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:

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b p_n(x)\mathrm{d}x.$$

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

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

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*

$$p_n(x_i) = f(x_i) \quad \textit{for } i = 0, 1, \ldots, n. \tag{5.1}$$

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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 $p_2(x_1) = f(x_1)$.

Definition 1. The kth ($k = 0,1,\dots,n$) Lagrange polynomial is a polynomial of degree n defined by

$$L_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \left(\frac{x-x_i}{x_k-x_i}\right).$$

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

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

Example 3. For $n=1$, we have

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

and

$$\begin{aligned} p_1(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) = f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0} \\ &= f(x_0)\frac{x_0-x_1+x-x_1-(x_0-x_1)}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0} \\ &= f(x_0) + \frac{f(x_1)-f(x_0)}{x_1-x_0}(x-x_0). \end{aligned}$$

Example 4. We consider the case $n=2$ and for simplicity set $x_0 = -1, x_1 = 0, x_2 = 1$. We have

$$L_0(x) = \left(\frac{x-x_1}{x_0-x_1}\right)\left(\frac{x-x_2}{x_0-x_2}\right) = \frac{(x-0)(x-1)}{(-1-0)(-1-1)} = \frac{1}{2}x^2 - \frac{1}{2}x,$$

$$L_1(x) = \left(\frac{x-x_0}{x_1-x_0}\right)\left(\frac{x-x_2}{x_1-x_2}\right) = \frac{(x-(-1))(x-1)}{(0-(-1))(0-1)} = -x^2+1,$$

$$L_2(x) = \left(\frac{x-x_0}{x_2-x_0}\right)\left(\frac{x-x_1}{x_2-x_1}\right) = \frac{(x-(-1))(x-0)}{(1-(-1))(1-0)} = \frac{1}{2}x^2 + \frac{1}{2}x.$$

Hence,

$$\begin{aligned} p_2(x) &= f(-1)\left(\frac{1}{2}x^2 - \frac{1}{2}x\right) + f(0)\left(-x^2+1\right) + f(1)\left(\frac{1}{2}x^2 + \frac{1}{2}x\right) \\ &= \frac{f(-1)-2f(0)+f(1)}{2}x^2 + \frac{f(1)-f(-1)}{2}x + f(0). \end{aligned}$$

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

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

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 kth 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

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

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,

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

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

$$f[x_0,x_1,x_2] = \frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0} = a_2, \quad f[x_1,x_2,x_3] = \frac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}, \quad \text{etc.}$$

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,

$$\begin{aligned} p_{n-1}(x) &= f[x_0] + f[x_0,x_1](x-x_0) + \cdots + f[x_0,x_1,\ldots,x_{n-1}](x-x_0)(x-x_1)\cdots(x-x_{n-2}), \\ q_{n-1}(x) &= f[x_1] + f[x_1,x_2](x-x_1) + \cdots + f[x_1,x_2,\ldots,x_n](x-x_1)(x-x_2)\cdots(x-x_{n-1}). \end{aligned}$$

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

$$g(x_0) = p_{n-1}(x_0) = f(x_0), \qquad g(x_n) = q_{n-1}(x_n) = f(x_n),$$

and

$$g(x_k) = \frac{x_k-x_0}{x_n-x_0} q_{n-1}(x_k) + \frac{x_n-x_k}{x_n-x_0} p_k(x_k) = \frac{x_k-x_0}{x_n-x_0} f(x_k) + \frac{x_n-x_k}{x_n-x_0} f(x_k) = f(x_k),$$

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

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

□

Example 5. For $f(x) = \dfrac{1}{1+9x^2}$, $x_0 = -1, x_1 = 0, x_2 = 1$, 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,

$$p_2(x) = \frac{1}{10} + \frac{9}{10}(x+1) - \frac{9}{10}(x+1)x. \tag{5.3}$$

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 $f(x) = \left(1+9x^2\right)^{-1}$. Consider the following integrals.

