Abstract—We derive basic statistics for the least squares piecewise monotonic approximation to noisy data. It is known that this approximation is the solution of a combinatorial problem, which is decomposed quite efficiently into separate monotonic approximation problems. Each monotonic section consists of disjoint intervals of adjacent equal components. We provide a B-spline representation of the solution and state the associated linear regression model. It is shown that the dispersion matrix of the model estimated coefficients is a positive definite diagonal matrix. Hence, confidence intervals and tests for the coefficients of the linear model are derived immediately and stably. A numerical example illustrates some technical aspects of an optimal fit, and demonstrates the estimation capability of the linear model. Our results suggest some subjects for future work.

Index Terms—approximation, B-spline, data fitting, first divided difference, least squares, linear regression model, piecewise monotonic approximation to noisy data. It is known that this approximation is the solution of a combinatorial problem, which is decomposed quite efficiently into separate monotonic approximation problems. Each monotonic section consists of disjoint intervals of adjacent equal components. We provide a B-spline representation of the solution and state the associated linear regression model. It is shown that the dispersion matrix of the model estimated coefficients is a positive definite diagonal matrix. Hence, confidence intervals and tests for the coefficients of the linear model are derived immediately and stably. A numerical example illustrates some technical aspects of an optimal fit, and demonstrates the estimation capability of the linear model. Our results suggest some subjects for future work.

1. INTRODUCTION

The purpose of this paper is to examine some basic statistics for the regression coefficients of the least squares piecewise monotonic fit to discrete data. Piecewise monotonicity enters in terms of sign changes in the first divided differences of the data.

Let \( \{ \phi_i : i = 1, 2, \ldots, n \} \) be measurements of the real function values \( \{ f(x_i) : i = 1, 2, \ldots, n \} \), where the abscissae \( \{ x_i : i = 1, 2, \ldots, n \} \) are in the strictly ascending order \( x_1 < x_2 < \cdots < x_n \). Demetriou and Powell [8] take the view that there are errors in the data that require corrections if the number of sign changes in the sequence \( \{ \phi_{i+1} - \phi_i : i = 1, 2, \ldots, n-1 \} \) is much greater than the number in the sequence \( \{ f(x_{i+1}) - f(x_i) : i = 1, 2, \ldots, n-1 \} \). Specifically, given a positive integer \( k \), they seek numbers \( \{ y_i : i = 1, 2, \ldots, n \} \) that minimize the objective function

\[
\Phi(y_1, y_2, \ldots, y_n) = \sum_{i=1}^{n} (y_i - \phi_i)^2
\]

subject to the constraints that there exist integers \( \{ t_j : j = 0, 1, \ldots, k \} \) satisfying the conditions

\[
1 = t_0 \leq t_1 \leq \cdots \leq t_k = n,
\]

such that the inequalities

\[
\begin{align*}
y_{t_j-1} \leq y_{t_j-1+1} \leq \cdots \leq y_{t_j}, & \quad \text{if } j \text{ is odd} \\
y_{t_j-1} \geq y_{t_j-1+1} \geq \cdots \geq y_{t_j}, & \quad \text{if } j \text{ is even}
\end{align*}
\]

hold.

The integers \( \{ t_j : j = 1, 2, \ldots, k-1 \} \) are also variables of the optimization calculation. We regard the data \( \{ \phi_i : i = 1, 2, \ldots, n \} \) and the smoothed values \( \{ y_i : i = 1, 2, \ldots, n \} \) as components of the vectors \( \phi \) and \( y \) in \( \mathbb{R}^n \), and we denote by \( y^T = (y_1, y_2, \ldots, y_n) \) the transpose of vector \( y \). We call vector \( y \) an optimal piecewise monotonic approximation to \( \phi \).

This is a challenging optimization problem that requires \( O(n^{k-1}) \) combinations of integers in order to find an optimal combination. However, Demetriou and Powell [8] have developed a dynamic programming method that generates the solution in only \( O(n^2 + kn \log_2 n) \) computer operations when \( k \geq 3 \) and in \( O(n) \) when \( k = 1 \) or 2. For a detailed presentation of the method, the reader may consult the reference. In order to consider the test statistics of the piecewise monotonic fit to the data, as stated at the beginning of the section, we give the following properties.

The important property of the least squares piecewise monotonic approximation problem is that it is decomposed into monotonic approximation problems (case \( k = 1 \)) to disjoint sets of adjacent data. Now, we have \( y_t = \phi_t \), where \( t \) is any element of the set \( \{ t_1, t_2, \ldots, t_k-1 \} \). It follows from the decomposition statement of Demetriou [6] that the particular monotonic problem on \( [x_{t_{j-1}}, x_{t_j}] \) requires the minimization of the sum of squares

\[
\sum_{i=t_{j-1}}^{t_j} (y_i - \phi_i)^2
\]

subject to the monotonicity constraints (3). Therefore, the components of \( y \) are defined by a separate quadratic programming calculation for each section. Further, the optimal values \( \{ y_i : i = t_{j-1}, \ldots, t_j \} \) consist of ranges of equal components. We consider these ranges by adopting the definition by Cullinan and Powell [2]. Specifically, if \( j \) is odd and, \( s \) and \( t \) are integers such that \( t_{j-1} \leq s < t \leq t_j + 1 \), then \( \eta \) is defined to be the real number \( \sum_{i=s}^{t-1} \phi_i/(t-s) \) that minimizes the expression

\[
\sum_{i=s}^{t-1} (\eta - \phi_i)^2.
\]

