Chapter 5
Interpolation

Polynomial approximation

Let us consider an integral of a given function \( f(x) \). We want to approximate \( f(x) \) by a polynomial \( p_n(x) \) of degree \( n \):

\[
\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx.
\]

One way to find such an approximation is to use the Taylor series:

\[
p_n(x) = f(a) + f'(a)(x-a) + \frac{1}{2} f''(a)(x-a)^2 + \cdots + \frac{1}{n!} f^{(n)}(a)(x-a)^n.
\]

**Example 1.** The function \( f(x) = \frac{1}{1 + 9x^2} \) is easy to expand if we recall that \((1-r)(1+r+r^2+\cdots) = 1\) and so, the geometric series \( \frac{1}{1-r} = 1 + r + r^2 + \cdots \) converges for \(|r| < 1\). We obtain

\[
\frac{1}{1 + 9x^2} = \frac{1}{1 - (-9x^2)} = 1 + (-9x^2) + (-9x^2)^2 + \cdots \text{ for } |x| < 1/3.
\]

In this case, we have \( p_0 = 1, p_2 = 1 - 9x^2, p_4 = 1 - 9x^2 + 81x^4 \), and so on.

The Taylor polynomial \( p_n(x) \) is a good approximation to \( f(x) \) when \( x \) is close to \( a \). In general, however, we need to consider other methods.

Polynomial interpolation

**Theorem 1.** Let \( x_0, x_1, \ldots, x_n \) be \( n + 1 \) distinct points. Then there exists a unique polynomial \( p_n(x) \) of degree \( \leq n \) which interpolates a given function \( f(x) \) at the given points such that

\[
p_n(x_i) = f(x_i) \quad \text{for } i = 0, 1, \ldots, n.
\]
Example 2. If \( n = 1 \) and we give \( x_0, x_1 \), we can choose the polynomial \( p_1 \) as
\[
p_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0} (x - x_0).
\]
In general \( f(x) \) and \( p_1(x) \) are different, but they agree at the given points, i.e., \( p_1(x_0) = f(x_0) \) and \( p_1(x_1) = f(x_1) \).

**Definition 1.** The \( k \)th \((k = 0, 1, \ldots, n)\) Lagrange polynomial is a polynomial of degree \( n \) defined by
\[
L_k(x) = \prod_{i=0}^{n} \left( \frac{x - x_i}{x_k - x_i} \right).
\]

**Remark 1.** We note that \( L_k(x_i) = \delta_{ik} \) for \( i = 0, 1, \ldots, n \).

For a given \( f(x) \), the Lagrange form of the interpolating polynomial is given by
\[
p_n(x) = f(x_0)L_0(x) + f(x_1)L_1(x) + \cdots + f(x_n)L_n(x) = \sum_{k=0}^{n} f(x_k)L_k(x).
\]

**Remark 2.** Note that \( p_n(x_i) = \sum_{k=0}^{n} f(x_k)L_k(x_i) = \sum_{k=0}^{n} f(x_k)\delta_{ik} = f(x_i) \) for \( i = 0, 1, \ldots, n \).

Example 3. For \( n = 1 \), we have
\[
L_0(x) = \frac{x - x_1}{x_0 - x_1}, \quad L_1(x) = \frac{x - x_0}{x_1 - x_0},
\]
and
\[
p_1(x) = f(x_0)L_0(x) + f(x_1)L_1(x) = f(x_0) \frac{x - x_1}{x_0 - x_1} + f(x_1) \frac{x - x_0}{x_1 - x_0}
= f(x_0) \frac{x - x_1 + x - x_1 - (x_0 - x_1)}{x_0 - x_1} + f(x_1) \frac{x - x_0}{x_1 - x_0}
= f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0} (x - x_0).
\]

