Numerical Analysis

Daming Li

Department of Mathematics, Shanghai JiaoTong University,
Shanghai, 200240, China
Email: lidaming@sjtu.edu.cn

October 14, 2014

In this chapter, the problem of representing functions within a computer is discussed. Several different subproblems will be considered. They differ according to the type of function being represented, whether known at relatively few points or at many (or all) points. The representation chosen (whether a polynomial, a spline function, a continued fraction, etc.) also determines the nature of the theory.

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. Here is the theorem that governs this problem.
If $x_0, x_1, \cdots, x_n$ are distinct real numbers, then for arbitrary values $y_0, y_1, \cdots, y_n$ there is a unique polynomial p_n of degree at most n such that

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

Proof. Let us prove the unicity first. Suppose there were two such polynomials, p_n and q_n. Then the polynomial $p_n - q_n$ would have the property that $(p_n - q_n)(x_i) = 0$ for $0 \le i \le n$. Since the degree of $p_n - q_n$ can be at most n, this polynomial can have at most n zeros if it is not the zero polynomial. Since the x_i, are distinct, $p_n - q_n$ has $n \times 1$ zeros; it must therefore be zero. Hence, $p_n = q_n$. For the existence part of the theorem, we proceed inductively. For $n = 0$, the existence is obvious since a constant function p_0 (polynomial of degree 0) can be chosen so that $p_0(x_0) = y_0$. Now suppose that we have obtained a polynomial p_{k-1} of degree $\le k - 1$ with $p_{k-i}(x_i) = y_i$ for $0 \le i \le k - 1$. We try to construct p_k in the form

$$p_k(x) = p_{k-1}(x) + c(x - x_0)(x - x_1) \cdots (x - x_{k-1})$$

Obviously,

$$P_k(x_i) = P_{k-1}(x_i) = y_i \quad (0 \le i \le k - 1)$$

Polynomial Interpolation

The coefficient c is determined by

$$P_k(x_k) = y_k$$

The polynomials $p_0, p_1, \cdots, , p_n$ constructed in the proof have the property that each p_k is obtained simply by adding a single term to p_{k-1}

$$\begin{aligned} p_k(x) &= c_0 + c_1(x - x_0)(x - x_1) + \cdots + c_k(x - x_0)\cdots(x - x_{k-1}) \\ &= \sum_{i=0}^{k} c_i \prod_{j=0}^{i-1}(x - x_j) \end{aligned}$$

These polynomials are called the interpolation polynomials in Newton's form. The coefficients c_k are written as

$$c_k = \frac{y_k - p_{k-1}(x_k)}{(x_k - x_0)(x_k - x_1)\cdots(x_k - x_{k-1})}$$

Polynomial Interpolation

The nested multiplication or Horner's algorithm is used to calculate

$$\begin{aligned} u &= \sum_{i=0}^{k} c_i \prod_{j=0}^{i-1} d_j = c_0 + c_1 d_0 d_1 + \cdots + c_k d_0 \cdots d_{k-1} \\ &= (\cdots(((c_k)d_{k-1} + c_{k-1})d_{k-2} + c_{k-2})d_{k-3} + \cdots + c_1) + c_0 \end{aligned}$$

$$u = c_k, \quad u \leftarrow u d_i + c_i, \quad i = k-1, \cdots, 0$$

If we choose $d_j = (x - x_j)$, this algorithm is used to calculate $p_k(x)$.

Polynomial Interpolation

Alternative method for construct the interpolation polynomial p_n in the Lagrange form

$$p_n(x) = \sum_{k=0}^{n} y_k l_k(x)$$

Here $l_0, \cdots, l_n$ are polynomials that depend on the nodes $x_0, x_1, \cdots, x_n$ but not on the ordinates $y_0, y_1, \cdots, y_n$. To ensure $p_n(x_i) = y_i$ for all $i = 0, \cdots, n$, the Lagrange basis function l_i satisfies

$$l_i(x_j) = \delta_{ij}, \quad i, j = 0, 1, \cdots, n$$

i.e.,

$$l_i(x) = \prod_{i \neq j = 0}^{n} \frac{x - x_j}{x_i - x_j}, \quad i = 0, 1, \cdots, n$$

