Theory and Applications of Spline Functions

Edited by T. N. E. Greville

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Proceedings of an Advanced Seminar
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Foreword

This volume is the proceedings of an advanced seminar conducted by the Mathematics Research Center, United States Army. It was held at the Wisconsin Center on the campus of the University of Wisconsin in Madison, October 7-9, 1968.

The seminar was opened with words of welcome by Professor J. Barkley Rosser, Director of the Mathematics Research Center. The program was divided into five sessions, each session consisting of two one-hour talks. The seminar was informally conducted, and the undersigned, as chairman of the organizing committee, acted as chairman of all the sessions.

This volume contains six articles, as two or more consecutive one-hour talks have been combined into a single article in some instances. The first article is a general introduction to spline functions. The second, third and fifth articles are concerned primarily with applications, the respective areas of application being initial value problems in ordinary differential equations, approximation of functions, and boundary value and eigenvalue problems. The fifth article, however, contains also a theoretical section concerned with generalizations of spline functions in several directions. The fourth describes numerical algorithms for interpolation and approximation by spline functions, and the sixth and last treats in some depth the intimate relationship between monosplines and quadrature formulae.

The organizing committee, chaired by the editor, included Professors J. W. Jerome of Case Western Reserve University and L. L. Schumaker of the University of Texas, who were visiting at the Mathematics Research Center during the preceding year, and Professor I. J. Schoenberg of the University of Wisconsin; Mrs. Gladys Moran served ably as seminar secretary. The preparation of the manuscripts for publication was under the capable supervision of Mrs. Dorothy Bowar. The editor wishes also to express his gratitude to the staff of Academic Press, Inc.

The efforts of the speakers and all who worked toward the success of the seminar are warmly appreciated.

Madison, Wisconsin
December 1968

T. N. E. Greville

Preface

Spline functions are a class of piecewise polynomial functions satisfying continuity properties only slightly less stringent than those of polynomials, and thus they are a natural generalization of polynomials. They are found to have highly desirable characteristics as approximating, interpolating, and curve-fitting functions. In fact, the solutions of a number of simple optimization problems are spline functions, and they are intimately related to the approximation of linear functionals.

Though spline functions, without being so called, were used previously in a few isolated instances, they were named and singled out for special study for the first time by Schoenberg in the middle 1940's. He has said that their fundamental properties are so simple and the mathematics involved so elementary that it is remarkable they were not discovered earlier. It is only in the 1960's that they have attracted wide attention, but in recent years the literature in this area has proliferated rapidly.

In 1968 a survey of the most interesting and useful available information about spline functions would have required extensive literature research, and some of the information would not have been found in a form very convenient and accessible for application-oriented users. It was the purpose of the advanced seminar held in October 1968 to instruct Army mathematicians in the more fundamental aspects of the theory and applications of spline functions. This volume makes the same information available to the general reader.

Madison, Wisconsin
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T. N. E. Greville

Contents

Introduction to Spline Functions

T. N. E. GREVILLE

1. Definition of spline function. Given a strictly increasing sequence of real numbers, $x_1, x_2, \ldots, x_n$, a spline function $S(x)$ of degree m with the knots $x_1, x_2, \ldots, x_n$ is a function defined on the entire real line having the following two properties.

(i) In each interval (x_i, x_{i+1}) for $i = 0, 1, \ldots, n$ (where $x_0 = -\infty$ and $x_{n+1} = \infty$), $S(x)$ is given by some polynomial of degree m or less.

(ii) $S(x)$ and its derivatives of orders $1, 2, \ldots, m-1$ are continuous everywhere.

Thus, a spline function is a piecewise polynomial function satisfying certain conditions regarding continuity of the function and its derivatives. When $m = 0$, condition (ii) is not operative, and a spline function of degree 0 is a step function. A spline function of degree 1 is a polygon.

While, in general, $S(x)$ is given by different polynomials in adjoining intervals (x_{i-1}, x_i) and (x_i, x_{i+1}), the definition does not require this. In a very special case, $S(x)$ might be given by a single polynomial on the entire real line. In other words, the class $\mathcal{S}_m(x_1, x_2, \ldots, x_n)$ of spline functions of degree m having the knots $x_1, x_2, \ldots, x_n$ includes all polynomials of degree m or less.

