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A METHOD FOR COMPUTING THE EFFECT OF AN ADDITIONAL
OBSERVATION ON A PREVIOUS LEAST-SQUARES ESTIMATE

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A METHOD FOR COMPUTING THE EFFECT OF AN ADDITIONAL
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SUMMARY

In the application of the method of least squares to data reduction, it may be desired to compute the effect of a single additional observation on the regression coefficients and their covariance matrix obtained previously. Simple exact formulas by which the new observation may be included are derived in this report for the case where the observation errors are uncorrelated. The starting point for the derivation is the matrix formulation of the well-known least-squares solution, and succeeding steps in the derivation do not require any further application of statistical theory. The resulting recursion expressions are identical to those developed from statistical filter theory for the case of uncorrelated errors.

INTRODUCTION

In the application of the method of least squares to data reduction, it would be desirable to be able to calculate the effect of an additional observation on a previous estimate of the (so-called) regression coefficients without resorting to the lengthy process of matrix inversion. Also, if one or more of the observations which have entered into the solution should appear, upon later examination, to be "wild," a simple procedure for removing these observations would be useful. Such procedures would permit rapid calculations of the type needed for smoothing and extrapolating time histories, as is done in the processing of radar measurements, for example.

This report describes how simple recursion formulas for both adding and subtracting observations may be derived from the well-known least-squares normal equations by simple applications of matrix algebra. In the derivation, the unknown quantities to be estimated are assumed to be constants. It is possible, however, to extend the formulas to the problem of estimating the state variables of a simple form of dynamic system. The resulting formulas are then the same as those derived by the application of optimal control theory to the problem of estimation and filtering in reference 1. References 2 and 3 present different derivations of the recursion formulas and applications of them to space navigation. Reference 4 is an early treatment of the application of least squares to data reduction.

SYMBOLS

A^*	known coefficients in regression equation
A	coefficients of weighted regression equation
X	true regression coefficients
x_n	original least-squares estimate of regression coefficients
x_{n+1}	revised estimate of regression coefficients
Y^*	observed quantities from which x_n was determined
Y	weighted observations
y^*	additional observation
y	weighted value of y^*
a^*	known coefficients corresponding to added observation
a	weighted values of a^*
ϵ_{Y^*}	true errors in observed quantities Y^*
ϵ_{y^*}	true error in y^*
σ_{y^*}	probable error in y^*
$[C_n]$	original covariance matrix
$[C_{n+1}]$	revised covariance matrix
$[\Delta C]$	difference between $[C_n]$ and $[C_{n+1}]$
$[I]$	identity matrix
w	weight for added observation equation
t	time

Matrix symbols:

$\{ \}$	column matrix
$[\]$	row matrix
$\ \ \ $	rectangular matrix
$[\]$	square matrix
$[\]$	diagonal matrix

Prime denotes transposition of a matrix. (Example: The notation $\{a'\}$ denotes the column matrix formed by transposing the row matrix $[a]$.)

DERIVATION OF METHOD

The derivation of the method of this report begins with a brief statement of the least-squares solution. Succeeding steps in the derivation are elementary matrix operations.

Let the system of simultaneous equations relating observations $\{Y^*\}$ to the unknowns $\{X\}$ be

$$\{Y^*\} = [A^*] \{X\} + \{\epsilon_{Y^*}\} \quad (1)$$

The number of observations n is greater than the number of elements of $\{X\}$, and the errors ϵ_{Y^*} are assumed to be random with a Gaussian distribution, zero mean, variance σ_y , and not correlated. Under these conditions, the probable value of $\{X\}$, obtained from n equations and denoted by $\{x_n\}$, is obtained by weighting each observation equation by multiplying it by the reciprocal of the variance σ_y of the corresponding observation, and then solving for coefficients $\{x_n\}$ which will minimize the sum of the squares of the weighted residuals. If

the weighted observations are denoted by $\{Y\}$ and the weighted observation coefficients by $\|A\|$, the probable value of $\{X\}$ is (see ref. 5)

