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CUBIC SPLINES

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Contents

1. Introduction

Spline functions are an important and powerful tool for a number of approximation tasks such as interpolation, data fitting and the solution of boundary value problems for differential equations.

Definition 1.1. Given the *knots* $\{x_j\}_{j=0}^{n}$ with

$$-\infty < x_0 < \cdots < x_n < \infty \ .$$

The function s belongs to the set $\widehat{\mathcal{S}}_m(x_0, \ldots, x_n)$ of *spline functions of degree m* over knots $x_0, \ldots, x_n$ if

1° s is a polynomial of degree at most m in each of the intervals $]-\infty, x_0[, \quad [x_0, x_1[, \quad \ldots, \quad [x_{n-1}, x_n], \quad]x_n, \infty[$.

2° s and its first $m{-}1$ derivatives vary continuosly across the knots:

$$s^{(p)}(x_i-) = s^{(p)}(x_i+), \qquad \begin{cases} p = 0, 1, \ldots, m{-}1 \\ i = 0, 1, \ldots, n \end{cases} \tag{1.1}$$

It is seen, that any polynomial of degree at most m belongs to $\widehat{\mathcal{S}}_m(x_0, \ldots, x_n)$. Generally, however, s is a *piecewise polynomial,* i.e. a new polynomial in each subinterval, and these polynomials are "glued together" so that $s \in \widehat{\mathcal{S}}_m(x_0,\ldots,x_n) \Rightarrow s \in \mathsf{C}^{m-1}(-\infty, \infty)$. The definition implies that $s^{(m)}$ is constant in each knot interval. The value $s^{(m)}(x)$ normally jumps when x passes a knot.

The socalled *natural spline functions* are of special interest,

Definition 1.2. The function s belongs to $\widehat{\mathcal{S}}_m^{\mathcal{N}}(x_0, \ldots, x_n)$, the set of *natural spline functions* of degree m over knots $x_0, \ldots, x_n$, if

1° $s \in \widehat{\mathcal{S}}_m(x_0,\ldots,x_n)$,

2° m is odd, i.e. $m = 2k{-}1$, where k is a positive integer,

3° s is a polynomial of degree at most $k{-}1$ for $-\infty < x < x_0$ and $x_n < x < \infty$.

Exercise 1.1. Show that $s \in \widehat{\mathcal{S}}_{2k-1}^{\mathcal{N}}(x_0,\ldots,x_n)$ satisfies

$$s^{(p)}(x_0) = s^{(p)}(x_n) = 0 \quad \text{for} \quad p = k, k{+}1, \ldots 2k{-}2 \ . \tag{1.2}$$

Example 1.2. The simplest natural spline is given by $m = k = 1$. In this case s is a piecewise linear function for $x_0 \le x \le x_n$ and constant outside this region. This is illustrated in Figure 1.1, where s interpolates 10 given points (x_0, y_0), $\ldots$, (x_9, y_9), and the abscissae are chosen as knots. In Figure 1.2 the same points are interpolated by a natural cubic spline function, i.e. $k = 2$, $m = 3$.

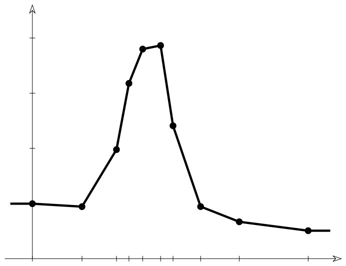

Figure 1.1. *Natural spline of degree one*

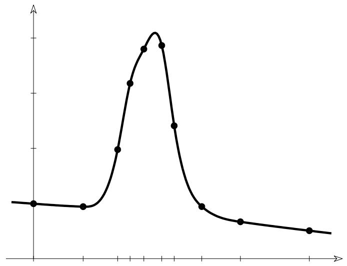

Figure 1.2. *Natural cubic spline*

Example 1.3. A *physical spline* has been used for centuries by draughtsmen. It is a thin, flexible rod, which is held fixed at certain points. The shape of the rod will be a smooth curve similar to Figure 1.2, cf. the front page.

In an ordinary Cartesian system let (x_i, y_i), $i = 0, 1, \ldots, n$ be the points of fixture and let $F(x)$ describe the shape of the spline. Assume that the fixtures are made without friction. Then F is twice continuously differentiable, while $F'''(x)$ has jumps across the points of fixture. Each jump reflects the force needed to fix the rod at this point.

The function obviously satisfies

$$F(x_i) = y_i, \quad i = 0, 1, \ldots, n \ , \tag{1.3a}$$

and the shape of the rod will be so that it has *minimum potential energy.* This energy can be expressed as

$$E_p = \frac{1}{2}\int_0^L \frac{M^2}{EI} ds = \frac{EI}{2}\int_a^b \frac{(F''(x))^2}{(1 + (F'(x))^2)^{\frac{5}{2}}} dx \ . \tag{1.3b}$$

Here, L and EI are the length of the rod and its bending stiffness, while M is the bending moment and s is the arc length; a and b are the projections of the end points onto the X-axis.

It is readily seen that outside the extreme fixture points the rod must be straight: $F''(x) = 0$ for $x < a$ and $x > b$, implying that the second integral in (1.3b) only has contribution from the interval $[x_0, x_n]$.

Example 1.4. A natural cubic spline function has a number of similarities with a physical spline: Both are twice continuously differentiable, the third derivative can have jumps across the knots, and both the physical spline and $s(x) \in \widehat{\mathcal{S}}_3^{\mathcal{N}}(x_0,\ldots,x_n)$ are straight lines outside $[x_0, x_n]$.

Also the minimum potential energy has an analogue: Let $G = \{g\}$ be the set of functions satisfying

$$g(x_i) = y_i, \quad i = 0, 1, \ldots, n \quad \text{and} \quad g \in \mathsf{C}^2(-\infty, \infty) \; .$$

It can be shown [1] that with $a \le x_0$ and $b \ge x_n$, then

$$\underset{\mathrm{g} \in \mathrm{G}}{\operatorname{argmin}} \Big\{ \int_a^b \big(g''(x)\big)^2 \, dx \Big\}$$

is the natural cubic spline function $s \in \widehat{\mathcal{S}}_3^{\mathcal{N}}(x_0,\ldots,x_n)$ interpolating the given points.

Example 1.5. Figure 1.3 shows the same points as in Figures 1.1 – 1.2, but now we have interpolated by a natural spline function of degree 5 and a polynomial of degree 9.

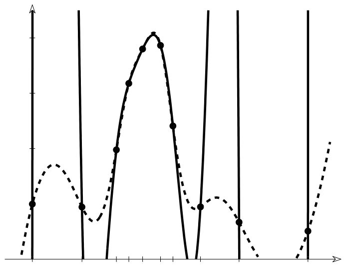

Figure 1.3. *Interpolation by a polynomial (full line) and a natural spline of degree 5 (dotted line)*

The emphasis in these notes is on cubic spline functions. Figure 1.2 shows that this degree is sufficiently high to give a smooth curve – the eye cannot see jumps in the third derivative – and Figure 1.3 indicates that a higher degree can result in undesirable laxity.

The behaviour outside the region $[x_0, x_n]$ is rarely of practical interest, and in the remainder of these notes we concentrate on $s \in \mathcal{S}_m(\boldsymbol{x}_{0:n})$, the class of degree m spline functions restricted to $x_0 \le x \le x_n$. This piecewise mth order polynomial can be expressed in the form

$$\begin{aligned} s(x) = d_{0,j} + d_{1,j}(x - x_{j-1}) + \cdots + d_{m,j}(x - x_{j-1})^m \\ \text{for} \quad x_{j-1} \le x < x_j, \quad j = 1, \ldots, n \end{aligned} \tag{1.4}$$

(with the right-hand inequality closed for $j = n$). This representation involves the $n \cdot (m+1)$ coefficients $\{d_{k,j}\}_{k=0,}^{m}{}_{j=1}^{n}$. They cannot be chosen freely, however, but must satisfy the conditions

$$\left.\begin{aligned} s(x_i-) &= s(x_i+) \\ s'(x_i-) &= s'(x_i+) \\ &\vdots \\ s^{(m-1)}(x_i-) &= s^{(m-1)}(x_i+) \end{aligned}\right\} \quad i = 1, \ldots, n-1 \; . \tag{1.5}$$

There are $(n-1) \cdot m$ conditions, and we are left with

$$\nu = n(m+1) - (n-1)m = n + m \tag{1.6}$$

degrees of freedom. This means that we need $n+m$ linearly independent conditions to get a unique $s \in \mathcal{S}_m(\boldsymbol{x}_{0:n})$ that does the desired job – i.e. approximates the actual function.

Similarly, $\mathcal{S}_m^{\mathcal{N}}(\boldsymbol{x}_{0:n})$ denotes the set of natural mth order spline functions restricted to $[x_0, x_n]$. Again, we can use (1.4) and (1.5), but a natural spline further has to satisfy the boundary conditions (1.2),

$$s^{(p)}(x_0) = s^{(p)}(x_n) = 0 \quad \text{for} \quad p = k, k+1, \ldots m-1; \;\; m = 2k - 1 \; .$$

Thus, a natural spline has $2(m - k) = m-1$ extra conditions to satisfy, and we are left with

$$\nu_N = n + 1 \tag{1.7}$$

degrees of freedom. A natural spline is e.g. uniquely defined by demanding that it interpolates knot values of the function.

We shall also deal with *periodic splines:*

Definition 1.3. The function s belongs to $\mathcal{S}_m^{\mathcal{P}}(\boldsymbol{x}_{0:n})$, the set of *periodic spline functions* of degree m over knots $x_0, \ldots, x_n$, if

1° $s \in \mathcal{S}_m(\boldsymbol{x}_{0:n})$,

2° $s^{(p)}(x_n) = s^{(p)}(x_0)$ for $p = 0, 1, \ldots, m-1$.

By subtracting the number m of extra conditions from ν in (1.6) we see that a periodic spline has

$$\nu_P = n \tag{1.8}$$

degrees of freedom. It is e.g. uniquely defined by demanding that it interpolates the values $s(x_1) = y_1, \ldots, s(x_n) = y_n$.

How to find an approximating spline in different contexts is discussed in Chapters 4 – 6. Before that, however, we discuss other representations in Chapter 2 and approximation errors in Chapter 3.

2. Representation of Splines

We consider a *cubic spline*, $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$. In (1.4) we saw that we can write it in the form

$$\begin{aligned} s(x) = d_{0,j} + d_{1,j}(x - x_{j-1}) + d_{2,j}(x - x_{j-1})^2 + d_{3,j}(x - x_{j-1})^3 \\ \text{for} \quad x_{j-1} \le x < x_j, \quad j = 1, \ldots, n \quad . \end{aligned} \tag{2.1}$$

Given the $4n$ coefficients $\{d_{k,j}\}$, this representation is well suited for evaluating the spline and/or derivatives of it. It is, however, unsuited for the determination of the spline that approximates the function in question.

Example 2.1. As indicated in connection with (1.4), we can set up a linear system of equations in the $4n$ unkonown coefficients. $3(n-1)$ of these equations are given by (1.5), specifying that s is twice continuously differentiable, and only $n+3$ – about a quarter of the number of equations – specify the actual job of the spline. In the remainder of this chapter we give representations that are better suited for this.

2.1. Hermite and Moment Interpolation

These two representations have built in the continuity of s and of respectively s' and s''. Let

$$h_j = x_j - x_{j-1}, \quad j = 1, \ldots, n \ , \tag{2.2}$$

$$s_i = s(x_i), \quad s'_i = s'(x_i), \quad s''_i = s''(x_i), \quad i = 0, 1, \ldots, n \ . \tag{2.3}$$

We can write

Hermite: for $j = 1, \ldots, n$, for $0 \le t \le 1$:

$$\begin{aligned} s(x_{j-1} + h_j t) = (1-t)^2 \left((1+2t)s_{j-1} + h_j t s'_{j-1}\right) \\ + t^2 \left((3-2t)s_j - h_j(1-t)s'_j\right) \quad . \end{aligned} \tag{2.4}$$

Moment:[1] for $j=1,\ldots,n$, for $0 \le t \le 1$:

$$s(x_{j-1}+h_j t) = (1-t)\left(s_{j-1} + \tfrac{1}{6}h_j^2\left((1-t)^2-1\right)s''_{j-1}\right) \qquad (2.5)$$
$$+\; t\left(s_j + \tfrac{1}{6}h_j^2\left(t^2-1\right)s''_j\right) \qquad .$$

Exercise 2.2. Show that the conditions

$$(s(x_i),\ s'(x_i)) = (s_i,\ s'_i)\,, \quad i=0,1,\ldots,n$$

are satisfied by (2.4), and that (2.5) ensures

$$(s(x_i),\ s''(x_i)) = (s_i,\ s''_i)\,, \quad i=0,1,\ldots,n\ .$$

The Hermite representation (2.4) involves $2n+2$ parameters and according to Exercise 2.2 it satisfies the continuity equations (1.5) for $p=0$ and $p=1$. The continuity of $s''(x)$ leads to the following $n-1$ conditions,

$$\begin{aligned} &h_{i+1}s'_{i-1} + 2(h_i+h_{i+1})s'_i + h_i s'_{i+1} \\ &\quad = 3\left(\frac{h_{i+1}}{h_i}(s_i-s_{i-1}) + \frac{h_i}{h_{i+1}}(s_{i+1}-s_i)\right), \quad i=1,\ldots,n-1\ . \end{aligned} \qquad (2.6)$$

Similarly, the continuity of $s'(x)$ leads to the following $n-1$ conditions on the $2n+2$ parameters in the Moment representation (2.5),[2]

$$\begin{aligned} &h_i s''_{i-1} + 2(h_i+h_{i+1})s''_i + h_{i+1}s''_{i+1} \\ &\quad = 6\left(\frac{1}{h_{i+1}}(s_{i+1}-s_i) - \frac{1}{h_i}(s_i-s_{i-1})\right), \quad i=1,\ldots,n-1\ . \end{aligned} \qquad (2.7)$$

Exercise 2.3. Prove (2.6) and (2.7).

In Chapter 3 we use the Hermite representation because it allows a simple derivation of error estimates, and in Chapter 4 we use (2.5) for interpolation between knot-values of a given function.

Exercise 2.4. Assume that we know $\{s_i,\ s'_i\}_{i=0}^n$. Write a function that computes the coefficients $\{d_{k,j}\}$ in the representation (2.1).

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[1] The second derivative is related to the physical bending moment, cf. Example 1.3, and (2.5) is derived from linear interpolation between the knot values of s''.

[2] Note that with both representations we find $\nu = 2n+2-(n-1) = n+3$ in agreement with (1.6).

2.2. B-Splines

A cubic spline has $n+3$ degrees of freedom, and we can write it in the form

$$s(x) = \sum_{j=1}^{n+3} c_j N_j(x)\ , \quad x_0 \le x \le x_n\ , \qquad (2.8)$$

where the $\{N_j\}$ are linearly independent, normalized cubic B-splines (or basis-splines).

Example 2.5. The concept generalizes to splines of any degree. The first order spline from Example 1.2 can be written in the form

$$s(x) = \sum_{j=1}^{n+1} c_j N_{1,j}(x)\ , \quad x_0 \le x \le x_n\ , \qquad (2.9)$$

where the $\{N_{1,j}\}$ are first order B-splines, given by

$$N_{1,i}(x) = \begin{cases} (x-x_{i-2})/h_{i-1} & \text{for } x_{i-2} \le x \le x_{i-1}\ , \\ (x_{i-1}-x)/h_i & \text{for } x_{i-1} \le x \le x_i\ , \\ 0 & \text{otherwise}\ . \end{cases}$$

These socalled *hat functions* are shown below.

Figure 2.1. *Hat Functions*

The $\{N_{1,j}\}$ are first order splines since they are continuous, piecewise polynomials of degree one. Each $N_{1,j}(x)$ is nonzero only in two consecutive knot intervals; we say that they have *local support*. They obviously are linearly independent, and since the number of them equals the number of degrees of freedom, any first order spline can be written in the form (2.9).

Note also, that for any $x \in [x_0, x_n]$ at most two $N_{1,j}(x) \ne 0$. Especially $N_{1,k+1}(x_k) = 1$ is the only nonzero contribution to the sum in (2.9) for $x = x_k$, and the choice $c_j = y_{j-1}$, $j=1,\ldots,n+1$ gives the piecewise linear interpolation in Figure 1.1.

The general B-spline of degree m can be introduced in different ways. We have chosen to give a constructive formulation and restrict the presentation to cubic splines:

Theorem 2.1. Let
$$x_{-2} \le x_{-1} \le x_0 < x_1 < \cdots < x_n \le x_{n+1} \le x_{n+2}$$
be an *augmented knot set*. The $\{M_{r,i}(x)\}_{i=1}^{n+r}$ defined by the recurrence

$$M_{0,i}(x) = \begin{cases} 1/(x_i - x_{i-1}) & \text{for } x_{i-1} \le x < x_i \\ 0 & \text{otherwise} \end{cases} \tag{2.10a}$$

$$M_{r+1,i}(x) = \frac{(x - x_{i-2-r})M_{r,i-1}(x) + (x_i - x)M_{r,i}(x)}{x_i - x_{i-2-r}} \quad \text{for } r = 0,1,2 \tag{2.10b}$$

are splines of degree r defined on $[x_0, x_n]$. They satisfy

$$M_{r,i}(x) = 0 \quad \text{for } x_0 \le x < x_{i-1-r} \text{ and } x_i \le x \le x_n \ , \tag{2.11a}$$

$$M_{r,i}(x) > 0 \quad \text{for } x_{i-1-r} < x < x_i \ , \tag{2.11b}$$

and their derivatives can be computed from

$$M'_{r+1,i}(x) = (r+1)\frac{M_{r,i-1}(x) - M_{r,i}(x)}{x_i - x_{i-2-r}} \ ; \quad r = 0,1,2 \ . \tag{2.11c}$$

The normalized cubic B-splines are given by

$$N_i(x) = (x_i - x_{i-4})M_{3,i}(x) \ . \tag{2.12a}$$

They satisfy

$$\sum_{j=1}^{n+3} N_j(x) = 1 \quad \text{for } x_0 \le x \le x_n \ . \tag{2.12b}$$

Proof: See Appendix B.1. □

The augmented knot set involves two extra knots at both ends, $x_{-2} \le x_{-1} \le x_0$ and $x_{n+2} \ge x_{n+1} \ge x_n$. The spline is independent of the choice of these extra knots, but the $\{N_j\}$ and the coefficients $\{c_j\}$ in (2.8) depend on the choice. If the interior knots are equidistant, $x_i = x_0 + ih,\ i = 1, \ldots, n$, then it is natural to extend this property to the extra knots, cf. Example 2.6. In Section 2.3 we discuss the choice of extra knots for periodic splines.

In the general case it has certain advantages to choose *multiple end knots:* $x_{-2} = x_{-1} = x_0$ and $x_{n+2} = x_{n+1} = x_n$. Figure 2.2 shows the B-splines corresponding to a mixture of choice of extra knots.

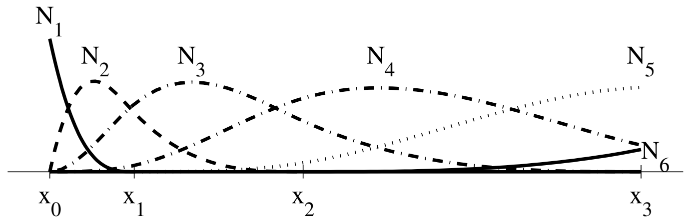


Figure 2.2. *Cubic B-splines for $n = 3$. $x_{-2} = x_{-1} = x_0 = 0.5$, $x_1 = 1,\ x_2 = 2,\ x_3 = 4,\ x_4 = 6,\ x_5 = 8$.*

From Theorem 2.1 it follows that each $N_i(x)$ is nonzero only in four consecutive knot intervals, and in the typical interval $[x_{j-1}, x_j[$ only $N_j(x)$, $N_{j+1}(x)$, $N_{j+2}(x)$ and $N_{j+3}(x)$ are nonzero. The nonzero values in the recurrence are illustrated in Figure 2.3, and in Appendix A.1 we give explicit expressions for these values and for the first two derivatives of $N_{j:j+3}(x)$.

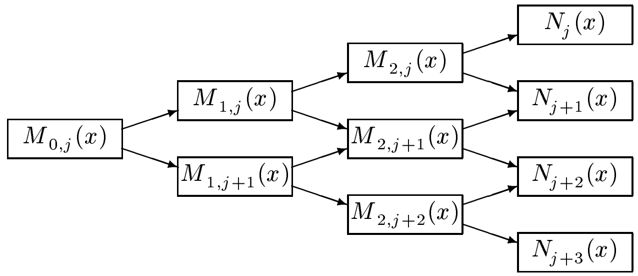


Figure 2.3. *Nonzero values in recurrence for cubic B-splines*

Example 2.6. Let the knots be equidistant with spacing h, i.e. $x_i = x_0 + ih$, $i = -2, -1, \ldots, n+2$. Using the expressions from Appendix A.1 it is easily verified that in the interval $[x_{j-1}, x_j]$ $(1 \le j \le n)$ the four nonzero B-splines can be written

$$N_j(x) = \tfrac{1}{6}u^3, \qquad N_{j+1}(x) = \tfrac{1}{6} + \tfrac{1}{2}u(1 + tu)$$
$$N_{j+2}(x) = \tfrac{1}{6} + \tfrac{1}{2}t(1 + tu), \qquad N_{j+3}(x) = \tfrac{1}{6}t^3 \ ,$$

where $t = (x - x_{j-1})/h, \quad u = (x_j - x)/h = 1 - t$.

Exercise 2.7. Consider a multiple end knot $x_{-2} = x_{-1} = x_0$, and let $h_1 = x_1 - x_0$, $h_2 = x_2 - x_1$. Show that

$$\begin{aligned}
&N_1(x_0) = 1, \quad N_1'(x_0) = -3/h_1, \quad N_1''(x_0) = 6/h_1^2,\\
&N_2(x_0) = 0, \quad N_2'(x_0) = 3/h_1, \quad N_2''(x_0) = -N_1''(x_0) - N_3''(x_0),\\
&N_3(x_0) = 0, \quad N_3'(x_0) = 0 \qquad N_3''(x_0) = 6/\left(h_1(h_1+h_2)\right) .
\end{aligned}$$

The B-spline representation seems more complicated than (2.1) and (2.4–5). The advantage, however, is that the number of parameters equals the number of degrees of freedom, so that the size of the system of equations defining the actual spline is as small as possible. Also, it should be noted that all quantities in (2.10) are positive. This implies that the recurrence is numerically stable.

Another advantage is that the B-spline representation is very versatile: In some applications it may be desirable to allow jumps in the second or first derivative, and this can be obtained simply by using *multiple interior knots:* The knot x_k has multiplicity q if

$$x_{k-1} < x_k = x_{k+1} = \cdots = x_{k+q-1} < x_{k+q} . \tag{2.13}$$

Theorem 2.2. Let x_k be an interior knot of multiplicity q.

