An adaptive curve fitting algorithm for one dimensional data sets is developed and tested. This algorithm is a modification of two earlier curve fitting packages using the least squares (L2) or the L1 approximation operator. This new algorithm performs a look ahead strategy in the "backing off" routine for locating the knots joining the polynomial approximating pieces.
AN ADAPTIVE PIECEWISE CURVE-FITTING PACKAGE USING A LOOK-AHEAD STRATEGY

by

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1. **Introduction**

This paper presents an adaptive curve fitting algorithm based upon a look-ahead strategy. This algorithm is a modification of two earlier curve fitting packages. In the first section a discussion of the capabilities of the original routines is given and in the second section the new adaptive algorithm is described. The last section of the paper presents some numerical testing results.

2. **Original \( \ell_1, \ell_2 \) Packages**

In [1], a FORTRAN program is given which computes a smooth piecewise polynomial approximation, \( p \), to a finite one-dimensional data set \( \{(x_i, y_i)\}_{i=1}^m \) using the least squares (\( \ell_2 \)) or the \( \ell_1 \) approximation operator. In order to describe these algorithms it is convenient to use a functional notation. Thus, let \( X = \{x_i\}_{i=1}^m \) and \( f \) be the function defined on \( X \) by \( f(x_i) = y_i, \ for \ i = 1, \ldots, m \). Let \( a = \min\{x: x \in X\} \) and \( b = \max\{x: x \in X\} \) and, for any function \( g \) defined on \( Y \subseteq X \) we use the notation \( \|g\|_Y \) to represent \( \max\{|g(x)|: x \in Y\} \).

A user of the code given in [1] must supply certain input parameters beyond the data \( \{(x_i, y_i)\}_{i=1}^m \). These additional parameters include \( N \) and \( SMTH \), where \( N - 1 \) is the desired degree of each approximating polynomial piece and \( SMTH \) is the desired smoothness or number of continuous derivatives of the fit on \([a, b] \). The user must also input a value for the desired percent error, \( PE \), which is used to calculate the tolerance, \( TOL \), which the approximating pieces must meet. That is, each approximating polynomial piece must fit the data in its interval of definition with a maximum absolute pointwise error less than \( TOL \). In addition, the parameter \( NPTS \) must be supplied. This parameter allows the addition of artificial data.
points. In particular, for a sparse data set, the user can add additional data points by setting NPTS > 0. In this case, the subroutine LINEAR will add NPTS new points by linear interpolating between consecutive data points.

In this context, the $L_1$ and $L_2$ packages will calculate an approximation $p$ to $f$ and a set of points (knots) $\{t_i\}_{i=0}^k \subseteq X$ with $a = t_0 < t_1 < \ldots < t_{k-1} < t_k = b$ such that

a. $p$ restricted to $[t_{i-1}, t_i]$ is a polynomial $p_i \in \pi_{N-1} = \{q: q$ is a real algebraic polynomial of degree $\leq N - 1}\}.

b. $p$ has SMTH continuous derivatives.

c. $\|f - p\|_X \leq TOL$.

The first step in the $L_1$ and $L_2$ packages is to determine the location of the first knot $t_1$. In order to do this, the codes find $\hat{c}_1$, the largest point in $X$ such that

a. $[a, \hat{c}_1] \cap X$ contains at least $\max(2, N + 1)$ points, and

b. If $p_1$ is the best approximation to $f$ from $\pi_{N-1}$ on $S_1 = [a, \hat{c}_1] \cap X$, then $\|f - p_1\|_{S_1} \leq TOL$.

If $\hat{c}_1 = b$, the algorithm successfully terminates with no interior knots.

If no such $\hat{c}_1$ exists, then the algorithm aborts and an appropriate error message is printed.

If $t_1$ exists, $a < \hat{c}_1 < b$, and SMTH $\geq 1$, then the right endpoint of the first polynomial piece is determined by "backing off" from $\hat{c}_1$ to a suitable point in $S_1$ using the following procedure.

