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Numerical Smoothing and Differentiation by Finite Differences

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Numerical Smoothing and Differentiation by Finite Differences

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NUMERICAL SMOOTHING AND DIFFERENTIATION BY FINITE DIFFERENCES

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ABSTRACT. General formulae are derived for digital polynomial smoothing and digital polynomial differentiation of data observed at equal abscissa spacings. The operations are performed by a moving fit of polynomials to small overlapping subsets of the data. Results are also derived for the special situation in which the moving fit approaches the boundary of the data set. Brief discussions indicate how the formulae are applied in practical situations and include a description of an error detection and correction technique which is very closely related to smoothing.

1. Introduction. The purpose of this paper is to present the theoretical results arising in the solution to the problems of digital polynomial smoothing and digital polynomial differentiation of observed (hence, noisy) data with equally spaced argument values. The method of smoothing is a simple moving fit of polynomials of a fixed, but arbitrary, degree to the data. At each step, the polynomial is fitted to a limited subset of consecutive data points, whose size is related to the degree of the polynomial. Furthermore, the moving fit is used to evaluate the polynomial at only the central point of the subset at each step. Smoothing is accomplished by replacing the original datum at the current central position by the polynomial value.

The results for polynomial smoothing extend in a natural way to the derivatives of the fitted polynomials, thereby yielding a method for the numerical differentiation of the data. Differentiation is accomplished in the same manner as smoothing in that again a moving fit is applied to subsets of consecutive data points and the fit is used to evaluate the derivative of the polynomial at the central point of the subset of data at each step. The polynomial derivative is then taken to be the derivative of the subset of data points at the central point of the subset. Again, the size of the subsets and the degree of the fitted polynomials are related.

There is an exception to the use of only the central point of each subset of data. When points near the boundaries of the full data set are encountered, results for both smoothing and differentiation must be extended to additional points at and near the boundaries in those subsets.

The advantages of digital polynomial smoothing and differentiation for data having equidistant arguments are that the formulae are independent of the specific data set to which they are applied, and the formulae use only finite differences of the data and, hence, are computationally efficient. In fact the coefficients of the finite differences are strictly rational numbers and so only integer arithmetic is involved.

While it is clear that the smoothing and differentiation operators are both linear filters, this paper will not develop that approach. Furthermore, this paper is limited to the derivation of the basic formulae and brief discussions of their application. Background and details on the smoothing and differentiation procedures and their practical implementation will be given in a series of three papers by Fleming and Hill, [1], [2], and [3]. Specific examples and extensions to higher dimensions also will be reserved for those papers.

2. Preliminaries. In practice, the numerical smoothing and differentiation procedures are applied to the entire data set by a moving fit, but for our purposes it is sufficient to restrict our results to a typical subset S of data referred to in Section 1. We require S to contain 2n+1 data points y_i and we may assume without loss of generality that the equally spaced abscissae have unit spacing at integer values. In fact, there is also no loss in generality if for simplicity we choose the integer values to be fixed and centered on zero, that is,

$$S = \{y_i = y(i) : i = -n, \ldots, o, \ldots, n\} \tag{1}$$

At the heart of this paper is the following problem.

PROBLEM 1. *Fit the polynomial*

$$P(x) = c_0 + c_1 x + c_2 x^2 + \ldots + c_{2n-2} x^{2n-2}$$

by least squares to the set S, that is, minimize the sum

$$\sum_{i=-n}^{n} [P(i) - y_i]^2$$

<u>to find explicit expressions for c_0 and c_1 in terms of the elements of S.</u> Since $P(0) = c_0$ and $P'(0) = c_1$, the basic devices for smoothing and differentiating in terms of S will have been established by the solution to this problem.

Before going into the solution, we state some definitions and two well-known properties from combinatorial analysis that are needed in the sequel. The notation for the binomial coefficients is given the following expanded definition for non-negative integers i and n:

$$(2) \qquad \binom{n}{i} = \begin{cases} \dfrac{n!}{i!(n-i)!} & \text{for } 0 \leqq i \leqq n, \\ 0 & \text{otherwise.} \end{cases}$$

It also will be useful to remember that $\binom{n}{i} = \binom{n}{n-i}$. Forward differences for the set S of (1) are defined as follows:

$$(3) \qquad (-1)^n \Delta^{2n-1} y_0 = \sum_{i=-n}^{n-1} (-1)^i \binom{2n-1}{n+i} y_i$$

and

$$(4) \qquad (-1)^n \Delta^{2n-1} y_1 = \sum_{i=-n}^{n-1} (-1)^i \binom{2n-1}{n+i} y_{i+1}$$

are the differences of order 2n-1 for the points y_0 and y_1, respectively, of S, while

$$(5) \qquad (-1)^n \Delta^{2n} y_0 = \sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} y_i$$

is the <u>2n</u>th difference of y_0. It follows from these three definitions that

(6) $$\Delta^{2n} y_0 = \Delta^{2n-1} y_0 - \Delta^{2n-1} y_1 .$$

For non-negative integers i, k, m, and n, the two combinatorial properties are

(7) $$\sum_{i=0}^{k} \binom{m}{i}\binom{n}{k-i} = \binom{m+n}{k}$$

for $k \leqq m+n$, and

(8) $$\sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} (x+i)^m = 0$$

for $m < 2n$ and arbitrary x. Identity (7) follows from a comparison of the coefficients of the term x^k on both sides of the identity $(1+x)^m (1+x)^n = (1+x)^{m+n}$, while (8) is just an expression of the well-known fact that the finite difference of order n of a polynomial of degree less than n is zero.

