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A Local Algorithm for Constructing Non-negative Cubic Splines

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An interpolating spline which interpolates positive function values is not necessarily positive for all arguments; a typical example of this occurs in the spline interpolation of the normal density function of probability theory. We describe an algorithm which produces non-negative interpolating splines provided the function to be interpolated is positive. We start with the interpolating natural spline and redefine it in those intervals for which the spline has negative values; we do this by adding few extra knots to those intervals. First we show that for any choice of extra knots it is possible to construct a spline which is non-negative. We call such a spline feasible. Second we show that within the set of feasible splines there is a best spline, in the sense that the functional which reflects the strain energy is minimized. Finally, by using a necessary optimality criterion we obtain an *optimal* spline which minimizes the strain energy also with respect to the free knots. The resulting formulae give explicit results and are very simple. Our numerical results show that the final step of selecting the interior knots appropriately gives very satisfactory results in a very efficient manner. The algorithm can be applied also to produce splines which stay below upper or stay above lower constant bounds. It is also very useful as a starting procedure for finding the globally best spline.

1. INTRODUCTION

Shape-preserving approximation is nowadays understood as an approximation which preserves relevant properties of the underlying function. These properties may be non-negativity (positivity), monotonicity

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(strict monotonicity), boundedness of the first derivative, etc.; in certain cases the goal is simply to produce "visually pleasing" approximations (cf. Carlson [6]).

Not so long ago several of these types of approximations were broadly referred to as monotone approximations (cf. Lorentz and Zeller [21]). The concept and subject of monotone approximation, a major trend in approximation theory, were introduced by Shisha [29] (see also [20] in this connection). In particular preservation of (ordinary) convexity has attracted several authors. One of the early papers is by Hornung [19]. More recent results are by Burmeister, Hess, and J. W. Schmidt in several papers [5, 16, 25, 26]. Convergence rates for monotone spline interpolation were given by Utreras [31].

We are concerned here with the preservation of non-negativity by using interpolating cubic splines. One immediate application is a class of problems arising in non-parametric statistics. Let $X_1, X_2, ..., X_n$ be the order statistics from a random sample of independent and identically distributed random variables arising from a population with unknown continuous density function f. Consider the problem of obtaining an estimate $\hat{f}$ of f, based on the sample and on some simple assumptions regarding the degree of smoothness of f. The first attempt at a solution of this problem was made by Boneva, Kendall, and Stefanov [3]. Using an area-matching condition on the histogram, they constructed a quadratic spline approximation to f. This work was extended by Schoenberg [27], who used the area-matching condition to construct cubic and quintic spline approximations to the cumulative distribution function F. In all of these applications, the constraint $f \geqslant 0$ was ignored.

More recently de Montricher, Tapia, and Thompson [14] developed the theory of a maximum penalized likelihood estimator of f in which the constraint $f \geqslant 0$ was incorporated in the analysis. However, there was no numerical implementation.

Another important statistical application, where the non-negativity constraint has been ignored, is the construction of smoothing spline approximations to the spectral density of a second order stationary random process. Cogburn and Davis [7] developed the theory of periodic smoothing L-splines, which in a particular case yielded a polynomial spline approximation to the spectral density . Wahba [32] developed a smoothing periodic polynomial spline approximation to the logarithm of the spectral density, and she has also done considerable research on the practical problem of estimating the optimal value of the Lagrange multiplier. De Figueiredo and Thompson [11] constructed smoothing cubic spline approximations to the spectral density. All of the above authors started with the periodogram of the random process which was then smoothed in some manner.

Another area in which non-negative polynomial splines are applicable is in the construction of quadrature rules with non-negative weights. Although no use of splines was made, Davis [8] gave a constructive proof of a result by Tchakaloff [30] on the existence of non-negative quadrature formulas. Applications of shape-preserving interpolation were made by Hill and Passow [17].

The rapid development of digital microprocessors has increased the area of feasibility for digital signal processing. Communications engineers are becoming aware of the potentialities of the use of splines, as evidenced, for example, in the work of Polge and Bhagavan [23], in which polynomial spline approximations to various signal waveforms were constructed. Many functions considered in this subject, such as the signal envelope and the ambiguity function, are non-negative functions [24].

