Comparison of the Method of Averages with the Method of Least Squares

By G. Dahlquist, B. Sjöberg and P. Svensson

Abstract. It is shown that the computationally simple method of averages can yield a surprisingly good solution of an overdetermined system of linear equations, provided that the grouping of the equations is done in an appropriate way. The notion of angle between linear subspaces is applied in a general comparison of this method and the method of least squares. The optimal application of the method is treated for the test problem of fitting a polynomial of degree less than six.

1. Introduction. Consider the overdetermined set of linear equations

$$Fx \approx z \tag{1.1}$$

where $z \in \boldsymbol{E}^n$, $x \in \boldsymbol{E}^m$, $n > m$ and F is a $n \times m$ matrix, whose columns are assumed to be linearly independent.

Several methods have been proposed to obtain a "solution" of such systems with less computation than that involved in the method of least squares. As an example, we mention Cauchy's method, described by Linnik [6, p. 345]. Guest [1] also uses some methods for reducing least-squares problems.

As early as in the eighteenth century overdetermined systems of equations were treated by a method, later known as the *method of averages* (MA). (Whittaker and Robinson [12, p. 258] refer to Tobias Mayer, who described it in 1748.)

This method means that the equations are separated into m groups and after that, group-wise summed. Hence the overdetermined set of equations is replaced by the system

$$G^T F y = G^T z \tag{1.2}$$

where G^T is an $m \times n$ matrix of the form

$$G^T = \begin{bmatrix} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots & \cdots & 0 & 0 & \cdots & 0 \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & \cdots & 1 & 1 & \cdots & 1 \end{bmatrix}. \tag{1.3}$$

The matrix G will be called a summation matrix, which is supposed to be chosen such that $G^T F$ is nonsingular.

In geometrical terms, (1.2) means that in MA the error vector $Fy - z$ is made orthogonal to the m-dimensional subspace $\boldsymbol{G}$ spanned by the columns of G, while in the method of least squares (MLS) the error vector is made orthogonal to the

Received July 19, 1967.

m-dimensional subspace $\boldsymbol{F}$, spanned by the columns of F, by solving the normal equations

$$F^T F x = F^T z \,. \tag{1.4}$$

In the following x and y will always denote the linear vector functions of z, which are defined by (1.4) and (1.2), respectively.

MA is attractive because of the simple arithmetic involved in the reduction to the $m \times m$ set of equations. In fact, (1.2) is obtained by $n(m+1)$ additions, while (1.4) requires $\frac{1}{2}m(m+3)n$ multiplications and about the same number of additions.

We shall now study how to choose G in order that the application of MA should give as good results as possible. First we need a measure of the goodness of the result obtained by MA and a method for computing this measure. The choice of measure depends on the nature of the errors in the overdetermined set of equations. We shall consider two measures, associated with the following problems: Let x and y be defined by (1.4) and (1.2), respectively, and let $\|\cdot\|$ be the Euclidean vector norm.

Problem 1. Determine, for a given summation matrix G,

$$\eta = \inf_z \left(\|z - Fx\|^2 / \|z - Fy\|^2\right) \qquad (z \in \boldsymbol{E}^n) \,.$$

η will be called the *characteristic ratio*. Then determine how to choose G so as to get η as large as possible.

Note that $0 \leqq \eta \leqq 1$, following directly from the definition of MLS. This measure seems to be adequate when "systematic" errors are dominant, i.e., when a vector $z \notin \boldsymbol{F}$ is given exactly and we want to obtain a simplified, approximate representation of z by a vector in $\boldsymbol{F}$, e.g., when a complicated analytic function is to be approximately represented by a polynomial.

Theorems 1 and 2 (see Section 2) indicate a general method for the calculation of η, formulated as an eigenvalue problem for a symmetric $m \times m$ matrix, $m \leqq n$. The optimal choice of G will be treated in Section 3 for the test problem of polynomial approximation, i.e., we shall determine numerically the "best" summation matrix under certain simplifying conditions. Numerical results are given for polynomial degree not exceeding five. Our results generalize those of Morduchow [7], and Morduchow & Levin [8] for polynomials of first and second degree respectively. The latter paper was the starting point of the present investigations.

When the errors are of a statistical nature, a different measure of goodness is adequate. The following formulation covers a common situation.

Problem 2. Let $z \in \boldsymbol{E}^n$ be a random vector, such that $E(z) \in \boldsymbol{F}$, say $E(z) = F\xi$ where $\xi \in \boldsymbol{E}^m$. Let the covariance matrix be $E((z - F\xi)(z - F\xi)^T) = \sigma^2 I$, where σ is a scalar constant and I the $n \times n$ unit matrix.

For a given summation matrix G, determine

$$\begin{aligned} \eta' &= E(\|Fx - F\xi\|^2)/E(\|Fy - F\xi\|^2) \\ &= \sum_{i=1}^{n} E((Fx - F\xi)_i^2) / \sum_{i=1}^{n} E((Fy - F\xi)_i^2) \,. \end{aligned}$$

η' will be called the *efficiency*. As in Problem 1, then determine G so as to get η' as large as possible.