If $1 \le q \le 3$, then

$$s^{(p)}(x_k-) = s^{(p)}(x_k+) \quad \text{for } p = 0, 1, \ldots, 3-q ,$$

while $s^{(4-q)}(x)$ may have a jump across x_k.

If $q \ge 4$, then the spline splits into to disjoint splines.

Proof: See Appendix B.2. □

Strictly speaking, the function

$$s(x) = \sum_{j=1}^{n+3} c_j N_j(x) , \quad x_0 \le x \le x_n$$

is not a cubic spline if one or more interior knots are multiple. Because of the applicability, however, we shall include this in the discussion. Note that the representations (2.4) and (2.5) do not allow any $h_j = 0$, but in the recurrence (2.10) there is no risk of division by zero.

2.3. Periodic Splines

According to the definition on page 6, a spline $s \in \mathcal{S}_3^{\mathcal{P}}(\boldsymbol{x}_{0:n})$ satisfies

$$s(x_0) = s(x_n) , \quad s'(x_0) = s'(x_n) , \quad s''(x_0) = s''(x_n) . \tag{2.14}$$

The Moment representation (2.5) can be used for this purpose: This representation has the $2(n+1)$ parameters $\{s_j\}$ and $\{s_j''\}$ and built-in continuity of s and s'', while the $n-1$ conditions (2.6),

$$\begin{aligned}
&h_i s_{i-1}'' + 2(h_i + h_{i+1}) s_i'' + h_{i+1} s_{i+1}''\\
&\quad = 6\left(\frac{y_{i+1} - y_i}{h_{i+1}} - \frac{y_i - y_{i-1}}{h_i}\right) \equiv d_i , \quad i = 1, \ldots, n-1
\end{aligned} \tag{2.15a}$$

ensure continuity of $s'(x)$ across the interior knots. If we let $s_0 = s_n$ and $s_0'' = s_n''$, then the first and third of the conditions in (2.14) are satisfied, and by means of (C.2) we see that the only remaining condition, $s'(x_0+) = s'(x_n-)$ leads to

$$\frac{s_1 - s_0}{h_1} + \tfrac{1}{6} h_1(-2s_0'' - s_1'') = \frac{s_n - s_{n-1}}{h_n} + \tfrac{1}{6} h_n(s_{n-1}'' + s_n'') ,$$

or, exploiting that $s_0 = s_n$ and $s_0'' = s_n''$,

$$\begin{aligned}
&h_1 s_1'' + h_n s_{n-1}'' + 2(h_1 + h_n) s_n''\\
&\quad = 6\left(\frac{s_1 - s_n}{h_1} - \frac{s_n - s_{n-1}}{h_n}\right) \equiv d_n .
\end{aligned} \tag{2.15b}$$

This respresentation is further discussed in Section 4.2.2.

Also the B-spline representation is easily modified to a periodic spline: Choose the extra knots as

$$\begin{aligned}
x_{-1} &= x_0 - h_n , \qquad & x_{-2} &= x_{-1} - h_{n-1} ,\\
x_{n+1} &= x_n + h_1 , \qquad & x_{n+2} &= x_{n+1} + h_2 .
\end{aligned} \tag{2.16}$$

Then it is easily verified by means of the formulae in Appendix A.1 that the only nonzero values at x_0 and x_n satisfy

$$N_k^{(p)}(x_0) = N_{n+k}^{(p)}(x_n) \quad \text{for} \quad \begin{cases} k = 1,2,3 \\ p = 0,1,2 \end{cases} . \tag{2.17}$$

Therefore, if we let

$$c_{n+k} = c_k \quad \text{for} \quad k = 1,2,3 , \tag{2.18}$$

then the spline is periodic. This respresentation is further discussed in Sections 4.3.2 and 5.1.3.

Example 2.8. In chapters 4 and 5 we discuss the computation of the B-spline coefficients $\{c_j\}$ in (2.8). For a periodic spline this can be reformulated to

$$s(x) = \sum_{j=1}^{3} c_j \left(N_j(x) + N_{n+j}(x)\right) + \sum_{j=4}^{n} c_j N_j(x) . \tag{2.19}$$

If $n < 3$, then this expression is simplified further:

For $n = 2$:

$$s(x) = c_1 \left(N_1(x) + N_3(x) + N_5(x)\right) + c_2 \left(N_2(x) + N_4(x)\right) . \tag{2.20a}$$

For $n = 1$ the choice of extra knots, (2.16), is not defined. This, however, does not matter, since the general periodic spline over one knot interval is a constant:

$$s(x) = c_1 \left(N_1(x) + N_2(x) + N_3(x) + N_4(x)\right) = c_1 . \tag{2.20b}$$

Here we have used (2.12b).

---

3. Approximation Error

In this chapter we treat the problem: how well can a function f be approximated by a cubic spline $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$ with $x_0 = a < x_n = b$? To answer that question we look at the *error function*

$$e(x) = f(x) - s(x) , \quad a \le x \le b . \tag{3.1}$$

We first look at the *local* behaviour of the error, i.e. inside one knot interval, and then at the *glocal* behaviour, i.e. in the whole range $[a, b]$.

Theorem 3.1. (Local error). Let $f \in \mathsf{C}^4[a, b]$ and $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$. In the knot interval $I_j \equiv [x_{j-1}, x_j]$ the error satisfies

$$\begin{aligned} \max_{x \in I_j} \left\{|e(x)|\right\} \le \tfrac{1}{384} h_j^4 F_j^{iv} + \tfrac{1}{4} h_j \max\left\{|e'_{j-1}|,\ |e'_j|\right\} \\ + \max\left\{|e_{j-1}|,\ |e_j|\right\} , \end{aligned} \tag{3.2a}$$

where

$$\begin{aligned} &h_j = x_j - x_{j-1}, \qquad F_j^{iv} = \max_{x \in I_j} \left\{|f''''(x)|\right\} , \\ &e_k = e(x_k), \qquad e'_k = e'(x_k) . \end{aligned} \tag{3.2b}$$

The first three derivatives are bounded by

$$\begin{aligned} \max_{x \in I_j} \left\{|e^{(p)}(x)|\right\} \le \alpha_p h_j^{4-p} F_j^{iv} + \beta_p h_j^{1-p} \max\left\{|e'_{j-1}|,\ |e'_j|\right\} \\ + \gamma_p h_j^{-p} |e_j - e_{j-1}| , \end{aligned} \tag{3.3a}$$

where

$$\begin{aligned} &\alpha_1 = \tfrac{\sqrt{3}}{216} , \qquad \beta_1 = 1 , \qquad \gamma_1 = \tfrac{3}{2} , \\ &\alpha_2 = \tfrac{1}{12} , \qquad \beta_2 = 6 , \qquad \gamma_2 = 6 , \\ &\alpha_3 = \tfrac{1}{2} , \qquad \beta_3 = 12 , \qquad \gamma_3 = 12 . \end{aligned} \tag{3.3b}$$

Proof: See Appendix B.3. □

From Theorem 3.1 we immediately see that

$$\max_{a\le x\le b}\{|e(x)|\} \le \tfrac{1}{384}\max_j\{h_j^4 F_j^{iv}\} + \tfrac14\max_j\{h_j|e_j'|\} + \max_j\{|e_j|\} \ . \tag{3.4}$$

This estimate is not directly useful, however, since it requires knowledge of both the error function and its derivative at all knots. However, just as (2.6) relates the values $\{s_j\}$ and $\{s_j'\}$, there are relations between the error contributions in (3.2):

Lemma 3.2. Let $f\in \mathsf{C}^4[a,b]$ and $s\in\mathcal{S}_3(\boldsymbol{x}_{0:n})$. Then

$$\max_{j=1,\ldots,n-1}\{|e_j'|\} \le \tfrac{1}{24}\max_j\{h_j^3F_j^{iv}\} + E_b' + \frac{6E}{h} \ , \tag{3.5a}$$

where $h=\min_j\{h_j\}$ and

$$E=\max_j\{|e_j|\}\ ,\quad E_b'=\max\{|e_0'|,\ |e_n'|\} \ . \tag{3.5b}$$

Proof: See Appendix B.4. □

Combining this with (3.4) we get

Theorem 3.3. (Global error). The approximation error satisfies

$$\max_{a\le x\le b}\{|e(x)|\} \le \frac{5H}{384}\max_j\{h_j^3F_j^{iv}\} + \frac{H}{4}E_b' + \big(1+1.5\frac{H}{h}\big)E \ , \tag{3.6}$$

where $H=\max_j\{h_j\}$.

If all $e_i=0$ and the knots are equidistant, $h_i\equiv h=(b-a)/n$, then Theorem 3.3 shows that

$$|e(x)| \le O(h^4) + O(hE_b') \ . \tag{3.7}$$

We discuss this further in Chapter 4.

Example 3.1. The estimate in Theorem 3.2 hides the *"local nature"* of a spline, but this is the subject of the present example:

Let the knots be equidistant with spacing $h=(b-a)/n$. Then Equation (B.10a) for the knot values of e' takes the form

$$\begin{aligned} 4e_1' + e_2' &= \psi_1 \\ e_{i-1}' + 4e_i' + e_{i+1}' &= \psi_i, \quad i=2,\ldots,n-2 \\ e_{n-2}' + 4e_{n-1}' &= \psi_{n-1} \end{aligned} \tag{3.8a}$$

where

$$\begin{aligned} \psi_1 &= -e_0' + 4(d_1+\varphi_1) \\ \psi_i &= 4(d_i+\varphi_i), \quad i=2,\ldots,n-2 \\ \psi_{n-1} &= -e_n' + 4(d_{n-1}+\varphi_{n-1}) \end{aligned} \ . \tag{3.8b}$$

The solution to this linear system of equations can be written in the form

$$e_i' = \sum_{k=1}^{n-1}\xi_{ik}\psi_k \ , \quad i=1,\ldots,n-1 \ , \tag{3.9}$$

where ξ_{ik} is the ith element of the solution to (3.8a) with $\psi_k=1$ as the only nonzero right-hand side. It is easily verified by insertion that

$$\xi_{ik} = A\left(r^{|i-k|} - Br^{k+i} - Cr^{2n-k-i}\right) \ , \tag{3.10a}$$

where

$$r=\sqrt{3}-2 \simeq -0.268 \tag{3.10b}$$

is a solution of the second order equation

$$r^2+4r+1=0 \ , \tag{3.10c}$$

and

$$A=\frac{1}{4+2r},\qquad B=\frac{1-r^{2n-2k}}{1-r^{2n}},\qquad C=\frac{1-r^{2k}}{1-r^{2n}} \ . \tag{3.10d}$$

The resulting contribution to the error function in the jth interval is found from Appendix B.3

$$\psi_k\omega_k(x_{j-1}+h_jt) = \psi_k h\left((1-t)^2t\xi_{j-1,k} - t^2(1-t)\xi_{j,k}\right) \ . \tag{3.11}$$

This is illustrated below.

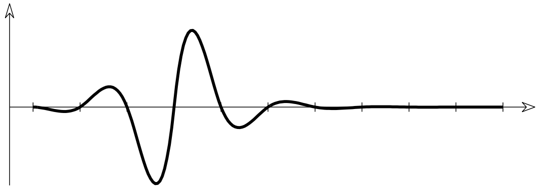


Figure 3.1. $\omega_3(x)$ *for* $n=10$

Note that the effect decays rapidly as we move away from the kth knot ($k=3$ above). The reason is that $\xi_{i,k}$ is dominated by $Ar^{|i-k|}$, which is reduced by a factor $r\simeq-\frac14$ as each knot is passed.

The result of the above example can be generalized: The derivative e_i' of the error function is dominated by the error contributions from the adjacent knot intervals. Especially as regards the contribution from the variation in $f(x)$ – i.e. the term with F_j^{iv} – the relevant quantity is $\max\{h_j^4 F_j^{iv}\}$ rather than $H \cdot \max\{h_j^3 F_j^{iv}\}$. This leads to the following guideline for obtaining a good approximation.

Rule of Thumb no. 1. The interior knots should be distributed so that $h_j^4 F_j^{iv}$ has the same order of magnitude throughout the entire range $[a, b]$.

This rule should not be used too literally, however: A rapid variation in knot spacing may induce “ripples” in the spline, as illustrated in the next example.

Example 3.2. Consider a problem with $h_i = h$ for $i = 1, \ldots, p$ and $h_i = H$ for $i = p{+}1, \ldots, n$.

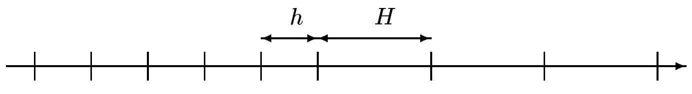


Figure 3.2. *Jump in knot spacing*

The values e_j' satisfy the following system of equations

$$\begin{aligned} 4e_1' + e_2' &= \psi_1 \\ e_{i-1}' + 4e_i' + e_{i+1}' &= \psi_i, \quad i = 2, \ldots, p{-}1 \\ 2(1{-}\eta)e_{p-1}' + 4e_p' + 2\eta e_{p+1}' &= \psi_p \\ e_{i-1}' + 4e_i' + e_{i+1}' &= \psi_i, \quad i = p{+}1, \ldots, n{-}2 \\ e_{n-2}' + 4e_{n-1}' &= \psi_{n-1} \end{aligned} \tag{3.12a}$$

where $\eta = h/(h{+}H) \;\Leftrightarrow\; 1{-}\eta = H/(h{+}H)$ and the right-hand sides are as in (3.8),

$$\begin{aligned} \psi_1 &= -e_0' + 4(d_1 + \varphi_1) \\ \psi_i &= 4(d_i + \varphi_i), \quad i = 2, \ldots, n{-}2 \\ \psi_{n-1} &= -e_n' + 4(d_{n-1} + \varphi_{n-1}) \end{aligned} \quad . \tag{3.12b}$$

Again, we express the solution in the form (3.9), and if $p = k$, then ξ_{ik} has the form (3.10a) with the same B and C, but with A changed to

$$\widetilde{A} = \frac{1}{4 + 2r} \; \frac{1}{1 + (1{-}2\eta)\,(Br^{2k} - Cr^{2n-2k})} \; .$$

Except for very small values of k or $n{-}k$ we have $B \simeq C \simeq 1$ and $\widetilde{A} \simeq A$.

For $p \neq k$ we can write

$$\begin{aligned} \xi_{ik} &= A\left(r^{|i-k|} - Br^{k+i} - Cr^{2n-k-i}\right) \\ &\quad + D\left(r^{|i-p|} - Gr^{p+i} - Kr^{2n-p-i}\right) \ , \end{aligned} \tag{3.13a}$$

where A, B, C are given by (3.10d),

$$G = \frac{1 - r^{2n-2p}}{1 - r^{2n}}, \qquad K = \frac{1 - r^{2p}}{1 - r^{2n}} \ , \tag{3.13b}$$

and

$$D = \frac{A(1{-}2\eta)\left(r^{|p-k|} - Br^{p+k} + Cr^{2n-k-p}\right)}{1 + (1{-}2\eta)\left(Gr^{2p} - Hr^{2n-2p}\right)} \ . \tag{3.13c}$$

Except for very small values of k, $n{-}k$, p or $n{-}p$ we have

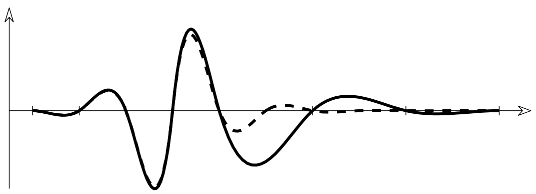
$$D \simeq A(1{-}2\eta)r^{|p-k|} \ .$$

As a particular example, let $p = k{+}1$. Then $D \simeq r(1{-}2\eta)A$ and

$$\widetilde{\xi}_{kk} \simeq \left(1 + r^2(1{-}2\eta)\right)\xi_{kk}, \qquad \widetilde{\xi}_{kp} \simeq 2(1{-}\eta)\xi_{kp} \ .$$

This is illustrated below by showing the error contribution $\omega_k(x)$ defined in (3.11). For comparison we also give the contribution in the equidistant knot case (dotted line).

Figure 3.3. $\omega_3(x)$ *for* $n = 7$, $p = 4$, $H = 2h$



In the fine part of the knot mesh the effect of the jump in spacing dies quickly. In the coarse part it takes longer, partly because the reduction by the factor r needs a longer distance.

The above example should not lead to undue pessimism. Normally, the ripples induced by a jump in knot spacing will “drown” in the local contributions to the error. It is generally recommended, however, to accompany the first rule of thumb by

Rule of Thumb no. 2. The interior knots should be distributed so that $\frac{1}{2} \le h_{i-1}/h_i \le 2$, and a change between small and large h_j-values should not take place too often.

Example 3.3. Powell [10] recommends to have at least three knots between jumps in knot spacing. The present author [9] found it advantageous in a special application to let h_i be a monotonely increasing function of i, cf. Example 4.7.

Example 3.4. The points used in the examples of Chapter 1 are taken from the function

$$f(x) = 2 - 0.1x + \frac{2(x-1)}{(x-4)^4+1} \,. \tag{3.14}$$

Figure 3.4 shows two spline approximations to this function. Both splines satisfy

$$s(x_i) = f(x_i),\ i=0,1,\ldots,n \quad \text{and} \quad s'(x_0) = f'(x_0),\ s'(x_n) = f'(x_n)$$

with $n=10$, $x_0=0$ and $x_n=10$, but they differ in the choice of interior knots: The knots of the dotted spline are equidistant, while the knots of the full line spline are distributed with respect to the different "nature" of f in different subregions, cf. Figure 3.5.

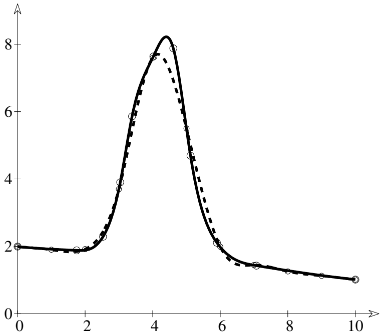


Figure 3.4. *Interpolating splines*

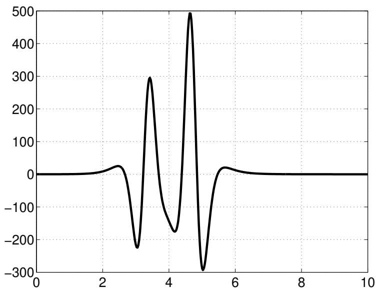


Figure 3.5. $f''''(x)$

Finally, Figures 3.6–7 show the error curves and the values of $\{h_j^4 F_j^{iv}\}$ for the two splines.

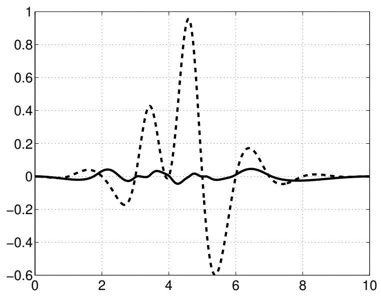


Figure 3.6. $e(x) = f(x) - s(x)$

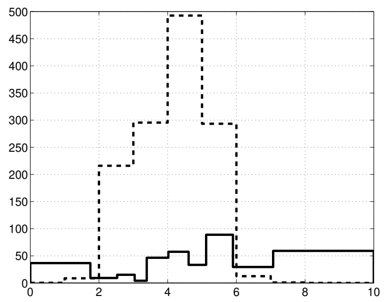


Figure 3.7. $h_j^4 F_j^{iv}$

The "full line spline" satisfies $|e(x)| < 0.05$.

4. Interpolation

Given the points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ with $x_0 < x_1 < \ldots < x_n$. We wish to interpolate between the points, i.e. to find a function $g \in \mathsf{C}[x_0, x_n]$ that satisfies $g(x_i) = y_i$ for $i = 0, 1, \ldots, n$. This problem does not have a unique solution. Two simple choices are the interpolating polynomial (of degree n) or the piecewise linear function obtained by linear interpolation between neighbouring points. These two choices are illustrated in Figures 1.3 and 1.1.

Often, however, neither the kinks in Figure 1.1 nor the "overswings" in Figure 1.3 are desirable. Rather, we want a smooth function, characterized by being at least twice continuously differentiable, and the risk of overswings is reduduced if we demand that $\int_{x_0}^{x_n} (g''(x))^2 \, dx$ should be as small as possible.

In Chapter 1 we saw that these goals are met by choosing g as the natural cubic spline $g = s \in \mathcal{S}_3^{\mathcal{N}}(\boldsymbol{x}_{0:n})$, satisfying

$$s(x_i) = y_i \ , \quad i = 0, 1, \ldots, n \ , \tag{4.1a}$$

$$s''(x_0) = s''(x_n) = 0 \ . \tag{4.1b}$$

The simplest way of determining the spline is via the Moment representation (2.5),

$$\begin{aligned} &\text{for } j = 1, \ldots, n: \quad h_j = x_j - x_{j-1}, \quad \text{for } 0 \le t \le 1 \ : \\ &\quad s(x_{j-1} + h_j t) = (1-t)\left(s_{j-1} + \tfrac{1}{6} h_j^2 \left((1-t)^2 - 1\right) s''_{j-1}\right) \\ &\qquad\qquad + t\left(s_j + \tfrac{1}{6} h_j^2 \left(t^2 - 1\right) s''_j\right) \quad . \end{aligned} \tag{4.2}$$

Here, the parameters $\{s_i\}$ are given by (4.1a),

$$s_i = y_i \ , \quad i = 0, 1, \ldots, n \ . \tag{4.3a}$$

The natural spline conditions (4.1b) lead to

$$s''_0 = s''_n = 0 \ , \tag{4.3b}$$

and finally, the continuity of $s'(x)$ leads to the equations (2.7). By means of (4.3a) they are seen to take the form

$$\begin{aligned} &h_i s''_{i-1} + 2(h_i + h_{i+1}) s''_i + h_{i+1} s''_{i+1} \\ &\quad = 6\left(\frac{y_{i+1} - y_i}{h_{i+1}} - \frac{y_i - y_{i-1}}{h_i}\right) \equiv d_i \ , \quad i = 1, \ldots, n-1 \ . \end{aligned} \tag{4.3c}$$

This is a linear system of equations, and exploiting (4.3b) in the first and the last equation we can write it in the form

$$\begin{bmatrix} 2(h_1+h_2) & h_2 & & \\ h_2 & 2(h_2+h_3) & h_3 & \\ & \cdot & \ddots & \cdot \\ & & h_{n-1} & 2(h_{n-1}+h_n) \end{bmatrix} \begin{bmatrix} s''_1 \\ s''_2 \\ \vdots \\ s''_{n-1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_{n-1} \end{bmatrix} , \tag{4.4a}$$

or, for short

$$\boldsymbol{A} \boldsymbol{s}''_{1:n-1} = \boldsymbol{d} \ . \tag{4.4b}$$

The matrix is tridiagonal, symmetric and positive definite. The last property follows because it is diagonally dominant and it implies that simple Gaussian elimination (i.e. without row interchanges) is numerically stable. The system can be solved by the *tridiagonal algorithm* given in Appendix A.2. The computational cost is about $8n$ flops.