$$\{x_n\} = [A'A]^{-1} \|A'\| \{Y\} \quad (2)$$

The matrix $[A'A]^{-1}$ in equation (2) is the covariance matrix of $\{x_n\}$. A proof of this statement appears in the appendix. For convenience, it will be denoted by $[C_n]$. Statistically, the covariance matrix is the expected value of the product formed by postmultiplying the difference between $\{x_n\}$ and its expected value by the transpose of the difference. The diagonal elements of the covariance matrix $[C_n]$ are the squares of the probable errors in the corresponding elements of $\{x_n\}$. Because of its statistical significance, it is generally desirable to compute the covariance matrix, even though the solution for $\{x_n\}$ could be performed without actual matrix inversion (by Crout's method, for example).

It will be assumed that a set of observation equations has been solved, as in equation (2), to obtain $\{x_n\}$ and the covariance matrix $[C_n]$. Suppose that an additional observation is then made and it is desired to compute the effect of this observation on the probable value of $\{X\}$ and on the covariance matrix. The additional observation y^* is related to $\{X\}$ by the equation

$$y^* = [a^*] \{X\} + \epsilon_y^* \quad (3)$$

The weighted equation corresponding to equation (3) is:

$$y = [a] \{X\} + \frac{\epsilon_y^*}{\sigma_y^*} \quad (4)$$

Revising the Estimate of $\{X\}$ Without Matrix Inversion

The least-squares solution for the revised estimate $\{x_{n+1}\}$ may be written:

$$\{x_{n+1}\} = \left[\begin{array}{c|c} \mathbb{A}' & \mathbf{a}' \\ \hline \mathbb{A}' & \mathbf{a}' \end{array} \right]^{-1} \left[\begin{array}{c} \mathbf{Y} \\ y \end{array} \right] \quad (5)$$

where partitioning has been used to show the added elements. The matrix

$\left[\begin{array}{c|c} \mathbb{A}' & \mathbf{a}' \\ \hline \mathbb{A}' & \mathbf{a}' \end{array} \right]^{-1}$ is the revised covariance matrix $[\bar{C}_{n+1}]$. This matrix may be written as

$$[\bar{C}_{n+1}] = \left[\mathbb{A}'\mathbb{A} + \{\mathbf{a}'\}[\mathbf{a}] \right]^{-1} \quad (6)$$

or

$$[\bar{C}_{n+1}] = \left[[\bar{C}_n]^{-1} + \{\mathbf{a}'\}[\mathbf{a}] \right]^{-1} \quad (7)$$

Equation (5) may then be written

$$\{x_{n+1}\} = \left[[\bar{C}_n]^{-1} + \{\mathbf{a}'\}[\mathbf{a}] \right]^{-1} \left\{ \mathbb{A}'\{\mathbf{Y}\} + \{\mathbf{a}'\}y \right\} \quad (8)$$

An expression for $\{x_{n+1}\}$ in terms of $\{x_n\}$ may be written as follows.

Equation (8) may be written as

$$\left[[\bar{C}_n]^{-1} + \{\mathbf{a}'\}[\mathbf{a}] \right] \{x_{n+1}\} = \mathbb{A}'\{\mathbf{Y}\} + \{\mathbf{a}'\}y \quad (9)$$

If equation (9) is multiplied through by $[\bar{C}_n]$, there is obtained the equation

$$\left[[\bar{I}] + [\bar{C}_n] \{\mathbf{a}'\}[\mathbf{a}] \right] \{x_{n+1}\} = [\bar{C}_n] \mathbb{A}'\{\mathbf{Y}\} + [\bar{C}_n] \{\mathbf{a}'\}y \quad (10)$$

By equation (2),

$$[\bar{C}_n] \mathbb{A}'\{\mathbf{Y}\} = \{x_n\} \quad (11)$$

For convenience, let $[\bar{C}_n] \{\mathbf{a}'\} = \{\mathbf{k}'\}$. Then equation (10) may be written

$$\left[[\bar{I}] + \{\mathbf{k}'\}[\mathbf{a}] \right] \{x_{n+1}\} = \{x_n\} + \{\mathbf{k}'\}y \quad (12)$$

