JOURNAL OF APPROXIMATION THEORY **18**, 39–49 (1976)

Variations on a Theme by Schoenberg

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Communicated by Oved Shisha

Received September 9, 1974

In this note we discuss three types of polynomial spline approximation: (i) Schoenberg's variation-diminishing approximation, (ii) simple variation-diminishing approximation, and (iii) a natural extrapolated approximation which can be obtained by taking the appropriate linear combination of the first two. The latter method, although not variation diminishing itself, has a number of practical advantages over either (i) or (ii), including higher-order convergence properties with respect to mesh gauge and in order of derivative, specifically, for C^2 functions defined on finite intervals, it exhibits uniform convergence behavior in value, slope, and curvature, whereas the other methods break down on the last and sometimes critical "shape-getting property," namely, convergence in curvature.

1. SCHOENBERG'S VARIATION-DIMINISHING SPLINE APPROXIMATION

Let knots $x_0 \leqslant x_1 \leqslant \cdots \leqslant x_{n+m+1}$ be given and let $N_{j,m+1}(x)$, $j = 0, 1,..., n$, be the associated B-spline basis of degree m (cf. [7, 8]). For a function $f(x)$ defined on the interval $[x_0, x_{n+m+1}]$ Schoenberg's variation-diminishing spline approximation to $f(x)$ is given by

$$S_\Delta f(x) = \sum_{j=0}^{n} f(\xi_j)\, N_{j,m+1}(x), \tag{1}$$

where

$$\xi_j = \sum_{i=1}^{m} x_{j+i}/m, \qquad j = 0, 1,..., n. \tag{2}$$

In this formulation we allow for the possible coincidence of the knots up to the mth order (of coincidence).

This method of approximation was introduced by Schoenberg as the "natural" extension to splines of the classical Bernstein polynomial approximation to a function $f(x)$ defined on a finite interval $[a, b]$.

Specifically, the preservation of linear functions and the variation-diminishing character of the Bernstein polynomial approximation have been made the basis for this extension to splines. Similar extensions have been made to splines defined with respect to more general Tchebycheff systems of functions by Marsden [5], and Karlin and Karon [2]. In this paper we consider only the ordinary or piecewise polynomial spline case.

Let $v(f)$ denote the number of sign changes of $f(x)$ on the interval $[\xi_0, \xi_n]$. Then formula (1) defines an approximation with the properties

$$v(S_\Delta f) \leqslant v(f) \tag{3}$$

and

$$S_\Delta f(x) = c + dx \qquad \text{on } [x_m, x_{n+1}] \tag{4}$$

for every

$$f(x) = c + dx \qquad \text{on } [\xi_0, \xi_n]. \tag{5}$$

In general the interval $[x_m, x_n]$ is strictly contained in the interval $[\xi_0, \xi_n]$ unless $a = x_0 = \cdots = x_m$ and $b = x_{n+1} = \cdots = x_{n+m+1}$, in which case both intervals coincide with $[a, b]$. This latter assumption is usually made in connection with Schoenberg's method of approximation on a finite interval because (3) may then be strengthened to

$$v(S_\Delta f - c - dx) \leqslant v(f - c - dx) \tag{6}$$

on $[a, b]$. Hence, the total variation $T(f)$ of f on $[a, b]$ satisfies

$$T(S_\Delta f) \leqslant T(f). \tag{7}$$

As a particular case, if $n = m$, then Schoenberg's method reduces to the classical Bernstein polynomial approximation of degree m on the interval $[a, b]$. Essentially, because of (6) and (7), the spline variation-diminishing method shares many of the related properties of its special case, the Bernstein method. Notably these include the so-called shape-preserving properties such as positivity, monotonicity, and convexity [4, 8]. In addition, the spline method has convergence properties on both the knot spacing and the degree of the spline [4, 5, 7].

2. Simple Variation-Diminishing Spline Approximation

We consider a second type of variation-diminishing approximation which is, in some ways, more natural than Schoenberg's method. In the notation of the previous section we define

$$s_\Delta f(x) = \sum_{j=0}^{n} \left[\left(\sum_{i=1}^{m} f(x_{i+j}) \right) \Big/ m \right] N_{j,m+1}(x). \tag{8}$$

From well-known properties of the B-spline basis it follows immediately that (8) preserves linear functions $f(x) = a + bx$ (cf. [8]). The number of sign changes in the ordered set of coefficients

$$a_j = \sum_{i=1}^{m} f(x_{i+j})/m, \qquad j = 0, 1,..., n,$$

is not greater than in the set $f(x_k)$, $k = 1, 2,..., n + m$, hence, in $f(x)$ itself.