There have been two main attempts on this problem in the literature. One concept was followed by de Boor and Daniel [10]. It consisted of representing a spline by non-negative linear combinations of B-splines. Naturally such a spline is non-negative.

The other concept was to use quadratic Bernstein-polynomials. In this area there have been many investigations, both theoretical and numerical, including those of Akima [2], Briggs and Rubel [4], Deimel, Doss, Fornuaro, McAllister, and Roulier [12], Deimel, McAllister, and Roulier [13] and Schumaker [28].

The latter concept has been also applied in CAD (see [15]).

The present authors use an entirely different approach to the construction of non-negative interpolating cubic splines. They consider first the natural spline which satisfies only the obvious constraint of passing through the data points.

In the second step in each subinterval between two successive knots in which this spline assumes negative values, the relevant portion of the spline is replaced by a non-negative cubic spline. This is carried out by the addition of extra knots, the location of which is variable and depends only on the values of the original spline and of its derivatives at the end points of the relevant subintervals. Hence, the fixing up procedure is entirely local in nature. In a first step one can determine a best non-negative spline, in the sense that the strain energy integral in each such sub-interval is minimized under the assumption that the extra knots are fixed.

In the last step the knots are also varied, again with the goal of minimizing the strain energy integral which require to solve a nonlinear (but not too difficult) equation. Here we make use of a characterization of such splines as given in Opfer and Oberle [22].

As a by-product we obtain an algorithm which can be used to produce splines which stay locally (i.e., between two consecutive knots) below or above a given constant.

The results can be extended to splines of arbitrary degree without difficulties.

2. Preliminaries

We present here a few well known results on cubic splines that we shall require. This material is treated well in [1].

We consider an interval $[a, b]$, $a<b$, and subdivide it by a mesh of points Δ, where

$$\Delta : a=x_1<x_2< \cdots <x_n=b.$$

An associated set of ordinates $y=\{y_i \mid i=1, 2, ..., n\}$ is prescribed. A cubic spline is a function $S_\Delta(y; \cdot)$ which is continuous together with its first and second derivatives on $[a, b]$, and which coincides with a cubic polynomial in each subinterval $[x_{j-1}, x_j]$, $j=2, 3, ..., n$, and satisfies the interpolation conditions $S_\Delta(y; x_j)=y_j$, $j=1, 2, ..., n$. The points $\{x_j \mid j=1, 2, ..., n\}$ are termed the *knots* of the spline. Moreover, a *natural* cubic spline is one satisfying the boundary conditions $S''_\Delta(y; x_1)=S''_\Delta(y; x_n)=0$. The existence and uniqueness of an interpolating natural cubic spline is well established. Moreover, we denote by $W_2^{(2)}$ the Sobolev space of real valued functions on $[a, b]$ with absolutely continuous first derivative and square integrable second derivative. The first result that we require is a theorem due to Holladay [18].

THEOREM 2.1. *Let $\Delta : a=x_1=x_2< \cdots <x_n=b$ and $y=\{y_i \mid i=1, 2, ..., n\}$ be given. Then of all functions f in $W_2^{(2)}$ such that $f(x_i)=y_i$, the natural cubic spline $S_\Delta(y; \cdot)$ minimizes*

$$\int_a^b f''^2(x)\, dx$$

uniquely.

The second result that we shall require is termed the first integral relation or simply Theorem of Pythagoras (cf. de Boor [9, p. 66]):

$$\int_a^b f''^2(x)\, dx - \int_a^b S''^2_\Delta(y; x)\, dx = \int_a^b |f''(x) - S''_\Delta(y; x)|^2\, dx \qquad (2.1)$$

for all $f \in W_2^{(2)}$ which passes through the data points. And clearly (2.1) is valid if in addition $f \geqslant 0$.

