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Lecture 6 Notes

These notes correspond to Sections 6.4 and 6.5 in the text.

Hermite Interpolation

Suppose that the interpolation points are perturbed so that two neighboring points x_i and x_{i+1}, $0 \leq i < n$, approach each other. What happens to the interpolating polynomial? In the limit, as $x_{i+1} \to x_i$, the interpolating polynomial $p_n(x)$ not only satisfies $p_n(x_i) = y_i$, but also the condition

$$p_n'(x_i) = \lim_{x_{i+1} \to x_i} \frac{y_{i+1} - y_i}{x_{i+1} - x_i}.$$

It follows that in order to ensure uniqueness, the data must specify the value of the derivative of the interpolating polynomial at x_i.

In general, the inclusion of an interpolation point x_i k times within the set $x_0, \ldots, x_n$ must be accompanied by specification of $p_n^{(j)}(x_i)$, $j = 0, \ldots, k-1$, in order to ensure a unique solution. These values are used in place of divided differences of identical interpolation points in Newton interpolation.

Interpolation with repeated interpolation points is called *osculatory interpolation*, since it can be viewed as the limit of distinct interpolation points approaching one another, and the term "osculatory" is based on the Latin word for "kiss".

In the case where each of the interpolation points $x_0, x_1, \ldots, x_n$ is repeated exactly once, the interpolating polynomial for a differentiable function $f(x)$ is called the *Hermite polynomial* of $f(x)$, and is denoted by $H_{2n+1}(x)$, since this polynomial must have degree $2n+1$ in order to satisfy the $2n+2$ constraints

$$H_{2n+1}(x_i) = f(x_i), \quad H_{2n+1}'(x_i) = f'(x_i), \quad i = 0, 1, \ldots, n.$$

To satisfy these constraints, we define, for $i = 0, 1, \ldots, n$,

$$\begin{aligned} H_i(x) &= [L_i(x)]^2(1 - 2L_i'(x_i)(x - x_i)), \\ K_i(x) &= [L_i(x)]^2(x - x_i), \end{aligned}$$

where, as before, $L_i(x)$ is the ith Lagrange polynomial for the interpolation points $x_0, x_1, \ldots, x_n$.

It can be verified directly that these polynomials satisfy, for $i, j = 0, 1, \ldots, n$,

$$H_i(x_j) = \delta_{ij}, \quad H_i'(x_j) = 0,$$

$$K_i(x_j) = 0, \quad K_i'(x_j) = \delta_{ij},$$

where δ_{ij} is the *Kronecker delta*

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$$

It follows that

$$H_{2n+1}(x) = \sum_{i=0}^{n} [f(x_i)H_i(x) + f'(x_i)K_i(x)]$$

is a polynomial of degree $2n+1$ that satisfies the above constraints.

To prove that this polynomial is the *unique* polynomial of degree $2n+1$, we assume that there is another polynomial $\tilde{H}_{2n+1}$ of degree $2n+1$ that satisfies the constraints. Because $H_{2n+1}(x_i) = \tilde{H}_{2n+1}(x_i) = f(x_i)$ for $i = 0, 1, \ldots, n$, $H_{2n+1} - \tilde{H}_{2n+1}$ has at least $n+1$ zeros. It follows from Rolle's Theorem that $H_{2n+1}' - \tilde{H}_{2n+1}'$ has n zeros that lie within the intervals (x_{i-1}, x_i) for $i = 0, 1, \ldots, n-1$.

Furthermore, because $H_{2n+1}'(x_i) = \tilde{H}_{2n+1}'(x_i) = f'(x_i)$ for $i = 0, 1, \ldots, n$, it follows that $H_{2n+1} - \tilde{H}_{2n+1}$ has $n+1$ additional zeros, for a total of at least $2n+1$. However, $H_{2n+1}' - \tilde{H}_{2n+1}'$ is a polynomial of degree $2n+1$, and the only way that a polynomial of degree $2n+1$ can have $2n+1$ zeros is if it is identically zero. Therefore, $H_{2n+1} = \tilde{H}_{2n+1}$, and the Hermite polynomial is unique.

Using a similar approach as for the Lagrange interpolating polynomial, combined with ideas from the proof of the uniqueness of the Hermite polynomial, the following result can be proved.

