Numerical analysis: polynomial interpolation

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1 Definition, existence and uniqueness

The subject of interpolation is fundamental across the scientific disciplines.

Algebraic polynomials of degree at most n:

$$\Pi_n := \{P_n(x) = a_0 + a_1 x + \cdots + a_n x^n\}$$

Polynomials are extremely important mathematical objects, which posess both algebraic simplicity and analytic power. We will use polynomials as devices of approximating complicated functions, derivatives etc. The degree n serves as a measure of complexity, and usually we would expect better approximations as we increase the degree.

Some facts:

1. For any $f(x)$ differentiable $n+1$ times, its Taylor polynomial of degree n around x_0 , $P_n(x) \in \Pi_n$ satisfies
$$\begin{array}{l} P_n\left(x_0\right) = f\left(x_0\right) + \frac{f'(x_0)}{1!}\left(x - x_0\right) + \frac{f''(x_0)}{2!}\left(x - x_0\right)^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}\left(x - x_0\right)^n, \\ P_n^{(k)}\left(x_0\right) = f^{(k)}\left(x_0\right), k = 0, 1, \ldots, n, \quad f(x) = P_n(x) + \frac{f^{(n+1)}(c)}{(n+1)!}\left(x - x_0\right)^{n+1} \end{array}$$
2. $P_n(x) = a_0 + a_1 x + \cdots + a_n x^n$ is the Taylor polynomial around $x_0 = 0$ of the function
$$a_0 = f(0), a_1 = \frac{f'(0)}{1!}, a_2 = \frac{f''(0)}{2!}, \ldots, a_n = \frac{f^{(n)}(0)}{n!}\cdot$$
3. $P(x) = a_0 + a_1 x + \cdots + a_n x^n$ and $Q(x) = b_0 + b_1 x + \cdots + b_n x^n$ are equal if and only if $a_k = b_k$ for $k = 0, 1, \ldots, n$.

Exercise. Write Taylor expansion of $p(x) = 1 + x + x^2$ around $x_0 = 1$: $p(x) = a_0 + a_1(x-1) + a_2(x-1)^2$.

Definition 1. The **interpolation polynomial** of a function $f(x)$ at **interpolation points/nodes** $x_0, \ldots, x_n$ is a polynomial $P_n(x) \in \Pi_n$ which satisfies the **interpolation conditions**

$$P_n(x_k) = f(x_k) \qquad k = 0, 1, \ldots, n. \tag{1}$$

Theorem 1. *If $x_0, \ldots, x_n$ are pairwise distinct, then there exists a unique interpolation polynomial $P_n \in \Pi_n$ satisfying (1).*

First proof. Let us write the linear system with respect to the unknown coefficients:

$$\begin{cases} P_n(x_0) = a_0 + a_1 x_0 + a_1 x_0^2 + \cdots + a_n x_0^n = f(x_0) \\ P_n(x_1) = a_0 + a_1 x_1 + a_1 x_1^2 + \cdots + a_n x_1^n = f(x_1) \\ \cdots \\ P_n(x_n) = a_0 + a_1 x_n + a_1 x_n^2 + \cdots + a_n x_n^n = f(x_n) \end{cases} \tag{2}$$

Write this in matrix form:

$$\underbrace{\begin{bmatrix} 1 & x_0 & \cdot & \cdot & x_0^n \\ 1 & x_1 & & & x_1^n \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 1 & x_n & \cdot & \cdot & x_n^n \end{bmatrix}}_{\text{coefficient matrix} A} \begin{bmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \cdot \\ \cdot \\ f(x_n) \end{bmatrix}$$

The matrix A is called Vandermonde matrix (van der Monde). Well-known fact: $|A| = \prod_{i>j}(x_i - x_j)$. Because the points are distinct, the linear system (2) has a unique solution. ☐

Second proof. The homogeneous system corresponding to (2) reads

$$P_n(x_0) = 0, P_n(x_1) = 0, \cdots, P_n(x_n) = 0.$$

By the fundamental theorem of algebra, a nonzero polynomial of degree n has at most n distinct zeros. Therefore $P_n \equiv 0$, i.e. the homogeneous system has only the trivial solution. Therefore the inhomogeneous system has a unique solution. ☐

2 Lagrange form of interpolation polynomial

The idea of the Lagrange form is to use the values $f(x_i)$ as coefficients in the expression

$$P_n(x) = \ell_0(x) f(x_0) + \ell_1(x) f(x_1) + \cdots + \ell_n(x) f(x_n) = \sum_{i=0}^{n} \ell_i(x) f(x_i)$$

where $\ell_i(x)$ are polynomials depending on the points $x_0, \ldots, x_n$, which satisfy the Lagrange interpolation conditions

$$\ell_i(x_j) = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}, \quad \forall 0 \le i, j \le n.$$

Check that $P_n(x_i) = f(x_i)$ for all $i = 0, 1, \ldots, n$. Therefore, P_n is indeed the interpolation polynomial according to theorem 1.

