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NONLINEAR REGRESSION WITH EMPHASIS ON SPLINE METHODS

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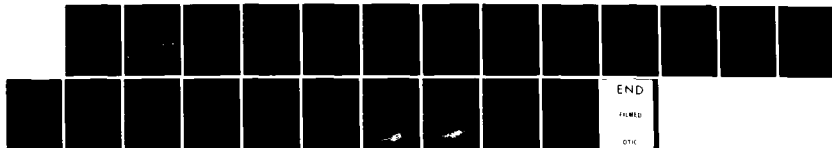
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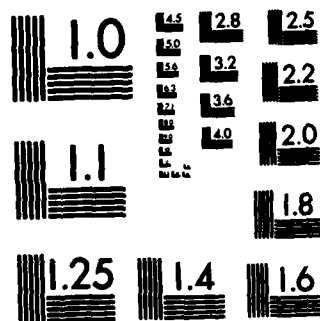
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Spline functions with variable knots have been very useful in nonlinear regression and approximation. For example, shape-preserved curve fitting can be adjusted to give optimal degree of approximation, and uniqueness, computational methods etc. have also been studied. To further investigate the local behavior of best approximants, the idea of best local approxi- mation was introduced. This relates the original problem to three important areas of research, namely: Padé approximants, recursive digital filter		

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20. (continued)

realization, and certain minimax approximation problems. In order to give meaningful investigation into these areas, techniques from Functional Analysis and Operator Theory have been used, and related but quite general results on Approximation Theory have also been found. In studying multi-variable regression, it was noted that tensor-product splines have very limited applications. Hence, basic theory and results concerning dimensions, bases, B-splines, interpolation, etc. on bivariate, and sometimes multi-variate, non-tensor product splines have been obtained.



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Nonlinear Regression With
Emphasis on Spline Mehods

FINAL REPORT

by

CHARLES K. CHUI

(in cooperation with P. W. Smith and J. D. Ward)

Aug. 2, 1984

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I. List of manuscripts submitted or published under ARO sponsorship.

- 1976 [1] C. K. Chui, P. W. Smith, and J. D. Ward, On uniqueness of piecewise polynomial approximation. 21st Conf. of Army Math., Vol. 76-I (1976), pp. 141-147.
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BRIEF OUTLINE OF RESEARCH FINDINGS

During the period supported by ARO Grant and Contract Numbers DAHC04-75-G0186, DAAG 29-78-G-0097, and DAAG 29-81-K-0133, we have obtained many results in the area of Nonlinear Regression with emphasis on Spline Methods. Our results have been published (or will be published) as listed on pages 1-4. In order to avoid redundancy, this list will also be used as references to this outline of research findings. Many of the results that have been reported in our Semi Annual Progress Reports will not be repeated here. Only some of the most important results are outlined. These results can be roughly divided into five areas.

1. Splines in nonlinear regression and approximation

Our first result in this direction is the study of how smooth are best (least-squares) splines approximants with a fixed number of (variable) knots when the data functions they approximate belong to some smoothness class. These results appeared in 1977 [1]. We proved, for example, that if the data function is continuous, then all best spline approximants (with n knots, say) are also continuous and, however, there exists an infinitely differentiable function which has no twice continuously differentiable best L_2 (or least-squares) spline approximants with n (variable) knots. The (first) continuously differentiable case is not yet settled.

We next considered the uniqueness problem of best L^2 approximation from second order spline manifolds with n (variable) knots. The main results appeared in 1977 [4] and 1978 [4]. We proved, for example, that if the data function f is strictly convex with concave $\log f''$, then there is uniqueness, and that there is no uniqueness if the concavity condition on $\log f''$ is omitted. We also introduced the idea of eventual uniqueness and proved that "eventually" (i.e. for sufficiently many knots) we do not require the concavity condition to guarantee uniqueness. Our results here have been generalized by our Ph.D. student Jeff Chow in his Ph.D. thesis ([5]).