3. Local Argument for the Construction of Non-negative Splines

In this paper we consider the obvious constraint that the prescribed vector y is positive; i.e., $y_i > 0$, $i = 1, 2, \ldots, n$. In view of Holladay's theorem, the minimizer of (2.1) is the natural cubic spline $S_\Delta(y; \cdot)$, but this does not in general satisfy the non-negativity constraint. In the sequel, for brevity, we abbreviate by $S_\Delta(y; \cdot)$ the unconstrained interpolating spline, since all splines under consideration pass necessarily through the data points.

To search for a non-negative function f in the subset of $W_2^{(2)}$ consisting of all non-negative cubic splines (passing through the data points) that minimizes the semi-norm $\int_a^b f''^2(x)\,dx$ would require the repeated computation of natural splines on finer grids than the given Δ.

If $S_\Delta(y; \cdot) \geqslant 0$, $f = S_\Delta(y; \cdot)$ minimizes $\int_b^a f''^2(x)\,dx$ and then our problem is solved.

Therefore we consider the case in which $S_\Delta(y; \cdot)$ has two distinct zero crossings in just one interval, say $[x_j, x_{j+1}]$. Also we set $R_j = [a, x_j] \cup [x_{j+1}, b]$. In view of the first integral relation, we have

$$\int_a^b f''^2(x)\,dx - \int_a^b S_\Delta''^2(y; x)\,dx$$
$$= \int_{R_j} |f''(x) - S_\Delta''(y; x)|^2\,dx + \int_{x_j}^{x_{j+1}} |f''(x) - S_\Delta''(y; x)|^2\,dx. \quad (3.1)$$

A consequence of the first integral relation is that the minimum of $\int_a^b |f''(x) - S_\Delta''(y; x)|^2\,dx$ can be computed by minimizing $\int_a^b f''^2(x)\,dx$ alone.

In order to obtain a local minimizing procedure which depends only on the interval $[x_j, x_{j+1}]$ we set $f(x) = S_\Delta(y; x)$ for all $x \in R_j$. Since in this case $\int_{R_j} |f''(x) - S_\Delta''(y; x)|^2\,dx = 0$, it remains to minimize

$$\int_{x_j}^{x_{j+1}} f''^2(x)\,dx. \quad (3.2)$$

We have put $f(x) = S_\Delta(y; x)$ for all $x \in R_j$. In order that the resulting spline is still in C^2, the minimizer of (3.2) has to be restricted to the conditions

$$\begin{aligned} f(x) &\geqslant 0 \qquad \text{for all} \quad x \in [x_j, x_{j+1}], \\ f^{(k)}(x_l) &= S_\Delta^{(k)}(y; x_l); \qquad k = 0, 1, 2; \quad l = j, j+1. \end{aligned} \quad (3.3)$$

Moreover, we see that, regardless of the number of intervals in $[a, b]$ in which $S_\Delta(y; \cdot)$ possesses negative values, the above considerations may be applied separately to each such interval and result in each case in minimizing (3.2) subject to (3.3). We emphasize also that we have not established as yet the existence of such an non-negative spline. We have, however, shown that if such a cubic spline exists, then it is determined in each interval solely by the boundary conditions on $S_\Delta(y; \cdot)$ in that interval.

Thus we seek a non-negative cubic spline f in $[x_j, x_{j+1}]$ which matches $S_\Delta(y; \cdot)$, $S'_\Delta(y; \cdot)$, and $S''_\Delta(y; \cdot)$ at the endpoints and minimizes (3.2). It is plausible that such an f, if it exists at all, should have the x-axis as a tangent at some interior $\hat{x} \in]x_j, x_{j+1}[$ and $f''(\hat{x}) \geqslant 0$.

It should be emphasized that our local algorithm suggested will not solve the global problem of minimizing $\int_b^a f''(x)^2\,dx$ subject to $f \geqslant 0$. However, it will produce—as we will see from the examples—a visually pleasing non-negative spline with little expense.

4. Construction of Feasible and Best Cubic Splines

Let j be an index such that the natural cubic spline $S_\Delta(y; \cdot)$ has negative values in $I_j = [x_j, x_{j+1}]$. Since the second derivatives $S''_\Delta(y; x_j)$ and $S''_\Delta(y; x_{j+1})$ are already uniquely determined by the four values $S_\Delta(y; x_j)$, $S'_\Delta(y; x_j)$, $S_\Delta(y; x_{j+1})$, $S'_\Delta(y; x_{j+1})$ we cannot expect to find a non-negative spline in I_j which matches all six boundary conditions mentioned in (3.3) and minimizes (3.2) as well.