An explicit form of the polynomials ℓ_i is the following:

$$\ell_i(x) = \frac{(x - x_0)(x - x_2)\cdots(x - x_{i-1})(x - x_{i+1})\cdots(x - x_n)}{(x_i - x_0)(x_i - x_2)\cdots(x_i - x_{i-1})(x_i - x_{i+1})\cdots(x_i - x_n)} = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

Example 1. Find the interpolation polynomial of degree ≤ 2 to the function $f(x) = \sqrt[3]{x}$ at the interpolation points $x_0 = 0, x_1 = 1, x_2 = -1$. What is the absolute and relative error of approximation at the point $x = 0.125$?

Solution. We have

$$\begin{array}{c} \ell_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-1)(x-(-1))}{(0-1)(0-(-1))} = -(x-1)(x+1) = -x^2+1 \\ \ell_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-0)(x+1)}{(1-0)(1+1)} = \frac{1}{2}x(x+1) = \frac{1}{2}x^2 + \frac{1}{2}x \\ \ell_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-0)(x-1)}{(-1-0)(-1-1)} = \frac{1}{2}x(x-1) = \frac{1}{2}x^2 - \frac{1}{2}x \end{array}.$$

Therefore $P_2(x) = \left(-x^2+1\right)\cdot 0 + \left(\frac{1}{2}x^2 + \frac{1}{2}x\right)\cdot 1 + \left(\frac{1}{2}x^2 - \frac{1}{2}x\right)\cdot(-1) = x$. At the point $x = 0.125$ we get

$$0.5 = (0.125)^{1/3} \approx P_2(0.125) = 0.125,$$

and so the absolute error is 0.375, relative error 60%.

Question: is the same polynomial also the interpolating polynomial for the functions $f(x) = x^3, x^5, x^7$ at the same interpolation points $x_0 = 0, x_1 = 1, x_2 = -1$?

Example 2. Compute the interpolation polynomial for $f(x) = 4^x$ which coincides with it at the points $x_0 = 0, x_1 = 1/2, x_2 = 1$.

Solution. We get

$$\begin{array}{c} \ell_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-0.5)(x-1)}{(0-0.5)(0-1)} = 2(x-0.5)(x-1) = 2x^2-3x+1 \\ \ell_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-0)(x-1)}{(0.5-0)(0.5-1)} = -4x(x-1) = -4x^2+4x \\ \ell_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-0)(x-0.5)}{(1-0)(1-0.5)} = 2x(x-0.5) = 2x^2-x \end{array}.$$

Therefore $P_2(x) = \left(2x^2-3x+1\right)\cdot 1 + \left(-4x^2+4x\right)\cdot 2 + \left(2x^2-x\right)\cdot 4 = 2x^2+x+1$.

For $x = 1/3$ we get $4^{1/3} = \sqrt[3]{4} \approx P_2(1/3) = 2\cdot\frac{1}{9} + \frac{1}{3} + 1 = \frac{14}{9} = 1.55555\ldots\ldots$, and from the calculator: $4^{1/3} = \sqrt[3]{4} = 1.58740105\ldots$ which is close. By increasing the degree of the polynomial we can expect to increase the accuracy.

Exercise 1. If $f(x)$ is even (odd) and the interpolation poits are symmetric around 0, prove that the interpolation polynomial is also even (odd).

Exercise 2. Prove that $\sum_{i=0}^{n} x_i \ell_i(x) \equiv x, \sum_{i=0}^{n} \ell_i(x) \equiv 1$. Compute $\sum_{i=0}^{n} x_i^k \ell_i(x)$ (hint: use the Lagrange form for the polynomial x^k).

3 Newton form of interpolation polynomial

Disadvantages of Lagrange form of interpolation polynomial:

1. Large complexity (order n^2);
2. Loss of numerical accuracy when points are close - subtracting close numbers! (compare with Taylor approximation);

3. Cannot reuse computations when adding new points.

Next we will see how the Newton form solves some of these issues.

Remark 1. There is an improved version of Lagrange interpolation, called *barycentric Lagrange interpolation,* which solves the above problems and is more stable, see e.g. [1, 4].

3.1 The general form

The Newton form seeks the (unique) interpolation polynomial in the form

$$\begin{aligned} P_n(x) &= A_0 q_0(x) + \dots A_n q_n(x) \\ q_0(x) &= 1 \\ q_1(x) &= x - x_0 \\ q_k(x) &= \prod_{i=0,\dots,k-1} (x - x_i) \Rightarrow \deg q_k = k \end{aligned}$$

- Check that the polynomials $\{q_0(x), \dots, q_n(x)\}$ are a basis for the space Π_n.
- Define $p_k(x) = A_0 q_0(x) + \dots + A_k q_k(x)$. Notice that for each k, A_k is the leading coefficient of $p_k(x)$.

Claim 1. If P_n is the interpolation polynomial at the nodes $x_0, \dots, x_n$ to the function $f(x)$, then $p_k(x)$ is the interpolation polynomial (to the same function $f(x)$) at the nodes $x_0, \dots, x_k$, for every $k = 0, 1, \dots, n$.