From equation (12),

$$\{x_{n+1}\} = \left[\overline{I} + \{k'\} [a] \right]^{-1} \{x_n\} + \left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} y \quad (13)$$

By making use of the identity,

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \left[\overline{I} + \{k'\} [a] \right] = \overline{I} \quad (14)$$

simple expressions for the terms

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \{x_n\} \quad \text{and} \quad \left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\}$$

in equation (13) may be obtained. Expansion of equation (14) gives:

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} + \left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} [a] = \overline{I} \quad (15)$$

Postmultiplication of equation (15) by $\{k'\}$ gives:

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} + \left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} [a] \{k'\} = \{k'\} \quad (16)$$

The product $[a] \{k'\}$ is a scalar quantity. Let this quantity be denoted by B . Then equation (16) may be written

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} (1 + B) = \{k'\} \quad (17)$$

Therefore,

$$\left[\overline{I} + \{k'\} [a] \right] \{k'\} = \frac{1}{1 + B} \{k'\} \quad (18)$$

Postmultiplication of equation (15) by $\{x_n\}$ gives

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \{x_n\} + \left[\overline{I} + \{k'\} [a] \right]^{-1} \{k'\} [a] \{x_n\} = \{x_n\} \quad (19)$$

By equation (18), equation (19) may be written

$$\left[\overline{I} + \{k'\} [a] \right]^{-1} \{x_n\} + \frac{1}{1 + B} \{k'\} [a] \{x_n\} = \{x_n\} \quad (20)$$

from which

$$\left[\mathbb{I} + \{k'\} [a] \right]^{-1} \{x_n\} = \{x_n\} - \frac{1}{1+B} \{k'\} [a] \{x_n\} \quad (21)$$

By equations (18) and (21), equation (13) may now be written as

$$\{x_{n+1}\} = \{x_n\} - \frac{1}{1+B} \{k'\} [a] \{x_n\} + \frac{1}{1+B} \{k'\} y \quad (22)$$

or

$$\{x_{n+1}\} = \{x_n\} + \frac{1}{1+B} \{k'\} \left(y - [a] \{x_n\} \right) \quad (23)$$

Equation (23) furnishes the means for revising the estimate of $\{X\}$. However, the matrix $\{k'\}$ and the scalar B are derived from the covariance matrix of the previous estimate. Therefore, if another observation is to be added, the revised covariance matrix $[C_{n+1}]$ must also be computed. This computation can also be done without matrix inversion.

Evaluating $[C_{n+1}]$

Let $[\Delta C]$ be the difference between $[C_{n+1}]$ and $[C_n]$ so that

$$[C_{n+1}] = [C_n] + [\Delta C] \quad (24)$$

By definition of the inverse of a matrix,

$$[C_{n+1}]^{-1} [C_n] + [C_{n+1}]^{-1} [\Delta C] = [\mathbb{I}] \quad (25)$$

From equation (7) it is seen that

$$[C_{n+1}]^{-1} = \left[[C_n]^{-1} + \{a'\} [a] \right] \quad (26)$$

Therefore, equation (25) may be written

$$[\mathbb{I}] + \{a'\} [a] [C_n] + [C_n]^{-1} [\Delta C] + \{a'\} [a] [\Delta C] = [\mathbb{I}] \quad (27)$$

or

$$\{a'\} [a] [C_n] + [C_n]^{-1} [\Delta C] + \{a'\} [a] [\Delta C] = [0] \quad (28)$$

Multiplication by $[C_n]$ and solving for $[\Delta C]$ gives:

$$[\Delta C] = - \left[[I] + [C_n] \{a'\} [a] \right]^{-1} [C_n] \{a'\} [a] [C_n] \quad (29)$$