The polynomial p_n can also be expressed in powers of x

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

The coefficients satisfies

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

The coefficient matrix here is called a Vandermonde matrix. It is nonsingular. The Vandermonde matrix is often ill conditioned, and the coefficients a_i may therefore be inaccurately determined by solving the above system. Therefore, this approach is not recommended.

f be a function in $C^{n+1}[a,b]$, and let p be the polynomial of degree $\leq n$ that interpolates the function f at $n+1$ distinct points $x_0, x_1, \cdots, x_n$ in the interval $[a,b]$. To each x in $[a,b]$ there corresponds a point ξ_x in (a,b) such that

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

Proof. If x is one of the nodes of interpolation x_i, the assertion is obviously true. So, let x be any point other than a node. Put

$$w(t) \equiv \prod_{i=0}^{n} (t - x_i), \quad \phi \equiv f - p - \lambda w$$

where λ is the real number that makes $\phi(x) = 0$. Thus,

$$\lambda = \frac{f(x) - p(x)}{w(x)}$$

Polynomial Interpolation

Now $\phi \in C^{n+1}[a,b]$, and ϕ vanishes at the $n+2$ points $x, x_0, x_1, \cdots, x_n$. By Rolle's Theorem, $\phi^{(n+1)}$ has at least one zero, say ξ_x, in (a,b)

$$0 = \phi^{(n+1)}(\xi_x) = f^{(n+1)}(\xi_x) - (n+1)!\lambda = f^{(n+1)}(\xi_x) - (n+1)! \frac{f(x) - p(x)}{w(x)}$$

In the above theorem, there is a term that can be optimized by choosing the nodes in a special way. An analysis of this problem was first given by the great Russian mathematician Chebyshev. The optimization process leads naturally to a system of polynomials called Chebyshev polynomials, and we begin with their definition and basic properties.

Chebyshev polynomials (of the first kind) are defined recursively as follows:

$$\begin{cases} T_0(x) = 1, \quad T_1(x) = x \\ T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \end{cases}$$

For x in the interval $[-1, 1]$, the Chebyshev polynomials have this closed-form expression

$$T_n(x) = \cos(n \arccos(x)) \quad (n \geq 0)$$

This is because

$$\cos((n+1)\theta) = 2\cos\theta\cos(n\theta) - \cos((n-1)\theta), \quad \theta = \arccos(x)$$

Polynomial Interpolation

From this formula, we obtain further properties of the Chebyshev polynomial

$$|T_n(x)| \leq 1, \quad -1 \leq x \leq 1$$

$$T_n(\cos(j\pi/n)) = (-1)^j, \quad 0 \leq j \leq n$$

$$T_n(\cos((2j-1)\pi/(2n))) = 0, \quad 1 \leq j \leq n$$

A monic polynomial is one in which the term of highest degree has coefficient unity. From the definition of the Chebyshev polynomials, we see that in $T_n(x)$ the term of highest degree is $2^{n-1}x^n$. Therefore, $2^{1-n}T_n$ is a monic polynomial.

If p is a monic polynomial of degree n, then

$$||p||_\infty = \max_{-1 \leq x \leq 1} |p(x)| \geq 2^{1-n}$$

Proof. We proceed by contradiction. Suppose that

$$|p(x)| < 2^{1-n} \quad (|x| \leq 1)$$

The inequality becomes equality if $p = 2^{1-n}T_n$.
Let $q = 2^{1-n}T_n$ be a monic polynomial of degree of n and $x_i = \cos(i\pi/n)$.

$$(-1)^i p(x_i) \leq |p(x_i)| < 2^{1-n} = (-1)^i q(x_i)$$

Consequently,

$$(-1)^i [q(x_i) - p(x_i)] > 0 \quad (0 \leq i \leq n)$$

This shows that the polynomial $q - p$ oscillates in sign $n + 1$ times on the interval $[-1, 1]$. It therefore must have at least n roots in $(-1, 1)$. But this is not possible, because $q - p$ has degree at most $n - 1$.