Now, if \( y_s = y_{s+1} = \cdots = y_{t-1-1} \) if \( s = t_{j-1} \) or \( y_{s-1} < y_s \), and if \( t = t_j + 1 \) or \( y_{t-1} < y_t \), then

\[
y_s = y_{s+1} = \cdots = y_{t-1} = \eta
\]

Analogously, we may consider the case when \( j \) is even.

The analysis of the statistics is addressed in Sections II and III. Section II gives the B-spline representation of the solution of the optimization problem, namely the optimal piecewise monotonic approximation to the data. This representation is an equivalent formulation of the solution by a constant spline with certain knots. Here we take advantage
of the fact that the coefficients of the B-spline representation of the constant spline consist of ranges of equal components and can be derived from a system of normal equations that has a positive definite diagonal coefficient matrix.

Section III states the linear regression model that is associated with the B-spline representation of the solution, and considers some common test statistics and confidence intervals for the model coefficients. Now the matrix structure obtained by the B-spline form of the solution gives immediately and stably these statistics.

Section IV presents numerical results obtained by fitting measurements of a known function contaminated by random errors. We apply the method to the data for certain values of k, providing some technical aspects of each fit, discuss on the spline representation of the optimal fit, and derive some statistics for the coefficients of the associated linear model. With the aim of guiding the use of the method, the results are instructively analyzed. Hence, the advantages derived by the spline representation of the optimal fit and the estimation capability of the linear regression model are demonstrated.

Section V reviews the results and discusses on future directions of this research.

All the experiments were run by L2WPMA, the Fortran program of Demetriou [5], which implements the method of [4].

The piecewise monotonic approximation problem arises in many important applications such as medical practices, spectroscopy, cancer research, and energy (references are included in Demetriou [7]). We emphasize the work that made by Lazaropoulos [10] on smart grid and renewable energy topologies.

II. THE SPLINE REPRESENTATION OF THE OPTIMAL FIT

In this section, we state a spline representation of the optimal fit, which we next employ in Section III for estimating purposes concerning the associated linear model.

The user provides the data \( y \in \mathbb{R}^n \) and the integer \( k \), and the method at the end of the calculation, supplies the optimal integers \( \{ t_j : j = 1, 2, \ldots, k-1 \} \) and the associated optimal components \( \{ y_i : i = 1, 2, \ldots, n \} \). As noted already, these components are calculated by independent monotonic approximation calculations between successive \( t_j \). Specifically, they are monotonic increasing on \([1, t_1]\) and on \([t_j-1, t_j]\) for odd \( j \) in \([2, k]\) and monotonic decreasing on \([t_j-1, t_j]\) for even \( j \) in \([2, k]\).

We recall from the paragraph that includes relations (6) that the optimal fit \( \{ y_i : i = 1, 2, \ldots, n \} \) consists of intervals of equal components, let \( I_j \) be the subset of indices of the constraints (3) such that

\[
I_j = \begin{cases} 
\{ i : y_{i-1} < y_i, \; i = t_j-1 + 1, \ldots, t_j \}, & \text{if } j \text{ is odd} \\
\{ i : y_{i-1} > y_i, \; i = t_j-1 + 1, \ldots, t_j \}, & \text{if } j \text{ is even} 
\end{cases}
\]

and let \( I \) be the union of the subsets

\[
I = \{ t_0 \} \cup I_1 \cup I_2 \cup \cdots \cup I_k.
\]

We denote by \( \{ s(x) : x_1 \leq x \leq x_n \} \) the piecewise interpolating function to the optimal values. It follows that \( s(x) \) is a constant spline whose knots are all in the set \( \{ x_i : i \in I \} \). Further, we set \( \kappa = |I| \), where \(|I|\) is the number of elements of \( I \), and let \( S \) be the space of all constant splines defined on the points \( \{ \xi_i : i = 1, 2, \ldots, \kappa \} \), the points being the set \( \{ x_i : i \in I \} \).

Provided that the knots \( \{ \xi_i \} \) are given, the calculation of \( y \) is equivalent to finding the function \( s \) that minimizes the sum of squares

\[
\sum_{i=1}^n [s(x_i) - \phi_i]^2, \quad s \in S.
\]

Then the components of \( y \) have the values \( \{ y_i = s(x_i) : i = 1, 2, \ldots, n \} \). We express \( s \) in the form

\[
s(x_i) = \sum_{j=1}^k c_j B_j(x_i), \quad i = 1, 2, \ldots, n,
\]

where \( \{ B_j : j = 1, 2, \ldots, \kappa \} \) is the first-order B-spline basis (see, for example, de Boor [1]: p.89) of the space \( S \) of all constant splines, with

\[
B_j(x) = \begin{cases} 
1, & \xi_j \leq x < \xi_{j+1} \\
0, & \text{otherwise},
\end{cases}
\]

except that when \( j = \kappa \) we define \( \xi_{\kappa+1} = x_n \) and replace the inequalities in formula (9) by \( \xi_\kappa \leq x \leq \xi_{\kappa+1} \).

