

CHAPTER 9

Approximation of Functions

The class of polynomials is undoubtedly the simplest class of functions. In this chapter we shall discuss how to use polynomials to approximate continuous functions. Piecewise polynomial functions (splines) will also be discussed. Attention will be primarily confined to real-valued functions of a single variable x .

9.1. WEIERSTRASS APPROXIMATION

We may recall from Section 4.3 that if a function $f(x)$ has derivatives of all orders in some neighborhood of the origin, then it can be represented by a power series of the form $\sum_{n=0}^{\infty} a_n x^n$. If ρ is the radius of convergence of this series, then the series converges uniformly for $|x| \leq r$, where $r < \rho$ (see Theorem 5.4.4). It follows that for a given $\epsilon > 0$ we can take sufficiently many terms of this power series and obtain a polynomial $p_n(x) = \sum_{k=0}^n a_k x^k$ of degree n for which $|f(x) - p_n(x)| < \epsilon$ for $|x| \leq r$. But a function that is not differentiable of all orders does not have a power series representation. However, if the function is continuous on the closed interval $[a, b]$, then it can be approximated uniformly by a polynomial. This is guaranteed by the following theorem:

Theorem 9.1.1 (Weierstrass Approximation Theorem). Let $f: [a, b] \rightarrow \mathbb{R}$ be a continuous function. Then, for any $\epsilon > 0$, there exists a polynomial $p(x)$ such that

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

Proof. Without loss of generality we can consider $[a, b]$ to be the interval $[0, 1]$. This can always be achieved by making a change of variable of the form

$$t = \frac{x - a}{b - a}.$$

As x varies from a to b , t varies from 0 to 1. Thus, if necessary, we consider that such a linear transformation has been made and that t has been renamed as x .

For each n , let $b_n(x)$ be defined as a polynomial of degree n of the form

$$b_n(x) = \sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} f\left(\frac{k}{n}\right), \quad (9.1)$$

where

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

We have that

$$\sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} = 1, \quad (9.2)$$

$$\sum_{k=0}^n \frac{k}{n} \binom{n}{k} x^k (1-x)^{n-k} = x, \quad (9.3)$$

$$\sum_{k=0}^n \frac{k^2}{n^2} \binom{n}{k} x^k (1-x)^{n-k} = \left(1 - \frac{1}{n}\right) x^2 + \frac{x}{n}. \quad (9.4)$$

These identities can be shown as follows: Let Y_n be a binomial random variable $B(n, x)$. Thus Y_n represents the number of successes in a sequence of n independent Bernoulli trials with x the probability of success on a single trial. Hence, $E(Y_n) = nx$ and $\text{Var}(Y_n) = nx(1-x)$ (see, for example, Harris, 1966, page 104; see also Exercise 5.30). It follows that

$$\sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} = P(0 \leq Y_n \leq n) = 1. \quad (9.5)$$

Furthermore,

$$\sum_{k=0}^n k \binom{n}{k} x^k (1-x)^{n-k} = E(Y_n) = nx, \quad (9.6)$$

$$\begin{aligned} \sum_{k=0}^n k^2 \binom{n}{k} x^k (1-x)^{n-k} &= E(Y_n^2) = \text{Var}(Y_n) + [E(Y_n)]^2 \\ &= nx(1-x) + n^2 x^2 = n^2 \left[\left(1 - \frac{1}{n}\right) x^2 + \frac{x}{n} \right]. \end{aligned} \quad (9.7)$$

Identities (9.2)–(9.4) follow directly from (9.5)–(9.7).

Let us now consider the difference $f(x) - b_n(x)$, which with the help of identity (9.2) can be written as

$$f(x) - b_n(x) = \sum_{k=0}^n \left[f(x) - f\left(\frac{k}{n}\right) \right] \binom{n}{k} x^k (1-x)^{n-k}. \quad (9.8)$$

Since $f(x)$ is continuous on $[0, 1]$, then it must be bounded and uniformly continuous there (see Theorems 3.4.5 and 3.4.6). Hence, for the given $\epsilon > 0$, there exist numbers δ and m such that

$$|f(x_1) - f(x_2)| \leq \frac{\epsilon}{2} \quad \text{if } |x_1 - x_2| < \delta$$

and

$$|f(x)| < m \quad \text{for all } x \in [0, 1].$$

From formula (9.8) we then have

$$|f(x) - b_n(x)| \leq \sum_{k=0}^n \left| f(x) - f\left(\frac{k}{n}\right) \right| \binom{n}{k} x^k (1-x)^{n-k}.$$

If $|x - k/n| < \delta$, then $|f(x) - f(k/n)| < \epsilon/2$; otherwise, we have $|f(x) - f(k/n)| < 2m$ for $0 \leq x \leq 1$. Consequently, by using identities (9.2)–(9.4) we obtain

$$\begin{aligned} |f(x) - b_n(x)| &\leq \sum_{|x - k/n| < \delta} \frac{\epsilon}{2} \binom{n}{k} x^k (1-x)^{n-k} \\ &\quad + \sum_{|x - k/n| \geq \delta} 2m \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \frac{\epsilon}{2} + 2m \sum_{|x - k/n| \geq \delta} \frac{(k/n - x)^2}{(k/n - x)^2} \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \frac{\epsilon}{2} + \frac{2m}{\delta^2} \sum_{|x - k/n| \geq \delta} \left(\frac{k}{n} - x \right)^2 \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \frac{\epsilon}{2} + \frac{2m}{\delta^2} \sum_{k=0}^n \left(\frac{k^2}{n^2} - \frac{2kx}{n} + x^2 \right) \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \frac{\epsilon}{2} + \frac{2m}{\delta^2} \left[\left(1 - \frac{1}{n} \right) x^2 + \frac{x}{n} - 2x^2 + x^2 \right]. \end{aligned}$$

Hence,

$$\begin{aligned} |f(x) - b_n(x)| &\leq \frac{\epsilon}{2} + \frac{2m}{\delta^2} \frac{x(1-x)}{n} \\ &\leq \frac{\epsilon}{2} + \frac{m}{2n\delta^2}, \end{aligned} \quad (9.9)$$

since $x(1-x) \leq \frac{1}{4}$ for $0 \leq x \leq 1$. By choosing n large enough that

$$\frac{m}{2n\delta^2} < \frac{\epsilon}{2},$$

we conclude that

$$|f(x) - b_n(x)| < \epsilon$$

for all $x \in [0, 1]$. The proof of the theorem follows by taking $p(x) = b_n(x)$. $\square$

Definition 9.1.1. Let $f(x)$ be defined on $[0, 1]$. The polynomial $b_n(x)$ defined by formula (9.1) is called the Bernstein polynomial of degree n for $f(x)$. $\square$

By the proof of Theorem 9.1.1 we conclude that the sequence $\{b_n(x)\}_{n=1}^{\infty}$ of Bernstein polynomials converges uniformly to $f(x)$ on $[0, 1]$. These polynomials are useful in that they not only prove the existence of an approximating polynomial for $f(x)$, but also provide a simple explicit representation for it. Another advantage of Bernstein polynomials is that if $f(x)$ is continuously differentiable on $[0, 1]$, then the derivative of $b_n(x)$ converges also uniformly to $f'(x)$. A more general statement is given by the next theorem, whose proof can be found in Davis (1975, Theorem 6.3.2, page 113).

Theorem 9.1.2. Let $f(x)$ be p times differentiable on $[0, 1]$. If the p th derivative is continuous there, then

$$\lim_{n \rightarrow \infty} \frac{d^p b_n(x)}{dx^p} = \frac{d^p f(x)}{dx^p}$$

uniformly on $[0, 1]$.

Obviously, the knowledge that the sequence $\{b_n(x)\}_{n=1}^{\infty}$ converges uniformly to $f(x)$ on $[0, 1]$ is not complete without knowing something about the rate of convergence. For this purpose we need to define the so-called *modulus of continuity* of $f(x)$ on $[a, b]$.

Definition 9.1.2. If $f(x)$ is continuous on $[a, b]$, then, for any $\delta > 0$, the modulus of continuity of $f(x)$ on $[a, b]$ is

$$\omega(\delta) = \sup_{|x_1 - x_2| \leq \delta} |f(x_1) - f(x_2)|,$$

where x_1 and x_2 are points in $[a, b]$. $\square$

On the basis of Definition 9.1.2 we have the following properties concerning the modulus of continuity:

Lemma 9.1.1. If $0 < \delta_1 \leq \delta_2$, then $\omega(\delta_1) \leq \omega(\delta_2)$.

Lemma 9.1.2. For a function $f(x)$ to be uniformly continuous on $[a, b]$ it is necessary and sufficient that $\lim_{\delta \rightarrow 0} \omega(\delta) = 0$.

The proofs of Lemmas 9.1.1 and 9.1.2 are left to the reader.

Lemma 9.1.3. For any $\lambda > 0$, $\omega(\lambda\delta) \leq (\lambda + 1)\omega(\delta)$.

Proof. Suppose that $\lambda > 0$ is given. We can find an integer n such that $n \leq \lambda < n + 1$. By Lemma 9.1.1, $\omega(\lambda\delta) \leq \omega[(n + 1)\delta]$. Let x_1 and x_2 be two points in $[a, b]$ such that $x_1 < x_2$ and $|x_1 - x_2| \leq (n + 1)\delta$. Let us also divide the interval $[x_1, x_2]$ into $n + 1$ equal parts, each of length $(x_2 - x_1)/(n + 1)$, by means of the partition points

$$y_i = x_1 + i \frac{(x_2 - x_1)}{n + 1}, \quad i = 0, 1, \dots, n + 1.$$

Then

$$\begin{aligned} |f(x_1) - f(x_2)| &= |f(x_2) - f(x_1)| \\ &= \left| \sum_{i=0}^n [f(y_{i+1}) - f(y_i)] \right| \\ &\leq \sum_{i=0}^n |f(y_{i+1}) - f(y_i)| \\ &\leq (n + 1) \omega(\delta), \end{aligned}$$

since $|y_{i+1} - y_i| = [1/(n + 1)]|x_2 - x_1| \leq \delta$ for $i = 0, 1, \dots, n$. It follows that

$$\omega[(n + 1)\delta] = \sup_{|x_1 - x_2| \leq (n + 1)\delta} |f(x_1) - f(x_2)| \leq (n + 1) \omega(\delta).$$

Consequently,

$$\begin{aligned}\omega(\lambda\delta) &\leq \omega[(n+1)\delta] \leq (n+1)\omega(\delta) \\ &\leq (\lambda+1)\omega(\delta). \quad \square\end{aligned}$$

Theorem 9.1.3. Let $f(x)$ be continuous on $[0, 1]$, and let $b_n(x)$ be the Bernstein polynomial defined by formula (9.1). Then

$$|f(x) - b_n(x)| \leq \frac{3}{2} \omega\left(\frac{1}{\sqrt{n}}\right)$$

for all $x \in [0, 1]$, where $\omega(\delta)$ is the modulus of continuity of $f(x)$ on $[0, 1]$.

