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FINAL REPORT

PROJECT A-700

METHODS OF FITTING MULTIVARIANT FUNCTIONAL MODELS
IN THE AREA OF LARGE COMPUTER EXPLOITATION

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D. E. PETERSON, AND J. W. WALKER

Performed for
George C. Marshall Space Flight Center
National Aeronautics and Space Administration
Huntsville, Alabama

Engineering Experiment Station

GEORGIA INSTITUTE OF TECHNOLOGY

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GEORGE C. MARSHALL SPACE FLIGHT CENTER
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The Astrodynamics and Guidance Theory Division of the Aero-Astrodynamics Laboratory of the Marshall Space Flight Center is examining the role of large computers as they may be exploited in the prediction of missile performance. The Georgia Institute of Technology and its Rich Electronic Computer Center have been studying such exploitation as it applies to the fitting of the Multivariant Functional Models under Contract No. NAS8-5365. Under this contract, attention has been focused on models which describe missile performance under various conditions and in response to various guidance methods.

The problem under consideration may be stated in the following manner. Let $x(t)$ be the instantaneous state vector with n components $x_i(t)$ $i = 1,2,\ldots,n$. The equations of motion may be taken as

$$F(\dot{x}(t),\ x(t),\ t,\ u(t)) = 0\ ,$$

where F stands for a set of functions and $u(t)$ is the guidance or control function. Terminal conditions at some time t_c may be taken as

$$G(x(t_c),\ t_c) = 0\ ,$$

where G represents a set of functions. The set of functions G are the mission requirements. It is desired to choose $u(t)$ in some class of functions in order to minimize t_c. Clearly, the optimum $u(t)$ depends on the initial conditions $x(t_0) = x_0$ and t_0. The optimum guidance function shall be denoted by $u(t;\ x_0,\ t_0)$.

If an optimum guidance function $u(t;\ x_0,\ t_0)$ is chosen and an optimum trajectory is followed, then at some future time t_1 with state vector

$x(t_1) = x_1$ the new optimum guidance function $u(t; x_1, t_1)$ must be identical with the old guidance function $u(t; x_0, t_0)$ for $t \geq t_1$. In other words, the optimum guidance function is invariant with respect to the state vector $x(t)$ and the time t.

Since various factors in the system cannot be accounted for, in practice the optimum trajectory may not be followed. It is important then to determine the optimum guidance function $u(t; x_0, t_0)$ as a function of the state vector x_0 and the time t_0. The determination of this function of the initial conditions is called a synthesis of the optimum guidance function $u(t; x_0, t_0)$.

As an approach to the synthesis problem one could select a number of initial conditions (x_i, t_i) and utilize a computer to find the corresponding $u(t; x_i, t_i)$. An approximation technique can then be employed to find a functional relationship between the $u(t; x_i, t_i)$ and the (x_i, t_i). Because of simplicity, an approximating polynomial could be assumed. Since the number of state variables is large (more than six), the number of coefficients in the model would be very large even for polynomials of low degree. Practical considerations forbid such procedures.

As a first approach to this problem, a balanced polynomial balanced design model was studied. It was shown that the least squares fit which involved the inversion of a large order matrix could be reduced to the inversion of many small order matrices. This procedure is reported in detail in Appendix 1. While this approach overcame the computational difficulties, there still remained the objections of the need for a tremendous number of data points and approximating polynomials with several hundred terms.

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To overcome these objections a "step-up" procedure was developed. In the language of regression analysis, psychologists and other investigators have for some time studied the problem of selecting out of n predictor variables that subset of k of them which will contribute most to the sum of squares due to regression (leaving the smallest sum of squares due to error).

The procedure starts with a model which assumes the guidance function as a linear combination of n terms (not necessarily polynomials). The procedure attempts to select a subset k of the n terms which best fit the observational data in the sense of least squares. First, that term is taken for which the greatest reduction in the error sum of squares is effected. The next term is selected again on the basis of the greatest reduction in the error sum of squares. By continuing in this way, the most significant terms may be obtained one by one. Stopping criteria can be devised in terms of the final number of terms desired and/or essentially insignificant improvement in the reduction of the error sum of squares. This procedure is reported in detail in Appendix 2.

Preliminary experience with the "step-up" procedure indicated that efficient stopping and throwout criteria depended on the class of problems under consideration. Accordingly, it was necessary to develop experience with this tool. Data was obtained from the Astrodynamics and Guidance Theory Division on some seventy-five trajectories. These data were analyzed and the "step-up" procedure applied to the fitting of the guidance functions. This analysis is reported in detail in Appendix 3.

In order to gain further insight into the synthesis problem, the flat earth problem was studied and an interesting graphical synthesis developed. This study is reported in detail in Appendix 4.

The studies reported in Appendices 2 through 4 indicate that the step-wise regression procedure shows considerable promise in the fitting of Multivariant Functional Models. Further experience with the procedure is necessary in order to resolve questions of roundoff and throwout criteria, precision requirements, and sensitivity to the data base.

It is recommended that in addition to the fitting problem, the performance of the various approximations be evaluated. Since complex problems tend to limit the degree of experimentation, it is felt that the flat earth problem investigated in Appendix 4 be utilized for further study. Controlled, but representative, data could be generated by the method discussed in Appendix 4 or by a general numerical integration program for solving the two point boundary value problem resulting from the Pontryagin formulation. The various data fits can be compared in actual control simulations using the identical equations of motion, etc., as those used in the data generation. Thus, various error analyses studies can be made comparing such items as terminal accuracy and the degree of optimality achieved by the various data fits.

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Respectfully submitted,

I. E. Perlin
Project Director

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APPENDIX 1

LEAST SQUARES ESTIMATION OF REGRESSION COEFFICIENTS
IN A SPECIAL CLASS OF POLYNOMIAL MODELS

I. INTRODUCTION

The problem with which we are concerned is that of approximating a real valued function of several real variables given a collection of points in the domain of the function and the corresponding values of the function at these points. Furthermore, we are considering a polynomial approximation of the function and are assuming the least squares criterion for the best approximation. Theoretically, then, our problem is easy -- simply use the polynomial of the chosen degree with the least squares estimates of the coefficients. However, from the practical point of view the problem is not so easy. Actually finding the least squares coefficients may be an almost impossible task when one is fitting a polynomial of several variables and modest degree. The inversion of the coefficient matrix of the normal equations is the usual problem.

The general methods for finding the least squares coefficients can be divided into two major categories--those which apply for arbitrarily chosen data points and those which depend on some special arrangement or design of the data points. The methods thus far proposed for arbitrarily chosen data points do not seem substantially to reduce the calculational difficulties from those of inverting the coefficient matrix of the normal equations. However, if one is willing to allow any apriori design of the data points, it is possible to have a design which will yield an easily invertable coefficient matrix. There is, of course, a middle ground between that of no restriction on the arrangement of data points (design) and that of the very severe restrictions needed to produce an easily invertable coefficient matrix. It is in this area of moderate restrictions on the design of the data points that we have had some success. We shall call our design of the data points a rectangular design. In the statistical literature this design is called a factorial design.

By using a rectangular design and a special form of polynomial called a balanced polynomial we have been able to calculate the least squares coefficients with a considerable reduction in calculational difficulty in the sense that several lower order matrices are easier to invert than one of higher order. The process by which we calculate the least squares coefficients will be called the step procedure.

II. RECTANGULAR DESIGNS

Suppose the domain of the function to be approximated is a subset of π-dimensional Euclidian space. Let $(x^{(1)}, \ldots, x^{(\pi)})$ be a typical point and define

$$D_i = \left\{ x_{t_i}^{(i)} : t_i = 1, \ldots, T_i, \quad x_{t_i} \neq x_{s_i} \text{ if } t_i \neq s_i \right\}.$$

Then the cartesian product

$$D_1 \times D_2 \times \ldots \times D_\pi = D$$

will be a subset of π-dimensional Euclidian space. We define a rectangular design to be any such D. Note that the T_i's need not be equal and the $x_{t_i}^{(i)}$ need not be equally spaced.