Example 4. We consider the case \( n = 2 \) and for simplicity set \( x_0 = -1, x_1 = 0, x_2 = 1 \). We have
\[
L_0(x) = \left( \frac{x - x_1}{x_0 - x_1} \right) \left( \frac{x - x_2}{x_0 - x_2} \right) = \frac{(x - 0)(x - 1)}{(-1 - 0)(-1 - 1)} = \frac{1}{2}x^2 - \frac{1}{2}x,
\]
\[
L_1(x) = \left( \frac{x - x_0}{x_1 - x_0} \right) \left( \frac{x - x_2}{x_1 - x_2} \right) = \frac{(x - (-1))(x - 1)}{(0 - (-1))(0 - 1)} = -x^2 + 1,
\]
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\[ L_2(x) = \left( \frac{x-x_0}{x_2-x_0} \right) \left( \frac{x-x_1}{x_2-x_1} \right) = \frac{(x-(-1))(x-0)}{(1-(-1))(1-0)} = \frac{1}{2} x^2 + \frac{1}{2} x. \]

Hence,

\[ p_2(x) = f(-1) \left( \frac{1}{2} x^2 - \frac{1}{2} x \right) + f(0) \left( -x^2 + 1 \right) + f(1) \left( \frac{1}{2} x^2 + \frac{1}{2} x \right) \]

\[ = \frac{f(-1) - 2f(0) + f(1)}{2} x^2 + \frac{f(1) - f(-1)}{2} x + f(0). \]

In particular if \( f(x) = \frac{1}{1+9x^2} \), then

\[ p_2(x) = \frac{\frac{1}{10} - 2(1) + \frac{1}{10}}{2} x^2 + \frac{\frac{1}{10} - \frac{1}{10}}{2} x + 1 = \frac{9}{10} x^2 + 1. \] (5.2)

Note that \( 1 - 9x^2 \) in the previous section satisfies \( 1 - 9(0)^2 = f(0) \) but has \( 1 - 9(\pm 1)^2 = -8 \neq f(\pm 1) \).

Remark 3. The interpolating polynomial \( p_n(x) \) is unique, but \( p_n(x) \) can be written in different forms.

**Newton’s form**

We can rewrite the interpolating polynomial \( p_n(x) = a_0 + a_1 x + \cdots + a_n x^n \) using the interpolation points \( x_0, \ldots, x_{n-1} \) as

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

This form is called the Newton form. The coefficients are obtained by (5.1):

\[ a_0 = f(x_0), \quad a_0 + a_1 (x_1 - x_0) = f(x_1), \quad \text{etc.} \]

To explore the coefficients, let us introduce divided differences.

**Definition 2.** Let \( f \) be a function defined at the distinct points \( x_0, x_1, \ldots, x_n \). The \( k \)th divided difference (\( 0 \leq k \leq n \)) with respect to \( x_i, x_{i+1}, \ldots, x_{i+k} \) is given by

\[ f[x_i] = f(x_i), \]

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

For example, we have
We make use of the above relations, and introduce polynomials \( p_n(x) \) and \( q_n(x) \), which interpolate \( f(x) \) at \( x_0, \ldots, x_n \) and \( x_0, x_1, \ldots, x_{n-1} \), respectively. Theorem 2. The coefficients in Newton form of \( p_n(x) \) are given by

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

Therefore we have

\[
p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \cdots + f[x_0, x_1, \ldots, x_n](x - x_0) \cdots (x - x_{n-1}).
\]

Here,

\[
f[x_0] = f(x_0) = a_0, \quad f[x_1] = f(x_1), \quad f[x_2] = f(x_2), \quad \text{etc.},
\]

\[
f[x_0, x_1] = f[x_1] - f[x_0] = a_1, \quad f[x_1, x_2] = f[x_2] - f[x_1] = a_2, \quad \text{etc.}
\]

Proof. Suppose

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

We introduce polynomials \( p_{n-1}(x) \) which interpolates \( f(x) \) at \( x_0, \ldots, x_{n-1} \) and \( q_{n-1}(x) \) which interpolates \( f(x) \) at \( x_1, \ldots, x_n \). The degrees of \( p_{n-1} \) and \( q_{n-1} \) are at most \( n - 1 \). Hence,

\[
p_{n-1}(x) = f[x_0] + f[x_0, x_1](x - x_0) + \cdots + f[x_0, x_1, \ldots, x_{n-1}](x - x_0) \cdots (x - x_{n-2}),
\]

\[
q_{n-1}(x) = f[x_1] + f[x_1, x_2](x - x_1) + \cdots + f[x_1, x_2, \ldots, x_n](x - x_1) \cdots (x - x_{n-1}).
\]

