

Interpolation and Polynomial Approximation

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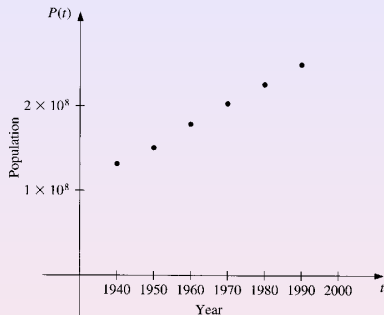


Outline

- 1 Interpolation and the Lagrange polynomial
- 2 Divided Differences
- 3 Hermite Interpolation
- 4 Cubic spline interpolation



Introduction



Question

In reviewing these data, how to provide a reasonable estimate of the population, say, in 1965, or even in 2010.



Interpolation

Suppose we do not know the function f , but a few information (data) about f , now we try to compute a function g that approximates f .

Theorem (Weierstrass Approximation Theorem)

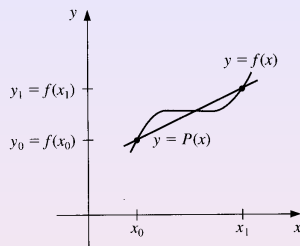
Suppose that f is defined and continuous on $[a, b]$. For any $\varepsilon > 0$, there exists a polynomial $P(x)$, defined on $[a, b]$, with the property that

$$|f(x) - P(x)| < \varepsilon, \quad \text{for all } x \text{ in } [a, b].$$

Reason for using polynomial

- 1 They uniformly approximate continuous function (Weierstrass Theorem)
- 2 The derivatives and indefinite integral of a polynomial are easy to determine and are also polynomials.

Interpolation and the Lagrange polynomial



Property

The linear function passing through $(x_0, f(x_0))$ and $(x_1, f(x_1))$ is unique.

Let

$$L_0(x) = \frac{x - x_1}{x_0 - x_1}, \quad L_1(x) = \frac{x - x_0}{x_1 - x_0}$$

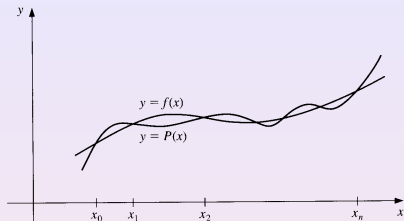
and

$$P(x) = L_0(x)f(x_0) + L_1(x)f(x_1).$$

Then

$$P(x_0) = f(x_0), \quad P(x_1) = f(x_1).$$





Question

How to find the polynomial of degree n that passes through $(x_0, f(x_0)), \dots, (x_n, f(x_n))$?

Theorem

If (x_i, y_i) , $x_i, y_i \in \mathbb{R}$, $i = 0, 1, \dots, n$, are $n + 1$ distinct pairs of data point, then there is a unique polynomial P_n of degree at most n such that

$$P_n(x_i) = y_i, \quad (0 \leq i \leq n). \quad (1)$$



Proof of Existence (by mathematical induction)

- 1 The theorem clearly holds for $n = 0$ (only one data point (x_0, y_0)) since one may choose the constant polynomial $P_0(x) = y_0$ for all x .
- 2 Assume that the theorem holds for $n \leq k$, that is, there is a polynomial P_k , $\deg(P_k) \leq k$, such that $y_i = P_k(x_i)$, for $0 \leq i \leq k$.
- 3 Next we try to construct a polynomial of degree at most $k + 1$ to interpolate (x_i, y_i) , $0 \leq i \leq k + 1$. Let

$$P_{k+1}(x) = P_k(x) + c(x - x_0)(x - x_1) \cdots (x - x_k),$$

where

$$c = \frac{y_{k+1} - P_k(x_{k+1})}{(x_{k+1} - x_0)(x_{k+1} - x_1) \cdots (x_{k+1} - x_k)}.$$

Since x_i are distinct, the polynomial $P_{k+1}(x)$ is well-defined and $\deg(P_{k+1}) \leq k + 1$. It is easy to verify that

$$P_{k+1}(x_i) = y_i, \quad 0 \leq i \leq k + 1.$$



Proof of Uniqueness

Suppose there are two such polynomials P_n and Q_n satisfying (1). Define

$$S_n(x) = P_n(x) - Q_n(x).$$

Since both $\deg(P_n) \leq n$ and $\deg(Q_n) \leq n$, $\deg(S_n) \leq n$. Moreover

$$S_n(x_i) = P_n(x_i) - Q_n(x_i) = y_i - y_i = 0,$$

for $0 \leq i \leq n$. This means that S_n has at least $n + 1$ zeros, it therefore must be $S_n = 0$. Hence $P_n = Q_n$. □



Idea

Construct polynomial $P(x)$ with $\deg(P) \leq n$ as

$$P(x) = L_{n,0}(x)f(x_0) + \cdots + L_{n,n}(x)f(x_n),$$

where

- 1 $L_{n,k}(x)$ are polynomial with degree n for $0 \leq k \leq n$.
- 2 $L_{n,k}(x_k) = 1$ and $L_{n,k}(x_i) = 0$ for $i \neq k$.