Note that $0 \leqq \eta' \leqq 1$, a consequence of the Gauss-Markoff theorem [10, p. 560], according to which the least-squares estimate is a minimum-variance estimate for any linear function of ξ. Hence, in particular, each component of Fx is a minimum-variance estimate of the corresponding component of $F\xi$. In view of this, η' indicates that proportion of the observations, which is utilized efficiently when MA is applied.

In Theorem 3, η' is expressed as a function of the eigenvalues for the same matrix that appears in Problem 1. Therefore, the same general approach can be used to solve both problems, but we have not yet carried through the computations for η'. According to Theorem 4, however, $\eta' \geqq \eta$.

2. General Results.

2.1. *Geometrical analysis of Problem* 1. Problem 1 can be treated either by using formal matrix algebra or by the application of the notion of an angle (gap) between two linear subspaces of a Euclidean space. We prefer the latter approach, since we believe that this natural but neglected notion can be useful in other problems of numerical analysis. This belief is confirmed by the fact that Varah [11], independent of our work, recently used it in a different context. Closely related concepts have been used in functional analysis, see e.g. [5, p. 197].

At first, we look at the case $n = 3$, $m = 2$. Here $\boldsymbol{F}$ and $\boldsymbol{G}$ are planes in $\boldsymbol{E}^3$. By (1.2) and (1.4), $z - Fx$ and $z - Fy$ are perpendicular to $\boldsymbol{F}$ and $\boldsymbol{G}$ respectively, which means that the angle between the two vectors equals the angle between $\boldsymbol{F}$ and $\boldsymbol{G}$, which we denote $[\boldsymbol{F}, \boldsymbol{G}]$. Therefore,

$$\|z - Fx\|/\|z - Fy\| = \cos\,[\boldsymbol{F}, \boldsymbol{G}]\,.$$

Next we take $n = 3$, $m = 1$. Here the geometrical interpretation shows that the minimum value of $\|z - Fx\|/\|z - Fy\|$, $z \in \boldsymbol{E}^3$, is $\cos\,[\boldsymbol{F}, \boldsymbol{G}]$. See also Fig. 1.

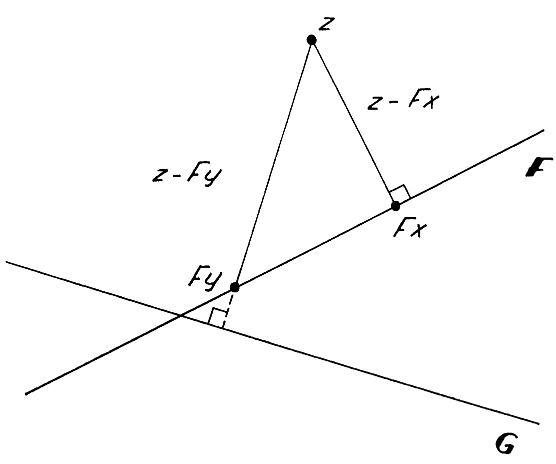

FIGURE 1

Now we look at the general case. Let $\boldsymbol{F}$ and $\boldsymbol{G}$ be linear subspaces of $\boldsymbol{E}^n$, and let A and B be two rectangular matrices, whose columns form *orthonormal* bases for $\boldsymbol{F}$ and $\boldsymbol{G}$ respectively, i.e. $A^TA = I$, $B^TB = I$. The orthogonal complements of $\boldsymbol{F}$ and $\boldsymbol{G}$ are denoted by $\boldsymbol{F}'$ and $\boldsymbol{G}'$ respectively. In our application $\boldsymbol{F}$ and $\boldsymbol{G}$ are of equal dimension, but this restriction is not necessary in this section.

The matrices

$$P_F = AA^T\,, \qquad P_{F'} = I - AA^T\,, \qquad P_G = BB^T\,, \qquad P_{G'} = I - BB^T$$

are orthogonal projections, [2, p. 8], for the spaces $\boldsymbol{F}$, $\boldsymbol{F}'$, $\boldsymbol{G}$ and $\boldsymbol{G}'$ respectively. The projections satisfy the relations

$$P^2 = P\,, \qquad P^T = P\,. \tag{2.1}$$

Definition.

$$\cos\,[\boldsymbol{F}, \boldsymbol{G}] = \min_{f \in \boldsymbol{F}} \|P_G f\|/\|f\|\,, \qquad 0 \leqq [\boldsymbol{F}, \boldsymbol{G}] \leqq \pi/2\,.$$

Comment. This definition is consistent with the ordinary definition of angle between subspaces of $\boldsymbol{E}^2$ and $\boldsymbol{E}^3$, if and only if the dimension of $\boldsymbol{F}$ is less than or equal to the dimension of $\boldsymbol{G}$. Cf. Lemma 2, below.

We shall now prove the following theorems.

THEOREM 1. $\eta = \cos^2\,[\boldsymbol{F}, \boldsymbol{G}]$.

THEOREM 2. $\cos^2\,[\boldsymbol{F}, \boldsymbol{G}]$ *is equal to the smallest eigenvalue of the matrix* A^TBB^TA.

