A note on numerical procedures for approximation by spline functions

by Ian Barrodale and Andrew Young*

A spline function is a piecewise polynomial of degree m joined smoothly so that it has m-1continuous derivatives. When used as an approximating function the spline provides a smooth yet flexible curve of relatively low degree.

The purpose of this note is to show how standard numerical procedures can be used without change to calculate the best (L_1 and L_∞) spline approximation, of given degree and joints, to a discrete point set.

Introduction

Definition. $S_{m, k}(x)$ is a spline function of degree m with joints at $x_1 < x_2 < \ldots < x_k$ if and only if it possesses the following two properties:

- (a) $S_{m,k}(x)$ is a polynomial of degree m in each of the intervals $(-\infty, x_1), [x_1, x_2), \ldots, [x_k, \infty)$. (b) $S_{m, k}(x) \in C^{m-1}$ i.e. it has continuous derivatives
- up to order m 1.

The set of splines of a given degree and with given joints is closed under addition and subtraction, while integration (differentiation) converts a spline into another spline with the same joints but of the next higher (lower) degree. The spline avoids the discontinuities in slope that occur with ordinary piecewise polynomials, while the relaxation of the requirement of continuity in the mth derivative allows it flexibility.

In the theory of interpolation the use of piecewise polynomials predates Newton. The restriction to smooth jointed interpolation formulae appeared in actuarial literature of the 19th century under the heading of osculatory interpolation. This appears to have been first introduced by Sprague (c. 1880); an example is provided by Hermite's interpolation formula. Further development in methods of osculatory interpolation, including the derivation of a smoothing formula which interpolates by means of spline functions, was undertaken by Jenkins (1927). However, the term "spline functions" was introduced some twenty years ago by Schoenberg to whom credit is due for much of the recent study of their properties.

Much interest has been centred on the role of the spline as an interpolating function, where it is required to fit a set of data points exactly. Necessary and sufficient conditions have been given by Schoenberg and Whitney (1953) for a spline $S_{m,k}$ to interpolate an arbitrary set of m + k + 1 points. In addition to some numerical interpolation procedures, Greville (1964) discusses the case where the given data points coincide with the joints of a spline function and there are m + 1 special conditions imposed.

There exists a unique cubic spline S, with k joints x_i contained in an interval [a, b], possessing the following minimal property: among all $f \in C^2[a, b]$ which interpolate a given function F at the points x_i the integral $\int_{0}^{0} [f''(x)]^{2} dx$ is minimized by S. Further properties of cubic splines and periodic splines are given by Walsh, Ahlberg and Nilson (1962), extensions to odd degree splines by De Boor (1963), and to splines of arbitrary degree by Schoenberg (1964).

The term elementary spline functions has been given to functions of the type $(x - a)^m_+$ where, for any real constant a.

$$(x-a)_+^m = \begin{cases} (x-a)^m & \text{if } x \ge a \\ 0 & \text{if } x < a \end{cases}$$

The *m*th derivative of an elementary spline function is m! H(x - a), where H is the Heaviside function. The mth derivative therefore has a discontinuity at x = a, where there is a step of m!. The suitability of these functions for the representation of any spline function was noted by Schoenberg and Whitney (1953). Every spline function can be represented uniquely as the sum of a polynomial and a linear combination of elementary spline functions.

Thus,
$$S_{m,k}(x) = P_m(x) + \sum_{i=1}^k c_i (x - x_i)_+^m$$
 (A)

where P_m is a polynomial of degree *m*, and the product of c_i and m! gives the step in the mth derivative of $S_{m,k}(x)$ at the *i*th joint.

The following result from the theory of Chebyshev approximation by spline functions involves monosplines (for which there is an analogue of the fundamental theorem of algebra (Schoenberg (1958)) and also (Schoenberg (1965)) a one-one correspondence with quadrature formulae). A monospline of degree m with joints $x_1 < x_2 < \ldots < x_k$ is a function M of the form

$$M_{m,k}(x) = x^m + S_{m-1,k}(x)$$

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where S is a spline function of degree m-1 with the same k joints. Johnson (1960) has proved that for all values of m and k satisfying $m \ge 1$ and $k \ge 0$, there exists a unique monospline $M_{m,k}^*$ which deviates least from zero on [-1, 1]. Clearly the Chebyshev polynomial $T_m = M_{m,0}^*$.

When the joints are specified splines and monosplines are linear approximating functions. Moreover, the representation (A) allows best approximations to be easily computed using existing algorithms.

Numerical procedures

The L_1 and L_{∞} (or Chebyshev) linear approximation problems for a discrete point set were stated as follows by Barrodale and Young (1966).

Given a function f(x) defined on $X = \{x_1, \ldots, x_N\}$ and an approximating function $F(A, x) = \sum_{j=1}^{n} a_j \phi_j(x)$, determine

- (i) $\min_{A \in E^n} \sum_{x \in X} |F(A, x) f(x)|$ (L₁ problem)
- (ii) $\min_{A \in E^n} \max_{x \in X} |F(A, x) f(x)|$ (L_{∞} problem)

Both were restated as problems in linear programming, and in either case the structure of the resulting matrix of coefficients allows the simplex algorithm to be used on a condensed tableau. We supplied the ALGOL procedures *MINSUMMOD* and *MINMAXMOD* which perform all the necessary computations.

In view of the representation (A) it is obvious that a spline $S_{m, k}$ is a linear approximating function. Using the above notation

$$F(A, x) = \sum_{j=1}^{n} a_{j}\phi_{j}(x) = \sum_{j=1}^{m+1} a_{j}x^{j-1} + \sum_{\substack{i=m+2\\j=m+2}}^{m+k+1} a_{j}(x-x_{j-m-1})^{m}_{+}$$

We can therefore determine best approximations by splines $S_{m, k}$ using the procedures *MINSUMMOD* and *MINMAXMOD* unaltered. The storage space is the same as for a polynomial of degree m + k, while numerical experiments we have done show that frequently less computing time is needed for the spline approximations.