We make \( g(x) \) as follows.

\[
g(x) = \frac{x - x_0}{x_n - x_0} q_{n-1}(x) + \frac{x_n - x}{x_n - x_0} p_{n-1}(x).
\]

Note that

\[
g(x_0) = p_{n-1}(x_0) = f(x_0), \quad g(x_n) = q_{n-1}(x_n) = f(x_n),
\]

and

\[
g(x_k) = \frac{x_k - x_0}{x_n - x_0} q_{n-1}(x_k) + \frac{x_n - x_k}{x_n - x_0} p_{n-1}(x_k) = \frac{x_k - x_0}{x_n - x_0} f(x_k) + \frac{x_n - x_k}{x_n - x_0} f(x_k) = f(x_k),
\]

where \( k = 1, 2, \ldots, n - 1 \). Therefore,

\[
g(x) = p_n(x) = a_0 + a_1 (x - x_0) + \cdots + a_n (x - x_0) \cdots (x - x_{n-1}).
\]

Using the expression for \( g(x) \), we obtain \( a_n \), which is the coefficient for \( x^n \), as
a_n = \frac{f[x_1, \ldots, x_n]}{x_n - x_0} - \frac{f[x_0, \ldots, x_{n-1}]}{x_n - x_0} = f[x_0, \ldots, x_n].

Indeed a_0 = f[x_0] for k = 0. Thus we recursively show that
\[ a_k = f[x_0, x_1, \ldots, x_k], \quad k = 0, 1, \ldots, n. \]

\[ \Box \]

Example 5. For \( f(x) = \frac{1}{1 + 9x^2} \), \( x_0 = -1, x_1 = 0, x_2 = 1 \), we have
\[ p_2(x) = f[x_0] + f[x_0, x_1](x-x_0) + f[x_0, x_1, x_2](x-x_0)(x-x_1). \]

Divided differences are computed as follows.
\[ f[x_0] = f(-1) = \frac{1}{10}, \quad f[x_1] = f(0), \quad f[x_2] = f(1), \]
\[ f[x_0, x_1] = \frac{f(0) - f(-1)}{0 - (-1)} = \frac{9}{10}, \quad f[x_1, x_2] = \frac{f(1) - f(0)}{1 - 0}, \]
\[ f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{1 - (-1)} = -\frac{9}{10}. \]

Hence,
\[ p_2(x) = \frac{1}{10} + \frac{9}{10}(x+1) - \frac{9}{10}(x+1)x. \] (5.3)

We can easily check that (5.2) = (5.3).

Optimal interpolation points

We have obtained \( p_2(x) = -\frac{9}{10}x^2 + 1 \) as an interpolating polynomial for \( f(x) = (1 + 9x^2)^{-1} \). Consider the following integrals.
\[ \int_{-1}^{1} f(x) \, dx = \left[ \frac{1}{3} \tan^{-1}(3x) \right]_{-1}^{1} = \frac{2}{3} \tan^{-1}(3) = 0.832697, \] (5.4)
\[ \int_{-1}^{1} p_2(x) \, dx = \frac{7}{5} = 1.4. \]

Thus \( p_2(x) \) is a poor approximation to \( f(x) \). Here we will consider how we can do better.

First, we try increasing \( n \). We have
\[ n = 2 \Rightarrow x_0 = -1, \ x_1 = 0, \ x_2 = 1, \]
\[ n = 4 \Rightarrow x_0 = -1, \ x_1 = -0.5, \ x_2 = 0, \ x_3 = 0.5, \ x_4 = 1, \]
\[ n = 8 \Rightarrow x_i = -1 + 0.25i, \quad i = 0, 1, \ldots, 8 \]
\[ n = 16 \Rightarrow x_i = -1 + 0.125i, \quad i = 0, 1, \ldots, 16. \]

We obtain
\[
\int_{-1}^{1} p_4(x) \, dx = 0.735385,
\]
\[
\int_{-1}^{1} p_8(x) \, dx = 0.738204,
\]
\[
\int_{-1}^{1} p_{16}(x) \, dx = 0.667583.
\]

The approximations are still not good.

