MA 3021: Numerical Analysis I
Interpolation and Polynomial Approximation

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Interpolation

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

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

- **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., $\overline{\mathcal{P}} = C[a,b]$.

- **Why not Taylor polynomials?**
  - need to calculate $f'(x), f''(x), \cdots$
  - accurate near at a specific point, not on entire interval.

Polynomial interpolation

- 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

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

- Such a polynomial is said to interpolate the data.

Lagrange polynomial

- Given $(x_0, f(x_0))$ and $(x_1, f(x_1))$, $x_0 \neq x_1$.

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

  Then *degree* $p(x) \leq 1$ and $p(x_0) = f(x_0)$, $p(x_1) = f(x_1)$.
- Given $n+1$ distinct numbers $x_0, x_1, \cdots, x_n$. For each $k = 0, 1, \cdots, n$, 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 $k = 0, 1, \cdots, n$,

$$\begin{aligned} L_{n,k}(x) &= \frac{(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0)(x_k - x_1) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)} \\ &= \prod_{i=0, i \neq k}^{n} \frac{x - x_i}{x_k - x_i}. \end{aligned}$$

Theorem on polynomial interpolation

Given $n+1$ distinct real (or complex) numbers $x_0, x_1, \cdots, x_n$ and their function values $f(x_0), f(x_1), \cdots, f(x_n)$. Then $\exists!$ polynomial $p(x)$, degree $p(x) \le n$, such that

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

In fact,

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

(The n-th Lagrange interpolating polynomial)

Proof. (uniqueness) Assume that

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n.$$

The interpolation conditions, $p(x_k) = f(x_k)$ for $0 \le k \le n$, 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 $\det X = \prod_{0 \le i < j \le n}(x_j - x_i) \neq 0$, (but is often ill conditioned.)

Example

- **Notation:** $L_k(x) := L_{n,k}(x)$ when there is no confusion.
- **Example:** $x_0 = 2, f(x_0) = 0.5, x_1 = 2.5, f(x_1) = 0.4, x_2 = 4, f(x_2) = 0.25$ (in fact, $f(x) = 1/x$). Find the second ($n = 2$) Lagrange interpolating polynomial.

$$
\begin{aligned}
L_{2,0}(x) &= L_0(x) = \frac{(x-2.5)(x-4)}{(2-2.5)(2-4)} = \frac{x^2-6.5x+10}{1}, \\
L_{2,1}(x) &= L_1(x) = \frac{(x-2)(x-4)}{(2.5-2)(2.5-4)} = \frac{x^2-6x+8}{-0.75}, \\
L_{2,2}(x) &= L_2(x) = \frac{(x-2)(x-2.5)}{(4-2)(4-2.5)} = \frac{x^2-4.5x+5}{3}. \\
\therefore p(x) &= 0.5\left(\frac{x^2-6.5x+10}{1}\right) + 0.4\left(\frac{x^2-6x+8}{-0.75}\right) + 0.25\left(\frac{x^2-4.5x+5}{3}\right) \\
&= 0.05x^2 - 0.425x + 1.15. \\
\therefore \frac{1}{3} &= f(3) \approx p(3) = 0.325.
\end{aligned}
$$

Theorem on polynomial interpolation error

Let f be a given real-valued function in $C^{n+1}[a,b]$. Let $x_0, x_1, \cdots, x_n \in [a,b]$ 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. Given $x \in [a,b]$. If $x = x_k$ for some $0 \le k \le n$. Then the assertion holds. Let $x \neq x_k$ for any $k = 0, 1, \cdots, n$. Define $g : [a,b] \to \mathbb{R}$ by

$$\begin{aligned} g(t) &= f(t) - p(t) - \lambda w(t) \qquad \text{(function in } t\text{)}, \\ \lambda &= \frac{f(x) - p(x)}{w(x)} \qquad \text{(a constant that makes } g(x) = 0\text{)}, \\ w(t) &= \prod_{i=0}^{n} (t - x_i) \qquad \text{(polynomial in } t\text{)}. \end{aligned}$$

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

Theorem on polynomial interpolation error (continued)

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

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

This completes the proof.