Example 4.1. Given the points

i	x_i	y_i
0	−1	−0.6861
1	0	1.0000
2	1	−0.2524
3	2	−0.2405
4	3	0.2142

The knots are equidistant, $h_j \equiv h = 1$, and (4.4) takes the form

$$\begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 4 \end{bmatrix} \begin{bmatrix} s''_1 \\ s''_2 \\ s''_3 \end{bmatrix} = \begin{bmatrix} -17.631 \\ 7.586 \\ 2.657 \end{bmatrix} \quad \text{with the solution} \quad \boldsymbol{s}''_{1:3} = \begin{bmatrix} -5.217 \\ 3.237 \\ -0.145 \end{bmatrix} .$$

The graph of s is shown in Example 4.5.

4.1. Error Analysis

We first consider the sensitivity of s with respect to small changes in the data.

Theorem 4.1. Let $s(x)$ and $s(x)+\delta s(x)$ be the natural splines that interpolate $(x_0,y_0),\ \ldots,\ (x_n,y_n)$ and $(x_0,y_0+\delta y_0),\ \ldots,\ (x_n,y_n+\delta y_n)$, respectively. Then

$$\max_{x_0\le x\le x_n}\{|\delta s(x)|\} \le \left(1+1.5\left(\frac{H}{h}\right)^2\right)\max_i\{|\delta y_i|\} \;,$$

where $h=\min\{h_i\}$, $H=\max\{h_i\}$.

Proof: See Appendix B.5. □

This modest effect of disturbances reflects the fact that the determination of a cubic spline is well conditioned. In Appendix B.5 we also show that the condition number of the matrix $\boldsymbol{A}$ in (4.4) satisfies

$$\kappa_\infty(\boldsymbol{A}) = \|\boldsymbol{A}\|_\infty\|\boldsymbol{A}^{-1}\|_\infty \le 3\frac{H}{h} \;. \tag{4.5}$$

If the number of knots is increased without changing the ratio between the largest and smallest h_i, then this condition number is independent of n.

4.1.1. Interpolation Errors. Assume now that the data points are from some function f, i.e. $y_i = f(x_i),\ i=0,1,\ldots,n$. We wish to see how close $s(x)$ is to $f(x)$.

Theorem 4.2. Let $y_i = f(x_i),\ i=0,1,\ldots,n$ for some function $f\in \mathsf{C}^4[x_0,x_n]$. Then the interpolating natural cubic spline satisfies

$$\max_{x_0\le x\le x_n}\{|f(x)-s(x)|\} \le \frac{13H}{384}\max_j\{h_j^3F_j^{iv}\} + \frac{H^2}{8}\max_{z=x_0,x_n}\{|f''(z)-s''(z)|\} \;,$$

where $h_j = x_j - x_{j-1}$, $H=\max\{h_j\}$ and F_j^{iv} is defined in Theorem 3.1.

Proof: See Appendix B.6. □

Spline interpolation has a number of applications. One is when $f(x)$ is hard to compute and we exploit the simple evaluation of an approximating spline. In this connection it is important to know the behaviour if the knot mesh is refined, i.e. $n\to\infty$, while the end points $x_0=a$ and $x_n=b$ stay fixed. We assume that the refinement is done so that $H=\max\{h_j\}\to 0$ as $n\to\infty$. Then, combining Theorems 3.3 and 4.2 we see that the interpolating natural spline satisfies

$$\max_{a\le x\le b}\{|f(x)-s(x)|\} \le \begin{cases} O(H^4) & \text{if } f''(a)=f''(b)=0 \;, \\ O(H^2) & \text{otherwise} \;. \end{cases} \tag{4.6}$$

Thus, if $f''(a)\ne 0$ or $f''(b)\ne 0$, then we loose two powers of H by using a natural spline. In Section 4.2 we shall see how it is possible to get a better performance.

Example 4.2. The estimate (4.6) ignores the local nature of the spline. If – as in Example 3.1 – the knots are equidistant, $h_i = H = (b-a)/n$, then the effect in the jth knot interval of the error e_0'' decays as r^j, where $r\simeq -0.268$. Thus, for a fixed $x\in\,]a,b[$ the effect is $O(H^2)\cdot r^{(x-a)/H}$, and except for x very close to a we will find $|r^{(x-a)/H}| < H^2$, and the local error (which is $O(H^4)$) dominates. A similar argument holds for the effect of e_n'', so in practice the error $|e(x)|$ is $O(H^4)$ in the major part of the range $[a,b]$. This is illustrated in Example 4.6.

4.2. Other Boundary Conditions

We consider the case where $f(x)$ can be computed for any $x\in[a,b]$ and seek an approximating spline without the loss of accuracy near a and b, which was discussed above.

We still use the conditions

$$s(x_i) = f(x_i)\;,\quad i=0,1,\ldots,n\;, \tag{4.7}$$

(the rules of thumb from Chapter 3 should be used to distribute the interior knots $x_{1:n-1}$), and need two more conditions to get a uniqe determination of $s\in\mathcal{S}_3(\boldsymbol{x}_{0:n})$. In the case of a natural spline these extra conditions were $s''(a)=s''(b)=0$. Now, we shall exploit the knowledge of f.

If $f'(x)$ or $f'(x)$ is available at the ends, then we supply (4.7) with

$$s^{(p)}(x_0) = f^{(p)}(a), \quad\text{and}\quad s^{(p)}(x_n) = f^{(p)}(b)\;, \tag{4.8}$$

where $p=1$ or $p=2$. From Theorem 3.3 (when $p=1$) or Theorem 4.2 (when $p=2$) it follows that the interpolation error behaves as $O(H^4)$ for $H \to 0$.

If derivative information is not available, then we can supply (4.7) with

$$\begin{aligned} s(x_{1.5}) - s(x_{0.5}) &= f(x_{1.5}) - f(x_{0.5}) \ , \\ s(x_{n-0.5}) - s(x_{n-1.5}) &= f(x_{n-0.5}) - f(x_{n-1.5}) \ , \end{aligned} \tag{4.9}$$

where $x_{k-0.5} \equiv x_k - \frac{1}{2}h_k$. These conditions are derived from central difference approximations to $s'(x) = f'(x)$ for $x = x_1$ and $x = x_{n-1}$. Also in this case we get $O(H^4)$ convergence of the approximating spline, see [5].

It should be mentioned that even for a small value of n the approximation obtained with the boundary conditions (4.8) or (4.9) is normally better than the natural spline approximation, cf. Example 4.5 below. Also, the modified systems discussed in Section 4.2.1 are as robust as stated in Theorem 4.1.

4.2.1. Practical Details. We still use the representation (4.2), and (4.3a) is still valid. The interior knot values of s'' satisfy the equations

$$\widetilde{\boldsymbol{A}}\boldsymbol{s}''_{1:n-1} = \widetilde{\boldsymbol{d}} \ , \tag{4.10}$$

where $\widetilde{\boldsymbol{A}}$ and $\widetilde{\boldsymbol{d}}$ are obtained by minor modifications of the matrix and right-hand side in (4.4). The modifications depend on the boundary conditions:

If $f''(x)$ is known at the ends, then $\widetilde{\boldsymbol{A}} = \boldsymbol{A}$ and $\widetilde{d}_i = d_i$ except for

$$\widetilde{d}_1 = d_1 - h_1 f''(x_0) \ , \qquad \widetilde{d}_{n-1} = d_{n-1} - h_n f''(x_n) \ , \tag{4.11a}$$

corresponding to

$$s''_0 = f''(x_0) \quad \text{and} \quad s''_n = f''(x_n) \ . \tag{4.11b}$$

If $f'(x)$ is used at the ends, then $\widetilde{\boldsymbol{A}}$ and $\widetilde{\boldsymbol{d}}$ differ from $\boldsymbol{A}$ and $\boldsymbol{d}$ only in the elements

$$\begin{aligned} &\widetilde{a}_{11} = 1.5h_1 + 2h_2 \ , \qquad \widetilde{a}_{n-1,n-1} = 2h_{n-1} + 1.5h_n \\ &\widetilde{d}_1 = d_1 - 3\left(\frac{s_1 - s_0}{h_1} - f'(x_0)\right) \ , \\ &\widetilde{d}_{n-1} = d_{n-1} + 3\left(\frac{s_n - s_{n-1}}{h_n} - f'(x_n)\right) \ , \end{aligned} \tag{4.12a}$$

and after having solved (4.10) we compute

$$\begin{aligned} s''_0 &= -\tfrac{1}{2}s''_1 + \frac{3}{h_1}\left(\frac{s_1 - s_0}{h_1} - f'(x_0)\right) \\ s''_n &= -\tfrac{1}{2}s''_{n-1} - \frac{3}{h_n}\left(\frac{s_n - s_{n-1}}{h_n} - f'(x_n)\right) \ . \end{aligned} \tag{4.12b}$$

Exercise 4.3. Use (4.2) – (4.3) to prove that the spline computed by (4.10) and (4.12) satisfies $s(x_i) = f(x_i),\ i = 0, \ldots, n$ and $s'(x_k) = f'(x_k),\ k = 0, n$.

Example 4.4. If we use the conditions (4.9), then the modified elements in $\boldsymbol{A}$ and $\boldsymbol{d}$ are

$$\begin{aligned} &\widetilde{a}_{1,1} = h_1 + \left(2 + \frac{h_2}{h_1}\right)h_2 \ , \quad \widetilde{a}_{1,2} = \left(1 + \frac{h_2}{h_1}\right)h_2 \ , \\ &\widetilde{a}_{n-1,n-2} = \left(1 + \frac{h_{n-1}}{h_n}\right)h_{n-1} \ , \\ &\widetilde{a}_{n-1,n-1} = \left(2 + \frac{h_{n-1}}{h_n}\right)h_{n-1} + h_n \ , \end{aligned} \tag{4.13a}$$

$$\begin{aligned} \widetilde{d}_1 &= d_1 + \frac{8}{h_1}\left(s_2 - s_0 - 2\left(f(x_{1.5}) - f(x_{0.5})\right)\right) \ , \\ \widetilde{d}_{n-1} &= d_{n-1} - \frac{8}{h_n}\left(s_n - s_{n-2} - 2\left(f(x_{n-0.5}) - f(x_{n-1.5})\right)\right) \ . \end{aligned} \tag{4.13b}$$

After having solved (4.10) the boundary values of s'' are found from

$$\begin{aligned} s''_0 &= -\left(2(h_1+h_2)s''_1 + h_2 s''_2 - d_1\right)/h_1 \ , \\ s''_n &= -\left(2(h_{n-1}+h_n)s''_{n-1} + h_{n-1}s''_{n-2} - d_{n-1}\right)/h_n \ . \end{aligned} \tag{4.13c}$$

In contrast with (4.11) or (4.12) the tridiagonal matrix $\widetilde{\boldsymbol{A}}$ is not symmetric in this case. The symmetry can be recovered by dividing the first and last equation by $1 + h_2/h_1$ and $1 + h_{n-1}/h_n$, respectively.

Example 4.5. The points in Example 4.1 are taken from the function

$$f(x) = \mathrm{e}^{-\frac{1}{2}x}\cos 2x \ , \tag{4.14}$$

for which $f'(-1) = 3.3414, \quad f'(3) = 0.0176$. We apply these boundary conditions for s, and (4.10) takes the form

$$\begin{bmatrix} 3.5 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 3.5 \end{bmatrix}\begin{bmatrix} s''_1 \\ s''_2 \\ s''_3 \end{bmatrix} = \begin{bmatrix} -12.665 \\ 7.586 \\ 3.968 \end{bmatrix} \quad \text{with the solution} \quad \boldsymbol{s}''_{1:3} = \begin{bmatrix} -4.458 \\ 2.937 \\ 0.294 \end{bmatrix} \ ,$$

and (4.12c) gives $s''_0 = -2.737\ , \quad s''_4 = -1.459$.

In Figure 4.1 we show this spline together with f and the natural spline from

Example 4.1.

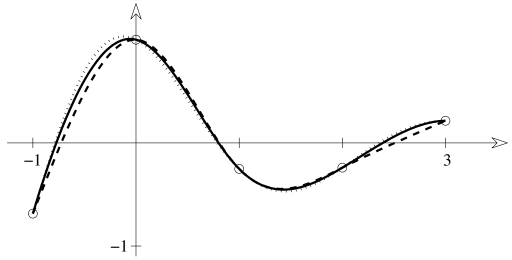


Figure 4.1. *f given by (4.14) (dotted line)*
Natural spline from Example 4.1 (dashed line)
Spline from this example (full line)

Example 4.6. For the function from the previous example we have computed the interpolating spline with equidistant knots on the range $[a,b]=[-1,3]$ and with three choices of boundary conditions

1° $s'(a)=f'(a)$ and $s'(b)=f'(b)$,

2° $s''(a)=f''(a)$ and $s''(b)=f''(b)$,

3° $s''(a)=s''(b)=0$, i.e. s is a natural spline.

In the first table below we give the error

$$\varepsilon_k = \max_{-1\le x\le 3}\{|f(x)-s(x)|\} = |f(u_k)-s(u_k)|$$

for increasing values of n. Here, the index k refers to the choice of boundary condition.

n	ε_1	u_1	ε_2	u_2	ε_3	u_3
2	5.12e-01	-0.064	1.50e+00	-0.160	1.54e+00	-0.168
4	8.85e-02	-0.456	1.93e-01	-0.536	2.13e-01	-0.544
8	3.82e-03	-0.232	8.99e-03	-0.776	1.41e-02	-0.784
16	2.69e-04	-0.624	4.68e-04	-0.888	2.94e-03	2.904
32	1.53e-05	-0.560	2.69e-05	-0.944	7.17e-04	2.952
64	9.46e-07	-0.656	1.59e-06	-0.976	1.78e-04	2.976
128	5.89e-08	-0.640	9.62e-08	-0.984	4.09e-05	2.984

For $n\ge 16$ we see that $\varepsilon_k(2n)\simeq \frac{1}{16}\varepsilon_k(n)$ for $k=1,2$, while $\varepsilon_3(2n)\simeq\frac{1}{4}\varepsilon_3(n)$. This is in agreement with (3.7) and (4.6). Note that both for $k=2$ and $k=3$ the point of maximum error gets increasingly close to an end point of the region.

We have similarly looked at the maximum error in the strictly interior part of the region. More specificly, we have found

$$\delta_k = \max_{-0.5\le x\le 2.5}\{|f(x)-s(x)|\} = |f(v_k)-s(v_k)| \ .$$

The results are given below

n	δ_1	v_1	δ_2	v_2	δ_3	v_3
2	5.12e-01	-0.064	1.50e+00	-0.160	1.54e+00	-0.168
4	8.85e-02	-0.456	1.92e-01	-0.496	2.10e-01	-0.496
8	3.82e-03	-0.232	2.53e-03	-0.216	2.54e-03	2.344
16	2.24e-04	-0.368	2.44e-04	-0.376	3.31e-04	-0.376
32	1.43e-05	-0.440	1.44e-05	-0.440	1.60e-05	-0.440
64	8.89e-07	-0.472	8.89e-07	-0.472	8.91e-07	-0.472
128	5.28e-08	-0.424	5.28e-08	-0.424	5.28e-08	-0.424

With all three choices of boundary conditions we find that the error behaves as $O(H^4)$ in agreement with Example 4.2. Also note that the point of maximum error is (almost) independent of k.

Example 4.7. We shall use the first rule of thumb from Chapter 3 to distribute the knots,

$$h_j^4 F_j^{iv} = const \ . \qquad (4.15)$$

With f given by (4.14) we find $f''''(x)=\frac{1}{16}\mathrm{e}^{-\frac{1}{2}x}\,(161\cos 2x - 240\sin 2x)$. Thus, F_j^{iv} varies as $\mathrm{e}^{-\frac{1}{2}x_{j-1}}$, and (4.15) leads to

$$h_j^4\ \mathrm{e}^{-\frac{1}{2}x_{j-1}} = const\ , \qquad x_j = a+\sum_{k=1}^{j} h_k\ , \qquad x_n = b\ .$$

This is a nonlinear problem, and experience indicates that it may not be worth the trouble to find the true solution. Instead, we approximate the condition by

$$\frac{h_{j+1}}{h_j} = \frac{\mathrm{e}^{x_j/8}}{\mathrm{e}^{x_{j-1}/8}} = \mathrm{e}^{h_j/8} \simeq \mathrm{e}^{(b-a)/(8n)} \equiv \alpha\ . \qquad (4.16a)$$

This implies

$$b-a = h_1+\cdots+h_n = h_1\left(1+\alpha+\cdots+\alpha^{n-1}\right) = \frac{\alpha^n-1}{\alpha-1}\,h_1\ , \qquad (4.16b)$$

from which we can find h_1, followed by $h_j=\alpha h_{j-1}$, $j=2,\ldots,n$.

For $a=-1$, $b=3$, $n=4$ we get $\alpha=1.1331$, $h_1=0.8210$ and the interior knots $x_1=-0.1790$, $\quad x_2=0.7513$, $\quad x_3=1.806$.

We have computed the interpolating spline with these knots and the boundary conditions $s'(x_k) = f'(x_k),\ k=0,n$. As compared with the equidistant knot spline from the previous example, the maximum value of $|e(x)|$ was reduced from `8.84e-02` to `6.50e-02`.

The reason for this small pay-off is that the "nature" of f does not change drastically over the interval $[a,b] = [-1,3]$. If we change this to $[a,b] = [-1,7]$ and also increase the number of knots to $n=10$, then $\max\{|e(x)|\} =$ `3.17e-02` for the equidistant knot spline, while the above approach leads to $\max\{|e(x)|\} =$ `1.02e-02`. The error curves are shown below.

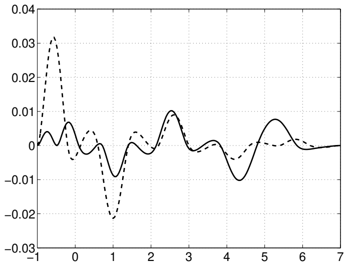


Figure 4.2. *Error curves.*
Equidistant knots (dashed)
Knots distributed by (4.16) (full line)

Example 4.8. In some applications a *parametric representation* of a curve is needed. This means the the points on the curve are expressed as

$$(u(p), v(p)) \quad \text{for} \quad a \le p \le b\ ,$$

where u and v are given functions of the parameter p.

Suppose that we are given $n{+}1$ distinct points on the curve, $(u_0, v_0), \ldots, (u_n, v_n)$. We can approximate the curve by $(U(p), V(p))$, where U and V are cubic splines over knots $p_0, \ldots, p_n$, determined by interpolation to the points $(p_0, u_0), \ldots, (p_n, u_n)$ and $(p_0, v_0), \ldots, (p_n, v_n)$, respectively.

We can choose the knots as $p_i = i,\ i=0,\ldots,n$, corresponding to the spacing $h_i = 1$, and the Moment representation (4.2) takes the form

$$\begin{aligned} &\text{for } j=1,\ldots,n: \quad \text{for } 0 \le t \le 1\ : \\ &\quad U(j{-}1+t) = (1{-}t)\left(U_{j-1} + \tfrac{1}{6}\left((1{-}t)^2 - 1\right)U''_{j-1}\right) \\ &\qquad\qquad + t\left(U_j + \tfrac{1}{6}\left(t^2-1\right)U''_j\right)\ , \end{aligned}$$

and similar for V. According to (4.3) the spline parameters should satisfy

$$\begin{aligned} &U_i = u_i\ , \quad i=0,1,\ldots,n \\ &U''_{i-1} + 4U''_i + U''_{i+1} = 6(u_{i-1} - 2u_i + u_{i+1})\ , \quad i=1,\ldots,n{-}1\ , \end{aligned}$$

and if we choose a natural spline, then the two remaining conditions are $U''_0 = U''_n = 0$. Similar expressions hold for V.

Other boundary conditions are possible. Suppose e.g. that we want the curve to have vertical tangents at the ends. Then we can use a natural spline for V, but for U we replace the natural spline conditions by $U'(0) = U'(n) = 0$, and use (4.12) to compute this spline.

We show two spline approximations to a parametic curve "given" by 6 points. The curve to the left uses natural splines for both U and V, while the other curve has vertical tangents at the ends.

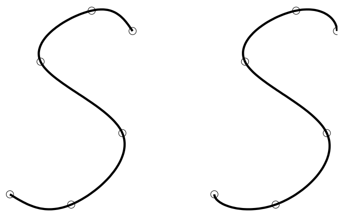


Figure 4.3. *Parametic curves*

4.2.2. Periodic Splines. If the data is periodic – e.g. describing a dayly, weekly or yearly variation – then it is desirable to let the spline share this property. This means that we seek $s \in \mathcal{S}_3^{\mathcal{P}}(\boldsymbol{x}_{0:n})$, cf. page 6.

Combining the results from Section 2.3 with (4.3c), we see that the periodic spline interpolating $\{(x_i, y_i)\}_{i=0}^{n}$ with $y_0 = y_n$ is determined by

$$s_i = y_i, \quad i=0,1,\ldots,n\ , \tag{4.17a}$$

and

$$\widetilde{\boldsymbol{A}}\boldsymbol{s}''_{1:n} = \boldsymbol{d}_{1:n}\ , \tag{4.17b}$$

where

$$\widetilde{\boldsymbol{A}} = \begin{bmatrix} 2(h_1{+}h_2) & h_2 & & & h_1 \\ h_2 & 2(h_2{+}h_3) & h_3 & & 0 \\ & \cdot & \cdot & \cdot & \vdots \\ & & h_{n-1} & 2(h_{n-1}{+}h_n) & h_n \\ h_1 & 0 & \cdots & h_n & 2(h_1{+}h_n) \end{bmatrix}. \tag{4.17c}$$

The system in (4.17b) can be solved by the algorithm given in Appendix A.3, followed by letting $s''_0 = s''_n$.

Example 4.9. Periodic splines are e.g. useful for a parametric representation of a closed, smooth curve. Given points $(u_1, v_1), \ldots, (u_n, v_n)$. As in Example 4.8 we approximate the curve by $(U(p), V(p))$ for $0 \le p \le n$, where U and V are cubic splines interpolating the points $(0, u_n), (1, u_1), \ldots, (n, u_n)$ and

$(0, v_n), (1, v_1), \ldots, (n, v_n)$, respectively. To get a smooth closed curve we demand that the splines be periodic, and use (4.17) with $h_i \equiv 1$ to determine the two splines.