The $L = N - \text{SMTH} - 1$ largest extreme points of the error function $f(x) - p_1(x)$ are selected from the interval $S_1$ and one of them will be used for the knot $t_1$. The knot is chosen in this manner because, in the continuous setting, if $f$ is differentiable and $\xi$ is an interior relative
extreme point of \( f(x) - p_1(x) \), then \( f'(\xi) - p'_1(\xi) = 0 \) so that \( f'(\xi) = p'_1(\xi) \).

Thus, joining \( p_2 \) to \( p_1 \) at \( \xi \) smoothly will force \( p_2 \) to have the same direction as \( f \) at the knot and should damp out unwanted oscillations.

In order to decide which extreme point to use for \( t_1 \), the code first computes the values \( f'(\xi_1), f'(\xi_2), \ldots, f'(\xi_v) \) where \( f'(\xi_v) \) is an approximation for the "slope" of the data at \( \xi_v \) determined by the centered quadratic interpolation of the data at \( \xi_v \) and its two immediate neighbors. The code then chooses the largest \( \xi \) such that \( |f'(\xi_v) - p'_1(\xi_v)| < \text{TOL} \). If no such \( \xi_v \) exists, then \( t_1 \) is chosen to be the largest \( \xi \), at which \( |f'(\xi_v) - p'_1(\xi_v)| \) attains its minimum. This procedure is repeated on the intervals \([t_1, b], \ldots, [t_n, b]\) until \( t_n = b \).

3. The New Algorithm

The original \( \xi_1 \) and \( \xi_2 \) packages approximated with polynomial pieces in standard form (e.g., \( p_1(x) = \sum_{n=1}^{N} c_n x^{n-1} \)). In the new algorithm, the polynomial pieces are of the form \( p_i(x) = \sum_{n=1}^{N} c_n (x - x^*)^{n-1} \) where \( x^* \) is the left endpoint of the subinterval on which \( p_i(x) \) is defined. However, the main focus of this algorithm is a new "backing off" strategy. This new "backing off" strategy can be characterized as a look-ahead strategy.