Polynomial Interpolation

Assume that the interpolation nodes are in the interval $[-1, 1]$. We have the following interpolation error

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

By the above theorem,

$$\max_{|x|\le 1} |\prod_{i=0}^{n} (x - x_i)| \ge 2^{-n}$$

The minimum value will be attained if $\prod_{i=0}^{n}(x - x_i)$ is the monic multiple of T_{n+1}; that is, $2^n T_{n+1}$. The nodes then will be the roots of T_{n+1}. These are

$$x_i = \cos\left(\frac{2i+1}{2n+2}\pi\right) \quad (0 \le i \le n)$$

Polynomial Interpolation

If the nodes x_i are the root of the Chebyshev polynomial T_{n+1}, then the interpolation error becomes (for $|x| \leq 1$)

$$|f(x) - p(x)| = \frac{1}{2^n(n+1)!} \max_{|t|\leq 1} |f^{(n+1)}(t)|$$

For any prescribed system of nodes

$$a \leq x_0 < x_1 < \cdots < x_n \leq b \quad (n \geq 0)$$

there exists a continuous function f on $[a, b]$ such that the interpolating polynomials for f using these nodes fail to converge uniformly to f.

Exercises: P.291

1(a)(b),6,7,9,10,11,21

Divided Differences

Assume that the interpolation nodes $\{x_i\}_{i=0}^n$ are distinct. the Lagrange basis functions are

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

The coefficients of the Newton form of the interpolation polynomial

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

satisfies

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

which is a lower triangular system for the unknowns $\{c_i\}_{i=0}^n$ due to $q_j(x_i) = 0$ for $i < j$.

Moreover, c_n depends on f at $x_0, x_1, \cdots, x_n$. Thus the notation

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

which is the coefficient of q_n when $\sum_{k=0}^{n} c_k q_k$ interpolates f at $x_0, x_1, \cdots, x_n$. We can also say that $f[x_0, x_1, \cdots, x_n]$ is the coefficient of x^n in the polynomial of degree at most n that interpolates f at $x_0, x_1, \cdots, x_n$. The expressions $f[x_0, x_1, \cdots, x_n]$ are called divided differences of f. The first few divided difference

$$f[x_0] = f(x_0)$$

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

This gives a hint as to why the term divided difference was adopted.

The Newton interpolating polynomial can also be written as

$$p(x) = \sum_{k=0}^{n} f[x_0, x_1, \cdots, x_k] \prod_{j=0}^{k-1} (x - x_j)$$

Divided Differences

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. First, let p_k denote the polynomial of degree at most k that interpolates f at the nodes $x_0, x_1, \cdots, x_k$. Let q denote the polynomial of degree at most $n - 1$ that interpolates f at $x_1, x_2, \cdots, x_n$. Then we have

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

This equation is proved by noting first that on both sides stands a polynomial of degree at most n. Then we verify that the values of these polynomials on the right and the left are the same at the points $x_0, x_1, \cdots, x_n$. Hence, the polynomials must be identical.

Divided Differences

The preceding theorem gives us these particular formulae:

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

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$

In these formulas, $x_0, x_1, \cdots$ can be interpreted as independent variables. Because of that, we also have equations such as

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

Here $f[x_i]$, $f[x_i, x_j]$, $f[x_i, x_j, x_k]$, etc, are difference of order $0, 1, 2, 3$, etc, respectively.

Divided Differences

$$
\begin{array}{lllll}
x_0 & f[x_0] & f[x_0, x_1] & f[x_0, x_1, x_2] & f[x_0, x_1, x_2, x_3] \\
x_1 & f[x_1] & f[x_1, x_2] & f[x_1, x_2, x_3] & \\
x_2 & f[x_2] & f[x_2, x_3] & & \\
x_3 & f[x_3] & & &
\end{array}
$$

Compute a divided difference table for these function values:

$$
\begin{array}{ccccc}
3 & 1 & 2 & -3/8 & 7/40 \\
1 & -3 & 5/4 & 3/20 & \\
5 & 2 & 2 & & \\
6 & 4 & & &
\end{array}
$$

Divided Differences

For $i = 0, 1, \cdots, n$, Do:
    $d_i \leftarrow f(x_i)$
EndDo
For $j = 1, \cdots, n$, Do:
    For $i = j, \cdots, n$, Do:
        $d_{ij} \leftarrow (d_i - d_{i-1})/(x_i - x_{i-j})$
    EndDo
EndDo

the conclusion of this algorithm the vector d contains the coefficients of the polynomial:

$$p(x) = \sum_{i=0}^{n} d_i \prod_{j=0}^{i-1} (x - x_j)$$

The divided difference is a symmetric function of its arguments. Thus, 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. The divided difference on the left side of Equation is the coefficient of x^n in the polynomial of degree at most n interpolating f at the points $z_0, z_1, \cdots, z_n$. The divided difference on the right is the coefficient of x^n in the polynomial of degree at most n that interpolates f at the points $x_0, x_1, \cdots, x_n$. These two polynomials are, of course, the same.