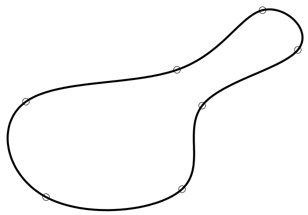


Figure 4.4. Closed parametric curve

4.3. Interpolation with B-Splines

The representation (4.2) is practical only if the data abscissae coincide with the knots. If we use the representation

$$s(x) = \sum_{j=1}^{n+3} c_j N_j(x) \ , \quad x_0 \le x \le x_n \ , \tag{4.18}$$

then we do not need this restriction, and it may be advantageous to be able to choose the knots so that the rules of thumb from Chapter 3 are taken into account. Also, it may be desirable to allow jumps in s'' or s' in certain points or to specify values of s'' or s' at some interior points.

Theorem 4.3. Given the data

$$s^{(p_i)}(t_i) = u_i \quad \text{with } p_i \in \{0, 1, 2\} \ ; \quad i = 1, \ldots, n+3 \tag{4.19}$$

and the knots

$$x_0 < x_1 \le x_2 \le \cdots \le x_{n-1} < x_n \ . \tag{4.20}$$

The data uniquely define $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$ if the following conditions are satisfied

1° $x_0 \le t_1 \le t_2 \le \cdots \le t_{n+3} \le x_n$.

2° $t_i < t_{i+1}$ if $p_i = p_{i+1}$.

3° $t_k < x_k < t_{k+4}$ for $k = 1, \ldots, n-1$.

4° At least one $p_i = 0$.

Proof: See [3]. □

Example 4.10. In normal practice most of the $p_i = 0$. If point 4° is not satisfied, but at least one $p_i = 1$, then we can add an arbitrary constant to the function.

Condition 3° is known as the *Schoenberg–Whitney condition*. It implies that there must be at least one data point with $t_i \in [x_0, x_1[$ – otherwise we have no information about c_1, since $N_1(x) \equiv 0$ for $x \ge x_1$. Similarly, there must be at least one $t_i \in]x_{n-1}, x_n]$. Also note that for $1 < j \le n-1$ the knot interval $[x_{j-1}, x_j]$ can be empty of data points. There may be at most three consecutive empty knot intervals.

A multiple interior knot gives rise to empty interval(s), and it folowws that the multiplicity can be at most four.

4.3.1. Practical Details. From (4.18) and (4.19) it follows that the B-splines coefficints $\{c_j\}$ should satisfy

$$\sum_{j=1}^{n+3} N_j^{(p_i)}(t_i) c_j = u_i \quad \text{for } \ i = 1, \ldots, n+3 \ . \tag{4.21a}$$

This is a linear system of equations, which we write in the form

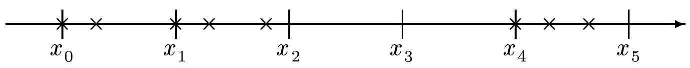
$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{u} \tag{4.21b}$$

with $\boldsymbol{c}, \boldsymbol{u} \in I\!R^{n+3}$ containing the $\{c_j\}$ and $\{u_i\}$, while $\boldsymbol{A} \in I\!R^{(n+3)\times(n+3)}$ has the elements

$$a_{ij} = N_j^{(p_i)}(t_i) \ , \quad i, j = 1, \ldots, n+3 \ . \tag{4.21c}$$

From Theorem 2.1 it follows that $\boldsymbol{A}_{i,:}$ has at most four nonzero elements. If the conditions in Theorem 4.3 are satisfied, then the matrix $\boldsymbol{A}$ has full rank, implying that the solution $\boldsymbol{c}$ is unique. Further, [3] shows that simple Gaussian elimination is stable. This implies that the "band structure" is preserved, and can be exploited.

Example 4.11. Let $n = 5$, $p_i = 0$ for all 8 data points and let the data abscissae be distributed as indicated below



Assume, that the end knots are multiple (cf. Exercise 2.7), then the nonzeros in $\boldsymbol{A}$ are distributed as shown below,

$$
\boldsymbol{A} = \begin{bmatrix}
x & & & & & & & \\
x & x & x & x & & & & \\
 & x & x & x & & & & \\
 & x & x & x & x & & & \\
 & x & x & x & x & & & \\
 & & & & x & x & x & \\
 & & & & x & x & x & x \\
 & & & & x & x & x & x
\end{bmatrix} .
$$

Example 4.12. In terms of (4.19) the problem of Example 4.1 with the boundary conditions from Example 4.5 is given by

i	t_i	p_i	u_i
1	−1	0	−0.6861
2	−1	1	3.3414
3	0	0	1.0000
4	1	0	−0.2524
5	2	0	−0.2405
6	3	0	0.2142
7	3	1	0.0176

We use the knots $x_{-3:6} = (-3,\ -2,\ \ldots, 5)$, and by means of Example 2.6 we see that the only nonzero values for $N_j(x_i)$ and $N_j'(x_i)$ are

$$N_{i+1}(x_i) = N_{i+3}(x_i) = \frac{1}{6}\,, \quad N_{i+2}(x_i) = \frac{4}{6}\,; \quad -N'_{+1}(x_i) = N'_{+3}(x_i) = \frac{1}{2h}\,.$$

The system (4.21) takes the form

$$
\frac{1}{6}\begin{bmatrix}
1 & 4 & 1 & & & & \\
-3 & 0 & 3 & & & & \\
 & 1 & 4 & 1 & & & \\
 & & 1 & 4 & 1 & & \\
 & & & 1 & 4 & 1 & \\
 & & & & 1 & 4 & 1 \\
 & & & & -3 & 0 & 3
\end{bmatrix} \boldsymbol{c} = \begin{bmatrix} -0.6861 \\ 3.3414 \\ 1.0000 \\ -0.2524 \\ -0.2405 \\ 0.2142 \\ 0.0176 \end{bmatrix} \quad \begin{array}{l}\text{with the}\\ \text{solution}\end{array} \quad \boldsymbol{c} = \begin{bmatrix} -4.9398 \\ -0.2299 \\ 1.7430 \\ -0.7420 \\ -0.2895 \\ 0.4573 \\ -0.2544 \end{bmatrix} .
$$

4.3.2. Periodic Splines. As discussed in Section 2.3, the periodicity of the spline is ensured by the special choice (2.16) of the extra knots, and by letting

$$c_{n+k} = c_k \quad \text{for} \quad k = 1, 2, 3\,. \tag{4.22}$$

This spline has n degrees of freedom, and is e.g. uniquely defined by demanding that $s(x_i) = y_i$ for $i = 1, \ldots, n$. According to Appendix A.1 these conditions take the form

$$N_{i+1}(x_i)c_{i+1} + N_{i+2}(x_i)c_{i+2} + N_{i+3}(x_i)c_{i+3} = y_i\,, \quad i = 1, \ldots, n\,. \tag{4.23}$$

It always holds that $N_{i+2}(x_i)$ is the largest of the three factors in (4.23), and this leads us to choose $\boldsymbol{c}_{3:n+2}$ as the "primary unknowns". Then (4.23) can be written in the form

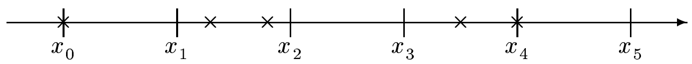
$$\widetilde{\boldsymbol{A}}\boldsymbol{c}_{3:n+2} = \boldsymbol{y}_{1:n}\,, \tag{4.24a}$$

where (omitting the argument (x_i) in the ith row)

$$
\widetilde{\boldsymbol{A}} = \begin{bmatrix}
N_3 & N_4 & & & N_2 \\
N_3 & N_4 & N_5 & & 0 \\
 & \cdot & \cdot & \cdot & \vdots \\
N_{n+3} & 0 & \cdots & N_{n+1} & N_{n+2}
\end{bmatrix} . \tag{4.24b}
$$

The matrix is diagonally dominant and (4.24a) can be solved by the algorithm in Appendix A.3, followed by letting $c_1 = c_{n+1}$, $c_2 = c_{n+2}$ and $c_{n+3} = c_3$.

Example 4.13. It is possible also to find a periodic spline that satisfies more general conditions as in Theorem 4.3. We shall not give details, but mention that with the same knots as in Example 4.11 ($n = 5$) we get a unique determination of a periodic spline e.g. when the data points are distributed as indicated below



We choose $\boldsymbol{c}_{2:6}$ as the "primary unknowns' and get a system of the form $\widetilde{\boldsymbol{A}}\boldsymbol{c}_{2:6} = \boldsymbol{b}$, where $\widetilde{\boldsymbol{A}}$ has the nonzero structure

$$
\widetilde{\boldsymbol{A}} = \begin{bmatrix}
x & x & & & x \\
x & x & x & x & \\
x & x & x & x & \\
x & & x & x & x \\
x & & & x & x
\end{bmatrix} .
$$

Again, this can be solved by the algorithm of Appendix A.3. Now, however, the matrix $\boldsymbol{A}$ of (A.4) is pentadiagonal.

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5. Curve Fitting

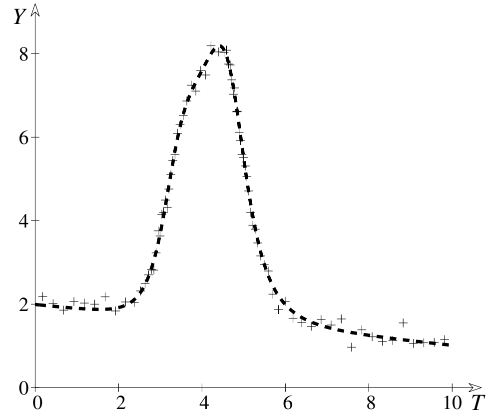


Figure 5.1. *Data points and underlying function*

Given points (t_1, y_1), ..., (t_m, y_m), that are assumed to satisfy

$$y_i = f(t_i) + \varepsilon_i \quad i = 1, \ldots, m \ . \tag{5.1a}$$

Here, f is the socalled *underlying function* and the $\{\varepsilon_i\}$ are (measurement) errors, which we assume to be *"white noise"*, i.e. to have the *expected values*

$$E(\varepsilon_i) = 0 \ , \qquad E(\varepsilon_i \varepsilon_j) = \begin{cases} \sigma^2 & \text{for } i = j \\ 0 & \text{otherwise} \end{cases} \ . \tag{5.1b}$$

Let $\varphi(\boldsymbol{p}, t)$ denote a *model* for f, depending on t and some *parameters* $\boldsymbol{p} \in \mathbb{R}^q$. The white noise assumption warrants that the best choice of parameters is the *least-squares solution* defined by

$$\boldsymbol{p}^* = \underset{\boldsymbol{p} \in \mathbb{R}^q}{\operatorname{argmin}} \left\{ \sum_{i=1}^{m} r_i(\boldsymbol{p})^2 \right\} \ , \tag{5.2a}$$

where $r_i(\boldsymbol{p})$ is the ith *residual*,

$$r_i(\boldsymbol{p}) = y_i - \varphi(\boldsymbol{p}, t_i) \ . \tag{5.2b}$$

The corresponding estimate of the *variance* σ^2 is

$$V = \frac{1}{m - q} \sum_{i=1}^{m} r_i(\boldsymbol{p}^*)^2 \ . \tag{5.3}$$

From (5.1a) and (5.2b) it follows that

$$r_i(\boldsymbol{p}^*) = f(t_i) - \varphi(\boldsymbol{p}^*, t_i) + \varepsilon_i \ . \tag{5.4}$$

Thus, the ith residual is the sum of *approximation error* $f(t_i) - \varphi(\boldsymbol{p}^*, t_i)$ and data (measurement) error ε_i. It follows, that the estimated variance V is a good approximation to σ^2 only if the average approximation error is small compared with the "noise level" σ.

Example 5.1. We have used polynomials,

$$\varphi(\boldsymbol{p}, t) = \sum_{j=1}^{q} p_j P_{j-1}(t) \ ,$$

(with $P_k(t)$ denoting a kth degree polynomial) to fit the 78 data points in Figure 5.1. In Figure 5.2 we show the estimated variance as a function of q.

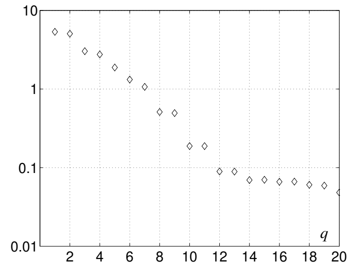


Figure 5.2. *Estimated variance for polynomial fits to data from Figure 5.1*

For small values of q the approximation error dominates (most of) the residuals, but for $q \geq 14$ the estimated variance is almost constant, indicating that the "noise" dominates in (5.4). The best polynomial fit is of degree $q_{\text{opt}} - 1 = 13$ and is shown in Figure 5.3.

By comparison with Figure 5.1 we see that the middle part is quite well approximated – with a smooting of the peak, however. Near both ends there are undesirable oscillations. This behaviour is typical for polynomial fits to data, where the underlying function has "different nature" in different regions.

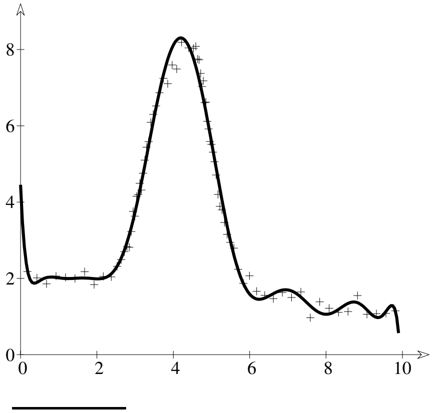


Figure 5.3. *Data points from Figure 5.1 and polynomial fit of degree 13*

In the remainder of this chapter we discuss fit with cubic splines,

$$\varphi(\boldsymbol{p}, t) = s(t) \ , \quad \text{where} \quad s \in \mathcal{S}_3(\boldsymbol{x}_{0:n}) \ . \tag{5.5}$$

The parameters in this case are the knots $x_{0:n}$ <u>and</u> the spline coefficients. In Section 5.1 we discuss the computation of the fitting spline in the case where the knots are given, and in Section 5.2 we discuss methods for iterative determination of the number $n+1$ and the distribution of the knots.

Provided that there is an adequate number of data points and that they are suitably distributed over the range (preferably closest where f varies most rapidly), then we shall see that it is possible to determine the number of knots and their distribution so that we get an approximation, which is satisfactory both locally and globally.

To ease the discussion we shall assume that the data points are ordered by increasing value of the abscissa, i.e.

$$a \le t_1 \le t_2 \le \cdots \le t_m \le b \ . \tag{5.6}$$

5.1. Computing the Fitting Spline

In this section we assume that we are given n and the knots $\boldsymbol{x}_{0:n}$ with $x_0 = a$, $x_n = b$. The only practical representation of the spline is in terms of B-splines, cf. Section 2.2,

$$s(t) = \sum_{j=1}^{n+3} c_j N_j(t) \ . \tag{5.7}$$

The *residual vector* $\boldsymbol{r}(\boldsymbol{c})$, whose ith component is $r_i(\boldsymbol{c}) = y_i - s(t_i)$, takes the form

$$\boldsymbol{r}(\boldsymbol{c}) = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{c} \tag{5.8a}$$

with

$$\boldsymbol{y} = [y_1, \ \ldots, \ y_m]^T, \quad \boldsymbol{c} = [c_1, \ \ldots, \ c_{n+3}]^T \ , \tag{5.8b}$$

and the elements in $\boldsymbol{A} \in \mathbb{R}^{m \times (n+3)}$ are

$$a_{ij} = N_j(t_i) \ , \quad i = 1, \ldots, m; \quad j = 1, \ldots, n+3 \ . \tag{5.8c}$$

We assume that $n+3 < m$, so that $\boldsymbol{r}(\boldsymbol{c}) \simeq \boldsymbol{0} \iff \boldsymbol{A}\boldsymbol{c} \simeq \boldsymbol{y}$ is an *overdetermined system of equations.* In Section 5.1.1 we show how to find the least-squares solution $\boldsymbol{c}^*$.

Theorem 5.1. Problem (5.8) has a unique least-squares solution $\boldsymbol{c}^*$ if $m \ge n+3$ and a subset $T_1, \ldots, T_{n+3}$ of the data abscissae $t_1, \ldots, t_m$ satisfies

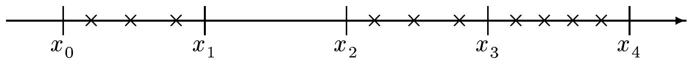
$$T_k < x_k < T_{k+4} \quad \text{for} \quad k = 1, \ldots, n-1 \ . \tag{5.9}$$

Proof: See [3]. □

This theorem is similar with Theorem 4.3, and the comments in Example 4.10 are still valid.

5.1.1. Practical Details. It follows from the local support of the B-splines, Figure 2.3, that each row of $\boldsymbol{A}$ contains at most four nonzero elements; for $t_i \in [x_{j-1}, x_j]$ this is the elements $\boldsymbol{A}_{i,j:j+3}$. They can be computed by the formulae given in Appendix A.1.

Example 5.2. The nonzero elements can be stored in an $m \times 4$ array `RA` plus and integer array `CA` with m elements, where `CA(i)` is the column number of the first nonzero element in $\boldsymbol{A}_{i,:}$. As an example consider the knots and data abscissae indicated below ($n = 4$, $m = 10$).



The structure of $\boldsymbol{A}$ and the contents of `CA` are

$$\boldsymbol{A} = \begin{bmatrix} x & x & x & x & & & \\ x & x & x & x & & & \\ x & x & x & x & & & \\ & & x & x & x & x & \\ & & x & x & x & x & \\ & & x & x & x & x & \\ & & & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \\ & & & x & x & x & x \end{bmatrix}, \qquad \mathtt{CA} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 3 \\ 3 \\ 3 \\ 4 \\ 4 \\ 4 \\ 4 \end{bmatrix} .$$

The least-squares solution can be found via *orthogonal transformation*[1)] determined so that the transformed matrix is upper triangular,

$$\boldsymbol{Q}\boldsymbol{r}(\boldsymbol{c}) = \boldsymbol{Q}\boldsymbol{y} - \boldsymbol{Q}\boldsymbol{A}\boldsymbol{c} = \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} - \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{0} \end{bmatrix} \boldsymbol{c} \,, \tag{5.10}$$

where $\boldsymbol{R} \in \mathbb{R}^{(n+3)\times(n+3)}$ has zeros below the diagonal. An orthogonal transformation does not change the 2-norm. This implies that

$$\begin{aligned} \sum_{i=1}^{m} r_i(\boldsymbol{c})^2 &= \|\boldsymbol{r}(\boldsymbol{c})\|_2^2 \\ &= \|\boldsymbol{Q}\boldsymbol{r}(\boldsymbol{c})\|_2^2 = \|\boldsymbol{u} - \boldsymbol{R}\boldsymbol{c}\|_2^2 + \|\boldsymbol{v} - \boldsymbol{0}\|_2^2 \,. \end{aligned}$$

This is minimal when $\boldsymbol{u} - \boldsymbol{R}\boldsymbol{c} = \boldsymbol{0}$, so the minimizer $\boldsymbol{c}^*$ is found by back substitution in the upper triangular system

$$\boldsymbol{R}\boldsymbol{c}^* = \boldsymbol{u} \,, \tag{5.11}$$

and the corresponding estimate (5.3) of the variance is

$$V = \tfrac{1}{m-(n+3)}\,\|\boldsymbol{v}\|_2^2 = \tfrac{1}{m-(n+3)}\,\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}^*\|_2^2 \,. \tag{5.12}$$

The transformation can e.g. be done by *Householders method* as described in Appendix A.4. There is no need for (column) pivoting, and the "band" structure of $\boldsymbol{A}$ can be exploited in the transformation, e.g. as shown in Example 5.3 below. The resulting $\boldsymbol{R}$ also has at most four nonzeros per row. Further, when (5.9) is satisfied, then all the diagonal elements in $\boldsymbol{R}$ are nonzero, and (5.11) has a unique solution.

1) See [6, Section 5.3.3] or [8, Section 6.2.1].

Example 5.3. The orthogonal transformation can be split into subtransformations, each of which handles the contributions from data points in one knot interval. Let $\boldsymbol{A}_{(j)}$ and $\boldsymbol{y}_{(j)}$ hold the contributions corresponding to $x_{j-1} \le t_i < x_j$ (with the right-hand inequality closed for $j = n$). The unknowns involved are $c_{j:j+3}$, and we let $\boldsymbol{R}_{(j-1)}$ and $\boldsymbol{u}_{(j-1)}$ denote the currently transformed matrix and right-hand side, involving $c_{j:j+2}$. The jth subtransformation takes the following form, sketched with three rows in $\boldsymbol{A}_{(j)}$ and $\boldsymbol{y}_{(j)}$ (marked by "+"), while an element that is changed by the subtransformation is marked by "z".

$$\boldsymbol{Q}_{(j)} \begin{bmatrix} \boldsymbol{R}_{(j-1)} & \boldsymbol{u}_{(j)} \\ \boldsymbol{A}_{(j)} & \boldsymbol{y}_{(j)} \end{bmatrix} = \boldsymbol{Q}_{(j)} \begin{bmatrix} \backslash & \backslash & \backslash & \backslash & & & | \\ & x & x & x & x & & x \\ & & x & x & x & & x \\ & & & x & x & & x \\ & & & & x & & x \\ & & + & + & + & + & + \\ & & + & + & + & + & + \\ & & + & + & + & + & + \\ & & + & + & + & + & + \end{bmatrix}$$

$$= \begin{bmatrix} \backslash & \backslash & \backslash & \backslash & & & | \\ & x & x & x & x & & x \\ & & z & z & z & z & z \\ & & & z & z & z & z \\ & & & & z & z & z \\ & & & & & z & z \\ & & & & & & * \\ & & & & & & * \end{bmatrix} = \begin{bmatrix} \boldsymbol{R}_{(j)} & \boldsymbol{u}_{(j)} \\ \boldsymbol{0} & \boldsymbol{w} \end{bmatrix} .$$

The vector $\boldsymbol{w}$ (marked by "*") contributes to $\boldsymbol{v}$, (5.10). The algorithm is initialized by computing $\boldsymbol{R}_{(1)}$ and $\boldsymbol{u}_{(1)}$ by transformation of $[\boldsymbol{A}_{(1)} \;\; \boldsymbol{y}_{(1)}]$ and terminates with $\boldsymbol{R} = \boldsymbol{R}_{(n)}$ and $\boldsymbol{u} = \boldsymbol{u}_{(n)}$.