Then

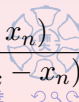
$$P(x_k) = f(x_k) \quad \text{for } k = 0, 1, \dots, n.$$

- 1 $\deg(L_{n,k}) = n$ and $L_{n,k}(x_i) = 0$ for $i \neq k$:

$$L_{n,k}(x) = c_k(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)$$

- 2 $L_{n,k}(x_k) = 1$:

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



Theorem

If x_0, x_1, \dots, x_n are $n + 1$ distinct numbers and f is a function whose values are given at these numbers, then a unique polynomial of degree at most n exists with

$$f(x_k) = P(x_k), \quad \text{for } k = 0, 1, \dots, n.$$

This polynomial is given by

$$P(x) = \sum_{k=0}^n f(x_k) L_{n,k}(x)$$

which is called the n th Lagrange interpolating polynomial.

Note that we will write $L_{n,k}(x)$ simply as $L_k(x)$ when there is no confusion as to its degree.



Example

Given the following 4 data points,

x_i	0	1	3	5
y_i	1	2	6	7

find a polynomial in Lagrange form to interpolate these data.

Solution: The interpolating polynomial in the Lagrange form is

$$P_3(x) = L_0(x) + 2L_1(x) + 6L_2(x) + 7L_3(x) \quad \text{with}$$

$$L_0(x) = \frac{(x-1)(x-3)(x-5)}{(0-1)(0-3)(0-5)} = -\frac{1}{15}(x-1)(x-3)(x-5),$$

$$L_1(x) = \frac{(x-0)(x-3)(x-5)}{(1-0)(1-3)(1-5)} = \frac{1}{8}x(x-3)(x-5),$$

$$L_2(x) = \frac{(x-0)(x-1)(x-5)}{(3-0)(3-1)(3-5)} = -\frac{1}{12}x(x-1)(x-5),$$

$$L_3(x) = \frac{(x-0)(x-1)(x-3)}{(5-0)(5-1)(5-3)} = \frac{1}{40}x(x-1)(x-3).$$



Question

What's the error involved in approximating $f(x)$ by the interpolating polynomial $P(x)$?

Theorem

Suppose

- 1 x_0, \dots, x_n are distinct numbers in $[a, b]$,
- 2 $f \in C^{n+1}[a, b]$.

Then, $\forall x \in [a, b]$, $\exists \xi(x) \in (a, b)$ such that

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

Proof: If $x = x_k$, for any $k = 0, 1, \dots, n$, then $f(x_k) = P(x_k)$ and (2) is satisfied.



If $x \neq x_k$, for all $k = 0, 1, \dots, n$, define

$$g(t) = f(t) - P(t) - [f(x) - P(x)] \prod_{i=0}^n \frac{t - x_i}{x - x_i}.$$

Since $f \in C^{n+1}[a, b]$ and $P \in C^\infty[a, b]$, it follows that $g \in C^{n+1}[a, b]$.
Since

$$g(x_k) = [f(x_k) - P(x_k)] - [f(x) - P(x)] \prod_{i=0}^n \frac{x_k - x_i}{x - x_i} = 0,$$

and

$$g(x) = [f(x) - P(x)] - [f(x) - P(x)] \prod_{i=0}^n \frac{x - x_i}{x - x_i} = 0,$$

it implies that g is zero at x, x_0, x_1, \dots, x_n . By the Generalized Rolle's Theorem, $\exists \xi \in (a, b)$ such that $g^{n+1}(\xi) = 0$. That is



$$\begin{aligned}
 0 &= g^{(n+1)}(\xi) \\
 &= f^{(n+1)}(\xi) - P^{(n+1)}(\xi) - [f(x) - P(x)] \frac{d^{n+1}}{dt^{n+1}} \left[\prod_{i=0}^n \frac{(t - x_i)}{(x - x_i)} \right]_{t=\xi}.
 \end{aligned} \tag{3}$$

Since $\deg(P) \leq n$, it implies that $P^{(n+1)}(\xi) = 0$. On the other hand, $\prod_{i=0}^n [(t - x_i)/(x - x_i)]$ is a polynomial of degree $(n + 1)$, so

$$\prod_{i=0}^n \frac{(t - x_i)}{(x - x_i)} = \left[\frac{1}{\prod_{i=0}^n (x - x_i)} \right] t^{n+1} + (\text{lower-degree terms in } t),$$

and

$$\frac{d^{n+1}}{dt^{n+1}} \left[\prod_{i=0}^n \frac{(t - x_i)}{(x - x_i)} \right] = \frac{(n + 1)!}{\prod_{i=0}^n (x - x_i)}.$$



Equation (3) becomes

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

i.e.,

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



Example

- 1 Goal: Prepare a table for the function $f(x) = e^x$ for $x \in [0, 1]$.
- 2 $x_{j+1} - x_j = h$ for $j = 0, 1, \dots, n-1$.
- 3 What should h be for linear interpolation to give an absolute error of at most 10^{-6} ?



Suppose $x \in [x_j, x_{j+1}]$. Equation (2) implies that

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



Let

$$g(x) = (x - jh)(x - (j + 1)h), \quad \text{for } jh \leq x \leq (j + 1)h.$$

Then

$$\max_{x_j \leq x \leq x_{j+1}} |g(x)| = \left| g \left(\left(j + \frac{1}{2} \right) h \right) \right| = \frac{h^2}{4}.$$

Consequently,

$$|f(x) - P(x)| \leq \frac{eh^2}{8} \leq 10^{-6},$$

which implies that

$$h < 1.72 \times 10^{-3}.$$

Since $n = (1 - 0)/h$ must be an integer, one logical choice for the step size is $h = 0.001$.



Difficulty for the Lagrange interpolation

- 1 If more data points are added to the interpolation problem, all the cardinal functions L_k have to be recalculated.
- 2 We shall now derive the interpolating polynomials in a manner that uses the previous calculations to greater advantage.