But $[C_n] \{a'\} = \{k'\}$ by previous definition. Also, because $[C_n]$ is symmetrical, $[a] [C_n] = [k]$. Thus, equation (29) may be written:

$$[\Delta C] = - \left[[I] + \{k'\} [a] \right]^{-1} \{k'\} [k] \quad (30)$$

By use of equation (18), equation (30) becomes

$$[\Delta C] = - \frac{1}{1+B} \{k'\} [k] \quad (31)$$

The expression for calculating $[C_{n+1}]$ without matrix inversion may therefore be written

$$[C_{n+1}] = [C_n] - \frac{1}{1+B} \{k'\} [k] \quad (32)$$

In order to keep the weighting process flexible, the final equations may be written in terms of the unweighted observation equation and a weighting factor w by making the following substitutions in equations (23) and (32):

$$y = wy^*$$

$$[a] = w [a^*]$$

$$[k] = w [a^*] [C_n]$$

$$B = w^2 [a^*] [C_n] \{a^{*'}\}$$

Now let

$$[a^*] [C_n] = [k^*]$$

and

$$[a^*][C_n]\{a^{*'}\} = B^*$$

Equation (32) may then be written

$$[\Delta C] = \frac{-w^2}{1 + w^2 B^*} [(k^{*'})' k^*] \quad (33)$$

Equation (23) becomes

$$\{x_{n+1}\} = \{x_n\} + \frac{w^2}{1 + w^2 B^*} \{(k^{*'})'\} (y^* - a^* \{x_n\}) \quad (34)$$

When the weighting factor is chosen to be the reciprocal of the probable error of the observation σ_y^* , equations (33) and (34) become

$$[\Delta C] = \frac{1}{\sigma_y^{*2} + B^*} [k^{*'} k^*] \quad (35)$$

and

$$\{x_{n+1}\} = \{x_n\} + \frac{1}{\sigma_y^{*2} + B^*} \{(k^{*'})'\} (y^* - [a^*] \{x_n\}) \quad (36)$$

Recursion Formulas for Deleting an Observation

These formulas are derived by assuming that $[C_{n+1}]$ and $\{x_{n+1}\}$ are known and solving for $[C_n]$ and $\{x_n\}$. The observation to be deleted is y , and its corresponding observation coefficients are $[a]$. From equation (7), it may be seen that

$$[C_n] = \left[[C_{n+1}]^{-1} - \{a'\} [a] \right]^{-1} \quad (37)$$

where $[a]$ is now the row of coefficients in the observation equation to be deleted.

By equation (2),

$$\{x_n\} = \left[[C_{n+1}]^{-1} - \{a'\} [a] \right]^{-1} \|A'\| \{Y\} \quad (38)$$

or

$$\left[\bar{C}_{n+1} \right]^{-1} - \{a'\} [a] \{x_n\} = \|A'\| \{Y\} \quad (39)$$

In order to obtain an expression involving $\{x_{n+1}\}$, the matrix $\{a'\} y$ is added to and subtracted from the right-hand side of equation (39), and the resulting expression is multiplied through by $\left[\bar{C}_{n+1} \right]$. Thus, equation (39) becomes

$$\left[\bar{I} \right] - \left[\bar{C}_{n+1} \right] \{a'\} [a] \{x_n\} = \left[\bar{C}_{n+1} \right] \left\{ \|A'\| \{Y\} + \{a'\} y - \{a'\} y \right\} \quad (40)$$

By equations (7) and (8),

$$\left[\bar{C}_{n+1} \right] \left\{ \|A'\| \{Y\} + \{a'\} y \right\} = \{x_{n+1}\} \quad (41)$$

Therefore, equation (40) may be written

$$\left[\bar{I} \right] - \left[\bar{C}_{n+1} \right] \{a'\} [a] \{x_n\} = \{x_{n+1}\} - \left[\bar{C}_{n+1} \right] \{a'\} y \quad (42)$$

Let $\left[\bar{C}_{n+1} \right] \{a'\} = \{k_1'\}$. Then equation (42) becomes

$$\left[\bar{I} \right] + \{k_1'\} [a] \{x_n\} = \{x_{n+1}\} - \{k_1'\} y \quad (43)$$

Equation (43) is similar in form to equation (12). By the same procedure used in simplifying equation (12), it may be shown that equation (43) can be written as

$$\{x_n\} = \{x_{n+1}\} + \frac{1}{1 - B_1} \{k_1'\} \left([a] \{x_{n+1}\} - y \right) \quad (44)$$

where $B_1 = [a] \{k_1'\}$.