For a proof to follow, we also will need to know explicitly the first two rows of the inverse of the square matrix $\underset{\sim}{B}$, which is of the form

(9) $$\underset{\sim}{B} = [b_{ij} = i^j : i = -n, \ldots, n;\ j=0, 1, \ldots, 2n].$$

The details are given in the following lemma.

LEMMA 1. <u>Given the unit basis vectors of dimension 2n+1, $\underset{\sim}{e}_1 = [1, 0, 0, \ldots, 0]^T$ and $\underset{\sim}{e}_2 = [0, 1, 0, \ldots, 0]^T$, and the matrix $\underset{\sim}{B}$ of (9), there exist unique vectors $\underset{\sim}{v}_1$ and $\underset{\sim}{v}_2$ of dimension 2n+1 with the property</u>

(10) $$\underset{\sim}{B}^T \underset{\sim}{v}_\ell = \underset{\sim}{e}_\ell,\ \ell = 1, 2.$$

In fact, $\underset{\sim}{v}_1$ and $\underset{\sim}{v}_2$ are given by

(11) $$v_{1i} = \begin{Bmatrix} 1, & i=0, \\ 0, & i=\pm 1, \ldots, \pm n, \end{Bmatrix}$$

and

(12) $$v_{2i} = (-1)^{i+1} i \sum_{k=|i|}^{n} \frac{(k-1)!(k-1)!}{(k-i)!(k+i)!}$$

Proof. The validity of (10) for $\ell=1$ is established by inspection. The proof for $\ell=2$ is by induction. For n=1, (9) and (12) applied to (10) become

$$\sum_{i=-1}^{1} v_{2i} b_{ij} = \tfrac{1}{2}[-(-1)^j + (1)^j] = \delta_{1j}, \; j=0, 1, 2,$$

where δ_{ij} is the Kronecker delta.

Now assume that the Lemma holds for n, that is,

(13) $$\delta_{1j} = \sum_{i=-n}^{n} (-1)^{i+1} i \sum_{k=|i|}^{n} \frac{(k-1)!(k-1)!}{(k-i)!(k+i)!} i^j$$

$$= \sum_{k=1}^{n} \frac{[(k-1)!]^2}{(2k)!} \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{j+1}$$

Hence, to prove the Lemma for n+1, we must show that

(14) $$\sum_{k=1}^{n+1} \frac{[(k-1)!]^2}{(2k)!} \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{j+1} = \delta_{1j}.$$

Notice first that the sum over i in (14) is zero whenever $j+1 < 2k$ by virtue of property (8). Therefore, the term with $k = n+1$ in the first sum in (14) is zero for $j = 0, 1, \ldots, 2n$, and so (14) reduces to (13) and is satisfied by the induction hypothesis. This leaves only the cases j = 2n+1 and 2n+2 to be proved, but the sum over i in (14) vanishes for any even value of j because the terms having indices i and -i cancel. Thus, there remains only the case j = 2n+1, that is, we must show that

$$(15)\qquad \sum_{k=1}^{n+1} \frac{[(k-1)!]^2}{(2k)!} \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{2n+2} = 0.$$

Let

$$(16)\qquad C_{k,n} = \frac{[(k-1)!]^2}{(2k)!} \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{2n}$$

for $k \leqq n+1$. We verify that

$$(17)\qquad C_{k,n+1} = k^2 C_{k,n} - (k-1)^2 C_{k-1,n} .$$

Definition (16) yields

$$k^2 C_{k,n} - (k-1)^2 C_{k-1,n}$$

$$= \frac{[(k-1)!]^2}{(2k)!} \left\{ k^2 \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{2n} - (2k)(2k-1) \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k-2}{k+i-1} i^{2n} \right\}$$

$$= \frac{[(k-1)!]^2}{(2k)!} \left\{ [k^2 - (k+i)(k-i)] \sum_{i=-k}^{k} (-1)^{i+1} \binom{2k}{k+i} i^{2n} \right\}$$

$$= C_{k,n+1} ,$$

where the second half of definition (2) was used in the second sum of the first line.

Applying (16) and (17) to (15), we have

$$\sum_{k=1}^{n+1} C_{k,n+1} = \sum_{k=1}^{n+1}\left[k^2 C_{k,n} - (k-1)^2 C_{k-1,n}\right]$$

$$= (n+1)^2 C_{n+1,n} + \sum_{k=1}^{n} k^2 C_{k,n} - \sum_{k=1}^{n} k^2 C_{k,n} - 0^2 C_{0,n}$$

$$= (n+1)^2 C_{n+1,n}.$$

However, $C_{n+1,n}$ is zero because the sum in (16) is the finite difference of order 2n+2 of a polynomial whose degree is less than 2n+2. Therefore, the double sum in (15) is indeed zero.

Finally, the uniqueness of vectors $\underset{\sim}{v}_1$ and $\underset{\sim}{v}_2$ follows from the existence of the inverse of the matrix $\underset{\sim}{B}$. □

3. Principal Results. We now derive the solutions to Problem 1.

THEOREM 1. <u>If a polynomial of degree 2n-2 is fitted to the data set S of (1) by least squares, then there exists a rational number θ_n such that the constant term c_0 of the polynomial has the form</u>

(18) $$c_0 = y_0 - \theta_n (-1)^n \Delta^{2n} y_0,$$

<u>where</u>

(19) $$\theta_n = \binom{2n}{n} \Big/ \binom{4n}{2n} = \frac{\prod_{i=1}^{n} (2i-1)}{\prod_{i=1}^{n} (2n+2i-1)} .$$