$$\int_{-1}^{1} f(x)\mathrm{d}x = \left[\frac{1}{3}\tan^{-1}(3x)\right]_{-1}^{1} = \frac{2}{3}\tan^{-1}(3) = 0.832697, \tag{5.4}$$

$$\int_{-1}^{1} p_2(x)\mathrm{d}x = \frac{7}{5} = 1.4.$$

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

$$
\begin{aligned}
n = 2 &\Rightarrow x_0 = -1,\ x_1 = 0,\ x_2 = 1, \\
n = 4 &\Rightarrow x_0 = -1,\ x_1 = -0.5,\ x_2 = 0,\ x_3 = 0.5,\ x_4 = 1, \\
n = 8 &\Rightarrow x_i = -1 + 0.25i, \quad i = 0, 1, \ldots, 8 \\
n = 16 &\Rightarrow x_i = -1 + 0.125i, \quad i = 0, 1, \ldots, 16.
\end{aligned}
$$

We obtain

$$
\begin{aligned}
\int_{-1}^{1} p_4(x)\mathrm{d}x &= 0.735385, \\
\int_{-1}^{1} p_8(x)\mathrm{d}x &= 0.738204, \\
\int_{-1}^{1} p_{16}(x)\mathrm{d}x &= 0.667583.
\end{aligned}
$$

The approximations are still not good.

Given $f(x)$ on $-1 \le x \le 1$, 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

$$
\begin{aligned}
n = 2 &\Rightarrow \theta_0 = 0,\ \theta_1 = \frac{\pi}{2},\ \theta_2 = \pi, \\
n = 4 &\Rightarrow \theta_0 = 0,\ \theta_1 = \frac{\pi}{4},\ \theta_2 = \frac{\pi}{2},\ \theta_3 = \frac{3\pi}{4},\ \theta_4 = \pi, \\
n = 8 &\Rightarrow \theta_i = \frac{i\pi}{8}, \quad i = 0, 1, \ldots, 8 \\
n = 16 &\Rightarrow \theta_i = \frac{i\pi}{16}, \quad i = 0, 1, \ldots, 16.
\end{aligned}
$$

For these Chebyshev points, we obtain

$$\int_{-1}^{1} p_2(x)\mathrm{d}x = 1.4,$$
$$\int_{-1}^{1} p_4(x)\mathrm{d}x = 1.00727,$$
$$\int_{-1}^{1} p_8(x)\mathrm{d}x = 0.844188,$$
$$\int_{-1}^{1} p_{16}(x)\mathrm{d}x = 0.832759. \tag{5.5}$$

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

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

Error analysis

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

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

Proof. For each x, we consider

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

Note that

$$g(x_j) = f(x_j) - p_n(x_j) - 0 = 0, \qquad j = 0,1,\dots,n,$$

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

[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 $f'(c) = 0$.