In the first step, the code will attempt to fit the entire data set on \( S = [a, b] \cap X \) with a polynomial \( p \in \pi_{N-1} \) such that \( \|f - p\|_S \leq \text{TOL} \). If this is not possible, then the algorithm will find the largest element of \( X, \xi_1 \), such that the best approximation \( p_1 \) to \( f \) on \( S_1 = [a, \xi_1]\) satisfies \( \|f - p_1\|_{S_1} \leq \text{TOL} \). This is done via a halving procedure.
Specifically, if it is found that the best approximation on \([a, b]\) does not satisfy the tolerance criterion then the code attempts to fit the data on the first \(N + 1\) points of \(X\). If it is unable to satisfy the tolerance criterion on this set, the code aborts, printing an appropriate error message. If the error criterion is satisfied on this small set then the point \(\hat{t}_1\) is computed via "bisection" initialized with the right endpoint of this small set and \(b\). The code will then attempt to fit the rest of the data using \(\hat{t}_1\) as the current left endpoint. Specifically, the best approximation \(p_2\) to \(f\) on \(S_2 = [\hat{t}_1, b] \cap X\) subject to \(p_2^{(j)}(\hat{t}_1) = p_1^{(j)}(\hat{t}_1), j = 0, 1, \ldots, NSMTH\) is calculated. If \(\|f - p_2\|_{S_2} \leq TOL\) holds, then the code successfully terminates with \(\hat{t}_1\) taken as our knot \(t_1\). If \(\|f - p_2\|_{S_2} > TOL\) then the bisection procedure is invoked once again to find \(\hat{t}_2 \in X\) such that \(\hat{t}_2\) is the largest element of \(X\) for which the best approximation \(p_2\) to \(f\) on \(S_2 = [\hat{t}_1, \hat{t}_2] \cap X\) subject to \(p_2^{(j)}(\hat{t}_1) = p_1^{(j)}(\hat{t}_1), j = 0, 1, \ldots, NSMTH\) satisfies \(\|f - p_2\|_{S_2} \leq TOL\). The code stores the current second subinterval \([\hat{t}_1, \hat{t}_2]\) and the polynomial piece \(p_2\) as the current knots and the best approximation to date. The code will then "back off" one point from \(\hat{t}_1\) to \(t'\), the point of \(X\) immediate preceding \(\hat{t}_1\). Then the above procedure is applied to \([a, \hat{t}_1]\). That is, \(\hat{t}_2 \in X\) is calculated such that \(\hat{t}_2\) is the largest element of \(X\) for which the best approximation \(\hat{p}_2\) to \(f\) on \(\hat{S}_2 = [\hat{t}_1, \hat{t}_2] \cap X\) subject to \(\hat{p}_2^{(j)}(\hat{t}_1) = p_1^{(j)}(\hat{t}_1), j = 0, \ldots, NSMTH\) satisfies \(\|f - \hat{p}_2\|_{\hat{S}_2} \leq TOL\). If \(\hat{t}_2 = b\) then the algorithm successfully terminates with the two polynomial pieces \(p_1\) and \(\hat{p}_2\) and the knot \(\hat{t}_1\) as the desired fit. If \(\hat{t}_2 < b\) occurs the \(p_1\) and \(\hat{p}_2\) and the knot \(\hat{t}_1\) remains the current candidate for the first two pieces and common knot for the final fit. If \(\hat{t}_1 > \hat{t}_2\) occurs then \(p_2\), \(\hat{t}_1\) and \(\hat{t}_2\) are replaced by
$\hat{t}_2$, $\hat{t}_1$, and $\hat{t}_2$, respectively, and the above backing off procedure is continued. At this point two options are available. In the first option, denoted as COMPUT I, the code will continue backing off, one point at a time, and store the current $\hat{t}_1$, $\hat{t}_2$ and the approximating polynomial piece, $p_2$, that approximates farthest to the right subject to the smoothness constraints and tolerance criterion as the current knots and best second approximation piece replacing any previous lesser attempts. If the code backs off two consecutive points without fitting farther to the right subject to the smoothness constraints and given tolerance, then the code will accept the current $\hat{t}_1$, $\hat{t}_2$ and $p_2$ as the knots and best approximation for the second subinterval and begin work on a third subinterval which has $\hat{t}_i$ as its left endpoint prior to "backing off". In the second option, denoted as COMPUT II, the code will back off a fixed number of points in an attempt to improve the current approximation. This fixed number is the greatest integer less than 1/2 the number of points in $[a, \hat{t}_1] \cap X$, $\hat{t}_1 = \text{the initial value for } \hat{t}_1$.

4. **Numerical Results**

In most cases, the original $\ell_1$ and $\ell_2$ packages and the modified algorithms presented here produced similar results. Precisely, in 68 out of 79 data sets tested with the $\ell_1$ packages and in 64 out of 83 data sets tested with the $\ell_2$ packages similar results were produced by the original and the new algorithms. Some examples illustrating this are shown in Figures 1-12 on six given data sets.

In our testing we found that the original $\ell_1$ and $\ell_2$ packages produced better results than the new versions in a small but significant number of
cases. We believe that this is primarily due to the fact that the new versions are designed with the objective of reducing the number of knots by extending the length of each subinterval as far as possible subject to the given smoothness and tolerance requirements. In doing this, the new methods try to be too perfect too soon and are unable to recover later on in the approximation. One could say that our methods suffer from greediness. An example of this behavior is given by the Titanium data tested with the $\ell_2$ packages (Figures 15, 16). Here the new method causes piecewise interpolation to result. Note that this instability of the new algorithm is not found in the original algorithm. On the other hand, for a few data sets, such as the data set Test 50000 the new algorithm for the $\ell_2$ package (Figures 13, 14) reduced the number of knots needed. Thus, we cannot claim that the original $\ell_1$ and $\ell_2$ packages will always produce better fits than the revised versions. Likewise, there were five data sets where the original $\ell_1$ package is superior to the new $\ell_1$ package. However, there were also six data sets where the new $\ell_1$ package produced a better fit than the original $\ell_1$ package. For example, the ABS(SIN(X)) data set with noise and bad points was tested using the $\ell_1$ packages (Figures 17, 18). Here the original package attempted to fit some of the bad points, whereas the new version did not.