As a specific example, consider the problem from Example 5.2, where the second knot interval is empty of data points.

$$\boldsymbol{R}_{(1)} = \boldsymbol{R}_{(2)} = \begin{bmatrix} x & x & x & x \\ & x & x & x \\ & & x & x \end{bmatrix} ,$$

$$\boldsymbol{Q}_{(3)} \begin{bmatrix} x & x & x & x & & & x \\ & x & x & x & & & x \\ & & x & x & & & x \\ & & + & + & + & + & + \\ & & + & + & + & + & + \\ & & + & + & + & + & + \end{bmatrix} = \begin{bmatrix} x & x & x & x & & & x \\ & x & x & x & & & x \\ & & z & z & z & z & z \\ & & & z & z & z & z \\ & & & & z & z & z \\ & & & & & z & z \end{bmatrix} ,$$

$$
\boldsymbol{Q}_{(4)}\begin{bmatrix}
\mathtt{x} & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & & & \mathtt{x}\\
 & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & & & \mathtt{x}\\
 & & \mathtt{x} & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & \mathtt{x}\\
 & & & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & \mathtt{x}\\
 & & & & \mathtt{x} & \mathtt{x} & & & \mathtt{x}\\
 & & & & & \mathtt{x} & & & \mathtt{x}\\
 & & & + & + & + & + & & +\\
 & & & + & + & + & + & & +\\
 & & & + & + & + & + & & +\\
 & & & + & + & + & + & & +
\end{bmatrix} = \begin{bmatrix}
\mathtt{x} & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & & & \mathtt{x}\\
 & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & & & \mathtt{x}\\
 & & \mathtt{x} & \mathtt{x} & \mathtt{x} & \mathtt{x} & & & \mathtt{x}\\
 & & & \mathtt{z} & \mathtt{z} & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & & & \mathtt{z} & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & & & & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & & & & & \mathtt{z} & & \mathtt{z}\\
 & & & & & & & & *\\
 & & & & & & & & *\\
 & & & & & & & & *
\end{bmatrix} .
$$

5.1.2. Boundary Conditions. Inspection of the data in Figure 5.1 indicates that the underlying function is almost a stright line at both ends. Therefore, it would be appropriate to approximate it by a *natural spline*, $s''(x_0) = s''(x_n) = 0$. This is a special case of more general boundary conditions,

$$
\begin{aligned}
\beta_{1,1}s(x_0) + \beta_{1,2}s'(x_0) + \beta_{1,3}s''(x_0) &= \beta_{1,4} ,\\
\beta_{2,1}s(x_n) + \beta_{2,2}s'(x_n) + \beta_{2,3}s''(x_n) &= \beta_{2,4} ,
\end{aligned}
\tag{5.13}
$$

where the $\{\beta_{k,j}\}$ are given.[2] Inserting (5.7) and exploiting that at a knot x_i the only nonzero $N_j^{(p)}(x_i)$-values are $N_{i+1:i+3}^{(p)}(x_i)$ we see that (5.13) is equivalent with

$$
\begin{aligned}
&\sum_{j=1}^{3}\alpha_{1,j}c_j = \beta_{1,4};\quad \alpha_{1,j} = \left(\beta_{1,1}N_j + \beta_{1,2}N_j' + \beta_{1,3}N_j''\right)_{x\,=\,x_0} ,\\
&\sum_{j=n+1}^{n+3}\alpha_{2,j}c_j = \beta_{2,4};\ \alpha_{2,j} = \left(\beta_{2,1}N_j + \beta_{2,2}N_j' + \beta_{2,3}N_j''\right)_{x\,=\,x_n} .
\end{aligned}
\tag{5.14}
$$

Now, assume that $\alpha_{1,1} \neq 0$ and $\alpha_{2,n+3} \neq 0$. Then (5.14) shows that the spline coefficients must satisfy

$$
\begin{aligned}
c_1 &= \gamma_1 - \widehat{\alpha}_{1,2}c_2 - \widehat{\alpha}_{1,3}c_3 ,\\
c_{n+3} &= \gamma_2 - \widehat{\alpha}_{2,n+1}c_{n+1} - \widehat{\alpha}_{2,n+2}c_{n+2} ,
\end{aligned}
\tag{5.15a}
$$

where

---

[2] The natural spline conditions are obtained with all $\beta_{k,j} = 0$ except for $\beta_{1,3} = \beta_{2,3} = 1$.

$$
\begin{aligned}
\left(\gamma_1, \widehat{\alpha}_{1,j}\right) &= \left(\beta_{1,4}, \alpha_{1,j}\right)/\alpha_{1,1} ,\\
\left(\gamma_2, \widehat{\alpha}_{2,j}\right) &= \left(\beta_{2,4}, \alpha_{2,j}\right)/\alpha_{2,n+3} .
\end{aligned}
\tag{5.15b}
$$

The residuals can be written

$$
r_i(\boldsymbol{c}) = y_i - c_1N_1(t_i) - c_{n+3}N_{n+3}(t_i) - \textstyle\sum_{j=2}^{n+2} c_jN_j(t_i) ,
$$

and by means of (5.15) we see that (5.8) is changed to

$$
\boldsymbol{r}(\widetilde{\boldsymbol{c}}) = \widetilde{\boldsymbol{y}} - \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{c}} , \tag{5.16a}
$$

with $\widetilde{\boldsymbol{c}} = \boldsymbol{c}_{2:n+2}$ and $\widetilde{\boldsymbol{y}}, \widetilde{\boldsymbol{A}}$ constructed as follows,

$$
\begin{aligned}
\widetilde{\boldsymbol{y}} &:= \boldsymbol{y} - \gamma_1\boldsymbol{A}_{:,1} - \gamma_2\boldsymbol{A}_{:,n+3}\\
\widetilde{\boldsymbol{A}} &:= \boldsymbol{A}_{:,2:n+2}\\
\widetilde{\boldsymbol{A}}_{:,j} &:= \widetilde{\boldsymbol{A}}_{:,j} - \widehat{\alpha}_{1,j}\boldsymbol{A}_{:,1} , \qquad j = 1, 2\\
\widetilde{\boldsymbol{A}}_{:,j} &:= \widetilde{\boldsymbol{A}}_{:,j} - \widehat{\alpha}_{2,j+1}\boldsymbol{A}_{:,n+3} , \qquad j = n, n+1
\end{aligned}
\tag{5.16b}
$$

The least-sqares fit is determined by $\boldsymbol{c}^*$, found as $\boldsymbol{c}^*_{2:n+2} = \widetilde{\boldsymbol{c}}^*$ and c_1^*, c_{n+3}^* computed by (5.15). Here, $\widetilde{\boldsymbol{c}}^*$ is computed by applying (5.10) – (5.11) to the reduced problem (5.16). The estimated variance is

$$
V = \tfrac{1}{m-(n+1)}\,\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}^*\|_2^2 . \tag{5.17}
$$

Compared with (5.12) the denominator is increased by 2 because the conditions reduce the number of degrees of freedoms of the spline.

Example 5.4. The strategy from Example 5.3 is easily modified to cope with the reduced problem (5.16). Since $(\boldsymbol{A})_{i,1} = (\boldsymbol{A})_{i,n+3} = 0$ for $x_1 \le t_i \le x_{n-1}$, the modifications in (5.16b) only affect $\widetilde{\boldsymbol{A}}_{(k)}$ and $\widetilde{\boldsymbol{y}}_{(k)}$ for $k = 1, n$.

As a specific example, consider the problem from Example 5.2, subject to boundary conditions. Letting "m" indicate an element in $\widetilde{\boldsymbol{A}}$ or $\widetilde{\boldsymbol{y}}$, which is modified by (5.16b), we get

$$
\boldsymbol{Q}_{(1)}\begin{bmatrix}
\mathtt{m} & \mathtt{m} & \mathtt{x} & & \mathtt{m}\\
\mathtt{m} & \mathtt{m} & \mathtt{x} & & \mathtt{m}\\
\mathtt{m} & \mathtt{m} & \mathtt{x} & & \mathtt{m}
\end{bmatrix} = \begin{bmatrix}
\mathtt{z} & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & \mathtt{z} & & \mathtt{z}
\end{bmatrix} = \begin{bmatrix} \widetilde{\boldsymbol{R}}_{(1)} & \widetilde{\boldsymbol{u}}_{(1)} \end{bmatrix} .
$$

The second knot interval has no data points, so $\widetilde{\boldsymbol{R}}_{(2)} = \widetilde{\boldsymbol{R}}_{(1)}$, $\widetilde{\boldsymbol{u}}_{(2)} = \widetilde{\boldsymbol{u}}_{(1)}$.

$$
\boldsymbol{Q}_{(3)}\begin{bmatrix}
\mathtt{x} & \mathtt{x} & \mathtt{x} & & & & \mathtt{x}\\
 & \mathtt{x} & \mathtt{x} & & & & \mathtt{x}\\
 & & \mathtt{x} & & & & \mathtt{x}\\
 & + & + & + & + & & +\\
 & + & + & + & + & & +\\
 & + & + & + & + & & +
\end{bmatrix} = \begin{bmatrix}
\mathtt{x} & \mathtt{x} & \mathtt{x} & & & & \mathtt{x}\\
 & \mathtt{z} & \mathtt{z} & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & \mathtt{z} & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & & \mathtt{z} & \mathtt{z} & & \mathtt{z}\\
 & & & & \mathtt{z} & & \mathtt{z}\\
 & & & & & & *
\end{bmatrix} = \begin{bmatrix} \widetilde{\boldsymbol{R}}_{(3)} & \widetilde{\boldsymbol{u}}_{(3)}\\ \boldsymbol{0} & w \end{bmatrix} .
$$

$$
\boldsymbol{Q}_{(4)} \begin{bmatrix} \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \mathrm{x} \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & + & \mathrm{m} & \mathrm{m} & \mathrm{m} \\ & & + & \mathrm{m} & \mathrm{m} & \mathrm{m} \\ & & + & \mathrm{m} & \mathrm{m} & \mathrm{m} \\ & & + & \mathrm{m} & \mathrm{m} & \mathrm{m} \end{bmatrix} = \begin{bmatrix} \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \mathrm{x} \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & \mathrm{z} & \mathrm{z} & \mathrm{z} & \mathrm{z} \\ & & & \mathrm{z} & \mathrm{z} & \mathrm{z} \\ & & & & \mathrm{z} & \mathrm{z} \\ & & & & & * \\ & & & & & * \\ & & & & & * \\ & & & & & * \end{bmatrix} = \begin{bmatrix} \widetilde{\boldsymbol{R}} & \widetilde{\boldsymbol{u}} \\ \boldsymbol{0} & \boldsymbol{w} \end{bmatrix} .
$$

5.1.3. Periodic Spline. If the underlying function is periodic, then we should use a periodic spline. In Section 2.3 we showed that it is obtained by computing the extra knots by (2.16),

$$
\begin{aligned} x_{-1} &= x_0 - h_n \,, & x_{-2} &= x_{-1} - h_{n-1} \,, \\ x_{n+1} &= x_n + h_1 \,, & x_{n+2} &= x_{n+1} + h_2 \,. \end{aligned}
$$

and letting

$$
c_{n+j} = c_j \quad \text{for} \quad j = 1, 2, 3 \,. \tag{5.18}
$$

We choose $\widetilde{\boldsymbol{c}} = \boldsymbol{c}_{1:n}$ as the "primary unknowns" and write the residual vector in the form

$$
\boldsymbol{r}(\widetilde{\boldsymbol{c}}) = \boldsymbol{y} - \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{c}} \,, \tag{5.19a}
$$

where $\widetilde{\boldsymbol{A}}$ has the structure

$$
\widetilde{\boldsymbol{A}} = \begin{bmatrix} \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \\ \vdots & \vdots & \vdots & \vdots & & & \\ \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & \\ & \vdots & \vdots & \vdots & \vdots & & \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & \\ & & \backslash & \backslash & \backslash & \backslash & \\ & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & \vdots & \vdots & \vdots & \vdots \\ & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ \mathrm{x} & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ \vdots & & & & \vdots & \vdots & \vdots \\ \mathrm{x} & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ \mathrm{x} & \mathrm{x} & & & & \mathrm{x} & \mathrm{x} \\ \vdots & \vdots & & & & \vdots & \vdots \\ \mathrm{x} & \mathrm{x} & & & & \mathrm{x} & \mathrm{x} \\ \mathrm{x} & \mathrm{x} & \mathrm{x} & & & & \mathrm{x} \\ \vdots & \vdots & \vdots & & & & \vdots \\ \mathrm{x} & \mathrm{x} & \mathrm{x} & & & & \mathrm{x} \end{bmatrix} \qquad \begin{array}{c} x_0 \le t_i < x_1 \\[2ex] x_1 \le t_i < x_2 \\[2ex] \vdots \\[2ex] x_{n-4} \le t_i < x_{n-3} \\[2ex] x_{n-3} \le t_i < x_{n-2} \\[2ex] x_{n-2} \le t_i < x_{n-1} \\[2ex] x_{n-1} \le t_i \le x_n \end{array} \tag{5.20}
$$

Again, we use orthogonal transformation, and the resulting $\widetilde{\boldsymbol{R}}$ will have the following structure (shown for $n = 10$),

$$
\widetilde{\boldsymbol{R}} = \begin{bmatrix} \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & & & & & \mathrm{x} & \mathrm{x} \\ & & & & & & & & & \mathrm{x} \end{bmatrix} .
$$

The strategy of Example 5.3 can be modified to cope with this structure. Note, that if $n \le 7$, then $\widetilde{\boldsymbol{R}}$ is a dense upper triangular matrix, and that we must use (2.20) if $n < 3$.

The orthogonal transformation also yields $\boldsymbol{u} \in \mathbb{R}^n$, and the least-sqares fit is determined by

$$
\boldsymbol{c}^*_{1:n} = \widetilde{\boldsymbol{R}}^{-1}\boldsymbol{u}, \qquad \boldsymbol{c}^*_{n+1:n+3} = \boldsymbol{c}^*_{1:3} \,.
$$

The estimated variance is

$$
V = \tfrac{1}{m-n} \, \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}^*\|_2^2 \,. \tag{5.21}
$$

The denominator reflects the fact that the number of degrees of freedoms of a periodic spline is n.

5.2. Choice of Knots

We want to find the cubic spline $s(t)$, which is the best approximation to $f(t)$ on the range $[a, b]$. Thus, for a given value of n the end knots are $x_0 = a$, $x_n = b$.

In the framework of a *model* $\varphi(\boldsymbol{p}, t)$, the vector $\boldsymbol{p}$ has $2n+2$ elements: the values of the interior knots plus the B-spline coefficients,

$$
\boldsymbol{p} = [x_1, \ \ldots, \ x_{n-1}, \ c_1, \ \ldots, \ c_{n+3}]^T \,.
$$

We want to find

$$
\begin{aligned} \boldsymbol{p}^* &= \operatorname*{argmin}_{\boldsymbol{p} \in \mathbb{R}^{2n+2}} \left\{ \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n+3} p_{n-1+j} N_j(\boldsymbol{p}_{1:n-1}, t_i) \right)^2 \right\} \,, \\ &\text{subject to} \quad a < p_1 \le p_2 \le \cdots \le p_{n-1} < b \,. \end{aligned}
$$

In contrast to the problem discussed in Section 5.1, this is a nonlinear problem and must be solved by iteration. Experience (see e.g. [4]) shows that often there is problems with the solution: The iteration may stop because the *Schoenberg-Whitney conditions* (5.9) are violated, or the solution found is a local rather than a global minimum.

Generally, a better result is obtained by successive adjustment of n and the distribution of the interior knots. The adjustments are heuristic, based on the interpretation

$$s(t) = s_F(t) + s_E(t) \tag{5.22}$$

of the spline computed as described in Section 5.1. Here, s_F is the approximation to f that we would get in the absence of errors, and s_E fits the $\{\varepsilon_i\}$. The residuals take the form

$$r_i(\boldsymbol{c}^*) = y_i - s(t_i) = e_F(t_i) + \varepsilon_i - s_E(t_i) \ , \tag{5.23}$$

where $e_F(t_i) = f(t_i) - s_F(t_i)$ is the achievable approximation error. Elaborating on the comment on (5.4), we see that the ith residual has contributions from approximation error $e_F(t_i)$, measurement error ε_i and *induced effect* of all the $\{\varepsilon_j\}$.

The goal of the heuristics is to find n and the interior knots so that the spline is lax enough to follow the variations in f, but not so lax that the effect of $\{\varepsilon_j\}$ dominates in any part of the region.

The basic idea is as follows: For a given n and knots $\boldsymbol{x}_{0:n}$ compute the fitting spline and estimate *trends*, i.e indication that approximation error dominates locally, Section 5.2.1. If this is the case, then insert a new knot (Section 5.2.2), i.e. augment n and we have a new knot set with which the process is repeated. Before giving details, we shall look at some examples.

Example 5.5. For the data of Figure 5.1 we have found the fitting cubic spline with $a = 0$, $b = 10$ and equidistant interior knots. Below we show results for $n = 4$ and $n = 16$.

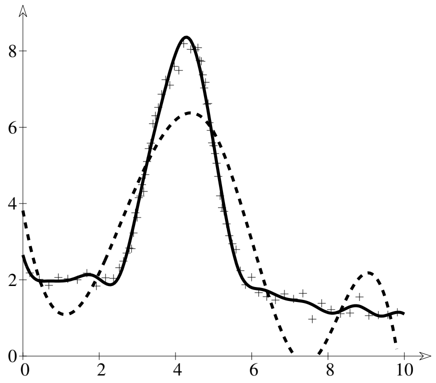


Figure 5.4. *Data points from Figure 5.1 and fit with cubic splines over equidistant knots. Dashed line: $n = 4$ Full line: $n = 16$*

The fit with $n = 4$ is too stiff. It does not give the peak at $t = 4.5$ and there is significant overswing at the ends.

The fit with $n = 16$ has many resemblances with the polynomial fit in Figure 5.3: The peak is quite well approximated (although the finer details are missing), but there is undesirable oscillations for $t < 2$ and $t > 7$.

These characteristics are enhanced and easier to quantify if we consider the residuals $r_i = y_i - s(t_i)$. See Figure 5.5; Notice the difference in scaling.

For $n = 4$ there are long stretches with constant sign of the residuals. According to (5.1b) and (5.23) the only possible explanation is that approximation error dominates. The spline is too stiff and must be relaxed by inserting more knots.

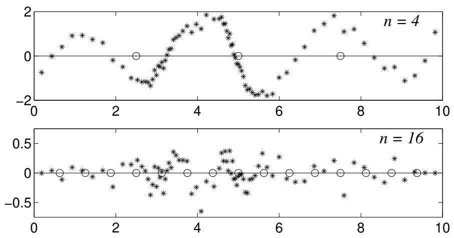


Figure 5.5. *Residuals for the fits in Figure 5.4*

For $n = 16$ the picture is less clear. For $t < 2$ the signs of the residuals seem to be random, indicating that the $\{\varepsilon_i\}$ dominate. Around the peak, however, there is indication that approximation error dominates.

Example 5.6. Similar to Example 5.1 we have computed the fitting spline with equidistant knots for $n = 1, 2, \ldots, 20$. The estimated variances are shown in Figure 5.6 together with the variances for the corresponding natural spline. Note, that in most cases the two variances are almost equal, and that the behaviour is similar to the behaviour shown in Figure 5.2, although it is not monotone.

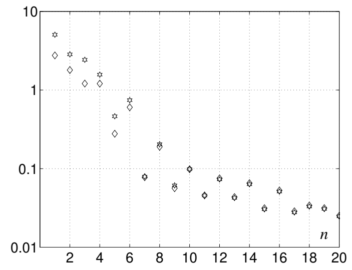


Figure 5.6. *Estimated variance for equidistant knots spline fits to data from Figure 5.1.*
$\diamond$: $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$
$\star$: $s \in \mathcal{S}_3^{\mathcal{N}}(\boldsymbol{x}_{0:n})$

The results indicate that $n = 11$ is the best choice, and the corresponding fits are shown below. Note that they are indistinguishable except near the ends, where the natural spline is best.

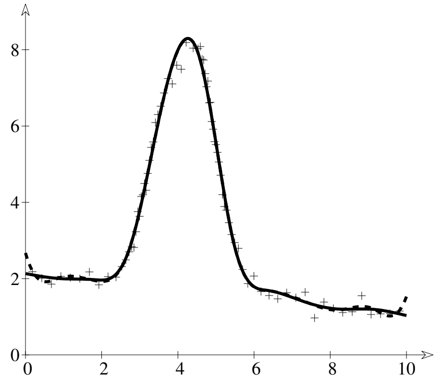


Figure 5.7. *Data points from Figure 5.1 and spline fits with* $n = 11$, *equidistant knots.*
Dashed line: $s \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$
Full line: $s \in \mathcal{S}_3^{\mathcal{N}}(\boldsymbol{x}_{0:n})$

Example 5.7. The underlying function for the data in Figure 5.1 is given by (3.14),

$$f(x) = 2 - 0.1x + \frac{2(x-1)}{(x-4)^4 + 1} \ .$$

To see, how well we can approximate this by fitting a cubic spline to the data points, we have distributed the knots as in Example 3.4 ($n = 10$) and used natural spline conditions. The estimated variance is $V = 0.0234$, while the true variance is $\sigma^2 = 0.0225$. The fit is shown in Figure 5.8.

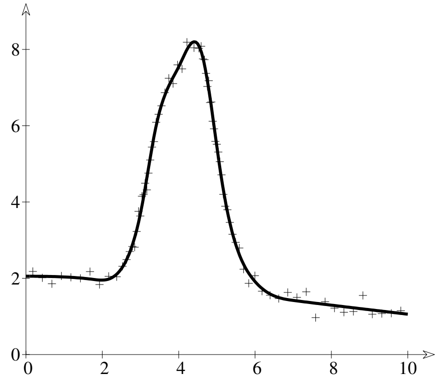
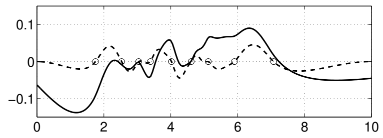


Figure 5.8. *Data points from Figure 5.1 and natural spline fit with* $n = 10$, *knots distributed as in Example 3.4*

Note that now we see some of the finer details of the peak. In Figure 5.9 we give the error $e(t) = f(t) - s(t)$. For comparison we also show the error curve

for the interpolating spline over the same knots, cf. Figure 3.4.

Figure 5.9. *Error curves.*
Interior knots marked by circles.
Dashed line: Interpolating spline from Example 3.4
Full line: Fitting natural spline



5.2.1. Trends. The information in the residuals can be quantified in different ways. Our presentation shares the main ideas with [10] and [4].

In the current knot set we let p_j denote the number of data points in the jth knot interval and q_j+1 is the index of the first of these; i.e.[3)]

$$x_{j-1} \le t_{q_j+1} \le \cdots \le t_{q_j+p_j} \le x_j < t_{q_j+p_j+1} \ . \tag{5.24}$$

The *local correlation* of the residuals is defined as

$$R_j = \textbf{if } \ p_j < 2 \ \textbf{then } \ 0 \ \textbf{else } \ \frac{1}{(p_j-1)V_j} \sum_{k=q_j+1}^{q_j+p_j-1} r_k r_{k+1} \ , \tag{5.25a}$$

where V_j is the estimate of *local variance*,

$$V_j = \max\left\{V, \ \frac{1}{p_j} \sum_{k=q_j+1}^{q_j+p_j} r_k^2\right\} \ . \tag{5.25b}$$

Here, V is the *global variance*, as estimated by (5.12), (5.17) or (5.21).