Example

$f(x) = e^x, x \in [0,1]$.

Let $x_0, x_1, \cdots, x_n$ be a uniform partition of $[0,1]$ with step size $h = 1/n$.

Consider $[x_j, x_{j+1}]$ for some $0 \le j \le n-1$. Let $p(x)$ be the first Lagrange interpolating polynomial on $[x_j, x_{j+1}]$.

Then for $x \in [x_j, x_{j+1}]$,

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

If $|f(x) - p(x)| \le (eh^2)/8 \le 10^{-6}$ then $h < 1.72 \times 10^{-3}$. We can choose $h = 0.001$.

Divided differences

- Let f be a function whose values are known at points (nodes) $x_0, x_1, \cdots, x_n$.
- We assume that these nodes are distinct, but they need not be ordered.
- 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 $1, x, x^2, \cdots, x^n$.

Divided differences (continued)

We should use the Newton form of the interpolating polynomial:

$$
\begin{aligned}
q_0(x) &= 1, \\
q_1(x) &= (x - x_0), \\
q_2(x) &= (x - x_0)(x - x_1), \\
q_3(x) &= (x - x_0)(x - x_1)(x - x_2), \\
&\vdots \\
q_n(x) &= (x - x_0)(x - x_1)(x - x_2)\cdots(x - x_{n-1}).
\end{aligned}
$$

Then the nth Lagrange interpolating polynomial p can be expressed as

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

Divided differences (continued)

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

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

- The elements of the coefficient matrix are

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

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

$$q_j(x) = \prod_{k=0}^{j-1} (x - x_k).$$

$$\Longrightarrow \quad a_{ij} = q_j(x_i) = \prod_{k=0}^{j-1} (x_i - x_k) = 0 \quad \text{if } i \le j-1.$$

Divided differences (continued)

- For example, consider the case of three nodes with

$$\begin{aligned} p(x) &= c_0 q_0(x) + c_1 q_1(x) + c_2 q_2(x) \\ &= c_0 + c_1(x - x_0) + c_2(x - x_0)(x - x_1). \end{aligned}$$

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

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

- Thus, c_n depends on f at $x_0, x_1, \cdots, x_n$, and define the notation

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

The expressions $f[x_0, x_1, \cdots, x_n]$ are called divided differences of f.

Divided differences (continued)

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

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

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

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

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

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

($\because$ same values at $x_0, x_1, \cdots, x_n$ and same degree $\leq n$)
Examining the coefficient of x^n on the both sides, we arrive at the assertion.

Table of divided differences

- 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:

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

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

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

- 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.

x_i	$f[x_i]$	$f[x_i, x_{i+1}]$	$f[x_i, \cdots, x_{i+2}]$	$f[x_i, \cdots, x_{i+3}]$	$f[x_i, \cdots, x_{i+4}]$
$x_0 = 1.0$	0.7651977	-0.4837057	-0.1087339	0.0658784	0.0018251
$x_1 = 1.3$	0.6200860	-0.5489460	-0.0494433	0.0680685	
$x_2 = 1.6$	0.4454022	-0.5786120	0.0118183		
$x_3 = 1.9$	0.2818186	-0.5715210			
$x_4 = 2.2$	0.1103623				

- The Newton interpolatory divided-difference formula can be written as

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

Properties of divided differences

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

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

Proof.

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

Osculating polynomial

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

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

- **Note:**
  - 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 $i = 0, 1, \cdots, n$, then $p(x) = n$-th Lagrange interpolating polynomial of $f(x)$ at $x_0, x_1, \cdots, x_n$.
  - If $m_i = 1$ for $i = 0, 1, \cdots, n$, then $p(x)$ is the Hermite interpolating polynomial.