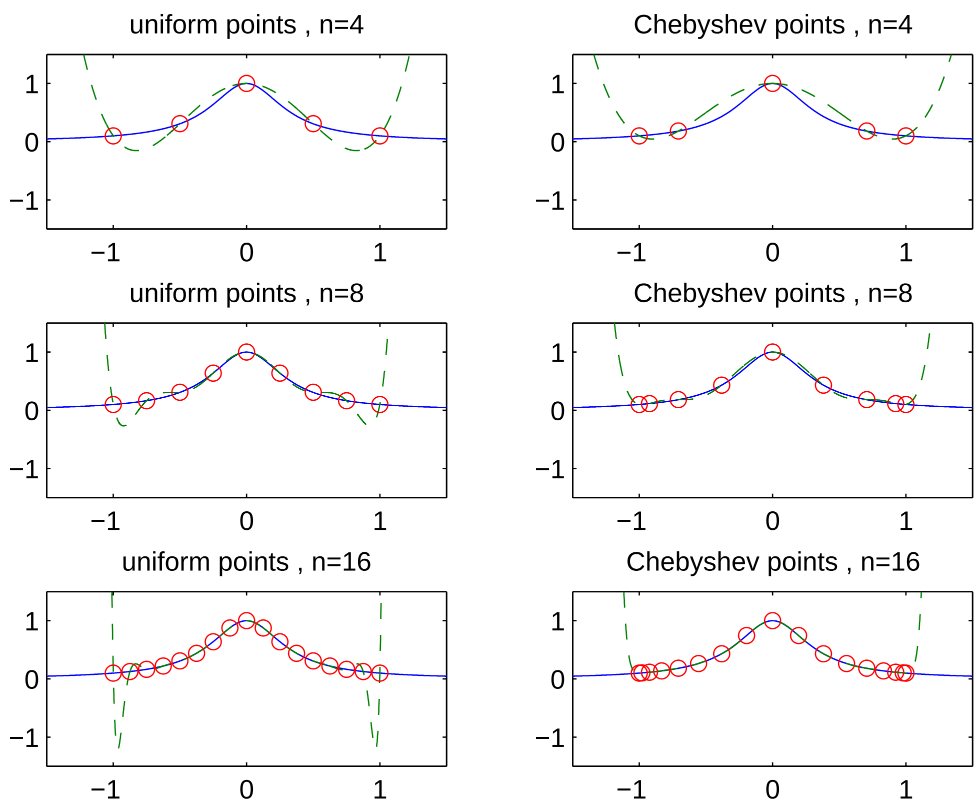

Fig. 5.1 Interpolating polynomials for the function $f(x) = \dfrac{1}{1+9x^2}$.

$$g^{(n+1)}(\xi) = 0.$$

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

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

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. □

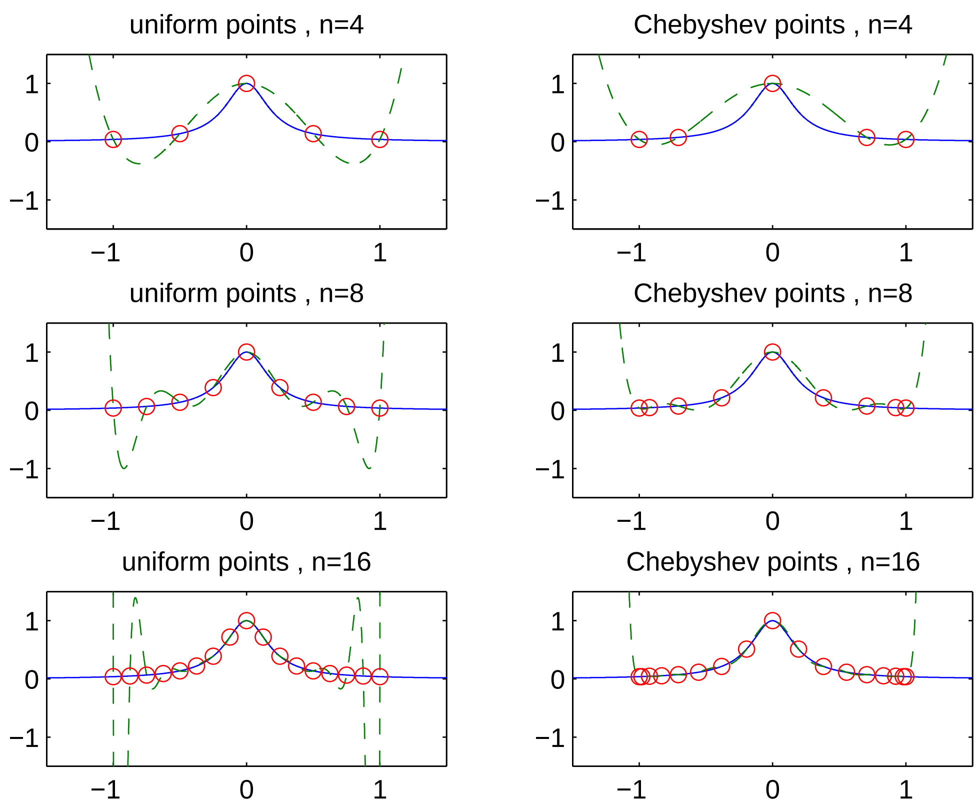

Fig. 5.2 Interpolating polynomials for the function $f(x) = \dfrac{1}{1+25x^2}$.