It is easily seen that R_j lies in the range $-1 \le R_j \le 1$ and that values close to $+1$ are obtained when r_k and r_{k+1} have the same sign in most cases. This indicates that approximation errors dominate, as in the upper part of Figure 5.5. From statistics, the value

$$\tau_j = \frac{1}{\sqrt{2(p_j-1)}} \tag{5.26}$$

is the threshold for significant correlation.

Summarizing, we get the following *measure of trend* in the jth knot interval,

3) If a data abscissa coincides with x_j, then this point belongs to both $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$, and then $\sum p_j > m$, the total number of data points.

$$T_j = \begin{cases} 0 & \text{if } p_j \le 1 \\ R_j/\tau_j & \text{otherwise} \end{cases} \quad . \tag{5.27}$$

A value $T_j \ge 1$ indicates that locally the spline is too stiff, and an extra knot should the inserted in the interval $[x_{j-1}, x_j]$, see Section 5.2.2.

Example 5.8. Figure 5.10 shows the trends for the fits of Figures 5.4–5. These T_j-values are a quantitative confirmation of the qualitative statements in Example 5.5: For for both values of n the trends indicate that further relaxation is required.

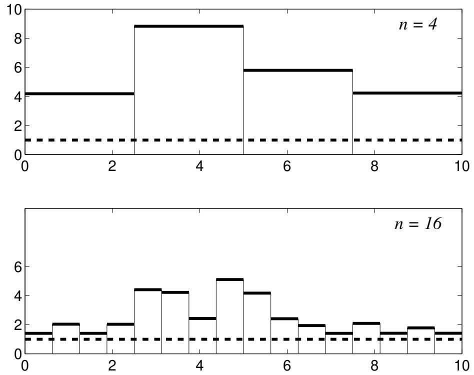


Figure 5.10. *Trends for the fits in Figures 5.4–5*

5.2.2. Knot Insertion. There exist a number of strategies for inserting extra knots. We shall give a simple version, which often leads to good results. In algorithmic form we can describe it as shown in (5.28) below.

Basically, the knot adjustment is to choose an interval – the kth (see below) – insert a new knot in the middle of it (thus increasing n by one) and maybe move the "old" knots x_{k-1} and x_k a little, according to the algorithm

$$\begin{aligned} &\textbf{if } T_{k-1} \ge 1 \textbf{ then } x_{k-1} := x_{k-1} - 0.1h_{k-1} \\ &\textbf{if } T_{k+1} \ge 1 \textbf{ then } x_k := x_k + 0.1h_{k+1} \end{aligned} \tag{5.29}$$

Artificial variables $T_0 = T_{n+1} = 0$ ensure that the end knots stay fixed.

The interval chosen has $T_k > 1$, and if one or both of its neighbours also show a need for "softening", then this strategy attemps to satisfy the needs

Given data $\{t_i, y_i\}_{i=1}^m$ and range $[a, b]$
  (with all $t_i \in [a, b]$)
Choose initial n and knots
  (with $x_0 = a$ and $x_n = b$)
repeat
  Compute fitting spline {Section 5.1}
  if $V_{\text{new}} > V_{\text{old}}$ **then**
    return with previous knot set
  Compute trends $T_{1:n}$ { (5.27) }
  $M :=$ argmax$\{T_j\}$
  if $T_M \ge 1$ **then** adjust knots and n {See below}
until $T_M < 1$ (5.28)

also for the neighbour(s). In order to enhance this possibility we compute

$$L := \text{argmax}\{T_j \mid T_{j-1} \ge 1 \text{ and } T_{j+1} \ge 1\} \ , \tag{5.30}$$

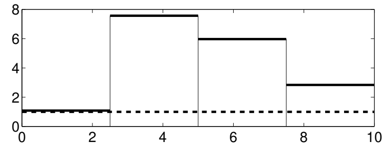
and choose

$$k = \begin{cases} L & \text{if } T_L \ge \max\{1,\ \tfrac{1}{2}T_M\} \\ M & \text{otherwise} \end{cases} \quad . \tag{5.31}$$

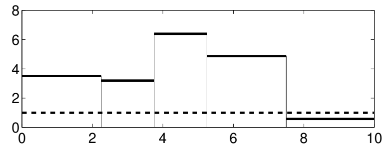
It should be noted that the trend measure (5.27) favours intervals with many data points. This enhances the probability that the reduced intervals still contain a fair amount of data points.

Example 5.9. We have used algorithm (5.28) – (5.31) to fit a natural spline to the data of Figure 5.1. As the starting point we chose $n = 4$ and equidistant knots. We got the following results.

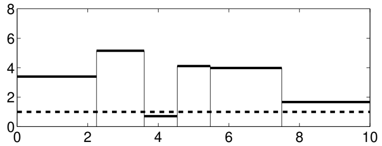
$n = 4$: $V = 1.5710$
$M = L = k = 2$.



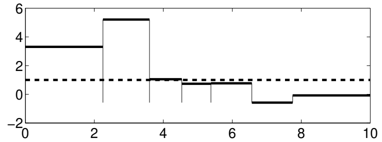
$n = 5$: $V = 0.6200$
$M = L = k = 3$.



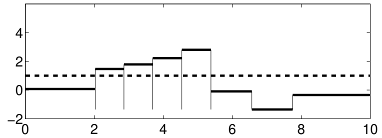
$n = 6: \quad V = 0.1556$
$\qquad M = 2, \ L = k = 5.$



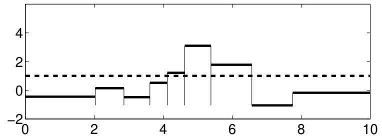
$n = 7: \quad V = 0.0896$
$\qquad M = L = k = 2.$



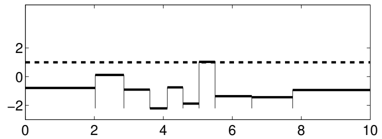
$n = 8: \quad V = 0.0477$
$\qquad M = 5, \ L = k = 4.$



$n = 9: \quad V = 0.0356$
$\qquad M = L = k = 6.$



$n = 10: \quad V = 0.0223$
$\qquad M = k = 7.$



$n = 11, \quad V = 0.0225$

The algorithm stops because the variance estimate increases. The optimal fit with $n = 10$ is almost indistinguishable from Figure 5.8. Below we give the errors for this fit and the fit in Example 5.7.

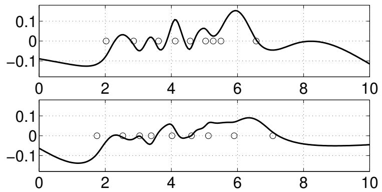


Figure 5.11. *Error curves.*
Interior knots marked by circles.
Above: Present spline
Below: Spline from Example 5.7

In both cases the maximum error is about 0.015, which is the standard deviation of the data.

6. Boundary Value Problems

Consider the linear second order differential equation

$$y''(x) + f(x)y'(x) + g(x)y(x) = r(x) \ , \quad a \le x \le b \tag{6.1a}$$

with boundary conditions

$$\alpha_1 y(a) + \beta_1 y'(a) = \gamma_1, \qquad \alpha_2 y(b) + \beta_2 y'(b) = \gamma_2 \ . \tag{6.1b}$$

Here, f, g and r are given functions, and $(\alpha_k, \beta_k) \ne (0,0)$ for $k = 1$ and $k = 2$. We assume that this boundary value problem has a unique solution y, and wish to find an approximating cubic spline s.

We give two methods for determining the spline, *collocation* and *Galerkins method*. In both cases we use the representation

$$s(x) = \sum_{j=1}^{n+3} c_j N_j(x) \ , \quad a \le x \le b \ , \tag{6.2}$$

where the $\{N_j\}$ are cubic B-splines defined on the knots
$x_{-2} \le x_{-1} \le x_0 = a < x_1 \le x_2 \le \cdots \le x_{n-1} < x_n = b \le x_{n+1} \le x_{n+2}$.

Also, in both cases we find the spline coefficents by setting up and solving a linear system of equations

$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{d} \ . \tag{6.3}$$

In this system the first and the last equation express that s should satisfy the boundary conditions,

$$\sum_{j=1}^{n+3} \bigl(\alpha_1 N_j(a) + \beta_1 N_j'(a)\bigr)\, c_j = \gamma_1 \ , \tag{6.4a}$$

and

$$\sum_{j=1}^{n+3} \bigl(\alpha_2 N_j(b) + \beta_2 N_j'(b)\bigr)\, c_j = \gamma_2 \ , \tag{6.4b}$$

respectively, while rows $2,\ldots,n{+}2$ in $\boldsymbol{A}\in\mathbb{R}^{(n+3)\times(n+3)}$ and $\boldsymbol{d}\in\mathbb{R}^{n+3}$ depend on the method.

The difference between the solution and the approximating spline,

$$D(x) = y(x) - s(x)\ , \quad a \le x \le b\ , \tag{6.5}$$

is the socalled *discretization error*. It depends on the problem, the method used to find s, and on the choice of knots. We only give examples of the behaviour of D and refer to [11] or [12] for a thorough discussion.

6.1. Collocation

With this method the spline is found so that it satisfies the differential equation in discrete points, the socalled *collocation points*, $z_1,\ldots,z_{n+1}$. Thus, the $n{+}1$ "interior" equations in (6.3) have the form

$$\sum_{j=1}^{n+3}\left(N_j''(z_i)+f(z_i)N_j'(z_i)+g(z_i)N_j(z_i)\right)c_j = r(z_i)\ , \qquad i=1,\ldots,n{+}1\ . \tag{6.6}$$

By proper choice of the collocation points the matrix $\boldsymbol{A}$ is nonsingular and the spline is uniquely determined. A specially simple choice, where this condition is satisfied, is given by the knots, $z_i = x_{i-1}$, $i=1,\ldots,n$. In this case, Theorem 2.1 shows that each equation in (6.3) has at most three nonzero contributions. Further, if we choose *multiple end knots*, then Exercise 2.7 shows that the "boundary equations" (6.4a–b) have at most two nonzero contributions, and the system is tridiagonal,

$$\begin{bmatrix} \mathrm{x} & \mathrm{x} & & & & \\ \mathrm{x} & \mathrm{x} & \mathrm{x} & & & \\ & \mathrm{x} & \mathrm{x} & \mathrm{x} & & \\ & & \cdot & \cdot & \cdot & \\ & & & \mathrm{x} & \mathrm{x} & \mathrm{x} \\ & & & & \mathrm{x} & \mathrm{x} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \\ \cdot \\ c_{n+3} \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ r(x_0) \\ \cdot \\ \cdot \\ r(x_n) \\ \gamma_2 \end{bmatrix}\ . \tag{6.7}$$

Example 6.1. Consider the problem

$$\begin{aligned} &y''(x)+y'(x)+4.25y(x) = 0\ , \quad -1\le x\le 3\ , \\ &y(-1) = \mathrm{e}^{0.5}\cos 2 \simeq -0.6861\ , \\ &y(3)+2y'(3) = -4\mathrm{e}^{-1.5}\sin 6 \simeq 0.2494\ . \end{aligned} \tag{6.8}$$

It is easily verified that the solution is $y(x) = \mathrm{e}^{-\frac{1}{2}x}\cos 2x$, cf. Examples 4.1, and 4.5 – 4.7.

We shall use equidistant interior knots

$$x_i = -1 + ih, \quad i=0,1,\ldots,n; \quad h = \frac{4}{n}\ , \tag{6.9a}$$

and multiple end knots

$$x_{-2} = x_{-1} = -1, \quad x_{n+1} = x_{n+2} = 3\ . \tag{6.9b}$$

For $n=4$ we get $h=1$, and (6.7) takes the form (at most 2 decimals are shown in the elements)

$$\begin{bmatrix} 1 & & & & & & \\ 7.25 & -6 & 3 & & & & \\ & 1.81 & 0.23 & 2.21 & & & \\ & & 1.21 & 0.83 & 2.21 & & \\ & & & 1.21 & -0.27 & 3.31 & \\ & & & & 3 & -12 & 13.25 \\ & & & & & -6 & 7 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \end{bmatrix} = \begin{bmatrix} -0.69 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.25 \end{bmatrix}\ .$$

The solution (shown with 4 digits) is

$$\boldsymbol{c} = \begin{bmatrix} -0.6861 \\ -0.8830 \\ 0.1078 \\ -0.2187 \\ -0.2863 \\ -0.2098 \end{bmatrix}\ ,$$

and the corresponding spline is shown in Figure 6.1 (full line) together wtih the true solution (dotted line).

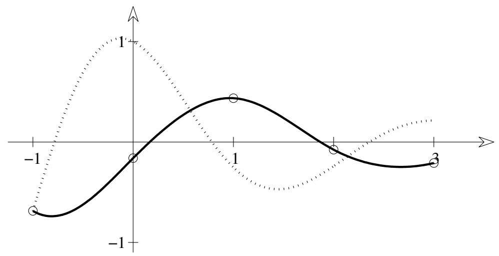


Figure 6.1.

Example 6.2. For the problem of the previous example and the knots given by (6.9) we have used knot collocation for increasing values of n – i.e. decreasing values of h. In the table we give the following measures for the *discretization error*, cf. Example 4.6,

$$\eta_n = \max_{-1\le x\le 3}\{|D(x)|\} = |D(u_n)|\ . \tag{6.10}$$

n	η_n	u_n
4	1.42e+00	−0.320
8	3.45e+00	−0.320
16	1.08e+00	−0.320
32	1.77e-01	−0.320
64	4.07e-02	−0.320
128	9.98e-03	−0.320
256	2.48e-03	−0.320

In all cases the point of maximum error is the same, and for the larger values of n we see that $\eta_{2n} \simeq \frac{1}{4}\eta_n$, corresponding to

$$|D(x)| \leq O(h^2) \ .$$

The results in Example 6.2 agree with [11, Chapter 8]: Under mild restrictions on the functions f, g and r and on the ratio $H/h = \max\{h_j\}/\min\{h_j\}$ the discretization error with knot collocation behaves as $O(H^2)$. It is also discussed how to choose the collocation points to achieve $O(H^4)$ convergence.

6.2. Galerkins Method

For the differential equation (6.1a) and a function φ we define the *residual function*

$$R(\varphi, x) = \varphi''(x) + f(x)\varphi'(x) + g(x)\varphi(x) - r(x) \ , \quad a \leq x \leq b \ . \tag{6.11}$$

Note that for the solution we have $R(y,x) \equiv 0$, and with the collocation method the spline is found so that

$$R(s, z_i) = 0 \ , \quad i = 1, \ldots, n{+}1 \ ,$$

where $\{z_i\}$ are the collocation points. With Galerkins method we try to make R small over the entire interval by demanding that

$$\int_a^b \psi_k(x) R(s,x) dx = 0 \ , \quad k = 1, \ldots, n{+}1 \ , \tag{6.12}$$

where the $\{\psi_k\}$ er linearly independent, socallad *test functions*.

By inserting (6.2) in (6.11) we see that

$$R(s,x) = -r(x) + \sum_{j=1}^{n+3} c_j \left(N_j''(x) + f(x)N_j'(x) + g(x)N_j(x)\right) \ ,$$

and in each of the conditions (6.12) the left hand side involves a linear combination of the $\{c_j\}$. Letting the kth condition in (6.12) correspond to the $(k{+}1)$st row in (6.3), we see that the elements in rows $2, \ldots, n{+}1$ of $\boldsymbol{A}$ and $\boldsymbol{d}$ are given by

for $k = 1, \ldots, n{+}1$:

$$a_{k+1,j} = \int_a^b \psi_k(x) \left(N_j''(x) + f(x)N_j'(x) + g(x)N_j(x)\right) dx \qquad j = 1, \ldots, n{+}3 \ , \tag{6.13a}$$

$$d_{k+1} = \int_a^b \psi_k(x) r(x) dx \ . \tag{6.13b}$$

These elements – and therefore the resulting spline s – depend on the choice of test functions. The simplest choice is

$$\psi_k(x) = N_{k+1}(x) \ , \quad k = 1, \ldots, n{+}1 \ , \tag{6.14}$$

in which case (6.13) takes the form

for $k = 2, \ldots, n{+}2$:

$$a_{k,j} = \int_a^b N_k(x) \left(N_j''(x) + f(x)N_j'(x) + g(x)N_j(x)\right) dx \qquad j = 1, \ldots, n{+}3 \ , \tag{6.15a}$$

$$d_k = \int_a^b N_k(x) r(x) dx \ . \tag{6.15b}$$

6.2.1. Practical Details. As usual we exploit the local support of B-splines: $N_i(x)$ is nonzero only for $x_{i-4} < x < x_i$. This implies that the integral in (6.15a) is nonzero only for $k{-}3 \leq j \leq k{+}3$, i.e. each row of $\boldsymbol{A}$ has at most 7 nonzero elements.

It is rarely possible to evaluate the integrals exactly. Instead we can use *numerical integration*, e.g. a two point *Gauss-Legendre* formula, where

$$I = \int_a^b G(x) dx \tag{6.16a}$$

is approximated by

$$I_n = \tfrac{1}{2}\sum_{i=1}^{n} h_i \left(G(x_{i-1} + \tfrac{3-\sqrt{3}}{6}h_i) + G(x_i - \tfrac{3-\sqrt{3}}{6}h_i)\right) \ . \tag{6.17}$$

This can be used for the elements in both $\boldsymbol{A}$ and $\boldsymbol{d}$, and has the effect, that (6.3) is replaced by

$$\widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{c}} = \widetilde{\boldsymbol{d}} \ . \tag{6.18}$$

If $H = \max\{h_i\}\searrow 0$ and the functions f, g, r are at least piecewise continuous, then the errors $\boldsymbol{A} - \widetilde{\boldsymbol{A}}$, $\boldsymbol{d} - \widetilde{\boldsymbol{d}}$ and $\boldsymbol{c} - \widetilde{\boldsymbol{c}}$ all behave as $O(H^4)$. This is of the same order of magnitude as the best possible discretization error with Galerkins method, [11, Chapter 7].

Example 6.3. A simpler approximation to the integrals is provided by the *trapezoidal rule*, where I in (6.16a) is approximated by

$$T_n = \tfrac{1}{2}\sum_{i=1}^{n} h_i\left(G(x_{i-1}) + G(x_i)\right) \ .$$

Thus, only knot values of the integrand are involved. This has the effect that we loose contributions with the coupling of N_k and $N_{k\pm3}$, and the matrix $\widetilde{\boldsymbol{A}}$ in (6.18) will have at most 5 nonzero elements per row.

This formula is not recommended, however, since it reduces the order of convergence from $O(H^4)$ to $O(H^2)$.

Example 6.4. We shall apply Galerkins method to the problem of Example 6.1. Again, we use equidistqant interior knots and multiple end knots. Further, we use the test functions $\{N_k\}_{k=2}^{n+2}$ and compute the elements by (6.16b). For $n = 4$ the system (6.18) takes the form (at most two decimals are shown in the elements)

$$\begin{bmatrix} 1 & & & & & & \\ 1.36 & -0.66 & 0.91 & 0.50 & 0.02 & & \\ 0.43 & 0.36 & 0.72 & 1.29 & 0.37 & 0.02 & \\ 0.05 & 0.28 & 0.69 & 1.37 & 1.29 & 0.50 & 0.07 \\ & 0.01 & 0.21 & 0.69 & 0.70 & 0.97 & 0.60 \\ & & 0.01 & 0.28 & 0.43 & -0.85 & 2.26 \\ & & & & & -6 & 7 \end{bmatrix} \widetilde{\boldsymbol{c}} = \begin{bmatrix} -0.69 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.25 \end{bmatrix} .$$

The solution (shown with 4 digits) is

$$\boldsymbol{c} = \left[\,-0.6861,\ \ 0.0414,\ \ 1.3030,\ \ -0.4339,\ \ -0.2754,\ \ 0.1302,\ \ 0.1472\,\right]^T \ ,$$

and the corresponding spline is shown in Figure 6.2.

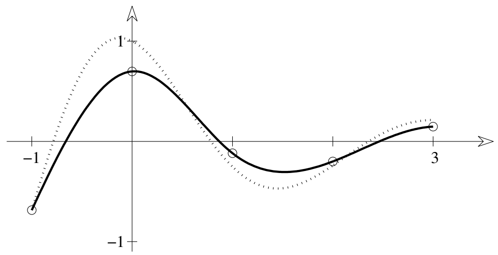


Figure 6.2. Galerkin solution to (6.9). $n = 4$. (Full line)

Dotted line: True solution.

Example 6.5. As in Example 6.2 we have investigated the discretization error for Galerkins method.

The point of maximum error varies between -0.480 and -0.250, and in Figure 6.3 (double logarithmic scale) we show the maximum discretization error for collocation (marked by $\diamond$) and Galerkins method (marked by $\star$).

The errors from Galerkins method behave as $O(h^4)$. This is in accordance with [11, Chapter 7].

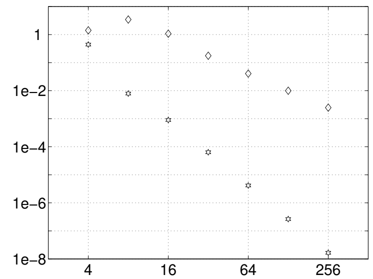


Figure 6.3.

Example 6.6. As the last demonstration of the versatility of cubic splines, consider the problem

$$y''(x) + g(x)y(x) = r(x) \ , \quad 0 \le x \le 2; \quad y(0) = y(2) = 0 \ , \tag{6.19a}$$

with

$$g(x) = \begin{cases} 4 \ , & 0 \le x < 1 \ , \\ 1 \ , & 1 < x \le 2 \ . \end{cases} \tag{6.19b}$$

This problem has a solution $y \in \mathsf{C}^1[0,2]$, but the second derivative has a jump across $x = 1$,

$$y''(1+) - y''(1-) = g(1-)y(1) - g(1+)y(1) = 3y(1) \ .$$

We can allow for this by placing a double knot at $x = 1$, cf. Theorem 2.2. This is easily handled by Galerkins method as described above – the vanishing knot interval is simply skipped in (6.16b).