Since $f = Ap$, $p \in \boldsymbol{E}^m$: $\|f\|^2 = p^TA^TAp = p^Tp = \|p\|^2$ and we have, since $B^TB = I$,

$$\cos^2\,[\boldsymbol{F}, \boldsymbol{G}] = \min_{\|p\|=1} \|P_G Ap\|^2 = \min_{\|p\|=1} p^TA^TBB^TAp\,. \tag{2.2}$$

Theorem 2 follows directly from this. Hence,

$$\sin^2\,[\boldsymbol{F}, \boldsymbol{G}] = 1 - \cos^2\,[\boldsymbol{F}, \boldsymbol{G}] = \max_{\|p\|=1} p^T(I - A^TBB^TA)p\,.$$

We denote the *spectral radius* of a matrix M by $\rho(M)$, cf. [2, p. 3]. Since $A^TA = I$ we have

$$\sin^2\,[\boldsymbol{F}, \boldsymbol{G}] = \max_{\|p\|=1} p^TA^T(I - BB^T)Ap = \rho(A^TP_{G'}A)\,. \tag{2.3}$$

We now need the following well-known and useful result, cf. [13, p. 54].

LEMMA 1. *Let U be a $m \times n$ matrix, let V be a $n \times m$ matrix, $n \geqq m$. Then the eigenvalues of UV are eigenvalues of VU as well. In particular, UV and VU have equal spectral radius, and the nonzero eigenvalues have equal multiplicity in UV and VU.*

If $n > m$, then the latter matrix has $n - m$ additional eigenvalues, equal to zero.

The application of Lemma 1 to (2.3) yields the equation

$$\sin^2\,[\boldsymbol{F}, \boldsymbol{G}] = \rho(AA^TP_{G'}) = \rho(P_FP_{G'})\,. \tag{2.4}$$

LEMMA 2. *If $\boldsymbol{F}$ and $\boldsymbol{G}$ have equal dimension, then $[\boldsymbol{F}, \boldsymbol{G}] = [\boldsymbol{G}, \boldsymbol{F}]$. If $\boldsymbol{F}$ has lower dimension than $\boldsymbol{G}$, then $[\boldsymbol{F}, \boldsymbol{G}] \leqq [\boldsymbol{G}, \boldsymbol{F}] = \pi/2$.*

Proof. Put $U = A^TB$, $V = B^TA$. By Theorem 2, $\cos^2\,[\boldsymbol{F}, \boldsymbol{G}]$ and $\cos^2\,[\boldsymbol{G}, \boldsymbol{F}]$ are equal to the smallest eigenvalues of UV and VU respectively. The dimension of $\boldsymbol{F}$ is equal to the number of rows in UV, while the dimension of $\boldsymbol{G}$ is equal to the number of columns in VU. The statement then follows from Lemma 1.

LEMMA 3. $[\boldsymbol{G}', \boldsymbol{F}'] = [\boldsymbol{F}, \boldsymbol{G}]$.

Comment. The reader is advised to interpret this result in the three-dimensional case.

Proof. Substitute in (2.4) $\boldsymbol{G}'$ for $\boldsymbol{F}$ and $\boldsymbol{F}'$ for $\boldsymbol{G}$. Then apply Lemma 1 and (2.4) again:

$$\sin^2 [\boldsymbol{G}', \boldsymbol{F}'] = \rho(P_{G'}P_F) = \rho(P_F P_{G'}) = \sin^2 [\boldsymbol{F}, \boldsymbol{G}] .$$

We are now in a position to prove Theorem 1. We first remark that the vector Fx defined by (1.4) is equal to $P_F z$, according to the theory of MLS, [2, p. 8]. Furthermore, $P_{F'}Fy = 0$ since $Fy \in \boldsymbol{F}$.

Hence,

$$P_{F'}(z - Fy) = P_{F'}z = (I - P_F)z = z - Fx .$$

$$\therefore \|z - Fx\|/\|z - Fy\| = \|P_{F'}(z - Fy)\|/\|z - Fy\| .$$

By (1.2), $z - Fy \in \boldsymbol{G}'$ for any $z \in \boldsymbol{E}^n$. Conversely, any vector $v \in \boldsymbol{G}'$ can be expressed in the form $v = z - Fy$. For if $z = v$ then, by (1.2), $y = 0$, and hence $z - Fy = v$. Hence,

$$\begin{aligned} \eta &= \inf_z \|z - Fx\|^2/\|z - Fy\|^2 \qquad (z \in \boldsymbol{E}^n) \\ &= \inf_v \|P_{F'}v\|^2/\|v\|^2 \qquad (v \in \boldsymbol{G}') \\ &= \cos^2 [\boldsymbol{G}', \boldsymbol{F}'] = \cos^2 [\boldsymbol{F}, \boldsymbol{G}] . \end{aligned}$$

Theorem 1 is thus proved.

2.2. *Algebraic analysis of Problem* 2. Again, let the columns of A and B form orthonormal bases of the spaces $\boldsymbol{F}$ and $\boldsymbol{G}$ respectively, which are now assumed to be of equal dimension m. Introduce the vectors $\hat{x}$, $\hat{y}$, $\hat{\xi}$ defined by $A\hat{x} = Fx$, $A\hat{y} = Fy$, $A\hat{\xi} = F\xi$. Then (1.4) and (1.2) are equivalent to $\hat{x} = A^T z$ and $B^T A\hat{y} = B^T z$, respectively. In the introduction we assumed that $G^T F$ is nonsingular. This implies that $B^T A$ is nonsingular, and hence $\hat{y} = (B^T A)^{-1} B^T z$.