Let p be the polynomial of degree at most n that interpolates a function f at a set of $n+1$ distinct nodes, $x_0, x_1, \cdots, x_n$. If t is a point different from the nodes, then

$$f(t) - p(t) = f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (t - x_j)$$

Proof. First, let q be the polynomial of degree at most $n+1$ that interpolates f at the nodes $x_0, x_1, \cdots, x_n, t$

$$q(x) = p(x) + f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (x - x_j)$$

Since $q(t) = f(t)$, we complete the proof.

Divided Differences

If f is n times continuously dijferentiable on $[a, b]$ and if $x_0, x_1, \cdots, x_n$ are distinct points in $[a, b]$, then there exists a point ξ in (a, b) such that

$$f[x_0, x_1, \cdots, x_n] = \frac{1}{n!} f^{(n)}(\xi)$$

Proof. First, let p be the polynomial of degree at most $n - 1$ that interpolates f at the nodes $x_0, x_1, \cdots, x_{n-1}$, then

$$f(x_n) - p(x_n) = \frac{1}{n!} f^{(n)}(\xi) \prod_{j=0}^{n-1} (x_n - x_j)$$

By the above theorem,

$$f(x_n) - p(x_n) = f[x_0, x_1, \cdots, x_n] \prod_{j=0}^{n-1} (x_n - x_j)$$

By comparing the above equality, we obtain the desired result.

Exercises: P.302

3,4,5,8,9,12,17,21

We require a polynomial of least degree that interpolates a function f and its derivative f' at two distinct points, say x_0 and x_1. The polynomial sought will satisfy

$$p(x_i) = f(x_i), \quad p'(x_i) = f'(x_i) \quad (i = 0, 1)$$

We want to find

$$p(x) = a + b(x - x_0) + c(x - x_0)^2 + d(x - x_0)^2(x - x_1)$$

Find a polynomial p that assumes these values: $p(0) = 0$, $p(1) = 1$, $p'(1/2) = 2$. Since there are three conditions, we try a quadratic,

$$p(x) = a + bx + cx^2$$

condition $p(0) = 0$ leads to $a = 0$. The other two conditions lead to

$$1 = p(1) = b + c$$

$$2 = p'(\frac{1}{2}) = b + c$$

Thus, no quadratic solves our problem. We now try a cubic polynomial for the same problem: $p(x) = a + bx + cx^2 + dx^3$, we discover that there exists a solution but it is not unique.

The nodes be $x_0, x_1, \cdots, x_n$, and suppose that at node x_i, these Hermite interpolation conditions are given:

$$p^{(j)}(x_0) = c_{ij} \quad (0 \leq j \leq k_i - 1, \quad 0 \leq i \leq n)$$

The total number of conditions on is denoted by $m + 1$, and therefore

$$m + 1 = k_0 + k_1 + \cdots + k_n$$

There exists a unique polynomial p in Π_m fulfilling the Hermite interpolation conditions.

Hermite Interpolation

Proof. The polynomial p is sought in the space Π_m, and it therefore has $m+1$ coefficients. The number of interpolatory conditions is also $m+1$. Thus, we have a square system of $m+1$ equations in $m+1$ unknowns to solve, and we wish to be assured that the coefficient matrix is nonsingular. To prove that a square matrix is nonsingular it suffices to prove that the homogeneous equation has only the zero solution. The homogeneous problem is to find $p \in \Pi_m$ such that

$$p^{(j)}(x_i) = 0 \quad (0 \le j \le k_i - 1, \quad 0 \le i \le n)$$

Such a polynomial has a zero of multiplicity k_i at x_i $(0 \le i \le n)$ and must therefore be a multiple of the polynomial q given by $q(x) = \prod_{i=0}^{n}(x - x_i)^{(k_i)}$ with degree $m + 1 = \sum_{i=0}^{n} k_i$, while p is to be of degree at most m. We therefore conclude that $p = 0$.