<u>Furthermore, the second term in the polynomial is given by</u>

(20) $$c_1 = \sum_{k=1}^{n} \frac{(-1)^k}{k} \binom{2k}{k}^{-1} \left[2\Delta^{2k-1} y_0 - \Delta^{2k} y_0\right] - \alpha_{2n-2} (-1)^n \left[2\Delta^{2n-1} y_0 - \Delta^{2n} y_0\right],$$

where

$$\alpha_{2n-2} = \binom{4n-2}{2n-1}^{-1} \sum_{k=1}^{n} \frac{2n}{k(n+k)} \binom{2k}{k}^{-1} \binom{2n+2k-2}{n+k-1}.$$

Proof. Define the matrix $\underset{\sim}{A} = [a_{ij} = i^j: \ i=-n, \ldots, n; \ j = 0, 1, \ldots, 2n-2]$, the vector of coefficients of the polynomial by $\underset{\sim}{c} = [c_j: j = 0, 1, \ldots, 2n-2]$, and the vector of data points of the set S in (1) by $\underset{\sim}{y} = [y_i: \ i=-n, \ldots, n]$. Then the coefficients are determined by the solution to the system of normal equations

(21) $$\underset{\sim}{A}^T \underset{\sim}{A} \underset{\sim}{c} = \underset{\sim}{A}^T \underset{\sim}{y}.$$

Since we wish to determine only the pair of coefficients c_0 and c_1, we need only to find vectors $\underset{\sim}{u}_1$ and $\underset{\sim}{u}_2$ of dimension 2n-1 satisfying

(22) $$\underset{\sim}{u}_\ell^T \underset{\sim}{A}^T \underset{\sim}{A} = \underset{\sim}{e}_\ell^T$$

for $\ell = 1, 2$, where $\underset{\sim}{e}_1 = [1, 0, 0, \ldots, 0]^T$ and $\underset{\sim}{e}_2 = [0, 1, 0, \ldots, 0]^T$ are the unit basis vectors of dimension 2n-1. It follows from (21) that

(23) $$c_{\ell-1} = \underset{\sim}{u}_\ell^T \underset{\sim}{A}^T \underset{\sim}{y}$$

for $\ell = 1, 2$.

Finding the unique vectors $\underset{\sim}{u}_\ell$ is by (22) tantamount to finding the first two rows of the inverse of $\underset{\sim}{A}^T \underset{\sim}{A}$ for general n. How to do this by direct mean is not at all obvious. Instead, we seek any pair of vectors $\underset{\sim}{v}_1$ and $\underset{\sim}{v}_2$ of dimension 2n+1 for which

(24) $$\underset{\sim}{A}^T \underset{\sim}{v}_\ell = \underset{\sim}{e}_\ell,$$

for $\ell = 1, 2$. Lemma 1 provides us with just such a pair of vectors. Now if $\underset{\sim}{v}_\ell$ were $\underset{\sim}{A}\underset{\sim}{u}_\ell$, we could use $\underset{\sim}{v}_\ell$ to find $c_{\ell-1}$ via (23). This is not the case, but we can use $\underset{\sim}{v}_\ell$ to find $\underset{\sim}{u}_\ell$. It has the form

$$(25) \qquad \underset{\sim}{u}_\ell = (\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T\underset{\sim}{v}_\ell,$$

since by (24)

$$\underset{\sim}{A}^T\underset{\sim}{A}\underset{\sim}{u}_\ell = \underset{\sim}{A}^T\underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T\underset{\sim}{v}_\ell = \underset{\sim}{e}_\ell,$$

thereby satisfying (22). Thus, all we need to know to calculate $c_{\ell-1}$ by (23) is the vector $\underset{\sim}{A}\underset{\sim}{u}_\ell$, which by (25) is

$$(26) \qquad \underset{\sim}{A}\underset{\sim}{u}_\ell = \underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T\underset{\sim}{v}_\ell.$$

Fortunately, the inverse matrix in (26) can be avoided because $\underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}$ is the projection operator on the linear manifold of a (2n+1)-dimensional Euclidean space R_{2n+1} spanned by the 2n-1 linearly independent columns of $\underset{\sim}{A}$. Hence, the orthogonal complement of this linear manifold is a linear manifold of R_{2n+1} spanned by two linearly independent vectors orthogonal to each of the columns of $\underset{\sim}{A}$. Convenient choices for this pair of vectors are the vector of coefficients of the finite difference operator of order 2n, namely

$$(27) \qquad \underset{\sim}{w}_1 = \left[w_{1i} = (-1)^i\binom{2n}{n+i}: \ i = -n, \ldots, n\right],$$

and a linear combination of vectors of coefficients of the finite difference operator of order 2n-1, that is,

$$(28) \qquad \underset{\sim}{w}_2 = \left[w_{2i} = (-1)^i\left\{\binom{2n-1}{n+i} - \binom{2n-1}{n+i-1}\right\} = (-1)^{i+1}\,\frac{i}{n}\binom{2n}{n+i}: \ i=-n, \ldots, n\right].$$

These vectors are orthogonal to the columns of $\underset{\sim}{A}$ because the inner products of $\underset{\sim}{w}_1$ and $\underset{\sim}{w}_2$ with the columns of $\underset{\sim}{A}$ yield, respectively, the $\underline{2n}$th and $\underline{2n-1}$st differences of i^j, which are zero for $j = 0, 1, \ldots, 2n-2$ by (8). In addition, the elements of $\underset{\sim}{w}_1$ possess the symmetry property $w_{1i} = w_{1,-i}$, while the elements of $\underset{\sim}{w}_2$ were specifically chosen to have the anti-symmetry property $w_{2,-i} = -w_{2i}$ so that $\underset{\sim}{w}_1$ and $\underset{\sim}{w}_2$ are guaranteed to be orthogonal to each other as well.