Letting the other knots be equidistant, we have

$$n = 2m+1; \qquad h = 1/m;$$

$$x_i = \begin{cases} ih & i = 0,1,\ldots,m \quad , \\ 1 & i = m+1 \quad , \\ (i-1)h & i = m+1,\ldots,n \ . , \end{cases}$$

We have computed the solution for increasing values of m, and let

$$Y_{i,m} = s(t_i); \quad t_i = \frac{i}{10}, \quad i = 1,\ldots,19 \ ,$$

where s is the spline computed with $h = 1/m$. Selected results are shown in the table below.

t_i	$m = 16$	$m = 24$	$m = 36$	$m = 54$
0.2	2.04491851	2.04491629	2.04491581	2.04491572
0.4	3.83803341	3.83803010	3.83802943	3.83802930
0.6	5.08835902	5.08835467	5.08835383	5.08835366
0.8	5.59060363	5.59059760	5.59059641	5.59059617
1.0	5.25757812	5.25757146	5.25757014	5.25756988
1.2	4.42959580	4.42959016	4.42958905	4.42958883
1.4	3.45691295	3.45690856	3.45690770	3.45690752
1.6	2.37033407	2.37033105	2.37033045	2.37033033
1.8	1.20520421	1.20520266	1.20520235	1.20520229

Note that each new m-value is $\rho = 1.5$ times the previous value.

Assume that

$$Y_{i,m} \simeq y(t_i) + A_i h^q \tag{6.20a}$$

for some constant A_i and *convergence exponent* q, which is independent of t_i. It is easily veryfied that

$$\rho^q \simeq \frac{Y_{i,\rho m} - Y_{i,m}}{Y_{i,\rho^2 m} - Y_{i,\rho m}} \equiv w_{\rho^2 m} \ , \tag{6.20b}$$

and that the *Richardson extrapolation*

$$\widetilde{Y}_{i,\rho m} = Y_{i,\rho m} + \Delta_{i,\rho m}; \quad \Delta_{i,\rho m} = \frac{Y_{i,\rho m} - Y_{i,m}}{\rho^q - 1} \tag{6.20c}$$

is a better approximation.

These observations assume that the "$\simeq$" in (6.20a) is almost an equality. For small values of m higher order powers of h have domonating influence and for large values of m the effect of rounding errors may spoil the results. If

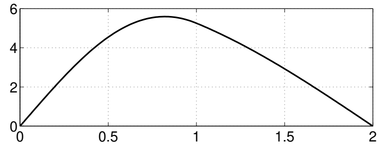
the computed value for q agrees with the expected value or if it is repeated with the next value of m, then we assume that the assumptions hold, and $\Delta_{i,m}$ will be a good estimate of the error $y(t_i) - Y_{i,m}$.

In the above table we have results for four m-values, and can use (6.20b) twice for each i. The results are given below – with $q_m = \log w_m / \log \rho$.

t_i	w_{36}	q_{36}	w_{54}	q_{54}
0.2	4.580	3.75	5.400	4.16
0.4	4.902	3.92	5.169	4.05
0.6	5.134	4.03	5.012	3.98
0.8	5.075	4.01	5.054	4.00
1.0	5.061	4.00	5.062	4.00
1.2	5.067	4.00	5.060	4.00
1.4	5.067	4.00	5.060	4.00
1.6	5.056	4.00	5.067	4.00
1.8	5.039	3.99	5.078	4.01

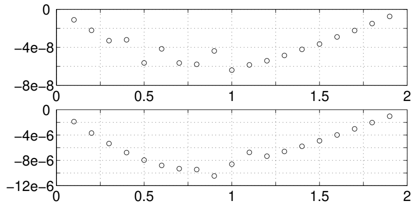
These results show that the discretization error behaves as s $O(h^4)$. Figure 6.4 shows the spline computed with $m = 54$, and the estimated errors are given in Figure 6.5.

Figure 6.4. Solution to (6.19)



We have also used Galerkins method on (6.19) with simple, equidistant knots, corresponding to $n = 2m$. A similar investigation shows that the discretization error in this case behaves as $O(h^3)$, and in Figure 6.5 we show errors from the finest knot mesh.

Figure 6.5. *Discretization errors. Above: Double knot at $x = 1$. $n = 109$. Below: Simple equidistant knots. $n = 108$*



Appendix A. Selected Details

A.1. Computation of B-Splines

In this section we give the expressions that are needed for evaluating a spline in the form (2.8). It follows (e.g. from Figure 2.3) that for any $x \in [x_0, x_n]$ there are (at most) four nonzero contributions

$$s^{(p)}(x) = \sum_{k=j}^{j+3} c_k N_k^{(p)}(x) \qquad \text{for} \quad x_{j-1} \le x < x_j \ . \tag{A.1}$$

The values below are derived from (2.10), (2.11c) and (B.4). We omit the argument (x). Note that the computation involves the knots $x_{j-3:j+2}$.

$$\begin{aligned}
M_{0,j} &= 1/(x_j - x_{j-1}) \\[1ex]
M_{1,j} &= (x_j - x)M_{0,j}/(x_j - x_{j-2}) \\
M_{1,j+1} &= (x - x_{j-1})M_{0,j}/(x_{j+1} - x_{j-1}) \\[1ex]
M_{2,j} &= (x_j - x)M_{1,j}/(x_j - x_{j-3}) \\
M_{2,j+1} &= \big((x - x_{j-2})M_{1,j} + (x_{j+1} - x)M_{1,j+1}\big)\,/(x_{j+1} - x_{j-2}) \\
M_{2,j+2} &= (x - x_{j-1})M_{1,j+1}/(x_{j+2} - x_{j-1}) \\[1ex]
N_j &= (x_j - x)M_{2,j} \\
N_{j+1} &= (x - x_{j-3})M_{2,j} + (x_{j+1} - x)M_{2,j+1} \\
N_{j+2} &= (x - x_{j-2})M_{2,j+1} + (x_{j+2} - x)M_{2,j+2} \\
N_{j+3} &= (x - x_{j-1})M_{2,j+2} \\[1ex]
N'_j &= -3M_{2,j} \\
N'_{j+1} &= 3(M_{2,j} - M_{2,j+1}) \\
N'_{j+2} &= 3(M_{2,j+1} - M_{2,j+2}) \\
N'_{j+3} &= 3M_{2,j+2}
\end{aligned}$$

$$\begin{aligned}
N''_j &= 6M_{1,j}/(x_j - x_{j-3}) \\
N''_{j+1} &= -6\,\big(M_{1,j}/(x_j - x_{j-3}) + (M_{1,j} - M_{1,j+1})/(x_{j+1} - x_{j-2})\big) \\
N''_{j+2} &= 6\,\big((M_{1,j} - M_{1,j+1})/(x_{j+1} - x_{j-2}) - M_{1,j+1}/(x_{j+2} - x_{j-1})\big) \\
N''_{j+3} &= 6M_{1,j+1}/(x_{j+2} - x_{j-1})
\end{aligned}$$

The knot values are of special interest. The (possibly) nonzero values are

	$x_{k-1}+$	x_k-
$M_{0,k}$	$\dfrac{1}{x_k - x_{k-1}}$	$\dfrac{1}{x_k - x_{k-1}}$
$M_{1,k}$	$\dfrac{1}{x_k - x_{k-2}}$	0
$M_{1,k+1}$	0	$\dfrac{1}{x_{k+1} - x_{k-1}}$
$M_{2,k}$	$\dfrac{x_k - x_{k-1}}{x_k - x_{k-3}} M_{1,k}$	0
$M_{2,k+1}$	$\dfrac{x_{k-1} - x_{k-2}}{x_{k+1} - x_{k-2}} M_{1,k}$	$\dfrac{x_{k+1} - x_k}{x_{k+1} - x_{k-2}} M_{1,k+1}$
$M_{2,k+2}$	0	$\dfrac{x_k - x_{k-1}}{x_{k+2} - x_{k-1}} M_{1,k+1}$
N_k	$(x_k - x_{k-1})M_{2,k}$	0
N_{k+1}	$(x_{k-1} - x_{k-3})M_{2,k} + (x_{k+1} - x_{k-1})M_{2,k+1}$	$(x_{k+1} - x_k)M_{2,k+1}$
N_{k+2}	$(x_{k-1} - x_{k-2})M_{2,k+1}$	$(x_k - x_{k-2})M_{2,k+1} + (x_{k+2} - x_k)M_{2,k+2}$
N_{k+3}	0	$(x_k - x_{k-1})M_{2,k+2}$
N'_k	$-3M_{2,k}$	0
N'_{k+1}	$3(M_{2,k} - M_{2,k+1})$	$-3M_{2,k+1}$
N'_{k+2}	$3M_{2,k+1}$	$3(M_{2,k+1} - M_{2,k+2})$
N'_{k+3}	0	$3M_{2,k+2}$
N''_k	$\dfrac{6}{x_k - x_{k-3}} M_{1,k}$	0
N''_{k+1}	$-N''_k - N''_{k+2}$	$\dfrac{6}{x_{k+1} - x_{k-2}} M_{1,k+1}$
N''_{k+2}	$\dfrac{6}{x_{k+1} - x_{k-2}} M_{1,k}$	$-N''_{k+1} - N''_{k+3}$
N''_{k+3}	0	$\dfrac{6}{x_{k+2} - x_{k-1}} M_{1,k+1}$

A.2. Tridiagonal Algorithm

The solution to the linear system

$$\boldsymbol{A z} = \boldsymbol{y} \quad \text{with} \quad \boldsymbol{A} = \begin{bmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & \cdot & \ddots & \cdot & \\ & & b_{m-1} & a_{m-1} & c_{m-1} \\ & & & b_m & a_m \end{bmatrix} \tag{A.2}$$

can be found by the *Tridiagonal Algorithm:*

$d_1 := a_1$
for $i := 2, \ldots, m$
  $e_i := b_i / d_{i-1}$
  $d_i := a_i - e_i * c_{i-1}$
  $y_i := y_i - e_i * y_{i-1}$
end
$z_m := y_m / d_m$
for $i := m{-}1 \ldots, 2, 1$
  $z_i := \left(y_i - c_i * z_{i+1}\right) / d_i$

This is just simple Gaussian elimination (i.e. without row interchanges), and should be used only for systems, where this is a stable process. The computational cost is about $8m$ flops.

The algorithm can be expressed as a factorization

$$\boldsymbol{A} = \boldsymbol{L U} \ , \tag{A.3a}$$

where $\boldsymbol{L}$ and $\boldsymbol{U}$ are the bidiagonal matrices

$$\boldsymbol{L} = \begin{bmatrix} 1 & & & \\ e_2 & 1 & & \\ & \ddots & \ddots & \\ & & e_m & 1 \end{bmatrix} , \qquad \boldsymbol{U} = \begin{bmatrix} d_1 & c_1 & & \\ & d_2 & c_2 & \\ & & \ddots & \ddots \\ & & & d_m \end{bmatrix} . \tag{A.3b}$$

The elements in $\boldsymbol{L}$ and $\boldsymbol{U}$ are computed as above – leaving out the calculations on $\boldsymbol{y}$ and $\boldsymbol{z}$ – and after that we solve $\boldsymbol{A z} = \boldsymbol{y}$ by

for $i := 2, \ldots, m$
  $y_i := y_i - e_i * y_{i-1}$
$z_m := y_m / d_m$ (A.3c)
for $i := m{-}1 \ldots, 2, 1$
  $z_i := \left(y_i - c_i * z_{i+1}\right) / d_i$

A.3. Algorithm for Periodic System

The systems in (4.17) and (4.24) fit into the more general form

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{G} \\ \boldsymbol{H}^T & \boldsymbol{B} \end{bmatrix} \boldsymbol{z} = \boldsymbol{d} \ , \tag{A.4a}$$

where $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ is a band matrix, e.g. tridiagonal as in (A.2), $\boldsymbol{G}, \boldsymbol{H} \in \mathbb{R}^{m \times q}$, $\boldsymbol{B} \in \mathbb{R}^{q \times q}$ and $\boldsymbol{z}, \boldsymbol{d} \in \mathbb{R}^n$, with $n = m{+}q$. This problem reduces to

$$\begin{bmatrix} \boldsymbol{I} & \boldsymbol{V} \\ \boldsymbol{H}^T & \boldsymbol{B} \end{bmatrix} \boldsymbol{z} = \begin{bmatrix} \widetilde{\boldsymbol{d}}_{1:m} \\ \boldsymbol{d}_{m+1:n} \end{bmatrix} , \tag{A.4b}$$

where $\boldsymbol{V}$ and $\widetilde{\boldsymbol{d}}_{1:m}$ are the solutions to

$$\boldsymbol{A V} = \boldsymbol{G} \ , \qquad \boldsymbol{A} \widetilde{\boldsymbol{d}}_{1:m} = \boldsymbol{d}_{1:m} \ . \tag{A.4c}$$

If $\boldsymbol{A}$ is tridiagonal, then $\boldsymbol{V}$ and $\widetilde{\boldsymbol{d}}_{1:m}$ can be computed via the $\boldsymbol{LU}$-factorization (A.3) with a cost of about $(8{+}5q)m$ flops. The idea generalizes to larger bandwidths. Next, by block elimination in (A.4b) we see that the last q components in $\boldsymbol{z}$ satisfy the $q{\times}q$ system

$$(\boldsymbol{B} - \boldsymbol{H}^T \boldsymbol{V}) \boldsymbol{z}_{m+1:n} = \boldsymbol{d}_{m+1:n} - \boldsymbol{H}^T \widetilde{\boldsymbol{d}}_{1:m} \ . \tag{A.4d}$$

This is solved by Gaussian elimination, and finally,

$$\boldsymbol{z}_{1:m} = \widetilde{\boldsymbol{d}}_{1:m} - \boldsymbol{V} \boldsymbol{z}_{m+1:n} \ . \tag{A.4e}$$

In the special case where $\boldsymbol{A}$ is tridiagonal and $q = 1$, $m = n{-}1$, the total cost is about $24n$ flops.

It should be mentioned that the algorithm is just a formalization of simple Gaussian elimination exploiting the arrowhead structure. It should be used only if this is a stable process, and this condition is satisfied in our spline applications.

A.4. Orthogonal Transformation

Consider the linear system

$$\boldsymbol{A c} \simeq \boldsymbol{y} \ ,$$

where $\boldsymbol{A} \in \mathbb{R}^{m \times q}$, $\boldsymbol{c} \in \mathbb{R}^q$ and $\boldsymbol{y} \in \mathbb{R}^m$ with $m \geq q$. By means of an orthogonal transformation this can be transformed to the system

$$\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{0} \end{bmatrix} \boldsymbol{c} \simeq \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} \ .$$

One way of doing this is *Householders method*, cf. [6, Section 5.3.3] or [8, Section 4.3]. It can be described as follows,

$$
\begin{array}{l}
\boldsymbol{B} := \begin{bmatrix} \boldsymbol{A} & \boldsymbol{y} \end{bmatrix} \\
\textbf{for } k := 1, \dots, q \\
\quad \boldsymbol{w} := \boldsymbol{B}_{k:m,k}; \quad b_{k,k} := -\mathrm{sign}(b_{k,k}) * \|\boldsymbol{w}\|_2 \\
\quad w_1 := w_1 - b_{k,k}; \quad \beta := -1/(b_{k,k} * w_1) \\
\quad \textbf{for } j := k+1, \dots, q+1 \\
\quad\quad \boldsymbol{B}_{k:m,j} := \boldsymbol{B}_{k:m,j} - \left(\beta * \boldsymbol{w}^T \boldsymbol{B}_{k:m,j}\right) \boldsymbol{w} \\
\quad \textbf{end} \\
\textbf{end}
\end{array}
$$

For each k this is an orthogonal transformation that puts zeros below the diagonal in the kth column (without explicitly storing them). The resulting $\boldsymbol{B}$ holds $\boldsymbol{R}$ in the upper right triangle of the first q columns, while the last columns holds $\boldsymbol{B}_{1:q,q+1} = \boldsymbol{u}$ and $\boldsymbol{B}_{q+1:m,q+1} = \boldsymbol{v}$.

APPENDIX B. SELECTED PROOFS

B.1. Proof of Theorem 2.1

First, we consider the differentiation rule (2.11c): Differentiating (2.10b) we get

$$
\begin{aligned}
(x_i - x_{i-2-r})M'_{r+1,i}(x) = M_{r,i-1}(x) &+ (x - x_{i-2-r})M'_{r,i-1}(x) \\
&- M_{r,i}(x) + (x_i - x)M'_{0,i}(x) \ .
\end{aligned} \tag{B.1}
$$

The functions $M_{0,j}(x)$ are piecewise constant, and for $r=0$ we see that

$$
(x_i - x_{i-2})M'_{1,i}(x) = M_{0,i-1}(x) - M_{r,i}(x)
$$

in agreement with (2.11c). Next, assume that (2.11c) holds for $q \le r-1$. Then

$$
\begin{aligned}
&(x - x_{i-2-r})M'_{r,i-1}(x) + (x_i - x)M'_{r,i}(x) \\
&\quad = r\left(\frac{x - x_{i-2-r}}{x_{i-1} - x_{i-2-r}}\big(M_{r-1,i-2}(x) - M_{r-1,i-1}(x)\big) \right. \\
&\qquad\quad \left. + \frac{x_i - x}{x_i - x_{i-1-r}}\big(M_{r-1,i-1}(x) - M_{r-1,i}(x)\big)\right) \\
&\quad = r\left(\frac{(x - x_{i-2-r})M_{r-1,i-2}(x) + (x_{i-1} - x)M_{r-1,i-1}(x)}{x_{i-1} - x_{i-2-r}}\right. \\
&\qquad\quad - \frac{(x - x_{i-1-r})M_{r-1,i-1}(x) + (x_i - x)M_{r-1,i}(x)}{x_i - x_{i-1-r}} \\
&\qquad\quad \left. - \left(\frac{x - x_{i-2-r} + x_{i-1} - x}{x_{i-1} - x_{i-2-r}} - \frac{x_i - x + x - x_{i-1-r}}{x_i - x_{i-1-r}}\right) M_{r-1,i-1}(x)\right) \\
&\quad = r\left(M_{r,i-1}(x) - M_{r,i}(x)\right) \ .
\end{aligned} \tag{B.2}
$$

By inserting this in (B.1) we see that (2.11c) also holds for $q=r$, and we have proven (2.11c) by induction.

Next, we note that all terms in the recurrence (2.10) are nonnegative and therefore $M_{r,i}(x) \ge 0$, and (2.12a) shows that also $N_i(x) \ge 0$. To show that $M_{r,i} \in \mathcal{S}_r(\boldsymbol{x}_{0:n})$ we can proceed as follows:

For $r=0$ it suffices to see that (2.10a) implies that (2.11a–b) are satisfied.

For $r=1$ we get

$$M_{1,i} = \begin{cases} 0 & \text{for} \quad x_0 \le x < x_{i-2} \\ \dfrac{x-x_{i-2}}{h_{i-1}(x_i-x_{i-2})} & \text{for} \quad x_{i-2} \le x < x_{i-1} \\ \dfrac{x_i-x}{h_i(x_i-x_{i-2})} & \text{for} \quad x_{i-1} \le x < x_i \\ 0 & \text{for} \quad x_i \le x \le x_n \end{cases} \tag{B.3a}$$

This is a piecewise first order polynomial satisfying (2.11a–b). Further,

$$\begin{aligned} M_{1,i}(x_{i-2}-) &= M_{1,i}(x_{i-2}+) = 0 \ , \\ M_{1,i}(x_{i-1}-) &= M_{1,i}(x_{i-1}+) = 1/(x_i-x_{i-2}) \ , \\ M_{1,i}(x_i-) &= M_{1,i}(x_i+) = 0 \ . \end{aligned} \tag{B.3b}$$

This shows that $M_{1,i}$ is continuous, so $M_{1,i} \in \mathcal{S}_1(\boldsymbol{x}_{0:n})$.

Analogously, we see that $M_{2,i}$ is a piecewise second order polynomial, which vanishes for $x<x_{i-3}$ and $x>x_i$ and satisfies

$$\begin{aligned} M_{2,i}(x_{i-3}-) &= M_{2,i}(x_{i-3}+) = 0 \ , \\ M_{2,i}(x_{i-2}-) &= M_{2,i}(x_{i-2}+) = h_{i-2}/\big((x_{i-1}-x_{i-3})(x_i-x_{i-3})\big) \ , \\ M_{2,i}(x_{i-1}-) &= M_{2,i}(x_{i-1}+) = h_{i-1}/\big((x_i-x_{i-2})(x_i-x_{i-3})\big) \ , \\ M_{2,i}(x_i-) &= M_{2,i}(x_i+) = 0 \ . \end{aligned} \tag{B.3c}$$

Thus, $M_{2,i}$ is continuous, and (2.11c) and the continuity of $M_{1,j}$ shows that also $M'_{2,i}$ is continuous. Therefore, $M_{2,i} \in \mathcal{S}_2(\boldsymbol{x}_{0:n})$.

Similarly we see that $M_{3,i}$ is a piecewise 3rd order polynomial, which is nonzero only for $x_{i-4} < x < x_i$, and varies continuously across the knots $x_{i-4:i}$. The continuity of $M'_{3,i}$ follows from (2.11c) and the continuity of $M_{2,i}$. To get higher derivatives, repeated use of (2.11c) shows that

$$\begin{aligned} M''_{r+1,i}(x) &= \frac{r+1}{x_i-x_{i-2-r}}\big(M'_{r,i-1}(x)-M'_{r,i}(x)\big) \\ &= \frac{(r+1)r}{x_i-x_{i-2-r}}\left(\frac{M_{r-1,i-2}(x)-M_{r-1,i-1}(x)}{x_{i-1}-x_{i-2-r}} \right. \\ &\qquad \left. - \frac{M_{r-1,i-1}(x)-M_{r-1,i}(x)}{x_i-x_{i-1-r}}\right) \ . \end{aligned} \tag{B.4}$$

This shows that $M''_{3,i}$ is a linear combination of the continuous functions $M_{1,i-2:i}$, and we have shown that $M_{3,i} \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$.

Finally, the normalized cubic B-splines $N_i(x)$ are obtained by multiplying $M_{3,i}(x)$ by a scalar, so also $N_i \in \mathcal{S}_3(\boldsymbol{x}_{0:n})$.

As regards (2.12b), it follows from (2.11a–b) that $N_{3,i:i+3}(x)$ are the only nonzero contributions to the sum in (2.12b) for a given $x \in [x_{i-1}, x_i]$, and by use of (2.10) we get

$$\begin{aligned} \sum_{j=1}^{n+3} N_{3,j}(x) &= N_{3,i}(x) + N_{3,i+1}(x) + N_{3,i+2}(x) + N_{3,i+3}(x) \\ &= (x_i-x)M_{2,i}(x) \\ &\quad +(x-x_{i-3})M_{2,i}(x) + (x_{i+1}-x)M_{2,i+1}(x) \\ &\quad +(x-x_{i-2})M_{2,i+1}(x) + (x_{i+2}-x)M_{2,i+2}(x) \\ &\quad +(x-x_{i-1})M_{2,i+2}(x) \\ &= (x_i-x_{i-3})M_{2,i}(x) + (x_{i+1}-x_{i-2})M_{2,i+1}(x) \\ &\qquad +(x_{i+2}-x_{i-1})M_{2,i+2}(x) \\ &= \cdots \\ &= (x_i-x_{i-2})M_{1,i}(x) + (x_{i+1}-x_{i-1})M_{1,i+1}(x) \\ &= \cdots = (x_i-x_{i-1})M_{0,i}(x) = 1 \ . \end{aligned} \tag{B.5}$$

B.2. Proof of Theorem 2.2

With q defined by (2.13), $q=1$ is the normal case: s is twice continuously differentiable.