Example 6. Let us consider

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

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

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

Such oscillation is due to $\omega_{n+1}(x)$, takes large absolute values near the endpoints of the interval.

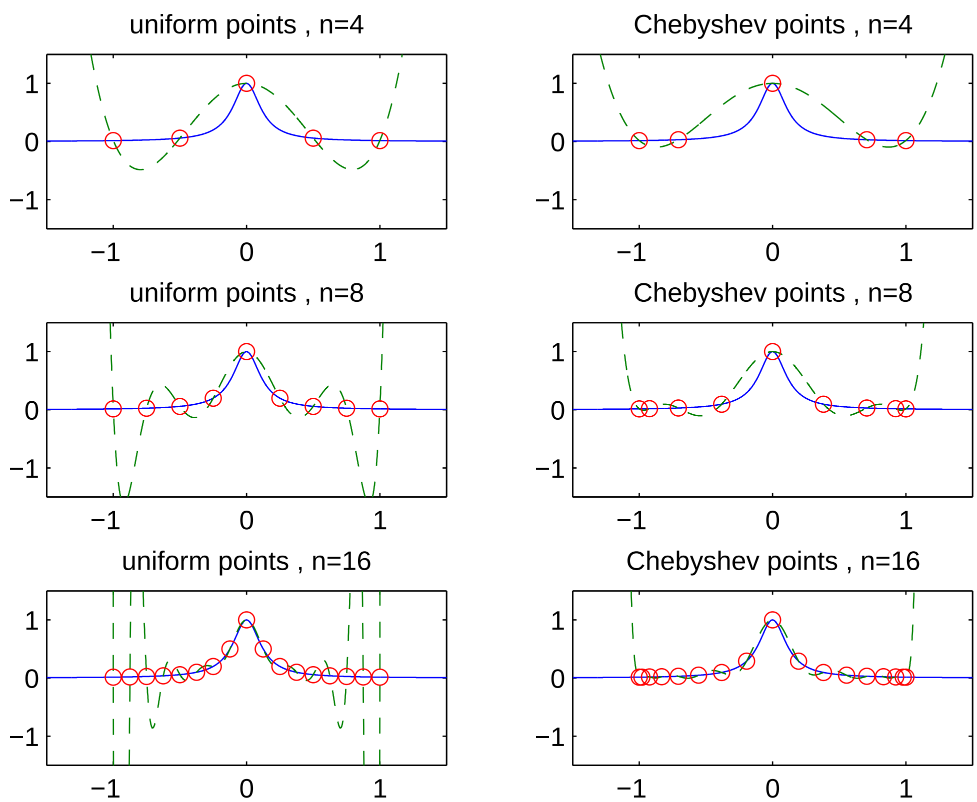

Fig. 5.3 Interpolating polynomials for the function $f(x) = \dfrac{1}{1+64x^2}$.

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

Taylor series. This is not a polynomial interpolation but we expect that qualitative behavior can be captured. We have $[1+(kx)^2]^{-1} = 1+[-(kx)^2]+[-(kx)^2]^2+\cdots$. 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 $[1+(kx)^2]^{-1}$, $|f^{(n+1)}(\xi)|$ 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 $a \le x \le b$. 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.

$$q(x) = f[x_i] + f[x_i, x_{i+1}](x - x_i), \quad \text{on } x_i \le x \le x_{i+1}.$$

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.

[2] The Gibbs phenomenon is oscillation which shows up at discontinuities. For example, let us consider the function $f(x)$:

$$f(x) = x - 2nL, \qquad \text{on } [(2n-1)L, (2n+1)L), \qquad n = 0, \pm 1, \pm 2, \ldots.$$

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

$$A_0 = \frac{1}{2L}\int_{-L}^{L} f(x)\mathrm{d}x, \quad A_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}\mathrm{d}x, \quad B_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}\mathrm{d}x.$$

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.

$$|f(x) - q(x)| \le \frac{1}{8} \max_{a\le x\le b} |f''(x)| \max_{0\le i\le n} |x_{i+1} - x_i|^2.$$

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 $x_i \le x \le x_{i+1}$.
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.

$$s(x) = \begin{cases} 0, & -1 \le x \le 0, \\ x^3, & 0 \le x \le 1. \end{cases}$$

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 $x_i \le x \le x_{i+1}$ $(i = 0, 1, \ldots, n-1)$, 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 $s_i''(x)$. Since $s(x)$ is (at most) of degree 3, $s_i''(x)$ is a linear polynomial. Using unknown constants a_i, a_{i+1}, we can write

[3] 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.