Let us simplify our notation by calling the above interval only $I = [u, v]$. The spline $S_\Delta(y; \cdot)$ restricted to I is a cubic polynomial and will be called p in the sequel of this section.

Two typical polynomials which are positive at the endpoints of I and negative somewhere in the interior are

$$p_1 = 1 - 7x + 4x^2 + 4x^3, \qquad x \in [0, 1], \tag{4.1a}$$

$$p_2 = 2 - 24x - 75x^2 + 50x^3, \qquad x \in [0, 1]. \tag{4.1b}$$

These polynomials will serve as test cases later on. The graphs are shown in Fig. 1. The relevant zeros of p_1 are $x_l = 0.15977540$, $x_r = 0.79886759$, and those of p_2 are $x_l = 0.61705073$, $x_r = 0.95110062$.

The problem of the preceding section can now be reformulated as finding a function $f \in W_2^2[u, v]$ with

$$\int_u^v f''^2(x)\,dx = \min \tag{4.2}$$

subject to

$$f(x) \geqslant 0 \qquad \text{for all} \quad x \in I = [u, v], \tag{4.3}$$

$$f(u) = \sigma_0, \qquad f'(u) = \sigma'_0, \qquad f(v) = \sigma_1, \qquad f'(v) = \sigma'_1, \tag{4.4}$$

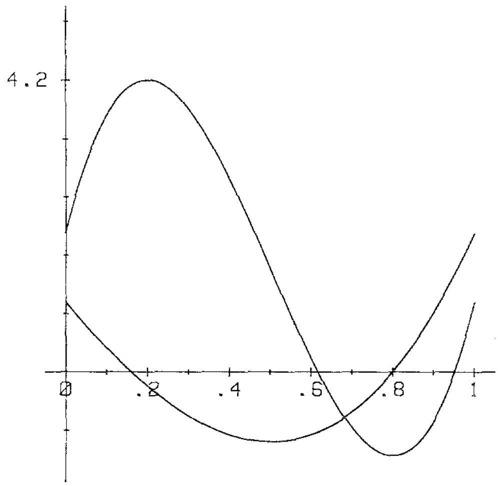

FIG. 1. Two test polynomials with positive endpoints and negative interior points.

where the four numbers σ are given by

$$\sigma_0 = p(u) > 0, \qquad \sigma_0' = p'(u), \qquad \sigma_1 = p(v) > 0, \qquad \sigma_1' = p'(v), \quad (4.5)$$

for a cubic polynomial p for which $p(x) < 0$ for some $x \in I$. Thus p has precisely two zeros $x_l < x_r$ in I. A necessary condition which is crucial in the construction of non-negative cubic spline which solves the above problem can be derived by variational techniques or by methods used in optimal control theory. The main information is contained in the following

THEOREM 4.1. *Let f solve the problem* (4.2) *to* (4.5). *Then f is a cubic C^2-spline with precisely one or two additional* (*simple*) *knots in the interior of I at which f vanishes. If there are two interior knots then f vanishes identically between these knots. Furthermore there are no zeros of f apart from or between the knots.*

Proof. Compare Opfer and Oberle [22]. ∎

A cubic spline with precisely one or two knots in the interior of I is called *feasible* if it matches the constraints (4.3) to (4.5). It is *optimal* it if solves the problem (4.2) to (4.5).

THEOREM 4.2. *The set of feasible splines is not empty.*

Proof. Let B be a cubic B-spline with vanishing values and vanishing first derivatives at the endpoints of I and with exactly one additional knot in the interior of I. For all $\alpha \in \mathbb{R}$, the spline

$$s = p + \alpha B \tag{4.6}$$

matches the boundary conditions (4.4) and (4.5). If α is sufficiently large it follows that $s(x) \geqslant 0$ for all $x \in I$. A similar construction is possible if we do have precisely two interior knots. ∎

COROLLARY 4.1. *There is a feasible spline s for which there exists a point* (called a contact point) $\hat{x} \in]u, v[$ *such that* $s(\hat{x}) = s'(\hat{x}) = 0$, $s''(\hat{x}) \geqslant 0$.