<u>Step Procedure</u>: The step procedure is most easily explained by an example. Let us consider a function of two variables, f, and consider an approximation of f by means of a second degree polynomial. Denoting $f(u,v)$ by y we have

$$y \approx (a_{11} + a_{21}u + a_{31}u^2) + (a_{12} + a_{22}u)v + a_{13}v^2 .$$

Suppose the data is in a rectangular design, say

$$D = D_1 \times D_2 , \quad D_1 = (u_1, \ldots, u_n) , \quad D_2 = (v_1, \ldots, v_m)$$

then we may use the step procedure to find estimates, not necessarily the best, of the a's. The procedure is as follows:

1. Hold u fixed at say u_i and define b_{i1}, b_{i2}, b_{i3} by

$$b_{i1} = a_{11} + a_{21}u_i + a_{31}u_i^2$$

$$b_{i2} = a_{12} + a_{22}u_i$$

$$b_{i3} = a_{13}$$

and consider

$$y_{ij} \approx b_{i1} + b_{i2}v_j + b_{i3}v_j^2$$

2. For each fixed i find the least squares estimates of b_{i1} , b_{i2} , b_{i3} .

3. Using these estimates as if they were observed values of $a_{11} + a_{21}u_i + a_{22}u_i^2$, $a_{12} + a_{22}u_i$, a_{13} respectively find the least squares estimates of a_{11} , a_{21} , a_{22} ; a_{12} , a_{22} ; and a_{13} .

Note that instead of a 6×6 matrix inversion as in the case of finding direct least squares estimates of the a's , we were only required to invert several smaller matrices of maximum size 3×3 . We could also have written the polynomial approximation as

$$y \approx (a_{11} + a_{12}v + a_{13}v^2) + (a_{21} + a_{22}v)u + a_{31}u^2$$

and used the procedure just as well. The estimates of the a's in this case would, in general, be different from those found above.

It is not difficult to show that in a general n^{th} degree polynomial of π variables the estimate of the coefficient of the highest power of the variable which appears in the first step of the step procedure is indeed the least squares estimate. We shall denote this result as theorem 1 . In general the estimates of the other coefficients do not have this property.

III. BALANCED POLYNOMIALS

As motivation for considering balanced polynomials, think of expanding a function of π variables, $x^{(1)}, \ldots, x^{(\pi)}$, in a power series in $x^{(\pi)}$ and approximate this by the first $L_\pi + 1$ terms; i.e., a polynomial in $x^{(\pi)}$ of degree L_π . Now expand the coefficients of this polynomial in power series in $x^{(\pi-1)}$ and approximate these series by their first $L_{\pi-1} + 1$ terms. Continue this process until all the variables have been used. Note this yields a polynomial in $x^{(1)}, \ldots, x^{(\pi)}$ of degree $L_1 L_2 \ldots L_\pi$ which is not the general polynomial of this degree. For example, if $\pi = 2$, $L_1 = L_2 = 2$ we have the balanced polynomial

$$(a_{11} + a_{21}u + a_{31}u^2) + (a_{12} + a_{22}u + a_{32}u^2)v + (a_{13} + a_{23}u + a_{33}u^2)v^2 \ .$$

This polynomial is a fourth degree polynomial in u, v but the u^4, u^3, v^4, v^3 , u^3v, v^3u terms are missing. Notice, however, that all the terms of the general second degree polynomial are present. So if higher degree terms are not objectionable, it would seem that if a general polynomial in π variables of degree L provides a reasonable approximation, a balanced polynomial in π variables with $\min_{j=1,\ldots,\pi} L_j \geq L$ would give an even better approximation.

In general a polynomial of the form

$$\sum_{\ell_1=1}^{L_1+1} \cdots \sum_{\ell_\pi=1}^{L_\pi+1} a_{\ell_1 \ldots \ell_\pi} \ x_{\ell_1}^{(1)} \ldots x_{\ell_\pi}^{(\pi)} \ , \quad x_{\ell_i}^{(i)} = \left(x^{(i)}\right)^{\ell_i - 1}$$

will be called a balanced polynomial. We show in theorem 2 that the step procedure applied to a balanced polynomial over a rectangular design will yield the least squares estimates of all the coefficients.

IV. PROPERTIES OF RECTANGULAR DESIGN AND BALANCED POLYNOMIALS

Consider the general d^{th} degree polynomial in the π variables $x^{(1)}, \ldots, x^{(\pi)}$ which we shall write as

$$(1) \quad a_{11\ldots1} + \ldots + a_{1\ldots i\ldots1}x_1^{(i)} + \ldots + (\text{terms in } x^{(1)}, \ldots, x^{(\pi)} \text{ of degree}$$
$$\leq d) + a_{1\ldots1d+1}(x^{(\pi)})^d .$$

We shall call $x^{(\pi)}$ the leading variable. Clearly this general polynomial may be written with any $x^{(i)}$ as the leading variable but in what follows we shall be concerned with the specific form of the polynomial in (1) and thus the leading variable will be $x^{(\pi)}$. If we use such a polynomial to approximate a real valued function f of π variables $x^{(1)}, \ldots, x^{(\pi)}$; we have the following result.

THEOREM 1: In the case of a general d^{th} degree polynomial in π variables the step procedure over a rectangular design yields the same estimate for the coefficient of the dth power of the leading variable as the least squares procedure over the same design.

Before presenting a proof of theorem 1 we shall exhibit an example which shows that theorem 1 is best possible in the sense that in general the step procedure estimates and the least squares estimates of the other coefficients do not agree. In particular this will justify the use of the specific form of (1) and the "leading variable" terminology.

Consider the general second degree polynomial in two variables

$$a_{11} + a_{21}u + a_{31}u^2 + (a_{12} + a_{22}u)v + a_{13}v^2$$

as an approximation of a real valued function f of two real variables u,v .

Let $y_{ij} = f(u_i , v_j)$ and thus suppose the expected value of y_{ij} given by

$$E(y_{ij}) = a_{11} + a_{21}u_i + a_{31}u_i^2 + (a_{12} + a_{22}u_i)v_j + a_{13}v_j^2$$

or in vector-matrix notation

$$E(\underline{y}) = X\,\underline{a}$$

where

$$\underline{y} = \begin{pmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{31} \\ y_{32} \\ y_{33} \end{pmatrix} \qquad X = \begin{pmatrix} 1 & u_1 & u_1^2 & u_1v_1 & v_1 & v_1^2 \\ 1 & u_1 & u_1^2 & u_1v_2 & v_2 & v_2^2 \\ 1 & u_1 & u_1^2 & u_1v_3 & v_3 & v_3^2 \\ 1 & u_2 & u_2^2 & u_2v_1 & v_1 & v_1^2 \\ 1 & u_2 & u_2^2 & u_2v_2 & v_2 & v_2^2 \\ 1 & u_2 & u_2^2 & u_2v_3 & v_3 & v_3^2 \\ 1 & u_3 & u_3^2 & u_3v_1 & v_1 & v_1^2 \\ 1 & u_3 & u_3^2 & u_3v_2 & v_2 & v_2^2 \\ 1 & u_3 & u_3^2 & u_3v_3 & v_3 & v_3^2 \end{pmatrix}$$

$$\underline{a} = \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{12} \\ a_{22} \\ a_{13} \end{pmatrix} \qquad\qquad \text{for} \quad i,j = 1, 2, 3 \ .$$

The least squares estimates of the coefficients may be found by solving the normal equations [1]

$$X'\,X\,\underline{a} = X'\,\underline{y} \quad .$$

If in our example we consider the rectangular design

$$D = D_1 \times D_2 \quad ; \quad D_1 = \left\{ -1,\ 0,\ 1 \right\} \qquad D_2 = \left\{ -2,\ 0,\ 1 \right\}$$

the normal equations become

$$
\begin{pmatrix}
9 & 0 & 6 & 0 & -3 & 15 \\
0 & 6 & 0 & -2 & 0 & 0 \\
6 & 0 & 6 & 0 & -2 & 10 \\
0 & -2 & 0 & 10 & 0 & 0 \\
-3 & 0 & -2 & 0 & 15 & -21 \\
15 & 0 & 10 & 0 & -21 & 51
\end{pmatrix}
\begin{pmatrix}
a_{11} \\ a_{21} \\ a_{31} \\ a_{12} \\ a_{22} \\ a_{13}
\end{pmatrix}
=
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & -1 & -1 & 0 & 0 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\
2 & 0 & -1 & 0 & 0 & 0 & -2 & 0 & 1 \\
-2 & 0 & 1 & -2 & 0 & 1 & -2 & 0 & 1 \\
4 & 0 & 1 & 4 & 0 & 1 & 4 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
y_{11} \\ y_{12} \\ y_{13} \\ y_{21} \\ y_{22} \\ y_{23} \\ y_{31} \\ y_{32} \\ y_{33}
\end{pmatrix}
$$