In the testing of these codes it was observed that the COMPUT I and COMPUT II options gave the same results for all 162 data sets tested. Our results may not be conclusive for all cases but we will assume the following statement is reasonable. In general, backing off until two consecutive attempts do not improve the fit subject to the smoothness constraints and given tolerance will suffice.
Further backing up will not allow the current approximating piece to extend farther to the right.

In summary, based upon the limited testing that we performed, it appears that the original \( z_1 \) and \( z_2 \) codes are preferable to the modified codes presented here. We believe this conclusion is warranted due to the fact that the original codes appear to be more robust than the new codes using the look-ahead strategy and that when both codes performed satisfactorily, they gave similar results.

As a final note we also wish to point out that our study also illustrates one problem facing a user of such software. Namely, at the outset there is no way to predict the effectiveness of a given data fitting code. A good illustration of this is given in the \( z_1 \) and \( z_2 \) fits of the Titanium data (Figures 19 and 20). Here the \( z_1 \) code was successful whereas the \( z_2 \) code was not. Since this particular data is not particularly unusual, it is somewhat surprising that these two codes should vary so widely on it. We believe that this is an indication of the need for more research on the many problems involved with data fitting.
L1 TANTALUM DATA

N=8, SMTH=6, TOL=.100. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L1 APPROX. OPERATOR

Figure 1
TANTALUM DATA

N=8, SIGMA 6, TOL= .100. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) LI APPROX. OPERATOR

Figure 2
L2 TANTALUM DATA
N=6, SMTH=1, TOL=.050. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPRX. USING (DISCRETE) L2 APPRX. OPERATOR

Figure 3
TANTALUM DATA

Piecwise polynomial approx. using (discrete) L2 approx. operator

Figure 4
L1 ARGON DATA
N=6, SMTH=1, TOL=.010. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L1 APPROX. OPERATOR

Figure 5
ARGON DATA
N=6, SMTH=1, TOL=.010. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING DISCRETE LI APPROX. OPERATOR

Figure 6
L1

SIN(X) ON (-3.14, 3.14)

N=6, SMTH=1, TBL=.200. KNOTS ARE INDICATED BY "X".

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L1 APPROX. OPERATOR

Figure 7
Figure 8
L2 \quad \text{EXP}(5x)

N = 6, SMTH = 1, TOL = 4.74. KNOTS ARE INDICATED BY *.

Figure 9
L2 \( \exp(5x) \)

\( \text{N=6, SMTH=1, TOL=14.741, KNOTS ARE INDICATED BY 0.} \)

**Figure 10**

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR
L2 CUBIC WITH NOISE
N=6. SMTH=2. TOL=2.042. KNOTS ARE INDICATED BY X.
L2 CUBIC WITH NOISE

NO. 6. WITH L2, T0, L0, 0.40, AND U ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR

Figure 12
L2 TEST 50000 DATA
N=6, SMTH=1, TOL=.100. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR

Figure 13

NPTS=200
Figure 14

PIECEWISE POLYNOMIAL APPROX. USING DISCRETE L2 APPROX. OPERATOR

TEST 50000 DATA
N=6, SMM=1, TOL=.100, XPTS ARE INDICATED BY X.
L2 TITANIUM DATA
N=6, SMTH= 2, TOL= .050, KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR

Figure 15
TITANIUM DATA
N=6, SMTH=2, TOL=.050. KNOTS ARE INDICATED BY X.

PIECESWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR.
L1 \text{ABS(SIN(X)) WITH NOISE}

N = 6, SMTH = 1, TOL = .100. KNOTS ARE INDICATED BY X.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L1 APPROX. OPERATOR

Figure 17
ABS(SIN(X)) WITH NOISE
N=6, SMTH=1, TOL=.130. HATS ARE INDICATED BY X.
PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) LI APPROX. OPERATOR

Figure 19
L2 TITANIUM DATA
N=6, SMTH: 2, TOL: .050, ROCKS ARE INDICATED BY "J.

PIECEWISE POLYNOMIAL APPROX. USING (DISCRETE) L2 APPROX. OPERATOR
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