

# MA 1018: Introduction to Scientific Computing

## Interpolation and Polynomial Approximation



Suh-Yuh Yang (楊肅煜)

Department of Mathematics, National Central University  
Jhongli District, Taoyuan City 320317, Taiwan

First version: November 09, 2025/Last updated: February 11, 2026

## Interpolation (插值)

---

- ① **Interpolation:** find a function that fits the given data

$$(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n).$$

- ② **Why polynomials?**

**The Weierstrass Approximation Theorem:**

Suppose that  $f \in C[a, b]$ . Then  $\forall \varepsilon > 0, \exists p(x)$  polynomial defined on  $[a, b]$  such that  $|f(x) - p(x)| < \varepsilon$  for all  $x \in [a, b]$ .

i.e., Every continuous function  $f$  on  $[a, b]$  is the uniform limit of polynomials; i.e.,  $\overline{\mathcal{P}} = C[a, b]$ .

- ③ **Why not Taylor polynomials?**

- need to calculate  $f'(x), f''(x), \dots$
- accurate near at a specific point, not on entire interval.

## Polynomial interpolation

---

- ① We solve the following problem: given a table of  $n + 1$  data points  $(x_i, y_i)$ ,

$x$	$x_0$	$x_1$	$x_2$	$\cdots$	$x_n$
$y$	$y_0$	$y_1$	$y_2$	$\cdots$	$y_n$

we seek a polynomial  $p$  of lowest possible degree for which

$$p(x_i) = y_i, \quad 0 \leq i \leq n.$$

- ② *Such a polynomial is said to “interpolate” the data.*

## Lagrange polynomial

---

- ① Given  $(x_0, f(x_0))$  and  $(x_1, f(x_1))$ ,  $x_0 \neq x_1$ , we consider

$$p(x) = \frac{x - x_1}{x_0 - x_1}f(x_0) + \frac{x - x_0}{x_1 - x_0}f(x_1) := L_{1,0}(x)f(x_0) + L_{1,1}(x)f(x_1).$$

*Then degree  $p(x) \leq 1$  and  $p(x_0) = f(x_0)$ ,  $p(x_1) = f(x_1)$ .*

- ② Given  $n + 1$  distinct numbers  $x_0, x_1, \dots, x_n$ , then for each  $k = 0, 1, \dots, n$ , how to construct a quotient  $L_{n,k}(x)$  such that

$$L_{n,k}(x_i) = \begin{cases} 1 & \text{if } i = k, \\ 0 & \text{if } i \neq k. \end{cases}$$

**Answer:** for  $k = 0, 1, \dots, n$ ,

$$\begin{aligned} L_{n,k}(x) &= \frac{(x - x_0) \cdots (x - x_{k-1}) (x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0) \cdots (x_k - x_{k-1}) (x_k - x_{k+1}) \cdots (x_k - x_n)} \\ &= \prod_{i=0, i \neq k}^n \frac{x - x_i}{x_k - x_i}. \end{aligned}$$

## Theorem on polynomial interpolation

---

**Lagrange Theorem:** Given  $n + 1$  distinct real (or complex) numbers  $x_0, x_1, \dots, x_n$  and their function values  $f(x_0), f(x_1), \dots, f(x_n)$ . Then there exists an unique polynomial  $p(x)$ , degree  $p(x) \leq n$ , such that

$$p(x_k) = f(x_k), \quad k = 0, 1, \dots, n.$$

In fact, this polynomial is given by

$$p(x) = f(x_0)L_{n,0}(x) + f(x_1)L_{n,1}(x) + \dots + f(x_n)L_{n,n}(x) = \sum_{k=0}^n f(x_k)L_{n,k}(x),$$

and we call  $p$  the  $n$ -th Lagrange interpolating polynomial.

## Proof of the Lagrange theorem

- 1 **Existence:** it is trivial. One can check that the given  $p(x)$  satisfies the requirements.
- 2 **Existence + Uniqueness:** assume that

$$p(x) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n.$$

The interpolation conditions,  $p(x_k) = f(x_k)$  for  $0 \leq k \leq n$ , lead to the following system of  $n + 1$  linear equations for determining  $a_0, a_1, \cdots, a_n$ :

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix}.$$

The coefficient matrix  $X$  is called the **Vandermonde matrix**. It is nonsingular with  $\det X = \prod_{0 \leq i < j \leq n} (x_j - x_i) \neq 0$ , (but it is often *ill-conditioned*).

## Example

- **Notation:**  $L_k(x) := L_{n,k}(x)$  when there is no confusion.
- **Example:** Given nodes and their function values:  $x_0 = 2$ ,  $f(x_0) = 0.5$ ,  $x_1 = 2.5$ ,  $f(x_1) = 0.4$ ,  $x_2 = 4$ ,  $f(x_2) = 0.25$ .