The solution of this system is

$$a_{11} = \frac{1}{54} \left(48 \sum_i y_{i1} + 30 \sum_i y_{i2} + 21 \sum_i y_{i3} - 18 \sum_j y_{1j} - 18 \sum_j y_{3j} \right)$$

$$a_{21} = \frac{1}{28} \left(-5 \sum_j y_{1j} + 5 \sum_j y_{3j} + 2 y_{11} - y_{13} - 2 y_{31} + y_{33} \right)$$

$$a_{31} = \frac{1}{54} \left(-18 \sum_i y_{i1} - 18 \sum_i y_{i2} - 18 \sum_i y_{i3} + 27 \sum_j y_{1j} + 27 \sum_j y_{3j} \right)$$

$$a_{12} = \frac{1}{28} \left(- \sum_j y_{1j} + \sum_j y_{3j} + 6 y_{11} - 3 y_{13} - 6 y_{31} + 3 y_{33} \right)$$

$$a_{22} = \frac{1}{54} \left(-3 \sum_i y_{i1} - 9 \sum_i y_{i2} + 12 \sum_i y_{i3} \right)$$

$$a_{13} = \frac{1}{54} \left(3 \sum_i y_{i1} - 9 \sum_i y_{i2} + 6 \sum_i y_{i3} \right)$$

Now consider the same design and use the step procedure to estimate the coefficients. Thus, write the polynomial as

$$b_1 + b_2 v + b_3 v^2$$

where

$$b_1 = a_{11} + a_{21}u + a_{31}u^2$$

$$b_2 = a_{12} + a_{22}u$$

$$b_3 = a_{13} \quad .$$

For fixed i find the least squares estimates of $b_{1i} = a_{11} + a_{21}u_i + a_{31}u_i^2$, $b_{2i} = a_{12} + a_{22}u_i$, $b_{3i} = a_{13}$. We obtain the normal equations in v alone:

$$(V'\,V)\,\underline{b}_i = V'\,\underline{y}_i$$

where

$$V = \begin{pmatrix} 1 & v_1 & v_1^2 \\ 1 & v_2 & v_2^2 \\ 1 & v_3 & v_3^2 \end{pmatrix} , \quad \underline{b}_i = \begin{pmatrix} b_{1i} \\ b_{2i} \\ b_{3i} \end{pmatrix} , \quad \underline{y}_i = \begin{pmatrix} y_{i1} \\ y_{i2} \\ y_{i3} \end{pmatrix} \quad .$$

The solution of this system is

$$b_{1i} = y_{i2}$$

$$b_{2i} = -\frac{1}{6} y_{i1} - \frac{1}{2} y_{i2} + \frac{2}{3} y_{i3}$$

$$b_{3i} = \frac{1}{6} y_{i1} - \frac{1}{2} y_{i2} + \frac{1}{3} y_{i3} \quad . \quad (i = 1, 2, 3)$$

The second step is to treat the u's as observations on the polynomials $a_{11} + a_{21}u + a_{31}u^2$, $a_{21} + a_{22}u$, a_{13} and find the least squares estimates of the a's. For b_1 the normal equations are

$$(U_1'\,U_1)\,\underline{a}_1 = U_1'\,\underline{b}_1$$

where

$$U_1 = \begin{pmatrix} 1 & u_1 & u_1^2 \\ 1 & u_2 & u_2^2 \\ 1 & u_3 & u_3^2 \end{pmatrix} , \quad \underline{a}_1 = \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} , \quad \underline{b}_1 = \begin{pmatrix} b_{11} \\ b_{12} \\ b_{13} \end{pmatrix} \quad .$$

The solution of this system is

$$a_{11} = b_{12} = y_{22}$$

$$a_{21} = -\frac{1}{2}(b_{11} + b_{13}) = -\frac{1}{2}(y_{12} + y_{32})$$

$$a_{31} = \frac{1}{2}(b_{11} + b_{13}) - b_{12} = \frac{1}{2}(y_{12} + y_{32}) - y_{22} \quad .$$

In the case of b_2 the normal equations are

$$(U_2' U_2)\, \underline{a}_2 = U_2'\, \underline{b}_2 \quad ,$$

where

$$U_2 = \begin{pmatrix} 1 & u_1 \\ 1 & u_2 \\ 1 & u_3 \end{pmatrix} \quad , \qquad \underline{a}_2 = \begin{pmatrix} a_{12} \\ a_{22} \end{pmatrix} \quad , \qquad \underline{b}_2 = \begin{pmatrix} b_{21} \\ b_{22} \\ b_{23} \end{pmatrix} \quad .$$

The solution of this system is

$$a_{12} = \frac{1}{3}\sum_{i=1}^{3} b_{1i} = \frac{1}{54}\left(-3\sum y_{i1} - 27\sum y_{i2} + 36\sum y_{i3}\right)$$

$$a_{22} = \frac{1}{2}(b_{13} - b_{11}) = \frac{1}{12}\left(-y_{31} - 3y_{32} + 4y_{33} + y_{11} + 3y_{12} - 4y_{13}\right) \quad .$$

Note at this point that none of the step procedure estimates agrees with the least squares estimate.

Finally consider b_3 and the normal equations

$$(U_3' U_3)\, \underline{a}_3 = U_3'\, \underline{b}_3$$

where

$$U_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad , \qquad \underline{a}_3 = a_{13} \quad , \qquad \underline{b}_3 = \begin{pmatrix} b_{31} \\ b_{32} \\ b_{33} \end{pmatrix}$$

so that

$$a_{13} = \frac{\sum\limits_{j=1}^{3} b_{3j}}{3} = \frac{1}{54} (3 \sum y_{i1} - 9 \sum y_{i2} + 6 \sum y_{i3})$$

which does agree with the least squares estimate of a_{13} .

Thus, we see that the step procedure for estimating the coefficients of a general polynomial over a rectangular design is not equivalent to least squares estimation over the same design. However, in theorem 2 we shall give conditions sufficient for the equivalence of the two procedures. We now present a proof of theorem 1 in the case $d = 2$, $\pi = 2$. (For the general proof see Appendix B.)

Consider the rectangular design

$$D = D_1 \times D_2 \quad ; \quad D_1 = \left\{ u_1 , u_2 , u_3 \right\} \quad ; \quad D_2 = \left\{ v_1 , v_2 , v_3 \right\}$$

and the polynomial

$$(*) \quad (a_{11} + a_{21}u + a_{31}u^2) + (a_{12} + a_{22}u)v + a_{13}v^2$$

written in preparation for the first step of the step procedure as

$$b_1 + b_2 v + b_3 v^2$$

where $b_1 = a_{11} + a_{21}u + a_{31}u^2$, $b_2 = a_{12} + a_{22}u$, $b_3 = a_{13}$. Let $y_{ij} = f(u_i v_j)$ where f is the function to be approximated by the polynomial $(*)$.

If we can demonstrate that the step procedure estimate of $a_{13} = b_3$ is a linear combination of the components of $X'\underline{y}$, using the notation of the example, and show that such an estimate is unbiased; then the step procedure estimate is the least squares estimate. (See Appendix A)

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Since the first step of the step procedure is a least squares estimation, the step procedure estimate of b_3, $\hat{b}_3$, is unbiased. Furthermore,

$$
\begin{pmatrix} \hat{b}_{1i} \\ \hat{b}_{2i} \\ \hat{b}_{3i} \end{pmatrix} = (V'V)^{-1} \begin{pmatrix} \sum_j y_{ij} \\ \sum_j v_j y_{ij} \\ \sum_j v_j^2 y_{ij} \end{pmatrix}
$$

that is, $\hat{b}_{3i}$ is a linear combination of

$$
\sum_j y_{ij} \quad , \quad \sum_j v_j y_{ij} \quad , \quad \sum_j v_j^2 y_{ij}
$$

for each i. Since $b_{3i} = a_{13}$ for each i the second step of the step procedure gives

$$
\frac{\sum_{i=1}^{3} \hat{b}_{3i}}{3}
$$

as the step procedure estimate of a_{13}. Clearly this is unbiased if $\hat{b}_{3i}$ is and this estimate is a linear combination of

$$
\sum_i \sum_j y_{ij} \quad , \quad \sum_i \sum_j v_j y_{ij} \quad , \quad \sum_i \sum_j v_j^2 y_{ij} \quad .
$$

However, the components of $X'\underline{y}$ are

$$
\sum_i \sum_j y_{ij} \quad , \quad \sum_{ij} u_i y_{ij} \quad , \quad \sum_{ij} u_i^2 y_{ij} \quad , \quad \sum_{ij} u_i v_j y_{ij} \quad , \quad \sum_{ij} v_j y_{ij} \quad , \quad \sum_{ij} v_j^2 y_{ij}
$$

so that the step procedure estimate of a_{13} is a linear combination of these components, specifically of the first, fifth and sixth. Thus, the proof is complete for this special case.