Proof. Using formula (9.1) and identity (9.2), we have that

$$\begin{aligned}|f(x) - b_n(x)| &= \left| \sum_{k=0}^n \left[f(x) - f\left(\frac{k}{n}\right) \right] \binom{n}{k} x^k (1-x)^{n-k} \right| \\ &\leq \sum_{k=0}^n \left| f(x) - f\left(\frac{k}{n}\right) \right| \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \sum_{k=0}^n \omega\left(\left|x - \frac{k}{n}\right|\right) \binom{n}{k} x^k (1-x)^{n-k}.\end{aligned}$$

Now, by applying Lemma 9.1.3 we can write

$$\begin{aligned}\omega\left(\left|x - \frac{k}{n}\right|\right) &= \omega\left(n^{1/2}\left|x - \frac{k}{n}\right|n^{-1/2}\right) \\ &\leq \left(1 + n^{1/2}\left|x - \frac{k}{n}\right|\right) \omega(n^{-1/2}).\end{aligned}$$

Thus

$$\begin{aligned}|f(x) - b_n(x)| &\leq \sum_{k=0}^n \left(1 + n^{1/2}\left|x - \frac{k}{n}\right|\right) \omega(n^{-1/2}) \binom{n}{k} x^k (1-x)^{n-k} \\ &\leq \omega(n^{-1/2}) \left[1 + n^{1/2} \sum_{k=0}^n \left|x - \frac{k}{n}\right| \binom{n}{k} x^k (1-x)^{n-k}\right].\end{aligned}$$

But, by the Cauchy–Schwarz inequality (see part 1 of Theorem 2.1.2), we have

$$\begin{aligned}
 & \sum_{k=0}^n \left| x - \frac{k}{n} \right| \binom{n}{k} x^k (1-x)^{n-k} \\
 &= \sum_{k=0}^n \left| x - \frac{k}{n} \right| \left[\binom{n}{k} x^k (1-x)^{n-k} \right]^{1/2} \left[\binom{n}{k} x^k (1-x)^{n-k} \right]^{1/2} \\
 &\leq \left[\sum_{k=0}^n \left(x - \frac{k}{n} \right)^2 \binom{n}{k} x^k (1-x)^{n-k} \right]^{1/2} \left[\sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} \right]^{1/2} \\
 &= \left[\sum_{k=0}^n \left(x - \frac{k}{n} \right)^2 \binom{n}{k} x^k (1-x)^{n-k} \right]^{1/2}, \quad \text{by identity (9.2)} \\
 &= \left[x^2 - 2x^2 + \left(1 - \frac{1}{n} \right) x^2 + \frac{x}{n} \right]^{1/2}, \quad \text{by identities (9.3) and (9.4)} \\
 &= \left[\frac{x(1-x)}{n} \right]^{1/2} \\
 &\leq \left[\frac{1}{4n} \right]^{1/2}, \quad \text{since } x(1-x) \leq \frac{1}{4}.
 \end{aligned}$$

It follows that

$$|f(x) - b_n(x)| \leq \omega(n^{-1/2}) \left[1 + n^{1/2} \left(\frac{1}{4n} \right)^{1/2} \right],$$

that is,

$$|f(x) - b_n(x)| \leq \frac{3}{2} \omega(n^{-1/2})$$

for all $x \in [0, 1]$. $\square$

We note that Theorem 9.1.3 can be used to prove Theorem 9.1.1 as follows: If $f(x)$ is continuous on $[0, 1]$, then $f(x)$ is uniformly continuous on $[0, 1]$. Hence, by Lemma 9.1.2, $\omega(n^{-1/2}) \rightarrow 0$ as $n \rightarrow \infty$.

Corollary 9.1.1. If $f(x)$ is a Lipschitz continuous function $\text{Lip}(K, \alpha)$ on $[0, 1]$, then

$$|f(x) - b_n(x)| \leq \frac{3}{2} K n^{-\alpha/2} \quad (9.10)$$

for all $x \in [0, 1]$.

Proof. By Definition 3.4.6,

$$|f(x_1) - f(x_2)| \leq K|x_1 - x_2|^\alpha$$

for all x_1, x_2 in $[0, 1]$. Thus

$$\omega(\delta) \leq K\delta^\alpha.$$

By Theorem 9.1.3 we then have

$$|f(x) - b_n(x)| \leq \frac{3}{2}Kn^{-\alpha/2}$$

for all $x \in [0, 1]$. □

Theorem 9.1.4 (Voronovsky's Theorem). If $f(x)$ is bounded on $[0, 1]$ and has a second-order derivative at a point x_0 in $[0, 1]$, then

$$\lim_{n \rightarrow \infty} n[b_n(x_0) - f(x_0)] = \frac{1}{2}x_0(1-x_0)f''(x_0).$$

Proof. See Davis (1975, Theorem 6.3.6, page 117). □

We note from Corollary 9.1.1 and Voronovsky's theorem that the convergence of Bernstein polynomials can be very slow. For example, if $f(x)$ satisfies the conditions of Voronovsky's theorem, then at every point $x \in [0, 1]$ where $f''(x) \neq 0$, $b_n(x)$ converges to $f(x)$ just like c/n , where c is a constant.

EXAMPLE 9.1.1. We recall from Section 3.4.2 that $f(x) = \sqrt{x}$ is $\text{Lip}(1, \frac{1}{2})$ for $x \geq 0$. Then, by Corollary 9.1.1,

$$|\sqrt{x} - b_n(x)| \leq \frac{3}{2n^{1/4}},$$

for $0 \leq x \leq 1$, where

$$b_n(x) = \sum_{k=0}^n \binom{n}{k} x^k (1-x)^{n-k} \left(\frac{k}{n}\right)^{1/2}.$$

9.2. APPROXIMATION BY POLYNOMIAL INTERPOLATION

One possible method to approximate a function $f(x)$ with a polynomial $p(x)$ is to select such a polynomial so that both $f(x)$ and $p(x)$ have the same values at a certain number of points in the domain of $f(x)$. This procedure is called interpolation. The rationale behind it is that if $f(x)$ agrees with $p(x)$ at some known points, then the two functions should be close to one another at intermediate points.

Let us first consider the following result given by the next theorem.

Theorem 9.2.1. Let $a_0, a_1, \dots, a_n$ be $n + 1$ distinct points in R , the set of real numbers. Let $b_0, b_1, \dots, b_n$ be any given set of $n + 1$ real numbers. Then, there exists a unique polynomial $p(x)$ of degree $\leq n$ such that $p(a_i) = b_i$, $i = 0, 1, \dots, n$.

Proof. Since $p(x)$ is a polynomial of degree $\leq n$, it can be represented as $p(x) = \sum_{j=0}^n c_j x^j$. We must then have

$$\sum_{j=0}^n c_j a_i^j = b_i, \quad i = 0, 1, \dots, n.$$

These equations can be written in vector form as

$$\begin{bmatrix} 1 & a_0 & a_0^2 & \cdots & a_0^n \\ 1 & a_1 & a_1^2 & \cdots & a_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & a_n & a_n^2 & \cdots & a_n^n \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}. \quad (9.11)$$

The determinant of the $(n + 1) \times (n + 1)$ matrix on the left side of equation (9.11) is known as Vandermonde's determinant and is equal to $\prod_{i > j} (a_i - a_j)$. The proof of this last assertion can be found in, for example, Graybill (1983, Theorem 8.12.2, page 266). Since the a_i 's are distinct, this determinant is different from zero. It follows that this matrix is nonsingular. Hence, equation (9.11) provides a unique solution for $c_0, c_1, \dots, c_n$. $\square$

Corollary 9.2.1. The polynomial $p(x)$ in Theorem 9.2.1 can be represented as

$$p(x) = \sum_{i=0}^n b_i l_i(x), \quad (9.12)$$

where

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - a_j}{a_i - a_j}, \quad i = 0, 1, \dots, n. \quad (9.13)$$

Proof. We have that $l_i(x)$ is a polynomial of degree n ($i = 0, 1, \dots, n$). Furthermore, $l_i(a_j) = 0$ if $i \neq j$, and $l_i(a_i) = 1$ ($i = 0, 1, \dots, n$). It follows that $\sum_{i=0}^n b_i l_i(x)$ is a polynomial of degree $\leq n$ and assumes the values $b_0, b_1, \dots, b_n$ at $a_0, a_1, \dots, a_n$, respectively. This polynomial is unique by Theorem 9.2.1. $\square$

Definition 9.2.1. The polynomial defined by formula (9.12) is called a *Lagrange interpolating polynomial*. The points $a_0, a_1, \dots, a_n$ are called points

of interpolation (or nodes), and $l_i(x)$ in formula (9.13) is called the i th Lagrange polynomial associated with the a_i 's. $\square$

The values $b_0, b_1, \dots, b_n$ in formula (9.12) are frequently the values of some function $f(x)$ at the points $a_0, a_1, \dots, a_n$. Thus $f(x)$ and the polynomial $p(x)$ in formula (9.12) attain the same values at these points. The polynomial $p(x)$, which can be written as

$$p(x) = \sum_{i=0}^n f(a_i)l_i(x), \quad (9.14)$$

provides therefore an approximation for $f(x)$ over $[a_0, a_n]$.