In fact,  $f(x) = 1/x$ .

Find the second ( $n = 2$ ) Lagrange interpolating polynomial.

$$L_{2,0}(x) = L_0(x) = \frac{(x-2.5)(x-4)}{(2-2.5)(2-4)} = \frac{x^2 - 6.5x + 10}{1},$$

$$L_{2,1}(x) = L_1(x) = \frac{(x-2)(x-4)}{(2.5-2)(2.5-4)} = \frac{x^2 - 6x + 8}{-0.75},$$

$$L_{2,2}(x) = L_2(x) = \frac{(x-2)(x-2.5)}{(4-2)(4-2.5)} = \frac{x^2 - 4.5x + 5}{3}.$$

$$\begin{aligned} \therefore p(x) &= 0.5 \left( \frac{x^2 - 6.5x + 10}{1} \right) + 0.4 \left( \frac{x^2 - 6x + 8}{-0.75} \right) \\ &\quad + 0.25 \left( \frac{x^2 - 4.5x + 5}{3} \right) = 0.05x^2 - 0.425x + 1.15. \end{aligned}$$

We have  $1/3 = f(3) \approx p(3) = 0.325$ .

## Theorem on polynomial interpolation error

Let  $f$  be a given real-valued function in  $C^{n+1}[a, b]$ . Let  $x_0, x_1, \dots, x_n \in [a, b]$  be  $n + 1$  distinct numbers. Then for each  $x$  in  $[a, b]$ ,  $\exists \xi(x) \in (a, b)$  such that

$$f(x) = p(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi(x)) \prod_{i=0}^n (x - x_i),$$

where  $p(x)$  is the  $n$ -th Lagrange interpolating polynomial.

*Proof.* Let  $x \in [a, b]$ .

If  $x = x_k$  for some  $0 \leq k \leq n$ , then the assertion holds.

Let  $x \neq x_k$  for any  $k = 0, 1, \dots, n$ . Define  $g : [a, b] \rightarrow \mathbb{R}$  by

$$g(t) = f(t) - p(t) - \lambda w(t) \quad (\text{function in } t),$$

$$\lambda = (f(x) - p(x)) / w(x) \quad (\text{a constant that makes } g(x) = 0),$$

$$w(t) = \prod_{i=0}^n (t - x_i) \quad (\text{polynomial in } t).$$

## Theorem on polynomial interpolation error (cont'd)

We can check that  $g \in C^{n+1}[a, b]$  and  $g$  vanishes at the  $n + 2$  points  $x, x_0, x_1, \dots, x_n$ . By generalized Rolle's Theorem,  $g'$  has at least  $n + 1$  distinct zeros in  $(a, b)$ .

Repeating this process, we conclude eventually that  $g^{(n+1)}$  has at least one zero  $\xi(x) \in (a, b)$ .

$$g^{(n+1)}(t) = f^{(n+1)}(t) - p^{(n+1)}(t) - \lambda w^{(n+1)}(t) = f^{(n+1)}(t) - (n + 1)! \lambda.$$

Hence, we have

$$\begin{aligned} 0 &= g^{(n+1)}(\xi(x)) = f^{(n+1)}(\xi(x)) - (n + 1)! \lambda \\ &= f^{(n+1)}(\xi(x)) - (n + 1)! \frac{f(x) - p(x)}{w(x)}. \end{aligned}$$

Therefore, we obtain

$$f(x) - p(x) = \frac{1}{(n + 1)!} f^{(n+1)}(\xi(x)) \prod_{i=0}^n (x - x_i).$$

This completes the proof.  $\square$

## Example

$f(x) = e^x, x \in [0, 1]$ . Let  $x_0, x_1, \dots, x_n$  be a uniform partition of  $[0, 1]$  with step size  $h = 1/n$ .

Consider  $[x_j, x_{j+1}]$  for some  $j$ . Let  $p(x)$  be the first Lagrange interpolating polynomial on  $[x_j, x_{j+1}]$ . Then for  $x \in [x_j, x_{j+1}]$ ,

$$\begin{aligned} |f(x) - p(x)| &= \left| \frac{f''(\xi)}{2!} (x - x_j)(x - x_{j+1}) \right| \\ &\leq \frac{e^\xi}{2} \left| (x - jh)(x - (j+1)h) \right|, \quad \xi \in (x_j, x_{j+1}) \\ &\leq \frac{1}{2} \max_{\xi \in [0,1]} e^\xi \max_{x \in [x_j, x_{j+1}]} \left| (x - jh)(x - (j+1)h) \right| \\ &\leq \frac{1}{2} e \frac{h^2}{4} = \frac{eh^2}{8}. \end{aligned}$$

If  $|f(x) - p(x)| \leq (eh^2)/8 \leq 10^{-6}$  then  $h < 1.72 \times 10^{-3}$ .