THEOREM 3. *$\eta' = m/\sum_{i=1}^m \lambda_i^{-1}$, where λ_i are the eigenvalues of $A^T BB^T A$.*

Proof. By definition,

$$\eta' = E(\|A\hat{y} - A\hat{\xi}\|^2)/E(\|A\hat{y} - A\hat{\xi}\|^2) .$$

We shall denote the trace of a matrix M by tr M.

$$E(\|A\hat{y} - A\hat{\xi}\|^2) = E(\|\hat{y} - \hat{\xi}\|^2) = \operatorname{tr} E((\hat{y} - \hat{\xi})(\hat{y} - \hat{\xi})^T) .$$

Since $\hat{y} - \hat{\xi} = (B^T A)^{-1} B^T z - \hat{\xi} = (B^T A)^{-1} B^T (z - A\hat{\xi})$, we obtain

$$\begin{aligned} E(\|A\hat{y} - A\hat{\xi}\|^2) &= \operatorname{tr} (B^T A)^{-1} B^T \cdot E((z - A\hat{\xi})(z - A\hat{\xi})^T) \cdot B(A^T B)^{-1} \\ &= \operatorname{tr} (B^T A)^{-1} B^T \sigma^2 I B (A^T B)^{-1} \\ &= \sigma^2 \operatorname{tr} (A^T BB^T A)^{-1} = \sigma^2 \sum_{i=1}^m \lambda_i^{-1} , \end{aligned}$$

where λ_i are the eigenvalues of the positive definite matrix $A^T BB^T A$ (see Remark 1, below).

Similarly, or simply by putting B equal to A, since $\hat{x} = A^T A\hat{x} = A^T z$,

$$E(\|A\hat{x} - A\hat{\xi}\|^2) = \sigma^2 \operatorname{tr}(A^TAA^TA)^{-1} = \sigma^2 m .$$

Hence,

$$\eta' = m/ \sum_{i=1}^{m} \lambda_i^{-1} . \tag{2.5}$$

Theorem 3 is thus proved.

THEOREM 4. $\eta' \geqq \eta/(1 - (1 - \eta)\cdot\dim(\boldsymbol{F} \cap \boldsymbol{G})/m) \geqq \eta$. *Here the same summation matrix is assumed for* η *and* η'.

Proof. We note that $f \in \boldsymbol{F} \Rightarrow AA^Tf = f$, $f \in \boldsymbol{G} \Rightarrow BB^Tf = f$. Hence, $f \in \boldsymbol{F} \cap \boldsymbol{G} \Rightarrow AA^TBB^Tf = AA^Tf = f$, i.e. $\boldsymbol{F} \cap \boldsymbol{G}$ is a (possibly empty) space of eigenvectors of AA^TBB^T belonging to the eigenvalue 1. In any case, the multiplicity of this eigenvalue is at least equal to $\dim(\boldsymbol{F} \cap \boldsymbol{G})$. By Lemma 1 the same conclusion holds for the matrix B^TAA^TB. By Theorem 1, the remaining λ_i are not less than η. By Theorem 3,

$$m/\eta' = \sum_{i=1}^{m} \lambda_i^{-1} \leqq \dim(\boldsymbol{F} \cap \boldsymbol{G})\cdot 1 + (m - \dim(\boldsymbol{F} \cap \boldsymbol{G}))\cdot\frac{1}{\eta} ,$$

valid also when $\boldsymbol{F} \cap \boldsymbol{G} = \phi$. Theorem 4 follows immediately from this inequality.

Remark 1. In the proofs of Theorems 1–4, no use is made of the special form of the matrix G. They therefore hold for an arbitrary matrix G, such that G^TF is nonsingular, and so their application is not restricted to MA. It should also be noted that $\eta' \to 0$, $\eta \to 0$ when G^TF tends to a singular matrix. The assumption of nonsingularity therefore means no restriction in the search for the summation matrices which maximize η or η'. If G^TF is singular for all summation matrices, e.g., if all the column sums of F are equal to zero, then MA has to be modified, e.g., by reversing the signs in some of the rows of F.

Remark 2. The inequality $\eta' \leqq 1$, which was mentioned in the introduction as a consequence of the Gauss-Markoff theorem follows easily from (2.5), since

$$0 < \lambda_i \leqq \|F^TGG^TF\| \leqq \|F^T\|\cdot\|G^T\|\cdot\|F\| \leqq 1 ,$$

for all i.

Remark 3. The first three theorems can be summarized in the form

$$1/\eta = \|(G^TF)^{-1}\|_2^2 , \qquad 1/\eta' = \|(G^TF)^{-1}\|_F^2/m .$$

Here we denote the Frobenius norm of a matrix by $\|\cdot\|_F$.

The inequality $\eta' \geqq \eta$ of Theorem 4 then follows from the well-known inequality $\|\cdot\|_F^2 \leqq m\|\cdot\|_2^2$.