Proof. Notice that $q_k(x) = q_{k-1}(x)(x - x_{k-1})$. Write

$$\begin{aligned} P_n(x) &= p_k(x) + A_{k+1} q_{k+1}(x) + \dots + A_n q_n(x) \\ &= p_k(x) + q_{k+1}(x) \underbrace{(A_{k+1} + A_{k+2}(x - x_{k+1}) + \dots + A_n (x - x_{k+1}) \cdots (x - x_{n-1}))}_{:=r(x),\ \deg r \le n-k-1}. \end{aligned} \tag{3}$$

For $i = 0, 1, \dots, k$ we get $f(x_i) = P_n(x_i) = p_k(x_i) + \underbrace{q_{k+1}(x_i)}_{=0} r(x_i) = p_k(x_i)$. Clearly $\deg p_k \le k$. ☐

Applying (3) with $k = n - 1$ we obtain the following recursion formula.

Corollary 1. *If P_n, P_{n-1} are the interpolation polynomials at $\{x_0, \dots, x_n\}$ and $\{x_0, \dots, x_{n-1}\}$ respectively, then*

$$P_n(x) = P_{n-1}(x) + A_n q_n(x). \tag{4}$$

So we can construct P_n by starting with $P_0(x) = f(x_0) = A_0$ and building all the $P_1, \dots, P_n$ successively.

Claim. We can see that each coefficient A_k should depend only on the points $x_0, \dots, x_k$ and the values of f at these points.

3.2 Computing the coefficients A_k

1. $n=0$: already saw that $P_0(x)=f(x_0)=A_0$ (degree 0). Define the symbol $f[x_0]=f(x_0)$ (divided difference of order 0)

2. $n=1$: $P_1(x)=f(x_0)+A_1(x-x_0)$. From interpolation condition: $P_1(x_1)=f(x_1)$ we get

$$A_1=\frac{f(x_1)-f(x_0)}{x_1-x_0}:=\underbrace{f[x_0,x_1]}_{\text{divided difference of order 1}}$$

Definition 2. Given $x_0,\ldots,x_k$ and $f(x_0),\ldots,f(x_k)$, the **divided difference of order** k is the coefficient A_k of x^k (and also of q_k in the Newton form) of the (unique) interpolation polynomial $p_k(x)\equiv P_k(x)$ (of degree $\le k$) to f at the points $x_0,\ldots,x_k$. Notation:

$$A_k=f[x_0,\ldots,x_k].$$

Therefore we can write the Newton form of the interpolation polynomial as follows:

$$P_n(x)=\sum_{k=0}^{n}f[x_0,\ldots,x_k]\,q_k(x). \tag{5}$$

Claim 2. $f[x_0,\ldots,x_n]$ does not depend on the ordering of $x_0,\ldots,x_n$.

Proof. Follows from the uniqueness of the interpolation polynomial. □

Claim 3 (Recursion formula for the divided differences).

$$f[x_0,x_1,\ldots,x_k]=\frac{f[x_1,\ldots,x_k]-f[x_0,\ldots,x_{k-1}]}{x_k-x_0},\quad x_k\neq x_0;\quad k=1,2,\ldots$$

Proof. Let P_{k-1} be the interpolation polynomial at the points $x_0,\ldots,x_{k-1}$ and Q_{k-1} be the interpolation polynomial at the points $x_1,\ldots,x_k$. Consider

$$p(x)=\frac{1}{x_k-x_0}\left\{(x-x_0)\,Q_{k-1}(x)+(x_k-x)\,P_{k-1}(x)\right\}. \tag{6}$$

We can check that:

1. For $i=1,\ldots,k-1$ we have $Q_{k-1}(x_i)=P_{k-1}(x_i)=f(x_i)$ and therefore $p(x_i)=\frac{f(x_i)}{x_k-x_0}\{x_i-x_0+x_k-x_i\}=f(x_i)$.

2. $p(x_0)=P_{k-1}(x_0)=f(x_0)$

3. $p(x_k)=Q_{k-1}(x_k)=f(x_k)$.

Therefore $p(x)=P_k(x)$, and its leading coefficient should be equal to A_k. By (3) it is also equal to

$$f[x_0,\ldots,x_k]=A_k=\frac{1}{x_k-x_0}\left\{f[x_1,\ldots,x_k]-f[x_0,\ldots,x_{k-1}]\right\}.$$

□

Example 3. Let us compute the Newton form for $f(x) = 4^x$ at $x_0 = 0, x_1 = 1/2, x_2 = 1$ as in Example 2. The divided differences are as follows:

$$\begin{array}{llcll}
x_0 = 0 & f[x_0] = 1 & & & \\
 & & & f[x_0, x_1] = \frac{2-1}{0.5-0} = 2 & \\
x_1 = 0.5 & f[x_1] = 2 & , & & f[x_0, x_1, x_2] = \frac{4-2}{1-0} = 2 \\
 & & & f[x_1, x_2] = \frac{4-2}{1-0.5} = 4 & \\
x_2 = 1 & f[x_2] = 4 & & &
\end{array}$$

and so we get $P_2(x) = 1 + 2(x-0) + 2(x-0)(x-0.5) = 2x^2 + x + 1$, exactly as before.