Based upon expression (8), we represent the optimal fit \( y \) by the triple \((\kappa, \omega, \varsigma)\). Here, \( \kappa \) is a positive integer, and \( \omega \) and \( \varsigma \) are vectors in \( \mathbb{R}^\kappa \), where the components of \( \omega \) are positive integers whose sum is \( n \), and the components of \( \varsigma \) are the coefficients of the spline expression (8). This triple denotes the vector \( y = y(\kappa, \omega, \varsigma) \in \mathbb{R}^n \) that has \( \omega_1 \) components equal to \( c_1, \omega_2 \) components equal to \( c_2 \) and so on up to \( \omega_\kappa \) components equal to \( c_\kappa \). Hence we define the knots \( \xi_1 = x_1, \xi_2 = x_{\omega_1+1}, \xi_3 = x_{\omega_1+\omega_2+1} \) and so on up to \( \xi_\kappa = x_{\omega_1+\omega_2+\cdots+\omega_{\kappa-1}+1} \), and we let \( c_1 = y_1, c_2 = y_{\omega_1+1}, c_3 = y_{\omega_1+\omega_2+1} \) and so on up to \( c_\kappa = y_{\omega_1+\omega_2+\cdots+\omega_{\kappa-1}+1} \).

As noted above, we use the L2WPMA software [5] for the calculation of the optimal piecewise monotonic approximation. By design, L2WPMA, at the end of the calculation, delivers the data indices of the knots, and the components of the optimal fit \( y \) that define the triple \((\kappa, \omega, \varsigma)\). So, in view of set \( I \), we may immediately obtain the sequences \( \{ \xi_j : j = 1, 2, \ldots, \kappa \} \) and \( \{ \xi_j : j = 1, 2, \ldots, \kappa \} \). It follows that the components of \( y \) between two successive interior knots, say \( \xi_j \) and \( \xi_{j+1} \), are

\[
y_i = c_j, \quad \omega_1 + \omega_2 + \cdots + \omega_{j-1} + 1 \leq i \leq \omega_1 + \omega_2 + \cdots + \omega_j,
\]

and similarly for the other cases.

Of course, given the knots, the coefficients satisfy the normal equations associated with the minimization of the objective function (1),

\[
\sum_{j=1}^\kappa \left[ \sum_{i=1}^n B_{\ell}(x_i) B_j(x_i) \right] c_j = \sum_{i=1}^n B_{\ell}(x_i) \phi_i, \quad \ell = 1, 2, \ldots, \kappa,
\]

which is a crucial part of our analysis. Indeed, since

\[
\sum_{i=1}^n B_{\ell}(x_i) B_j(x_i) = 0, \quad \text{for } |\ell - j| > 0,
\]

system (10) simplifies to the diagonal system of equations
\[
\begin{bmatrix}
  e_1 \\
  e_2 \\
  \vdots \\
  e_k
\end{bmatrix}
= \begin{bmatrix}
  c_1 \\
  c_2 \\
  \vdots \\
  c_k
\end{bmatrix}
\begin{bmatrix}
  b_1 \\
  b_2 \\
  \vdots \\
  b_k
\end{bmatrix},
\]
(12)

where for \( j = 1, 2, \ldots, k \)
\[
e_j = \sum_{x_i \in \{j, j+1\}} |B_j(x_i)|^2 = \omega_j,
\]
(13)

and
\[
b_j = \sum_{x_i \in \{j, j+1\}} B_j(x_i)\phi_i = \sum_{x_i \in \{j, j+1\}} \phi_i.
\]

Besides that the coefficient matrix of system (12) is diagonal, is positive definite as well. Thus, not only it is straightforward to solve for \( \{c_j : j = 1, 2, \ldots, k\} \), but also to stably obtain the test statistics of the linear model.

III. THE LINEAR MODEL

We now turn to the discussion of expressing function (8) as a linear regression model in order to derive some statistics that are useful in the practical application of the piecewise monotonic data approximation method. We shall see that our particular problem has some computational advantages over the well known general linear regression problem. Here, presentation and notation follows Kendall and Stuart [9], but the subject of linear regression is treated in almost any textbook of statistics (see, for instance, [3] for an exposition from the point of view of econometrics).