Since $\underset{\sim}{w}_1$ and $\underset{\sim}{w}_2$ span the orthogonal complement of the space spanned by the columns of $\underset{\sim}{A}$, we can write the projection operator in terms of the projection on the orthogonal complement, namely

$$(29) \qquad \underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T = \underset{\sim}{I} - \frac{\underset{\sim}{w}_1\underset{\sim}{w}_1^T}{\|\underset{\sim}{w}_1\|^2} - \frac{\underset{\sim}{w}_2\underset{\sim}{w}_2^T}{\|\underset{\sim}{w}_2\|^2} ,$$

where $\underset{\sim}{I}$ is the identity matrix.

The formal solution to our problem is now in hand. Apply (29) to (26), and in turn apply that result to (23) to obtain the following representations for coefficients c_0 and c_1:

$$(30) \qquad c_{\ell-1} = \underset{\sim}{v}_\ell^T\underset{\sim}{y} - \frac{(\underset{\sim}{v}_\ell^T\underset{\sim}{w}_1)(\underset{\sim}{w}_1^T\underset{\sim}{y})}{\|\underset{\sim}{w}_1\|^2} - \frac{(\underset{\sim}{v}_\ell^T\underset{\sim}{w}_2)(\underset{\sim}{w}_2^T\underset{\sim}{y})}{\|\underset{\sim}{w}_2\|^2}$$

for $\ell = 1, 2$.

To make (30) explicit, we first evaluate the normed quantities the denominators. By (27), (28), and repeated use of (2) and (7),

$$(31) \qquad \underset{\sim}{w}_1^T\underset{\sim}{w}_1 = \sum_{i=-n}^{n} \binom{2n}{n+i}\binom{2n}{n+i} = \sum_{j=0}^{2n} \binom{2n}{j}\binom{2n}{2n-j} = \binom{4n}{2n},$$

and

$$(32)\qquad \underset{\sim}{w}_2^T \underset{\sim}{w}_2 = \sum_{i=-n}^{n} \left[\binom{2n-1}{n+i} - \binom{2n-1}{n+i-1}\right]\left[\binom{2n-1}{n-i-1} - \binom{2n-1}{n-i}\right]$$

$$= \sum_{k=0}^{2n-1} \binom{2n-1}{k}\binom{2n-1}{2n-1-k} - \sum_{k=0}^{2n} \binom{2n-1}{2n-k}\binom{2n-1}{k}$$

$$- \sum_{k=0}^{2n-2} \binom{2n-1}{k}\binom{2n-1}{2n-2-k} + \sum_{k=0}^{2n-1} \binom{2n-1}{2n-1-k}\binom{2n-1}{k}$$

$$= \binom{4n-2}{2n-1} - \binom{4n-2}{2n} - \binom{4n-2}{2n-2} + \binom{4n-2}{2n-1}$$

$$= 2\left[\binom{4n-2}{2n-1} - \binom{4n-2}{2n}\right] = \frac{1}{n}\binom{4n-2}{2n-1}.$$

In addition, we will need the scalar $\underset{\sim}{v}_2^T \underset{\sim}{w}_2$. For this we write v_{2i} of (12) in the equivalent form

$$(33)\qquad v_{2i} = (-1)^i \sum_{k=|i|}^{n} \frac{1}{k}\binom{2k}{k}^{-1}\left[\binom{2k-1}{k+i} - \binom{2k-1}{k-1+i}\right],$$

so that again by the repeated use of (2) and (7),

$$(34)\qquad \underset{\sim}{v}_2^T \underset{\sim}{w}_2 = \sum_{i=-n}^{n} \left[\binom{2n-1}{n+i} - \binom{2n-1}{n+i-1}\right] \sum_{k=|i|}^{n} \frac{1}{k}\binom{2k}{k}^{-1}\left[\binom{2k-1}{k+i} - \binom{2k-1}{k-1+i}\right]$$

$$= \sum_{k=1}^{n} \frac{1}{k}\binom{2k}{k}^{-1} \sum_{i=-k}^{k} \left[\binom{2n-1}{n+i} - \binom{2n-1}{n-1+i}\right]\left[\binom{2k-1}{k-1-i} - \binom{2k-1}{k-i}\right]$$

$$= \sum_{k=1}^{n} \frac{1}{k}\binom{2k}{k}^{-1}\left[\sum_{j=0}^{n+k-1}\binom{2n-1}{n+k-1-j}\binom{2k-1}{j} - \sum_{j=0}^{n+k}\binom{2n-1}{n+k-j}\binom{2k-1}{j}\right.$$

$$\left. - \sum_{j=0}^{n+k-2}\binom{2n-1}{n+k-2-j}\binom{2k-1}{j} + \sum_{j=0}^{n+k-1}\binom{2n-1}{n+k-1-j}\binom{2k-1}{j}\right]$$

$$= \sum_{k=1}^{n} \frac{1}{k}\binom{2k}{k}^{-1}\left[\binom{2n+2k-2}{n+k-1} - \binom{2n+2k-2}{n+k} - \binom{2n+2k-2}{n+k-2} + \binom{2n+2k-2}{n+k-1}\right]$$

$$= \sum_{k=1}^{n} \frac{2}{k}\binom{2k}{k}^{-1}\left[\binom{2n+2k-2}{n+k-1} - \binom{2n+2k-2}{n+k}\right]$$