Definition 3 (The divided differences table)**.**

$$\begin{array}{lllll}
f[x_0] & & & & \\
 & f[x_0, x_1] & & & \\
f[x_1] & & \ddots & & \\
 & f[x_1, x_2] & & f[x_0, x_1, \ldots, x_{n-1}] & \\
\vdots & & & & f[x_0, x_1, \ldots, x_n] \\
 & & & f[x_1, x_2, \ldots, x_n] & \\
f[x_{n-1}] & & \iddots & & \\
 & f[x_{n-1}, x_n] & & & \\
f[x_n] & & & &
\end{array}$$

The table is used to compute the coefficients of all interpolation polynomials up to degree n in Newton form. Adding x_{n+1} would result in addition of a row at the bottom, and removing x_n would result in removal of the last row.

Exercise 3. Without further computations, write down the interpolation polynomial for $f(x) = 4^x$ at $x_0 = 0, x_1 = 1/2$ and at $x_1 = 1/2, x_2 = 1$.

4 Interpolation error formula

Definition 4. Suppose $f(x)$ is sampled at distinct points $x_0, \ldots, x_n$. The interpolation error associated with approximating f by its interpolation polynomial is the quantity

$$\begin{aligned} e(x) &= f(x) - P_n(x) \\ &= f(x) - \sum_{k=0}^{n} f[x_0, \ldots, x_k]\, q_k(x). \end{aligned}$$

Claim 4. The interpolation error formula can be written as

$$e(x) = f[x_0, \ldots, x_n, x] \underbrace{q_{n+1}(x)}_{\prod_{k=0}^{n}(x-x_k)}, \quad x \notin \{x_0, \ldots, x_n\}. \tag{7}$$

Proof. Let $\bar{x} = x_{n+1}$ be distinct from $x_0, \ldots, x_n$, and consider $P_{n+1}(x)$ the interpolation polynomial at $x_0, \ldots, x_{n+1} = \bar{x}$. We have

$$\begin{aligned} P_{n+1}(x) &= P_n(x) + f[x_0, \ldots, x_n, \bar{x}]\, q_{n+1}(x) \\ f(\bar{x}) = f(x_{n+1}) = P_{n+1}(x_{n+1}) = P_{n+1}(\bar{x}) &= P_n(\bar{x}) + f[x_0, \ldots, x_n, \bar{x}]\, q_{n+1}(\bar{x}) \\ f(\bar{x}) - P_n(\bar{x}) &= f[x_0, \ldots, x_n, \bar{x}]\, q_{n+1}(\bar{x}). \end{aligned}$$

This proves the claim. □

Remark. The error formula (7) is also valid for $x_i \in \{x_0, \ldots, x_n\}$ provided we can define the divided differences for repeated nodes (as we shall do in the next lecture). In this case clearly

$$f(x_i) - P_n(x_i) = e(x_i) = f[x_0, \ldots, x_n, x_i]\, q_{n+1}(x_i) = 0$$

and therefore the formula is trivially valid.

Claim 5. Suppose that $f(x)$ and its first $k-1$ derivatives are continuous in some interval $I = [a, b]$ containing all the interpolation points, and the k-th derivative $f^{(k)}$ exists in the open inverval (a, b). Then there exists $c \in (a, b)$ such that

$$f[x_0, \ldots, x_k] = \frac{f^{(k)}(c)}{k!}.$$

Proof. Without loss of generality $a < x_0 < \cdots < x_k < b$. The function $e(x) = f(x) - P_k(x)$ is k times differentiable in (a, b), and it has $k+1$ zeros, since $e(x_i) = 0$ for $i = 0, 1, \ldots, k$. Then by **Rolle's theorem**, there is an internal point $c \in (a, b)$ where $e^{(k)}(c) = 0$. But

$$\begin{aligned} e^{(k)}(x) &= f^{(k)}(x) - P_k^{(k)}(x) \\ 0 = e^{(k)}(c) &= f^{(k)}(c) - k! A_k \\ f[x_0, \ldots, x_k] = A_k &= \frac{f^{(k)}(c)}{k!} \end{aligned}$$

which proves the claim. □

Combining the preceding two claims we obtain the interpolation error formula.

Theorem 2. *Let f be n times continuously differentiable in $I = [a, b]$ and suppose $f^{(n+1)}$ exists in the open inverval (a, b). Let $x_0, \ldots, x_n \subset I$ be pairwise distinct and let $x \in I$. Then there exists $c = c(x) \in (a, b)$ such that*

$$e(x) = f(x) - P_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!} q_{n+1}(x). \tag{8}$$

Remark 2. It is in fact not necessary to require continuity of f and its n first derivatives at the endpoints.