Consequently, as in [8],

$$v(s_\Delta f(x)) \leqslant v(a_i) \leqslant v(f), \qquad i = 0, 1,..., n. \tag{9}$$

The preservation of linear functions allows one to strengthen (9) to

$$v(s_\Delta f(x) - c - dx) \leqslant v(f - c - dx) \tag{10}$$

for all c, d. Therefore,

$$T(s_\Delta f) \leqslant T(f) \tag{11}$$

on the interval $[a, b]$; i.e., $s_\Delta f(x)$ is an alternative variation-diminishing spline approximation to $f(x)$ which we call *simple* variation-diminishing spline approximation.

What we mean by the phrase "more natural" above is simply that the evaluations of the function take place at the knots rather than on the m-fold average of the knots as in Schoenberg's method. The striking resemblance of the two variation-diminishing formulas is made clear by rewriting (1) as

$$S_\Delta f(x) = \sum_{j=0}^{n} f\left[\left(\sum_{i=1}^{m} x_{i+j}\right)\Big/ m\right] N_{j,m+1}(x). \tag{12}$$

Of course, either approximation method preserves positivity, monotonicity, and convexity. However, the property of convexity has to be qualified somewhat in the case of formula (8): strict convexity is not always preserved. For example, in the special case of no interior knot, $s_\Delta f$ reduces to the straight line connecting the end points of $f(x)$. However, if there is at least one interior knot strict convexity is also preserved. In addition to not containing Bernstein polynomial approximation as a special case, this method does not converge to the function with respect to the degree m for a fixed set of interior knots. Rather, it always converges to the straight line joining the end points of the function.

THEOREM 1. *Let* $a < y_1 \leqslant y_2 \leqslant \cdots \leqslant y_k < b$. *Define knots by setting* $x_0 = x_1 = \cdots = x_m = a$, $x_{m+i} = y_i$, $i = 1, 2,..., k$, *and* $x_{m+k+1} = x_{m+k+2} =$

$\cdots = x_{2m+k+1} = b$. *Then* $s_\Delta f \to f(a) + [f(b) - f(a)]((x-a)/(b-a))$ *as* $m \to \infty$.

Proof. Formula (8) specializes to

$$s_\Delta f(x) = f(a) \sum_{i=0}^{m-1} N_i(x) + \sum_{l=1}^{k} f(y_l)/m \sum_{i=0}^{m-1} N_{i+l}(x)$$

$$+ f(b)/m \sum_{i=0}^{m-1} (i+1)\, N_{k+i+1}(x) - f(a)/m \sum_{i=1}^{m-1} iN_i(x).$$

The result follows from the limit identities

$$\lim_{m\to\infty} \sum_{i=0}^{m-1} N_i(x) = 1$$

and

$$\lim_{m\to\infty} (1/m) \sum_{i=0}^{m-1} (i+1)\, N_{k+i+1}(x) = \lim_{m\to\infty} (1/m) \sum_{i=0}^{m+k} iN_i(x) = (x-a)/(b-a).$$

When compared on the basis of knot spacing, the methods are somewhat less distinguishable.

THEOREM 2. *Let* $f \in C^2[a,b]$, $\| f'' \| = \max_{a \leqslant x \leqslant b} | f''(x)|$ *and* $\| \Delta \|$ *be the mesh gage. Then*

$$| s_\Delta f(x) - S_\Delta f(x)| \leqslant (m^2 - 1)/24 \| f'' \| \cdot \| \Delta \|^2. \tag{13}$$