For $m > 0$, a spline function of degree m could equally well be defined as a function in C^{m-1} whose m-th derivative is a step function. Even more concisely, a spline function of degree m is any m-th order indefinite integral of a step function.

A spline is a mechanical device used by draftsmen to draw a smooth curve consisting of a strip or rod of some flexible material to which weights are attached, so that it can be constrained to pass through or near certain plotted points on a graph. The term "spline function" (first used in [1]) is intended to suggest that the graph of such a function is similar to a curve drawn by a mechanical spline. Indeed, it has been shown [1, p. 67] that, to a first order of approximation, the curve produced by a spline is a cubic (i. e., third-degree) spline function.

Some writers use "spline" as a synonym for "spline function" and we shall sometimes do so.

2. Usefulness of spline functions. Polynomials have long been the functions most widely used to approximate other functions, mainly because they have the simplest mathematical properties. However, it is a common observation that a polynomial of moderately high degree fitted to a fairly large number of given data points tends to exhibit more numerous, and more severe undulations than a curve drawn with a spline or a French curve. There is now considerable evidence that in many circumstances a spline function is a more adaptable approximating function than a polynomial involving a comparable number of parameters. This conclusion is based in part on actual numerical experience, and in part on mathematical demonstrations that the solutions of a variety of problems of "best" approximation actually turn out to be spline functions. Examples of both kinds of evidence will be found in the articles in this volume. Also indicated will be applications of spline functions as interpolating functions, as approximating functions, in approximating linear functionals, especially definite integrals, and as approximations to solutions of ordinary differential equations.

3. Representation by truncated power functions. A particularly simple type of spline function is the truncated power function x_+^m defined by

$$x_+^m = \begin{cases} x^m & (x > 0) \\ 0 & (x \leq 0) \end{cases} .$$

For $m = 0$ this is the well known Heaviside function.

It is easily seen (see [2]) that any function $S \in \mathcal{S}_m(x_1, x_2, \ldots, x_n)$ has a unique representation of the form

$$S(x) = p(x) + \sum_{j=1}^{n} c_j (x - x_j)_+^m , \tag{3.1}$$

where $p \in \pi_m$. Here π_m denotes the class of polynomials of degree m or less. The representation (3.1) was first given in [3].

4. Natural splines. A spline $s(x)$ of odd degree $2k-1$ with the knots $x_1, x_2, \ldots, x_n$ is called a natural spline if it is given in each of the two intervals $(-\infty, x_1), (x_n, \infty)$ by some polynomial of degree $k-1$ (rather than $2k-1$) or less (in general, not the same polynomial in the two intervals). It is a matter of simple algebra to show [2, 4] that s is a natural spline of degree $2k-1$ with the indicated knots if and only if the representation (3.1) assumes the form

$$s(x) = p(x) + \sum_{j=1}^{n} c_j (x - x_j)_+^{2k-1} \qquad (p \in \pi_{k-1}) \tag{4.1}$$

and the coefficients c_j satisfy the relations

$$\sum_{j=1}^{n} c_j x^r = 0 \qquad (r = 0, 1, \ldots, k-1). \tag{4.2}$$

We shall denote by $\mathfrak{n}_{2k-1}(x_1, x_2, \ldots, x_n)$ the class of natural splines of degree $2k-1$ having the knots $x_1, x_2, \ldots, x_n$. Evidently this class contains π_{k-1}.

5. Spline integration formula. Hereafter we shall often be concerned with integrals in which a spline function appears as a kernel function. The following lemma facilitates the evaluation of such integrals. In this connection, the reader will note that it follows from the definition of a spline function that the derivative of a spline function of degree greater than zero is a spline function of the next lower degree with the same knots. Consequently, k-fold differentiation of a spline of degree k or more reduces the degree by k.

Lemma 5.1. Let S be given by (3.1) with $m = 2k-1$, where

(5.1) $$a \le x_1 < x_2 < \dots < x_n \le b,$$

and let f be a function having the following properties.

(i) $f \in C^{k-1}[a,b]$ and $f^{(k)}$ is continuous in each open interval (x_i, x_{i+1}), $i = 0, 1, \dots, n$, with $x_0 = a$ and $x_{n+1} = b$, when appropriate.