The linear model behind equation (8) in matrix notation is
\[
\hat{\phi} = X\phi + \varepsilon,
\]
(14)

where \( X \) is an \( n \times k \) matrix with elements \( \{B_j(x_i) : i = 1, 2, \ldots, n\} \) for \( j = 1, 2, \ldots, k \), vector \( \phi \) has the components \( \{c_j : j = 1, 2, \ldots, k\} \), and \( \varepsilon \) is an \( n \)-vector of “error” random variables \( \varepsilon_i \) with zero mean and variance \( \sigma^2 \). For example, if \( n = 8, k = 3 \) and \( \xi_1 = 1, \xi_2 = 5 \) and \( \xi_3 = 8 \), then matrix \( X \) of system (14) is
\[
X = \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\

\end{bmatrix},
\]
(15)

The usual results of regression analysis apply. The least squares method requires the unconstrained minimization of the sum of squares
\[
S(\varepsilon) = (\hat{\phi} - X\phi)^T(\hat{\phi} - X\phi)
\]
(16)
in the components of \( \varepsilon \). Differentiating gives
\[
2X^T(\hat{\phi} - X\phi) = 0,
\]
(17)

which is equivalent to the normal equations (10). Solving (17) gives the least squares estimator of \( \varepsilon \)
\[
\hat{\varepsilon} = (X^TX)^{-1}X^T\hat{\phi},
\]
(18)

because, in view of elements (13), matrix \( (X^TX) \) is the \( k \times k \) diagonal and positive definite coefficient matrix that occurs at system (12), thus invertible.

Since \( X \) is constant, expression (18) is written as
\[
\hat{\varepsilon} = (X^TX)^{-1}X^T(\phi + \varepsilon) = \hat{\phi} + (X^TX)^{-1}X^T\varepsilon,
\]
(19)

In addition, we take into account the expected value \( E(\varepsilon) = 0 \), and obtain \( E(\hat{\varepsilon}) = \hat{\phi} \). Further, by assumption, the dispersion matrix is
\[
V(\varepsilon) = E(\varepsilon\varepsilon^T) = \sigma^2I,
\]
(20)

where \( I \) is the \( n \times n \) identity matrix. Hence, the dispersion matrix of \( \hat{\varepsilon} \) is
\[
V(\hat{\varepsilon}) = \sigma^2(X^TX)^{-1}.
\]
(21)

Now we remember the definitions of matrix \( X \) and elements \( \{e_j : j = 1, 2, \ldots, k\} \), and obtain
\[
V(\hat{\varepsilon}) = \sigma^2 \begin{bmatrix}
1/e_1 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 1/e_k
\end{bmatrix}.
\]
(22)

Although expression (18) has only theoretical value, because the estimated coefficients are derived by the piecewise monotonic approximation method mentioned in Section II, we see that the inversion of matrix \( (X^TX) \) is straightforward. Hence, we obtain a highly useful structure for deriving the following statistics.

To start with, since
\[
E[(\hat{\phi} - X\phi)(\hat{\phi} - X\phi)^T] = \sigma^2(n - k),
\]
we have the unbiased estimator of \( \sigma^2 \)
\[
s^2 = \frac{1}{n - k}(\hat{\phi} - X\phi)(\hat{\phi} - X\phi)^T.
\]
(23)

Further, we assume that \( \varepsilon \) is a vector of normal error variables and we may set confidence intervals and test hypothesis for any component of the parameter vector \( \phi \) (see, for example, [9]: p. 377).

Any estimator \( \hat{c}_j \) is a linear function of the data components and is therefore normally distributed with mean \( c_j \) and variance, from (22),
\[
\text{var}(\hat{c}_j) = \sigma^2[(X^TX)^{-1}]_{jj} = \sigma^2e_j^{-1}.
\]
(24)

As \( s^2 \) is distributed independently of \( \varepsilon \) and hence of any component of \( \varepsilon \), the distribution of \((n - k)s^2/\sigma^2\) is of the \( \chi^2 \) form with \( n - k \) degrees of freedom. It follows that the statistic
\[
t = (\hat{c}_j - c)/(s^2[(X^TX)^{-1}]_{jj})^{1/2} = (\hat{c}_j - c)/(s^2e_j^{-1/2})^{1/2},
\]
(25)

which is the ratio of a standardized normal variate to the square root of an independent \( \chi^2/\nu \) variate, has a Student’s \( t \)-distribution with \( \nu = n - k \) degrees of freedom. Hence, we may set confidence intervals for \( c_j \) or to test hypotheses concerning its value. We denote by \( \alpha \) the confidence level, and the central confidence interval with coefficient \( 1 - \alpha \) is
\[
\hat{c}_j \pm t_{1 - \frac{\alpha}{2}}\left(s^2[(X^TX)^{-1}]_{jj}\right)^{1/2},
\]
or
\[
\tilde{e}_j \pm t_{1-\frac{1}{2}\alpha}\left(s^2\hat{e}_j^{-1}\right)^{\frac{1}{2}},
\]
(26)
where \(t_{1-\frac{1}{2}\alpha}\) is a value of Student’s \(t\) for \(\nu\) degrees of freedom.