If we are willing to restrict ourselves to balanced polynomials, we may use the following result.

THEOREM 2: The step procedure when applied to a balanced polynomial approximation of a real function of several real variables over a rectangular design will yield the least squares estimates of the coefficients.

Consider the special case of a balanced polynomial in two variables each with maximum degree 2 ,

$$(a_{11} + a_{21}u + a_{31}u^2) + (a_{12} + a_{22}u + a_{32}u^2)\, v + (a_{13} + a_{23}u + a_{33}u^2)\, v^2 \; ,$$

as an approximation of a real function f of two real variables u,v over the rectangular design

$$D = D_1 \times D_2 \; , \quad D_1 = \left\{ u_1 \, , \, u_2 \, , \, u_3 \right\} \; , \quad D_2 = \left\{ v_1 \, , \, v_2 \, , \, v_3 \right\} \; .$$

Let $y_{t_1 t_2} = f(u_{t_1} \, , \, v_{t_2})$; $t_1 = 1, 2, 3$; $t_2 = 1, 2, 3$.

First we shall consider the least squares criterion for estimates of the a's and generate the normal equations ; then we shall show that the step procedure estimates of the a's satisfy the normal equations and are, therefore, least squares estimates.

Define S by

$$S = \sum_{t_1=1}^{3} \sum_{t_2=1}^{3} \left\{ y_{t_1 t_2} - \sum_{\ell_2=1}^{3} \sum_{\ell_1=1}^{3} a_{\ell_1 \ell_2} u_{t_1}^{\ell_1 - 1} v_{t_2}^{\ell_2 - 1} \right\}^2$$

and calculate $\dfrac{\partial}{\partial a_{\alpha_1 \alpha_2}} S$. Setting this partial derivative equal to zero, we arrive at the equation

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$$\sum_{t_1=1}^{3} \sum_{t_2=1}^{3} y_{t_1 t_2} u_{t_1}^{\alpha_1 - 1} v_{t_2}^{\alpha_2 - 1} = \sum_{\ell_2=1}^{3} \sum_{\ell_1=1}^{3} a_{\ell_1 \ell_2} \left\{ \sum_{t_1=1}^{3} \sum_{t_2=1}^{3} u_{t_1}^{\ell_1 - 1} u_{t_1}^{\alpha_1 - 1} v_{t_2}^{\ell_2 - 1} v_{t_2}^{\alpha_2 - 1} \right\} .$$

Now employing the properties of the rectangular design we have

$$(4) \quad \sum_{t_1=1}^{3} \sum_{t_2=1}^{3} y_{t_1 t_2} u_{t_1}^{\alpha_1 - 1} v_{t_2}^{\alpha_2 - 1} = \sum_{\ell_1=1}^{3} \sum_{\ell_2=1}^{3} a_{\ell_1 \ell_2} \left\{ \left(\sum_{t_1=1}^{3} u_{t_1}^{\ell_1 - 1} u_{t_1}^{\alpha_1 - 1} \right) \left(\sum_{t_2=1}^{3} v_{t_2}^{\ell_2 - 1} v_{t_2}^{\alpha_1 - 1} \right) \right\} .$$

We shall define the matrices U, V as follows

$$U = \begin{pmatrix} 1 & u_1 & u_1^2 \\ 1 & u_2 & u_2^2 \\ 1 & u_3 & u_3^2 \end{pmatrix} \qquad V = \begin{pmatrix} 1 & v_1 & v_1^2 \\ 1 & v_2 & v_2^2 \\ 1 & v_3 & v_3^2 \end{pmatrix}$$

Then clearly $\sum_{t_1=1}^{3} u_{t_1}^{\ell_1 - 1} u_{t_1}^{\alpha_1 - 1}$ is in the ℓ_1, α_1 position of the matrix $U'U$.

Similarly for $\sum_{t_2=1}^{3} v_{t_2}^{\ell_2 - 1} v_{t_2}^{\alpha_2 - 1}$. Thus define

$$U_{\ell_1 \alpha_1} = \sum_{t_1=1}^{3} u_{t_1}^{\ell_1 - 1} u_{t_1}^{\alpha_1 - 1}$$

$$V_{\ell_2 \alpha_2} = \sum_{t_2=1}^{3} v_{t_2}^{\ell_2 - 1} v_{t_2}^{\alpha_2 - 1}$$

and (4) becomes

$$(5) \quad \sum_{t_1=1}^{3} \sum_{t_2=1}^{3} y_{t_1 t_2} u_{t_1}^{\alpha_1 - 1} v_{t_2}^{\alpha_2 - 1} = \sum_{\ell_1=1}^{3} \sum_{\ell_2=1}^{3} A_{\ell_1 \ell_2} U_{\ell_1 \alpha_1} V_{\ell_2 \alpha_2}$$

Equation (5) is a typical equation from the set of normal equations.

We shall now use the step procedure to estimate a coefficient, $A_{s_1 s_2}$. In order to facilitate the writing down of this estimate, we shall have

need of the following notation. Let

$$(U^{\ell_1 s_1}) = (U'U)^{-1} \qquad \ell_1 = 1, 2, 3 \quad s_1 = 1, 2, 3$$

$$(V^{\ell_2 s_2}) = (V'V)^{-1} \qquad \ell_2 = 1, 2, 3 \quad s_2 = 1, 2, 3$$

and note $u_{r_1}^{\ell_1-1}$ is in the ℓ_1, r_1 position of U' and similarly for $v_{r_2}^{\ell_2-1}$.

The first step of the step procedure for finding an estimate of $A_{s_1 s_2}$ is

$$A_{t_1 s_2}^{(1)} = (V'V)^{-1} V' \underline{Y}_{t_1}$$

$$= \sum_{r_2=1}^{3} \left\{ \sum_{\ell_2=1}^{3} V^{\ell_2 s_2} v_{r_2}^{\ell_2-1} \right\} y_{t_1 r_2}$$

where $\underline{Y}_{t_1} = (y_{t_1 1}, y_{t_1 2}, y_{t_1 3})$. The second and in this case final step is then

$$A_{s_1 s_2} = (U'U)^{-1} U' a_{s_2}^{(1)}$$

$$= \sum_{r_1=1}^{3} \left\{ \sum_{\ell_1=1}^{3} U^{\ell_1 s_1} u_{r_1}^{\ell_1-1} \right\} a_{r_1 s_2}^{(1)}$$

$$= \sum_{r_1=1}^{3} \sum_{\ell_1=1}^{3} U^{\ell_1 s_1} u_{r_1}^{\ell_1-1} \sum_{r_1=1}^{3} \sum_{\ell_2=1}^{3} V^{\ell_2 s_2} v_{r_2}^{\ell_2-1} y_{r_1 r_2}$$

Using the fact that we have a balanced polynomial over a rectangular design we may write

$$A_{s_1 s_2} = \sum_{r_1=1}^{3} \sum_{r_2=1}^{3} \left\{ y_{r_1 r_2} \sum_{\ell_1=1}^{3} \sum_{\ell_2=1}^{3} U^{\ell_1 s_1} V^{\ell_2 s_2} u_{r_1}^{\ell_1-1} v_{r_2}^{\ell_2-1} \right\} .$$

If we substitute $A_{s_1 s_2}$ for $A_{\ell_1 \ell_2}$ in equation (5), the right hand side becomes

$$\sum_{s_1=1}^{3} \sum_{s_2=1}^{3} A_{s_1 s_2} U_{s_1 \alpha_1} V_{s_2 \alpha_2} =$$

$$\sum_{r_1=1}^{3} \sum_{r_2=1}^{3} y_{r_1 r_2} \left\{ \sum_{\ell_1=1}^{3} \sum_{\ell_2=1}^{3} [u_{r_1}^{\ell_1-1} v_{r_2}^{\ell_2-1} (\sum_{s_1=1}^{3} U^{\ell_1 s_1} U_{s_1 \alpha_1})(\sum_{s_2=1}^{3} V^{\ell_2 s_2} V_{s_2 \alpha_2})] \right\} \ .$$

However $\sum_{s_1=1}^{3} U^{\ell_1 s_1} U_{\ell_1 \alpha_1} = \delta_{\ell_1 \alpha_1} = 0$ or 1 depending on whether $\ell_1 \neq \alpha_1$ or $\ell_1 = \alpha_1$. Similarly, $\sum_{s_2=1}^{3} V^{\ell_2 s_2} V_{s_2 \alpha_2} = \delta_{\ell_2 \alpha_2}$. So that we have the right hand side of (5) equal to

$$\sum_{r_1=1}^{3} \sum_{r_2=1}^{3} y_{r_1 r_2} \left\{ \sum_{\ell_1=1}^{3} \sum_{\ell_2=1}^{3} u_{r_1}^{\ell_1-1} v_{r_2}^{\ell_2-1} \delta_{\ell_1 \alpha_1} \delta_{\ell_2 \alpha_2} \right\} =$$

$$\sum_{r_1=1}^{3} \sum_{r_2=1}^{3} y_{r_1 r_2} u_{r_1}^{\alpha_1-1} v_{r_2}^{\alpha_2-1}$$

which is the left hand side of equation (5) . Thus $A_{s_1 s_2}$ is a solution of the normal equations and the proof of theorem 2 is complete for this special case.