We can choose  $h = 0.001$ .

## Divided differences (均差)

---

- 1 Let  $f$  be a function whose values are known at points (nodes)  $x_0, x_1, \dots, x_n$ . We assume that these nodes are distinct, but they need not be ordered.
- 2 We know there is a unique polynomial  $p$  of degree at most  $n$  such that

$$p(x_i) = f(x_i) \quad \text{for } 0 \leq i \leq n.$$

$p$  can be constructed as a linear combination of  $1, x, x^2, \dots, x^n$ .

## Divided differences (cont'd)

---

We should use the Newton form of the interpolating polynomial:

$$q_0(x) = 1,$$

$$q_1(x) = (x - x_0),$$

$$q_2(x) = (x - x_0)(x - x_1),$$

$$q_3(x) = (x - x_0)(x - x_1)(x - x_2),$$

$$\vdots$$

$$q_n(x) = (x - x_0)(x - x_1)(x - x_2) \cdots (x - x_{n-1}).$$

The  $n$ th Lagrange interpolating polynomial  $p$  can be expressed as

$$p(x) = \sum_{j=0}^n c_j q_j(x).$$

## Divided differences (cont'd)

---

- 1 The interpolation conditions give rise to a linear system of equations for the unknown coefficients:

$$\sum_{j=0}^n c_j q_j(x_i) = f(x_i) \quad \text{for } 0 \leq i \leq n.$$

- 2 The elements of the coefficient matrix are

$$a_{ij} = q_j(x_i) \quad \text{for } 0 \leq i, j \leq n.$$

- 3 *The  $(n + 1) \times (n + 1)$  matrix  $A = (a_{ij})$  is a lower triangular matrix because*

$$q_j(x) = \prod_{k=0}^{j-1} (x - x_k) \implies a_{ij} = q_j(x_i) = \prod_{k=0}^{j-1} (x_i - x_k) = 0 \text{ if } i \leq j - 1.$$

## Divided differences (cont'd)

---

- ① For example, consider the case of three nodes with

$$\begin{aligned} p(x) &= c_0q_0(x) + c_1q_1(x) + c_2q_2(x) \\ &= c_0 + c_1(x - x_0) + c_2(x - x_0)(x - x_1). \end{aligned}$$

Setting  $x = x_0$ ,  $x = x_1$ , and  $x = x_2$ , we have a lower triangular system

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & (x_1 - x_0) & 0 \\ 1 & (x_2 - x_0) & (x_2 - x_0)(x_2 - x_1) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \end{bmatrix}.$$

- ② Thus,  $c_n$  depends on  $f$  at  $x_0, x_1, \dots, x_n$ . Define the notation

$$c_n := f[x_0, x_1, \dots, x_n].$$

We call  $f[x_0, x_1, \dots, x_n]$  a divided difference of  $f$ .

## Divided differences (cont'd)

- ①  $f[x_0, x_1, \dots, x_n]$  is the coefficient of  $q_n$  when  $\sum_{k=0}^n c_k q_k$  interpolates  $f$  at  $x_0, x_1, \dots, x_n$ . For example,

$$f[x_0] = f(x_0), \quad f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}.$$

- ② **Theorem on Higher-Order Divided Differences:** In general, divided differences satisfy the equation:

$$f[x_0, x_1, \dots, x_n] = \frac{f[x_1, x_2, \dots, x_n] - f[x_0, x_1, \dots, x_{n-1}]}{x_n - x_0}.$$

*Proof.* Let  $p_k$  be the polynomial of degree  $\leq k$  that interpolates  $f$  at  $x_0, x_1, \dots, x_k$ . Let  $q$  denote the polynomial of degree  $\leq n-1$  that interpolates  $f$  at  $x_1, x_2, \dots, x_n$ . Then

$$p_n(x) = q(x) + \frac{x - x_n}{x_n - x_0} (q(x) - p_{n-1}(x)).$$

( $\because$  same values at  $x_0, x_1, \dots, x_n$  and same degree  $\leq n$ )

Examining the coefficient of  $x^n$  on the both sides, we arrive at the assertion.  $\square$

## Table of divided differences

- 1 If a table of function values  $(x_i, f(x_i))$  is given, we can construct from it a table of divided differences as follows: ( $n = 3$ )

---

$x_0$	$f[x_0]$			
		$f[x_0, x_1]$		
$x_1$	$f[x_1]$		$f[x_0, x_1, x_2]$	
		$f[x_1, x_2]$		$f[x_0, x_1, x_2, x_3]$
$x_2$	$f[x_2]$		$f[x_1, x_2, x_3]$	
		$f[x_2, x_3]$		
$x_3$	$f[x_3]$			

---

- 2 The following formula is called Newton's interpolatory divided-difference formula:

$$p_n(x) = f[x_0] + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](x - x_0) \cdots (x - x_{k-1}).$$

- 3 The coefficients required in the Newton interpolatory divided-difference formula occupy the top row in the divided difference table.