Definition

- 1 f is a function defined at x_0, x_1, \dots, x_n
- 2 Suppose that m_1, m_2, \dots, m_k are k distinct integers with $0 \leq m_i \leq n$ for each i .

The Lagrange polynomial that interpolates f at the k points $x_{m_1}, x_{m_2}, \dots, x_{m_k}$ is denoted $P_{m_1, m_2, \dots, m_k}(x)$.



Theorem

Let f be defined at distinct points x_0, x_1, \dots, x_k , and $0 \leq i, j \leq k$, $i \neq j$.
Then

$$P(x) = \frac{(x - x_j)}{(x_i - x_j)} P_{0,1,\dots,j-1,j+1,\dots,k}(x) - \frac{(x - x_i)}{(x_i - x_j)} P_{0,1,\dots,i-1,i+1,\dots,k}(x)$$

describes the k -th Lagrange polynomial that interpolates f at the $k + 1$ points x_0, x_1, \dots, x_k .

Proof: Since

$$\deg(P_{0,1,\dots,j-1,j+1,\dots,k}) \leq k - 1$$

and

$$\deg(P_{0,1,\dots,i-1,i+1,\dots,k}) \leq k - 1,$$

it implies that $\deg(P) \leq k$. If $0 \leq r \leq k$ and $r \neq i, j$, then



$$\begin{aligned}
 P(x_r) &= \frac{(x_r - x_j)}{(x_i - x_j)} P_{0,1,\dots,j-1,j+1,\dots,k}(x_r) - \frac{(x_r - x_i)}{(x_i - x_j)} P_{0,1,\dots,i-1,i+1,\dots,k}(x_r) \\
 &= \frac{(x_r - x_j)}{(x_i - x_j)} f(x_r) - \frac{(x_r - x_i)}{(x_i - x_j)} f(x_r) = f(x_r).
 \end{aligned}$$

Moreover

$$\begin{aligned}
 P(x_i) &= \frac{(x_i - x_j)}{(x_i - x_j)} P_{0,1,\dots,j-1,j+1,\dots,k}(x_i) - \frac{(x_i - x_i)}{(x_i - x_j)} P_{0,1,\dots,i-1,i+1,\dots,k}(x_i) \\
 &= f(x_i)
 \end{aligned}$$

and

$$\begin{aligned}
 P(x_j) &= \frac{(x_j - x_j)}{(x_i - x_j)} P_{0,1,\dots,j-1,j+1,\dots,k}(x_j) - \frac{(x_j - x_i)}{(x_i - x_j)} P_{0,1,\dots,i-1,i+1,\dots,k}(x_j) \\
 &= f(x_j).
 \end{aligned}$$

Therefore $P(x)$ agrees with f at all points x_0, x_1, \dots, x_k . By the uniqueness theorem, $P(x)$ is the k -th Lagrange polynomial that interpolates f at the $k + 1$ points x_0, x_1, \dots, x_k , i.e., $P \equiv P_{0,1,\dots,k}$.



Neville's method

The theorem implies that the Lagrange interpolating polynomial can be generated recursively. The procedure is called the Neville's method.

- 1 Denote

$$Q_{i,j} = P_{i-j,i-j+1,\dots,i-1,i}.$$

- 2 Hence $Q_{i,j}$, $0 \leq j \leq i$, denotes the interpolating polynomial of degree j on the $j + 1$ points $x_{i-j}, x_{i-j+1}, \dots, x_{i-1}, x_i$.
- 3 The polynomials can be computed in a manner as shown in the following table.

x_0	$P_0 = Q_{0,0}$					
x_1	$P_1 = Q_{1,0}$	$P_{0,1} = Q_{1,1}$				
x_2	$P_2 = Q_{2,0}$	$P_{1,2} = Q_{2,1}$	$P_{0,1,2} = Q_{2,2}$			
x_3	$P_3 = Q_{3,0}$	$P_{2,3} = Q_{3,1}$	$P_{1,2,3} = Q_{3,2}$	$P_{0,1,2,3} = Q_{3,3}$		
x_4	$P_4 = Q_{4,0}$	$P_{3,4} = Q_{4,1}$	$P_{2,3,4} = Q_{4,2}$	$P_{1,2,3,4} = Q_{4,3}$	$P_{0,1,2,3,4} = Q_{4,4}$	

x_0	$P_0 = Q_{0,0}$							
x_1	$P_1 = Q_{1,0}$	$P_{0,1} = Q_{1,1}$						
x_2	$P_2 = Q_{2,0}$	$P_{1,2} = Q_{2,1}$	$P_{0,1,2} = Q_{2,2}$					
x_3	$P_3 = Q_{3,0}$	$P_{2,3} = Q_{3,1}$	$P_{1,2,3} = Q_{3,2}$	$P_{0,1,2,3} = Q_{3,3}$				
x_4	$P_4 = Q_{4,0}$	$P_{3,4} = Q_{4,1}$	$P_{2,3,4} = Q_{4,2}$	$P_{1,2,3,4} = Q_{4,3}$	$P_{0,1,2,3,4} = Q_{4,4}$			

$$P_{0,1}(x) = \frac{(x - x_1)P_0(x) - (x - x_0)P_1(x)}{x_0 - x_1},$$

$$P_{1,2}(x) = \frac{(x - x_2)P_1(x) - (x - x_1)P_2(x)}{x_1 - x_2},$$

⋮

$$P_{0,1,2}(x) = \frac{(x - x_2)P_{0,1}(x) - (x - x_0)P_{1,2}(x)}{x_0 - x_2}$$

⋮



Example

Compute approximate value of $f(1.5)$ by using the following datas:

