CMDA 4604: Intermediate Topics in Mathematical Modeling
Lecture 19: Interpolation and Quadrature

In this lecture we make a brief diversion into the areas of *interpolation* and *quadrature*.

Given a function $f \in C[a,b]$, we say that a polynomial p *interpolates* f at the point $\widehat{x} \in [a,b]$ if

$$f(\widehat{x}) = p(\widehat{x}).$$

In the context of today's lecture, we aim to use interpolation as a way to construct good polynomial approximations to f. The next lecture we will put today's results into the broader context of the course: we will show how the approximate solutions constructed by the finite element method can be related to interpolating polynomials, and so the accuracy of interpolating polynomials will lead to error bounds for the finite element method.

We have three goals today: (1) construct interpolating polynomials p_n; (2) bound the error $f(x) - p_n(x)$; (3) integrate interpolating polynomials to approximate the integral of f

1. Constructing Interpolating Polynomials.

We seek to solve the following problem:

Polynomial interpolation problem. Given a function $f \in C[a,b]$ and points $x_0, \ldots, x_n \in [a,b]$, construct a polynomial p_n of degree not exceeding n such that

$$p_n(x_j) = f(x_j), \qquad j = 0, \ldots, n.$$

In any numerical analysis course, one learns that a unique solution p_n to this problem always exists, and be constructed in various ways. Here we shall just detail one elegant way to develop the interpolant, called the *Lagrange form*.

The idea behind the Lagrange form is simple. Consider the functions

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

Note that each L_k is a degree-n polynomial. (For each value of k, the product contains n terms of the form $(x - x_j)/(x_k - x_j)$. Each of these terms is a degree-1 polynomial. The product of n degree-1 polynomials is a degree-n polynomial.) Moreover, these polynomials have a very special property: by construction, L_k takes the value 1 at x_k and has roots at each of the points x_j, $j \neq k$:

$$L_k(x_j) = \begin{cases} 1, & j = k \\ 0, & j \neq k. \end{cases}$$

These $n+1$ polynomials $L_0, \ldots, L_n$ form a basis for the $n+1$ dimensional vector space of polynomials having degree n or less.

These *Lagrange basis functions* make it trivial to construct the solution p_n to the polynomial interpolation function:

$$p_n(x) = \prod_{k=0}^{n} f(x_k)L_k(x).$$

Since p_n is the sum of degree-n polynomials, it too is a degree-n polynomial. The property that $L_k(x_i) = 0$ for $i \neq k$ ensures that at the interpolation point x_j,

$$p_n(x_j) = \prod_{k=0}^{n} f(x_k)L_k(x_j) = f(x_j)L_j(x_j) = f(x_j).$$

Thus the polynomial p_n passes through f at the designated points. But how accurately does p_n approximate f at the other points in the interval $[a, b]$ where we have not specified the interpolation condition?

2. Interpolation Error Analysis.

We now seek to characterize the maximum error

$$\max_{x\in[a,b]} |f(x) - p_n(x)|.$$

The characterization of this error is one of the most fundamental results in numerical analysis.

Theorem (Interpolation Error Bound). Suppose $f \in C^{n+1}[a, b]$ and let $p_n \in \mathcal{P}_n$ denote the polynomial that interpolates f at the points $x_0, \ldots, x_n \in [a, b]$ for $j = 0, \ldots, n$. The for every $x \in [a, b]$ there exists $\xi \in [a, b]$ such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j).$$

This result yields a bound for the worst error over the interval $[a, b]$:

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

Proof. Consider some arbitrary point $\widehat{x} \in [a, b]$. We seek a descriptive expression for the error $f(\widehat{x}) - p_n(\widehat{x})$. If $\widehat{x} = x_j$ for some $j \in \{0, \ldots, n\}$, then $f(\widehat{x}) - p_n(\widehat{x}) = 0$ and there is nothing to prove. Thus, suppose for the rest of the proof that $\widehat{x}$ is not one of the interpolation points.

To describe $f(\widehat{x}) - p_n(\widehat{x})$, we shall build the polynomial of degree $n + 1$ that interpolates f at $x_0, \ldots, x_n$, and also $\widehat{x}$. Of course, this polynomial will give zero error at $\widehat{x}$, since it interpolates f there. From this polynomial we can extract a formula for $f(\widehat{x}) - p_n(\widehat{x})$ by measuring how much the degree $n + 1$ interpolant improves upon the degree-n interpolant p_n at $\widehat{x}$.