As was pointed out already, the diagonal matrix \((X^\top X)\) in our problem is self-solving, so in practice we would not expect any computational errors, due to rounding-off of the elements of \((X^\top X)\). On the other hand, in general least squares calculations, the numerical calculation of the inverse of this matrix can become highly ill-conditioned. However, in the least squares estimation problem, the entries of \((X^\top X)^{-1}\) give information about the kinds and sizes of errors in the data. Therefore, the inverse \((X^\top X)^{-1}\) is needed for obtaining some useful statistics. Fortunately, in our case, \((X^\top X)\) has the highly helpful diagonal structure that is defined in Section II and matrix (22) is particularly simple.

IV. AN EXAMPLE ON SIMULATED DATA

This section presents some numerical results on simulated data to demonstrate the advantages gained by the spline representation of the optimal piecewise monotonic fit in obtaining and using the statistics of Section III. We let,

\[
f(x) = \sin(4x) + 0.5x^2, \quad 0 \leq x \leq 2\pi,
\]
(27)
\(n = 75\) and the abscissae be the equally spaced values
\(x_i = \frac{2i}{n-1}, \quad i = 1, 2, \ldots, n\). Each of the components \(\{\phi_i : i = 1, 2, \ldots, n\}\) was generated by adding to \(f(x_i)\) a random number from the uniform distribution on \([-0.5, 0.5]\). We have chosen the magnitude of the added error to be as large as needed in order that the reader may easily follow the presentation of the results. By using the sine function, we know the number of underlying monotonic sections and therefore we can judge whether the obtained fit is suitable to the data. We see that function (27) has five monotonic sections.

We fed the data to L2WPMA and we let the number of monotonic sections take the values \(k = 1, 2, 3, 4\) and 5. The corresponding optimal piecewise monotonic fits are presented in Figs. 1, 2 and 3. We note that the optimal approximations for \(k = 1\) and \(k = 2\) coincide, where in the case \(k = 2\) the monotonic decreasing section degenerates to the \(n\)-th data point. The same holds when \(k = 3\) and \(k = 4\). By comparing the fits in these three figures, we see that the optimal approximation with \(k = 5\) monotonic sections reveals well the underlying trends of the data. Thus, it is considered to be an appropriate approximation.

Some calculated results are presented in Table I. Table I consists of a triplex of columns for the cases \(k = 1, k = 3, k = 5\). Each triplex gives the components of \(\omega\) and \(\xi\) of the triple \(y(k, \omega, \xi)\), one column for each vector, and two more columns for the components of \(\xi\) and the corresponding data indices. The sum of squares of residuals and the maximum absolute residual of the fits associated with these cases are added at the bottom of Table I. The optimal fit with \(k = 1\) monotonic section consists of \(\kappa = 14\) different intervals of equal components where the \(j\)-th interval contains \(\omega_j\) components equal to \(c_j\) for \(j = 1, 2, \ldots, 14\). Increasing \(k\) should increase the number of intervals of equal components at the solution as well, otherwise a contradiction would be obtained. At the same time, it is expected that the number of equal components within each interval should be decreasing on average as they are distributed across the range of data. In fact, the optimal fit with \(k = 3\) monotonic sections consists of 29 different intervals of equal components, and the optimal fit with \(k = 5\) monotonic sections consists of 39 such intervals. It is worth noticing that as \(k\) increases and the components of \(y\) are distributed across more intervals, their values are modified and the optimal fit comes closer to the measurements. Certainly, this is indicated from the reduction of the sum of squares of residuals and the decrease of the maximum absolute residual of the associated fits.

Further, the spline representation of the solution, which is presented in Table I, is provided by the L2WPMA output. The indices of the knots (see column “knot index”) correspond to the sequence of the knots (see column “\(\xi_j\)” and therefore the values of first order B-splines in expression (9) are calculated accordingly. Furthermore, having available the first order B-splines, they can then be utilized as explanatory variables in the linear regression model (14). Hence, the coefficients \(c_j\) may be derived from formula (18). The main advantage of this consideration is that the estimated regression coefficients \(\hat{c}_j\) inherit some statistical properties due to the estimation process. Thus, both the derivation of some basic statistics and the implementation of statistical inferences are allowed. It is worthy of attention that the linear regression formulation (14) would not be possible, if the optimal piecewise monotonic approximation was not available. Indeed, the optimal approximation is the solution of a highly nonlinear combinatorial problem, while linear regression is the representation of this solution. Thus, the data analysis of this paper follows the use of the piecewise approximation to the data.

We illustrate the data analysis output by presenting in Table II the results of the linear model (14) that was derived by the optimal piecewise monotonic fit with \(k = 5\) monotonic sections. A multiple linear regression was performed ab initio to predict the true values \(\{y_i : i = 1, 2, \ldots, 75\}\) given the measurements \(\{\phi_i : i = 1, 2, \ldots, 75\}\) and the regressors \(\{B_j(x_j), j = 1, 2, \ldots, 39\}\). The overall regression was statistically significant with \(F(39, 36) = 194\) \((p\text{-value} = 0.00)\), and coefficient of determination \(R^2\) equal to 0.9953. Of course, the estimated coefficients \(\{\hat{c}_j : j = 1, 2, \ldots, 39\}\) are identical to the components \(\{c_j : j = 1, 2, \ldots, 39\}\) provided by the L2WPMA software (see the rightmost column of Table I).