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



1 The first-degree approximation:

$$\begin{aligned} Q_{1,1}(1.5) &= \frac{(x - x_0)Q_{1,0} - (x - x_1)Q_{0,0}}{x_1 - x_0} \\ &= \frac{(1.5 - 1.0)Q_{1,0} - (1.5 - 1.3)Q_{0,0}}{1.3 - 1.0} = 0.5233449, \end{aligned}$$

$$\begin{aligned} Q_{2,1}(1.5) &= \frac{(x - x_1)Q_{2,0} - (x - x_2)Q_{1,0}}{x_2 - x_1} \\ &= \frac{(1.5 - 1.3)Q_{2,0} - (1.5 - 1.6)Q_{1,0}}{1.6 - 1.3} = 0.5102968, \end{aligned}$$

$$\begin{aligned} Q_{3,1}(1.5) &= \frac{(x - x_2)Q_{3,0} - (x - x_3)Q_{2,0}}{x_3 - x_2} \\ &= \frac{(1.5 - 1.6)Q_{3,0} - (1.5 - 1.9)Q_{2,0}}{1.9 - 1.6} = 0.5132634, \end{aligned}$$

$$\begin{aligned} Q_{4,1}(1.5) &= \frac{(x - x_3)Q_{4,0} - (x - x_4)Q_{3,0}}{x_4 - x_3} \\ &= \frac{(1.5 - 1.9)Q_{4,0} - (1.5 - 2.2)Q_{3,0}}{2.2 - 1.9} = 0.5104270. \end{aligned}$$



① The second-degree approximation:

$$\begin{aligned} Q_{2,2}(1.5) &= \frac{(x - x_1)Q_{2,1} - (x - x_2)Q_{1,1}}{x_2 - x_1} \\ &= \frac{(1.5 - 1.3)Q_{2,1} - (1.5 - 1.6)Q_{1,1}}{1.6 - 1.3} = 0.5124715, \end{aligned}$$

$$\begin{aligned} Q_{3,2}(1.5) &= \frac{(x - x_2)Q_{3,1} - (x - x_3)Q_{2,1}}{x_3 - x_2} \\ &= \frac{(1.5 - 1.6)Q_{3,1} - (1.5 - 1.9)Q_{2,1}}{1.9 - 1.6} = 0.5112857, \end{aligned}$$

$$\begin{aligned} Q_{4,2}(1.5) &= \frac{(x - x_3)Q_{4,1} - (x - x_4)Q_{3,1}}{x_4 - x_3} \\ &= \frac{(1.5 - 1.9)Q_{4,1} - (1.5 - 2.2)Q_{3,1}}{2.2 - 1.9} = 0.5137361. \end{aligned}$$



x	$f(x)$	1st-deg	2nd-deg	3rd-deg	4th-deg
1.0	0.7651977				
1.3	0.6200860	0.5233449			
1.6	0.4554022	0.5102968	0.5124715		
1.9	0.2818186	0.5132634	0.5112857	0.5118127	
2.2	0.1103623	0.5104270	0.5137361	0.5118302	0.5118200

Table: Results of the higher-degree approximations

x	$f(x)$	1st-deg	2nd-deg	3rd-deg	4th-deg	5th-deg
1.0	0.7651977					
1.3	0.6200860	0.5233449				
1.6	0.4554022	0.5102968	0.5124715			
1.9	0.2818186	0.5132634	0.5112857	0.5118127		
2.2	0.1103623	0.5104270	0.5137361	0.5118302	0.5118200	
2.5	-0.0483838	0.4807699	0.5301984	0.5119070	0.5118430	0.5118277

Table: Results of adding $(x_5, f(x_5))$



Divided Differences

- Neville's method: generate successively higher-degree polynomial approximations at a specific point.
- Divided-difference methods: successively generate the polynomials themselves.

Suppose that $P_n(x)$ is the n th Lagrange polynomial that agrees with f at distinct x_0, x_1, \dots, x_n . Express $P_n(x)$ in the form

$$P_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots + a_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}).$$

- Determine constant a_0 :

$$a_0 = P_n(x_0) = f(x_0)$$

- Determine a_1 :

$$f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1) \Rightarrow a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

- The zero divided difference of the function f with respect to x_i :

$$f[x_i] = f(x_i)$$

- The first divided difference of f with respect to x_i and x_{i+1} is denoted and defined as

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}.$$

- The second divided difference of f is defined as

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}.$$

- The k -th divided difference relative to $x_i, x_{i+1}, \dots, x_{i+k}$ is given by

$$f[x_i, x_{i+1}, \dots, x_{i+k}] = \frac{f[x_{i+1}, x_{i+2}, \dots, x_{i+k}] - f[x_i, x_{i+1}, \dots, x_{i+k-1}]}{x_{i+k} - x_i}$$



As might be expected from the evaluation of a_0, a_1, \dots, a_n in $P_n(x)$, the required coefficients are given by

$$a_k = f[x_0, x_1, \dots, x_k], \quad k = 0, 1, \dots, n.$$

Therefore $P_n(x)$ can be expressed as

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

This formula is known as the Newton's divided-difference formula.

x_i	$k = 0$	$k = 1$	$k = 2$	$k = 3$
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	$f[x_3]$			

Table: Outline for the generation of the divided differences



Example

Given the following 4 points ($n = 3$)

x_i	0	1	3	5
y_i	1	2	6	7

find a polynomial of degree 3 in Newton's form to interpolate these data.