Given \( f(x) \) on \(-1 \leq x \leq 1\), we consider two options to choose the interpolation points \( x_0, \ldots, x_n \). In uniform points, we take \( x_i \) as
\[
x_i = -1 + ih, \quad h = \frac{2}{n}, \quad i = 0, 1, \ldots, n.
\]

We can also choose \( x_i \) as follows.

**Chebyshev points:**
\[
x_i = -\cos \theta_i, \quad \theta_i = ih, \quad h = \frac{\pi}{n}, \quad i = 0, 1, \ldots, n.
\]

The Chebyshev points are clustered near the endpoints of the interval.

We have
\[
\begin{align*}
n = 2 \Rightarrow \theta_0 &= 0, \ \theta_1 = \frac{\pi}{2}, \ \theta_2 = \pi, \\
n = 4 \Rightarrow \theta_0 &= 0, \ \theta_1 = \frac{\pi}{4}, \ \theta_2 = \frac{\pi}{2}, \ \theta_3 = \frac{3\pi}{4}, \ \theta_4 = \pi, \\
n = 8 \Rightarrow \theta_i &= \frac{i\pi}{8}, \quad i = 0, 1, \ldots, 8 \\
n = 16 \Rightarrow \theta_i &= \frac{i\pi}{16}, \quad i = 0, 1, \ldots, 16.
\end{align*}
\]

For these Chebyshev points, we obtain
\[\int_{-1}^{1} p_2(x) dx = 1.4,\]
\[\int_{-1}^{1} p_4(x) dx = 1.00727,\]
\[\int_{-1}^{1} p_8(x) dx = 0.844188,\]
\[\int_{-1}^{1} p_{16}(x) dx = 0.832759.\] (5.5)

We see that (5.5) \(\approx\) (5.4).

Let us look at numerical results. In Fig. 5.1, interpolations for \(f(x) = \frac{1}{1 + 9x^2}\) are shown. Let us also look at results from similar functions. In Fig. 5.2 and Fig. 5.3, we plot interpolations for \(f(x) = \frac{1}{1 + 25x^2}\) and \(f(x) = \frac{1}{1 + 64x^2}\).

**Error analysis**

**Theorem 3.** Let \(p_n(x)\) be the interpolating polynomial for a given smooth function \(f(x)\) with interpolation points \(x_0, \ldots, x_n\). Then for each \(x \in [x_0, x_n]\) there exists \(\xi(x) \in [x_0, x_n]\) such that

\[f(x) = p_n(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \omega_{n+1}(x), \quad \omega_{n+1}(x) = (x-x_0)(x-x_1)\cdots(x-x_n).\]

**Proof.** For each \(x\), we consider

\[g(t) = f(t) - p_n(t) - [f(x) - p_n(x)]\prod_{i=0}^{n} \frac{t-x_i}{x-x_i}, \quad x_0 \leq x \leq x_n.\]

Note that

\[g(x_j) = f(x_j) - p_n(x_j) - 0 = 0, \quad j = 0, 1, \ldots, n,\]

and

\[g(x) = f(x) - p_n(x) - [f(x) - p_n(x)] \cdot 1 = 0.\]

Therefore \(g(t)\) has \(n+2\) roots on \([x_0, x_n]\). By repeatedly using Rolle’s theorem\(^1\), we see that there exists \(\xi \in [x_0, x_n]\) such that

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\(^1\) If \(f\) is continuous on \([a, b]\) and differentiable on \((a, b)\) with \(f(a) = f(b) = 0\), then there exists \(c \in (a, b)\) such that \(f'(c) = 0\).
Fig. 5.1 Interpolating polynomials for the function $f(x) = \frac{1}{1 + 9x^2}$.