Proof. From Taylor's theorem,

$$f(x_{i+j}) = f(\xi_j) + (x_{i+j} - \xi_j)\, f'(\xi_j) + (x_{i+j} - \xi_j)^2/2f''(\xi_{ij}^*),$$

where ξ_{ij}^* is between x_{i+j} and ξ_j. Therefore,

$$\sum_{i=1}^{m} f(x_{i+j})/m = f(\xi_j) + \sum_{i=1}^{m} (x_{i+j} - \xi_j)^2/2mf''(\xi_{ij}^*),$$

from which it follows that

$$s_\Delta f = S_\Delta f + \sum_{j=0}^{n} \left[\sum_{i=1}^{m} (x_{i+j} - \xi_j)^2/2mf''(\xi_{ij}^*) \right] N_j(x)$$

or

$$| s_\Delta f - S_\Delta f | \leqslant \left\{ \sum_{j=0}^{n} \left[\sum_{i=1}^{m} (x_{i+j} - \xi_j)^2/2m \right] N_j(x) \right\} \| f'' \|.$$

In terms of the mesh gage $\| \Delta \|$ we have

$$\sum_{i=1}^{m} (x_{i+j} - \xi_j)^2/2m \leqslant (m^2 - 1)/24 \, \| \Delta \|^2$$

for all j. Hence,

$$| s_\Delta f(x) - S_\Delta f(x) | \leqslant (m^2 - 1)/24 \, \| f'' \| \cdot \| \Delta \|^2. \qquad \text{Q.E.D.}$$

For Schoenberg's method we know that

$$| S_\Delta f(x) - f(x) | \leqslant (m + 1)/24 \, \| f''(x) \| \cdot \| \Delta \|^2. \tag{14}$$

Using the triangle inequality on (13) and (14), we see that the error in simple variation-diminishing approximation is bounded by

$$| s_\Delta f(x) - f(x) | \leqslant (m^2 + m)/24 \, \| f'' \| \cdot \| \Delta \|^2. \tag{15}$$

Although both methods have the same quadratic order of convergence on the mesh spacing (for C^2 functions), one might expect the Schoenberg method to be generally better (by a factor of $1/m$) and this is born out in a numerical comparison of the two methods (maximum error) on the function $f(x) = e^x$, summarized in Table I. The number of equally spaced knots n and the degree of the spline m is given by the pair (n, m).

The theory of this second kind of variation-diminishing approximation method parallels that of Schoenberg's method. For example, a minor modification of Marsden's proof [4] leads to

THEOREM 3. *Let the $\{x_i\}$ be defined as above and $\{\bar{N}_j(x)\}$ the B-spline basis of degree $m - 2$ on the reduced set of knots $\{ y_i \}$, where $y_i = x_{i+2}$, $i = 0, 1, \ldots, n + m - 3$. Then*

$$\frac{d^2}{dx^2} s_\Delta f = \sum_{j=2}^{n-1} f''(\eta_j) \frac{(x_{j+m} + x_j - x_{j-1+m} - x_{j-1})}{2(\bar{\xi}_j - \bar{\xi}_{j-1})} \bar{N}_j(x),$$

where

$$\bar{\xi}_j = \left(\sum_{i=1}^{m-1} x_{j+i} \right) \Big/ (m - 1) \qquad \text{and} \qquad x_{j-1} < \eta_j < x_{j+m}.$$

The analog of the convergence results for first and second derivatives is

THEOREM 4. *If $f \in C^1[0, 1]$ and m is fixed, then $(d/dx)\, s_\Delta f \to df/dx$ uniformly on $[0, 1]$ as $\| \Delta \| \to 0$. If $f \in C^2\,[0, 1]$ and $x_i = i/n$, then (d^2/dx^2)*

$s_\Delta f \to d^2f/dx^2$ *pointwise in the open interval* (0, 1) and uniformly on compact subsets of (0, 1) *as* $n \to \infty$. *At the ends of the interval,*

$$\lim_{n\to\infty} \frac{d^2}{dx^2} s_\Delta f(0) = (m-1)/2 \frac{d^2}{dx^2} f(0)$$

and

$$\lim_{n\to\infty} \frac{d^2}{dx^2} s_\Delta f(1) = (m-1)/2 \frac{d^2}{dx^2} f(1).$$

As in Schoenberg's method, we have convergence to second derivatives at the end points only for $m = 3$, i.e., the cubic spline case.