Theorem Let f be $2n+2$ times continuously differentiable on $[a, b]$, and let H_{2n+1} denote the Hermite polynomial of f with interpolation points $x_0, x_1, \ldots, x_n$ in $[a, b]$. Then there exists a point $\xi(x) \in [a, b]$ such that

$$f(x) - H_{2n+1}(x) = \frac{f^{(2n+2)}(\xi(x))}{(2n+2)!}(x - x_0)^2(x - x_1)^2 \cdots (x - x_n)^2.$$

The representation of the Hermite polynomial in terms of Lagrange polynomials and their derivatives is not practical, because of the difficulty of differentiating and evaluating these polynomials. Instead, one can construct the Hermite polynomial using a Newton divided-difference table, in which each entry corresponding to two identical interpolation points is filled with the value of $f'(x)$ at the common point. Then, the Hermite polynomial can be represented using the Newton divided-difference formula.

Differentiation

We now discuss how polynomial interpolation can be applied to help solve a fundamental problem from calculus that frequently arises in scientific applications, the problem of computing the derivative of a given function $f(x)$.

Finite Difference Approximations

Recall that the derivative of $f(x)$ at a point x_0, denoted $f'(x_0)$, is defined by

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This definition suggests a method for approximating $f'(x_0)$. If we choose h to be a small positive constant, then

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}.$$

This approximation is called the *forward difference formula.*

To estimate the accuracy of this approximation, we note that if $f''(x)$ exists on $[x_0, x_0 + h]$, then, by Taylor's Theorem, $f(x_0 + h) = f(x_0) + f'(x_0)h + f''(\xi)h^2/2$, where $\xi \in [x_0, x_0 + h]$. Solving for $f'(x_0)$, we obtain

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

so the error in the forward difference formula is $O(h)$. We say that this formula is *first-order accurate.*

The forward-difference formula is called a *finite difference approximation* to $f'(x_0)$, because it approximates $f'(x)$ using values of $f(x)$ at points that have a small, but finite, distance between them, as opposed to the definition of the derivative, that takes a limit and therefore computes the derivative using an "infinitely small" value of h. The forward-difference formula, however, is just one example of a finite difference approximation. If we replace h by $-h$ in the forward-difference formula, where h is still positive, we obtain the *backward-difference formula*

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}.$$

Like the forward-difference formula, the backward difference formula is first-order accurate.

If we average these two approximations, we obtain the *centered-difference formula*

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h}.$$

To determine the accuracy of this approximation, we assume that $f'''(x)$ exists on the interval $[x_0 - h, x_0 + h]$, and then apply Taylor's Theorem again to obtain

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f'''(\xi_+)}{6}h^3,$$

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 - \frac{f'''(\xi_-)}{6}h^3,$$

where $\xi_+ \in [x_0, x_0 + h]$ and $\xi_- \in [x_0 - h, x_0]$. Subtracting the second equation from the first and solving for $f'(x_0)$ yields

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{f'''(\xi_+) + f'''(\xi_-)}{12} h^2.$$

By the Intermediate Value Theorem, $f'''(x)$ must assume every value between $f'''(\xi_-)$ and $f'''(\xi_+)$ on the interval (ξ_-, ξ_+), including the average of these two values. Therefore, we can simplify this equation to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{f'''(\xi)}{6} h^2,$$

where $\xi \in [x_0 - h, x_0 + h]$. We conclude that the centered-difference formula is *second-order accurate.* This is due to the cancellation of the terms involving $f''(x_0)$.

Example Consider the function

$$f(x) = \frac{\sin^2\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)}{\sin\left(\frac{\sqrt{x}-1}{\sqrt{x^2+1}}\right)}.$$

Our goal is to compute $f'(0.25)$. Differentiating, using the Quotient Rule and the Chain Rule, we obtain

$$\begin{aligned} f'(x) &= \frac{2\sin\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)\cos\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)\left[\frac{2x+1}{2\sqrt{x^2+1}(\cos x - x)} + \frac{\sqrt{x^2+1}(\sin x + 1)}{(\cos x - x)^2}\right]}{\sin\left(\frac{\sqrt{x}-1}{\sqrt{x^2+1}}\right)} - \\ &\quad \frac{\sin\left(\frac{\sqrt{x^2+x}}{\cos x - x}\right)\cos\left(\frac{\sqrt{x}-1}{\sqrt{x^2+1}}\right)\left[\frac{1}{2\sqrt{x}\sqrt{x^2+1}} - \frac{x(\sqrt{x}-1)}{(x^2+1)^{3/2}}\right]}{\sin^2\left(\frac{\sqrt{x}-1}{\sqrt{x^2+1}}\right)}. \end{aligned}$$

Evaluating this monstrous function at $x = 0.25$ yields $f'(0.25) = -9.066698770$.