$$= \sum_{k=1}^{n} \frac{2}{k(n+k)}\binom{2k}{k}^{-1}\binom{2n+2k-2}{n+k-1}.$$

Next, we note that since the elements of $\underset{\sim}{v}_1$ and $\underset{\sim}{w}_1$ are arranged symmetrically about the center element and those of $\underset{\sim}{v}_2$ and $\underset{\sim}{w}_2$ are arranged anti-symmetrically, it follows that $\underset{\sim}{v}_1^T\underset{\sim}{w}_2 = 0$ and $\underset{\sim}{v}_2^T\underset{\sim}{w}_1 = 0$. Also, by (11) and (27), $\underset{\sim}{v}_1^T\underset{\sim}{w}_1 = \binom{2n}{n}$. Finally, by (1), (11), (33), (37), (28), (31), (34), and the foregoing, we may write (30) as follows:

$$c_0 = y_0 - \binom{2n}{n}\binom{4n}{2n}^{-1}\sum_{i=-n}^{n}(-1)^i\binom{2n}{n+i}y_i,$$

which by (5) yields (18) and (19), and

(35)
$$c_1 = \sum_{i=-n}^{n}(-1)^i\sum_{k=|i|}^{n}\frac{1}{k}\binom{2k}{k}^{-1}\left[\binom{2k-1}{k+i} - \binom{2k-1}{k-1+i}\right]y_i$$

$$-\binom{4n-2}{2n-1}^{-1}\left[\sum_{k=1}^{n}\frac{2n}{k(n+k)}\binom{2k}{k}^{-1}\binom{2n+2k-2}{n+k-1}\right]\sum_{i=-n}^{n}(-1)^i\left[\binom{2n-1}{n+i} - \binom{2n-1}{n+i-1}\right]y_i$$

$$= \sum_{k=1}^{n} \frac{1}{k}\binom{2k}{k}^{-1}\left[\sum_{i=-k}^{k-1}(-1)^i\binom{2k-1}{k+i}y_i + \sum_{i=-k}^{k-1}(-1)^i\binom{2k-1}{k+i}y_{i+1}\right]$$

$$- \binom{4n-2}{2n-1}^{-1}\left[\sum_{k=1}^{n}\frac{2n}{k(n+k)}\binom{2k}{k}^{-1}\binom{2n+2k-2}{n+k-1}\right]\left[\sum_{i=-n}^{n-1}(-1)^i\binom{2n-1}{n+i}(y_i + y_{i+1})\right],$$

which by (3), (4), and (6) is (20). The identity in (19) follows from the relationship

$$(36) \qquad \binom{2n}{n}\binom{4n}{2n}^{-1} = \frac{(2n)!(2n)!(2n)!}{n!n!(4n)!}$$

$$= \frac{2^n n![(2n-1)(2n-3)\ldots 1]}{n!} \times \frac{[2n(2n-1)\ \ldots\ (n+1)]n!}{n!}$$

$$\times \frac{(2n)!}{2^n[2n(2n-1)\ \ldots\ (n+1)][(4n-1)(4n-3)\ \ldots\ (2n+1)](2n)!}. \qquad \square$$

The machinery developed in the proof of Theorem 1 can be used to advantage in developing results analogous to those in Theorem 1 for polynomials of degree 2n-1.

COROLLARY 1. <u>If the degree of the polynomial in Theorem 1 is raised from 2n-2 to 2n-1, all the results of that theorem remain valid, with the exception that $\alpha_{2n-1} \equiv 0$ replaces α_{2n-2} in (20), that is,</u>

$$(37) \qquad c_1 = \sum_{k=1}^{n} \frac{(-1)^k}{k}\binom{2k}{k}^{-1}\left[2\Delta^{2k-1}y_0 - \Delta^{2k}y_0\right].$$

<u>Proof</u>. Use the proof of Theorem 1, but with the range of the index j increased from 2n-2 to 2n-1, that is, j = 0, 1, ..., 2n-1 in the definition of $\underset{\sim}{A}$, $\underset{\sim}{c}$, $\underset{\sim}{e}_\ell$ and $\underset{\sim}{u}_\ell$. The proof goes through as before,

except that now $\underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T$ is the projection operator on the linear manifold of R_{2n+1} spanned by 2n linearly independent columns of $\underset{\sim}{A}$. Consequently, the orthogonal complement of this linear manifold is spanned by a single vector orthogonal to each of the columns of $\underset{\sim}{A}$. That vector is $\underset{\sim}{w}_1$ of (27). In other words, (29) becomes

$$(38) \qquad \underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T = \underset{\sim}{I} - \frac{\underset{\sim}{w}_1\underset{\sim}{w}_1^T}{\|\underset{\sim}{w}_1\|^2},$$

and so (30) reduces to

$$(39) \qquad c_{\ell-1} = \underset{\sim}{v}_\ell^T\underset{\sim}{y} - \frac{\underset{\sim}{v}_\ell^T\underset{\sim}{w}_1 \; \underset{\sim}{w}_1^T\underset{\sim}{y}}{\|\underset{\sim}{w}_1\|^2}$$

for $\ell = 1, 2$.