However, apart from the point estimation of the coefficients, a number of additional statistics are produced for the model coefficients that take advantage of the constant spline representation (8) of the optimal fit. The standard error of the estimated coefficients, the 95% confidence interval of the coefficients and the \(t\)-statistic for the statistical significance of each coefficient are presented in Table II. If we take a significance level \(\alpha = 0.05\), then we see that all the coefficients are significantly different from zero, except \(c_{11}, c_{11}, c_{16}\) and \(c_{17}\). The knots \(\xi_0 = 0, \xi_{11} = 0.93, \xi_{16} = 1.27\) and \(\xi_{17} = 1.40\), which are associated with the non significant coefficients, are located in the neighborhood of the points where the function intersects the horizontal axis. Now, the 95% confidence interval of the model coefficients indicates that there is 95% probability for the true value of the estimated coefficients.
TABLE 1
EXAMPLE OF SECTION IV: COMPONENTS OF ω and c of the triple \(g(k, \omega, c)\) for the optimal fit with \(k = 1, 3\) and \(5\) monotonic sections, and components of \(ξ\) with the corresponding data indices ("knot index") of expression (8)

<table>
<thead>
<tr>
<th>(k = 1)</th>
<th>(k = 3)</th>
<th>(k = 5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\omega_j)</td>
<td>knot index</td>
<td>(\xi_j)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>35</td>
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<tr>
<td>4</td>
<td>3</td>
<td>37</td>
</tr>
<tr>
<td>5</td>
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<td>40</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
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</tr>
<tr>
<td>7</td>
<td>2</td>
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<td>8</td>
<td>22</td>
<td>47</td>
</tr>
<tr>
<td>9</td>
<td>1</td>
<td>69</td>
</tr>
<tr>
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<td>1</td>
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<td>2</td>
<td>73</td>
</tr>
<tr>
<td>14</td>
<td>1</td>
<td>75</td>
</tr>
</tbody>
</table>

\[\sum_{1 \leq i \leq 75} (y_i - \phi_i)^2 = 11.9935\]

\[\max_{1 \leq i \leq 75} |y_i - \phi_i| = 1.2273\]

\[\sum_{1 \leq i \leq 75} (y_i - \phi_i)^2 = 2.9266\]

\[\max_{1 \leq i \leq 75} |y_i - \phi_i| = 0.6450\]

\[\sum_{1 \leq i \leq 75} (y_i - \phi_i)^2 = 1.6976\]

\[\max_{1 \leq i \leq 75} |y_i - \phi_i| = 0.3637\]

to lie between the given lower and upper limits, which are shown in Fig 3. Furthermore, we present in Fig. 4 this 95% confidence interval together with the true function values \(\{f(x_i): i = 1, 2, \ldots, 75\}\). We see that five times (namely at the points \(x_{10} = 0.38, x_{12} = 0.47, x_{13} = 0.51, x_{14} = 0.55, x_{30} = 1.49\)) the true values violate the upper confidence interval limit and three times (namely at the points \(x_{10} = 0.38, x_{37} = 1.53, x_{75} = 3.14\)) violate the lower limit by a negligible amount. Of note is that because we know the underlying function, we can immediately see the accuracy of our best approximation. Thus, this example illustrates the predictive ability of the piecewise monotonic approximation method.

V. Conclusion

In this paper we examined some basic statistics for the least squares piecewise monotonic fit to \(n\) discrete data contaminated by random errors, where \(k\) monotonic sections are desired.

For this analysis, the authors employed L2WPMA software, which is a Fortran package that solves the piecewise monotonic approximation problem. It is designed to provide also the knots for the constant spline representation of the solution. Having had this representation we proceeded to the definition of the associated linear model, and to the derivation of the \(t\)-statistics and relevant confidence intervals for the model coefficients.

We illustrated the estimation capability of the method by an example with simulated data, and we presented the results in a way that is instructive to the use of the method and the derivation of the statistics. The advantage of having a known underlying function, as in this example, is that we can have error estimates of the fit and therefore we can check the accuracy of the obtained approximation. The authors are going to consider the arduous problem of investigating the accuracy of the fit to the data and relating statistics when no more knowledge of the underlying function than providing integer \(k\) is required. For this case, only a-posteriori estimators like the sum of squares of residuals and the maximum distortion between fit and data are available.

Besides the standard output of the linear regression model that is presented in Table II, the spline representation of the piecewise monotonic approximation allows a number of additional statistical tests to be developed for the investigation.
Fig. 1. Best piecewise monotonic approximation (o) with \( k = 1 \) to 75 data (+) from \( f(x) = \sin(4x) + 0.5x^2 \), \( x \in [0, 2\pi] \), contaminated by numbers uniformly distributed in \([-0.5, 0.5]\). The piecewise linear interpolant illustrates the best fit.

Fig. 2. As in Fig. 1, but \( k = 3 \).