(ii) $f^{(k-r-1)}(x)\, S^{(k+r)}(x) = 0 \quad (r = 0, 1, \dots, k-2; x = a, b)$.

(iii) $f(a)\, S^{(2k-1)}(a-0) = f(b)\, S^{(2k-1)}(b+0) = 0$.

Then,

(5.2) $$\int_a^b f^{(k)}(x)\, S^{(k)}(x)\, dx = (-1)^k (2k-1)! \sum_{i=1}^{n} c_i\, f(x_i).$$

Proof. By successive integration by parts, we have

(5.3) $$\int_a^b f^{(k)}(x)\, S^{(k)}(x)\, dx = \sum_{r=0}^{k-2} (-1)^r [f^{(k-r-1)}(b)\, S^{(k+r)}(b) - f^{(k-r-1)}(a)\, S^{(k+r)}(a)] + (-1)^{k-1} \int_a^b f'(x)\, S^{(2k-1)}(x)\, dx.$$

The summation in the right member of (5.3) vanishes because of property (ii). Since $S^{(2k-1)}$ is a step function with the same knots as S, the integral in the right member of (5.3) is a sum of integrals of the form

(5.4) $$\eta_i \int_{x_i}^{x_{i+1}} f'(x)\, dx = \eta_i [f(x_{i+1}) - f(x_i)],$$

where η_i is the constant value of $S^{(2k-1)}$ in (x_i, x_{i+1}). Summing the right member of (5.4) with respect to i and rearranging terms gives

(5.5) $$\sum_{i=1}^{n} f(x_i) [S^{(2k-1)}(x_i - 0) - S^{(2k-1)}(x_i + 0)] + f(b)\, S^{(2k-1)}(b+0) - f(a)\, S^{(2k-1)}(a-0).$$

Now, the last two terms of (5.5) vanish by property (iii), while successive differentiation of (3.1) gives

(5.6) $$S^{(2k-1)}(x_i + 0) - S^{(2k-1)}(x_i - 0) = (2k-1)!\, c_i \quad (i = 1, 2, \dots, n).$$

In view of (5.5) and (5.6), (5.3) reduces to (5.2).

It may be remarked parenthetically that (5.2) is a particular case of a well known result in the theory of distributions of L. Schwartz (see formula (II, 2; 8), Tome I, p. 38, of [5]).

Corollary 5.2. If, in addition to the hypotheses of Lemma 5.1, f vanishes at every knot of S, then

$$\int_a^b f^{(k)}(x)\, S^{(k)}(x)\, dx = 0 .$$

Corollary 5.3. Let (5.1) hold, let s be a natural spline given by (4.1) with $k \geq 1$, and let $f \in C^{k-1}[a, b]$ be such that $f^{(k)}$ is continuous in each interval (x_i, x_{i+1}), $i = 0, 1, \ldots, n$, with $x_0 = a$ and $x_{n+1} = b$, when appropriate. Then

$$\int_a^b f^{(k)}(x)\, s^{(k)}(x)\, dx = (-1)^k (2k-1)! \sum_{i=1}^n c_i\, f(x_i) .$$

If, in addition, f vanishes at every knot of S,

$$\int_a^b f^{(k)}(x)\, s^{(k)}(x)\, dx = 0 .$$

Proof. Since $s \in \mathfrak{n}_{2k-1}(x_1, x_2, \ldots, x_n)$, it follows that $s^{(k)}$ is a spline of degree $k-1$ that vanishes identically for $x \leq x_1$ and for $x \geq x_n$. Consequently, conditions (ii) and (iii) of Lemma 5.1 are fulfilled, and the first conclusion follows. The last statement is a consequence of Corollary 5.2.

6. Uniqueness of interpolation by natural splines. We shall now show that for a given set of n data points

$$(6.1) \qquad (x_1, y_1),\ (x_2, y_2), \ldots, (x_n, y_n)$$

with distinct abscissas there is, if $1 \leq k \leq n$, a unique $s \in \mathfrak{n}(x_1, x_2, \ldots, x_n)$ that interpolates the given data points. In the proof we shall use the following lemma.