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V. IMPLICATIONS AND EXTENSIONS

Comparison to ANOVA

The analysis of variance model for a factorial design which includes all of the interaction terms is equivalent to a balanced polynomial model in which the degree of the polynomial in a given variable is one less than the number of levels of the factor corresponding to that variable. In the analysis of variance model we break up the degrees of freedom for a factor into each of the different levels and in a polynomial model we use the constant, linear, and quadratic parts. If we have a factor at levels a, b, and c then we may think of these three degrees of freedom as corresponding to the space spanned by

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad .$$

Equivalently, we may consider the space spanned by

$$\begin{pmatrix} 1 & a & a^2 \\ 1 & b & b^2 \\ 1 & c & c^2 \end{pmatrix} \quad .$$

The first is the analysis of variance model and the second is the polynomial model.

A factorial design in which all interactions above order d are assumed to be zero is equivalent to a polynomial model in which cross products involving more than d + 1 factor are omitted.

Relaxation of Balanced Polynomial Conditions

We have seen in theorem 1 that the rectangular design enables us to use the very easy step procedure to find the least squares estimate of the coefficients of the highest power of each variable in a model which is the general polynomial of degree d . In theorem 2 we see that the rectangular design enables us to use the step procedure to calculate the least squares estimates of all of the coefficients of a model which is a balanced polynomial. We may now ask; is it necessary to have a balanced polynomial to get all of the coefficients by the step procedure? Is it possible to have other polynomial models in which the step procedure gives the least squares estimates of some terms other than just the highest power?

To gain some insight into these questions we shall consider as an example the two factor model

$$E \, y_{ij} \; = \; P \, (u_i \, , \, v_j)$$

where P is a polynomial in u and v and the design is a rectangular design in which u has 4 values and v has 3 .

Now we apply the step procedure with leading variable v . We write $P \, (u, v)$ as a polynomial in v .

$$E \, y_{ij} \; = \; P_0(u_i) \; + \; v_j P_1(u_i) \; + \; v_j^2 P_2(u_i) \; .$$

Let $\quad v \; = \; \begin{pmatrix} 1 & v_1 & v_1^2 \\ 1 & v_2 & v_2^2 \\ 1 & v_3 & v_3^2 \end{pmatrix} \; .$ $\qquad$ Let $\quad y_i \; = \; \begin{pmatrix} y_{i1} \\ y_{i2} \\ y_{i3} \end{pmatrix} \; .$

Then the estimates of P_0, P_1, and P_2 are given by

$$
\begin{pmatrix}
\hat{P}_0(u_i) \\
\hat{P}_1(u_i) \\
\hat{P}_2(u_i)
\end{pmatrix}
= (v^T v)^{-1} v^T y_i \quad .
$$

In particular $\hat{P}_\ell(u_i) = L_\ell \begin{pmatrix} \sum\limits_j y_{ij} \\ \sum\limits_j v_j y_{ij} \\ \sum\limits_j v_j^2 y_{ij} \end{pmatrix}$ where L_ℓ stands for some linear

combination. If we assume that $P_0(u_i) = a_{00} + a_{10}u + a_{20}u^2$,

$P_1(u) = a_{01} + a_{11}u$, and $P_2(u) = a_{02}$ then we estimate a_{02} by

averaging $\hat{P}_2(u_i)$ over the values of u. That is

$$
\hat{a}_{02} = L_{02}
\begin{pmatrix}
\sum\limits_{ij} y_{ij} \\
\sum\limits_{ij} v_j y_{ij} \\
\sum\limits_{ij} v_j^2 y_{ij}
\end{pmatrix} \quad .
$$

Now this is a least squares estimate of a_{02} only if it is a linear combination of the right side of the least squares normal equations. That is, only if it is a linear combination of

$$
x^T y =
\begin{pmatrix}
\sum\limits_{ij} y_{ij} \\
\sum\limits_{ij} u_i y_{ij} \\
\sum\limits_{ij} u_i^2 y_{ij} \\
\sum\limits_{ij} v_j y_{ij} \\
\sum\limits_{ij} u_i v_j y_{ij} \\
\sum\limits_{ij} v_j^2 y_{ij}
\end{pmatrix} \quad .
$$

$\hat{a}_{02}$ is a linear combination of these terms.

We estimate a_{01} and a_{11} by

$$\begin{pmatrix} \hat{a}_{01} \\ \hat{a}_{11} \end{pmatrix} = \begin{pmatrix} 4 & \Sigma u_i \\ \Sigma u_i & \Sigma u_i^2 \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 & 1 & 1 \\ u_1 & u_2 & u_3 & u_4 \end{pmatrix} \begin{pmatrix} P_i(u_1) \\ P_i(u_2) \\ P_i(u_3) \\ P_i(u_4) \end{pmatrix}$$

$$= L \begin{pmatrix} \sum_{ij} y_{ij} \\ \sum_{ij} v_j\, y_{ij} \\ \sum_{ij} v_j^2\, y_{ij} \\ \sum_{ij} u_i\, y_{ij} \\ \sum_{ij} u_i\, v_j\, y_{ij} \\ \sum_{ij} u_i\, v_j^2\, y_{ij} \end{pmatrix} .$$

All of the components of this vector except the last one are in $x^T y$. Hence $\hat{a}_{01}$ or $\hat{a}_{11}$ are not least squares estimates unless the data points u_i , v_j are such that the linear combinations symbolized by L do not involve this last term.

Now we could also put $a_{12} uv^2$ in the model so as to put $\sum_{ij} u_i v_j^2 y_{ij}$ in the right side of the least squares normal equations. By continually putting terms in the model as needed in this example we find that to determine the least squares estimates of all of the coefficients by the step procedure inde- pendent of the data points (except that the design be rectangular) it is nec- essary that the polynomial in the model be balanced. This example also indi- cates how we would go about expanding the polynomial model so as to estimate certain coefficients by the step procedure. Having estimated some of the coef- ficients, we may eliminate them from y and do an ordinary least squares regression, if it is then practicable.

APPENDIX A: STATISTICAL BACKGROUND

It is assumed that the reader is familiar with such terms as expected value, random variable, variance, etc. If not, ready reference to these terms may be found in such books as Cramer [1] and Loève [2].

We shall be concerned here with independent random variables $y_1, \ldots, y_n$ such that the expected value of y_i is a linear function of m parameters $p_1, \ldots, p_m$ and the variance of y_i is σ^2, i.e.,

$$E(\underline{y}) = A \underline{p}$$

$$\text{Var}(y_i) = \sigma^2 \qquad i = 1, \ldots, n$$

where $\underline{y}' = (y_1, \ldots, y_n)$, $\underline{p}' = (p_1, \ldots, p_n)$ and $A = (a_{ij})$ is a known real $n \times m$ matrix. We shall be interested in estimating by functions of $y_1, \ldots, y_n$ certain linear functions of the parameters, say $\underline{\ell}'\underline{p}$ where $\underline{\ell}' = (\ell_1, \ldots, \ell_m)$. We call an estimate of $\underline{\ell}'\underline{p}$ which has expected value $\underline{\ell}'\underline{p}$ an unbiased estimate. If the estimate is also a linear function of the y's, say $\underline{c}'\underline{y}$, $\underline{c}' = (c_1, \ldots, c_n)$, we call it a linear unbiased estimate. Thus, $\underline{c}'\underline{y}$ is a linear unbiased estimate of $\underline{\ell}'\underline{p}$ if and only if

$$E(\underline{c}'\underline{y}) = \underline{\ell}'\underline{p} \quad .$$

Since $E(\underline{c}'\underline{y}) = \underline{c}'A \underline{p}$ we have from the previous equation

$$\underline{c}'A \underline{p} = \underline{\ell}'\underline{p}$$

as a necessary and sufficient condition for $\underline{c}'\underline{y}$ to be a linear unbiased estimate of $\underline{\ell}'\underline{p}$. Since we shall consider all of Euclidian m-space as the parameter space, we have equivalently

$$(5) \qquad \qquad \underline{c}'A = \underline{\ell}' \quad .$$

We define $V(A')$ to be the vector space generated by the rows of the $m \times n$, $m \leq n$, matrix A' and $V^*(A')$ to the vector space orthogonal to $V(A')$ in the n dimensional vector space over the real numbers.