Proof. If s is a feasible spline such that $s(\hat{x}) = 0$ for some interior point $\hat{x}$, then necessarily $s'(\hat{x}) = 0$ and $s''(\hat{x}) \geqslant 0$ since $\hat{x}$ is a local minimum of s. By varying α in (4.6) we can produce splines s with positive and with negative minima. Therefore there must be an α such that the corresponding s has minimum value zero. Since $s(u) = \sigma_0 > 0$, $s(v) = \sigma_1 > 0$ this minimum must be attained at an interior point $\hat{x}$. ∎

A feasible spline with a contact point $\hat{x}$ as described in Corollary 4.1 can be constructed easily. The non-negativity condition of s reads

$$s(x) = p(x) + \alpha B(x) \geqslant 0 \qquad \text{for all } x \in I.$$

Since $B(x) > 0$ for all $x \in]u, v[$ we must require that

$$\alpha \geqslant -p(x)/B(x) \qquad \text{for all} \quad x \in]u, v[.$$

Therefore the smallest α which defines a feasible spline is

$$\hat{\alpha} = \max_{x \in [x_l, x_r]} \{-p(x)/B(x)\}, \tag{4.7}$$

where

$$p(x_l) = p(x_r) = 0 \qquad \text{and} \qquad u < x_l < x_r < v. \tag{4.8}$$

Let $\hat{\alpha} = -p(\hat{x})/B(\hat{x})$; then clearly $s(\hat{x}) = p(\hat{x}) + \hat{\alpha} B(\hat{x}) = 0$ and $s(x) \geqslant 0$ for all $x \in I$.

For the two polynomials p_1, p_2 of (4.1) the corresponding curves $-p/B$ are sketched in Fig. 2.

For p_1 we obtain $\hat{\alpha} = 2.42814970$ and for p_2 we obtain $\hat{\alpha} = 18.9384921$ where the additional knot is taken at 0.3.

A feasible spline $\hat{s}$ is called a *best* spline if for fixed interior knot(s) it approximates the given polynomial best, i.e.,

$$\| p'' - \hat{s}'' \|_2 \leqslant \| p'' - s'' \|_2 \qquad \text{for all feasible } s, \tag{4.9}$$

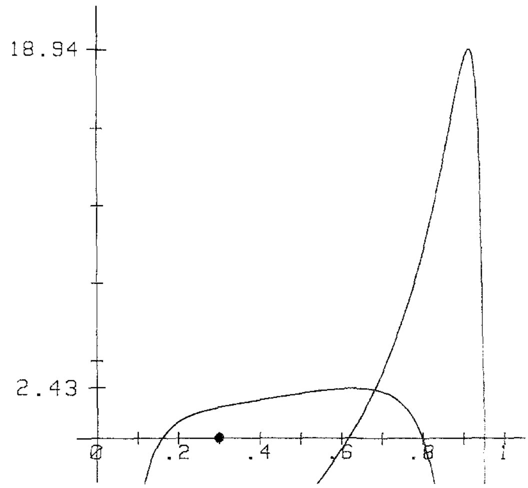

FIG. 2. Quotients $-p/B$ for the two test polynomials $p=p_1$ and $p=p_2$.

where $\| \ \|_2$ is the usual 2-norm. If we use $s=p+\alpha B$ from (4.6) then (4.9) reads $\hat{\alpha}\,\|B''\|_2 \leqslant \alpha\,\|B''\|_2$ for all α which define feasible splines. Since we have already computed the smallest α which defines a feasible spline, namely $\hat{\alpha}$ of (4.7), this $\hat{\alpha}$ also defines a best spline in the sense of (4.9).