The behavior for higher derivatives is very similar. Finally, the analog of the Voronowskaja result for equal knot spacing (cf. [4]) is

THEOREM 5. *If* $f \in C^2[0, 1]$ *and* x *fixed,* $0 < x < 1$, *then*

$$s_N f(x) - f(x) = \frac{m^2+m}{24n^2} f''(x) + o\left(\frac{m^2+m}{n^2}\right). \tag{16}$$

Here, $N = n + 1$ represents the number of knots counting the end points of the interval.

Remarks. If one seeks other linear combinations of B-spline basis functions which lead to "variation-diminishing" approximation methods, it is possible to find many alternative schemes of the form

$$S(x) = \sum_j f(\xi_j)\left(\sum_i w_{ij} N_j(x)\right),$$

i.e., if one fixes the knots in advance. Unfortunately, the $\{\xi_j\}$ and $\{w_{ij}\}$, in general, depend nonlinearly not only on the number and locations of the knots, but also on the degree of the spline. Exceptions to this are the iterates of these variation-diminishing methods, e.g., $S = S_\Delta(S_\Delta f)$, $S = S_\Delta(S_\Delta(S_\Delta f))$, etc. However, the two schemes above seem to be the most natural ones that can be devised of this genre.

3. EXTRAPOLATED APPROXIMATION

To motivate this section, we first consider Schoenberg's variation-diminishing approximation method of degree m with $N - 2$ equally spaced interior knots. Then $S_N f(x) = f(x) + E(x)$, where

$$E(x) = (m+1)/24n^2 f''(x) + o((m+1)/n^2). \tag{17}$$

The form of the error in (17) first suggested to us the application of the familiar Richardson extrapolation technique as it is ordinarily used throughout numerical analysis to speed up the convergence of a numerical process. Namely, computing two variation-diminishing approximations for different numbers, N_1 and N_2, of equally spaced knots, we take that linear combination which has the term involving $f''(x)$ eliminated from the error of approximation to $f(x)$. Specifically, with $n_1 = N_1 - 1$ and $n_2 = N_2 - 1$, this formula is given by

$$S_{N_1,N_2}f(x) \equiv (n_2^2 S_{N_2}f(x) - n_1^2 S_{N_1}f(x))/(n_2^2 - n_1^2). \tag{18}$$

Because of (16) one can do the same thing with the simple diminishing method; in fact, the same linear combination eliminates the $f''(x)$ term:

$$s_{N_1,N_2}f(x) \equiv (n_2^2 s_{N_2}f(x) - n_1^2 s_{N_1}f(x))/(n_2^2 - n_1^2). \tag{19}$$

Although of some practical interest we abandon these methods in favor of a better one. Guided by the above idea we can also eliminate the $f''(x)$ term by simply combining the two variation-diminishing schemes. From (16) and (17) we obtain the formula

$$T_N f(x) \equiv (mS_N f(x) - s_N f(x))/(m - 1). \tag{20}$$

We regard (20) as the natural extrapolated method for a variety of reasons. First, the knots of the resulting mth-degree spline are the same as in each of the terms, whereas (18) and (19) involve splines with different knots. More importantly, (20) reproduces quadratics and, relatedly, has higher-order convergence properties in function value and the first two derivatives. Finally, the same linear combination is valid for arbitrary knot spacing. We now consider this latter method, i.e.,

$$T_\Delta f(x) \equiv (mS_\Delta f(x) - s_\Delta f(x))/(m - 1). \tag{21}$$

As one might expect, the natural tools to use in the general case are the relations obtained from the Marsden identity connecting the B-spline basis with ordinary polynomials [4], namely:

$$\begin{aligned} 1 &\equiv \sum_{j=0}^{n} N_{j,m+1}(x), \\ x &\equiv \sum_{j=0}^{n} \xi_j N_{j,m+1}(x), \\ x^2 &\equiv \sum_{j=0}^{n} \xi_j^{(2)} N_{j,m+1}(x), \\ &\vdots \qquad \vdots \qquad \vdots \end{aligned} \tag{22}$$

where

$$\begin{aligned} \xi_j &= \sum_{i=1}^{m} x_{j+i}/m, \\ \xi_j^{(2)} &= \sum_{i<k} x_{j+i}x_{j+k}\Big/\binom{m}{2}, \\ &\vdots \qquad \vdots \quad \vdots \end{aligned} \tag{23}$$

etc. As noted above, either Schoenberg's method or the simple spline variation-diminishing method are both immediately derivable by considering the first two relations. It is a trivial matter to see that the formula in (21) satisfies the first three relations using the algebraic identity

$$\left[m\left(\sum_{i=1}^{m} y_i/m\right)^2 - \sum_{i=1}^{m} y_i^2/m\right]\Big/(m-1) = \sum_{i<j} y_i y_j\Big/\binom{m}{2}, \tag{24}$$

valid for all $m \geqslant 2$. Hence, when $f(x) = a + bx + cx^2$, $T_\Delta f(x) \equiv f(x)$.

