx u(x_j), \qquad j = 1, \dots, n-1.$$

and will instead use the polynomial $p_{2,j}$ that interpolates u_{j-1}, u_j, and u_{j+1}, giving

$$p''_{2,j}(x) = \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2}. \qquad (1.22)$$

Let us accumulate all our equations for $j = 0, \dots, n$:

$$\begin{aligned}
u_0 &= 0 \\
u_0 - 2u_1 + u_2 &= -h^2 g(x_1) \\
u_1 - 2u_2 + u_3 &= -h^2 g(x_2) \\
&\vdots \\
u_{n-3} - 2u_{n-2} + u_{n-1} &= -h^2 g(x_{n-2}) \\
u_{n-2} - 2u_{n-1} + u_n &= -h^2 g(x_{n-1}) \\
u_n &= 0.
\end{aligned}$$

Notice that this is a system of $n+1$ linear equations in $n+1$ variables $u_0, \dots, u_{n+1}$. Thus we can arrange this in matrix form as

$$\begin{bmatrix} 1 & & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \\ & & & & & & 1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 0 \\ -h^2 g(x_1) \\ -h^2 g(x_2) \\ \vdots \\ -h^2 g(x_{n-2}) \\ -h^2 g(x_{n-1}) \\ 0 \end{bmatrix}, \tag{1.23}$$

where the blank entries are zero. Notice that the first and last entries are trivial: $u_0 = u_n = 0$, and so we can trim them off to yield the slightly simpler matrix

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \begin{bmatrix} -h^2 g(x_1) \\ -h^2 g(x_2) \\ \vdots \\ -h^2 g(x_{n-2}) \\ -h^2 g(x_{n-1}) \end{bmatrix}. \tag{1.24}$$

Solve this $(n-1) \times (n-1)$ linear system of equations using Gaussian elimination. One can show that the solution to the differential equation inherits the accuracy of the interpolant: the error $|u(x_j) - u_j|$ behaves like $O(h^2)$ as $h \to 0$.

Ideally, use an efficient version of Gaussian elimination that exploits the banded structure of this matrix to give a solution in $O(n)$ operations.

Example 1.7 (Mixed boundary conditions)**.** Modify the last example to keep the same differential equation

$$-u''(x) = g(x), \qquad x \in [0, 1]$$

but not use *mixed* boundary conditions,

$$u'(0) = u(1) = 0.$$

The derivative condition on the left requires special attention. One might be tempted to use a simple linear interpolant to approximate the boundary condition on the left side, giving a variation on the formula (1.14):

$$\frac{u_1 - u_0}{h} = 0.$$