Theorem on the Hermite interpolation

Let $x_0, x_1, \cdots, x_n \in [a, b]$ 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 $x_0, x_1, \cdots, x_n$ 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

$$\begin{aligned} H_{n,j}(x) &= \Big(1 - 2(x - x_j) L'_{n,j}(x_j)\Big) L^2_{n,j}(x), \\ \widehat{H}_{n,j}(x) &= (x - x_j) L^2_{n,j}(x), \\ L_{n,j}(x) &= \frac{(x - x_0)(x - x_1)\cdots(x - x_{j-1})(x - x_{j+1})\cdots(x - x_n)}{(x_j - x_0)(x_j - x_1)\cdots(x_j - x_{j-1})(x_j - x_{j+1})\cdots(x_j - x_n)}. \end{aligned}$$

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

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

Proof of the existence

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

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

  $$H_{n,i}(x_i) = \Big(1 - 2(x_i - x_i)L'_{n,i}(x_i)\Big)L^2_{n,i}(x_i) = \Big(1 - 2(x_i - x_i)L'_{n,i}(x_i)\Big) = 1.$$

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

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

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

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

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

Proof of the existence (continued)

If $i = j$ then

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

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

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

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

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

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

$\therefore H_{2n+1}(x)$ agrees with $f(x)$ and $H'_{2n+1}(x)$ agrees with $f'(x)$ at $x_0, x_1, \cdots, x_n$.

Note: For the uniqueness and the error estimate, see page 137, Exercise # 11 (a)(b).

Example

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

$$
\begin{aligned}
L_{2,0}(x) &= \frac{(x-1.6)(x-1.9)}{(-0.3)(-0.6)} = \frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9}, \\
L'_{2,0}(x) &= \frac{100}{9}x - \frac{175}{9}; \\
L_{2,1}(x) &= \frac{(x-1.3)(x-1.9)}{(0.3)(-0.3)} = -\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9}, \\
L'_{2,1}(x) &= -\frac{200}{9}x + \frac{320}{9}; \\
L_{2,2}(x) &= \frac{(x-1.3)(x-1.6)}{(0.6)(0.3)} = \frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9}, \\
L'_{2,2}(x) &= \frac{100}{9}x - \frac{145}{9}.
\end{aligned}
$$

Example (continued)

$$
\begin{aligned}
H_{2,0}(x) &= (10x-12)(\frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9})^2, \\
H_{2,1}(x) &= 1(-\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9})^2, \\
H_{2,2}(x) &= 10(2-x)(\frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9})^2, \\
\widehat{H}_{2,0}(x) &= (x-1.3)(\frac{50}{9}x^2 - \frac{175}{9}x + \frac{152}{9})^2, \\
\widehat{H}_{2,1}(x) &= (x-1.6)(-\frac{100}{9}x^2 + \frac{320}{9}x - \frac{247}{9})^2, \\
\widehat{H}_{2,2}(x) &= (x-1.9)(\frac{50}{9}x^2 - \frac{145}{9}x + \frac{104}{9})^2.
\end{aligned}
$$

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

Divided-difference formula

- The Newton interpolatory divided-difference formula for the nth Lagrange polynomial at distinct numbers $x_0, x_1, \cdots, x_n$ is given by

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

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

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

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

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

Spline interpolation

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:** $f'(x_0), f'(x_1), \cdots, f'(x_n)$ are usually not available.

Goal:

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

$\Longrightarrow$ **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:

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

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 (continued)

- From condition (1), we have

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

- From condition (2), we have $S_0'(x_1) = S_1'(x_1)$.

  $\because S_0'(x) = b_0 + 2c_0(x - x_0)$ and $S_1'(x) = b_1 + 2c_1(x - x_1)$.

  $\therefore b_0 + 2c_0(x_1 - x_0) = b_1$.
- 6 unknowns, 5 equations $\Longrightarrow$ flexibility exists.
- If we require $S \in C^2[x_0, x_2]$, then $S_0''(x_1) = 2c_0, S_1''(x_1) = 2c_1 \Longrightarrow c_0 = c_1$

  $\Longrightarrow$ 5 unknowns and 5 equations $\Longrightarrow$ a solution may not exist!