3. An Application: Polynomial Fitting to Equidistant Data.

3.1. *Formulation of the problem.* A function $f(x)$ is known at n equidistant points,

$$x_k = -1 + 2k/(n - 1) , \qquad 0 \leqq k \leqq n - 1 . \tag{3.1}$$

We call this set of points a *grid*. This function is to be approximated by a polynomial $P(x)$ of degree $m - 1$,

$$P(x) = \sum_{j=0}^{m-1} r_j x^j , \qquad m < n .$$

Put

$$z = (f(x_0), f(x_1), \cdots, f(x_{n-1}))^T$$

$$y = (r_0, r_1, \cdots, r_{m-1})^T$$

$$F = \begin{bmatrix} 1 & x_0 & \cdots & x_0^{m-1} \\ 1 & x_1 & \cdots & x_1^{m-1} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 1 & x_{n-1} & \cdots & x_{n-1}^{m-1} \end{bmatrix} \tag{3.2}$$

from which we get

$$z - Fy = e\,, \tag{3.3}$$

where e is an error vector.

In order to obtain the MA approximation, we multiply the left-hand side of this equation by a matrix G^T of the form already mentioned in the introduction, cf. formulae (1.2), (1.3). Then we solve for y the matrix equation

$$G^T(Fy - z) = 0\,. \tag{3.4}$$

The summation matrix $G = (g_{ij}),\ i = 0, 1, \cdots, n - 1;\ j = 0, 1, \cdots, m - 1$, corresponds to a grouping of the equations, i.e., to a certain subdivision of the point set $\{x_k\}$.

According to Theorems 1 and 2, Problem 1 is therefore to calculate the angle between the space $\boldsymbol{F}$ of polynomials of degree $\leqq m - 1$ and the space $\boldsymbol{G}$ of step functions (with $m - 1$ discontinuities defined by the summation matrix G), and to allocate the discontinuities on the grid in order to make this angle as small as possible. An application of Rolle's theorem shows that the constants are the only functions which belong to both $\boldsymbol{F}$ and $\boldsymbol{G}$, provided that $n \geqq 2m - 1$. Hence

$$\dim(\boldsymbol{F} \cap \boldsymbol{G}) = 1 \tag{3.5}$$

if $n \geqq 2m - 1$.

We now proceed to define the orthonormal bases for $\boldsymbol{F}$ and $\boldsymbol{G}$. Let $\{a_j(x)\}_{j=0}^{m-1}$ be the set of polynomials, which are mutually orthonormal under summation over $\{x_k\}_{k=0}^{n-1}$. These polynomials were investigated by Chebyshev, Gram and Ch. Jordan [3], [4]. Let $A = (a_{kj})$, where $a_{kj} = a_j(x_k),\ 0 \leqq j \leqq m - 1, 0 \leqq k \leqq n - 1$. The columns of A span the same subspace $\boldsymbol{F}$ as the columns of F.

We now introduce the assumption that the subdivision of the grid is symmetric, i.e. that the number of 1's is the same in the jth row of G^T as in the $(m - 1 - j)$th row.

We shall determine the symmetric subdivision which yields the maximum characteristic ratio. We believe that no asymmetric subdivision is more efficient, although we have not proved this. We also believe that the characteristic ratio cannot be increased by permitting "nested" groups of equations, i.e., groups obtained by adding equations which do not arise from adjacent points of the grid.

Having made the assumption of symmetry, it is advantageous to replace G by a matrix B, whose columns span the same space as the columns of G and have parity properties similar to those of the orthogonal polynomials which occur in the columns of A.

Let $g_0, g_1, \cdots, g_{m-1}$ be the columns of G and let $b_0, b_1, \cdots, b_{m-1}$ be the columns of B. We then define

$$
\begin{aligned}
b_{m-2s-1} &= [(-1)^{m+1}\cdot g_s + g_{m-s-1}]/\|(-1)^{m+1}\cdot g_s + g_{m-s-1}\| , \\
b_{m-2s-2} &= [(-1)^{m} g_s + g_{m-s-1}]/\|(-1)^{m}\cdot g_s + g_{m-s-1}\| , \\
& \qquad s = 0, 1, \cdots, [(m-1)/2] .
\end{aligned} \tag{3.6}
$$

Because of the symmetry properties, b_i is orthogonal to a_j if $i - j$ is odd. Hence B^TA has a checkerboard structure, where the nonzero elements are of the form

$$d_j \cdot \sum_{k=p_j}^{q_j} a_i(x_k) .$$

An explicit formula for sums of this type will be derived in the next section. The calculation of the eigenvalues of A^TBB^TA is simplified because this matrix has a similar checkerboard structure, and therefore breaks down into two matrices, both of order $m/2$ if m is even, and of order $(m + 1)/2$ and $(m - 1)/2$ if m is odd.