## Example

Compute a divided difference table from

$x_i$	1.0	1.3	1.6	1.9	2.2
$f(x_i)$	0.7651977	0.6200860	0.4554022	0.2818186	0.1103623

*Solution:*

$i$	$x_i$	$f[x_i]$	$f[x_{i-1}, x_i]$	$f[x_{i-2}, x_{i-1}, x_i]$	$f[x_{i-3}, \dots, x_i]$	$f[x_{i-4}, \dots, x_i]$
0	1.0	0.7651977				
1	1.3	0.6200860	-0.4837057			
2	1.6	0.4554022	-0.5489460	-0.1087339		
3	1.9	0.2818186	-0.5786120	-0.0494433	0.0658784	
4	2.2	0.1103623	-0.5715210	0.0118183	0.0680685	0.0018251

The Newton interpolatory divided-difference formula is

$$\begin{aligned} p_4(x) = & 0.7651977 - 0.4837057(x - 1.0) \\ & - 0.1087339(x - 1.0)(x - 1.3) \\ & + 0.0658784(x - 1.0)(x - 1.3)(x - 1.6) \\ & + 0.0018251(x - 1.0)(x - 1.3)(x - 1.6)(x - 1.9). \end{aligned}$$

## Properties of divided differences

---

**Theorem.** If  $(z_0, z_1, \dots, z_n)$  is a permutation of  $(x_0, x_1, \dots, x_n)$ , then

$$f[z_0, z_1, \dots, z_n] = f[x_0, x_1, \dots, x_n].$$

*Proof:*

- $f[z_0, z_1, \dots, z_n]$  is the coefficient of  $x^n$  in the polynomial of degree  $\leq n$  that interpolates  $f$  at the nodes  $z_0, z_1, \dots, z_n$ .
- $f[x_0, x_1, \dots, x_n]$  is the coefficient of  $x^n$  in the polynomial of degree  $\leq n$  that interpolates  $f$  at the nodes  $x_0, x_1, \dots, x_n$ .
- These two polynomials are **the same**. This leads to the conclusion.

## Osculating polynomial (密切多項式)

- ① **Definition:** Let  $x_0, x_1, \dots, x_n \in [a, b]$  be  $n + 1$  distinct numbers. Let  $m_0, m_1, \dots, m_n \geq 0$  integers.  $m = \max\{m_0, m_1, \dots, m_n\}$ . Suppose that  $f \in C^m[a, b]$ . Then the osculating polynomial approximating  $f$  is the polynomial  $p(x)$  of least degree such that

$$\frac{d^k p(x_i)}{dx^k} = \frac{d^k f(x_i)}{dx^k} \quad \text{for } i = 0, 1, \dots, n \text{ and } k = 0, 1, \dots, m_i.$$

② **Remarks:**

- degree of  $p(x) \leq \left(\sum_{i=0}^n m_i\right) + n := M$ .
- If  $n = 0$ , then  $p(x) = m_0$ -th Taylor polynomial of  $f(x)$  at  $x_0$ .
- If  $m_i = 0$  for  $i = 0, 1, \dots, n$ , then  $p(x) = n$ -th Lagrange interpolating polynomial of  $f(x)$  at  $x_0, x_1, \dots, x_n$ .
- If  $m_i = 1$  for  $i = 0, 1, \dots, n$ , then  $p(x)$  is the Hermite interpolating polynomial.

## Theorem on the Hermite interpolation

**Hermite Theorem:** Let  $x_0, x_1, \dots, x_n \in [a, b]$  be  $n + 1$  distinct numbers and  $f \in C^1[a, b]$ . The the unique polynomial of least degree agreeing with  $f(x)$  and  $f'(x)$  at  $x_0, x_1, \dots, x_n$  is the Hermite polynomial of degree at most  $2n + 1$  given by

$$H_{2n+1}(x) = \sum_{j=0}^n f(x_j)H_{n,j}(x) + \sum_{j=0}^n f'(x_j)\widehat{H}_{n,j}(x),$$

where

$$H_{n,j}(x) = \left(1 - 2(x - x_j)L'_{n,j}(x_j)\right)L_{n,j}^2(x),$$

$$\widehat{H}_{n,j}(x) = (x - x_j)L_{n,j}^2(x),$$

$$L_{n,j}(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_{j-1})(x - x_{j+1}) \cdots (x - x_n)}{(x_j - x_0)(x_j - x_1) \cdots (x_j - x_{j-1})(x_j - x_{j+1}) \cdots (x_j - x_n)}.$$

Moreover, if  $f \in C^{2n+2}[a, b]$ , then

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

## Proof of the existence

---

① **Claim:**  $H_{2n+1}(x_i) = f(x_i)$  for all  $i = 0, 1, \dots, n$ .