THEOREM 6. *If* $f \in C^i[0, 1]$ *and* $m \geqslant 2$, *then* $(d^i/dx^i)\, T_\Delta f \to d^if/dx^i$ *uniformly on* $[0, 1]$ *as* $\| \Delta \| \to 0$ *for* $i = 0, 1, 2$.

Proof. For $i = 0, 1$ one can relate this directly to the established convergence behavior of the functions $S_\Delta f$ and $s_\Delta f$. For $i = 2$ a more detailed proof as found in [4] may be constructed. Specifically, one can show

$$(d^2/dx^2)\, T_\Delta f(x) = \sum_{j=2}^{n} A_j \bar{N}_j(x), \tag{25}$$

where $B_j = (m-1)(\bar{\xi}_j - \bar{\xi}_{j-1})\, A_j$ is given by

$$\begin{aligned} B_j = m[&(f(\xi_j) - f(\xi_{j-1}))/(\xi_j - \xi_{j-1}) - (f(\xi_{j-1}) - f(\xi_{j-2}))/(\xi_{j-1} - \xi_{j-2})] \\ &- [(f(x_{j+m}) - f(x_j))/(x_{j+m} - x_j) - (f(x_{j+m-1}) - f(x_{j-1}))/(x_{j+m-1} - x_{j-1})]. \end{aligned}$$

For C^2 functions A_j is simply an elaborate finite difference approximation to $f''(\bar{\xi}_j)$, i.e., $A_j = f''(\bar{\xi}_j) + \theta_j$ with θ_j bounded in terms of the modulus of continuity of $f''(x)$, e.g., $|\theta_j| \leqslant \omega(f'', (m+1)\|\Delta\|)$. With this interpretation it is a short step from (25) to the proof of uniform convergence in the second derivative as $\|\Delta\| \to 0$. For smoother functions, for example, those where the second derivative is Lipshitz continuous, the above results can be sharpened to: $T_\Delta^i f(x) \to f^i(x)$ with a rate of convergence given by $\|\Delta\|^{3-i}$, $i = 0, 1, 2$.

Remarks. For equally spaced knots the uniformity of convergence to second and higher derivatives breaks down at the end points of the interval for either variation-diminishing method. In the extrapolated approximation these phenomena begin with the third and higher derivatives. This is of interest because many applications require the approximation method to have the ability to represent data faithfully up through curvature. For example, in computer-aided design-related applications the merits of a fitted curve are often judged visually and curvature behavior is not only observable, but may be a crucial criterion. This is especially true if such a curve is to represent a highly stylized physical shape. On the other hand, there are strictly physical applications where first and second derivatives of an approximation, e.g., to experimental data representing a physical variable, are considered important and useful quantities (such as estimates of velocity and acceleration from displacement data). In these cases the behavior of higher-order derivatives ($\geqslant 3$) are much less relevant. Although the variation-diminishing spline approximation methods have a number of desirable overall shape-preserving and -smoothing properties, they are theoretically unable to approximate accurately the curvature of the data or function (except for $m = 3$). The above modification is intended and recommended as a practical compromise between the legitimate variation-diminishing methods and the many kinds of higher-order spline methods developed over the past several years which, typically, exhibit uniform convergence in all derivatives up to and including the degree of the spline. We call the reader's attention to the fact that this method consists of $m/(m-1)$ parts Schoenberg's method minus $1/(m-1)$ part of a comparable spline variation-diminishing approximation. In practice, at least for large enough m, we expect many of the qualitative difference between it and Schoenberg's method to disappear.