Since we wish to understand the relationship of the degree $n + 1$ interpolant to p_n, we shall write that degree $n + 1$ interpolant in a manner that explicitly incorporates p_n. Given this setting, use of the Newton form of the interpolant is natural; i.e., we write the degree $n + 1$ polynomial as

$$p_n(x) + \gamma \prod_{j=0}^{n} (x - x_j)$$

for some constant γ chosen to make the interpolant exact at $\widehat{x}$. For convenience, we write

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

and then denote the error of this degree $n+1$ interpolant by

$$\phi(x) \equiv f(x) - (p_n(x) + \gamma w(x)).$$

To make the polynomial $p_n(x) + \gamma w(x)$ interpolate f at $\widehat{x}$, we shall pick γ such that $\phi(\widehat{x}) = 0$. The fact that $\widehat{x} \notin \{x_j\}_{j=0}^{n}$ ensures that $w(\widehat{x}) \neq 0$, and so we can force $\phi(\widehat{x}) = 0$ by setting

$$\gamma = \frac{f(\widehat{x}) - p_n(\widehat{x})}{w(\widehat{x})}.$$

Furthermore, since $f(x_j) = p_n(x_j)$ and $w(x_j) = 0$ at all the $n+1$ interpolation points $x_0, \ldots, x_n$, we also have $\phi(x_j) = f(x_j) - p_n(x_j) - \gamma w(x_j) = 0$. Thus, ϕ is a function with at least $n+2$ zeros in the interval $[a, b]$. Rolle's Theorem[1] tells us that between every two consecutive zeros of ϕ, there is some zero of ϕ'. Since ϕ has at least $n+2$ zeros in $[a, b]$, ϕ' has at least $n+1$ zeros in this same interval. We can repeat this argument with ϕ' to see that ϕ'' must have at least n zeros in $[a, b]$. Continuing in this manner with higher derivatives, we eventually conclude that $\phi^{(n+1)}$ must have at least one zero in $[a, b]$; we denote this zero as ξ, so that $\phi^{(n+1)}(\xi) = 0$.

We now want a more concrete expression for $\phi^{(n+1)}$. Note that

$$\phi^{(n+1)}(x) = f^{(n+1)}(x) - p_n^{(n+1)}(x) - \gamma w^{(n+1)}(x).$$

Since p_n is a polynomial of degree n or less, $p_n^{(n+1)} \equiv 0$. Now observe that w is a polynomial of degree $n+1$. We could write out all the coefficients of this polynomial explicitly, but that is a bit tedious, and we do not need all of them. Simply observe that we can write $w(x) = x^{n+1} + q(x)$, for some $q \in \mathcal{P}_n$, and this polynomial q will vanish when we take $n+1$ derivatives:

$$w^{(n+1)}(x) = \left(\frac{d^{n+1}}{dx^{n+1}}\, x^{n+1}\right) + q^{(n+1)}(x) = (n+1)! + 0.$$

Assembling the pieces, $\phi^{(n+1)}(x) = f^{(n+1)}(x) - \gamma\,(n+1)!$. Since $\phi^{(n+1)}(\xi) = 0$, we conclude that

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

Substituting this expression into $0 = \phi(\widehat{x}) = f(\widehat{x}) - p_n(\widehat{x}) - \lambda w(\widehat{x})$, we obtain

$$f(\widehat{x}) - p_n(\widehat{x}) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n}(\widehat{x} - x_j). \qquad \blacksquare$$

[1]Recall the Mean Value Theorem from calculus: Given $d > c$, suppose $f \in C[c, d]$ is differentiable on (c, d). Then there exists some $\eta \in (c, d)$ such that $(f(d) - f(c))/(d - c) = f'(\eta)$. Rolle's Theorem is a special case: If $f(d) = f(c)$, then there is some point $\eta \in (c, d)$ such that $f'(\eta) = 0$.

This error bound has strong parallels to the remainder term in Taylor's formula. Recall that for sufficiently smooth h, the Taylor expansion of f about the point x_0 is given by

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \cdots + \frac{(x - x_0)^k}{k!} f^{(k)}(x_0) + \frac{f^{(k+1)}(\xi)}{(k+1)!}(x - x_0)^k.$$

Ignoring the remainder term at the end, note that the Taylor expansion gives a polynomial model of f, but one based on local information about f and its derivatives, as opposed to the polynomial interpolant, which is based on global information, but only about f, not its derivatives. Rearranging this expression, we have

$$f(x) - \left(f(x_0) + (x - x_0)f'(x_0) + \cdots + \frac{(x - x_0)^k}{k!} f^{(k)}(x_0)\right) = \frac{f^{(k+1)}(\xi)}{(k+1)!}(x - x_0)^k,$$

a perfect analogue of the interpolation error formula we have just proved.