If  $i \neq j$ , then  $H_{n,j}(x_i) = 0$  and  $\widehat{H}_{n,j}(x_i) = 0$ .

$$\begin{aligned}H_{n,i}(x_i) &= (1 - 2(x_i - x_i)L'_{n,i}(x_i))L_{n,i}^2(x_i) \\ &= (1 - 2(x_i - x_i)L'_{n,i}(x_i)) = 1.\end{aligned}$$

$$\widehat{H}_{n,i}(x_i) = (x_i - x_i)L_{n,i}^2(x_i) = 0.$$

$$\therefore H_{2n+1}(x_i) = \sum_{j=0, j \neq i}^n f(x_j)0 + f(x_i)1 + \sum_{j=0}^n f'(x_j)\widehat{H}_{n,j}(x_i) = f(x_i).$$

② **Claim:**  $H'_{2n+1}(x_i) = f'(x_i)$  for all  $i = 0, 1, \dots, n$ .

$$H'_{n,j}(x) = -2L'_{n,j}(x_j)L_{n,j}^2(x) + (1 - 2(x - x_j)L'_{n,j}(x_j))2L_{n,j}(x)L'_{n,j}(x).$$

If  $i \neq j$  then  $H'_{n,j}(x_i) = 0$ .

## Proof of the existence (cont'd)

---

If  $i = j$  then

$$\begin{aligned}H'_{n,j}(x_i) &= -2L'_{n,j}(x_j)L_{n,j}^2(x_i) + (1 - 2(x_i - x_j)L'_{n,j}(x_j))2L_{n,j}(x_i)L'_{n,j}(x_i) \\ &= -2L'_{n,j}(x_j)L_{n,j}^2(x_i) + 2L_{n,j}(x_i)L'_{n,j}(x_i) = -2L'_{n,j}(x_j) + 2L'_{n,j}(x_i) = 0.\end{aligned}$$

$$\widehat{H}'_{n,j}(x) = L_{n,j}^2(x) + (x - x_j)2L_{n,j}(x)L'_{n,j}(x).$$

If  $i \neq j$  then  $\widehat{H}'_{n,j}(x_i) = 0$ .

If  $i = j$  then  $\widehat{H}'_{n,j}(x_i) = L_{n,j}^2(x_i) + (x_i - x_j)2L_{n,j}(x_i)L'_{n,j}(x_i) = 1$ .

$$\therefore H'_{2n+1}(x) = \sum_{j=0}^n f(x_j)H'_{n,j}(x) + \sum_{j=1}^n f'(x_j)\widehat{H}'_{n,j}(x).$$

$\therefore H'_{2n+1}(x_i) = f'(x_i)$  for all  $i = 0, 1, \dots, n$ .

**Note:** For the uniqueness and error estimate, see page 143, #11 (a)(b).

## Example

Find the Hermite interpolating polynomial according the following table:

$k$	$x_k$	$f(x_k)$	$f'(x_k)$
0	1.3	0.6200860	-0.5220232
1	1.6	0.4554022	-0.5698959
2	1.9	0.2818186	-0.5811571

First, we compute

$$L_{2,0}(x) = \frac{(x-1.6)(x-1.9)}{(-0.3)(-0.6)} = \frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9}, \quad L'_{2,0}(x) = \frac{100}{9}x - \frac{175}{9}$$

$$L_{2,1}(x) = \frac{(x-1.3)(x-1.9)}{(0.3)(-0.3)} = -\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9}, \quad L'_{2,1}(x) = -\frac{200}{9}x + \frac{320}{9}$$

$$L_{2,2}(x) = \frac{(x-1.3)(x-1.6)}{(0.6)(0.3)} = \frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9}, \quad L'_{2,2}(x) = \frac{100}{9}x - \frac{145}{9}$$