4. Numerical Example

Table I illustrates the behavior of the maximum error for the three approximation methods applied to the function $f(x) = e^x$ on $[0, 1]$. The pair (n, m) represents the number of equally spaced knots and the degree of the spline, respectively. For smooth functions these results are typical and predictable from the theory. Comparison plots of these methods (cf. [6]) indicate that the extrapolated method is much more effective than either variation-diminishing method in accurately representing the function together with its first two derivatives on the whole interval.

5. Modified Bernstein Polynomial Approximation

We conclude this paper with a special case of the extrapolated spline approximation method that we have introduced, namely, the case of no interior knot. Set $0 = x_0 = x_1 = \cdots = x_{m-1}$ and $1 = x_m = x_{m+1} = \cdots =$

TABLE I

(n, m)	E_S	E_s	E_T
(2, 2)	0.108	0.212	0.014
(2, 3)	0.072	0.212	0.0096
(2, 4)	0.054	0.212	0.0072
(2, 5)	0.044	0.212	0.0058
(2, 10)	0.022	0.212	0.0029
(2, 15)	0.015	0.212	0.0019
(3, 2)	0.052	0.108	0.0031
(3, 3)	0.047	0.142	0.0024
(3, 4)	0.040	0.59	0.0028
(3, 5)	0.034	0.70	0.0028
(3, 10)	0.020	0.191	0.0021
(3, 15)	0.014	0.198	0.0016
(4, 2)	0.027	0.055	0.00091
(4, 3)	0.030	0.092	0.00079
(4, 4)	0.030	0.119	0.00125
(4, 5)	0.028	0.137	0.00157
(4, 10)	0.018	0.174	0.00163
(4, 15)	0.013	0.187	0.00135
(5, 2)	0.017	0.033	0.00038
(5, 3)	0.019	0.058	0.00036
(5, 4)	0.021	0.085	0.00054
(5, 5)	0.021	0.108	0.00081
(5, 10)	0.016	0.159	0.00126
(5, 15)	0.012	0.177	0.00115
(10, 2)	0.0037	0.0075	0.000035
(10, 3)	0.0046	0.0139	0.000032
(10, 4)	0.0054	0.0218	0.000055
(10, 5)	0.0062	0.0310	0.000078
(10, 10)	0.0088	0.0884	0.000257
(10, 15)	0.0086	0.1284	0.000489
(15, 2)	0.0016	0.0032	0.000011
(15, 3)	0.0020	0.0061	0.000007
(15, 4)	0.0024	0.0098	0.000011
(15, 5)	0.0028	0.0141	0.000018
(15, 10)	0.0044	0.0441	0.000065
(15, 15)	0.0055	0.0827	0.000150

x_{2m-2}. Then Schoenberg's method reduces to the ordinary Bernstein polynomial approximation of degree m, $B_m f(x) = \sum_{\nu=0}^{m} \binom{m}{\nu} f(\nu/m)\, x^\nu (1-x)^{m-\nu}$. Simple variation-diminishing spline approximation specializes to the straight line joining the end points of the function; $L(x) = f(0)(1-x) + f(1)\,x$. Therefore, the extrapolated approximation is of the form $T_m f(x) = (mB_m f(x) - L(x))/(m-1)$, also a polynomial of degree m. Although others (e.g., [1]) have considered linear combinations of Bernstein polynomials which have higher-order convergence properties, this slight modification of the ordinary Bernstein approximation may be new. Although not variation diminishing, it is partially shape preserving in the sense that it preserves convexity and strict convexity. From Voronowskaja's theorem,

$$\lim_{m\to\infty} (m-1)(T_m f(x) - f(x)) = (x(1-x)/2) f''(x) + f(x) - L(x), \quad (26)$$

which can be rewritten in mean value form as

$$\lim_{m\to\infty} (m-1)(T_m f(x) - f(x)) = (x(1-x)/2)(f''(x) - f''(\xi_x)), \quad (27)$$

where $0 < \xi_x < 1$. The rate of convergence to $f(x)$ is the same as that of $B_m f(x)(o(1/m))$. However, since it reproduces quadratics, one can often expect $T_m f(x)$ to be a better approximation, particularly for smooth functions. For $f(x) = e^x$ on $[0, 1]$ we see from Table I (entries $(2, m)$) that the computed maximum error is consistently 0.13 of the maximum error in the classical case.

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