For the case $\ell=1$, (39) and (30) are identical because $\underset{\sim}{v}_1^T\underset{\sim}{w}_2 = 0$ in (30). Hence, the remainder of the proof is identical to that given for Theorem 1. On the other hand, for the case $\ell= 2$, $\underset{\sim}{v}_2^T\underset{\sim}{w}_1 = 0$ in (39), so that $c_1 = \underset{\sim}{v}_2^T\underset{\sim}{y}$, which is the first double sum in (35) in the proof of Theorem 1, which in turn is (37). □

COROLLARY 2. <u>If the degree of the polynomial in Theorem 1 is raised from 2n-2 to 2n, then the constant term of the polynomial has the trivial relationship</u> $c_0 = y_0$, <u>but the second coefficient</u> c_1 <u>is identical to (37) of Corollary 1.</u>

<u>Proof.</u> In this case the matrix $\underset{\sim}{A}$ in the proof of Theorem 1 is $\underset{\sim}{B}$ of (9), and so by Lemma 1 we have that

$$c_{\ell-1} = \underset{\sim}{v}_\ell^T\underset{\sim}{y}$$

for $\ell = 1, 2$. The results follow from (11), (33), and the first double sum in (35). □

4. Additional Results. Two known results are presented for completeness and for consistency with our previous results and notation.

THEOREM 2. If a polynomial $P(x)$ of degree $2n-1$ is fitted exactly to the data set S of (1) with the point y_0 deleted (i.e., the set $S - \{y_0\}$), then the constant term of the polynomial is

$$(40) \qquad c_0 = y_0 - \binom{2n}{n}^{-1} (-1)^n \Delta^{2n} y_0 .$$

Proof. By hypothesis $y_i = P(i)$ for $i = -n, \ldots, -1, 1, \ldots, n$. Since it is not necessarily true that $y_0 = P(0)$, let $\delta = P(0) - y_0 = c_0 - y_0$. Then by (5) and (8)

$$(-1)^n \Delta^{2n} y_0 = \sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} y_i = \sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} P(i) - \binom{2n}{n}\delta$$

$$= 0 - \binom{2n}{n}\delta,$$

which yields (40), since $\delta = c_0 - y_0$. □

Theorem 2 states that the distance between the point y_0 of S and the polynomial of degree $2n-1$ that interpolates the $2n$ neighbors of y_0 is $\binom{2n}{n}^{-1} (-1)^n \Delta^{2n} y_0$.

Theorem 3. If each point of the extended set of data points $T = \{y_i = y(i): i = -2n, \ldots, 2n\}$ lies on a polynomial $P(x)$ of degree $2n-1$, except the point y_0 which lies a distance δ away from the polynomial, then the sum

(41) $$\sum_{k=-n}^{n} \Delta^{2n} y_k = 0,$$

where $\Delta^{2n} y_k$, defined by

(42) $$(-1)^n \Delta^{2n} y_k = \sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} y_{i+k} ,$$

is the 2nth forward difference of the point in S of (1). Furthermore, the maximum of the absolute values of these 2n+1 differences of the set S in T is $\Delta^{2n} y_0$.

Proof. By hypothesis $y_i = P(i)$ for $i = -2n, \ldots, -1, 1, \ldots, 2n$ and $y_0 = P(0) - \delta$. Therefore, by (42) and (8)

(43) $$(-1)^n \Delta^{2n} y_k = \sum_{i=-n}^{n} (-1)^i \binom{2n}{n+i} P(i+k) - (-1)^k \binom{2n}{n-k} \delta = (-1)^{k+1} \binom{2n}{n+k} \delta,$$

and so the sum

$$\sum_{k=-n}^{n} \Delta^{2n} y_k = \delta \sum_{k=-n}^{n} (-1)^{n+k+1} \binom{2n}{n+k} = 0$$

by (8). In addition, for $k = -n, \ldots, -1, 1, \ldots, n$,

(44) $$|\Delta^{2n} y_k| = \binom{2n}{n+k} |\delta| < \binom{2n}{n} |\delta| = |\Delta^{2n} y_0|,$$

by (43) and (40). □

5. Results Near Boundaries. When the moving polynomial-fit procedure for both smoothing and differentiation approaches a boundary of the full data set, the procedure breaks down because the central point of the subset S of (1) no longer has its full complement of 2n neighboring

points. The solution to this difficulty is to start and stop the moving fit n+1 points away from the boundary, and then simply use the resulting values P(i) of the fitted polynomial for i = -n, ..., -1, at the beginning of the data stream and for i = 1, ..., n at the end. The necessary details are now provided.

THEOREM 4. If the polynomial P(x) of degree 2n-2 is fitted to the data set S of (1) by least squares, the polynomial values for i = -n, ..., n are given by

$$(45)\qquad P(i) = y_i - (-1)^{n+i}\binom{2n}{n+i}\left\{\binom{4n}{2n}^{-1}\Delta^{2n} y_0 - i\binom{4n-2}{2n-1}^{-1}\left[2\Delta^{2n-1} y_0 - \Delta^{2n} y_0\right]\right\}.$$

Proof. Define the matrix $\underset{\sim}{A}$ and vectors $\underset{\sim}{c}$ and $\underset{\sim}{y}$ as in the proof of Theorem 1, then it follows that the vector of polynomial values

$$(46)\qquad \underset{\sim}{p} = [p_i = P(i):\ i = -n, \ldots, n]$$

can be written

$$(47)\qquad \underset{\sim}{p} = \underset{\sim}{A}\underset{\sim}{c}$$

Furthermore, the system of normal equations (21) can be written

$$\underset{\sim}{c} = (\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T\underset{\sim}{y};$$

therefore,

$$(48)\qquad \begin{aligned}\underset{\sim}{p}-\underset{\sim}{y} &= \underset{\sim}{A}\underset{\sim}{c}-\underset{\sim}{y}\\ &= [\underset{\sim}{A}(\underset{\sim}{A}^T\underset{\sim}{A})^{-1}\underset{\sim}{A}^T - \underset{\sim}{I}]\underset{\sim}{y}.\end{aligned}$$