## Example (cont'd)

Next, we compute

$$H_{2,0}(x) = (10x - 12)\left(\frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9}\right)^2$$

$$H_{2,1}(x) = 1\left(-\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9}\right)^2$$

$$H_{2,2}(x) = 10(2 - x)\left(\frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9}\right)^2$$

$$\hat{H}_{2,0}(x) = (x - 1.3)\left(\frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9}\right)^2$$

$$\hat{H}_{2,1}(x) = (x - 1.6)\left(-\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9}\right)^2$$

$$\hat{H}_{2,2}(x) = (x - 1.9)\left(\frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9}\right)^2$$

Therefore, we obtain

$$\begin{aligned} H_5(x) = & 0.6200860H_{2,0}(x) + 0.4554022H_{2,1}(x) + 0.2818186H_{2,2}(x) \\ & - 0.5220232\hat{H}_{2,0}(x) - 0.5698959\hat{H}_{2,1}(x) - 0.5811571\hat{H}_{2,2}(x). \end{aligned}$$

## Divided-difference formula

- ① The Newton interpolatory divided-difference formula for the  $n$ th Lagrange polynomial at distinct numbers  $x_0, x_1, \dots, x_n$  is given by

$$p_n(x) = f[x_0] + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](x - x_0) \cdots (x - x_{k-1}).$$

- ② Define  $z_0, z_1, \dots, z_{2n+1}$  by  $z_{2i} = z_{2i+1} = x_i$ , for  $i = 0, 1, \dots, n$ . Then the Newton interpolatory divided-difference formula for the Hermite interpolating polynomial at distinct numbers  $x_0, x_1, \dots, x_n$  is given by

$$H_{2n+1}(x) = f[z_0] + \sum_{k=1}^{2n+1} f[z_0, z_1, \dots, z_k](x - z_0)(x - z_1) \cdots (x - z_{k-1}),$$

where  $f[x_i, x_i] := f'(x_i)$ , since

$$\lim_{x \rightarrow x_i} f[x_i, x] = \lim_{x \rightarrow x_i} \frac{f(x) - f(x_i)}{x - x_i} = f'(x_i).$$

## Spline interpolation (樣條插值)

---

### Disadvantages of

- *Lagrange interpolating polynomial*: oscillation of high-degree polynomial.
- *Piecewise linear approximation*: no assurance of differentiability at each endpoints of the subintervals.
- *Piecewise Hermite interpolating polynomial  $H_3(x)$  of degree 3*:  $f'(x_0), f'(x_1), \dots, f'(x_n)$  are usually not available.

### Our goals:

- piecewise polynomial;
- no derivative information, except perhaps at  $x_0 (= a)$  and  $x_n (= b)$ ;
- $\in C^1[a, b]$ .

$\implies$  **spline interpolation**

## Quadratic spline

---

Let  $f$  be defined on  $[x_0, x_2]$ . Given  $f(x_0)$ ,  $f(x_1)$  and  $f(x_2)$ , a quadratic spline function  $S$  consists of the quadratic polynomials:

$$\begin{aligned} S_0(x) &= a_0 + b_0(x - x_0) + c_0(x - x_0)^2 && \text{on } [x_0, x_1], \\ S_1(x) &= a_1 + b_1(x - x_1) + c_1(x - x_1)^2 && \text{on } [x_1, x_2] \end{aligned}$$

such that

- (1)  $S(x_0) = f(x_0)$ ,  $S(x_1) = f(x_1)$  and  $S(x_2) = f(x_2)$ ;
- (2)  $S \in C^1[x_0, x_2]$ .

## Quadratic spline (cont'd)

---

- ① From condition (1), we have

$$\begin{aligned}a_0 &= f(x_0), \\a_0 + b_0(x_1 - x_0) + c_0(x_1 - x_0)^2 &= f(x_1), \\a_1 &= f(x_1), \\a_1 + b_1(x_2 - x_1) + c_1(x_2 - x_1)^2 &= f(x_2).\end{aligned}$$

- ② From condition (2), we have  $S'_0(x_1) = S'_1(x_1)$ .  
 $\therefore S'_0(x) = b_0 + 2c_0(x - x_0)$  and  $S'_1(x) = b_1 + 2c_1(x - x_1)$ .  
 $\therefore b_0 + 2c_0(x_1 - x_0) = b_1$ .
- ③ 6 unknowns, 5 equations  $\implies$  flexibility exists.
- ④ If we require  $S \in C^2[x_0, x_2]$ , then  $S''_0(x_1) = 2c_0, S''_1(x_1) = 2c_1$   
 $\implies c_0 = c_1 \implies$  5 unknowns and 5 equations  
 $\implies$  a solution may not exist!

## Cubic spline $\in C^2[x_0, x_n]$

① **Disadvantage:** the derivatives of the interpolant may not agree with the function  $f(x)$ , even at the nodes  $x_0, x_1, \dots, x_n$ .