Lemma 6.1. If a function g vanishes for $n \geq k$ distinct arguments and $g^{(k)}$ is identically zero, then g is identically zero.

Proof. Clearly $g \in \pi_{k-1}$, and the conclusion follows.

Theorem 6.2. If $1 \leq k \leq n$ and the abscissas $x_1, x_2, \ldots, x_n$ are distinct, there is a unique $s \in \mathfrak{n}_{2k-1}(x_1, x_2, \ldots, x_n)$ that interpolates the data points (6.1).

Proof. Clearly there is no loss of generality in assuming that (5.1) holds.

The statement that s interpolates the points (6.1) is tantamount to the assertion that the relations

$$s(x_i) = y_i \qquad (i = 1, 2, \ldots, n) \tag{6.2}$$

are satisfied. Expression (4.1) contains a total of $n+k$ coefficients, and substitution of this expression, with $x = x_i$, in the left member of (6.2) gives n linear equations in these coefficients, while (4.2) provides k further linear equations. The theorem will be proved if it can be shown that the overall linear system is nonsingular.

Now, this will be established if it can be shown that the corresponding homogeneous system has only the trival solution in which all $n + k$ coefficients vanish. In other words, we need only show that the only $s_0 \in \mathfrak{n}_{2k-1}(x_1, x_2, \ldots, x_n)$ that interpolates the data points

$$(x_1, 0), \ (x_2, 0), \ldots, (x_n, 0) \tag{6.3}$$

is the trivial one that is identically zero everywhere. To prove this let s_0 be a natural spline with the required properties, and consider the integral $\sigma(s_0)$ given by

$$\sigma(s_0) = \int_a^b [s_0^{(k)}(x)]^2 \, dx .$$

By Corollary 5.3, identifying both f and s with s_0, we conclude that $\sigma(s_0) = 0$. By the definition of $\sigma(s_0)$, this clearly implies that $s_0^{(k)}$ vanishes identically. Consequently, by Lemma 6.1, s_0 is identically zero, as required.

7. The smoothest interpolation problem. Consider the problem of finding the smoothest interpolating function g for the n data points (6.1), where by "smoothest" we mean that the integral

$$\sigma(g) = \int_a^b [g^{(k)}(x)]^2 \, dx \tag{7.1}$$

is minimized, with $k \geq 1$. We shall consider only interpolating functions $g \in C^{k-1}[a, b]$ such that $g^{(k)}$ is piecewise continuous. (This condition can be weakened somewhat; see [6].)

If $k = n$, it is well known that there is a unique polynomial $L(x)$ of degree $k-1$ that interpolates the points (6.1). This is given by Lagrange's formula [7]

$$L(x) = \sum_{j=1}^{n} \frac{P_j(x)}{P_j(x_j)} y_j ,$$

where

$$P(x) = (x - x_1)(x - x_2) \ldots (x - x_n) ,$$

and $P_j(x)$ is the product obtained by deleting the factor $x - x_j$ from $P(x)$. For $g = L$, (7.1) gives $\sigma = 0$, which is evidently its smallest possible value Conversely, $\sigma = 0$ implies that g is in π_{k-1}, and L is known to be the unique interpolating function of this class.

The case $k > n$ is not interesting, as there is then an infinite set of interpolating polynomials in π_{k-1}.

We shall show that for $k < n$ there is a unique smoothest interpolating function, which is, in fact, precisely the interpolating natural spline of degree $2k-1$ having the abscissas of the given data points as knots, whose existence is guaranteed by Theorem 6.2. For $k = 2$, this was first shown by J. C. Holladay [8], and for the general case by C. de Boor [9] and I. J. Schoenberg [6]. Corollary 7.2 below will be used in the proof. Lemma 7.1, which precedes it, will be needed subsequently.

Lemma 7.1. Let f_1, f_2 be piecewise continuous and such that

$$\int_a^b f_1(x)\, f_2(x)\, dx = 0 , \tag{7.2}$$

and let

$$f = f_1 + f_2 \tag{7.3}$$

and

$$\rho(g) = \int_a^b [g(x)]^2\, dx \quad (g \in L_2(a, b)). \tag{7.4}$$

Then

$$\rho(f_1) \leq \rho(f) , \tag{7.5}$$

with equality only if $f = f_1$ at all points of continuity of f_2.