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

- **Disadvantage:** the derivatives of the interpolant may not agree with the function $f(x)$, even at the nodes $x_0, x_1, \cdots, x_n$.
- **Definition:** Given $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$ and a set of function values $f(x_0), f(x_1), \cdots, f(x_n)$. A cubic spline interpolant S for f is a function that satisfies
  1. $S|_{[x_j, x_{j+1}]}$ is a cubic polynomial for $j = 0, 1, \cdots, n-1$ (denote $S|_{[x_j, x_{j+1}]}(x) = S_j(x)$);
  2. $S(x_j) = f(x_j)$, $j = 0, 1, \cdots, n$;
  3. $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$, $j = 0, 1, \cdots, n-2$;
  4. $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$, $j = 0, 1, \cdots, n-2$;
  5. $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$, $j = 0, 1, \cdots, n-2$;
  6. one of the following is satisfied:
     - $S''(x_0) = S''(x_n) = 0$, free or natural boundary conditions $\Rightarrow$ natural spline;
     - $S'(x_0) = f'(x_0), S'(x_n) = f'(x_n)$, clamped boundary conditions $\Rightarrow$ clamped spline.

Cubic spline (continued)

- Condition (1) $\Rightarrow$ denote $S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$, $j = 0, 1, \cdots, n-1$.
- Condition (2) $\Rightarrow$ $S_j(x_j) = a_j = f(x_j)$ (given), $j = 0, 1, \cdots, n-1$. Define $a_n := S_{n-1}(x_n) = f(x_n)$ (given).
- Condition (3) $\Rightarrow$ $a_{j+1} = S_{j+1}(x_{j+1}) = S_j(x_{j+1}) = a_j + b_j(x_{j+1} - x_j) + c_j(x_{j+1} - x_j)^2 + d_j(x_{j+1} - x_j)^3$, $j = 0, 1, \cdots, n-2$.

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

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

  $\because a_n = f(x_n) = S_{n-1}(x_n) = a_{n-1} + b_{n-1}(x_n - x_{n-1}) + c_{n-1}(x_n - x_{n-1})^2 + d_{n-1}(x_n - x_{n-1})^3$.

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

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

Cubic spline (continued)

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

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

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

Condition (4) $\Rightarrow b_{j+1} = S'_{j+1}(x_{j+1}) = S'_j(x_{j+1}) = b_j + 2c_j h_j + 3d_j h_j^2$, $j = 0, 1, \cdots, n-2$.

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

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

Cubic spline (continued)

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

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

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

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

$\Rightarrow 2c_{j+1} = 2c_j + 6d_jh_j$, $j = 0, 1, \cdots, n-2$.

$\Rightarrow c_{j+1} = c_j + 3d_jh_j$, $j = 0, 1, \cdots, n-2$.

$\Rightarrow c_{j+1} = c_j + 3d_jh_j$, $j = 0, 1, \cdots, n-2, n-1$. $\leftarrow$ (3.17)

Cubic spline (continued)

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

$(3.15) \Rightarrow$

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

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

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

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

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

Similarly, $(3.19) \Rightarrow b_j = b_{j-1} + h_{j-1}(c_{j-1} + c_j),\ j = 1, 2, \cdots, n. \leftarrow (*)$

Cubic spline (continued)

Combining (*) and (3.20) with the common index $j = 1, 2, \cdots, n-1$, we have

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

$$\Rightarrow h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_j c_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}),$$
$j = 1, 2, \cdots, n-1.$ $\leftarrow$ (3.21)

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 (continued)

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

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

$\Rightarrow 2h_0c_0 + h_0c_1 = \frac{3}{h_0}(a_1 - a_0) - 3b_0. \qquad (b_0 = f'(x_0)) \leftarrow$ (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) with $j = n - 1 \Rightarrow$
$f'(x_n) := b_n = \frac{1}{h_{n-1}}(a_n - a_{n-1}) - \frac{1}{3}h_{n-1}(2c_{n-1} + c_n) + h_{n-1}(c_{n-1} + c_n)$.

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

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

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

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