An alternative approach is to use a *centered difference* approximation,

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

Using this formula with $x = 0.25$ and $h = 0.005$, we obtain the approximation

$$f'(0.25) \approx \frac{f(0.255) - f(0.245)}{0.01} = -9.067464295,$$

which has absolute error 7.7×10^{-4}. While this complicated function must be evaluated twice to obtain this approximation, that is still much less work than using differentiation rules to compute $f'(x)$, and then evaluating $f'(x)$, which is much more complicated than $f(x)$. □

While Taylor's Theorem can be used to derive formulas with higher-order accuracy simply by evaluating $f(x)$ at more points, this process can be tedious. An alternative approach is to compute the derivative of the interpolating polynomial that fits $f(x)$ at these points. Specifically, suppose we want to compute the derivative at a point x_0 using the data

$$(x_{-j}, y_{-j}), \ldots, (x_{-1}, y_{-1}), (x_0, y_0), (x_1, y_1), \ldots, (x_k, y_k),$$

where j and k are known nonnegative integers, $x_{-j} < x_{-j+1} < \cdots < x_{k-1} < x_k$, and $y_i = f(x_i)$ for $i = -j, \ldots, k$. Then, a finite difference formula for $f'(x_0)$ can be obtained by analytically computing the derivatives of the Lagrange polynomials $\{\mathcal{L}_{n,i}(x)\}_{i=-j}^{k}$ for these points, where $n = j + k + 1$, and the values of these derivatives at x_0 are the proper weights for the function values $y_{-j}, \ldots, y_k$. If $f(x)$ is $n+1$ times continuously differentiable on $[x_{-j}, x_k]$, then we obtain an approximation of the form

$$f'(x_0) = \sum_{i=-j}^{k} y_i \mathcal{L}'_{n,i}(x_0) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=-j, i\neq 0}^{k} (x_0 - x_i),$$

where $\xi \in [x_{-j}, x_k]$.

Among the best-known finite difference formulas that can be derived using this approach is the second-order-accurate three-point formula

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{f'''(\xi)}{3}h^2, \quad \xi \in [x_0, x_0+2h],$$

which is useful when there is no information available about $f(x)$ for $x < x_0$. If there is no information available about $f(x)$ for $x > x_0$, then we can replace h by $-h$ in the above formula to obtain a second-order-accurate three-point formula that uses the values of $f(x)$ at x_0, $x_0 - h$ and $x_0 - 2h$.

Another formula is the five-point formula

$$f'(x_0) = \frac{f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)}{12h} + \frac{f^{(5)}(\xi)}{30}h^4, \quad \xi \in [x_0-2h, x_0+2h],$$

which is fourth-order accurate. The reason it is called a five-point formula, even though it uses the value of $f(x)$ at four points, is that it is derived from the Lagrange polynomials for the five points $x_0 - 2h, x_0 - h, x_0, x_0 + h$, and $x_0 + 2h$. However, $f(x_0)$ is not used in the formula because $\mathcal{L}'_{4,0}(x_0) = 0$, where $\mathcal{L}_{4,0}(x)$ is the Lagrange polynomial that is equal to one at x_0 and zero at the other four points.

If we do not have any information about $f(x)$ for $x < x_0$, then we can use the following five-point formula that actually uses the values of $f(x)$ at five points,

$$f'(x_0) = \frac{-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)}{12h} + \frac{f^{(5)}(\xi)}{5}h^4,$$

where $\xi \in [x_0, x_0 + 4h]$. As before, we can replace h by $-h$ to obtain a similar formula that approximates $f'(x_0)$ using the values of $f(x)$ at $x_0, x_0 - h, x_0 - 2h, x_0 - 3h$, and $x_0 - 4h$.