Solution:

x_i	$k = 0$	$k = 1$	$k = 2$	$k = 3$
0	1			
		> 1		
1	2		$> \frac{1}{3}$	
		> 2		$> -\frac{17}{120}$
3	6		$> -\frac{3}{8}$	
		$> \frac{1}{2}$		
5	7			

So,

$$P(x) = 1 + x + \frac{1}{3}x(x-1) - \frac{17}{120}x(x-1)(x-3).$$



Theorem

Suppose $f \in C^n[a, b]$ and x_0, x_1, \dots, x_n are distinct numbers in $[a, b]$. Then there exists $\xi \in (a, b)$ such that

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}.$$

Proof: Define

$$g(x) = f(x) - P_n(x).$$

Since $P_n(x_i) = f(x_i)$ for $i = 0, 1, \dots, n$, g has $n + 1$ distinct zeros in $[a, b]$. By the generalized Rolle's Theorem, $\exists \xi \in (a, b)$ such that

$$0 = g^{(n)}(\xi) = f^{(n)}(\xi) - P_n^{(n)}(\xi).$$

Note that

$$P_n^{(n)}(x) = n!f[x_0, x_1, \dots, x_n].$$

As a consequence

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}.$$



Let

$$h = \frac{x_n - x_0}{n} = x_{i+1} - x_i, \quad i = 0, 1, \dots, n-1.$$

Then each $x_i = x_0 + ih$, $i = 0, 1, \dots, n$. For any $x \in [a, b]$, write

$$x = x_0 + sh, \quad s \in \mathbb{R}.$$

Hence $x - x_i = (s - i)h$ and

$$\begin{aligned} P_n(x) &= f[x_0] + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](x - x_0)(x - x_1) \cdots (x - x_{k-1}) \\ &= f(x_0) + \sum_{k=1}^n f[x_0, x_1, \dots, x_k](s - 0)h(s - 1)h \cdots (s - k + 1)h \\ &= f(x_0) + \sum_{k=1}^n f[x_0, x_1, \dots, x_k]s(s - 1) \cdots (s - k + 1)h^k \\ &= f(x_0) + \sum_{k=1}^n f[x_0, x_1, \dots, x_k]k! \binom{s}{k} h^k, \end{aligned}$$



- The binomial formula

$$\binom{s}{k} = \frac{s(s-1)\cdots(s-k+1)}{k!}$$

- The forward difference notation Δ

$$\Delta f(x_i) = f(x_{i+1}) - f(x_i)$$

and

$$\Delta^k f(x_i) = \Delta^{k-1} f(x_{i+1}) - \Delta^{k-1} f(x_i) = \Delta \left(\Delta^{k-1} f(x_i) \right),$$

for $i = 0, 1, \dots, n-1$.

- With this notation,

$$\begin{aligned} f[x_0, x_1] &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1}{h} \Delta f(x_0) \\ f[x_0, x_1, x_2] &= \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} \\ &= \frac{\frac{1}{h} \Delta f(x_1) - \frac{1}{h} \Delta f(x_0)}{2h} = \frac{1}{2h^2} \Delta^2 f(x_0), \end{aligned}$$



- In general

$$f[x_0, x_1, \dots, x_k] = \frac{1}{k! h^k} \Delta^k f(x_0).$$

- The Newton forward-difference formula:

$$P_n(x) = f(x_0) + \sum_{k=1}^n \binom{s}{k} \Delta^k f(x_0).$$

- The interpolation nodes are arranged as x_n, x_{n-1}, \dots, x_0 :

$$\begin{aligned} P_n(x) &= f[x_n] + f[x_n, x_{n-1}](x - x_n) \\ &\quad + f[x_n, x_{n-1}, x_{n-2}](x - x_n)(x - x_{n-1}) + \dots \\ &\quad + f[x_n, \dots, x_0](x - x_n)(x - x_{n-1}) \cdots (x - x_1). \end{aligned}$$



- If the nodes are equally spaced with

$$h = \frac{x_n - x_0}{n}, \quad x_i = x_n - (n - i)h, \quad x = x_n + sh,$$

then

$$\begin{aligned} P_n(x) &= f[x_n] + \sum_{k=1}^n f[x_n, x_{n-1}, \dots, x_{n-k}]sh(s+1)h \cdots (s+k-1) \\ &= f(x_n) + \sum_{k=1}^n f[x_n, x_{n-1}, \dots, x_{n-k}](-1)^k k! \binom{-s}{k} h^k \end{aligned}$$

- Binomial formula:

$$\binom{-s}{k} = \frac{-s(-s-1) \cdots (-s-k+1)}{k!} = (-1)^k \frac{s(s+1) \cdots (s+k-1)}{k!}.$$