The following theorem is basic in the study of linear estimation.

THEOREM A: If $\underline{\ell}'\underline{p}$ is a linear combination of the parameters for which there exists a vector $\underline{d}'$ such that $E(\underline{d}'\underline{y}) = \underline{\ell}'\underline{p}$ then there exists exactly one vector $\underline{c}'$ in $V(A')$ for which $E(\underline{c}'\underline{y}) = \underline{\ell}'\underline{p}$. Furthermore, $\text{Var}(\underline{c}'\underline{y})$ minimizes the variance of $\underline{d}'\underline{y}$ over all $\underline{d}'$ such that $E(\underline{d}'\underline{y}) = \underline{\ell}'\underline{p}$.

PROOF: To prove the first assertion consider the decomposition

$$\underline{d}' = \underline{c}' + \underline{e}'$$

where $\underline{c}'$ is the projection of $\underline{d}'$ on $V(A')$ and $\underline{e}'$ the projection of $\underline{d}'$ on $V^*(A')$. Now by assumption

$$\underline{\ell}'\underline{p} = E(\underline{d}'\underline{y})$$

but

$$E(\underline{d}'\underline{y}) = \underline{d}'A\underline{p} = (\underline{c}' + \underline{e}')A\underline{p} = \underline{c}'A\underline{p} + \underline{e}'A\underline{p} = \underline{c}'A\underline{p} = E(\underline{c}'\underline{y})$$

since $\underline{e}'$ is orthogonal to the column vectors of A. Thus,

$$E(\underline{c}'\underline{y}) = E(\underline{d}'\underline{y}) = \underline{\ell}'\underline{p}.$$

Now suppose $\underline{c}_1'$ belongs to $V(A')$ and $E(\underline{c}_1'\underline{y}) = \underline{\ell}'\underline{p}$. Then for every p

$$E(\underline{c}_1'\underline{y}) = E(\underline{c}'\underline{y})$$

or

$$\underline{c}_1'A\underline{p} = \underline{c}'A\underline{p} \qquad \text{for all } p$$

which implies $(\underline{c}_1' - \underline{c}')$ is orthogonal to $V(A')$, i.e., belongs to $V^*(A')$. However, $\underline{c}_1' - \underline{c}'$ belongs to $V(A')$ since each does and thus $\underline{c}_1' - \underline{c}' = \underline{o}'$, i.e., $\underline{c}_1' \equiv \underline{c}'$. This completes the proof of the first assertion.

Now suppose $\underline{d}'\underline{y}$ is a linear unbiased estimate of $\ell'\underline{p}$. Then decompose $\underline{d}'$ into $\underline{c}_1'$ and $\underline{e}_1'$ where $\underline{c}_1'$ belongs to $V(A')$ and $\underline{e}_1'$ belongs to $V^*(A')$. As before $\underline{c}_1'\underline{y}$ is also a linear unbiased estimate of $\ell'\underline{p}$ and $\underline{c}_1'$ belongs to $V(A')$. By the uniqueness argument given previously $\underline{c}_1' = \underline{c}'$. Hence, $\underline{d}' = \underline{c}' + \underline{e}_1'$. Thus, $\mathrm{Var}(\underline{d}'\underline{y}) = \underline{d}'\sigma^2 I_n \underline{d} = \sigma^2 \underline{d}'\underline{d} = \sigma^2(\underline{c}' + \underline{e}_1')(\underline{c} + \underline{e}_1)$ $= \sigma^2 \underline{c}'\underline{c} + \sigma^2 \underline{e}_1'\underline{e}_1 = \mathrm{Var}(\underline{c}'\underline{y}) + \sigma^2 \underline{e}_1'\underline{e}_1$. Therefore $\mathrm{Var}(\underline{d}'\underline{y}) > \mathrm{Var}(\underline{c}'\underline{y})$ for $\underline{d}' \neq \underline{c}'$, i.e., $\underline{e}_1'\underline{e}_1 \neq 0$. This completes the proof.

We shall call this unique estimate which minimizes the variance over all linear unbiased estimates the best estimate of $\ell'\underline{p}$.

Theorem A says that if the "best" estimate of $\ell'p$ is $c'y$ then $c' = q'A'$ for some q'. From equation (5) we see that we must have $q'A'A = \ell'$. These equations are called the conjugate normal equations. Conversely, we have that if $q'A'A = \ell'$ then $q'A'y$ is the unique "best" estimate of $\ell'p$.

THEOREM B: (Gauss-Markov) If $\ell'p$ has an unbiased linear estimate then the best estimate is $\ell'\hat{p}$ where $\hat{p}$ are the least squares estimates of p.

PROOF: The least squares estimates of p are those values for p_1, p_2, $\cdots$, p_n which minimize the sum of squared deviations of y_1, y_2, $\cdots$, y_n from their (estimated) expected value. Thus

$$S^2 = \sum_{j=1}^{n} (y_j - a_{j1}p_1 - a_{j2}p_2 - \cdots - a_{jm}p_m)^2$$

is to be minimized by choice of p_1 , p_2 , $\cdots$ p_m . Now

$$S^2 = (y' - p'A')(y - Ap) = y'y - p'A'y - y'Ap + p'A'Ap = y'y - 2p'A'y + p'A'Ap \quad .$$

By differentiating S' with respect to each of the p's and setting these
m derivatives equal to zero we obtain

$$- 2A'y + 2A'Ap = \underline{0} \quad \text{or}$$

$$* \qquad\qquad A'Ap = A'y \quad .$$

Equations * are called the normal equations. Thus, if $\hat{p}$ satisfies the normal
equations then $\hat{p}$ is a critical point of S^2 . Now we shall show that it is
a minimum point.

Let y' be decomposed as $y' = m' + e'$ where m' is in $V(A')$ and e'
is in $V^*(A')$. Thus, $m' = x'A'$ and $e'A = 0$. Then, $y'A = x'A'A + e'A = x'A'A$
or $A'Ax = A'y$. Hence, $\underline{x}$ must satisfy the normal equations. Conversely
since $\hat{p}$ satisfies the normal equations, $\hat{p}'A'$ is the projection of y' on
$V(A')$ and hence $m' = \hat{p}'A'$. That is $(y' - \hat{p}'A')A = \underline{0}'$ and $\hat{p}'A'$ is
in $V(A')$.

COROLLARY: If $Eq'A'y = \ell'p$ then $q'A'y = \ell'\hat{p}$ where $\hat{p}$ are least
squares estimates of p .

PROOF: $q'A'$ is in $V(A')$ and by assumption $Eq'A'y = \ell'p$. Hence
by theorem A $q'A'y$ is the unique best estimate of $\ell'p$. By theorem B ,
$\ell'\hat{p}$ is the unique best estimate of $\ell'p$. Hence $q'A'y = \ell'\hat{p}$.

APPENDIX B: PROOF OF THEOREM 1

Consider the rectangular design

$$D = D_1 \ x \ \cdots \ x \ D_\pi \quad , \quad D_i = \left\{ x_{t_i}^{(i)} \ : \ t_i = 1 \ , \ \cdots \ , \ T_i \right\}$$

and the polynomial (2) written, in preparation for step one of the step procedure, as

$$(3) \quad b_1^{(\pi)} + b_2^{(\pi)} \ x^{(\pi)} + \cdots + b_d^{(\pi)} \ (x^{(\pi)})^{d-1} + b_{d+1}^{(\pi)} \ (x^{(\pi)})^d$$

where $b_k^{(\pi)}$ is a polynomial in $x^{(1)}, \ \cdots \ , \ x^{(\pi-1)}$ of degree $(d - (k-1))$.

Let $y_{t_1 \cdots t_\pi} = f(x_{t_1}^{(1)}, \ \cdots \ , \ x_{t_\pi}^{(\pi)})$ where f is the function to be approximated by the polynomial (2) .