EXAMPLE 9.2.1. Consider the function $f(x) = x^{1/2}$. Let $a_0 = 60$, $a_1 = 70$, $a_2 = 85$, $a_3 = 105$ be interpolation points. Then

$$p(x) = 7.7460l_0(x) + 8.3666l_1(x) + 9.2195l_2(x) + 10.2470l_3(x),$$

where

$$\begin{aligned} l_0(x) &= \frac{(x-70)(x-85)(x-105)}{(60-70)(60-85)(60-105)}, \\ l_1(x) &= \frac{(x-60)(x-85)(x-105)}{(70-60)(70-85)(70-105)}, \\ l_2(x) &= \frac{(x-60)(x-70)(x-105)}{(85-60)(85-70)(85-105)}, \\ l_3(x) &= \frac{(x-60)(x-70)(x-85)}{(105-60)(105-70)(105-85)}. \end{aligned}$$

Table 9.1. Approximation of $f(x) = x^{1/2}$ by the Lagrange Interpolating Polynomial $p(x)$

x	$f(x)$	$p(x)$
60	7.74597	7.74597
64	8.00000	7.99978
68	8.24621	8.24611
70	8.36660	8.36660
74	8.60233	8.60251
78	8.83176	8.83201
82	9.05539	9.05555
85	9.21954	9.21954
90	9.48683	9.48646
94	9.69536	9.69472
98	9.89949	9.89875
102	10.09950	10.09899
105	10.24695	10.24695

Using $p(x)$ as an approximation of $f(x)$ over the interval $[60, 105]$, tabulated values of $f(x)$ and $p(x)$ were obtained at several points inside this interval. The results are given in Table 9.1.

9.2.1. The Accuracy of Lagrange Interpolation

Let us now address the question of evaluating the accuracy of Lagrange interpolation. The answer to this question is given in the next theorem.

Theorem 9.2.2. Suppose that $f(x)$ has n continuous derivatives on the interval $[a, b]$, and its $(n + 1)$ st derivative exists on (a, b) . Let $a = a_0 < a_1 < \dots < a_n = b$ be $n + 1$ points in $[a, b]$. If $p(x)$ is the Lagrange interpolating polynomial defined by formula (9.14), then there exists a point $c \in (a, b)$ such that for any $x \in [a, b]$, $x \neq a_i$ ($i = 0, 1, \dots, n$),

$$f(x) - p(x) = \frac{1}{(n + 1)!} f^{(n+1)}(c) g_{n+1}(x), \quad (9.15)$$

where

$$g_{n+1}(x) = \prod_{i=0}^n (x - a_i).$$

Proof. Define the function $h(t)$ as

$$h(t) = f(t) - p(t) - [f(x) - p(x)] \frac{g_{n+1}(t)}{g_{n+1}(x)}.$$

If $t = x$, then $h(x) = 0$. For $t = a_i$ ($i = 0, 1, \dots, n$),

$$h(a_i) = f(a_i) - p(a_i) - [f(x) - p(x)] \frac{g_{n+1}(a_i)}{g_{n+1}(x)} = 0.$$

The function $h(t)$ has n continuous derivatives on $[a, b]$, and its $(n + 1)$ st derivative exists on (a, b) . Furthermore, $h(t)$ vanishes at x and at all $n + 1$ interpolation points, that is, it has at least $n + 2$ different zeros in $[a, b]$. By Rolle's theorem (Theorem 4.2.1), $h'(t)$ vanishes at least once between any two zeros of $h(t)$ and thus has at least $n + 1$ different zeros in (a, b) . Also by Rolle's theorem, $h''(t)$ has at least n different zeros in (a, b) . By continuing this argument, we see that $h^{(n+1)}(t)$ has at least one zero in (a, b) , say at the point c . But,

$$\begin{aligned} h^{(n+1)}(t) &= f^{(n+1)}(t) - p^{(n+1)}(t) - \frac{f(x) - p(x)}{g_{n+1}(x)} g_{n+1}^{(n+1)}(t) \\ &= f^{(n+1)}(t) - \frac{f(x) - p(x)}{g_{n+1}(x)} (n + 1)!, \end{aligned}$$

since $p(t)$ is a polynomial of degree $\leq n$ and $g_{n+1}(t)$ is a polynomial of the form $t^{n+1} + \lambda_1 t^n + \lambda_2 t^{n-1} + \cdots + \lambda_{n+1}$ for suitable constants $\lambda_1, \lambda_2, \dots, \lambda_{n+1}$. We thus have

$$f^{(n+1)}(c) - \frac{f(x) - p(x)}{g_{n+1}(x)} (n+1)! = 0,$$

from which we can conclude formula (9.15). $\square$

Corollary 9.2.2. Suppose that $f^{(n+1)}(x)$ is continuous on $[a, b]$. Let $\tau_{n+1} = \sup_{a \leq x \leq b} |f^{(n+1)}(x)|$, $\kappa_{n+1} = \sup_{a \leq x \leq b} |g_{n+1}(x)|$. Then

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq \frac{\tau_{n+1} \kappa_{n+1}}{(n+1)!}.$$

Proof. This follows directly from formula (9.15) and the fact that $f(x) - p(x) = 0$ for $x = a_0, a_1, \dots, a_n$. $\square$

We note that κ_{n+1} , being the supremum of $|g_{n+1}(x)| = |\prod_{i=0}^n (x - a_i)|$ over $[a, b]$, is a function of the location of the a_i 's. From Corollary 9.2.2 we can then write

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq \frac{\phi(a_0, a_1, \dots, a_n)}{(n+1)!} \sup_{a \leq x \leq b} |f^{(n+1)}(x)|, \quad (9.16)$$

where $\phi(a_0, a_1, \dots, a_n) = \sup_{a \leq x \leq b} |g_{n+1}(x)|$. This inequality provides us with an upper bound on the error of approximating $f(x)$ with $p(x)$ over the interpolation region. We refer to this error as interpolation error. The upper bound clearly shows that the interpolation error depends on the location of the interpolation points.

Corollary 9.2.3. If, in Corollary 9.2.2, $n = 2$, and if $a_1 - a_0 = a_2 - a_1 = \delta$, then

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq \frac{\sqrt{3}}{27} \tau_3 \delta^3.$$

Proof. Consider $g_3(x) = (x - a_0)(x - a_1)(x - a_2)$, which can be written as $g_3(x) = z(z^2 - \delta^2)$, where $z = x - a_1$. This function is symmetric with respect to $x = a_1$. It is easy to see that $|g_3(x)|$ attains an absolute maximum over $a_0 \leq x \leq a_2$, or equivalently, $-\delta \leq z \leq \delta$, when $z = \pm \delta/\sqrt{3}$. Hence,

$$\begin{aligned} \kappa_3 &= \sup_{a_0 \leq x \leq a_2} |g_3(x)| = \max_{-\delta \leq z \leq \delta} |z(z^2 - \delta^2)| \\ &= \left| \frac{\delta}{\sqrt{3}} \left(\frac{\delta^2}{3} - \delta^2 \right) \right| = \frac{2}{3\sqrt{3}} \delta^3. \end{aligned}$$

By applying Corollary 9.2.2 we obtain

$$\sup_{a_0 \leq x \leq a_2} |f(x) - p(x)| \leq \frac{\sqrt{3}}{27} \tau_3 \delta^3.$$

We have previously noted that the interpolation error depends on the choice of the interpolation points. This leads us to the following important question: How can the interpolation points be chosen so as to minimize the interpolation error? The answer to this question lies in inequality (9.16). One reasonable criterion for the choice of interpolation points is the minimization of $\phi(a_0, a_1, \dots, a_n)$ with respect to $a_0, a_1, \dots, a_n$. It turns out that the optimal locations of $a_0, a_1, \dots, a_n$ are given by the zeros of the Chebyshev polynomial (of the first kind) of degree $n + 1$ (see Section 10.4.1). $\square$

Definition 9.2.2. The Chebyshev polynomial of degree n is defined by

$$\begin{aligned} T_n(x) &= \cos(n \operatorname{Arccos} x) \\ &= x^n + \binom{n}{2} x^{n-2} (x^2 - 1) + \binom{n}{4} x^{n-4} (x^2 - 1)^2 + \dots, \\ &\quad n = 0, 1, \dots. \end{aligned} \quad (9.17)$$

Obviously, by the definition of $T_n(x)$, $-1 \leq x \leq 1$. One of the properties of $T_n(x)$ is that it has simple zeros at the following n points:

$$\zeta_i = \cos \left[\frac{(2i-1)}{2n} \pi \right], \quad i = 1, 2, \dots, n. \quad \square$$

The proof of this property is given in Davis (1975, pages 61–62).

We can consider Chebyshev polynomials defined on the interval $[a, b]$ by making the transformation

$$x = \frac{a+b}{2} + \frac{b-a}{2} t,$$

which transforms the interval $-1 \leq t \leq 1$ into the interval $a \leq x \leq b$. In this case, the zeros of the Chebyshev polynomial of degree n over the interval $[a, b]$ are given by

$$z_i = \frac{a+b}{2} + \frac{b-a}{2} \cos \left[\left(\frac{2i-1}{2n} \right) \pi \right], \quad i = 1, 2, \dots, n.$$

We refer to the z_i 's as Chebyshev points. These points can be obtained geometrically by subdividing the semicircle over the interval $[a, b]$ into n

equal arcs and then projecting the midpoint of each arc onto the interval (see De Boor, 1978, page 26).

Chebyshev points have a very interesting property that pertains to the minimization of $\phi(a_0, a_1, \dots, a_n)$ in inequality (9.16). This property is described in Theorem 9.2.3, whose proof can be found in Davis (1975, Section 3.3); see also De Boor (1978, page 30).