3.2. *A summation formula for the polynomials* $a_j(x)$. In order to compute $\sum_{k=p}^{q} a_j(x_k)$ we define a function $F(x)$ satisfying the relation (step-length $h = 2/(n - 1)$):

$$\Delta F(x) \equiv F(x + h) - F(x) = a_j(x) . \tag{3.7}$$

Then

$$\sum_{k=p}^{q} a_j(x_k) = F(x_q + h) - F(x_p) . \tag{3.8}$$

Jordan [3, p. 445] gives the following recurrence relation:

$$
\begin{aligned}
& a_j(x) = r_j\cdot x\cdot a_{j-1}(x) - s_j\cdot a_{j-2}(x) \\
& \text{where} \quad r_j = \frac{n-1}{j}\left(\frac{4j^2 - 1}{n^2 - j^2}\right)^{1/2}, \qquad s_j = r_j/r_{j-1} . \\
& \text{Initial values: } a_0 = n^{-1/2},\ a_1 = \left(\frac{3(n-1)}{n(n+1)}\right)^{1/2}\cdot x .
\end{aligned} \tag{3.9}
$$

According to Jordan [4, p. 315], we have for the chosen grid and with slight modifications (the operator Δ means differencing with respect to x):

$$c_j(j + 1)\,\Delta a_{j+1} = 2h(x + h)\,\Delta a_j + jh^2\Delta a_j + 2h^2(j + 1)a_j . \tag{3.10}$$

But $(x + h)\,\Delta a_j = \Delta(xa_j) - ha_j$, therefore

$$2jh^2a_j = \Delta[(j + 1)c_j\cdot a_{j+1} - h(2x + jh)a_j] .$$

$$\therefore F = \frac{j+1}{2jh^2}\,c_j\cdot a_{j+1} - \frac{2x + jh}{2jh}\,a_j + C ,$$

$$\text{where } c_j = C_j/C_{j+1},\ C_j^{-2} = h^{4j}\binom{2j}{j}\binom{n+j}{2j+1} .$$

Jordan [3, p. 445] gives

$$\frac{j+1}{2h} c_j a_{j+1} = \frac{2j+1}{j+1} x a_j - \frac{2j+1}{j+1} \cdot \frac{jh}{2} \left\{ \frac{n^2 - j^2}{4j^2 - 1} \right\}^{1/2} a_{j-1} ;$$

$$\text{(3.11)} \quad \therefore \quad F = \frac{2j+1}{jh(j+1)} x a_j - \frac{2j+1}{2(j+1)} \left\{ \frac{n^2 - j^2}{4j^2 - 1} \right\}^{1/2} a_{j-1} - \left\{ \frac{x}{jh} + \frac{1}{2} \right\} a_j + C$$

$$= \frac{1}{2h(j+1)} \left[(2x - jh - h) a_j - h \left\{ \frac{(2j+1)(n^2 - j^2)}{2j-1} \right\}^{1/2} a_{j-1} \right] + C .$$

We have used the formulae (3.8), (3.9) and (3.11) to calculate the elements of $B^T A$.

3.3. *The limit case with infinitely many observations.* When $n \to \infty$ the polynomials $\sqrt{n} \cdot a_j$ will approach the Legendre polynomials P_j normalized so that

$$\frac{1}{2} \int_{-1}^{1} P_i P_j dx = \delta_{ij} .$$

The step functions b_j will now be defined on the interval $[-1, 1]$ so that

$$\frac{1}{2} \int_{-1}^{1} b_i b_j dx = \delta_{ij} .$$

Essentially the b_j's are chosen as before.

If we put $a_j = (\Delta/h)\ (h \cdot F)$ and let $h \to 0$ in (3.11), then $a_j(x)$ tends to the normalized Legendre polynomial, and we obtain a well-known formula:

$$\text{(3.12)} \qquad \int a_j(x) dx = \frac{1}{j+1} \left(x \cdot a_j(x) - \left(\frac{2j+1}{2j-1} \right)^{1/2} \cdot a_{j-1}(x) \right) + C$$

which has been used analogously to (3.11) when computing the scalar products

$$(a_i, b_j) = \frac{1}{2} \int_{-1}^{1} a_i b_j dx .$$

3.4. *A simple example of the η-calculation.* Let $m = 2$ and n be even; then B is determined by the symmetry conditions:

$$b_{j0} = 1/\sqrt{n} , \qquad b_{j1} = \operatorname{sgn}(j - n/2)/\sqrt{n} , \qquad j = 0, 1, \cdots, n-1 .$$

According to formula (3.8) we have

$$A^T B = \begin{bmatrix} 1 & 0 \\ 0 & \frac{2}{\sqrt{n}} \left[F(1+h) - F\left(\frac{1}{n-1} \right) \right] \end{bmatrix} ,$$

where $F(x)$ is given by formula (3.11).

$$F(x) = \frac{1}{2 \cdot 2h} [(2x - 2h) a_1(x) - h(3(n^2 - 1))^{1/2} a_0(x)]$$

$$= \frac{1}{4h} \left[(2x - 2h) \left(\frac{3(n-1)}{n(n+1)} \right)^{1/2} x - h \cdot (3(n^2 - 1))^{1/2} / \sqrt{n} \right]$$

$$= \frac{1}{4h} \cdot \left(\frac{3(n-1)}{n(n+1)} \right)^{1/2} \cdot [2(x - h)x - h(n+1)] .$$

Finally we get

$$A^T B B^T A = \begin{bmatrix} 1 & 0 \\ 0 & 3/(4(1 - 1/n^2)) \end{bmatrix}$$

whereof

$$\eta = 3/(4 - 4n^{-2}) \, , \qquad \eta' = 6/(7 - 4n^{-2}) \tag{3.13}$$

$$\lim \eta = 0.75 \, , \qquad \lim \eta' = 0.86 \, .$$

TABLE 1

Characteristic ratios of MA *with optimal grouping (degree of polynomial* = *m* − 1). *See also Section* 3.4.