Now follow the proof of Theorem 1 from (21) through (29). Applying (29) to (48), we have

$$\underset{\sim}{p}-\underset{\sim}{y} = -\frac{(\underset{\sim}{w}_1^T\underset{\sim}{y})\underset{\sim}{w}_1}{\|\underset{\sim}{w}_1\|^2} - \frac{(\underset{\sim}{w}_2^T\underset{\sim}{y})\underset{\sim}{w}_2}{\|\underset{\sim}{w}_2\|^2}.$$

By (27), (28), (31) and (32), the elements of these vectors can be written

(49)
$$P(i) = y_i - \binom{4n}{2n}^{-1}\left[\sum_{k=-n}^{n}(-1)^k\binom{2n}{n+k}y_k\right](-1)^i\binom{2n}{n+i}$$
$$- n\binom{4n-2}{2n-1}^{-1}\left\{\sum_{k=-n}^{n}(-1)^k\left[\binom{2n-1}{n+k}-\binom{2n-1}{n+k-1}\right]y_k\right\}(-1)^{i+1}\frac{i}{n}\binom{2n}{n+i},$$

from which (45) results after applying (3), (4), (5) and (6). □

Note that for i=0, (45) becomes (18).

COROLLARY 3. <u>If a polynomial P(x) of degree 2n-1 is fitted to the data set S by least squares, the polynomial values for i = -n, ..., n are given by</u>

(50)
$$P(i) = y_i - (-1)^{n+i}\binom{2n}{n+i}\binom{4n}{2n}^{-1}\Delta^{2n}y_0.$$

<u>Proof</u>. Using the proof of Theorem 4 and the supporting arguments of Corollary 1 related to the increase in dimension, we can apply (38) to (48) and obtain

$$\underset{\sim}{p}-\underset{\sim}{y} = -\frac{(\underset{\sim}{w}_1^T\underset{\sim}{y})\underset{\sim}{w}_1}{\|\underset{\sim}{w}_1\|^2}.$$

The elements of these vectors are those given in the first line of (49), from which one obtains (50). □

Note that for i=0, (50) also becomes (18).

For the derivatives near boundaries, we need to determine the derivative of the polynomials $P_k(x)$ of degrees k = 2n-2, 2n-1 fitted by least squares to the set S, and of the exact-fit polynomial of degree k=2n, for x=i with i = -n, ..., n. The problem can be formulated as follows. Let $\underset{\sim}{p}'_k$ be the required vector of derivatives of the polynomial $P_k(x)$, that is,

$$\underset{\sim}{p}'_k = [p'_{ki} = P'_k(i): \; i = -n, \ldots, n],$$

and let $\underset{\sim}{D}_{k+1}$ be a (k+1)-dimensional superdiagonal matrix of the form

$$\underset{\sim}{D}_{k+1} = [d_{i,i+1} = i, \; i=1, \ldots, k; \; d_{ij} = 0, \text{ otherwise}: \; i, j=1, \ldots, k+1].$$

Then by the structure of the matrix $\underset{\sim}{A}$ and the vector of polynomial coefficients $\underset{\sim}{c}$, it follows that the vector of polynomial derivatives is precisely

(51) $$\underset{\sim}{p}'_k = \underset{\sim}{A}\underset{\sim}{D}_{k+1}\underset{\sim}{c}$$

for k = 2n-2, ..., 2n and where $\underset{\sim}{A}$ and $\underset{\sim}{c}$ are dimensioned accordingly.

Now we do not know the full vector $\underset{\sim}{c}$, but by (47) we do know

(52) $$\underset{\sim}{A}\underset{\sim}{c} = \underset{\sim}{p}_k \quad ,$$

where $\underset{\sim}{p}_k$ is the vector (46) of polynomial values. For polynomials of degree k = 2n-2, 2n-1, 2n, these values are given explicitly by (45), (50), and $P_{2n}(i) = y_i$, respectively. Since we know only $\underset{\sim}{A}\underset{\sim}{c}$, we first must find a (2n+1)-dimensional matrix $\underset{\sim}{E}$ such that

(53) $$\underset{\sim}{E}\underset{\sim}{A} = \underset{\sim}{A}\underset{\sim}{D}_{k+1}$$

The matrix $\underset{\sim}{E}$ obviously is not unique, but any $\underset{\sim}{E}$ that satisfies (53) will suffice. Unfortunately, we cannot give a general expression for a choice of the elements of $\underset{\sim}{E}$ as a function of n. All we can say is that given the matrix $\underset{\sim}{E}$, one finds the vector $\underset{\sim}{p}'_k$ from the relationship

(54) $$\underset{\sim}{p}'_k = \underset{\sim}{E}\underset{\sim}{A}\underset{\sim}{c} = \underset{\sim}{E}\underset{\sim}{p}_k$$

obtained from (51), (52), and (53), where $\underset{\sim}{p}_k$ is known as noted previously. Thus, the problem of finding the derivatives $P'_k(i)$ for all indices i in the set S reduces to that of finding an appropriate matrix $\underset{\sim}{E}$.

6. The Smoothing Procedure. For completeness we give a brief description of how the results of this paper apply to numerical smoothing. For complete details, see [1] and [2]. One begins by choosing values n and k for the number of points in the moving fit and the degree of polynomial, respectively. Let the complete data set be $Y = \{y_j = y(j): j=1, \ldots, N\}$, where usually n is picked so that $n \ll N$. Form consecutive, overlapping subsets $S_j = \{y_{j+i}: i = -n, \ldots, n\}$ for $j = n+1, \ldots, N-n$. Then the smoothed data set $\hat{Y} = \{\hat{y}_j: j=1, \ldots, N\}$ is obtained in the following manner.