Hermite Interpolation

The polynomial p that we seek must satisfy these equations:

$$p(x_i) = c_{i0}, \quad p'(x_i) = c_{i1}, \quad 0 \le i \le n$$

In analogy with the Lagrange formula, we write

$$p(x) = \sum_{i=0}^{n} c_{i0} A_i(x) + \sum_{i=0}^{n} c_{i1} B_i(x)$$

where the basis functions

$$A_i(x_j) = \delta_{ij}, \quad B_i(x_j) = 0$$

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

With the aid of Lagrange basis

$$l_i(x) = \prod_{i \ne j = 0}^{n} \frac{x - x_j}{x_i - x_j}, \quad 0 \le i \le n$$

$$A_i(x) = [1 - 2(x - x_i) l_i'(x_i)] l_i^2(x), \quad 0 \le i \le n$$

$$B_i(x) = (x - x_i) l_i^2(x), \quad 0 \le i \le n$$

If $n = 1$,

$$A_0(x) = [1 - 2(x - x_0)l_0'(x_0)]l_0^2(x)$$

$$A_1(x) = [1 - 2(x - x_1)l_1'(x_1)]l_1^2(x)$$

$$B_0(x) = (x - x_0)l_0^2(x)$$

$$B_1(x) = (x - x_1)l_1^2(x)$$

and

$$l_0(x) = \frac{x - x_1}{x_0 - x_1}, \quad l_1(x) = \frac{x - x_0}{x_1 - x_0}$$

Let $x_0, x_1, \cdots, x_n$ be distinct nodes in $[a, b]$ and let $f \in C^{2n+2}[a, b]$. If p is the polynomial of degree at most $2n+1$ such that

$$p(x_i) = f(x_i), \quad p'(x_i) = f'(x_i), \quad 0 \leq i \leq n$$

then to each x in [a, b] there corresponds a point ξ in (a, b) such that

$$f(x) - p(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \prod_{i=0}^{n} (x - x_i)^2$$

The proof is similar to that of the Lagrange interpolation error.

Exercises: P.314

2,3,6,12

A spline function consists of polynomial pieces on subintervals joined together with certain continuity conditions. Formally, suppose that $n+1$ points $t_0, t_1, \cdots, t_n$ have been specified and satisfy $t_0 < t_1 < \cdots < t_n$. These points are called knots. Suppose also that an integer $k \geq 0$ has been prescribed. A spline function of degree k having knots $t_0, t_1, \cdots, t_n$ is a function S such that (i) on each interval $[t_{i-1}, t_i)$, S is a polynomial of degree $\leq k$. (ii) S has a continuous $(k-1)$st derivative on $[t_0, t_n]$. Hence, S is a continuous piecewise polynomial of degree at most k having continuous derivatives of all orders up to $k-1$.

Splines of degree 0 are piecewise constants

$$S(x) = \begin{cases} c_0 & x \in [t_0, t_1) \\ c_1 & x \in [t_1, t_2) \\ \vdots & \vdots \\ c_{n-1} & x \in [t_{n-1}, t_n] \end{cases}$$

Splines of degree 1 are piecewise linear function

$$S(x) = \begin{cases} a_0 x + b_0 & x \in [t_0, t_1] \\ a_1 x + b_1 & x \in [t_1, t_2] \\ \vdots & \vdots \\ a_{n-1} x + b_{n-1} & x \in [t_{n-1}, t_n] \end{cases}$$

Splines of degree 3 (Cubic splines) are piecewise cubic polynomial

$$S(x) = \begin{cases} S_0(x) & x \in [t_0, t_1] \\ S_1(x) & x \in [t_1, t_2] \\ \vdots & \vdots \\ S_{n-1}(x) & x \in [t_{n-1}, t_n] \end{cases}$$

with $4n$ coefficients. The polynomials S_{i-1} and S_i interpolate the same value at the point t_i

$$S_{i-1}(t_i) = y_i = S_i(t_i) \quad (1 \leq i \leq n-1)$$

Hence, S is automatically continuous. Moreover, S' and S'' are assumed to be continuous, and these conditions will be used in the derivation of the cubic function. The continuity of S' and S'' provides the $2(n-1)$ conditions. On each interval $[t_i, t_{i+1}]$, there are 2 interpolating conditions, $S(t_i) = y_i$ and $S_{i+1} = y_{i+1}$, giving $2n$ conditions. Thus there are altogether $4n-2$ conditons for determining $4n$ coefficients. Two degrees of freedom remain.