By following procedures similar to those expressed in equations (24) to (32), it may be shown that

$$\left[\bar{C}_n \right] = \left[\bar{C}_{n+1} \right] - \frac{1}{1 - B_1} \{k_1'\} [k_1] \quad (45)$$

Application to Dynamic Systems

When the quantities to be estimated are variables which describe the instantaneous state of a dynamic system, and when the observed quantities are not occurring simultaneously, the method of least squares can be applied if the state variables at one time can be expressed in terms of those at another time in the following way:

$$\{X_{t,2}\} = [\Phi(t_2; t_1)] \{X_{t,1}\} \quad (46)$$

where the transition matrix $[\Phi(t_2; t_1)]$ is dependent only on the times t_2 and t_1 at which states $\{X_{t,2}\}$ and $\{X_{t,1}\}$ occur and may be calculated from a knowledge of the dynamics of the system. Under these conditions, the state at the time of any particular observation may be expressed in terms of the state at the time of the last observation. The necessary simultaneous equations, in the form of equation (1), can then be set up to obtain a least-squares estimate of the state at the time t_n of the nth observation. Then, considering the fact that at time t_{n+1}

$$\{X_{t,n+1}\} = [\Phi(t_{n+1}; t_n)] \{X_{t,n}\} \quad (47)$$

it is easily shown that the least-squares estimate $\{x_{t,n+1}\}$ is calculated by substituting $[\Phi(t_{n+1}; t_n)] \{x_{t,n}\}$ for $\{x_n\}$ and by substituting $[\Phi(t_{n+1}; t_n)] [C_n] [\Phi'(t_{n+1}; t_n)]$ for $[C_n]$ in equations (36) and (37) and in the definitions of $\{k^*\}$ and B^* . Thus,

$$\begin{aligned} \{x_{t,n+1}\} &= [\Phi(t_{n+1}; t_n)] \{x_{t,n}\} \\ &+ \frac{1}{\sigma_y^{*2} + B^*} \{k^*\} \left(y^* - [a^*] [\Phi(t_{n+1}; t_n)] \{x_{t,n}\} \right) \end{aligned} \quad (48)$$

where

$$\{k^*\} = [\Phi(t_{n+1}; t_n)] [C_n] [\Phi'(t_{n+1}; t_n)] \{a^{*'}\}$$

and

$$B^* = [a^*] [\Phi(t_{n+1}; t_n)] [C_n] [\Phi'(t_{n+1}; t_n)] \{a^{*'}\}$$

The covariance matrix of $\{x_{t,n+1}\}$ is

$$[C_{n+1}] = [\Phi(t_{n+1}; t_n)] [C_n] [\Phi'(t_{n+1}; t_n)] - \frac{1}{\sigma_y^{*2} + B^*} \{k^{*'}\} [k^*] \quad (49)$$

DISCUSSION

Uses of Recursion Formulas

In any experimental procedure where data are accumulated over a period of time and where the least-squares method is to be used, the data reduction may be started as soon as enough observations have been made to give a solution. The remaining observations may be accounted for as they are made. Each time the recursion formulas are applied, the revised solution forms a basis for adding a new observation. The solution may be checked for wild points by calculating the residuals of the observations which have entered the solution. If any observation has an excessively large residual, it may be deleted and replaced by another observation if desired.

In certain data-smoothing procedures, a small section of, for example, a time history of experimental data is fitted by a polynomial which would not fit the entire time history. As the data are accumulated, data points are added to one end of the small section and deleted from the other end. The recursion formulas in this report should be very useful in procedures of this sort.

Effects of Correlated Errors

In this report it has been assumed that the observation errors were uncorrelated. That is, a knowledge of the error in any one observation gives no information as to the probable error in any other observation.

When the observation errors are known to be correlated, different recursion formulas may be used if the correlation coefficients are known. The recursion formulas in references 2 and 3 take into account the possibility of correlated errors. In many practical cases, either the observation errors are not correlated or their correlation coefficients are not known. In these cases the ordinary weighted least-squares estimate is the best which can be obtained. Reference 6 treats the subject of correlated errors from the standpoint of least squares.