- Backward-difference:

$$\nabla^k f(x_i) = \nabla^{k-1} f(x_i) - \nabla^{k-1} f(x_{i-1}) = \nabla \left(\nabla^{k-1} f(x_i) \right),$$

then

$$f[x_n, x_{n-1}] = \frac{1}{h} \nabla f(x_n), \quad f[x_n, x_{n-1}, x_{n-2}] = \frac{1}{2h^2} \nabla^2 f(x_n),$$

and, in general,

$$f[x_n, x_{n-1}, \dots, x_{n-k}] = \frac{1}{k! h^k} \nabla^k f(x_n).$$

- Newton backward-difference formula:

$$P_n(x) = f(x_0) + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_k).$$



Hermite Interpolation

Given $n + 1$ data points $x_0 < x_1 < \cdots < x_n$, and

$$\begin{array}{ccccccc} y_0^{(0)} = f(x_0) & y_1^{(0)} = f(x_1) & \cdots & y_n^{(0)} = f(x_n) \\ y_0^{(1)} = f'(x_0) & y_1^{(1)} = f'(x_1) & \cdots & y_n^{(1)} = f'(x_n) \\ \vdots & \vdots & & \vdots \\ y_0^{(m_0)} = f^{(m_0)}(x_0) & y_1^{(m_1)} = f^{(m_1)}(x_1) & \cdots & y_n^{(m_n)} = f^{(m_n)}(x_n) \\ \downarrow & \downarrow & & \downarrow \\ m_0 + 1 \text{ conditions} & m_1 + 1 \text{ conditions} & \cdots & m_n + 1 \text{ conditions} \end{array}$$

for some function $f \in C^m[a, b]$ where $m = \max\{m_0, m_1, \dots, m_n\}$.



- Determine a polynomial P of degree at most N , where

$$N = \left(\sum_{i=0}^n m_i \right) + n, \quad (5)$$

to satisfy the following interpolation conditions:

$$P^{(k)}(x_i) = y_i^{(k)}, \quad k = 0, 1, \dots, m_i, \quad i = 0, 1, \dots, n. \quad (6)$$

- If $n = 0$, then P is the m_0 th Taylor polynomial for f at x_0 .
- If $m_i = 0$ for each i , then P is the n th Lagrange polynomial interpolating f on x_0, \dots, x_n .
- If $m_i = 1$ for each i , then P is called the Hermite polynomials.



Theorem

If $f \in C^1[a, b]$ and $x_0, \dots, x_n \in [a, b]$ are distinct, then the polynomial of least degree agreeing with f and f' at x_0, \dots, x_n is unique and is 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

$$H_{n,j}(x) = [1 - 2(x - x_j)L'_{n,j}(x_j)] L_{n,j}^2(x), \quad \widehat{H}_{n,j}(x) = (x - x_j)L_{n,j}^2(x),$$

and

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

Moreover, if $f \in \mathbb{C}^{2n+2}[a, b]$, then $\exists \xi(x) \in [a, b]$ s.t.

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

Proof:

Since

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

it implies that

$$H_{n,j}(x_i) = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j, \end{cases} \quad \widehat{H}_{n,j}(x_i) = 0 \quad \forall i, j.$$

As a consequence,

$$H_{2n+1}(x_i) = \sum_{j=0, j \neq i}^n f(x_j) \cdot 0 + f(x_i) \cdot 1 + \sum_{j=0}^n f'(x_j) \cdot 0 = f(x_i), \quad \forall i.$$

By definitions of $H_{n,j}(x)$ and $\widehat{H}_{n,j}(x)$,

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



It implies that if $i \neq j$,

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

and

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

Therefore, $\forall i$,

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

That is H_{2n+1} agrees with f and H'_{2n+1} with f' at x_0, \dots, x_n .



Proof of uniqueness:

- Since $\deg(P) \leq 2n + 1$, write

$$P(x) = a_0 + a_1x + \cdots + a_{2n+1}x^{2n+1}.$$

- $2n + 2$ coefficients, $a_0, a_1, \dots, a_{2n+1}$, to be determined and $2n + 2$ conditions given

$$P(x_i) = f(x_i), \quad P'(x_i) = f'(x_i), \quad \text{for } i = 0, \dots, n.$$

$\Rightarrow 2n + 2$ linear equations in $2n + 2$ unknowns to solve

\Rightarrow show that the coefficient matrix A of this system is nonsingular.

- To prove A is nonsingular, it suffices to prove that $Au = 0$ has only the trivial solution $u = 0$.
- $Au = 0$ iff

$$P(x_i) = 0, \quad P'(x_i) = 0, \quad \text{for } i = 0, \dots, n.$$

$\Rightarrow P$ is a multiple of the polynomial given by

$$q(x) = \prod_{i=0}^n (x - x_i)^2.$$



- However, $\deg(q) = 2n + 2$ whereas P has degree at most N .
- Therefore, $P(x) = 0$, i.e. $u = 0$.
- That is, A is nonsingular, and the Hermite interpolation problem has a unique solution. □



Divided Difference Method for Hermite Interpolation

Denote the $N + 1$ conditions pairs

$$(x_0, f(x_0)), (x_0, f'(x_0)), (x_1, f(x_1)), (x_1, f'(x_1)), \dots, (x_n, f(x_n)), (x_n, f'(x_n))$$

by consecutive coordinate pairs

$$(z_0, f(x_0)), (z_1, f'(x_0)), (z_2, f(x_1)), (z_3, f'(x_1)), \dots, (z_{N-1}, f(x_n)), (z_N, f'(x_n))$$

Note that $z_0 \leq z_1 \leq \dots \leq z_N$. The unique Hermite interpolating polynomial in Newton's form can then be written as

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

If $z_i \neq z_{i+k}$, then

$$f[z_i, z_{i+1}, \dots, z_{i+k}] = \frac{f[z_{i+1}, z_{i+2}, \dots, z_{i+k}] - f[z_i, z_{i+1}, \dots, z_{i+k-1}]}{z_{i+k} - z_i}$$