Spline Interpolation

Now we derive the equation for $S_i(x)$ on the interval $[t_i, t_{i+i}]$. First we define the numbers

$$z_i = \lim_{x \to t_i} S_i''(x) = \lim_{x \to t_i} S_{i+1}''(x)$$

Since S_i is a cubic polynomial on $[t_i, t_{i+1}]$, S'' is a linear function satisfying $S_i''(t_i) = z_i$ and $S_i''(t_{i+i}) = z_{i+1}$ and therefore is given by

$$S_i''(x) = \frac{z_i}{h_i}(t_{i+1} - x) + \frac{z_{i+1}}{h_i}(x - t_i)$$

where $h_i \equiv t_{i+1} - t_i$. If this is integrated twice,

$$S_i(x) = \frac{z_i}{6h_i}(t_{i+1} - x)^3 + \frac{z_{i+1}}{6h_i}(x - t_i)^3 + C(x - t_i) + D(t_{i+1} - x)$$

where C and D are constants of integration. The interpolation conditions $S_i(t_i) = y_i$ and $S_i(t_{i+1}) = y_{i+1}$ can now be imposed on S_i to determine C and D.

Spline Interpolation

The result is

$$S_i(x) = \frac{z_i}{6h_i}(t_{i+1}-x)^3 + \frac{z_{i+1}}{6h_i}(x-t_i)^3 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}h_i}{6}\right)(x-t_i) + \left(\frac{y_i}{h_i} - \frac{z_i h_i}{6}\right)(t_{i+1}-x)$$

To determine $z_1, z_2, \cdots, z_{n-1}$, we use the continuity conditions for S'. At the interior knots t_i, we must have $S'_{i-1}(t_i) = S'_i(t_i)$. Note that

$$S'_i(t_i) = -\frac{h_i}{3}z_i - \frac{h_i}{6}z_{i+1} - \frac{y_i}{h_i} + \frac{y_{i+1}}{h_i}$$

$$S'_{i-1}(t_i) = -\frac{h_{i-1}}{3}z_{i-1} + \frac{h_{i-1}}{3}z_i - \frac{y_{i-1}}{h_{i-1}} + \frac{y_i}{h_{i-1}}$$

The unknowns $\{z_i\}_{i=0}^n$ satisfies

$$h_{i-1}z_{i-1} + 2(h_i + h_{i-1})z_i + h_i z_{i+1} = \frac{6}{h_i}(y_{i+1}-y_i) - \frac{6}{h_{i-1}}(y_i - y_{i-1})$$

for $i = 1, 2, \cdots, n-1$. One excellent choice is $z_0 = z_n = 0$. The resulting spline function is called a natural cubic spline.

Let f'' be continuous in $[a, b]$ and let $a = t_0 < t_1 < \cdots < t_n = b$. If S is the natural cubic spline interpolating f at the knots t_i for $0 \leq i \leq n$ then

$$\int_a^b |S''(x)|^2 dx \leq \int_a^b |f''(x)|^2 dx$$

Proof. Let $g = f - S$. Then $g(t_i) = 0$ for $0 \leq i \leq n$ and

$$\int_a^b (f'')^2 dx = \int_a^b (S'')^2 dx + \int_a^b (g'')^2 dx + 2\int_a^b S''g'' dx$$

$$\begin{aligned}
\int_a^b S''g'' dx &= \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} S''g'' dx \\
&= \sum_{i=1}^{n} \left(\Big[(S''g')(t_i) - (S''g')(t_{i-1}) \Big] - \int_{t_{i-1}}^{t_i} S'''g' dx \right) \\
&= -\sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} S'''g' dx = -\sum_{i=1}^{n} c_i \int_{t_{i-1}}^{t_i} g' dx = 0
\end{aligned}$$

Exercises: P.327

6,7,8,13