In view of Theorem 4.1, splines with precisely two interior knots also must be taken into account. If we choose two interior knots, say $u<\xi_l<\xi_r<v$ arbitrarily, then we cannot expect to find a feasible C^2-spline which vanishes between the two given knots, since this would require finding two cubic polynomials each defined by five conditions. We will call a feasible C^2-spline with two interior knots which vanishes between these two knots a spline with a *contact line* (sometimes also called spline with *boundary arc*). It should be remarked here that by using a representation of the form $s=p+\alpha_1 B_1+\alpha_2 B_2$ it is not so easy to construct a feasible spline with two interior knots.

It should be observed that the evaluation of $\|B''\|_2$, if at all necessary, can be carried out exactly by applying Simpson's rule in the subintervals defined by the knots.

5. Optimal Knots Selection

Let us consider the same setting as before. The only difference now is that the interior knots are regarded as free. As measure of approximation we still use the semi-norm $\|p''-s''\|_2$. We have to distinguish between two

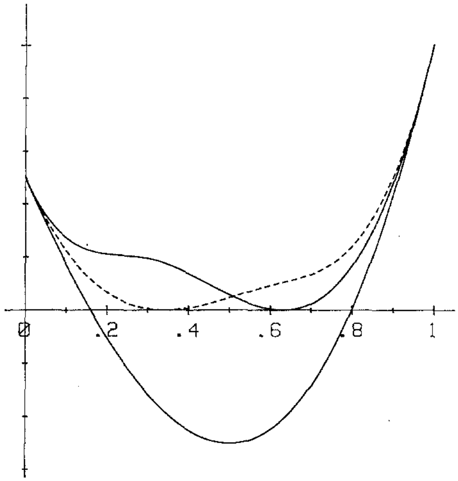

FIG. 3. Best splines for test polynomial p_1.

cases according to the number of interior knots. In Figs. 3 and 4 we present best splines for different placements of one additional knot which demonstrate that it is worthwhile to think about the placement of the interior knot(s).

A. *Case of Two Interior Knots*

The case of two interior knots $u < \xi_l < \xi_r < v$ turns out to be simpler. Therefore we treat this case first. For this case we apply Theorem 4.1 and

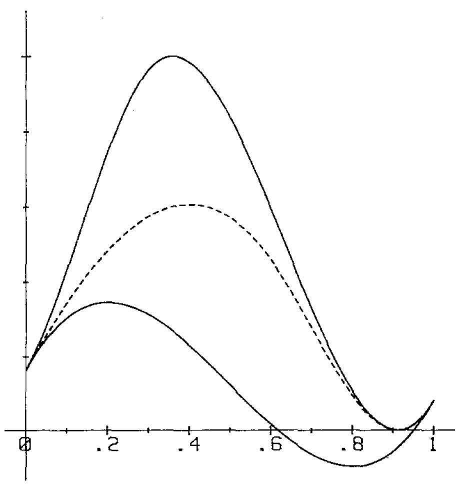

FIG. 4. Best splines for test polynomial p_2.

take the spline s in a form which is more convenient for our purpose, namely

$$s(x)=\begin{cases} s_l(x)=a_l(\xi_l-x)^3 & \text{for} \quad x\in[u,\xi_l], \\ 0 & \text{for} \quad x\in]\xi_l,\xi_r[, \\ s_r(x)=a_r(x-\xi_r)^3 & \text{for} \quad x\in[\xi_r,v]. \end{cases} \tag{5.1}$$

This representation makes s automatically a C^2-spline. We have to satisfy the conditions (4.4), (4.5) which read explicitly

$$s(u)=\sigma_0=a_l(\xi_l-u)^3, \qquad s'(u)=\sigma_0'=-3a_l(\xi_l-u)^2, \tag{5.2a}$$

$$s(v)=\sigma_1=a_r(v-\xi_r)^3, \qquad s'(v)=\sigma_1'=3a_r(v-\xi_r)^2. \tag{5.2b}$$