Example 4. Continuing Examples 2 and 3, the interpolation error for $f(x) = 4^x$ at $x_0 = 0, x_1 = 1/2, x_2 = 1$ can be bounded as follows (let's say at the point $x = 1/3$):

$$
\begin{aligned}
f(x) = 4^x \Rightarrow f'(x) = 4^x \ln 4 \Rightarrow f''(x) &= 4^x (\ln 4)^2 \Rightarrow f^{(3)}(x) = 4^x (\ln 4)^3 \\
e(x) = f(x) - P_2(x) &= \frac{4^c (\ln 4)^3}{6} x (x - 1/2)(x - 1) \\
e\left(\frac{1}{3}\right) &= \frac{4^c (\ln 4)^3}{6 \cdot 27} \\
(c < 1) &\le 0.0658.
\end{aligned}
$$

Recall that $P_2(x) = 2x^2 + x + 1$. The exact error is therefore $e(1/3) = 4^{1/3} - P_2(1/3) \approx 0.0318$ and so the bound is not so bad.

Example 5. Let us now bound the error uniformly in $[0,1]$. The polynomial $q_3(x) = x(x - 1/2)(x - 1)$ has extremal points at $\frac{1}{6}\left(3 \pm \sqrt{3}\right)$ and the extremal values are $\pm\frac{1}{12\sqrt{3}}$. This gives the bound

$$
\max_{x \in [0,1]} |e(x)| \le \frac{4 (\ln 4)^3}{6} \frac{1}{12\sqrt{3}} \approx 0.0855.
$$

Let us look at (8) again. If we can bound the $n+1$-st derivative uniformly in $[a,b]$ by $\sup_{x \in [a,b]} \left| \frac{f^{(n+1)}(x)}{(n+1)!} \right| \le M$, and denoting $h = b - a$ we have

$$
\sup_{x \in [a,b]} |e(x)| \le M h^{n+1}. \tag{9}
$$

Exercise 4. Let $f(x) = \cos 2x$. Denote $e_n(x) = f(x) - P_n(x)$.

1. Find $0 \le L \le 1$ such that the interpolation error in $[0,L]$ with 4 points $x_0, \ldots, x_3 \in [0,L]$ will be at most $|e_3(x)| \le 10^{-6}$.
2. Find n for which the interpolation error in $[0,1]$ will be at most $|e_n(x)| \le 10^{-6}$.

Solution. Using (9) we compute:

1. $\sup_{x \in [0,1]} \left| \frac{f^{(4)}(x)}{4!} \right| \le \frac{2^4}{4!} = \frac{2}{3}$ and so

$$
\begin{aligned}
\max_{x \in [0,1]} |e(x)| \le \frac{2}{3} L^4 &< 10^{-6} \\
L &< \left(\frac{3}{2}\right)^{\frac{1}{4}} 10^{-\frac{3}{2}} < 0.035.
\end{aligned}
$$

2. On the other hand,

$$
\max_{x \in [0,1]} |e_n(x)| \le \frac{2^{n+1}}{(n+1)!} \le 10^{-6}
$$

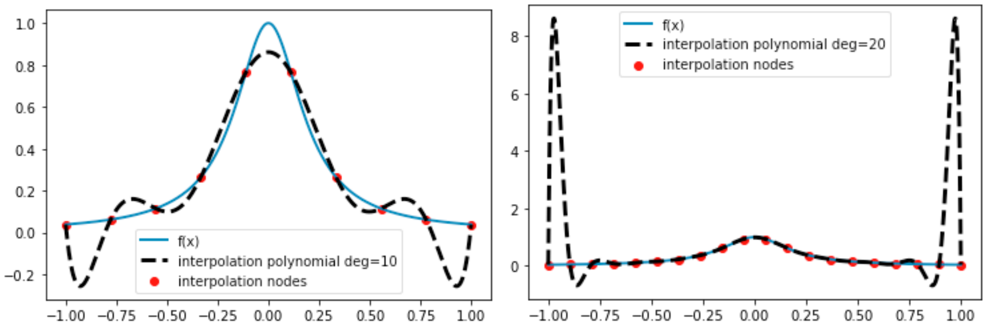

Figure 1: Runge's phenomenon

Since $a_n = \frac{2^{n+1}}{(n+1)!}$ is monotonically decreasing, we compute its value for first few n:

n	a_n
0	2.
1	2.
2	1.33333
3	0.666667
4	0.266667
5	0.0888889
6	0.0253968
7	0.00634921
8	0.00141093
9	0.000282187
10	0.0000513067
11	8.55112×10^{-6}
12	1.31556×10^{-6}
13	1.87937×10^{-7}
14	2.50582×10^{-8}
15	3.13228×10^{-9}

and so the minimal n is 13.