Theorem 9.2.3. The function

$$\phi(a_0, a_1, \dots, a_n) = \sup_{a \leq x \leq b} \left| \prod_{i=0}^n (x - a_i) \right|,$$

where the a_i 's belong to the interval $[a, b]$, achieves its minimum at the zeros of the Chebyshev polynomial of degree $n + 1$, that is, at

$$z_i = \frac{a+b}{2} + \frac{b-a}{2} \cos \left[\left(\frac{2i+1}{2n+2} \right) \pi \right], \quad i = 0, 1, \dots, n, \quad (9.18)$$

and

$$\min_{a_0, a_1, \dots, a_n} \phi(a_0, a_1, \dots, a_n) = \frac{2(b-a)^{n+1}}{4^{n+1}}.$$

From Theorem 9.2.3 and inequality (9.16) we conclude that the choice of the Chebyshev points given in formula (9.18) is optimal in the sense of reducing the interpolation error. In other words, among all sets of interpolation points of size $n + 1$ each, Chebyshev points produce a Lagrange polynomial approximation for $f(x)$ over the interval $[a, b]$ with a minimum upper bound on the error of approximation. Using inequality (9.16), we obtain the following interesting result:

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq \frac{2}{(n+1)!} \left(\frac{b-a}{4} \right)^{n+1} \sup_{a \leq x \leq b} |f^{(n+1)}(x)|. \quad (9.19)$$

The use of Chebyshev points in the construction of Lagrange interpolating polynomial $p(x)$ for the function $f(x)$ over $[a, b]$ produces an approximation which, for all practical purposes, differs very little from the best possible approximation of $f(x)$ by a polynomial of the same degree. This was shown by Powell (1967). More explicitly, let $p^*(x)$ be the best approximating polynomial of $f(x)$ of the same degree as $p(x)$ over $[a, b]$. Then, obviously,

$$\sup_{a \leq x \leq b} |f(x) - p^*(x)| \leq \sup_{a \leq x \leq b} |f(x) - p(x)|.$$

De Boor (1978, page 31) pointed out that for $n \leq 20$,

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq 4 \sup_{a \leq x \leq b} |f(x) - p^*(x)|.$$

This indicates that the error of interpolation which results from the use of Lagrange polynomials in combination with Chebyshev points does not exceed the minimum approximation error by more than a factor of 4 for $n \leq 20$. This is a very useful result, since the derivation of the best approximating polynomial can be tedious and complicated, whereas a polynomial approximation obtained by Lagrange interpolation that uses Chebyshev points as interpolation points is simple and straightforward.

9.2.2. A Combination of Interpolation and Approximation

In Section 9.1 we learned how to approximate a continuous function $f: [a, b] \rightarrow \mathbb{R}$ with a polynomial by applying the Weierstrass theorem. In this section we have seen how to interpolate values of f on $[a, b]$ by using Lagrange polynomials. We now show that these two processes can be combined. More specifically, suppose that we are given $n + 1$ distinct points in $[a, b]$, which we denote by $a_0, a_1, \dots, a_n$ with $a_0 = a$ and $a_n = b$. Let $\epsilon > 0$ be given. We need to find a polynomial $q(x)$ such that $|f(x) - q(x)| < \epsilon$ for all x in $[a, b]$, and $f(a_i) = q(a_i)$, $i = 0, 1, \dots, n$.

By Theorem 9.1.1 there exists a polynomial $p(x)$ such that

$$|f(x) - p(x)| < \epsilon' \quad \text{for all } x \in [a, b],$$

where $\epsilon' < \epsilon/(1 + M)$, and M is a nonnegative number to be described later. Furthermore, by Theorem 9.2.1 there exists a unique polynomial $u(x)$ such that

$$u(a_i) = f(a_i) - p(a_i), \quad i = 0, 1, \dots, n.$$

This polynomial is given by

$$u(x) = \sum_{i=0}^n [f(a_i) - p(a_i)] l_i(x), \quad (9.20)$$

where $l_i(x)$ is the i th Lagrange polynomial defined in formula (9.13). Using formula (9.20) we obtain

$$\begin{aligned} \max_{a \leq x \leq b} |u(x)| &\leq \sum_{i=0}^n |f(a_i) - p(a_i)| \max_{a \leq x \leq b} |l_i(x)| \\ &\leq \epsilon' M, \end{aligned}$$

where $M = \sum_{i=0}^n \max_{a \leq x \leq b} |l_i(x)|$, which is some finite nonnegative number. Note that M depends only on $[a, b]$ and $a_0, a_1, \dots, a_n$. Now, define $q(x)$ as $q(x) = p(x) + u(x)$. Then

$$q(a_i) = p(a_i) + u(a_i) = f(a_i), \quad i = 0, 1, \dots, n.$$

Furthermore,

$$\begin{aligned} |f(x) - q(x)| &\leq |f(x) - p(x)| + |u(x)| \\ &< \epsilon' + \epsilon' M \\ &< \epsilon \quad \text{for all } x \in [a, b]. \end{aligned}$$

9.3. APPROXIMATION BY SPLINE FUNCTIONS

Approximation of a continuous function $f(x)$ with a single polynomial $p(x)$ may not be quite adequate in situations in which $f(x)$ represents a real physical relationship. The behavior of such a function in one region may be unrelated to its behavior in another region. This type of behavior may not be satisfactorily matched by any polynomial. This is attributed to the fact that the behavior of a polynomial everywhere is governed by its behavior in any small region. In such situations, it would be more appropriate to partition the domain of $f(x)$ into several intervals and then use a different approximating polynomial, usually of low degree, in each subinterval. These polynomial segments can be joined in a smooth way, which leads to what is called a piecewise polynomial function.

By definition, a spline function is a piecewise polynomial of degree n . The various polynomial segments (all of degree n) are joined together at points called knots in such a way that the entire spline function is continuous and its first $n - 1$ derivatives are also continuous. Spline functions were first introduced by Schoenberg (1946).

9.3.1. Properties of Spline Functions

Let $[a, b]$ can be interval, and let $a = \tau_0 < \tau_1 < \cdots < \tau_m < \tau_{m+1} = b$ be partition points in $[a, b]$. A spline function $s(x)$ of degree n with knots at the points $\tau_1, \tau_2, \dots, \tau_m$ has the following properties:

- i. $s(x)$ is a polynomial of degree not exceeding n on each subinterval $[\tau_{i-1}, \tau_i]$, $1 \leq i \leq m + 1$.
- ii. $s(x)$ has continuous derivatives up to order $n - 1$ on $[a, b]$.

In particular, if $n = 1$, then the spline function is called a linear spline and can be represented as

$$s(x) = \sum_{i=1}^m a_i |x - \tau_i|,$$

where $a_1, a_2, \dots, a_m$ are fixed numbers. We note that between any two knots, $|x - \tau_i|$, $i = 1, 2, \dots, m$, represents a straight-line segment. Thus the graph of $s(x)$ is made up of straight-line segments joined at the knots.

We can obtain a linear spline that resembles Lagrange interpolation: Let $\theta_0, \theta_1, \dots, \theta_{m+1}$ be given real numbers. For $1 \leq i \leq m$, consider the functions

$$l_0(x) = \begin{cases} \frac{x - \tau_1}{\tau_0 - \tau_1}, & \tau_0 \leq x \leq \tau_1, \\ 0, & \tau_1 \leq x \leq \tau_{m+1}, \end{cases}$$

$$l_i(x) = \begin{cases} 0, & x \notin [\tau_{i-1}, \tau_{i+1}], \\ \frac{x - \tau_{i-1}}{\tau_i - \tau_{i-1}}, & \tau_{i-1} \leq x \leq \tau_i, \\ \frac{\tau_{i+1} - x}{\tau_{i+1} - \tau_i}, & \tau_i \leq x \leq \tau_{i+1}, \end{cases}$$

$$l_{m+1}(x) = \begin{cases} 0, & \tau_0 \leq x \leq \tau_m, \\ \frac{x - \tau_m}{\tau_{m+1} - \tau_m}, & \tau_m \leq x \leq \tau_{m+1}. \end{cases}$$

Then the linear spline

$$s(x) = \sum_{i=0}^{m+1} \theta_i l_i(x) \quad (9.21)$$

has the property that $s(\tau_i) = \theta_i$, $0 \leq i \leq m+1$. It can be shown that the linear spline having this property is unique.

Another special case is the cubic spline for $n = 3$. This is a widely used spline function in many applications. It can be represented as $s(x) = s_i(x) = a_i + b_i x + c_i x^2 + d_i x^3$, $\tau_{i-1} \leq x \leq \tau_i$, $i = 1, 2, \dots, m+1$, such that for $i = 1, 2, \dots, m$,

$$s_i(\tau_i) = s_{i+1}(\tau_i),$$

$$s'_i(\tau_i) = s'_{i+1}(\tau_i),$$

$$s''_i(\tau_i) = s''_{i+1}(\tau_i).$$

In general, a spline of degree n with knots at $\tau_1, \tau_2, \dots, \tau_m$ is represented as

$$s(x) = \sum_{i=1}^m e_i (x - \tau_i)_+^n + p(x), \quad (9.22)$$

where $e_1, e_2, \dots, e_m$ are constants, $p(x)$ is a polynomial of degree n , and

$$(x - \tau_i)_+^n = \begin{cases} (x - \tau_i)^n, & x \geq \tau_i, \\ 0, & x \leq \tau_i. \end{cases}$$

For an illustration, consider the cubic spline

$$s(x) = \begin{cases} a_1 + b_1x + c_1x^2 + d_1x^3, & a \leq x \leq \tau, \\ a_2 + b_2x + c_2x^2 + d_2x^3, & \tau \leq x \leq b. \end{cases}$$

Here, $s(x)$ along with its first and second derivatives must be continuous at $x = \tau$. Therefore, we must have

$$a_1 + b_1\tau + c_1\tau^2 + d_1\tau^3 = a_2 + b_2\tau + c_2\tau^2 + d_2\tau^3, \quad (9.23)$$

$$b_1 + 2c_1\tau + 3d_1\tau^2 = b_2 + 2c_2\tau + 3d_2\tau^2, \quad (9.24)$$

$$2c_1 + 6d_1\tau = 2c_2 + 6d_2\tau. \quad (9.25)$$

Equation (9.25) can be written as

$$c_1 - c_2 = 3(d_2 - d_1)\tau. \quad (9.26)$$

From equations (9.24) and (9.26) we get

$$b_1 - b_2 + 3(d_2 - d_1)\tau^2 = 0. \quad (9.27)$$

Using now equations (9.26) and (9.27) in equation (9.23), we obtain $a_1 - a_2 + 3(d_1 - d_2)\tau^3 + 3(d_2 - d_1)\tau^3 + (d_1 - d_2)\tau^3 = 0$, or equivalently,

$$a_1 - a_2 + (d_1 - d_2)\tau^3 = 0. \quad (9.28)$$

We conclude that

$$d_2 - d_1 = \frac{1}{\tau^3}(a_1 - a_2) = \frac{1}{3\tau^2}(b_2 - b_1) = \frac{1}{3\tau}(c_1 - c_2). \quad (9.29)$$

Let us now express $s(x)$ in the form given by equation (9.22), that is,

$$s(x) = e_1(x - \tau)_+^3 + \alpha_0 + \alpha_1x + \alpha_2x^2 + \alpha_3x^3.$$

In this case,

$$\alpha_0 = a_1, \quad \alpha_1 = b_1, \quad \alpha_2 = c_1, \quad \alpha_3 = d_1,$$

and

$$-e_1\tau^3 + \alpha_0 = a_2, \quad (9.30)$$

$$3e_1\tau^2 + \alpha_1 = b_2, \quad (9.31)$$

$$-3e_1\tau + \alpha_2 = c_2, \quad (9.32)$$

$$e_1 + \alpha_3 = d_2. \quad (9.33)$$

In light of equation (9.29), equations (9.30)–(9.33) have a common solution for e_1 given by $e_1 = d_2 - d_1 = (1/3\tau)(c_1 - c_2) = (1/3\tau^2)(b_2 - b_1) = (1/\tau^3)(a_1 - a_2)$.