However the divided-difference formula has to be modified because there may be repetitions among z_i . Since $z_{2i} = z_{2i+1} = x_i$ for each i , let

$$\xi_{2i} < \xi_{2i+1}$$

be distinct coordinates and $\xi_j \rightarrow z_j$, for $2i \leq j \leq 2i+1$. Then, by applying Theorem 3.6,

$$f[z_{2i}, z_{2i+1}] = \lim_{\substack{\xi_j \rightarrow z_j \\ 2i \leq j \leq 2i+1}} f[\xi_{2i}, \xi_{2i+1}] = f'(z_{2i}) = f'(x_i)$$



z	$f(z)$		
$z_0 = x_0$	$f[z_0] = f(x_0)$	$f[z_0, z_1] = f'(x_0)$	
$z_1 = x_0$	$f[z_1] = f(x_0)$	$f[z_1, z_2] = \frac{f[z_2] - f[z_1]}{z_2 - z_1}$	$f[z_0, z_1, z_2] = \frac{f[z_1, z_2] - f[z_0, z_1]}{z_2 - z_0}$
$z_2 = x_1$	$f[z_2] = f(x_1)$	$f[z_2, z_3] = f'(x_1)$	$f[z_1, z_2, z_3] = \frac{f[z_2, z_3] - f[z_1, z_2]}{z_3 - z_1}$
$z_3 = x_1$	$f[z_3] = f(x_1)$	$f[z_3, z_4] = \frac{f[z_4] - f[z_3]}{z_4 - z_3}$	$f[z_2, z_3, z_4] = \frac{f[z_3, z_4] - f[z_2, z_3]}{z_4 - z_2}$
$z_4 = x_2$	$f[z_4] = f(x_2)$	$f[z_4, z_5] = f'(x_2)$	$f[z_3, z_4, z_5] = \frac{f[z_4, z_5] - f[z_3, z_4]}{z_5 - z_3}$
$z_5 = x_2$	$f[z_5] = f(x_2)$		



Cubic spline interpolation

- The previous sections concern the approximation of an arbitrary function on a closed interval by a polynomial. However, the oscillatory nature of high-degree polynomials restricts their use.
- Piecewise polynomial interpolation: divide the interval into a collection of subintervals and construct different approximation on each subinterval.
- The simplest piecewise polynomial approximation is piecewise linear interpolation.
- A disadvantage of linear function approximation is that the interpolating function is not smooth at each of the endpoints of the subintervals. It is often required that the approximating function is continuously differentiable.
- An alternative procedure is to use a piecewise polynomial of Hermite type. However, to use Hermite piecewise polynomials for general interpolation, we need to know the derivatives of the function being approximated, which is frequently not available.



- The most common piecewise-polynomial use cubic polynomials between each successive pair of nodes and is called cubic spline interpolation.

Definition

Given a function f defined on $[a, b]$, and a set of nodes $a = x_0 < x_1 < \cdots < x_n = b$, a cubic spline interpolation S for f is a function that satisfies the following conditions:

- S is a cubic polynomial, denoted $S_j(x)$, on $[x_j, x_{j+1}]$ for each $j = 0, 1, \dots, n - 1$;
- $S_j(x_j) = f(x_j)$ and $S_j(x_{j+1}) = f(x_{j+1}) \forall j = 0, 1, \dots, n - 1$;
- $S_{j+1}(x_{j+1}) = S_j(x_{j+1}) \forall j = 0, 1, \dots, n - 2$;
- $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1}) \forall j = 0, 1, \dots, n - 2$;
- $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1}) \forall j = 0, 1, \dots, n - 2$;
- One of the following sets of boundary conditions is satisfied:
 - $S''(x_0) = S''(x_n) = 0$ (free or natural boundary);
 - $S'(x_0) = f'(x_0)$ and $S'(x_n) = f'(x_n)$ (clamped boundary).

Construction of cubic spline interpolation

Remark

In general, clamped boundary conditions lead to more accurate approximations since they include more information about the function.

Write

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

That is

$$a_j = S_j(x_j) = f(x_j).$$

Since $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$, it implies that

$$a_{j+1} = a_j + b_j(x_{j+1} - x_j) + c_j(x_{j+1} - x_j)^2 + d_j(x_{j+1} - x_j)^3.$$

Let

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

Then

$$a_{j+1} = a_j + b_j h_j + c_j h_j^2 + d_j h_j^3. \quad (7)$$



Define $b_n = S'(x_n)$ and observe that

$$S'_j(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2$$

implies that

$$b_j = S'_j(x_j), \quad \forall j = 0, 1, \dots, n-1.$$

Applying $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$ gives

$$b_{j+1} = b_j + 2c_j h_j + 3d_j h_j^2, \quad \forall j = 0, 1, \dots, n-1. \quad (9)$$

Defining $c_n = S''(x_n)/2$ and applying $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$, we get

$$c_{j+1} = c_j + 3d_j h_j, \quad \forall j = 0, 1, \dots, n-1.$$

Hence

$$d_j = \frac{c_{j+1} - c_j}{3h_j}.$$



Substituting d_j in (9) into (7) and (8), it obtains

$$a_{j+1} = a_j + b_j h_j + \frac{h_j^2}{3}(2c_j + c_{j+1}) \quad (10)$$

and

$$b_{j+1} = b_j + h_j(c_j + c_{j+1}). \quad (11)$$

Eq. (10) implies that

$$b_j = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}), \quad (12)$$

and then

$$b_{j-1} = \frac{1}{h_{j-1}}(a_j - a_{j-1}) - \frac{h_{j-1}}{3}(2c_{j-1} + c_j). \quad (13)$$



Substituting (12) and (13) into (11), we get

$$h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_jc_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}). \quad (14)$$

for each $j = 1, 2, \dots, n - 1$.