Significance of Covariance Matrix

It is obvious from equation (2) that the covariance matrix of the estimated coefficients does not contain any information obtained from the observations directly. The variances of the observed quantities, which enter as weighting factors, are presumed to be known. Consequently, the covariance matrix which results from the estimation of the unknown coefficients by any given set of

observations can be computed before any observations are made. Likewise, by means of the recursion expression, the effect of a single observation on the covariance matrix can be predicted without actually making the observation. If in some experimental program there is a choice of observations which may be added, the optimum observation may be chosen by precomputing the effect of each observation and choosing the one which gives the greatest reduction in the covariance matrix.

Langley Research Center,
National Aeronautics and Space Administration,
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APPENDIX

PROOF THAT $[C_n]$ IS COVARIANCE MATRIX OF $\{x_n\}$

If the weighting factors which were applied to equation (1) are arranged in a diagonal matrix denoted by $\left[\frac{1}{\sigma_Y}\right]$, it may be seen that $\left[\frac{1}{\sigma_Y}\right] \|A^*\| = \|A\|$ and equation (2) may be written

$$\{x_n\} = \left[\|A^{*'}\| \left[\frac{1}{\sigma_Y^2}\right] \|A^*\| \right]^{-1} \|A^{*'}\| \left[\frac{1}{\sigma_Y^2}\right] \{Y^*\} \quad (A1)$$

From the definition of a covariance matrix and under the condition previously assumed that the errors in the observations $\{Y^*\}$ are uncorrelated, it follows that the covariance matrix of $\{Y^*\}$ is the diagonal matrix $[\sigma_Y^2]$. Let this matrix be denoted by $\left[\sum_Y\right]$. Then equation (A1) may be written as

$$\{x_n\} = \left[\|A^{*'}\| \left[\sum_Y\right]^{-1} \|A^*\| \right]^{-1} \|A^{*'}\| \left[\sum_Y\right]^{-1} \{Y^*\} \quad (A2)$$

Let

$$\{y\} = \|A^{*'}\| \left[\sum_Y\right]^{-1} \{Y^*\} \quad (A3)$$

For example, in an equation of the form

$$\{p\} = \|q\| \{r\}$$

the covariance matrix of $\{p\}$ is given in terms of the covariance matrix of $\{r\}$ by the following relationship derived from the theory of the propagation of error:

$$\left[\sum_p\right] = \|q\| \left[\sum_r\right] \|q'\|$$

The covariance matrix of y is then

$$\left[\sum_y \right] = \left\| \left\| A^* \right\| \left[\sum_Y \right]^{-1} \left\| \left[\sum_Y \right] \left\| \left[\sum_Y \right]^{-1} \left\| A^* \right\| \right\| \right\| \quad (A4)$$

Because $\left[\sum_Y \right]^{-1}$ is symmetrical, equation (A4) becomes

$$\left[\sum_y \right] = \left\| A^* \right\| \left[\sum_Y \right]^{-1} \left[\sum_Y \right] \left[\sum_Y \right]^{-1} \left\| A^* \right\| \quad (A5)$$

or, by the definition of $[C_n]$ given in the text,

$$\left[\sum_y \right] = \left\| A^* \right\| \left[\sum_Y \right]^{-1} \left\| A^* \right\| = [C_n]^{-1} \quad (A6)$$

From equations (A2) and (A3), again making use of the definition of $[C_n]$,

$$\{x_n\} = [C_n] \{y\} \quad (A7)$$

Again, by the theory of the propagation of errors, and making use of the fact that the transpose of $[C_n]$ is $[C_n]$, the covariance matrix of $\{x_n\}$, denoted

by $\left[\sum_{x,n} \right]$, is

$$\left[\sum_{x,n} \right] = [C_n] \left[\sum_y \right] [C_n] \quad (A8)$$

Substituting $[C_n]^{-1}$ for $\left[\sum_y \right]$, according to equation (A6), equation (A8) becomes

$$\left[\sum_{x,n} \right] = [C_n] \quad (A9)$$

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