9.3.2. Error Bounds for Spline Approximation

Let $a = \tau_0 < \tau_1 < \dots < \tau_m < \tau_{m+1} = b$ be a partition of $[a, b]$. We recall that the linear spline $s(x)$ given by formula (9.21) has the property that $s(\tau_i) = \theta_i$, $0 \leq i \leq m+1$, where $\theta_0, \theta_1, \dots, \theta_{m+1}$ are any given real numbers. In particular, if θ_i is the value at τ_i of a function $f(x)$ defined on the interval $[a, b]$, then $s(x)$ provides a spline approximation of $f(x)$ over $[a, b]$ which agrees with $f(x)$ at $\tau_0, \tau_1, \dots, \tau_{m+1}$. If $f(x)$ has continuous derivatives up to order 2 over $[a, b]$, then an upper bound on the error of approximation is given by (see De Boor, 1978, page 40)

$$\max_{a \leq x \leq b} |f(x) - s(x)| \leq \frac{1}{8} \left(\max_i \Delta\tau_i \right)^2 \max_{a \leq x \leq b} |f^{(2)}(x)|,$$

where $\Delta\tau_i = \tau_{i+1} - \tau_i$, $i = 0, 1, \dots, m$. This error bound can be made small by reducing the value of $\max_i \Delta\tau_i$.

A more efficient and smoother spline approximation than the one provided by the linear spline is the commonly used cubic spline approximation. We recall that a cubic spline defined on $[a, b]$ is a piecewise cubic polynomial that is twice continuously differentiable. Let $f(x)$ be defined on $[a, b]$. There exists a unique cubic spline $s(x)$ that satisfies the following interpolatory constraints:

$$\begin{aligned} s(\tau_i) &= f(\tau_i), & i &= 0, 1, \dots, m+1, \\ s'(\tau_0) &= f'(\tau_0), \\ s'(\tau_{m+1}) &= f'(\tau_{m+1}), \end{aligned} \quad (9.34)$$

(see Prenter, 1975, Section 4.2).

If $f(x)$ has continuous derivatives up to order 4 on $[a, b]$, then information on the error of approximation, which results from using a cubic spline, can be obtained from the following theorem, whose proof is given in Hall (1968):

Theorem 9.3.1. Let $a = \tau_0 < \tau_1 < \cdots < \tau_m < \tau_{m+1} = b$ be a partition of $[a, b]$. Let $s(x)$ be a cubic spline associated with $f(x)$ and satisfies the constraints described in (9.34). If $f(x)$ has continuous derivatives up to order 4 on $[a, b]$, then

$$\max_{a \leq x \leq b} |f(x) - s(x)| \leq \frac{5}{384} \left(\max_i \Delta \tau_i \right)^4 \max_{a \leq x \leq b} |f^{(4)}(x)|,$$

where $\Delta \tau_i = \tau_{i+1} - \tau_i$, $i = 0, 1, \dots, m$.

Another advantage of cubic spline approximation is the fact that it can be used to approximate the first-order and second-order derivatives of $f(x)$. Hall and Meyer (1976) proved that if $f(x)$ satisfies the conditions of Theorem 9.3.1, then

$$\begin{aligned} \max_{a \leq x \leq b} |f'(x) - s'(x)| &\leq \frac{1}{24} \left(\max_i \Delta \tau_i \right)^3 \max_{a \leq x \leq b} |f^{(4)}(x)|, \\ \max_{a \leq x \leq b} |f''(x) - s''(x)| &\leq \frac{3}{8} \left(\max_i \Delta \tau_i \right)^2 \max_{a \leq x \leq b} |f^{(4)}(x)|. \end{aligned}$$

Furthermore, the bounds concerning $|f(x) - s(x)|$ and $|f'(x) - s'(x)|$ are best possible.

9.4. APPLICATIONS IN STATISTICS

There is a wide variety of applications of polynomial approximation in statistics. In this section, we discuss the use of Lagrange interpolation in optimal design theory and the role of spline approximation in regression analysis. Other applications will be seen later in Chapter 10 (Section 10.9).

9.4.1. Approximate Linearization of Nonlinear Models by Lagrange Interpolation

We recall from Section 8.6 that a nonlinear model is one of the form

$$y(\mathbf{x}) = h(\mathbf{x}, \boldsymbol{\theta}) + \epsilon, \quad (9.35)$$

where $\mathbf{x} = (x_1, x_2, \dots, x_k)'$ is a vector of k input variables, $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots, \theta_p)'$ is a vector of p unknown parameters, ϵ is a random error, and $h(\mathbf{x}, \boldsymbol{\theta})$ is a known function which is nonlinear in at least one element of $\boldsymbol{\theta}$.

We also recall that the choice of design for model (9.35), on the basis of the Box–Lucas criterion, depends on the values of the elements of $\boldsymbol{\theta}$ that appear nonlinearly in the model. To overcome this undesirable design dependence problem, one possible approach is to construct an approximation

to the mean response function $h(\mathbf{x}, \boldsymbol{\theta})$ with a Lagrange interpolating polynomial. This approximation can then be utilized to obtain a design for parameter estimation which does not depend on the parameter vector $\boldsymbol{\theta}$. We shall restrict our consideration of model (9.35) to the case of a single input variable x .

Let us suppose that the region of interest, R , is the interval $[a, b]$, and that $\boldsymbol{\theta}$ belongs to a parameter space Ω . We assume that:

- a. $h(x, \boldsymbol{\theta})$ has continuous partial derivatives up to order $r + 1$ with respect to x over $[a, b]$ for all $\boldsymbol{\theta} \in \Omega$, where r is such that $r + 1 \geq p$ with p being the number of parameters in model (9.35), and is large enough so that

$$\frac{2}{(r+1)!} \left(\frac{b-a}{4} \right)^{r+1} \sup_{a \leq x \leq b} \left| \frac{\partial^{r+1} h(x, \boldsymbol{\theta})}{\partial x^{r+1}} \right| < \delta \quad (9.36)$$

for all $\boldsymbol{\theta} \in \Omega$, where δ is a small positive constant chosen appropriately so that the Lagrange interpolation of $h(x, \boldsymbol{\theta})$ achieves a certain accuracy.

- b. $h(x, \boldsymbol{\theta})$ has continuous first-order partial derivatives with respect to the elements of $\boldsymbol{\theta}$.
- c. For any set of distinct points, $x_0, x_1, \dots, x_r$, such that $a \leq x_0 < x_1 < \dots < x_r \leq b$, where r is the integer defined in (a), the $p \times (r+1)$ matrix

$$\mathbf{U}(\boldsymbol{\theta}) = [\nabla h(x_0, \boldsymbol{\theta}) : \nabla h(x_1, \boldsymbol{\theta}) : \dots : \nabla h(x_r, \boldsymbol{\theta})]$$

is of rank p , where $\nabla h(x_i, \boldsymbol{\theta})$ is the vector of partial derivatives of $h(x_i, \boldsymbol{\theta})$ with respect to the elements of $\boldsymbol{\theta}$ ($i = 0, 1, \dots, r$).

Let us now consider the points $z_0, z_1, \dots, z_r$, where z_i is the i th Chebyshev point defined by formula (9.18). Let $p_r(x, \boldsymbol{\theta})$ denote the corresponding Lagrange interpolating polynomial for $h(x, \boldsymbol{\theta})$ over $[a, b]$, which utilizes the z_i 's as interpolation points. Then, by formula (9.14) we have

$$p_r(x, \boldsymbol{\theta}) = \sum_{i=0}^r h(z_i, \boldsymbol{\theta}) l_i(x), \quad (9.37)$$

where $l_i(x)$ is a polynomial of degree r which can be obtained from formula (9.13) by substituting z_i for a_i ($i = 0, 1, \dots, r$). By inequality (9.19), an upper bound on the error of approximating $h(x, \boldsymbol{\theta})$ with $p_r(x, \boldsymbol{\theta})$ is given by

$$\sup_{a \leq x \leq b} |h(x, \boldsymbol{\theta}) - p_r(x, \boldsymbol{\theta})| \leq \frac{2}{(r+1)!} \left(\frac{b-a}{4} \right)^{r+1} \sup_{a \leq x \leq b} \left| \frac{\partial^{r+1} h(x, \boldsymbol{\theta})}{\partial x^{r+1}} \right|.$$

However, by inequality (9.36), this upper bound is less than δ . We then have

$$\sup_{a \leq x \leq b} |h(x, \boldsymbol{\theta}) - p_r(x, \boldsymbol{\theta})| < \delta \quad (9.38)$$

for all $\boldsymbol{\theta} \in \Omega$. This provides the desired accuracy of approximation.

On the basis of the above arguments, an approximate representation of model (9.35) is given by

$$y(x) = p_r(x, \boldsymbol{\theta}) + \epsilon. \quad (9.39)$$

Model (9.39) will now be utilized in place of $h(x, \boldsymbol{\theta})$ to construct an optimal design for estimating $\boldsymbol{\theta}$.