The first two equations are equations for the unknowns a_l, ξ_l. The last two equations are equations for the unknowns a_r, ξ_r. These equations can be easily solved. And the solution is

$$\xi_l=u-\frac{3\sigma_0}{\sigma_0'}, \qquad a_l=-\frac{\sigma_0'^3}{27\sigma_0^2}, \qquad \xi_r=v-\frac{3\sigma_1}{\sigma_1'}, \qquad a_r=\frac{\sigma_1'^3}{27\sigma_1^2}. \tag{5.3}$$

Since we must have $u<\xi_l<\xi_r<v$, we obtain the requirements

$$\sigma_0'<0, \qquad \sigma_1'>0, \qquad v-u>3\left(\frac{\sigma_1}{\sigma_1'}-\frac{\sigma_0}{\sigma_0'}\right). \tag{5.4}$$

The first two conditions imply that the coefficients a_l, $a_r>0$ with the consequence that $s(x)\geqslant 0$ for all $x\in[u,v]$. They also say that p is convex on $[u,v]$. However, convexity alone does not imply the existence of a contact line. For, replacing p by $p+\text{const}$ does not change the convexity. But the last condition of (5.4) will not hold if the constant is only large enough. We turn now to the case of one interior knot.

B. *Case of One Interior Knot*

We use a similar representation as in the previous case, namely

$$s(x)=\begin{cases} s_l(x)=b_l(\xi-x)^2+a_l(\xi-x)^3 & \text{for} \quad x\in[u,\xi[, \\ s_r(x)=b_l(x-\xi)^2+a_r(x-\xi)^3 & \text{for} \quad x\in[\xi,v], \end{cases} \tag{5.5}$$

where ξ is the unknown knot. The representation (5.5) again makes s a C^2-spline. Since ξ is a contact point we must have $s''(\xi)/2=b_l\geqslant 0$. The spline must meet the four conditions (4.4). Therefore we have four equations for the unknowns a_l, a_r, b_l, ξ. From these four equations one can easily eliminate the quantities a_l, a_r and one is left with two equations for b_l, ξ which can be put into the form

$$b_l(\xi-u)^2(v-\xi)^2=(v-\xi)^2(3\sigma_0+\sigma_0'(\xi-u)), \tag{5.6a}$$

$$b_l(\xi-u)^2(v-\xi)^2=(\xi-u)^2(3\sigma_1-\sigma_1'(v-\xi)). \tag{5.6b}$$

Since $b_l \geqslant 0$ we must have

$$3\sigma_0+\sigma_0'(\xi-u)\geqslant 0, \quad 3\sigma_1-\sigma_1'(v-\xi)\geqslant 0 \tag{5.7}$$

in order that the above equations have a solution. Every solution is then a zero of the cubic polynomial

$$g(\xi)=(v-\xi)^2(3\sigma_0+\sigma_0'(\xi-u))-(\xi-u)^2(3\sigma_1-\sigma_1'(v-\xi)). \tag{5.8}$$

This polynomial always has at least one zero in $]u, v[$ since $g(u)>0$ and $g(v)<0$.

In dependence on the signs of σ_0' and σ_1' the conditions (5.7) are given in Table I.

From Table I we see that conditions (5.7) are valid exactly if conditions (5.4) are not valid.

If the given problem (4.2) to (4.5) would have two different solutions, any convex combination of these solutions would also be a solution. Thus we would have an infinite number of solutions. Our conditions, however, allow only finitely many solutions (namely at most three, corresponding to the zeros of g defined in (5.8)). Therefore only one solution is possible.

We summarize.

THEOREM 5.1. *Let p be a polynomial on $[u, v]$ with properties mentioned in* (4.5). *If p satisfies conditions* (5.4) *the optimal spline s is defined by two interior knots $u<\xi_l<\xi_r<v$ and it is given by* (5.1) *and* (5.3). *If the conditions*

TABLE I

Conditions (5.7) in Dependence on the Signs of the σ''s

Sign σ_0'	Sign σ_1'	Conditions (5.7)
+	+	$u\leqslant v-3\sigma_1/\sigma_1'\leqslant\xi\leqslant v$
+	−	Cannot occur
−	+	$v-3\sigma_1/\sigma_1'\leqslant\xi\leqslant u-3\sigma_0/\sigma_0'$
−	−	$\xi\leqslant u-3\sigma_0/\sigma_0'\leqslant v$

(5.4) *are not satisfied, then the optimal spline s is defined by precisely one interior knot* $u < \xi < v$, *and s is defined by* (5.5), (5.6), (5.8).