The strategy of differentiating Lagrange polynomials to approximate derivatives can be used to approximate higher-order derivatives. For example, the second derivative can be approximated using a centered difference formula,

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

which is second-order accurate.

Example We will construct a formula for approximating $f'(x)$ at a given point x_0 by interpolating $f(x)$ at the points x_0, $x_0 + h$, and $x_0 + 2h$ using a second-degree polynomial $p_2(x)$, and then approximating $f'(x_0)$ by $p_2'(x_0)$. Since $p_2(x)$ should be a good approximation of $f(x)$ near x_0, especially when h is small, its derivative should be a good approximation to $f'(x)$ near this point.

Using Lagrange interpolation, we obtain

$$p_2(x) = f(x_0)\mathcal{L}_{2,0}(x) + f(x_0 + h)\mathcal{L}_{2,1}(x) + f(x_0 + 2h)\mathcal{L}_{2,2}(x),$$

where $\{\mathcal{L}_{2,j}(x)\}_{j=0}^2$ are the Lagrange polynomials for the points x_0, $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$. Recall that these polynomials satisfy

$$\mathcal{L}_{2,j}(x_k) = \delta_{jk} = \left\{ \begin{array}{ll} 1 & \text{if } j = k \\ 0 & \text{otherwise} \end{array} \right. .$$

Using the formula for the Lagrange polynomials,

$$\mathcal{L}_{2,j}(x) = \prod_{i=0, i \neq j}^{2} \frac{(x - x_i)}{(x_j - x_i)},$$

we obtain

$$\begin{aligned}
\mathcal{L}_{2,0}(x) &= \frac{(x - (x_0 + h))(x - (x_0 + 2h))}{(x_0 - (x_0 + h))(x_0 - (x_0 + 2h))} \\
&= \frac{x^2 - (2x_0 + 3h)x + (x_0 + h)(x_0 + 2h)}{2h^2}, \\
\mathcal{L}_{2,1}(x) &= \frac{(x - x_0)(x - (x_0 + 2h))}{(x_0 + h - x_0)(x_0 + h - (x_0 + 2h))} \\
&= \frac{x^2 - (2x_0 + 2h)x + x_0(x_0 + 2h)}{-h^2}, \\
\mathcal{L}_{2,2}(x) &= \frac{(x - x_0)(x - (x_0 + h))}{(x_0 + 2h - x_0)(x_0 + 2h - (x_0 + h))} \\
&= \frac{x^2 - (2x_0 + h)x + x_0(x_0 + h)}{2h^2}.
\end{aligned}$$

It follows that

$$\begin{aligned}
\mathcal{L}'_{2,0}(x) &= \frac{2x - (2x_0 + 3h)}{2h^2} \\
\mathcal{L}'_{2,1}(x) &= -\frac{2x - (2x_0 + 2h)}{h^2} \\
\mathcal{L}'_{2,2}(x) &= \frac{2x - (2x_0 + h)}{2h^2}
\end{aligned}$$

We conclude that $f'(x_0) \approx p_2'(x_0)$, where

$$\begin{aligned}
p_2'(x_0) &= f(x_0)\mathcal{L}'_{2,0}(x_0) + f(x_0 + h)\mathcal{L}'_{2,0}(x_0) + f(x_0 + 2h)\mathcal{L}'_{2,0}(x_0) \\
&\approx f(x_0)\frac{-3}{2h} + f(x_0 + h)\frac{2}{h} + f(x_0 + 2h)\frac{-1}{2h} \\
&\approx \frac{3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h}.
\end{aligned}$$

Using Taylor's Theorem to write $f(x_0 + h)$ and $f(x_0 + 2h)$ in terms of Taylor polynomials centered at x_0, it can be shown that the error in this approximation is $O(h^2)$, and that this formula is exact when $f(x)$ is a polynomial of degree 2 or less. □

In a practical implementation of finite difference formulas, it is essential to note that roundoff error in evaluating $f(x)$ is bounded independently of the spacing h between points at which $f(x)$ is evaluated. It follows that the roundoff error in the approximation of $f'(x)$ actually *increases* as h decreases, because the errors incurred by evaluating $f(x)$ are divided by h. Therefore, one must choose h sufficiently small so that the finite difference formula can produce an accurate approximation, and sufficiently large so that this approximation is not too contaminated by roundoff error.