3. Interpolatory Quadrature Formulas.

The finite element method requires computations like

$$(f, \phi_k) = \int_0^1 f(x)\phi_k(x)\ \mathrm{d}x$$

to construct the load vector. It may be inconvenient (or even impossible for some f) to compute this inner product. For such cases we wish to approximate the integral.

We shall consider the generic problem of approximating

$$I(f) = \int_a^b f(x)\,\mathrm{d}x.$$

Polynomial interpolation provides a simple way to approximate the integral:

- Construct the polynomial interpolant p_n to f at designated points;
- Approximate $\int_a^b f(x)\,\mathrm{d}x$ by $\int_a^b p_n(x)\,\mathrm{d}x$.

If we construct p_n using the Lagrange form described above, this procedure becomes very simple:

- Construct the interpolating polynomial

$$p_n(x) = \sum_{j=0}^{n} f(x_j)L_j(x);$$

- Integrate the interpolating polynomial to obtain $I_n(f)$, approximating the exact integral $I(f)$:

$$\begin{aligned} I_n(f) &= \int_a^b p_n(x)\,\mathrm{d}x \\ &= \int_a^b \sum_{j=0}^{n} f(x_j)L_j(x)\,\mathrm{d}x \\ &= \sum_{j=0}^{n} f(x_j)\int_a^b L_j(x)\,\mathrm{d}x. \end{aligned}$$

Notice that the integrals that remain depend on the Lagrange basis functions L_j *but not on* f. We will call these integrals the *weights* of the quadrature rule:

$$w_j = \int_a^b L_j(x)\,\mathrm{d}x.$$

Then the quadrature rule takes the simple form

$$I_n(f) = \sum_{j=0}^{n} w_j f(x_j).$$

The points $x_0, \ldots, x_n$ are called the *nodes* of the quadrature rule. When you choose evenly spaced points over $[a, b]$, you recover familiar rules that you have already encountered in calculus:

- $n = 0$ ($x_0 = (a + b)/2$, $L_0(x) = 1$) gives
$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; (b - a)f(\tfrac{1}{2}(a + b));$$
- $n = 1$ ($x_0 = a$, $x_1 = b$) gives the trapezoid rule:
$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \frac{b-a}{2}\Big(f(a) + f(b)\Big);$$
- $n = 2$ ($x_0 = a$, $x_1 = (a + b)/2$, $x_2 = b$) gives Simpson's rule:
$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \frac{b-a}{6}\Big(f(a) + 4f(\tfrac{1}{2}(a + b)) + f(b)\Big).$$

The first rule approximates f with an interpolating constant; the trapezoid rule approximates f with an interpolating linear polynomial; Simpson's rule approximates f with an interpolating quadratic.

How does one quantify the error $I(f) - I_n(f)$? Simply integrate the error formula for polynomial interpolation! One must then calculate:

$$\begin{aligned} I(f) - I_n(f) &= \int_a^b f(x) - p_n(x)\,\mathrm{d}x \\ &= \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{j=0}^{n}(x - x_j)\,\mathrm{d}x. \end{aligned}$$

The error analysis for the trapezoid rule (where $x_0 = a$ and $x_1 = b$) follows from application of the mean value theorem for integrals:

$$\begin{aligned} \int_a^b f(x)\,\mathrm{d}x - \int_a^b p_1(x)\,\mathrm{d}x &= \int_a^b \tfrac{1}{2}f''(\xi(x))(x - a)(x - b)\,\mathrm{d}x \\ &= \tfrac{1}{2}f''(\eta)\int_a^b (x - a)(x - b)\,\mathrm{d}x \\ &= \tfrac{1}{2}f''(\eta)(\tfrac{1}{6}a^3 - \tfrac{1}{2}a^2b + \tfrac{1}{2}ab^2 - \tfrac{1}{6}b^3) \\ &= -\tfrac{1}{12}f''(\eta)(b - a)^3 \end{aligned}$$

for some $\eta \in [a,b]$. As we expect, if $f(x)$ is a linear polynomial, then $f''(x) = 0$ for all x, and hence the trapezoid rule will be exact.