Fig. 3. As in Fig. 1, but \( k = 5 \). In addition, the 95% confidence interval of the piecewise linear interpolant is illustrated with the dot lines.
Fig. 4. Piecewise linear interpolant to the 75 data points $(\phi)$ of $f(x) = \sin(4x) + 0.5x^2$, $x \in [0, 2\pi]$. In addition, the 95% confidence interval that occurs in Fig 3 is illustrated with the dot lines.

TABLE II
EXAMPLE OF SECTION IV: OUTPUT FROM LINEAR MODEL OF SECTION III FOR THE OPTIMAL PIECEWISE MONOTONIC APPROXIMATION WITH $k = 5$

<table>
<thead>
<tr>
<th>$j$</th>
<th>B-Spline Basis</th>
<th>Est. Coef. $c_j$</th>
<th>Std. Error</th>
<th>Confidence Interval (95%)</th>
<th>$t$-statistic</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$B_1$</td>
<td>-0.25</td>
<td>0.22</td>
<td>-0.69 - 0.19</td>
<td>1.33</td>
<td>0.26</td>
</tr>
<tr>
<td>2</td>
<td>$B_2$</td>
<td>0.37</td>
<td>0.13</td>
<td>0.12 - 0.62</td>
<td>3.57</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>$B_3$</td>
<td>0.49</td>
<td>0.22</td>
<td>0.05 - 0.93</td>
<td>5.10</td>
<td>0.03</td>
</tr>
<tr>
<td>4</td>
<td>$B_4$</td>
<td>0.71</td>
<td>0.13</td>
<td>0.46 - 0.97</td>
<td>32.36</td>
<td>0.00</td>
</tr>
<tr>
<td>5</td>
<td>$B_5$</td>
<td>1.09</td>
<td>0.22</td>
<td>0.65 - 1.53</td>
<td>25.12</td>
<td>0.00</td>
</tr>
<tr>
<td>6</td>
<td>$B_6$</td>
<td>1.55</td>
<td>0.22</td>
<td>1.11 - 1.99</td>
<td>50.79</td>
<td>0.00</td>
</tr>
<tr>
<td>7</td>
<td>$B_7$</td>
<td>2.27</td>
<td>0.22</td>
<td>0.78 - 1.66</td>
<td>31.47</td>
<td>0.00</td>
</tr>
<tr>
<td>8</td>
<td>$B_8$</td>
<td>0.74</td>
<td>0.10</td>
<td>0.54 - 0.94</td>
<td>58.14</td>
<td>0.00</td>
</tr>
<tr>
<td>9</td>
<td>$B_9$</td>
<td>0.68</td>
<td>0.15</td>
<td>0.37 - 0.99</td>
<td>19.52</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>$B_{10}$</td>
<td>0.20</td>
<td>0.11</td>
<td>-0.02 - 0.42</td>
<td>3.28</td>
<td>0.08</td>
</tr>
<tr>
<td>11</td>
<td>$B_{11}$</td>
<td>-0.04</td>
<td>0.22</td>
<td>-0.48 - 0.40</td>
<td>0.04</td>
<td>0.85</td>
</tr>
<tr>
<td>12</td>
<td>$B_{12}$</td>
<td>-0.46</td>
<td>0.15</td>
<td>-0.77 - -0.14</td>
<td>8.81</td>
<td>0.01</td>
</tr>
<tr>
<td>13</td>
<td>$B_{13}$</td>
<td>-0.47</td>
<td>0.22</td>
<td>-0.91 - -0.03</td>
<td>4.71</td>
<td>0.04</td>
</tr>
<tr>
<td>14</td>
<td>$B_{14}$</td>
<td>-0.75</td>
<td>0.22</td>
<td>-1.19 - -0.31</td>
<td>11.89</td>
<td>0.00</td>
</tr>
<tr>
<td>15</td>
<td>$B_{15}$</td>
<td>-0.25</td>
<td>0.13</td>
<td>-0.50 - 0.01</td>
<td>3.94</td>
<td>0.05</td>
</tr>
<tr>
<td>16</td>
<td>$B_{16}$</td>
<td>-0.01</td>
<td>0.13</td>
<td>-0.26 - 0.25</td>
<td>0.00</td>
<td>0.95</td>
</tr>
<tr>
<td>17</td>
<td>$B_{17}$</td>
<td>0.14</td>
<td>0.22</td>
<td>-0.30 - 0.58</td>
<td>0.42</td>
<td>0.52</td>
</tr>
<tr>
<td>18</td>
<td>$B_{18}$</td>
<td>0.40</td>
<td>0.15</td>
<td>0.09 - 0.71</td>
<td>6.80</td>
<td>0.01</td>
</tr>
<tr>
<td>19</td>
<td>$B_{19}$</td>
<td>1.42</td>
<td>0.13</td>
<td>1.17 - 1.68</td>
<td>126.49</td>
<td>0.00</td>
</tr>
<tr>
<td>20</td>
<td>$B_{20}$</td>
<td>2.01</td>
<td>0.15</td>
<td>1.70 - 2.32</td>
<td>170.83</td>
<td>0.00</td>
</tr>
<tr>
<td>21</td>
<td>$B_{21}$</td>
<td>2.27</td>
<td>0.13</td>
<td>2.02 - 2.52</td>
<td>326.83</td>
<td>0.00</td>
</tr>
<tr>
<td>22</td>
<td>$B_{22}$</td>
<td>2.81</td>
<td>0.15</td>
<td>2.50 - 3.12</td>