Proof. By the above considerations. ∎

We apply the above theorem to the two test polynomials p_1, p_2 defined in (4.1a), (4.1b), respectively. For p_1 we obtain

$$\sigma_0 = 1, \qquad \sigma_0' = -7, \qquad \sigma_1 = 2, \qquad \sigma_1' = 13$$

and condition (5.4) is valid. Thus the resulting spline s has a *contact line* and is defined in (5.1), (5.3) with

$$\xi_l = 3/7 = 0.4286, \qquad a_l = 7^3/27 = 12.7037, \tag{5.9a}$$

$$\xi_r = 7/13 = 0.5385, \qquad a_r = 13^3/108 = 20.3426, \tag{5.9b}$$

$$\|p'' - s''\|_2 = 13.88044188. \tag{5.9c}$$

From the last condition in (5.4) we deduce that we could replace p_1 with $p_1 + \text{const}$ without violating this condition as long as $\text{const} < 1/6$. For p_2 we have

$$\sigma_0 = 2, \qquad \sigma_0' = 24, \qquad \sigma_1 = 1, \qquad \sigma_1' = 24$$

and condition (5.4) is not valid. Thus the solution has only a *contact point* and is obtained from (5.8), (5.6), (5.5):

$$\xi = (2 + 3\sqrt{2})/7 = 0.89180581, \tag{5.10a}$$

$$\begin{gathered} b_l = 2340.968830, \qquad a_l = -2622.156167, \qquad a_r = -20{,}847.16817, \\ \hat{\alpha} = 4.05250462, \qquad \|p'' - s''\|_2 = 45.1936094, \end{gathered} \tag{5.10b}$$

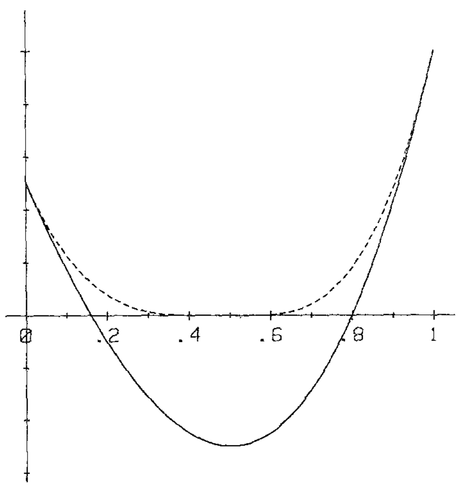

FIG. 5. Optimal spline for test polynomial p_1.

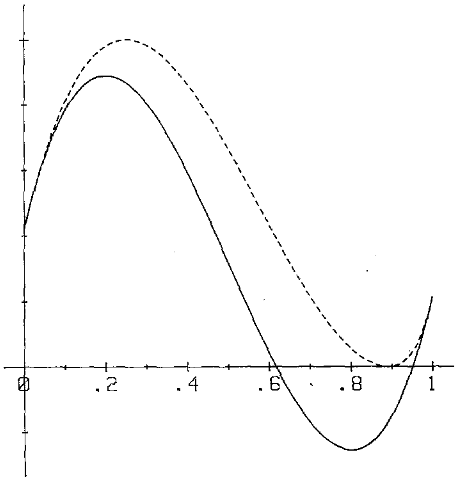

FIG. 6. Optimal spline for test polynomial p_2.

where $\hat{\alpha}$ refers to the former representation (4.6). The optimal splines are presented in Figs. 5 and 6.

C. *General Remarks*

The procedure described is very simple and the results are very satisfactory in many cases. The procedure may serve also another purpose. When computing non-negative splines according to a global strategy (cf. [22]) the start selection of knots turns out to be crucial, since these knots serve as initial values for a Newton-iteration. From our own numerical experience it is apparent that the optimal knots as described in this section are in general very useful as starting values for the above mentioned Newton-iteration, cf. Dauner and Reinsch.

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