Since $p_n(x)$ is a polynomial of degree at most $n$, we have $p_n^{(n+1)}(x) = 0$. Furthermore we have

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

Thus,

$$g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - [f(x) - p_n(x)] \frac{(n + 1)!}{(x - x_0) \cdots (x - x_n)} = 0.$$ 

Solving this equation for $f(x)$ completes the proof. □
Example 6. Let us consider

\[ f(x) = \frac{1}{1 + (kx)^2}, \quad x \in [-1, 1]. \]

In Fig. 5.1 (k = 3), Fig. 5.2 (k = 5), and Fig. 5.3 (k = 8), we see oscillation near the endpoints for uniform points. This is called the Runge phenomenon. Runge observed that

\[ \lim_{n \to \infty} \| f - p_n \|_\infty = \infty \quad \text{for } k > k_c, \quad k_c \approx 3.63. \]

Such oscillation is due to \( \omega_{n+1}(x) \), takes large absolute values near the endpoints of the interval.
Let us try to qualitatively understand the Runge phenomenon, i.e., oscillation near the endpoints in the above example. According to the above-mentioned theorem, the error at $x$ is given by

$$|f(x) - p_n(x)| = \frac{f^{(n+1)}(\xi)}{(n+1)!} \omega_{n+1}(x).$$

Since $\omega_{n+1}(x)$ is a polynomial of degree $n + 1$, $|\omega_{n+1}(x)| \to \infty$ as $|x| \to \infty$. The polynomial $\omega_{n+1}(x)$ has $n + 1$ distinct roots between $x_0$ and $x_n$, and so $|\omega_{n+1}(x)|$ doesn’t become too big on $[x_0, x_n]$. This is the first observation. In Fig. 5.4, we plot $\omega_5(x)$, $\omega_9(x)$, and $\omega_{17}(x)$ for uniform points and Chebyshev points. For Chebyshev points, many of $x_0, x_1, \ldots, x_n$ come near the endpoints to suppress oscillation. Secondly, let us take a look at $f^{(n+1)}(\xi)$. We consider the polynomial approximation by the
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Taylor series. This is not a polynomial interpolation but we expect that qualitative behavior can be captured. We have \[ 1 + (kx)^2 = 1 + [-1(kx)^2] + [-1(kx)^2]^2 + \cdots. \]
Thus we notice that the coefficients get larger and larger for higher-order terms. This implies \(|f^{(n+1)}(\xi)|\) is large for large \(n\). Of course if we consider functions other than \[ 1 + (kx)^2 - 1, \quad |f^{(n+1)}(\xi)| \] is not necessarily large. By these considerations, we can qualitatively understand the Runge phenomenon. This is a famous oscillation as well as the Gibbs phenomenon\(^2\).

Piecewise linear interpolation

Suppose a function \(f(x)\) is given on \(a \leq x \leq b\). We take \(n + 1\) distinct points as
\[ a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b. \]
The interpolating polynomial \(p_n(x)\) may not be a good approximation to \(f(x)\) on the entire interval. Therefore we consider the piecewise linear interpolation \(q(x)\).

We construct \(q(x)\) as follows by making a linear polynomial interpolation in each interval.
\[ q(x) = f[x_i] + f[x_i, x_{i+1}] (x - x_i), \quad \text{on } x_i \leq x \leq x_{i+1}. \]

We note that
\[ q(x_i) = f(x_i), \quad i = 0, 1, \ldots, n. \]
We also note that \(q(x)\) is continuous but it is not necessarily differentiable at \(x = x_i\).

We can estimate the error as follow.

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\(^2\) The Gibbs phenomenon is oscillation which shows up at discontinuities. For example, let us consider the function \(f(x)\): \[ f(x) = x - 2nL, \quad \text{on } [(2n-1)L, (2n+1)L), \quad n = 0, \pm 1, \pm 2, \ldots. \]

We express \(f(x)\) with the Fourier series:
\[ f(x) = A_0 + \sum_{n=1}^{\infty} \left( A_n \cos \frac{n\pi x}{L} + B_n \sin \frac{n\pi x}{L} \right), \]
where
\[ A_0 = \frac{1}{2L} \int_{-L}^{L} f(x) dx, \quad A_n = \frac{1}{L} \int_{-L}^{L} f(x) \cos \frac{n\pi x}{L} dx, \quad B_n = \frac{1}{L} \int_{-L}^{L} f(x) \sin \frac{n\pi x}{L} dx. \]

In practice, the sum is taken up to some finite number \(N\) and \(\sum_{n=1}^{\infty}\) is replaced by \(\sum_{n=1}^{N}\). There appear strong oscillations near discontinuities at \(x = (2n-1)L\) even for large \(N\). This is called the Gibbs phenomenon.
\[ |f(x) - q(x)| \leq \frac{1}{8} \max_{a \leq x \leq b} |f''(x)| \max_{0 \leq i \leq n} |x_{i+1} - x_i|^2. \]

Hence \( q(x) \) is second-order accurate.