Theorem

If f is defined at $a = x_0 < x_1 < \dots < x_n = b$, then f has a unique natural spline interpolant S on the nodes x_0, x_1, \dots, x_n that satisfies $S''(a) = S''(b) = 0$.

Proof: The boundary conditions imply that

$$\begin{aligned} c_n &= S''(x_n)/2 = 0, \\ 0 &= S''(x_0) = 2c_0 + 6d_0(x_0 - x_0) \Rightarrow c_0 = 0. \end{aligned}$$



Solving tridiagonal linear system

Let

$$A = LU \equiv \begin{bmatrix} l_{11} & & & & & \\ l_{21} & l_{22} & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & l_{n,n-1} & l_{nn} & \end{bmatrix} \begin{bmatrix} 1 & u_{12} & & & & \\ & 1 & u_{23} & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & u_{n-1,n} \\ & & & & & 1 \end{bmatrix}.$$

Comparing the coefficients of matrix in both sides, we have

$$\begin{aligned} a_{11} &= l_{11}, \\ a_{i,i-1} &= l_{i,i-1}, \quad \text{for } i = 2, 3, \dots, n, \\ a_{ii} &= l_{i,i-1}u_{i-1,i} + l_{ii}, \quad \text{for } i = 2, 3, \dots, n, \\ a_{i,i+1} &= l_{ii}u_{i,i+1}, \quad \text{for } i = 1, 2, \dots, n-1. \end{aligned}$$



It implies that

$$l_{11} = a_{11}, \quad u_{12} = a_{12}/l_{11},$$

and, for $i = 2, \dots, n-1$,

$$l_{i,i-1} = a_{i,i-1},$$

$$l_{ii} = a_{ii} - l_{i,i-1}u_{i-1,i},$$

$$u_{i,i+1} = a_{i,i+1}/l_{ii},$$

and

$$l_{n,n-1} = a_{n,n-1},$$

$$l_{nn} = a_{nn} - l_{n,n-1}u_{n-1,n}.$$



Forward substitution

Solve $Ly = b$

$$\Rightarrow \begin{cases} \ell_{11}y_1 &= b_1, \\ \ell_{21}y_1 + \ell_{22}y_2 &= b_2, \\ &\vdots \\ \ell_{n,n-1}y_{n-1} + \ell_{nn}y_n &= b_n. \end{cases}$$

$$\Rightarrow \begin{cases} y_1 &= b_1/\ell_{11}, \\ y_2 &= (b_2 - \ell_{21}y_1)/\ell_{22}, \\ &\vdots \\ y_n &= (b_n - \ell_{n,n-1}y_{n-1})/\ell_{nn}. \end{cases}$$

$$\Rightarrow \begin{cases} y_1 &= b_1/\ell_{11}, \\ y_i &= (b_i - \ell_{i,i-1}y_{i-1})/\ell_{ii}, \text{ for } i = 2, \dots, n. \end{cases}$$



Back substitution

Solve $Ux = y$,

$$\Rightarrow \begin{cases} x_1 + u_{12}x_2 = y_1, \\ \vdots \\ x_{n-1} + u_{n-1,n}x_n = y_{n-1}, \\ x_n = y_n, \end{cases}$$

$$\Rightarrow \begin{cases} x_n = y_n, \\ x_{n-1} = y_{n-1} - u_{n-1,n}x_n, \\ \vdots \\ x_1 = y_1 - u_{12}x_2, \end{cases}$$

$$\Rightarrow \begin{cases} x_n = y_n, \\ x_i = y_i - u_{i,i+1}x_{i+1}, \text{ for } i = n-1, \dots, 1. \end{cases}$$



Theorem

If f is defined at $a = x_0 < x_1 < \cdots < x_n = b$ and differentiable at a and b , then f has a unique clamped spline interpolant S on the nodes x_0, x_1, \dots, x_n that satisfies $S'(a) = f'(a)$ and $S'(b) = f'(b)$.

Proof. Since $f'(a) = S'(a) = S'(x_0) = b_0$, Eq. (12) with $j = 0$ implies

$$f'(a) = \frac{1}{h_0}(a_1 - a_0) - \frac{h_0}{3}(2c_0 + c_1).$$

Consequently,

$$2h_0c_0 + h_0c_1 = \frac{3}{h_0}(a_1 - a_0) - 3f'(a).$$

Similarly,

$$f'(b) = b_n = b_{n-1} + h_{n-1}(c_{n-1} + c_n),$$



so Eq. (12) with $j = n - 1$ implies that

$$\begin{aligned} f'(b) &= \frac{a_n - a_{n-1}}{h_{n-1}} - \frac{h_{n-1}}{3}(2c_{n-1} + c_n) + h_{n-1}(c_{n-1} + c_n) \\ &= \frac{a_n - a_{n-1}}{h_{n-1}} + \frac{h_{n-1}}{3}(c_{n-1} + 2c_n), \end{aligned}$$

and

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

Eq. (14) together with the equations

$$2h_0c_0 + h_0c_1 = \frac{3}{h_0}(a_1 - a_0) - 3f'(a)$$

and

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