One advantage that families of spline functions possess over other approximating manifolds arises from the nonlinear parameters (the knots) which can be concentrated in regions of somewhat complex structure of a function to be approximated. This had been recognized by de Boor and his student Dotson who developed heuristics to obtain an asymptotically optimal solution to an ordinary differential equation using collocation and knot redistribution. Our papers 1978 [5] and 1982 [3] represented the culmination of our research into the asymptotic behavior of best approximating splines with free knots. These results put the de Boor-Dotson work on a firm foundation. Perhaps surprisingly, the asymptotically optimal knot distribution is the same for splines as it is for (discontinuous) piecewise polynomials. Of course, the approximation rate is the same but the constants are different. The major result may be stated as follows. Let $E(n,k,p,f)$ be the L_p error ($1 \leq p < \infty$) of best approximation to a function $f \in C^k[0,1]$ (this smoothness assumption

can be weakened) from the C^{k-2} splines of order k with n variable knots. Then as $n \rightarrow \infty$ we have $n^k E(n, k, p, f) \rightarrow J(k, p, f^{(k)})$. Furthermore, we can exhibit an increasing function t depending on $f^{(k)}$ so that if we approximate by splines of order k (in C^{k-2}) with knots at $\{t(i/N)\}_{i=0}^N$, the error in best L_p approximation $E(n, k, p, f, t)$ satisfies $n^k E(n, k, p, f, t) \rightarrow J(k, p, f^{(k)})$.

Another area on nonlinear regression with emphasis on spline manifolds is shape-preservation approximation with optimal (i.e. Jackson) degree of approximation. Our results in this direction appeared in 1980 [2] and 1980 [4]. We extended DeVore's result in S[11] to all L_p spaces, $1 \leq p \leq \infty$, and gave an elementary and constructive proof. Our method of proof is now considered very important by others and has been used by many authors, including R. Beatson, D. Leviatan, H. N. Mhaskar, in obtaining various constraint approximation results.

2. Best local approximation, Padé approximants, and digital filters

In studying splines or piecewise polynomials with many knots, (or break-points) one is quickly lead to the problem of best approximation on ever decreasing intervals. We call this best local approximation. When rational functions are considered, J. L. Walsh (S[14], S[15]) already related this problem to Padé approximants. In S[10] (see also 1976 [2] in S[1]), we introduced the notion of best local approximation and in 1978 [1] we discovered various results in the L^2 setting. A detailed study was given by our student L. Y. Su in S[13]. For two and more points, the

best local approximation results for L^∞ were discovered in 1981 [1]. We noted in particular that this leads to a minimax approximation problem. We also conjectured that this would hold for any number of points, and this conjecture was recently confirmed in the L^p , $1 < p \leq \infty$, setting in S[9]. The multidimensional results hold analogously as shown in S[8] and S[9].

Since best local approximation relates to Padé approximants, we were lead to study problems in the later area. In 1977 [3], we introduced this idea to digital filter designs. Unfortunately, there was no guarantee on stability. A least-squares inverse studied in 1980 [3] now guarantees stability, or a two-sided approximation scheme (see 1977 [3] and S[4]) followed by certain all-pass filter also gives stability. To approximate the phase we introduced the ε -Herglotz transform which, together with methods from Approximation Theory, give very good results (cf. S[7]).

The design discussed above was studied in the frequency domain. In real-time tracking, it is more convenient to work in the time domain. Following the suggestions of Mr. W. L. Shepherd and Mr. R. E. Green, we studied the α - β - γ filter using limits of the Kalman gains and characterized limiting (or near) optimality. White noise processes were considered in S[6] and recently, in 1984 [11], we generalized the results in S[6] to the color input setting. This avoids the singularity as possibly encountered in the (colored noise) Kalman filtering.