**Spline interpolation**

Let \( x_0 < x_1 < \cdots < x_{n-1} < x_n \). A cubic spline is a function \( s(x) \) satisfying the following conditions.\(^3\)

1. \( s(x) \) is a cubic polynomial on each interval \( x_i \leq x \leq x_{i+1} \).
2. \( s(x) \) interpolates \( f(x) \) at \( x_0, \ldots, x_n \).
3. \( s(x), s'(x), s''(x) \) are continuous at the interior points \( x_1, \ldots, x_{n-1} \).

**Example 7.** The function \( s(x) \) with \( x_0 = -1, x_1 = 0, x_2 = 1 \) below is an example of a cubic spline.

\[
s(x) = \begin{cases} 
0, & -1 \leq x \leq 0, \\
x^3, & 0 \leq x \leq 1.
\end{cases}
\]

We can check that \( s(x) \) satisfies the above conditions 1 and 3.

For given function \( f(x) \) and \( x_0 < x_1 < \cdots < x_{n-1} < x_n \), let us consider how we can find the cubic spline \( s(x) \) that interpolates \( f(x) \) at the given points, i.e., \( s(x_i) = f(x_i) \), \( i = 0, 1, \ldots, n \).

On each interval \( x_i \leq x \leq x_{i+1} \) \((i = 0, 1, \ldots, n-1)\), we can write

\[
s(x) = s_i(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3.
\]

There are \( 4n \) unknown coefficients as a total. On each interval, we have two equations \( s(x_i) = f(x_i) \) and \( s(x_{i+1}) = f(x_{i+1}) \), and so there are \( 2n \) equations on the entire region. Moreover since \( s'(x) \) and \( s''(x) \) must be continuous at \( x = x_1, \ldots, x_{n-1} \), there are \( 2(n-1) \) equations. Thus we have \( 4n - 2 \) equations as a total. Hence we can impose two more conditions. Let us choose (although other choices are possible)

\[
s''(x_0) = s''(x_n) = 0.
\]

This choice gives the natural cubic spline interpolant.

For uniform points on \([-1, 1]\), let us determine the cubic spline. We note that

\[
x_i = -1 + ih, \quad h = \frac{2}{n}, \quad i = 0, 1, \ldots, n.
\]

**Step 1:** We first focus on \( s''(x) \). Since \( s(x) \) is (at most) of degree 3, \( s''(x) \) is a linear polynomial. Using unknown constants \( a_i, a_{i+1} \), we can write

\[^3\text{A function which satisfies conditions 1. and 3. is said to be a cubic spline. Here, of course, we consider interpolation with cubic splines. So, we also impose condition 2.}\]
Recall that we imposed Step 4: The above equation is summarized as

$$s''_i(x) = a_i \left( \frac{x_{i+1} - x}{h} \right) + a_{i+1} \left( \frac{x - x_i}{h} \right), \quad i = 0, 1, \ldots, n - 1.$$  

Note that $s'_i(x_i) = a_i$ and $s''_i(x_{i+1}) = a_{i+1}$. This implies that $s''_{i-1}(x_i) = a_i = s''_i(x_i)$. Thus $s''(x)$ is continuous at the interior points $x_1, \ldots, x_{n-1}$.