<td>333.88</td>
<td>0.00</td>
</tr>
<tr>
<td>23</td>
<td>$B_{23}$</td>
<td>3.00</td>
<td>0.15</td>
<td>2.69 - 3.32</td>
<td>381.83</td>
<td>0.00</td>
</tr>
<tr>
<td>24</td>
<td>$B_{24}$</td>
<td>3.31</td>
<td>0.22</td>
<td>2.87 - 3.75</td>
<td>231.63</td>
<td>0.00</td>
</tr>
<tr>
<td>25</td>
<td>$B_{25}$</td>
<td>3.20</td>
<td>0.22</td>
<td>2.76 - 3.64</td>
<td>216.49</td>
<td>0.00</td>
</tr>
<tr>
<td>26</td>
<td>$B_{26}$</td>
<td>3.03</td>
<td>0.22</td>
<td>2.59 - 3.47</td>
<td>194.10</td>
<td>0.00</td>
</tr>
<tr>
<td>27</td>
<td>$B_{27}$</td>
<td>2.97</td>
<td>0.10</td>
<td>2.77 - 3.17</td>
<td>931.2</td>
<td>0.00</td>
</tr>
<tr>
<td>28</td>
<td>$B_{28}$</td>
<td>2.71</td>
<td>0.15</td>
<td>2.40 - 3.03</td>
<td>311.68</td>
<td>0.00</td>
</tr>
<tr>
<td>29</td>
<td>$B_{29}$</td>
<td>2.18</td>
<td>0.22</td>
<td>1.74 - 2.62</td>
<td>100.48</td>
<td>0.00</td>
</tr>
<tr>
<td>30</td>
<td>$B_{30}$</td>
<td>2.59</td>
<td>0.15</td>
<td>2.28 - 2.90</td>
<td>283.64</td>
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</tr>
<tr>
<td>31</td>
<td>$B_{31}$</td>
<td>2.68</td>
<td>0.11</td>
<td>2.46 - 2.90</td>
<td>606.27</td>
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</tr>
<tr>
<td>32</td>
<td>$B_{32}$</td>
<td>2.75</td>
<td>0.15</td>
<td>2.43 - 3.06</td>
<td>318.61</td>
<td>0.00</td>
</tr>
<tr>
<td>33</td>
<td>$B_{33}$</td>
<td>2.81</td>
<td>0.22</td>
<td>2.37 - 3.25</td>
<td>166.94</td>
<td>0.00</td>
</tr>
<tr>
<td>34</td>
<td>$B_{34}$</td>
<td>2.93</td>
<td>0.22</td>
<td>2.49 - 3.37</td>
<td>181.50</td>
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</tr>
<tr>
<td>35</td>
<td>$B_{35}$</td>
<td>3.20</td>
<td>0.22</td>
<td>2.76 - 3.64</td>
<td>216.49</td>
<td>0.00</td>
</tr>
<tr>
<td>36</td>
<td>$B_{36}$</td>
<td>4.21</td>
<td>0.22</td>
<td>3.77 - 4.65</td>
<td>374.72</td>
<td>0.00</td>
</tr>
<tr>
<td>37</td>
<td>$B_{37}$</td>
<td>4.24</td>
<td>0.22</td>
<td>3.80 - 4.68</td>
<td>380.08</td>
<td>0.00</td>
</tr>
<tr>
<td>38</td>
<td>$B_{38}$</td>
<td>4.39</td>
<td>0.15</td>
<td>4.08 - 4.71</td>
<td>816.76</td>
<td>0.00</td>
</tr>
<tr>
<td>39</td>
<td>$B_{39}$</td>
<td>5.42</td>
<td>0.22</td>
<td>4.98 - 5.86</td>
<td>621.08</td>
<td>0.00</td>
</tr>
</tbody>
</table>

$R$-squared: 0.9935

Adjusted $R$-squared: 0.9901

df numerator ($F$-statistic): 39

df denominator ($F$-statistic): 36

No. observations: 75
of some interesting questions related to the tuning of the parameters of the piecewise monotonic fit. For example, one such question is whether an optimal piecewise monotonic fit with $k$ monotonic sections may be further smoothed by concatenating successive intervals of equal components that do not differ significantly.

Another question is whether a piecewise monotonic fit with more monotonic sections explains significantly better the variability of the data compared with an optimal fit with fewer monotonic sections. We have already developed some statistical tests (see [11] and [12]) that consider this question, while the analysis we presented in this paper shows that there is room for improvement.

These questions and more results on hypothesis testing, as well as the investigation of a parsimonious version of the linear model of Section III will be published separately from the authors.

REFERENCES