② **Definition:** given  $a = x_0 < x_1 < \dots < x_{n-1} < x_n = b$  and a set of function values  $f(x_0), f(x_1), \dots, f(x_n)$ , a cubic spline interpolant  $S$  for  $f$  is a function that satisfies

(1)  $S|_{[x_j, x_{j+1}]}$  is a cubic polynomial for  $j = 0, 1, \dots, n-1$ ,

denoted by  $S|_{[x_j, x_{j+1}]}(x) = S_j(x)$ ;

(2)  $S(x_j) = f(x_j)$ ,  $j = 0, 1, \dots, n$ ;

(3)  $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$ ,  $j = 0, 1, \dots, n-2$ ;

(4)  $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$ ,  $j = 0, 1, \dots, n-2$ ;

(5)  $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$ ,  $j = 0, 1, \dots, n-2$ ;

(6) one of the following is satisfied:

(i)  $S''(x_0) = S''(x_n) = 0$ , free or natural boundary conditions  $\Rightarrow$  natural spline;

(ii)  $S'(x_0) = f'(x_0)$ ,  $S'(x_n) = f'(x_n)$ , clamped boundary conditions  $\Rightarrow$  clamped spline.

## Cubic spline (cont'd)

- Condition (1)  $\Rightarrow$  denote

$$S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3, j = 0 : n - 1.$$

- Condition (2)  $\Rightarrow S_j(x_j) = a_j = f(x_j)$  (given),  $j = 0 : n - 1$ .

Define  $a_n := S_{n-1}(x_n) = f(x_n)$  (given).

- Condition (3)  $\Rightarrow a_{j+1} = S_{j+1}(x_{j+1}) = S_j(x_{j+1}) = a_j + b_j(x_{j+1} - x_j) + c_j(x_{j+1} - x_j)^2 + d_j(x_{j+1} - x_j)^3, j = 0 : n - 2$ .

Define  $h_j = x_{j+1} - x_j, j = 0 : n - 1$ .

$$\Rightarrow a_{j+1} = a_j + b_j h_j + c_j h_j^2 + d_j h_j^3, j = 0 : n - 2.$$

$$\because a_n = f(x_n) = S_{n-1}(x_n) =$$

$$a_{n-1} + b_{n-1}(x_n - x_{n-1}) + c_{n-1}(x_n - x_{n-1})^2 + d_{n-1}(x_n - x_{n-1})^3.$$

$$\therefore a_n = a_{n-1} + b_{n-1}h_{n-1} + c_{n-1}h_{n-1}^2 + d_{n-1}h_{n-1}^3.$$

$$\Rightarrow a_{j+1} = a_j + b_j h_j + c_j h_j^2 + d_j h_j^3, j = 0 : n - 1. \leftarrow (3.15)$$

## Cubic spline (cont'd)

---

Define  $b_n := S'(x_n) = S'_{n-1}(x_n)$ .

$$\because S'_j(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2, j = 0 : n - 1.$$

$$\Rightarrow S'_j(x_j) = b_j, j = 0 : n - 1.$$

Condition (4)  $\Rightarrow$

$$b_{j+1} = S'_{j+1}(x_{j+1}) = S'_j(x_{j+1}) = b_j + 2c_j h_j + 3d_j h_j^2, j = 0 : n - 2.$$

$$\begin{aligned} \because b_n &= S'_{n-1}(x_n) = b_{n-1} + 2c_{n-1}(x_n - x_{n-1}) + 3d_{n-1}(x_n - x_{n-1})^2 \\ &= b_{n-1} + 2c_{n-1}h_{n-1} + 3d_{n-1}h_{n-1}^2. \end{aligned}$$

$$\therefore b_{j+1} = b_j + 2c_j h_j + 3d_j h_j^2, j = 0 : n - 1. \leftarrow (3.16)$$

## Cubic spline (cont'd)

---

$$\because S_j''(x) = 2c_j + 6d_j(x - x_j), j = 0 : n - 1.$$

$$\Rightarrow S_j''(x_j) = 2c_j, j = 0 : n - 1.$$

$$\text{Define } c_n := \frac{1}{2}S_{n-1}''(x_n) = \frac{1}{2}(2c_{n-1} + 6d_{n-1}(x_n - x_{n-1})) = \frac{1}{2}(2c_{n-1} + 6d_{n-1}h_{n-1}).$$