Since ideal digital filter characteristics are piecewise linear functions, and in most applications, consist only of the pass and stop bands, these characteristics can easily be smoothed to C^∞ functions. The approximation order of such functions by rational functions (i.e.

filter realization) with all poles lying outside the unit circle (for stability) have now been obtained in 1984 [9]. In addition, the order of approximation by least-squares inverses which give an all-pole filter with guaranteed stability is also given in 1984 [9].

In another direction, the order of polynomial (FIR filters) approximations on two disjoint intervals (i.e. two pass bands) was studied in 1983 [5]. This study, however, was restricted to the real case only.

3. Applications of functional analysis and operator theory.

The topics in this section include approximation by minimum norm interpolants in the disc algebra, factorizations of operators, constrained approximation in L_p and certain properties of Toeplitz operators. In 1979 [2], we considered the problem of minimum norm interpolation in the disc algebra and obtained certain rates of convergence. The main result there can be stated as follows. Let $f \in A$ (the disc algebra) and let E_N , $N = 1, 2, \dots$ be closed subsets of the unit circle of measure zero such that $\gamma_N = \log(\|f\|_T / \|f\|_{E_N}) \rightarrow 0$. Then there exist minimal norm interpolants s_N of f satisfying $(f - s_N) \in M_N \equiv \{g \in A: g(E_N) = 0\}$ such that $\|f - s_N\| = O(\gamma_N)$. Moreover, this rate of convergence is sharp in the sense that $O(\gamma_N)$ cannot be replaced by $o(\gamma_N)$.

Papers 1982 [1], 1983 [10] and 1984 [5] deal with LU factorizations of invertible operators on certain Banach spaces. In 1983 [10], a cholesky factorization for positive definite bi-infinite matrices was presented. Applications to block Toeplitz matrices, signal processing and

spline interpolation are then derived. As a sample application, consider the following problem in spline interpolation. Let $\underline{t}$ be a bi-infinite partition of the real line which is periodic of order r . Consider the problem: find $s \in S_t^{2k} \cap L_\infty$ so that $s(t_i) = x_i$, $-\infty < i < \infty$ with $\|x\|_\infty < \infty$. We showed that the subspace of splines vanishing at all knots has a basis of exponentially growing (or decaying) splines and hence derive de Boor's result that the above interpolation has a unique solution. In another direction it was shown that column diagonally dominant invertible matrices A admit LU factorizations and that L and U are (strong) limits of the factorizations of the compressions of A . It was also shown that Gauss elimination performed on a matrix "enhances" its diagonal dominance. Finally in 1984 [3], we solved a class of constrained optimization problems which lead to algorithms for the construction of convex interpolants to convex data.

In 1981 [2] and [3], a factorization theorem for strictly m -banded totally positive matrices was derived. It was then shown that such a matrix is a product of m one-banded matrices with positive entries. Also for a certain class of block Toeplitz matrices, the smallest sector containing the zeros of the determinant for the corresponding symbol is identified. In 1984 [2] the null space of banded bi-infinite block Toeplitz matrices is determined in terms of the Kronecher canonical form. In 1984 [4], decay rates for inverses of band matrices are obtained. The rates are faster than exponential decay. We also remark that in 1983 [11] in S[3] a compendium of recent developments of infinite dimensional numerical linear algebra is given, most of the matrix problems dealt with arose from the study of spline interpolation on biinfinite meshes.

4. General Approximation Theory

In order to study various aspects of nonlinear regression (with emphasis on spline methods), we had to develop new directions and obtain related results in other areas of Approximation Theory.

Perhaps the most significant result here is the so-called "Problem of G. G. Lorentz." We solved this problem in 1978 [2], and even generalized this result in 1978 [6] and 1980 [5] in S[2]. The idea was based on the belief that "like best approximates like" and tells us which subspace should possibly be used for the best result in approximation. It has application to antenna design, by indicating the best location to place antennas for better performance. We also applied this idea in 1980 [1] to approximate derivatives from function values and proved its equivalence to approximation of one B-spline by linear combinations of others.