Comments

Fig. 1 is an example of spline approximations to a function with a discontinuous first derivative. The function f(x) was defined by 41 values of |x| for $x = -2(0 \cdot 1)2$. It has been approximated in both norms by a cubic spline with one joint at x = 0. These best approximations are symmetric to the y axis and only part of the complete graph is shown.

The choice of number and position of joints for any particular set of data is based on experience and intuition,

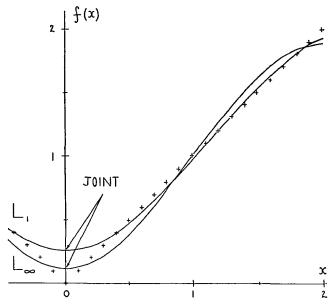


Fig. 1.—A section of the graph of best L_1 and L_∞ cubic spline approximations, with one joint at x = 0, to f(x) = |x| for x = -2(0.1)2 (indicated by +'s)

for, as Rice (1964) remarks, "the problems associated with the 'best joints' have not been investigated to any extent". For the set of data shown in Fig. 1 it is obvious that x = 0 is a good joint for an ordinary piecewise approximation, but perhaps a bad point at which to insist on continuous first and second derivatives. From empirical evidence it appears that the cubic spline with one joint at x = 0 gives a better L_{∞} approximation than any other cubic spline with one joint, or two joints (neither at x = 0), or even four joints where no joint is close to x = 0.

If a good choice of joints has been made then close spline approximations of low degree are often possible. Control of round-off error is a resulting practical advantage. A theoretical disadvantage of spline approximation arises because we are not dealing with Chebyshev sets. This does not affect the existence of best approximations, but can affect both uniqueness and characterization in the L_{∞} norm. See Rice (1964).

The requirement that a spline $S_{m,k}$ has all of the first m-1 derivatives continuous may be too stringent. In fact for a given function f(x), a spline $S_{m,k}$ may provide a better approximation than a spline $S_{m+1,k}$, where both splines have the same k joints. In practice it may be desirable to insist on continuity in only the first and second derivatives (say) but to use an approximating function of greater degree than the cubic. A "weak-spline" function of the form $F_{m,k,p}$, where

$$F_{m, k, p}(x) = P_m(x) + \sum_{i=1}^k c_i (x - x_i)_+^p$$
 where $p < m$

would provide a sequence of functions which (for given k joints and fixed p) has a monotonic decreasing error

of approximation with increasing m. These approximations can again be computed by using MINSUMMOD and MINMAXMOD without alteration.

Thus these algorithms provide adequate means of obtaining splines and similar approximations without recourse to special computing methods.

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Correspondence

To the Editor. The Computer Journal.

Sir,

Papers by Parker and Crank (1964) and Keast and Mitchell (1966) have recently considered the stability of Crank and Nicolson's procedure (Crank and Nicolson, 1947) for solving the parabolic partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

with u(x, 0) = f(x), $0 \le x \le 1$, and with boundary conditions

$$a_0 \frac{\partial u}{\partial x} + b_0 u = \lambda_0(t); x = 0, t > 0$$
$$a_1 \frac{\partial u}{\partial x} + b_1 u = \lambda_1(t); x = 1, t > 0.$$

Their results conceal what is an essentially simple situation. Consider the preparation of (1) for solution by a computer in the two following stages:

(a) The right-hand side of (1) is replaced by a suitable difference scheme in Δx , and the boundary conditions are incorporated to give (cf. Parker and Crank, 1964)

$$\dot{w} = \frac{1}{(\Delta x)^2} \left[-Uw + l \right]; w(0) = c$$
 (2)

where w(t) is a vector with N + 1 components approximating the value of u(x, t) at $x = 0, \Delta x, 2\Delta x, \dots, N\Delta x$. The

physics of the problem can be a valuable guide at this stage: indeed it is safest to set up (2) directly from a discrete physical model (see Rosenbrock and Storey, 1965, pp. 8-15).

(b) The time derivatives in (2) are replaced by a difference scheme to give (cf. Parker and Crank, 1964)

$$v^{n+1} - v^n = r\{\theta[-Uv^{n+1} + l^{n+1}] + (1-\theta)[-Uv^n + l^n]\}$$
(3)
$$[I + r\theta U]v^{n+1} = [I - r(1-\theta)U]v^n + k^n; v^0 = c$$
(4)

where v^n approximates $w(n\Delta t)$ and $r = \Delta t/(\Delta x)^2$. So far as this stage is concerned we have the following simple result:

If (2) is stable (resp. asymptotically stable), and if $\frac{1}{2} \le \theta \le 1$, r > 0 [or if $0 \le \theta < \frac{1}{2}$ and $0 < r \le 1/(\frac{1}{2} - \theta)\lambda_{max}(U)$] then (4) is stable (resp. asymptotically stable).

Thus all the real difficulties regarding the stability of (4) are associated with stage (a), which belongs to the physical formulation of the problem rather than to Crank and Nicolson's procedure. Of course if (2) is unstable (or stable but not asymptotically stable) we have no right to expect (4) to be stable (or asymptotically stable).

To prove the result stated it is only necessary to write

$$c = \sum_{i=0}^{N} \alpha_i z_i \tag{5}$$

$$Uz_i - \lambda_i z_i = 0 \tag{6}$$

(Continued on p. 324)

where