**Step 2:** By integrating $s''_i(x)$ twice, we obtain

$$s_i(x) = \frac{a_i(x_{i+1} - x)^3}{6h} + \frac{a_{i+1}(x - x_i)^3}{6h} + b_i \left( \frac{x_{i+1} - x}{h} \right) + c_i \left( \frac{x - x_i}{h} \right), \quad (5.6)$$  

where $b_i, c_i$ are constants. We have

$$s_i(x_i) = \frac{a_i h^2}{6} + b_i = f_i, \quad s_i(x_{i+1}) = \frac{a_{i+1} h^2}{6} + c_i = f_{i+1}.$$  

Hence,

$$b_i = f_i - \frac{a_i h^2}{6}, \quad c_i = f_{i+1} - \frac{a_{i+1} h^2}{6}.$$  

**Step 3:** By differentiating $s_i(x)$, we obtain

$$s'_i(x) = -\frac{a_i(x_{i+1} - x)^2}{2h} + \frac{a_{i+1}(x - x_i)^2}{2h} + \left( f_i - \frac{a_i h^2}{6} \right) - \frac{1}{h} + \left( f_{i+1} - \frac{a_{i+1} h^2}{6} \right) \frac{1}{h}.$$  

Since $s'_{i-1}(x_i) = s'_i(x_i)$ ($i = 1, \ldots, n - 1$) must be satisfied, we have

$$a_i h + \frac{f_{i-1}}{6} - \frac{a_i h}{6} + \frac{f_i}{6} - a_i h + \frac{a_i h}{6} = \frac{a_i h}{2} + \frac{f_i}{6} + \frac{a_i h}{6} + \frac{f_{i+1}}{6} - \frac{a_{i+1} h}{6}.$$  

The above equation is summarized as

$$a_{i-1} + 4a_i + a_{i+1} = \frac{6}{h^2} \left( f_{i-1} - 2f_i + f_{i+1} \right).$$  

**Step 4:** Recall that we imposed $s'_0(x_0) = s''_{n-1}(x_n) = 0$. Boundary values $a_0, a_n$ are obtained as

$$s'_0(x_0) = a_0 = 0, \quad s''_{n-1}(x_n) = a_n = 0.$$  

Therefore we obtain the following matrix-vector equation.

$$A \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{n-2} \\ a_{n-1} \end{bmatrix} = \frac{6}{h^2} \begin{bmatrix} f_0 - 2f_1 + f_2 \\ f_1 - 2f_2 + f_3 \\ \vdots \\ f_{n-3} - 2f_{n-2} + f_{n-1} \\ f_{n-2} - 2f_{n-1} + f_n \end{bmatrix}.$$
Here the matrix $A$ is symmetric, tridiagonal, and positive definite.

**Step 5:** By solving the linear system, we obtain $a_i$, $i = 1, \ldots, n-1$ ($a_0, a_n$ are already known). Thus all coefficients $a_i, b_i, c_i$ in (5.6) are found. Hence we obtain $s(x)$.

The procedure how to find $s(x)$ may be summarized as follows.

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Write $s''<em>i(x)$ using $a_i, a</em>{i+1}$, so that $s''_{i-1}(x_i) = s''_i(x_i)$.</td>
</tr>
<tr>
<td>2</td>
<td>Integrate $s''_i(x)$ twice and find $b_i, c_i$ by using $s_i(x_i) = f_i$.</td>
</tr>
<tr>
<td>3</td>
<td>Get a three-term recurrence relation by $s'_{i-1}(x_i) = s'_i(x_i)$.</td>
</tr>
<tr>
<td>4</td>
<td>Obtain a matrix by boundary conditions $s''<em>0(x_0) = s''</em>{n-1}(x_n) = 0$.</td>
</tr>
<tr>
<td>5</td>
<td>Find $a_i$ by the linear system and obtain $s(x)$.</td>
</tr>
</tbody>
</table>

There are final comments. Firstly, the error is estimated as

$$|f(x) - s(x)| \leq \frac{5}{384} \max_{a \leq x \leq b} |f^{(4)}(x)| h^4.$$ 

Thus, it is 4th order accurate. Secondly, the natural cubic spline interpolant has inflection points at the endpoints of the interval because we impose the boundary conditions $s''(x_0) = s''(x_n) = 0$. There are also inflection points in the interior of the interval which do not exist in the original $f(x)$. These inflection points are problematic in some applications.
Fig. 5.4 The polynomial $\omega_5(x)$, $\omega_9(x)$, and $\omega_{17}(x)$ are plotted for uniform points and Chebyshev points.