Example 6 (Runge's phenomenon)**.** The famous example by Runge shows that we may have diverging $\sup_{x\in[a,b]} |e_n(x)|$ as $n \to \infty$ even for a "nice" function such as $f(x) = \frac{1}{1+25x^2}$, but only when using equispaced interpolation nodes. The divergence happens towards the endpoints of the inverval (in the figure below, the interval is $[-1, 1]$).

Remark 3. To quote the paper [5]:

> For equispaced points, ..., polynomial interpolation fails. Even for analytic f, the interpolants do not always converge, let alone geometrically, as shown by Runge.... Moreover, the interpolation process is exponentially ill-conditioned, with Lebesgue constants of size about 2^n, ... This ill-conditioning means that even if f is entire, so that the interpolants converge in theory, they will diverge rapidly on a computer, at least for values of x near the endpoints, because of exponential amplification of rounding errors.

Remark 4. If we use so-called *Chebyshev nodes* for interpolation, the interpolation error will go to zero as $n \to \infty$ for sufficiently smooth functions.

5 Hermite interpolation

The basic form of polynomial interpolation requires equality of function values at the interoplation nodes ($P_n(x_k) = f(x_k)$). A more advanced form is to also require equality of the first order derivative (or several first derivatives, i.e. $P_n'(x_k) = f'(x_k), P_n''(x_k) = f''(x_k), \dots$ This is called *Hermite interpolation* [3]. In this more general case, if high order derivatives (up to $f^{(n)}$) need to be interpolated at a node x_k, this node will be repeated $n+1$ times.

Remark 5. If some of the derivatives are missing, e.g. $P_n(x_k) = f(x_k), P_n''(x_k) = f''(x_k)$, this is called *Hermite-Birkhoff interpolation*, but the theory is **much much more** complicated (in particular regarding existence and uniqueness).

Example. $\{x_0, x_0, x_0, x_1, x_2, x_2\}$ means that the (Hermite) interpolation polynomial $P(x)$ must satisfy the conditions

$$\begin{aligned}&P(x_0) = f(x_0), P'(x_0) = f'(x_0), P''(x_0) = f''(x_0),\\&P(x_1) = f(x_1)\\&P(x_2) = f(x_2), P'(x_2) = f'(x_2).\end{aligned}$$

Example. If the problem is given by $P_1(x_0) = f(x_0)$, $P_1'(x_0) = f'(x_0)$ (i.e. 2 equal nodes $\{x_0, x_0\}$) then

$$P_1(x) = f(x_0) + f'(x_0)(x - x_0).$$

This can be seen as the limiting case of the interpolation problem for the nodes $\{x_0, x_1\}$ when $x_1 \to x_0$ in the Newton form:

$$P_1(x) = f(x_0) + \underbrace{\frac{f(x_1) - f(x_0)}{x_1 - x_0}}_{\to f'(x_0)}(x - x_0).$$

Naturally, we will want to use Newton's form of interpolation polynomial to deal with this case, but we need to modify the definition of the divided differences for the case of repeated nodes.

Definition 5. If f is differentiable at x_0, then

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

For defining the general case, we will assume the nodes to be ordered in non-decreasing order.

Definition 6. Suppose that $x_0 \le x_1 \le \dots \le x_n$ (so that all possible repetitions are adjacent). If f has n continuous derivatives in an open neighborhood of x_0, then

$$f[x_0, \dots, x_n] = \begin{cases} \frac{f[x_1,\dots,x_n] - f[x_0,\dots,x_{n-1}]}{x_n - x_0} & x_0 < x_n \\ \frac{1}{n!} f^{(n)}(x_0) & x_0 = x_n. \end{cases} \tag{10}$$

This covers all cases (why?)

Exercise. Let f be twice continuously differentiable around x_0. Check that

$$f\left[x_0, x_0, x_0\right] = \lim_{h\to 0} f\left[x_0, x_0, x_0+h\right].$$

Remark. In fact, it can be shown that $f\left[x_0, x_1, \ldots, x_n\right]$ is a continuous function in all of its arguments, see e.g. [2, p. 51].

Example 7. If $x_0 < x_1$ then

$$f\left[x_0, x_0, x_1\right] = \frac{f\left[x_0, x_1\right] - f\left[x_0, x_0\right]}{x_1 - x_0} = \frac{\left(f\left(x_1\right) - f\left(x_0\right)\right)/\left(x_1 - x_0\right) - f'\left(x_0\right)}{x_1 - x_0}.$$

The Hermite interpolation problem

Let $y_0 \le y_1 \le \cdots \le y_n$ with possible repetitions, with $m+1$ distinct values $x_0, \ldots, x_m$ (where clearly $m \le n$). For each $i = 0, \ldots, m$ let the value x_i be repeated $k_i + 1$ times, then

$$\sum_{i=0}^{m} \left(k_i + 1\right) = n + 1.$$

For example: $\{y_0, y_1, y_2, y_3, y_4, y_5\} = \{x_0, x_0, x_0, x_1, x_2, x_2\}$ so that $n = 5, m = 2$ and $k_0 = 2, k_1 = 0, k_2 = 1$.