Another area is inverse approximation. The basic results were obtained in 1980 [3] and 1982 [5]. Various research problems were posed in 1980 [6] in S[2]. One application is to give an efficient design of a stable realizable digital filter, and another application is to give an all-pass filter which is used to stabilize not necessarily stable recursive digital filters.

The third area is approximation on disjoint intervals. The results we obtained 1983 [5] cannot be proved by using one-interval approximation results, showing that much research is needed in this area. Of course there are applications to design digital filters with more than one pass-bands.

As discussed in Section 2, we also introduced the idea of best local approximation in trying to understand local behaviors of splines with many knots.

5. Development of multivariate splines

Perhaps the most exciting recent development in Approximation Theory is Multivariate splines. This view is commonly shared by many leaders in the field, including Professor G. G. Lorentz (see S[12] p. 4111 of the Introduction: Approximation and Interpolation in the last 20 years). (Univariate) splines have proved to be extremely useful in the last two and a half decades in all applications in Engineering and Physical and Biological Sciences that require data analysis. For problems in higher dimensions, tensor-product splines (i.e. splines as linear combination of tensor-product B-splines) have been used. However, as all users would soon find out that such applications are not only restrictive (since rectangular grids are required), their utility is also limited due to the large number of parameters (since coordinate degrees are too high, for instance). So, multivariate splines which are non-tensor product splines are required. We have now many contributions in this area (for instance, see 1982 [6], 1983 [1], [2], [3], [4], [6], [7], [8], [9] and 1984 [1], [6], [7], [8], and [12]), and most our results have been reported in the previous Semi-annual Progress Reports. In this final report, we would like to report only those results not reported earlier.

In the paper 1984 [12] that will appear in the Proceedings of the Second Army Conference on Applied Mathematics which took place in May, 1984, we have shown that bivariate C^1 cubic B-splines have very unusual behaviors, and in general require very large supports. So to study scattered data, it is advisable to use higher degree bivariate C^1

splines. We have recently shown that the lowest degree for the existence of splines with one interior grid-point support for an arbitrary triangulation is four, and that degree four is, however, not useful for Lagrange-typed interpolation. Hence, we looked into bivariate C^1 splines with total degree five and have constructed all locally supported splines on an arbitrary triangulation. Using these splines, we can choose arbitrary subspaces for interpolation and approximation purposes. For instance, if only the function and first partial derivative values of the actual function in Fig. 1 are given at the sample points in Fig. 2, we have constructed the approximating surface shown in Fig. 3 by using three locally supported splines around each sample point in the Hermite interpolation process. The order of approximation can be proved to be at least two. We are still improving our techniques in this direction. We mention, in passing that there are important applications to image processing, data reduction, image enhancement, etc.

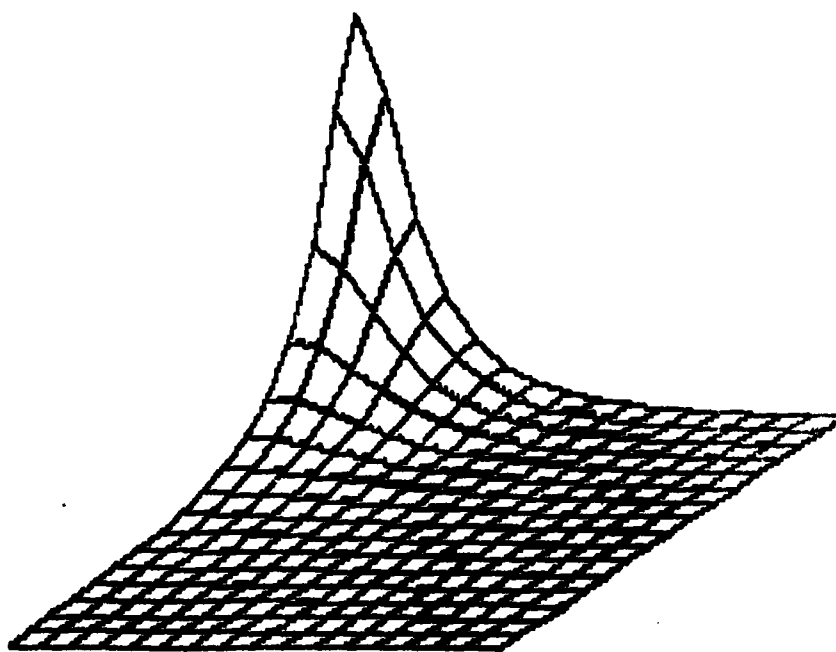


Fig. 1 (Actual function)