With $q=2$ we have to consider values at x_k- and $x_k+ = x_{k+1}+$. From the expressions in Appendix A.1 it follows that the only nonzero values of N_i, N'_i and N''_i are

$$\begin{aligned} N_{k+2}(x_k-) &= N_{k+2}(x_k+) = (x_{k+2}-x_k)/(x_{k+2}-x_{k-1}) \ , \\ N_{k+3}(x_k-) &= N_{k+3}(x_k+) = (x_k-x_{k-1})/(x_{k+2}-x_{k-1}) \ , \\ N'_{k+2}(x_k-) &= N'_{k+2}(x_k+) = -3/(x_{k+2}-x_{k-1}) \ , \\ N'_{k+3}(x_k-) &= N'_{k+3}(x_k+) = 3/(x_{k+2}-x_{k-1}) \ , \\ N''_{k+1}(x_k-) &= \frac{6}{h_k(x_{k+1}-x_{k-2})}, \quad N''_{k+3}(x_k-) = \frac{6}{h_k(x_{k+2}-x_{k-1})} \ , \\ N''_{k+2}(x_k-) &= -N''_{k+1}(x_k-) - N''_{k+3}(x_k-) \ , \end{aligned}$$

$$N''_{k+2}(x_k+) = \frac{6}{h_{k+2}(x_{k+2}-x_{k-1})}, \quad N''_{k+4}(x_k+) = \frac{6}{h_{k+2}(x_{k+3}-x_k)} \ ,$$

$$N''_{k+3}(x_k+) = -N''_{k+2}(x_k+) - N''_{k+4}(x_k+) \ .$$

Thus, s and s' are continuous, but

$$\begin{aligned} s''(x_k+) - s''(x_k-) = &-c_{k+1}N''_{k+1}(x_k-) + c_{k+2}\left(N''_{k+2}(x_k+) - N''_{k+2}(x_k-)\right) \\ &+c_{k+3}\left(N''_{k+3}(x_k+) - N''_{k+3}(x_k-)\right) + c_{k+4}N''_{k+4}(x_k+) \end{aligned}$$

is nonzero except for special combinations of $c_{k+1:k+4}$.

With $q=3$ we consider values at x_k- and $x_k+ = x_{k+2}+$, and the only nonzero values of N_i and N'_i are

$$N_{k+3}(x_k-) = N_{k+3}(x_k+) = 1 \ ,$$

$$N'_{k+2}(x_k-) = -N'_{k+3}(x_k-) = -3/(x_{k+2}-x_{k-1}) \ ,$$

$$N'_{k+3}(x_k+) = -N'_{k+4}(x_k+) = -3/(x_{k+3}-x_k) \ ,$$

Thus, s is continuous, but normally $s'(x_k-) \neq s'(x_k+)$.

Finally, for $q \geq 4$ we find

$$N_{k+3}(x_k-) = N_{k+q}(x_k+) = 1 \ ,$$

and $s(x_k+) - s(x_k-) = c_{k+q} - c_{k+3}$, which generally will be nonzero.

B.3. Proof of Theorem 3.1

We use the Hermite representation (2.4) for s and can similarly write

$$\begin{aligned} &\text{for } 0 \leq t \leq 1 \ : \\ &f(x_{j-1}+h_jt) = (1-t)^2\left((1+2t)f(x_{j-1}) + h_jtf'(x_{j-1})\right) \\ &\qquad + t^2\left((3-2t)f(x_j) - h_j(1-t)f'(x_j)\right) + R_j(t) \ , \end{aligned} \tag{B.6a}$$

where the error $R_j(t)$ according to [7, p. 104] can be expressed as

$$R_j(t) = \frac{1}{4!}h_j^4t^2(1-t)^2f''''(x_{j-1}+h_j\theta_t), \quad 0 \leq \theta_t \leq 1 \ . \tag{B.6b}$$

We introduce (B.6) and (3.2b) in (3.1) and get

$$\begin{aligned} \left|e(x_{j-1}+h_jt)\right| = &\Big|(1-t)^2\left((1+2t)e_{j-1} + th_je'_{j-1}\right) \\ &+ t^2\left((3-2t)e_j - (1-t)h_je'_j\right) \\ &+\frac{1}{4!}h_j^4\left|t^2(1-t)^2f''''(x_{j-1}+h_j\theta_t)\right| \\ \leq &\max\left\{|e_{j-1}|,|e_j|\right\}\cdot\max_{0\leq t\leq 1}\left\{|(1-t)^2(1+2t)| + |t^2(3-2t)|\right\} \\ &+h_j\max\left\{|e'_{j-1}|,|e'_j|\right\}\cdot\max_{0\leq t\leq 1}\left\{|(1-t)^2t| + |t^2(1-t)|\right\} \\ &+\frac{1}{4!}\cdot\max_{x\in I_j}\left\{|f''''(x)|\right\}\cdot\max_{0\leq t\leq 1}\left\{|t^2(1-t)^2|\right\} \ , \end{aligned}$$

and (3.2) follows immediately.

Similar to the above expression for $e(x_{j-1}+h_jt)$ we can write

$$\begin{aligned} e'(x_{j-1}+h_jt) = &\frac{6}{h_j}t(1-t)(e_j - e_{j-1}) \\ &+(1-t)(1-3t)e'_{j-1} - t(2-3t)e'_j + R_{1,j}(t) \ , \end{aligned} \tag{B.7a}$$

$$e''(x_{j-1}+h_jt) = \frac{6}{h_j^2}(1-2t)(e_j-e_{j-1}) - \frac{(4-6t)e'_{j-1} + (2-6t)e'_j}{h_j} + R_{2,j}(t) \ , \tag{B.7b}$$

$$e'''(x_{j-1}+h_jt) = \frac{-12}{h_j^3}(e_j - e_{j-1}) + \frac{6}{h_j^2}\left(e'_{j-1} + e'_j\right) + R_{3,j}(t) \ , \tag{B.7c}$$

where [2] show that the errors $R_{p,j}(t)$ – coming from Hermite interpolation of f – satisfy

$$\text{for } 0 \leq t \leq 1 : \quad |R_{p,j}(t)| \leq \alpha_p h_j^{4-p}F_j^{iv} \ , \tag{B.8}$$

with α_p given by (3.3b). The quantities β_p and γ_p are found by maximization of the other terms in (B.7).

B.4. Proof of Lemma 3.2

[12, pp 55–56] shows that

$$\begin{aligned} &h_{i+1}f'(x_{i-1}) + 2(h_i+h_{i+1})f'(x_i) + h_if'(x_{i+1}) \\ &\quad = 3\frac{h_{i+1}}{h_i}(f(x_i) - f(x_{i-1})) + 3\frac{h_i}{h_{i+1}}(f(x_{i+1}) - f(x_i)) \\ &\quad +2(h_i+h_{i+1})\varphi_i \ , \end{aligned} \tag{B.9a}$$

where

$$|2(h_i+h_{i+1})\varphi_i| \le \frac{1}{24}\left(h_{i+1}h_i^3F_i^{iv} + h_ih_{i+1}^3F_{i+1}^{iv}\right) \ . \tag{B.9b}$$

We subtract (2.6) from (B.9a), divide by $2(h_i+h_{i+1})$ and get the following tridiagonal linear system of equations for $\{e_j'\}$:

$$\tfrac{1}{2}(1-\eta_i)e_{i-1}' + e_i' + \tfrac{1}{2}\eta_i e_{i+1}' = d_i + \varphi_i \ , \quad i=1,\dots,n-1 \ , \tag{B.10a}$$

where

$$\begin{aligned} \eta_i &= \frac{h_i}{h_i+h_{i+1}} \quad \Leftrightarrow \quad 1-\eta_i = \frac{h_{i+1}}{h_i+h_{i+1}} \ , \\ d_i &= 1.5(1-\eta_i)\frac{e_i-e_{i-1}}{h_i} + 1.5\eta_i\frac{e_{i+1}-e_i}{h_{i+1}} \ . \end{aligned} \tag{B.10b}$$

We easily derive the following estimates

$$\frac{h}{h+H} \le \eta_i, \ 1-\eta_i \le \frac{H}{h+H} \ , \tag{B.11a}$$

$$|d_i| \le 1.5(1-\eta_i+\eta_i)\frac{2E}{h} = 3\frac{E}{h} \ , \tag{B.11b}$$

$$|\varphi_i| \le \tfrac{1}{48}\left((1-\eta_i)h_i^3F_i^{iv} + \eta_ih_{i+1}^3F_{i+1}^{iv}\right) \le \tfrac{1}{48}\max_j\left\{h_j^3F_j^{iv}\right\} \ , \tag{B.11c}$$

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

$$\begin{aligned} |e_i'| &\le \tfrac{1}{2}(1-\eta_i+\eta_i)\max\left\{|e_{i-1}'|,\ |e_{i+1}'|\right\} + |d_i| + |\varphi_i| \\ &\le \tfrac{1}{2}\max\left\{|e_{i-1}'|,\ |e_{i+1}'|\right\} + 3\frac{E}{h} + \tfrac{1}{48}\max_j\left\{h_j^3F_j^{iv}\right\} \ . \end{aligned} \tag{B.11d}$$

Now (3.5) follows immediately.

B.5. Proof of Theorem 4.1

The perturbed spline $s+\delta s$ is expressed by (4.2) in terms of $\{(s+\delta s)_j, (s''+\delta s'')_j\}$, and it follows that

$$\delta s_i = \delta y_i, \ i=0,\dots,n; \qquad \delta s_0'' = \delta s_n'' = 0 \ ,$$

while $\delta\boldsymbol{s}_{1:n-1}''$ satisfy the following system corresponding to (4.4),

$$\boldsymbol{A}\delta\boldsymbol{s}_{1:n-1}'' = \delta\boldsymbol{d} \ ,$$

where

$$\boldsymbol{A} = \boldsymbol{D}(\boldsymbol{I}+\boldsymbol{B}), \quad (\delta\boldsymbol{d})_i = 6\left(\frac{\delta y_{i+1}-\delta y_i}{h_{i+1}} - \frac{\delta y_i - \delta y_{i-1}}{h_i}\right)$$

with

$$\boldsymbol{D} = 2\mathrm{diag}(h_i+h_{i+1}), \quad \boldsymbol{B} = \begin{bmatrix} 0 & 1-\eta_1 & & \\ \eta_2 & 0 & 1-\eta_2 & \\ & \cdot & \ddots & \cdot \\ & & \eta_{n-1} & 0 \end{bmatrix} \ ,$$

and η_i is given by (B.10b). It follows that

$$\begin{aligned} \|\delta\boldsymbol{s}_{1:n-1}''\|_\infty &= \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\boldsymbol{D}^{-1}\delta\boldsymbol{d}\|_\infty \\ &\le \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\|_\infty\|\boldsymbol{D}^{-1}\|_\infty\|\delta\boldsymbol{d}\|_\infty \ . \end{aligned} \tag{B.12}$$

Before proceeding we need the following

Lemma B.1. Let $\|\cdot\|_p$ be any norm, in which $\|\boldsymbol{I}\|_p = 1$. If the matrix $\boldsymbol{B}$ satisfies $\|\boldsymbol{B}\|_p < 1$, then

$$\|(\boldsymbol{I}+\boldsymbol{B})^{-1}\|_p \le \frac{1}{1-\|\boldsymbol{B}\|_p} \ . \tag{B.13}$$

Proof:

$$\begin{aligned} 1 = \|\boldsymbol{I}\|_p &= \|(\boldsymbol{I}+\boldsymbol{B})^{-1}(\boldsymbol{I}+\boldsymbol{B})\|_p \\ &= \|(\boldsymbol{I}+\boldsymbol{B})^{-1} + (\boldsymbol{I}+\boldsymbol{B})^{-1}\boldsymbol{B}\|_p \\ &\ge \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\|_p - \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\boldsymbol{B}\|_p \\ &\ge \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\|_p\left(1-\|\boldsymbol{B}\|_p\right) \ , \end{aligned}$$

and (B.13) follows. □

Now, $\|\boldsymbol{B}\|_\infty = \tfrac{1}{2}\max\limits_i\{|\eta_i| + |1-\eta_i|\} = \tfrac{1}{2}$, and proceeding with (B.12) we get

$$\|\delta\boldsymbol{s}''\|_\infty \le \frac{1}{1-\frac{1}{2}}\cdot\frac{1}{4h}\cdot 6\cdot\frac{4}{h}\|\delta\boldsymbol{y}\|_\infty = \frac{12}{h^2}\|\delta\boldsymbol{y}\|_\infty \ . \tag{B.14}$$

Finally, by means of (4.2) we get

$$\begin{aligned} \max_{x_0\le x\le x_n}\{|\delta s(x)|\} &\le \|\delta\boldsymbol{y}\|_\infty \max_{0\le t\le 1}\{|1-t|+|t|\} \\ &\quad + \tfrac{1}{6}\|\delta\boldsymbol{s}''\|_\infty H^2 \max_{0\le t\le 1}\left\{|(1-t)\left((1-t)^2-1\right)| + |t(t^2-1)|\right\} \\ &= \|\delta\boldsymbol{y}\|_\infty + \tfrac{1}{6}\|\delta\boldsymbol{s}''\|_\infty H^2\cdot\tfrac{3}{4} \ , \end{aligned}$$

and Theorem 4.1 follows when we insert (B.14).

As regards the condition number, we see that

$$\|\boldsymbol{A}\|_\infty \|\boldsymbol{A}^{-1}\|_\infty \le \|\boldsymbol{A}\|_\infty \|\boldsymbol{D}^{-1}\|_\infty \|(\boldsymbol{I}+\boldsymbol{B})^{-1}\|_\infty \le 6H \cdot \frac{1}{4h} \cdot \frac{1}{1-\frac{1}{2}} ,$$

yielding (4.5).

B.6. Proof of Theorem 4.2

For the interpolating spline we have $e_i \equiv f(x_i) - s(x_i) = 0$, and Theorem 3.3 shows that

$$\max_{x_0 \le x \le x_n} \{|e(x)|\} \le \frac{5H}{384} \max_j \left\{h_j^3 F_j^{iv}\right\} + \frac{H}{4} \max\left\{|e_0'|, e_n'|\right\} . \tag{B.15}$$

We have to express the boundary contribution in terms of the second derivative of e, and use (B.7b) and (B.8) to get

$$e_0'' \ = -h_1^{-1}(4e_0' + 2e_1') + R_{2,1}(0) \quad \Rightarrow$$

$$\begin{aligned} |e_0'| &= |-\tfrac{1}{2}e_1' - \tfrac{1}{4}h_1\left(e_0'' - R_{2,1}(0)\right)| \\ &\le \tfrac{1}{2}|e_1'| + \tfrac{1}{4}h_1|e_0''| + \tfrac{1}{48}h_1^3 F_1^{iv} . \end{aligned}$$

Similarly we find

$$|e_n'| \le \tfrac{1}{2}|e_{n-1}'| + \tfrac{1}{4}h_n|e_n''| + \tfrac{1}{48}h_n^3 F_n^{iv} ,$$

and by combining this with Lemma 3.2 we get

$$\max\left\{|e_0'|, |e_n'|\right\} \le \tfrac{1}{12}\max\left\{h_j^3 F_j^{iv}\right\} + \tfrac{1}{2}H \max\left\{|e_0''|, |e_n''|\right\} .$$

The theorem follows by inserting this estimate in (B.15).

APPENDIX C. ANSWERS TO EXCERCISES

Exercise 1.1. The answer follows from 3° in Definition 1.2 and the continuity condition in Definition 1.1.

Exercise 2.2. With s given by (2.4) we see that

$$s(x_{j-1}) = s(x_{j-1} + h_j \cdot 0) = s_{j-1} \quad \text{and} \quad s(x_j) = s(x_{j-1} + h_j) = s_j .$$

The first derivative is found from

$$\begin{aligned} \frac{ds}{dx} &= h_j^{-1}\frac{ds}{dt} \\ &= 6h_j^{-1}t(t-t)(s_j - s_{j-1}) + (1-t)(1-3t)s_{j-1}' - t(2-3t)s_j' . \end{aligned} \tag{C.1}$$

Thus, $s'(x_{j-1}) = s_{j-1}'$ and $s'(x_j) = s_j'$.

Also with the representation (2.5) we easily see that $s(x_{j-1}) = s_{j-1}$ and $s(x_j) = s_j$, while

$$\begin{aligned} s'(x_{j-1} + h_j t) = h_j^{-1}(s_j - s_{j-1}) \\ + \tfrac{1}{6}h_j\left((1 - 3(1-t)^2)s_{j-1}'' - (1 - 3t^2)s_j''\right) , \end{aligned} \tag{C.2a}$$

$$s''(x_{j-1} + h_j t) = (1-t)s_{j-1}'' + ts_j'' . \tag{C.2b}$$

From the last expression we see that $s''(x_{j-1}) = s_{j-1}''$, $s''(x_j) = s_j''$.

Exercise 2.3. With s given by (2.4) and using (C.1) we find

$$s''(x_{j-1} + h_j t) = 6h_j^{-2}(1-2t)(s_j - s_{j-1}) + h_j^{-1}\left((6t-4)s_{j-1}' + (6t-2)s_j'\right) .$$

This implies

$$s''(x_i-) = -6h_i^{-2}(s_i - s_{i-1}) + 2h_i^{-1}(s_{i-1}' + 2s_i') ,$$

$$s''(x_i+) = \ \ 6h_{i+1}^{-2}(s_{i+1} - s_i) - 2h_{i+1}^{-1}(2s_i' + s_{i+1}') .$$

When we equate these two expressions, reorder and multiply by $\frac{1}{2}h_i h_{i+1}$, we get (2.6).

With s given by (2.5) we use (C.2a) to find

$$s'(x_i-) = h_i^{-1}(s_i - s_{i-1}) + \tfrac{1}{6}h_i(s''_{i-1} + 2s''_i) ,$$

$$s'(x_i+) = h_{i+1}^{-1}(s_{i+1} - s_i) - \tfrac{1}{6}h_{i+1}(2s''_i + s''_{i+1}) .$$

(2.7) follows by equating these two expressions, reordering and multiplying by 6.

Exercise 2.4. From (2.4) we see that

$$s(x_{j-1} + h_j t) = s_{j-1} + h_j s'_{j-1} t + \big(3(s_j - s_{j-1}) - h_j(2s'_{j-1} + s'_j)\big)\, t^2 + \big(2(s_{j-1} - s_j) + h_j(s'_{j-1} + s'_j)\big)\, t^3 ,$$

and with $x - x_{j-1} = h_j t$ we see that

$$d_{0j} = s_{j-1} ,$$

$$d_{1j} = s'_{j-1} ,$$

$$d_{2j} = 3h_j^{-2}(s_j - s_{j-1}) - h_j^{-1}(2s'_{j-1} + s'_j) ,$$

$$d_{3j} = -2h_j^{-3}(s_j - s_{j-1}) + h_j^{-2}(s'_{j-1} + s'_j) .$$

In MATLAB we can use the following function,

```
function d = Hermite2pp(x,s,ds)
    n1 = length(x);  n = n1-1;
    n2 = n+n;  n3 = n2 + n;
    x = x(:)';  s = s(:)';  ds = ds(:)';
    h = diff(x);  q = diff(s) ./ h^2;
    d = [s(1:n); ds(1:n); zeros(n2,1)];
    d(n2+[1:n]) = 3*q - (2*ds(1:n)+ds(2:n1))./h;
    d(n3+[1:n]) = -2*q./h + (ds(1:n) + ds(2:n1))./h.^2;
```

Exercise 2.7. The values are immediately obtained from the expressions in Appendix B.2 for values at x_k+ in the case $q=3$.

Exercise 4.3. From (C.2) we see that

$$s'(x_0) = (s_1 - s_0)/h_1 + \tfrac{1}{6}h_1\,(-2s''_0 - s''_1) ,$$

$$s'(x_n) = (s_n - s_{n-1})/h_n + \tfrac{1}{6}h_n\,\big(s''_{n-1} + 2s''_n\big) ,$$

and setting $s'(x_0) = f'(x_0)$, $s'(x_n) = f'(x_n)$ we get (4.12b). (4.12a) is obtained by using (4.12b) in (4.3c) for $i=1$ and $i=n-1$.

REFERENCES

[1] J.H. Ahlberg, E.N. Nilson and J.L. Walsh: *The Theory of Splines and their Applications.* Academic Press, New York. 1967.

[2] G. Birkhoff and A. Priver: *Hermite Interpolation Errors for Derivatives.* J. Math. and Physics **46**, 440 – 447. 1967.

[3] M.G. Cox: *The Incorporation of Boundary Conditions in Spline Approximation Problems.* NPL Report NAC 80. 1977.

[4] M.G. Cox: *Practical Spline Approximation.* NPL Report DITC 1/82.1982.

[5] A.R. Curtis: *The Approximation of a Function of One Variable by Cubic Splines.* Chapter 4 in J.G. Hayes (ed): *Numerical Approximation to Functions and Data.* Athlone Press, London. 1970.

[6] G.H. Golub and C.F. Van Loan: *Matrix Computations, 2nd edition.* John Hopkins University Press, Baltimore. 1989.

[7] R.W. Hamming: *Numerical Methods for Engineers and Scientists.* McGraw-Hill, New York. 1962.

[8] H.B. Nielsen: *Numerisk lineær algebra.* (textbook in Danish). IMM, DTU, DK-2800 Lyngby. 1996.

[9] H.B. Nielsen and H. True: *Numerical Solution of the Nonlinear Stability of an Incompressible Ekman Boundary Layer.* Lecture Notes in Physics **90**, 410 – 415. Springer, Berlin. 1975.

[10] M.J.D. Powell: *Curve Fitting by Splines in one Variable.* Chapter 6 in J.G. Hayes (ed): *Numerical Approximation to Functions and Data.* Athlone Press, London. 1970.

[11] P.M. Prenter: *Splines and Variational Methods.* Wiley, New York, 1975.

[12] M.H. Schultz: *Spline Analysis.* Prentice-Hall, Englewood Cliffs, N.J. 1973.

Further recommended reading:

[13] C. de Boor: *A Practical Guide to Splines.* Springer, New York. 1978.

[14] P. Dierckx: *Curve and Surface Fitting with Splines.* Clarendon Press, Oxford. 1993.

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