Let us now apply the Box–Lucas criterion described in Section 8.6 to approximate the mean response in model (9.39). In this case, the matrix $\mathbf{H}(\boldsymbol{\theta})$ [see model (8.66)] is an $n \times p$ matrix whose (u, i) th element is $\partial p_r(x_u, \boldsymbol{\theta}) / \partial \theta_i$, where x_u is the design setting at the u th experimental run ($u = 1, 2, \dots, n$) and n is the number of experimental runs. From formula (9.37) we then have

$$\frac{\partial p_r(x_u, \boldsymbol{\theta})}{\partial \theta_i} = \sum_{j=0}^r \frac{\partial h(z_j, \boldsymbol{\theta})}{\partial \theta_i} l_j(x_u), \quad i = 1, 2, \dots, p.$$

These equations can be written as

$$\nabla p_r(x_u, \boldsymbol{\theta}) = \mathbf{U}(\boldsymbol{\theta}) \boldsymbol{\lambda}(x_u),$$

where $\boldsymbol{\lambda}(x_u) = [l_0(x_u), l_1(x_u), \dots, l_r(x_u)]'$ and $\mathbf{U}(\boldsymbol{\theta})$ is the $p \times (r+1)$ matrix

$$\mathbf{U}(\boldsymbol{\theta}) = [\nabla h(z_0, \boldsymbol{\theta}) : \nabla h(z_1, \boldsymbol{\theta}) : \dots : \nabla h(z_r, \boldsymbol{\theta})].$$

By assumption (c), $\mathbf{U}(\boldsymbol{\theta})$ is of rank p . The matrix $\mathbf{H}(\boldsymbol{\theta})$ is therefore of the form

$$\mathbf{H}(\boldsymbol{\theta}) = \boldsymbol{\Lambda} \mathbf{U}'(\boldsymbol{\theta}),$$

where

$$\boldsymbol{\Lambda}' = [\boldsymbol{\lambda}(x_1) : \boldsymbol{\lambda}(x_2) : \dots : \boldsymbol{\lambda}(x_n)].$$

Thus

$$\mathbf{H}'(\boldsymbol{\theta}) \mathbf{H}(\boldsymbol{\theta}) = \mathbf{U}(\boldsymbol{\theta}) \boldsymbol{\Lambda}' \boldsymbol{\Lambda} \mathbf{U}'(\boldsymbol{\theta}). \quad (9.40)$$

If $n \geq r+1$ and at least $r+1$ of the design points (that is, $x_1, x_2, \dots, x_n$) are distinct, then $\boldsymbol{\Lambda}' \boldsymbol{\Lambda}$ is a nonsingular matrix. To show this, it is sufficient to prove that $\boldsymbol{\Lambda}$ is of full column rank $r+1$. If not, then there must exist constants $\alpha_0, \alpha_1, \dots, \alpha_r$, not all equal to zero, such that

$$\sum_{i=0}^r \alpha_i l_i(x_u) = 0, \quad u = 1, 2, \dots, n.$$

This indicates that the r th degree polynomial $\sum_{i=0}^r \alpha_i l_i(x)$ has n roots, namely, $x_1, x_2, \dots, x_n$. This is not possible, because $n \geq r + 1$ and at least $r + 1$ of the x_u 's ($u = 1, 2, \dots, n$) are distinct (a polynomial of degree r has at most r distinct roots). This contradiction implies that Λ is of full column rank and $\Lambda' \Lambda$ is therefore nonsingular.

Applying the Box–Lucas design criterion to the approximating model (9.37) amounts to finding the design settings that maximize $\det[\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})]$. From formula (9.40) we have

$$\det[\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})] = \det[\mathbf{U}(\boldsymbol{\theta}) \Lambda' \Lambda \mathbf{U}'(\boldsymbol{\theta})]. \quad (9.41)$$

We note that the matrix $\Lambda' \Lambda = \sum_{u=1}^n \boldsymbol{\lambda}(x_u) \boldsymbol{\lambda}'(x_u)$ depends only on the design settings. Let $\nu_{\min}(x_1, x_2, \dots, x_n)$ and $\nu_{\max}(x_1, x_2, \dots, x_n)$ denote, respectively, the smallest and the largest eigenvalue of $\Lambda' \Lambda$. These eigenvalues are positive, since $\Lambda' \Lambda$ is positive definite by the fact that $\Lambda' \Lambda$ is nonsingular, as was shown earlier. From formula (9.41) we conclude that

$$\begin{aligned} \det[\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})] \nu_{\min}^p(x_1, x_2, \dots, x_n) &\leq \det[\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})] \\ &\leq \det[\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})] \nu_{\max}^p(x_1, x_2, \dots, x_n). \end{aligned} \quad (9.42)$$

This double inequality follows from the fact that the matrices $\nu_{\max}(x_1, x_2, \dots, x_n) \mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta}) - \mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})$ and $\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta}) - \nu_{\min}(x_1, x_2, \dots, x_n) \mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})$ are positive semidefinite. An application of Theorem 2.3.19(1) to these matrices results in the double inequality (9.42) (why?). Note that the determinant of $\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})$ is not zero, since $\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})$, which is of order $p \times p$, is of rank p by assumption (c).

Now, from the double inequality (9.42) we deduce that there exists a number γ , $0 \leq \gamma \leq 1$, such that

$$\begin{aligned} \det[\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})] &= [\gamma \nu_{\min}^p(x_1, x_2, \dots, x_n) + (1 - \gamma) \nu_{\max}^p(x_1, x_2, \dots, x_n)] \\ &\quad \times \det[\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})]. \end{aligned}$$

If γ is integrated out, we obtain

$$\begin{aligned} \int_0^1 \det[\mathbf{H}'(\boldsymbol{\theta})\mathbf{H}(\boldsymbol{\theta})] d\gamma &= \frac{1}{2} [\nu_{\min}^p(x_1, x_2, \dots, x_n) + \nu_{\max}^p(x_1, x_2, \dots, x_n)] \\ &\quad \times \det[\mathbf{U}(\boldsymbol{\theta})\mathbf{U}'(\boldsymbol{\theta})]. \end{aligned}$$

Consequently, to construct an optimal design we can consider finding $x_1, x_2, \dots, x_n$ that maximize the function

$$\psi(x_1, x_2, \dots, x_n) = \frac{1}{2} [\nu_{\min}^p(x_1, x_2, \dots, x_n) + \nu_{\max}^p(x_1, x_2, \dots, x_n)]. \quad (9.43)$$

This is a modified version of the Box–Lucas criterion. Its advantage is that the optimal design is free of θ . We therefore call such a design a parameter-free design. The maximization of $\psi(x_1, x_2, \dots, x_n)$ can be conveniently carried out by using a FORTRAN program written by Conlon (1991), which is based on Price's (1977) controlled random search procedure.

EXAMPLE 9.4.1. Let us consider the nonlinear model used by Box and Lucas (1959) of a consecutive first-order chemical reaction in which a raw material A reacts to form a product B , which in turn decomposes to form substance C . After time x has elapsed, the mean yield of the intermediate product B is given by

$$h(x, \theta) = \frac{\theta_1}{\theta_1 - \theta_2} (e^{-\theta_2 x} - e^{-\theta_1 x}),$$

where θ_1 and θ_2 are the rate constants for the reactions $A \rightarrow B$ and $B \rightarrow C$, respectively.

Suppose that the region of interest R is the interval $[0, 10]$. Let the parameter space Ω be such that $0 \leq \theta_1 \leq 1$, $0 \leq \theta_2 \leq 1$. It can be verified that

$$\frac{\partial^{r+1} h(x, \theta)}{\partial x^{r+1}} = (-1)^{r+1} \frac{\theta_1}{\theta_1 - \theta_2} (\theta_2^{r+1} e^{-\theta_2 x} - \theta_1^{r+1} e^{-\theta_1 x}).$$

Let us consider the function $w(x, \phi) = \phi^{r+1} e^{-\phi x}$. By the mean value theorem (Theorem 4.2.2),

$$\theta_2^{r+1} e^{-\theta_2 x} - \theta_1^{r+1} e^{-\theta_1 x} = (\theta_2 - \theta_1) \frac{\partial w(x, \theta_*)}{\partial \phi},$$

where $\partial w(x, \theta_*)/\partial \phi$ is the partial derivative of $w(x, \phi)$ with respect to ϕ evaluated at θ_* , and where θ_* is between θ_1 and θ_2 . Thus

$$\theta_2^{r+1} e^{-\theta_2 x} - \theta_1^{r+1} e^{-\theta_1 x} = (\theta_2 - \theta_1) [(r+1)\theta_*^r e^{-\theta_* x} - \theta_*^{r+1} x e^{-\theta_* x}].$$

Hence,

$$\begin{aligned} \sup_{0 \leq x \leq 10} \left| \frac{\partial^{r+1} h(x, \theta)}{\partial x^{r+1}} \right| &\leq \theta_1 \theta_*^r \sup_{0 \leq x \leq 10} [e^{-\theta_* x} |r+1 - x\theta_*|] \\ &\leq \sup_{0 \leq x \leq 10} |r+1 - x\theta_*|. \end{aligned}$$

However,

$$|r + 1 - x\theta_*| = \begin{cases} r + 1 - x\theta_* & \text{if } r + 1 \geq x\theta_*, \\ -r - 1 + x\theta_* & \text{if } r + 1 < x\theta_*. \end{cases}$$

Since $0 \leq x\theta_* \leq 10$, then

$$\sup_{0 \leq x \leq 10} |r + 1 - x\theta_*| \leq \max(r + 1, 9 - r).$$

We then have

$$\sup_{0 \leq x \leq 10} \left| \frac{\partial^{r+1} h(x, \boldsymbol{\theta})}{\partial x^{r+1}} \right| \leq \max(r + 1, 9 - r).$$

By inequality (9.36), the integer r is determined such that

$$\frac{2}{(r + 1)!} \left(\frac{10}{4} \right)^{r+1} \max(r + 1, 9 - r) < \delta. \tag{9.44}$$

If we choose $\delta = 0.053$, for example, then it can be verified that the smallest positive integer that satisfies inequality (9.44) is $r = 9$. The Chebyshev points in formula (9.18) that correspond to this value of r are given in Table 9.2. On choosing n , the number of design points, to be equal to $r + 1 = 10$, where all ten design points are distinct, the matrix Λ in formula (9.40) will be nonsingular of order 10×10 . Using Conlon's (1991) FORTRAN program for the maximization of the function ψ in formula (9.43) with $p = 2$, it can be shown that the maximum value of ψ is 17.457. The corresponding optimal values of $x_1, x_2, \dots, x_{10}$ are given in Table 9.2.