The analysis for Simpson's rule is a bit more complicated. One can actually show something stronger than what you might expect from integrating the polynomial interpolation error:

$$\int_a^b f(x)\,\mathrm{d}x - \int_a^b p_2(x)\,\mathrm{d}x = -\frac{1}{90}\,\frac{(b-a)^5}{2^5}\,f^{(4)}(\eta)$$

for some $\eta \in [a,b]$. Notice that this bound involves $f^{(4)}$, rather than the expected $f^{(3)}$: *Simpson's rule will be exact for cubic polynomials, not just quadratics!*

If you want greater accuracy than these bounds suggest, you could simply increase the degree n, and there are some settings in which this makes great sense: but one must be careful about how to select the nodes $x_0, \ldots, x_n$, and uniformly spaced points are not the best choice.

Composite rules. As an alternative to integrating a high-degree polynomial, one can pursue a simpler approach that is often very effective, especially for problems that are not particularly smooth (e.g., our hat functions): Break the interval $[a,b]$ into subintervals, and apply the trapezoid rule or Simpson's rule on each subinterval. Applying the trapezoid rule gives

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{j=1}^{n} \int_{x_{j-1}}^{x_j} f(x)\,\mathrm{d}x \approx \sum_{j=1}^{n} \frac{(x_j - x_{j-1})}{2}\Big(f(x_{j-1} + f(x_j)\Big).$$

The standard implementation assumes that f is evaluated at uniformly spaced points between a and b, $x_j = a + jh$ for $j = 0, \ldots, n$ and $h = (b-a)/n$, giving the following famous formulation:

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \frac{h}{2}\Big(f(a) + 2\sum_{j=1}^{n-1} f(a+jh) + f(b)\Big).$$

(Of course, one can readily adjust this rule to cope with irregularly spaced points.) The error in the composite trapezoid rule can be derived by summing up the error in each application of the trapezoid rule:

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x - \frac{h}{2}\Big(f(a) + 2\sum_{j=1}^{n-1} f(a+jh) + f(b)\Big) \;&=\; \sum_{j=1}^{n}\Big(-\tfrac{1}{12}f''(\eta_j)(x_j - x_{j-1})^3\Big)\\ &=\; -\frac{h^3}{12}\sum_{j=1}^{n} f''(\eta_j)\end{aligned}$$

for $\eta_j \in [x_{j-1}, x_j]$. We can simplify these f'' terms by noting that $\frac{1}{n}(\sum_{j=1}^{n} f''(\eta_j))$ is the average of n values of f'' evaluated at points in the interval $[a,b]$. Naturally, this average cannot exceed the maximum or minimum value that f'' assumes on $[a,b]$, so there exist points $\xi_1, \xi_2 \in [a,b]$ such that

$$f''(\xi_1) \le \frac{1}{n}\sum_{j=1}^{n} f''(\eta_j) \le f''(\xi_2).$$

Thus the intermediate value theorem guarantees the existence of some $\eta \in [a,b]$ such that

$$f''(\eta) = \frac{1}{n}\sum_{j=1}^{n} f''(\eta_j).$$

The composite trapezoid error bound thus simplifies to

$$\int_a^b f(x)\,\mathrm{d}x - \frac{h}{2}\Big(f(a) + 2\sum_{j=1}^{n-1} f(a+jh) + f(b)\Big) = -\frac{h^2}{12}(b-a)f''(\eta).$$

Similar analysis can be performed to derive the composite Simpson's rule. We now must ensure that n is even, since each interval on which we apply the standard Simpson's rule has width $2h$. Simple algebra leads to the formula

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h}{3}\Big(f(a) \ + \ 4\sum_{j=1}^{n/2} f(a+(2j-1)h) \ + \ 2\sum_{j=1}^{n/2-1} f(a+2jh) \ + \ f(b)\Big).$$

Derivation of the error formula for the composite Simpson's rule follows the same strategy as the analysis of the composite trapezoid rule. One obtains

$$\int_a^b f(x)\,\mathrm{d}x - \frac{h}{3}\Big(f(a) \ + \ 4\sum_{j=1}^{n/2} f(a+(2j-1)h) \ + \ 2\sum_{j=1}^{n/2-1} f(a+2jh) \ + \ f(b)\Big) = -\frac{h^4}{180}(b-a)f^{(4)}(\eta)$$

for some $\eta \in [a,b]$.