This is also the number of interpolation conditions which will define our problem uniquely.

Let there be given the values $\left\{f\left(x_i\right), f'\left(x_i\right), \ldots, f^{(k_i)}\left(x_i\right)\right\}_{i=0}^{m}$. The Hermite interpolation polynomial P should satisfy the interpolation conditions

$$P^{(j)}\left(x_i\right) = f^{(j)}\left(x_i\right), \forall i = 0, \ldots, m, j = 0, 1, \ldots, k_i. \tag{11}$$

The following theorem is presented without complete proof.

Theorem 3. *There exists a unique polynomial $P_n \in \Pi_n$ satisfying the Hermite interpolation conditions (11). Moreover, P_n can be written in the Newton form (5), where the divided differences are defined by the recursive formula (10). The error formulas (7) and (8) hold for the case of Hermite interpolation as well, valid for all $x \in \mathbb{R}$.*

Remark 6. The existence and uniqueness of the Hermite polynomial can be shown as follows: write a polynomial $P_n\left(x\right) = \sum_{i=0}^{n} c_i x^i$ in the basis of monomials, and consider the linear system defined by the (11) with respect to the coefficients: $U\mathbf{c} = \mathbf{f}$. The matrix U is a generalization of the Vandermonde matrix from theorem 1, called the *confluent Vandermonde matrix.* Then this system has a unique solution if and only if the corresponding homogeneous system has only the trivial solution. However, the homogeneous system $U\mathbf{r} = 0$ is equivalent to the conditions (here $R\left(x\right) = \sum r_i x^i$ is the polynomial corresponding to the coefficient vector $\mathbf{r}$)

$$R^{(j)}\left(x_i\right) = 0,\ \forall i = 0, \ldots, m, j = 0, 1, \ldots, k_i.$$

This means that x_i is a zero of multiplicity $k_i + 1$ (why?), and consequently the polynomial $R\left(x\right)$ has at least $\sum_{i=0}^{m}\left(k_i + 1\right) = n + 1$ zeros *counting multiplicities.* Since $\deg R\left(x\right) \le n$ we conclude that $R\left(x\right) \equiv 0$.

Example. To illustrate the last claim in the proof above, consider $m = 1$ and $k_0 = k_1 = 1$, then in the previous construction we must have $R(x_0) = R(x_1) = 0$, therefore by Rolle's theorem $R'(c) = 0$ for some $c \in (x_0, x_1)$. But we also have $R'(x_0) = R'(x_1) = 0$ and so $R'(x)$ has at least 3 distinct zeros. However $\deg R' \leq 2$ and therefore $R'(x) \equiv 0$ and consequently $R(x) = \text{const} = 0$.

Example 8 (Hermite interpolation of degree ≤ 3)**.** Construct the Hermite interpolation polynomial for the node configuration $\{x_0, x_0, x_1, x_1\}$.

Solution. Compute the divided difference table:

1. $f[x_0, x_0] = f'(x_0), f[x_0, x_1] = \frac{f(x_1)-f(x_0)}{x_1-x_0}, f[x_1, x_1] = f'(x_1)$
2. $f[x_0, x_0, x_1] = \frac{f[x_0,x_1]-f[x_0,x_0]}{x_1-x_0} = \frac{(f(x_1)-f(x_0))/(x_1-x_0)-f'(x_0)}{x_1-x_0}$
3. $f[x_0, x_1, x_1] = \frac{f[x_1,x_1]-f[x_0,x_1]}{x_1-x_0} = \frac{f'(x_1)-(f(x_1)-f(x_0))/(x_1-x_0)}{x_1-x_0}$
4. $$\begin{aligned} f[x_0, x_0, x_1, x_1] =& \frac{f[x_0, x_1, x_1] - f[x_0, x_0, x_1]}{x_1 - x_0} = \\ =& \frac{\frac{f'(x_1)-(f(x_1)-f(x_0))/(x_1-x_0)}{x_1-x_0} - \frac{(f(x_1)-f(x_0))/(x_1-x_0)-f'(x_0)}{x_1-x_0}}{x_1 - x_0} \end{aligned}$$

The final result:

$$\begin{aligned} P_3(x) =& f(x_0) + f'(x_0)(x - x_0) + \frac{(f(x_1) - f(x_0))/(x_1 - x_0) - f'(x_0)}{x_1 - x_0}(x - x_0)^2 + \\ &+ \frac{f'(x_1) - 2(f(x_1) - f(x_0))/(x_1 - x_0) + f'(x_0)}{(x_1 - x_0)^2}(x - x_0)^2 (x - x_1). \end{aligned}$$

Check that $P_3(x_0) = f(x_0), P_3(x_1) = x_1, P_3'(x_0) = f'(x_0), P_3'(x_1) = f'(x_1)$.