If $k = 2n-1$ and an exact polynomial fit to $S_j - \{y_j\}$ is desired, use (40), that is,

(40) $$\hat{y}_j = y_j - \binom{2n}{n}^{-1}(-1)^n\Delta^{2n}y_j.$$

For $k = 2n-1$ (or $2n-2$) and a least squares polynomial fit to S_j, use (18), that is,

(18) $$\hat{y}_j = y_j - \theta_n (-1)^n \Delta^{2n} y_j$$

with θ_n given by (19). Recall that (40) and (18) provide elements for $\hat{Y}$ only for the indices $j = n+1, \ldots, N-n$. For the remaining points at and near the boundary of Y we use

$$\hat{y}_j = P_k(j),$$

where $P_k(j)$ is given by (50) if $k = 2n-1$, and by (45) if $k = 2n-2$. Note that in both (50) and (45), $\Delta^{2n} y_0$ must be replaced by $\Delta^{2n} y_{n+1}$ if $j < n+1$ and by $\Delta^{2n} y_{N-n}$ if $j > N-n$. This entire cycle can be repeated any number of times, depending upon the amount of smoothing that is required.

A procedure closely related to smoothing, but much more selective, is an error detection and correction procedure based in part on the work of Guerra and Tapia [4]. It takes advantage of the properties developed in Theorems 2 and 3. Error detection and correction differs from smoothing in that smoothing adjusts all points in Y, whereas the error detection and correction procedure corrects only those points in Y that are bad, that is, in error by an amount greater than the background noise level of the data, which we denote by ε.

Briefly, the error detection and correction procedure works as follows. Errors are detected by generating the difference $\Delta^{2n} y_j$ for each set S_j and by searching their absolute values for the maximum value, denoted $|\Delta^{2n} y_J|$, as a result of (44) and Theorem 3. If by (40), the difference

(55) $$|c_0 - y_J| = \left| \binom{2n}{n}^{-1} (-1)^n \Delta^{2n} y_J \right| > \varepsilon,$$

(i.e., the difference is larger than the background noise level) the point y_J is assumed to be in error. Furthermore, if in analogy to (41)

$$\left| \sum_{i=-n}^{n} \Delta^{2n} y_{J+i} \right| \leq (2n+1) \binom{4n}{2n}^{\frac{1}{2}} \varepsilon, \tag{56}$$

(see [1]) the error in y_J is an isolated one relative to the set S_J and, hence, can be corrected to the value $\hat{y}_J$ using (40) with c_0 and y_0 replaced by $\hat{y}_J$ and y_J, respectively.

On the other hand, if the test (56) fails, two or more points in the set S_J are in error. In this case, y_J is corrected to $\hat{y}_J$ by the least squares polynomial using (18).

After y_J has been replaced by $\hat{y}_J$ in Y, the entire set is searched again for the maximum of the absolute values of its differences of order 2n. The point corresponding to this new maximum value also is corrected by the foregoing procedures. This process is continued until all the absolute difference quantities in (55) are less than or equal to ε. This means that in the final set $\hat{Y}$ some of the points will remain unaltered from their original value in Y, while other points may have been changed several times. In [4], Guerra and Tapia prove that this process is guaranteed to be a finite process.

Finally, we have not discussed the treatment of points at and near the boundaries of Y that may be in error. This procedure is too involved to discuss here, but can be found in [1].

7. The Differentiation Procedure. To numerically differentiate the set Y, one simply does a moving fit of the polynomial $P_k(x)$ of degree k to the subsets S_j one at a time and evaluates the derivative of the polynomial $P_k'(x)$ for x=j. Specifically, the differentiated set $Y' = \{y_j': j=1,\ldots, N\}$ is obtained in the following manner.

For a polynomial of degree k=2n (or 2n-1), one obtains y_j' by setting $y_j' = c_1$ in (20) and replacing y_0 by y_j everywhere. If a polynomial of degree 2n-2 is desired, set $y_j' = c_1$ in (37) and replace both of the y_0 by y_j. Note that this procedure provides elements for the set Y' only for the indices $j = n+1, \ldots, N-n$. For the remaining points at and near the boundary of Y, we obtain the derivatives by finding an appropriate matrix E from (53), which is then applied to (54) to obtain the elements of $\underset{\sim}{p}'$.

8. Conclusions. We have developed theoretical results for numerically smoothing noisy data sets using polynomials of degree 2n-2 and 2n-1, and for numerically differentiating data sets using polynomials of degree 2n-2, 2n-1, and 2n, where n is related to the size of the subsets S of Y. In addition, we established an interesting result for fitting a polynomial of degree 2n-1 to the set $S - \{y_0\}$, which has application to error detection and correction. Also, brief descriptions were given on the practical application of smoothing and differentiation to noisy data sets. It should be pointed out that all results and procedures in this paper hold as well for central and backward differences.

Finally, we note that the three operations, error correction, smoothing and differentiation, taken together give one a set of very versatile tools. For example, smoothing is usually more effective if error detection is done first. Also, differentiation is usually more meaningful if the data are smoothed first. In fact, some of the best results can be obtained for differentiation if all three operations are performed in order.

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TECHNICAL SERVICE PUBLICATIC[...] ports containing data, observations, instru[...] A partial listing includes data serials; prediction and outlook periodicals; technical manuals, training papers, planning reports, and information serials; and miscellaneous technical publications.

TECHNICAL REPORTS — Journal quality with extensive details, mathematical developments, or data listings.

TECHNICAL MEMORANDUMS — Reports of preliminary, partial, or negative research or technology results, interim instructions, and the like.

Information on availability of NOAA publications can be obtained from:

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