If we can demonstrate that the step procedure estimate of a coefficient is a linear combination of the components of $X'\underline{y}$ --where the matrix X arises from writing the system

$$E(y_{t_1 \cdots t_\pi}) = a_{11 \cdots 1} + \cdots + a_{1 \cdots i \cdots 1} x_{t_i}^{(i)} + \cdots +$$

$$(\text{terms in } x_{t_1}^{(1)}, \ \cdots \ , \ x_{t_\pi}^{(\pi)} \text{ of degree} \leq d) +$$

$$a_{11 \cdots 1d+1}(x_{t_\pi}^{(\pi)})^d \quad , \quad t_i = 1 \ , \ \cdots \ , \ T_i$$

in the matrix form

$$E(\underline{y}) = X \underline{a}$$

as in the case of the preceding example--and show that such an estimate is unbiased; then the step procedure estimate is the least squares estimate [3] .

Since the first step of the step procedure is a least squares estimation of the $b^{(\pi)}$'s with $x^{(1)}, \ldots, x^{(\pi-1)}$ held fixed, the expected value of the estimate $\hat{b}^{(\pi)}_{d+1}$ of $b^{(\pi)}_{d+1}$ is $b^{(\pi)}_{d+1} = a_{1\ldots 1 d+1}$. Also the estimate $\hat{b}^{(\pi)}_{d+1}$ is itself a linear combination of

$$\sum_{t_\pi=1}^{T_\pi} y_{t_1\ldots t_\pi} \quad , \quad \sum_{t_\pi=1}^{T_\pi} x^{(\pi)}_{t_\pi} y_{t_1\ldots t_\pi} \quad , \quad \sum_{t_\pi=1}^{T_\pi} (x^{(\pi)}_{t_\pi})^d \, y_{t_1\ldots t_\pi} \quad .$$

Since $b^{(\pi)}_{d+1}$ is independent of $x^{(1)}, \ldots, x^{(\pi)}$ succeeding steps in the step procedure will at each stage give the mean of the result of the previous stage over the number of data points in the present stage so that the step procedure estimate of $b^{(\pi)}_{d+1}$ is

$$\frac{\displaystyle\sum_{t_1=1}^{T_1} \ldots \sum_{t_{\pi-1}=1}^{T_{\pi-1}} \hat{b}^{(\pi)}_{d+1}}{T_1 \, T_2 \, \ldots \, T_{\pi-1}} \quad .$$

Since $\hat{b}^{(\pi)}_{d+1}$ is unbiased, this estimate will be unbiased. This estimate will also be a linear combination of

$$\sum_{t_1=1}^{T_1} \ldots \sum_{t_\pi=1}^{T_\pi} y_{t_1\ldots t_\pi} \quad , \quad \sum_{t_1=1}^{T_1} \ldots \sum_{t_\pi=1}^{T_\pi} x^{(\pi)}_{t_\pi} y_{t_1\ldots t_\pi} \,, \ldots, \quad \sum_{t_1=1}^{T_1} \ldots \sum_{t_\pi=1}^{T_\pi} (x^{(\pi)}_{t_\pi})^d \, y_{t_1\ldots t_\pi} \quad ,$$

i.e., the components of $X'\underline{y}$. This completes the proof.

It is clear from the proof that by choosing $x^{(i)}$ as the leading variable the step procedure could be used to calculate the least squares estimate of the coefficient of $(x^{(i)})^d$. We are usually interested in the least squares estimate of all the coefficients and in this case theorem 1 is not very helpful.

APPENDIX C: PROOF OF THEOREM 2

Consider the balanced polynomial

$$\sum_{\ell_1 = 1}^{L_1 + 1} \cdots \sum_{\ell_\pi = 1}^{L_\pi + 1} a_{\ell_1 \cdots \ell_\pi} x_{\ell_1}^{(1)} \cdots x_{\ell_\pi}^{(\pi)} \quad , \quad x_{\ell_i}^{(i)} = \left(x^{(i)} \right)^{\ell_i - 1}$$

as an approximation of a real function f of π real variables $x^{(1)}, \ldots, x^{(\pi)}$ over the rectangular design

$$D = D_1 \times \cdots \times D_\pi \quad , \quad D_i = \left\{ x_{t_i}^{(i)} : t_i = 1, 2, \ldots, T_i \right|$$

$$\left. x_{t_i}^{(i)} \neq x_{s_i}^{(i)} , \quad t_i \neq s_i \right\} .$$

Let

$$y_{t_1 \cdots t_\pi} = f \left(x_{t_1}^{(1)}, \ldots, x_{t_\pi}^{(\pi)} \right) .$$

In what follows we shall use capital letters without affixes to denote the appropriate collection of lower case letters for subscripting purposes, e.g.

$$L = \left\{ \ell_1, \ldots, \ell_\pi \right\} .$$

First we shall consider the least squares criterion for estimates of the a's and generate the normal equations, then we shall show that the step procedure estimates of the a's satisfy the normal equations and are thus least squares estimates.

ACTUAL PROOF: Define S by

$$S \triangleq \sum_{t_1 \cdots t_\pi} \left\{ y_{t_1 \cdots t_\pi} - \sum_{\ell_1 \cdots \ell_\pi} a_{\ell_1 \cdots \ell_\pi} x_{t_1 \ell_1}^{(1)} \cdots x_{t_\pi \ell_\pi}^{(\pi)} \right\}^2$$

and calculate $\dfrac{\partial}{\partial a_{\alpha_1 \ldots \alpha_\pi}} S$. Setting this partial derivative equal to

zero, we arrive at the equation

$$\sum_T y_T \, x^{(1)}_{t_1 \alpha_1} \cdots x^{(\pi)}_{t_\pi \alpha_\pi} = \sum_L a_L \sum_T x^{(1)}_{t_1 \ell_1} x^{(1)}_{t_1 \alpha_1} \cdots x^{(\pi)}_{t_\pi \ell_\pi} x^{(\pi)}_{t_\pi \alpha_\pi} \quad .$$

Now employing the properties of the rectangular design we have

$$(4) \quad \sum_T y_T \, x^{(1)}_{t_1 \alpha_1} \cdots x^{(\pi)}_{t_\pi \alpha_\pi} = \sum_L a_L \left\{ \left(\sum_{t_1} x^{(1)}_{t_1 \ell_1} x^{(1)}_{t_1 \alpha_1} \right) \cdots \left(\sum_{t_\pi} x^{(\pi)}_{t_\pi \ell_\pi} x^{(\pi)}_{t_\pi \alpha_\pi} \right) \right\} \quad .$$

If we let the matrix $(x^{(i)}_{t_i \ell_i})$ be denoted by X_i , then we have that

$$x^{(i)}_{\ell_i \alpha_i} \triangleq \sum_{t_i} x^{(i)}_{t_i \ell_i} x^{(i)}_{t_i \alpha_i}$$

is the element in the ℓ_i , α_i position of the matrix $X'_i X_i$ and from (4)

$$(6) \quad \sum_T y_T \, x^{(1)}_{t_1 \alpha_1} \cdots x^{(\pi)}_{t_\pi \alpha_\pi} = \sum_L a_L \left(X^{(1)}_{\ell_1 \alpha_1} \cdots X^{(\pi)}_{\ell_\pi \alpha_\pi} \right) \quad .$$

Equation (6) is a typical equation from the normal equations.

We shall now use the step procedure to estimate a typical a, $a_{s_1 \ldots s_\pi}$.
In order to facilitate the writing down of this estimate we shall have
need of the following notation. Let

$$\left(z^{(i)}_{\ell_i r_i} \right) \triangleq X'_i \quad , \quad \ell_i = 1 , \ldots , L_i + 1 , \quad r_i = 1 , \ldots , T_i$$

$$\left(x^{\ell_i s_i}_{(i)} \right) \triangleq \left(X'_i X_i \right)^{-1} s_i , \quad \ell_i = 1 , \ldots , L_i + 1 \quad .$$

The first step of the step procedure for finding the estimate of $a_{s_1, \ldots, s_\pi}$ is

$$a^{(1)}_{t_1 \ldots t_{\pi-1} s_\pi} = (X'_\pi X_\pi)^{-1} X'_\pi Y_{t_1 \ldots t_{\pi-1}} = \sum_{r_\pi = 1}^{T_\pi} \left\{ \sum_{\ell_\pi = 1}^{L_\pi + 1} x^{\ell_\pi s_\pi}_{(\pi)} z^{(\pi)}_{\ell_\pi r_\pi} \right\} y_{t_1 \ldots t_{\pi-1} r_\pi}$$

where $Y'_{t_1 \ldots t_{\pi-1}} = (y_{t_1, \ldots, t_{\pi-1}, 1}, \cdots, y_{t_1, \ldots, t_{\pi-1}, T_\pi})$. The second step is then

$$a^{(2)}_{t_1 \ldots t_{\pi-2} s_{\pi-1} s_\pi} = (X'_{(\pi-1)} X_{(\pi-1)})^{-1} X'_{\pi-1} a^{(1)}_{t_1 \ldots t_{\pi-2} s_\pi}$$

$$= \sum_{r_{\pi-1}=1}^{T_{\pi-1}} \left\{ \sum_{\ell_{\pi-1}=1}^{L_{\pi-1}+1} X^{\ell_{\pi-1} s_{\pi-1}}_{(\pi-1)} Z^{(\pi-1)}_{\ell_{\pi-1} r_{\pi-1}} \right\} a^{(1)}_{t_1 \ldots t_{\pi-2} r_{\pi-1} s_\pi}$$