In the last example, we have

$$\begin{aligned} e(x) &= f(x) - P_3(x) \\ &= f[x_0, x_0, x_1, x_1, x](x - x_0)^2 (x - x_1)^2 \\ &= \frac{f^{(4)}(c)}{4!}(x - x_0)^2 (x - x_1)^2 \end{aligned}$$

Using the calculation in Example 10, set $h = x_1 - x_0$, then we can bound the last quantity by

$$\sup_{x \in [x_0, x_1]} |e(x)| \leq \frac{\sup_{x \in [x_0, x_1]} |f^4(x)|}{4!} \left(\frac{h^2}{4}\right)^2. \tag{12}$$

Example 9. Consider the Hermite interpolation problem for the function $f(x) = e^x$ with the nodes $\{x_0, x_0, x_1, x_1\}$ where $x_0 = 0, x_1 = 1$.

1. The divided differences table computation gives $f[x_0] = 1$, $f[x_0, x_0] = 1, f[x_0, x_0, x_1] = e - 2$ and $f[x_0, x_0, x_1, x_1] = 3 - e$, therefore

$$P_3(x) = 1 + 1 \cdot x + (e - 2)x^2 + (3 - e)x^2(x - 1).$$

2. Approximate $\sqrt{e}$ using $P_3(x)$:

   $$\sqrt{e} = e^{1/2} \approx P_3(1/2) \approx 1.6444$$

   On the calculator $\sqrt{e} \approx 1.6487$ so the error is $e(1/2) \approx 0.0044$

3. Using (12) we obtain the error bound

   $$\sup_{x\in[0,1]} |e^x - P_3(x)| \le \frac{e}{4!4^2} \approx 0.0071.$$

6 Spline functions

Definition 7. Let $a = x_0 < \cdots < x_n = b$. **Spline function** of degree k and smoothness m is a function which is a polynomial of degree k on each subinterval $[x_{i-1}, x_i]$ for $i = 1, \ldots, n$, and in addition has m continuous derivatives at <u>every point</u> in $[a, b]$.

Note that if $m \ge k$ then the polynomial pieces must have all k derivatives coinciding at each x_i, and therefore the pieces must be the same polynomial, in which case the entire spline is just a polynomial. The most common scenario is $m = k - 1$.

Example 10 (Piecewise linear interpolation, $m = 0, k = 1$)**.** . Let $f(x)$ be twice continuously differentiable, and $a = x_0 < \cdots < x_n = b$. At each $[x_{i-1}, x_i]$ the spline is just a linear polynomial of interpolation, connecting $(x_{i-1}, f(x_{i-1}))$ and $(x_i, f(x_i))$. At the inner points the derivative does not exist.

$$e_i(x) = \frac{f''(\xi_i)}{2!} \underbrace{(x - x_{i-1})(x - x_i)}_{\psi_i(x)}, \quad \xi_i, x \in (x_{i-1}, x_i).$$

$$|\psi_i(x)| \le \left|\psi_i\left(\frac{x_{i-1} + x_i}{2}\right)\right| = \frac{(x_i - x_{i-1})^2}{4}.$$

Adding more points and letting $h = \max_i |x_i - x_{i-1}|$ we get the bound

$$\max_{x\in[a,b]} |e(x)| \le \frac{h^2}{8} \max_{x\in[a,b]} |f''(x)|.$$

Example 11 (Cubic Hermite spline interpolation)**.** Consider the case $m = 2, k = 3$. Let $P_{3,i}(x)$ be the Hermite polynomial satisfying

$$\begin{aligned} P_{3,i}(x_{i-1}) &= f(x_{i-1}) \\ P'_{3,i}(x_{i-1}) &= f'(x_{i-1}) \\ P_{3,i}(x_i) &= f(x_i) \\ P'_{3,i}(x_i) &= f'(x_i) \end{aligned}$$

Let $S(x)$ be the piecewise-cubic polynomial defined to be equal to $P_{3,i}(x)$ on each piece $[x_{i-1}, x_i]$. Notice that $S(x)$ has one continuous derivative in $[a, b]$. Let $h = \max_{i=1}^n (x_i - x_{i-1})$, then by (12) on each piece $[x_{i-1}, x_i]$ the error is bounded by

$$\sup_{x\in[a,b]} |f(x) - S(x)| = \max_{i=1,\ldots,n} \sup_{x\in[x_{i-1},x_i]} |f(x) - P_{3,i}(x)| \le \frac{\sup_{x\in[a,b]} \left|f^4(x)\right|}{4!} \left(\frac{h^2}{4}\right)^2. \qquad (13)$$

In practice, the cubic splines are frequently used to draw a smooth curve $S(x)$ between data points (x_i, y_i), by requiring $S(x_i) = y_i$ and $S'(x_i) = z_i$ where the values z_i are chosen somehow (there is no unique choice). For example: $z_0 = z_{n+1} = 0$ and $z_i = \frac{y_{i+1}-y_{i-1}}{x_{i+1}-x_{i-1}}$ for $i = 1, \ldots, n-1$ (which is the central difference scheme for approximating the derivative, as we shall see in the next lecture).

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