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

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

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

where b_i, c_i are constants. We have

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

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

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

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.

$$\overbrace{\begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 4 \end{pmatrix}}^{A} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{n-2} \\ a_{n-1} \end{pmatrix} = \frac{6}{h^2} \begin{pmatrix} f_0 - 2f_1 + f_2 \\ f_1 - 2f_2 + f_3 \\ \vdots \\ f_{n-3} - 2f_{n-2} + f_{n-1} \\ f_{n-2} - 2f_{n-1} + f_n \end{pmatrix}.$$

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.

Step 1	Write $s_i''(x)$ using a_i, a_{i+1}, so that $s_{i-1}''(x_i) = s_i''(x_i)$.
Step 2	Integrate $s_i''(x)$ twice and find b_i, c_i by using $s_i(x_i) = f_i$.
Step 3	Get a three-term recurrence relation by $s_{i-1}'(x_i) = s_i'(x_i)$.
Step 4	Obtain a matrix by boundary conditions $s_0''(x_0) = s_{n-1}''(x_n) = 0$.
Step 5	Find a_i by the linear system and obtain $s(x)$.

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

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

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.

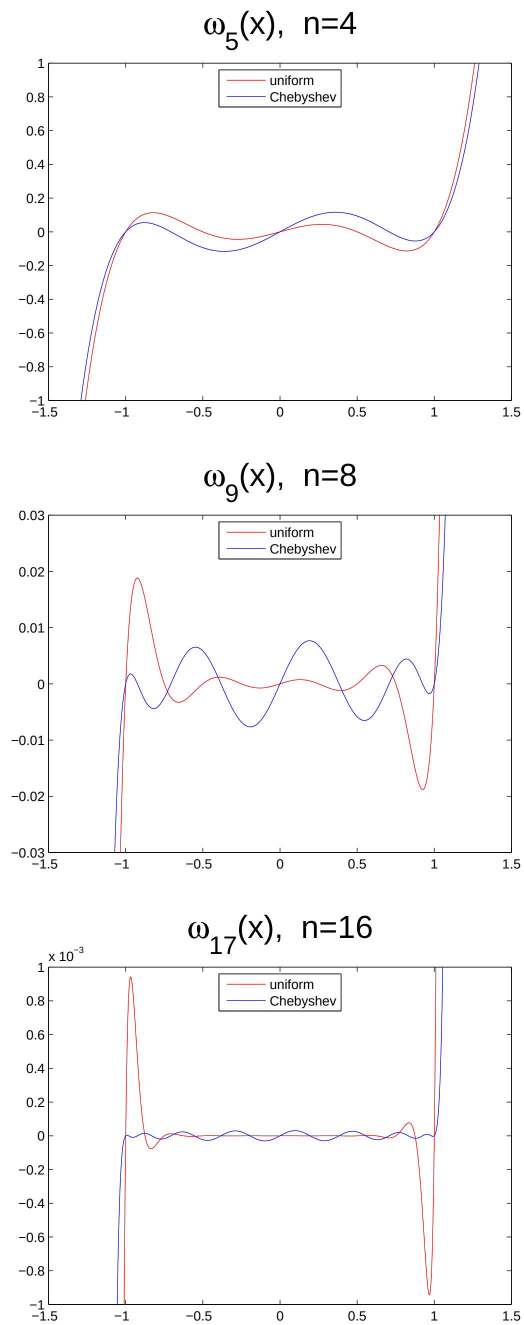

Fig. 5.4 The polynomial $\omega_5(x)$, $\omega_9(x)$, and $\omega_{17}(x)$ are plotted for uniform points and Chebyshev points.