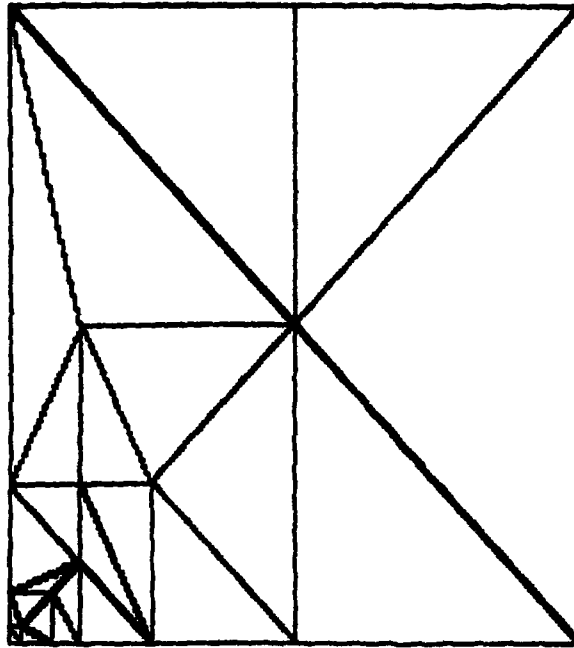


Fig. 2 (Sample points at vertices of all triangles)

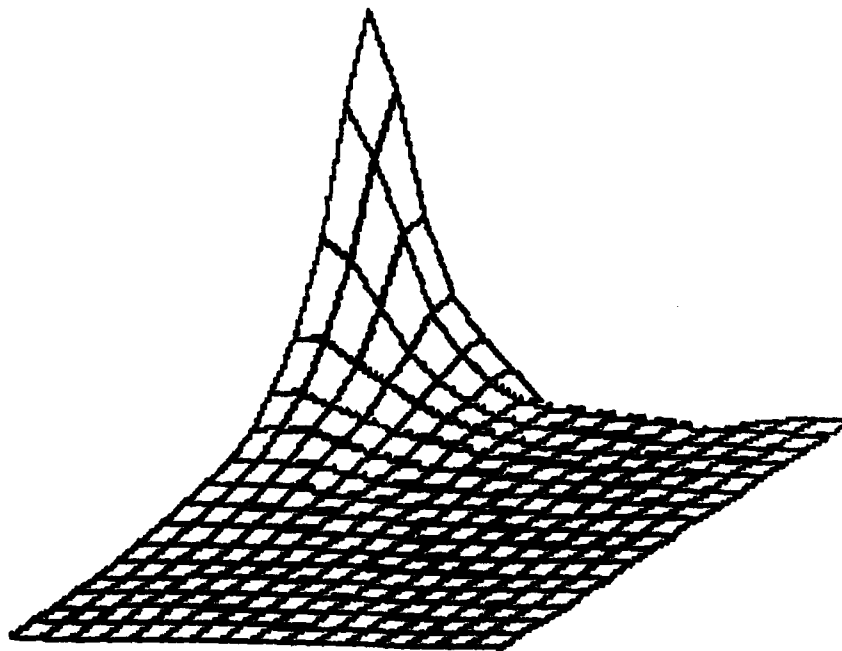


Fig. 3 (Approximate surface)

REFERENCES

The list of manuscripts submitted or published under ARO sponsorship on pages 1-4 is used for references. In addition, the following books and papers are also mentioned in this report.

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