Table 9.2. Chebyshev Points and Optimal Design Points for Example 9.4.1

Chebyshev Points	Optimal Design Points
9.938	9.989
9.455	9.984
8.536	9.983
7.270	9.966
5.782	9.542
4.218	7.044
2.730	6.078
1.464	4.038
0.545	1.381
0.062	0.692

9.4.2. Splines in Statistics

There is a broad variety of work on splines in statistics. Spline functions are quite suited in practical applications involving data that arise from the physical world rather than the mathematical world. It is therefore only natural that splines have many useful applications in statistics. Some of these applications will be discussed in this section.

9.4.2.1. The Use of Cubic Splines in Regression

Let us consider fitting the model

$$y = g(x) + \epsilon, \quad (9.45)$$

where $g(x)$ is the mean response at x and ϵ is a random error. Suppose that the domain of x is divided into a set of $m + 1$ intervals by the points $\tau_0 < \tau_1 < \dots < \tau_m < \tau_{m+1}$ such that on the i th interval ($i = 1, 2, \dots, m + 1$), $g(x)$ is represented by the cubic spline

$$s_i(x) = a_i + b_i x + c_i x^2 + d_i x^3, \quad \tau_{i-1} \leq x \leq \tau_i. \quad (9.46)$$

As was seen earlier in Section 9.3.1, the parameters a_i, b_i, c_i, d_i ($i = 1, 2, \dots, m + 1$) are subject to the following continuity restrictions:

$$a_i + b_i \tau_i + c_i \tau_i^2 + d_i \tau_i^3 = a_{i+1} + b_{i+1} \tau_i + c_{i+1} \tau_i^2 + d_{i+1} \tau_i^3, \quad (9.47)$$

that is, $s_i(\tau_i) = s_{i+1}(\tau_i)$, $i = 1, 2, \dots, m$;

$$b_i + 2c_i \tau_i + 3d_i \tau_i^2 = b_{i+1} + 2c_{i+1} \tau_i + 3d_{i+1} \tau_i^2, \quad (9.48)$$

that is, $s'_i(\tau_i) = s'_{i+1}(\tau_i)$, $i = 1, 2, \dots, m$; and

$$2c_i + 6d_i \tau_i = 2c_{i+1} + 6d_{i+1} \tau_i, \quad (9.49)$$

that is, $s''_i(\tau_i) = s''_{i+1}(\tau_i)$, $i = 1, 2, \dots, m$. The number of unknown parameters in model (9.45) is therefore equal to $4(m + 1)$. The continuity restrictions (9.47)–(9.49) reduce the dimensionality of the parameter space to $m + 4$. However, only $m + 2$ parameters can be estimated. This is because the spline method does not estimate the parameters of the s_i 's directly, but estimates the ordinates of the s_i 's at the points $\tau_0, \tau_1, \dots, \tau_{m+1}$, that is, $s_1(\tau_0)$ and $s_i(\tau_i)$, $i = 1, 2, \dots, m + 1$. Two additional restrictions are therefore needed. These are chosen to be of the form (see Poirier, 1973, page 516; Buse and Lim, 1977, page 64):

$$s''_1(\tau_0) = \pi_0 s''_1(\tau_1),$$

or

$$2c_1 + 6d_1 \tau_0 = \pi_0 (2c_1 + 6d_1 \tau_1), \quad (9.50)$$

and

$$s''_{m+1}(\tau_{m+1}) = \pi_{m+1} s''_{m+1}(\tau_m),$$

or

$$2c_{m+1} + 6d_{m+1}\tau_{m+1} = \pi_{m+1}(2c_{m+1} + 6d_{m+1}\tau_m), \quad (9.51)$$

where π_0 and π_{m+1} are known.

Let $y_1, y_2, \dots, y_n$ be n observations on the response y , where $n > m + 2$, such that n_i observations are taken in the i th interval $[\tau_{i-1}, \tau_i]$, $i = 1, 2, \dots, m + 1$. Thus $n = \sum_{i=1}^{m+1} n_i$. If $y_{i1}, y_{i2}, \dots, y_{in_i}$ are the observations in the i th interval ($i = 1, 2, \dots, m + 1$), then from model (9.45) we have

$$y_{ij} = g(x_{ij}) + \epsilon_{ij}, \quad i = 1, 2, \dots, m + 1; j = 1, 2, \dots, n_i, \quad (9.52)$$

where x_{ij} is the setting of x for which $y = y_{ij}$, and the ϵ_{ij} 's are distributed independently with means equal to zero and a common variance σ^2 . The estimation of the parameters of model (9.45) is then reduced to a restricted least-squares problem with formulas (9.47)–(9.51) representing linear restrictions on the $4(m + 1)$ parameters of the model [see, for example, Searle (1971, Section 3.6), for a discussion concerning least-squares estimation under linear restrictions on the fitted model's parameters]. Using matrix notation, model (9.52) and the linear restrictions (9.47)–(9.51) can be expressed as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad (9.53)$$

$$\mathbf{C}\boldsymbol{\beta} = \boldsymbol{\delta}, \quad (9.54)$$

where $\mathbf{y} = (\mathbf{y}'_1: \mathbf{y}'_2: \dots: \mathbf{y}'_{m+1})'$ with $\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{in_i})'$, $i = 1, 2, \dots, m + 1$, $\mathbf{X} = \text{Diga}(\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{m+1})$ is a block-diagonal matrix of order $n \times [4(m + 1)]$ with $\mathbf{X}_i$ being a matrix of order $n_i \times 4$ whose j th row is of the form $(1, x_{ij}, x_{ij}^2, x_{ij}^3)$, $j = 1, 2, \dots, n_i$; $i = 1, 2, \dots, m + 1$; $\boldsymbol{\beta} = (\boldsymbol{\beta}'_1: \boldsymbol{\beta}'_2: \dots: \boldsymbol{\beta}'_{m+1})'$ with $\boldsymbol{\beta}_i = (a_i, b_i, c_i, d_i)'$, $i = 1, 2, \dots, m + 1$; and $\boldsymbol{\epsilon} = (\boldsymbol{\epsilon}'_1: \boldsymbol{\epsilon}'_2: \dots: \boldsymbol{\epsilon}'_{m+1})'$, where $\boldsymbol{\epsilon}_j$ is the vector of random errors associated with the observations in the i th interval, $i = 1, 2, \dots, m + 1$. Furthermore, $\mathbf{C} = [\mathbf{C}'_0: \mathbf{C}'_1: \mathbf{C}'_2: \mathbf{C}'_3]'$, where, for $l = 0, 1, 2$,

$$\mathbf{C}_l = \begin{bmatrix} -\mathbf{e}'_{1l} & \mathbf{e}'_{1l} & \mathbf{0}' & \cdots & \mathbf{0}' & \mathbf{0}' \\ \mathbf{0}' & -\mathbf{e}'_{2l} & \mathbf{e}'_{2l} & \cdots & \mathbf{0}' & \mathbf{0}' \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0}' & \mathbf{0}' & \mathbf{0}' & \cdots & -\mathbf{e}'_{ml} & \mathbf{e}'_{ml} \end{bmatrix}$$

is a matrix of order $m \times [4(m+1)]$ such that $\mathbf{e}'_{i0} = (1, \tau_i, \tau_i^2, \tau_i^3)$, $\mathbf{e}'_{i1} = (0, 1, 2\tau_i, 3\tau_i^2)$, $\mathbf{e}'_{i2} = (0, 0, 2, 6\tau_i)$, $i = 1, 2, \dots, m$, and

$$\mathbf{C}_3 = \begin{bmatrix} 0 & 0 & 2(\pi_0 - 1) & 6(\pi_0\tau_1 - \tau_0) & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 2(\pi_{m+1} - 1) & 6(\pi_{m+1}\tau_m - \tau_{m+1}) \end{bmatrix}$$

is a $2 \times [4(m+1)]$ matrix. Finally, $\boldsymbol{\delta} = (\boldsymbol{\delta}'_0: \boldsymbol{\delta}'_1: \boldsymbol{\delta}'_2: \boldsymbol{\delta}'_3)' = \mathbf{0}$, where the partitioning of $\boldsymbol{\delta}$ into $\boldsymbol{\delta}_0$, $\boldsymbol{\delta}_1$, $\boldsymbol{\delta}_2$, and $\boldsymbol{\delta}_3$ conforms to that of $\mathbf{C}$. Consequently, and on the basis of formula (103) in Searle (1971, page 113), the least-squares estimator of $\boldsymbol{\beta}$ for model (9.53) under the restriction described by formula (9.54) is given by

$$\begin{aligned} \hat{\boldsymbol{\beta}}_r &= \hat{\boldsymbol{\beta}} - (\mathbf{X}'\mathbf{X})^{-1}\mathbf{C}'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{C}']^{-1}(\mathbf{C}\hat{\boldsymbol{\beta}} - \boldsymbol{\delta}) \\ &= \hat{\boldsymbol{\beta}} - (\mathbf{X}'\mathbf{X})^{-1}\mathbf{C}'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{C}']^{-1}\mathbf{C}\hat{\boldsymbol{\beta}}, \end{aligned}$$

where $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ is the ordinary least-squares estimator of $\boldsymbol{\beta}$.

This estimation procedure, which was developed by Buse and Lim (1977), demonstrates that the fitting of a cubic spline regression model can be reduced to a restricted least-squares problem. Buse and Lim presented a numerical example based on Indianapolis 500 race data over the period (1911–1971) to illustrate the implementation of their procedure.

Other papers of interest in the area of regression splines include those of Poirier (1973) and Gallant and Fuller (1973). The paper by Poirier discusses the basic theory of cubic regression splines from an economic point of view. In the paper by Gallant and Fuller, the knots are treated as unknown parameters rather than being fixed. Thus in their procedure, the knots must be estimated, which causes the estimation process to become nonlinear.

9.4.2.2. Designs for Fitting Spline Models

A number of papers have addressed the problem of finding a design to estimate the parameters of model (9.45), where $g(x)$ is represented by a spline function. We shall make a brief reference to some of these papers.

Agarwal and Studden (1978) considered a representation of $g(x)$ over $0 \leq x \leq 1$ by a linear spline $s(x)$, which has the form given by (9.21). Here, $g''(x)$ is assumed to be continuous. If we recall, the θ_i coefficients in formula (9.21) are the values of s at $\tau_0, \tau_1, \dots, \tau_{m+1}$.