$$\text{Condition (5): } S_{j+1}''(x_{j+1}) = S_j''(x_{j+1}), j = 0 : n - 2.$$

$$\Rightarrow 2c_{j+1} = 2c_j + 6d_j h_j, j = 0 : n - 2.$$

$$\Rightarrow c_{j+1} = c_j + 3d_j h_j, j = 0 : n - 2.$$

$$\Rightarrow c_{j+1} = c_j + 3d_j h_j, j = 0 : n - 1. \leftarrow (3.17)$$

## Cubic spline (cont'd)

$$(3.17) \Rightarrow d_j = \frac{1}{3h_j}(c_{j+1} - c_j), j = 0 : n - 1.$$

$$(3.15) \Rightarrow$$

$$a_{j+1} = a_j + b_j h_j + c_j h_j^2 + \frac{1}{3h_j}(c_{j+1} - c_j)h_j^3 = a_j + b_j h_j + \frac{h_j^2}{3}(2c_j + c_{j+1}),$$
$$j = 0 : n - 1. \leftarrow (3.18)$$

$$(3.16) \Rightarrow b_{j+1} = b_j + 2c_j h_j + 3 \frac{1}{3h_j}(c_{j+1} - c_j)h_j^2 = b_j + h_j(c_j + c_{j+1}),$$
$$j = 0 : n - 1. \leftarrow (3.19)$$

$$(3.18) \Rightarrow b_j h_j = (a_{j+1} - a_j) - \frac{h_j^2}{3}(2c_j + c_{j+1}), j = 0 : n - 1.$$

$$\Rightarrow b_j = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}), j = 0 : n - 1. \leftarrow (3.20)$$

$$\Rightarrow b_{j-1} = \frac{1}{h_{j-1}}(a_j - a_{j-1}) - \frac{h_{j-1}}{3}(2c_{j-1} + c_j), j = 1 : n.$$

$$\text{Similarly, } (3.19) \Rightarrow b_j = b_{j-1} + h_{j-1}(c_{j-1} + c_j), j = 1 : n. \leftarrow (\star)$$

## Cubic spline (cont'd)

---

Combining  $(\star)$  and (3.20) with the common index  $j = 1 : n - 1$ , we have

$$\begin{aligned} & \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}) = \\ & \frac{1}{h_{j-1}}(a_j - a_{j-1}) - \frac{h_{j-1}}{3}(2c_{j-1} + c_j) + h_{j-1}(c_{j-1} + c_j), j = 1 : n - 1. \\ \Rightarrow & h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_jc_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}), \\ & j = 1 : n - 1. \leftarrow (3.21) \end{aligned}$$

Consider (3.21), we have  $n + 1$  unknowns  $\{c_j\}_{j=0}^n$  and  $n - 1$  equations.

If we impose Condition 6 (i), natural boundary conditions,  $c_0 = 0$  and  $c_n = 0 \Rightarrow n - 1$  unknowns  $\{c_j\}_{j=1}^{n-1}$  and  $n - 1$  equations.

The resulting linear system is strictly diagonally dominant  
 $\Rightarrow \exists$  **unique natural spline.**

## Cubic spline (cont'd)

If we impose Condition 6 (ii), clamped boundary conditions,  $S'(x_0) = f'(x_0) (= b_0)$  and  $S'(x_n) = f'(x_n)$ .

$$(3.20) \text{ with } j = 0 \Rightarrow b_0 = \frac{1}{h_0}(a_1 - a_0) - \frac{h_0}{3}(2c_0 + c_1).$$

$$\Rightarrow 3b_0 - \frac{3}{h_0}(a_1 - a_0) = -h_0(2c_0 + c_1).$$

$$\Rightarrow 2h_0c_0 + h_0c_1 = \frac{3}{h_0}(a_1 - a_0) - 3b_0, b_0 = f'(x_0). \text{ (Additional Eqn1)}$$

$$(3.19) \Rightarrow S'(x_n) = f'(x_n) := b_n = b_{n-1} + h_{n-1}(c_{n-1} + c_n).$$

$$(3.20) \text{ with } j = n - 1 \Rightarrow$$

$$f'(x_n) := b_n = \frac{1}{h_{n-1}}(a_n - a_{n-1}) - \frac{1}{3}h_{n-1}(2c_{n-1} + c_n) + h_{n-1}(c_{n-1} + c_n).$$

$$\Rightarrow f'(x_n) := b_n = \frac{1}{h_{n-1}}(a_n - a_{n-1}) + \frac{1}{3}h_{n-1}(c_{n-1} + 2c_n).$$

$$\Rightarrow h_{n-1}c_{n-1} + 2h_{n-1}c_n = 3f'(x_n) - \frac{3}{h_{n-1}}(a_n - a_{n-1}). \text{ (Additional Eqn2)}$$

$$\Rightarrow n + 1 \text{ unknowns } \{c_j\}_{j=0}^n \text{ and } n + 1 \text{ equations.}$$

The resulting linear system is strictly diagonally dominant

$\Rightarrow \exists$  **unique clamped spline.**