	$m = 3$		$m = 4$		$m = 5$			$m = 6$		
n	P	η	P	η	P	Q	η	P	Q	η
4	1	.900								
5	1	.800	1	.667						
6	1	.714	1	.893	1	1	.794			
7	2	.694	1	.789	1	1	.595	1	1	.667
8	2	.763	1	.778	1	2	.742	1	1	.742
10	2	.776	1	.682	1	2	.654	1	2	.595
15	3	.771	2	.750	1	4	.666	1	3	.632
20	4	.769	3	.695	2	5	.690	1	4	.691
50	10	.768	6	.708	4	14	.683	3	10	.643
1000	200	.768	130	.728	82	270	.698	57	195	.670
n	a	η	a	η	a	b	η	a	b	η
∞	.200	.768	.130	.729	.082	.270	.699	.058	.194	.670

TABLE 2

Characteristic ratios of MA *with almost equal grouping.*

	$m = 3$		$m = 4$		$m = 5$			$m = 6$		
n	P	η	P	η	P	Q	η	P	Q	η
4	1	.900								
5	2	.357	1	.667						
6	2	.571	2	.143	1	1	.794			
7	2	.694	2	.208	1	1	.595	1	1	.667
8	3	.397	2	.384	2	1	.136	1	1	.742
10	3	.618	3	.185	2	2	.238	2	2	.022
20	7	.449	5	.314	4	4	.184	3	3	.194
50	17	.475	13	.272	10	10	.172	8	8	.117
n	a	η	a	η	a	b	η	a	b	η
∞	.333	.493	.250	.304	.200	.200	.170	.167	.167	.086

3.5. *Numerical calculation of characteristic ratios.* The construction of the *symmetric* subdivision of the grid, which gives as large characteristic ratio as possible, is a maximization problem for a function of $[(m - 1)/2]$ variables, which has been solved on a computer for $m \leqq 6$. A search technique was used. Details are given in [9]. See Table 1.

For comparison we have also computed the characteristic ratios obtained when the groups are made equally or almost equally large. It is obvious from Table 2 that the characteristic ratio is much lower than for optimal subdivision, especially when the polynomial's degree is high.

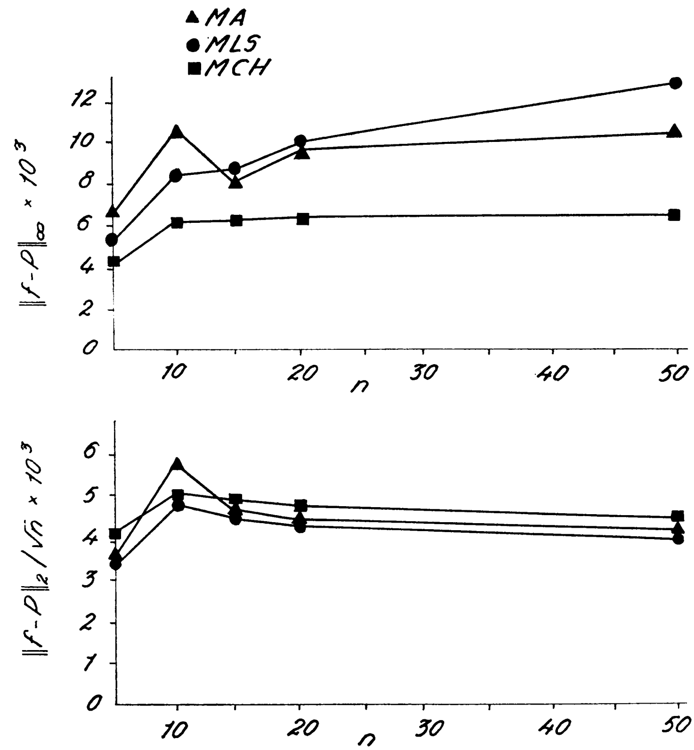

FIGURE 2. $f(x) = 1/(2 + x)$, $m = 4$.

The results of these test calculations show that MA can be very efficient if it is used in an appropriate way, and that it is profitable to spend some thought on the question how to group the equations.

We do not advocate the application of MA for polynomial approximation. The fact that the efficiency can be as high as it is in this test example indicates that MA deserves to be considered as a method for data reduction, in particular when small computers without built-in multiplication are used.

The parameters in the tables are:

m = the number of unknown coefficients in the polynomial (=degree + 1).

n = the number of observations (=the number of original equations).

P = the number of observations in the first group (and the last because the grouping is symmetric).

Q = the number of observations in the second group.
η = the characteristic ratio as defined in the introduction.

When n is odd and m is even, the equation corresponding to the origin is added with weight 1/2 to each of the two groups arising from the points adjacent to the origin.