Proof. In view of (7.2), (7.3) and (7.4),

$$\rho(f) = \rho(f_1) + \rho(f_2).$$

Since $\rho(g) \geq 0$ for any g, (7.5) follows at once. Equality holds in (7.5) only if $\rho(f_2) = 0$. But this implies $f_2 = 0$ at all points of continuity, and consequently $f = f_1$ at such points.

Corollary 7.2. Let $f_1, f_2 \in C^{k-1}[a, b]$ have piecewise continuous k-th derivatives such that

$$\int_a^b f_1^{(k)}(x)\ f_2^{(k)}(x)\ dx = 0 ,$$

and let f_2 vanish for $n \geq k$ distinct arguments in $[a, b]$. Let f be defined by (7.3), and $\sigma(g)$ by (7.1) for any g. Then

$$\sigma(f_1) \leq \sigma(f) , \tag{7.6}$$

with equality only if $f = f_1$.

Proof. Inequality (7.6) follows immediately from Lemma 7.1, with $f_1^{(k)}$, $f_2^{(k)}$, $f^{(k)}$ assuming the roles of f_1, f_2, f in that lemma. If equality holds in (7.6), then, by the continuity of $f^{(k-1)}$, $f^{(k)}(x) \equiv 0$. By Lemma 6.1, $f_2(x) \equiv 0$, and so $f = f_1$.

Theorem 7.3. Let (5.1) hold, let k satisfy $1 \leq k \leq n$, and let s be the unique natural spline interpolating function for the data points (6.1) given by Theorem 6.2. Let f be any interpolating function for the points (6.1) such that $f \in C^{k-1}[a, b]$, and $f^{(k)}$ is piecewise continuous. Then

$$\sigma(s) \leq \sigma(f)$$

with equality only if $f = s$.

Proof. Applying Corollary 5.3 and identifying f with $f - s$, we conclude that

$$\int_a^b s^{(k)}(x)[f^{(k)}(x) - s^{(k)}(x)]dx = 0 . \tag{7.7}$$

We next apply Corollary 7.2, identifying f_1 with s and f_2 with $f - s$. In view of (7.7), the hypotheses of the corollary are satisfied. The conclusion of the theorem follows at once.

The preceding proof parallels closely the proofs given by de Boor [9] and Schoenberg [6]. This completes the solution of the smoothest interpolation problem for the case $k \le n$, except for the numerical determination of the parameters of the smoothest interpolating spline s, which will be considered later.

It is easily seen that for $k = 1$ the smoothest interpolating function amounts to joining each pair of consecutive data points by a straight line and using the familiar straight-line interpolation.

8. <u>Peano's theorem.</u> We shall now see that the theorem of unique natural spline interpolation (Theorem 6.2) has an intimate relationship to approximation of linear functionals. Probably the most important mathematical tool for studying such approximations in a theorem due to G. Peano [10-12]. In order to state Peano's theorem, we shall need to describe precisely the class of linear functionals we are going to consider. Following [12], we choose the class defined by

$$\mathfrak{F}f = \int_a^b [a_0(x)f(x) + a_1(x)f'(x) + \ldots + a_m(x)f^{(m)}(x)]dx + \sum_{i=1}^{j_0} b_{i0}f(x_{i0}) + \sum_{i=1}^{j_1} b_{i1}f'(x_{i1}) + \ldots + \sum_{i=1}^{j_m} b_{im}f^{(m)}(x_{im}) \quad (8.1)$$

where the functions $a_i(x)$ are piecewise continuous over $[a, b]$ and the abscissas x_{ij} are in $[a, b]$. While this is not the most general class of functionals that might be considered, it is adequate for most purposes. Evidently included as particular cases are (i) the integral of f over $[a, b]$ or any subinterval, (ii) the r-th derivative of f evaluated for $x = \xi$, where $\xi \in [a, b]$ and $0 \le r \le m$, and (iii) any linear combination of ordinates of f with abscissas in $[a, b]$.

We shall say that $\mathfrak{F}$ annihilates f if $\mathfrak{F}f = 0$.

<u>Peano's theorem.</u> Let $\mathfrak{F}$ be a linear functional of the form (8.1) that annihilates all polynomials of degree m or