Let $x_1, x_2, \dots, x_r$ be r design points in $[0, 1]$. Let $\bar{y}_i$ denote the average of n_i observations taken at x_i ($i = 1, 2, \dots, r$). The vector $\boldsymbol{\theta} = (\theta_0, \theta_1, \dots, \theta_{m+1})'$ can therefore be estimated by

$$\hat{\boldsymbol{\theta}} = \mathbf{A}\bar{\mathbf{y}}, \quad (9.55)$$

where $\bar{\mathbf{y}} = (\bar{y}_1, \bar{y}_2, \dots, \bar{y}_r)'$ and $\mathbf{A}$ is an $(m+2) \times r$ matrix. Hence, an estimate of $g(x)$ is given by

$$\hat{g}(x) = \mathbf{l}'(x)\hat{\boldsymbol{\theta}} = \mathbf{l}'(x)\mathbf{A}\bar{\mathbf{y}}, \quad (9.56)$$

where $\mathbf{l}(x) = [l_0(x), l_1(x), \dots, l_{m+1}(x)]'$.

Now, $E(\hat{\boldsymbol{\theta}}) = \mathbf{A}\mathbf{g}_r$, where $\mathbf{g}_r = [g(x_1), g(x_2), \dots, g(x_r)]'$. Thus $E[\hat{g}(x)] = \mathbf{l}'(x)\mathbf{A}\mathbf{g}_r$, and the variance of $\hat{g}(x)$ is

$$\begin{aligned}\text{Var}[\hat{g}(x)] &= E[\mathbf{l}'(x)\hat{\boldsymbol{\theta}} - \mathbf{l}'(x)\mathbf{A}\mathbf{g}_r]^2 \\ &= \frac{\sigma^2}{n} \mathbf{l}'(x) \mathbf{A} \mathbf{D}^{-1} \mathbf{A}' \mathbf{l}(x),\end{aligned}$$

where $\mathbf{D}$ is an $r \times r$ diagonal matrix with diagonal elements $n_1/n, n_2/n, \dots, n_r/n$. The mean squared error of $\hat{g}(x)$ is the variance plus the squared bias of $\hat{g}(x)$. It follows that the integrated mean squared error (IMSE) of $\hat{g}(x)$ (see Section 8.4.3) is

$$\begin{aligned}J &= \frac{n\omega}{\sigma^2} \int_0^1 \text{Var}[\hat{g}(x)] dx + \frac{n\omega}{\sigma^2} \int_0^1 \text{Bias}^2[\hat{g}(x)] dx \\ &= V + B,\end{aligned}$$

where $\omega = (\int_0^1 dx)^{-1} = \frac{1}{2}$, and

$$\text{Bias}^2[\hat{g}(x)] = [g(x) - \mathbf{l}'(x)\mathbf{A}\mathbf{g}_r]^2.$$

Thus

$$\begin{aligned}J &= \frac{1}{2} \int_0^1 \mathbf{l}'(x) \mathbf{A} \mathbf{D}^{-1} \mathbf{A}' \mathbf{l}(x) dx + \frac{n}{2\sigma^2} \int_0^1 [g(x) - \mathbf{l}'(x)\mathbf{A}\mathbf{g}_r]^2 dx \\ &= \frac{1}{2} \text{tr}(\mathbf{A} \mathbf{D}^{-1} \mathbf{A}' \mathbf{M}) + \frac{n}{2\sigma^2} \int_0^1 [g(x) - \mathbf{l}'(x)\mathbf{A}\mathbf{g}_r]^2 dx,\end{aligned}$$

where $\mathbf{M} = \int_0^1 \mathbf{l}(x) \mathbf{l}'(x) dx$.

Agarwal and Studden (1978) proposed to minimize J with respect to (i) the design (that is, $x_1, x_2, \dots, x_r$ as well as $n_1, n_2, \dots, n_r$), (ii) the matrix $\mathbf{A}$, and (iii) the knots $\tau_1, \tau_2, \dots, \tau_m$, assuming that g is known.

Park (1978) adopted the D -optimality criterion (see Section 8.5) for the choice of design when $g(x)$ is represented by a spline of the form given by formula (9.22) with only one intermediate knot.

Draper, Guttman, and Lipow (1977) extended the design criterion based on the minimization of the average squared bias B (see Section 8.4.3) to situations involving spline models. In particular, they considered fitting first-order or second-order models when the true mean response is of the second order or the third order, respectively.

9.4.2.3. Other Applications of Splines in Statistics

Spline functions have many other useful applications in both theoretical and applied statistical research. For example, splines are used in nonparametric

regression and data smoothing, nonparametric density estimation, and time series analysis. They are also utilized in the analysis of response curves in agriculture and economics. The review articles by Wegman and Wright (1983) and Ramsay (1988) contain many references on the various uses of splines in statistics (see also the article by Smith, 1979). An overview of the role of splines in regression analysis is given in Eubank (1984).

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EXERCISES

In Mathematics

- 9.1. Let $f(x)$ be a function with a continuous derivative on $[0, 1]$, and let $b_n(x)$ be the n th degree Bernstein approximating polynomial of f . Then, for some constant c and for all n ,

$$\sup_{0 \leq x \leq 1} |f(x) - b_n(x)| \leq \frac{c}{n^{1/2}}.$$

- 9.2. Prove Lemma 9.1.1.

- 9.3. Prove Lemma 9.1.2.

- 9.4. Show that for every interval $[-a, a]$ there is a sequence of polynomials $p_n(x)$ such that $p_n(0) = 0$ and $\lim_{n \rightarrow \infty} p_n(x) = |x|$ uniformly on $[-a, a]$.

- 9.5. Suppose that $f(x)$ is continuous on $[0, 1]$ and that

$$\int_0^1 f(x) x^n dx = 0, \quad n = 0, 1, 2, \dots$$

Show that $f(x) = 0$ on $[0, 1]$.

[Hint: $\int_0^1 f(x) p_n(x) dx = 0$, where $p_n(x)$ is any polynomial of degree n .]

- 9.6. Suppose that the function $f(x)$ has $n + 1$ continuous derivatives on $[a, b]$. Let $a = a_0 < a_1 < \dots < a_n = b$ be $n + 1$ points in $[a, b]$. Then

$$\sup_{a \leq x \leq b} |f(x) - p(x)| \leq \frac{\tau_{n+1} h^{n+1}}{4(n+1)},$$

where $p(x)$ is the Lagrange polynomial defined by formula (9.14), $\tau_{n+1} = \sup_{a \leq x \leq b} |f^{(n+1)}(x)|$, and $h = \max(a_{i+1} - a_i)$, $i = 0, 1, \dots, n - 1$.
[Hint: Show that $|\prod_{i=0}^n (x - a_i)| \leq n!(h^{n+1}/4)$.]

- 9.7. Apply Lagrange interpolation to approximate the function $f(x) = \log x$ over the interval $[3.50, 3.80]$ using $a_0 = 3.50$, $a_1 = 3.60$, $a_2 = 3.70$, and $a_3 = 3.80$ as interpolation points. Compute an upper bound on the error of approximation.

- 9.8. Let $a = \tau_0 < \tau_1 < \dots < \tau_n = b$ be a partition of $[a, b]$. Suppose that $f(x)$ has continuous derivatives up to order 2 over $[a, b]$. Consider a

cubic spline $s(x)$ that satisfies

$$s(\tau_i) = f(\tau_i), \quad i = 0, 1, \dots, n,$$

$$s'(a) = f'(a),$$

$$s'(b) = f'(b).$$

Show that

$$\int_a^b [f''(x)]^2 dx \geq \int_a^b [s''(x)]^2 dx.$$

- 9.9.** Determine the cubic spline approximation of the function $f(x) = \cos(2\pi x)$ over the interval $[0, \pi]$ using five evenly spaced knots. Give an upper bound on the error approximation.

In Statistics

- 9.10.** Consider the nonlinear model

$$y(x) = h(x, \boldsymbol{\theta}) + \epsilon,$$

where

$$h(x, \boldsymbol{\theta}) = \theta_1(1 - \theta_2 e^{-\theta_3 x}),$$

such that $0 \leq \theta_1 \leq 50$, $0 \leq \theta_2 \leq 1$, $0 \leq \theta_3 \leq 1$. Obtain a Lagrange interpolating polynomial that approximates the mean response function $h(x, \boldsymbol{\theta})$ over the region $[0, 8]$ with an error not exceeding $\delta = 0.05$.

- 9.11.** Consider the nonlinear model

$$y = \alpha + (0.49 - \alpha) \exp[-\beta(x - 8)] + \epsilon,$$

where ϵ is a random error with a zero mean and a variance σ^2 . Suppose that the region of interest is the interval $[10, 40]$, and that the parameter space Ω is such that $0.36 \leq \alpha \leq 0.41$, $0.06 \leq \beta \leq 0.16$. Let $s(x)$ be the cubic spline that approximates the mean response, that is, $\eta(x, \alpha, \beta) = \alpha + (0.49 - \alpha) \exp[-\beta(x - 8)]$, over $[10, 40]$. Determine the number of knots needed so that

$$\max_{10 \leq x \leq 40} |\eta(x, \alpha, \beta) - s(x)| < 0.001$$

for all $(\alpha, \beta) \in \Omega$.

9.12. Consider fitting the spline model

$$y = \beta_0 + \beta_1 x + \beta_2 (x - \alpha)_+^2 + \epsilon$$

over the interval $[-1, 1]$, where α is a known constant, $-1 \leq \alpha \leq 1$. A three-point design consisting of x_1, x_2, x_3 with $-1 \leq x_1 < \alpha \leq x_2 < x_3 \leq 1$ is used to fit the model. Using matrix notation, the model is written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}.$$

where $\mathbf{X}$ is the matrix

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & 0 \\ 1 & x_2 & (x_2 - \alpha)^2 \\ 1 & x_3 & (x_3 - \alpha)^2 \end{bmatrix},$$

and $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2)'$. Determine x_1, x_2, x_3 so that the design is D -optimal, that is, it maximizes the determinant of $\mathbf{X}'\mathbf{X}$.
[Note: See Park (1978).]