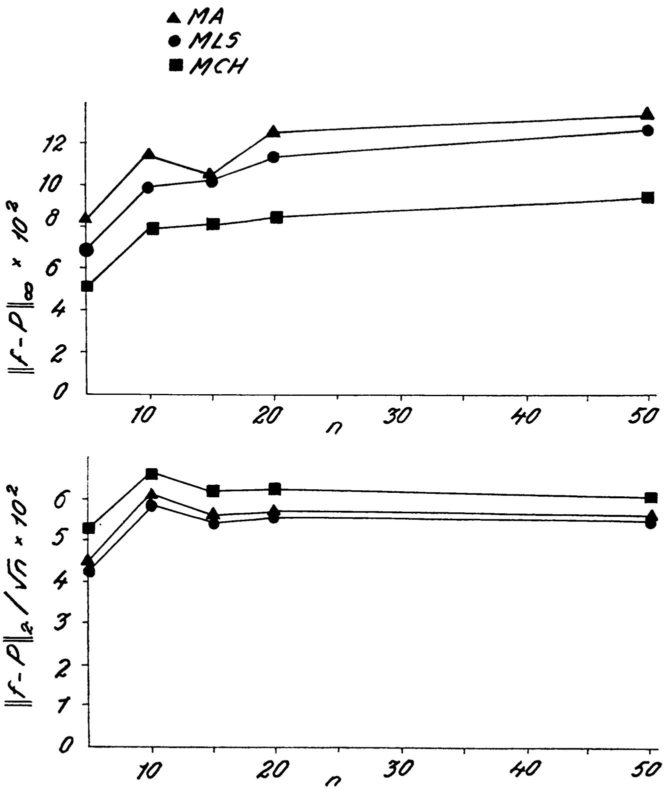

FIGURE 3. $f(x) = R(-0.1, 0.1)$, $m = 4$.

In the continuous case,

$$a = \lim_{n \to \infty} P(n)/n\,, \qquad b = \lim Q(n)/n\,.$$

For example, when $m = 6$, $n = \infty$, the points of variation of the step functions $b_j(x)$ are $-1 + 2a$, $-1 + 2(a + b)$, 0, $1 - 2(a + b)$, $1 - 2a$. Note that $P(n)$ and $Q(n)$ are always close to na and nb, respectively. The optimal subdivision for the case $n = \infty$ therefore indicates a good subdivision even for small values of n.

The efficiency η' has been computed in one case. For $m = 3$, $n = \infty$ we found $\eta'_{\max} = 0.838$ for $a = 0.22$. This should be compared to the bound given by Theorem 4, $\eta'_{\max} \geqq 0.832$, using the values $a = 0.2$ and $\eta = 0.768$ from Table 1.

It is believed that the errors in the values of a, b, η do not exceed 0.001.

3.6. *A numerical experiment.* In order to illustrate the two aspects discussed in the introduction, we have fitted polynomials of degree 3 to

(1) the function $f(x) = 1/(2 + x)$,

(2) sets of random numbers, uniformly distributed on $(-0.1, 0.1)$. In both cases, we used the grids $\{x_k = -1 + 2k/(n-1);\ k = 0, 1, \cdots, n-1\}$ for $n = 5, 10, 15, 20, 50$. Each fit was made with three different methods, namely MA with optimal grouping, MLS and Chebyshev approximation (MCH). The results are measured in both Euclidean and maximum norm on the grid. See Figs. 2, 3.

Royal Institute of Technology
Department of Numerical Analysis
Stockholm 70, Sweden

1. P. G. Guest, *Numerical Methods of Curve Fitting*, Cambridge Univ. Press, Cambridge, 1961. MR 22 #11511.

2. A. S. Householder, *The Theory of Matrices in Numerical Analysis*, Blaisdell, New York, 1964. MR **30** #5475.

3. Ch. Jordan, *Calculus of Finite Differences*, reprint of 2nd ed., Chelsea, New York, 1960. MR **1**, 74.

4. Ch. Jordan, "Approximation and graduation according to the principle of least squares by orthogonal polynomials," *Ann. Math. Statist.*, 1932, pp. 257–357.

5. T. Kato, *Perturbation Theory for Linear Operators*, Die Grundlehren der math. Wiss., Band 132, Springer-Verlag, New York, 1966. MR **34** #3324.

6. Yu. V. Linnik, *Method of Least Squares and Principles of the Theory of Observations*, Pergamon Press, New York, 1961. MR **23** #A1438.

7. M. Morduchow, "Method of averages and its comparison with the method of least squares," *J. Appl. Phys.*, v. 25, 1954, pp. 1260–1263. MR **16**, 403.

8. M. Morduchow & L. Levin, "Comparison of the method of averages with the method of least squares: fitting a parabola," *J. Math. and Phys.*, v. 38, 1959, pp. 181–192. MR **22** #1983.

9. B. Sjöberg & P. Svensson, *Medelvärdesmetodens Effektivitet vid Kurvanpassning*, Royal Institute of Technology Computer Science Dept. Report, Stockholm, 1964.

10. J. Todd (Editor), *Survey of Numerical Analysis*, McGraw-Hill, New York, 1962. MR **24** #B1271.

11. J. M. Varah, *The Computation of Bounds for the Invariant Subspaces of a General Matrix Operator*, Stanford University Computer Science Dept. Technical Report No. CS 66.

12. E. Whittaker & G. Robinson, *The Calculus of Observations*, 4th ed., Blackie, London, 1944.

13. J. H. Wilkinson, *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, 1965. MR **32** #1894.