The ith step is thus

$$a^{(i)}_{t_1 \ldots t_{\pi-i}, s_{\pi-i-1}, \ldots s_\pi} = (X'_{\pi-i-1} X_{\pi-i-1})^{-1} X'_{\pi-i-1} a^{(i-1)}_{t_1 \ldots t_{\pi-i}, s_{\pi-i-2}, \ldots s_\pi} .$$

Finally

$$a_{s_1 \ldots s_\pi} = (X'_1 X_1)^{-1} X'_{(1)} a^{(\pi-1)}_{s_2 \ldots s_\pi}$$

$$= \sum_{r_1=1}^{T_1} \left\{ \sum_{\ell_1=1}^{L_1+1} X^{\ell_1 s_1}_{(1)} Z^{(1)}_{\ell_1 r_1} \right\} a^{(\pi-1)}_{r_1 s_2 \ldots s_\pi}$$

$$= \sum_{r_1=1}^{T_1} \sum_{\ell_1=1}^{L_1+1} X^{\ell_1 s_1}_{(1)} Z^{(1)}_{\ell_1 r_1} \sum_{r_2=1}^{T_2} \sum_{\ell_2=1}^{L_2+1} X^{\ell_2 s_2}_{(2)} Z^{(2)}_{\ell_2 r_2} \cdot \cdot \cdot$$

$$\sum_{r_{\pi-1}=1}^{T_{\pi-1}} \sum_{\ell_{\pi-1}=1}^{L_{\pi-1}+1} X^{\ell_{\pi-1} s_{\pi-1}}_{(\pi-1)} Z^{(T-1)}_{\ell_{\pi-1} r_{\pi-1}} \sum_{r_\pi=1}^{T_\pi} \sum_{\ell_\pi=1}^{L_\pi+1} X^{\ell_\pi s_\pi}_{(\pi)} Z^{(\pi)}_{\ell_\pi r_\pi} y_{r_1 \ldots r_\pi} .$$

By using the fact that we have a balanced polynomial over a rectangular design we can write

$$a_s = a_{s_1 \ldots s_\pi} = \sum_R \left\{ y_R \sum_L X^{\ell_1 s_1}_{(1)} \ldots X^{\ell_\pi s_\pi}_{(\pi)} Z^{(1)}_{\ell_1 r_1} \ldots Z^{(\pi)}_{\ell_\pi r_\pi} \right\} .$$

If we substitute a_s for a_L in equation (6), the right hand side of (6) becomes

$$\sum_s \left\{ a_s \left(X_{s_1 \alpha_1}^{(1)} \cdots X_{s_\pi \alpha_\pi}^{(\pi)} \right) \right\} =$$

$$\sum_R y_R \left\{ \sum_L \left[\left(Z_{\ell_1 r_1}^{(1)} \cdots Z_{\ell_\pi r_\pi}^{(\pi)} \right) \left(\sum_{s_1} X_{(1)}^{\ell_1 s_1} X_{s_1 \alpha_1}^{(1)} \right) \cdots \left(\sum_{s_\pi} X_{(\pi)}^{\ell_\pi s_\pi} X_{s_\pi \alpha_\pi}^{(\pi)} \right) \right] \right\} .$$

However

$$\sum_{s_i} \left(X_{(i)}^{\ell_i s_i} X_{s_i \alpha_i}^{(i)} \right) = \delta_{\ell_i \alpha_i} = \begin{cases} 0 , & \ell_i \neq \alpha_i \\ 1 , & \ell_i = \alpha_i \end{cases} , \text{ so that we have the}$$

right hand side of (6) equal to

$$\sum_R y_R \left\{ \sum_L \left(Z_{\ell_1 r_1}^{(1)} \cdots Z_{\ell_\pi r_\pi}^{(\pi)} \right) \delta_{\ell_1 \alpha_1} \cdots \delta_{\ell_\pi \alpha_\pi} \right\} = \sum_R y_R \left(Z_{\alpha_1 r_1}^{(1)} \cdots Z_{\alpha_\pi r_\pi}^{(\pi)} \right)$$

which is the left hand side of equation (6) . Thus a_s is a solution to the normal equations and the proof is therefore complete.

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APPENDIX 2

APPROXIMATING OPTIMAL TRAJECTORIES: SELECTION OF SIGNIFICANT
ESTIMATION VARIABLES IN A LEAST SQUARES PROBLEM

APPROXIMATING OPTIMAL TRAJECTORIES: SELECTION OF SIGNIFICANT ESTIMATION VARIABLES IN A LEAST SQUARES PROBLEM

The Astrodynamic and Guidance Theory Division of the Aero-Astrodynamics Laboratory of the Marshall Space Flight Center is examining the role of "large computers" as they may be exploited in the control and guidance of missile performance. Under Contract No. NAS8-5365 the Georgia Institute of Technology and its Rich Electronic Computer Center have been studying such exploitation as it applies to the approximation of guidance functions with multivariate functional models. Under this contract attention so far has been focused on methods to reduce the computational and variable-selection problems in least squares models.

Background

The state vector, $x(t)$ (describing the flight of a missile through space) has the derivative $\dot{x}(t)$. These vectors along with a vector descriptive of the guidance function, $u(t)$, satisfy equations of motion, which may be expressed formally as

$$F[x(t), \dot{x}(t), t, u(t)] = 0$$

The missile is intended to satisfy certain mission requirements at some future time, t_c, and we may indicate these requirements in the equations describing terminal conditions:

$$G[x(t_c), \dot{x}(t_c), t_c] = 0$$

Note that the functions F and G are themselves vectors. The guidance problem may be expressed generally as that of choosing a "best" guidance function u out

of the class of possible guidance functions. In particular we may wish to choose a function u in such a way as to minimize

$$\int_o^{t_c} c(x,\dot{x},u,t)dt$$

In practical situations with real missiles we could not use the exact optimum guidance function as a function of time because of measurement errors and so on. The missile strays from the optimum path into a situation for which the chosen guidance function is no longer best. It then becomes necessary to calculate a new optimum guidance function based on new initial conditions. In short it is important to be able to synthesize the optimal guidance function, u, in terms of the state variables at each point in the phase space.

One approach to this synthesis which has been proposed consists in selecting a scatter of initial points (possibly organized in subregions of the phase space); using a large-scale computer to determine the corresponding values of the optimal guidance function; and then using some approximation technique to estimate the guidance function as a function of the state of the missile.

Various considerations, both practical and theoretical, suggest that such an approximation be based on the criterion of "least squares." Even, however, if attention is restricted to this well-known method, difficulties arise. In the first place fitting a function of several variables becomes very quickly a huge matrix inversion problem. In an earlier study done under this contract, entitled: "Least Squares Estimation of Regression Coefficients in a Special Class of Polynomial Models," techniques were described which reduced the large inversion problem to a sequence of low-order inversions, when fitting balanced polynomials to rectangular grids of data. While these techniques hold promise in special circumstances, evidently they have a limited usefulness.

A second major difficulty in least squares approximations arises in deciding which class of functions or which subset of a very large class of estimation variables will be used to approximate the unknown function. Evidently, a method which elects a relatively few highly efficient estimation variables also serves to keep the matrix-inversion problem under control, since that computation depends directly on the number of estimation variables used.

It happens that there is a method available by means of which the incorporation of estimation variables into the approximating functions can be sequenced in what seems usually to be an efficient manner. We shall call this formal procedure for activating estimation variables simply the step-up procedure. The procedure appears first to have been used by R. J. Wherry (Annal. of Math. Stat., 1931). More recent discussions have appeared by H. E. Anderson and B. Fruchter (Psychometrika, 1960), and E. F. Schultz, Jr. and J. F. Goggans (Bulletin of the Agricultural Exp. Station, Auburn Univ., 1961). Since examples can be constructed to show that the step-up procedure is not always optimal, the difficult problem of assessing its merit arises.

The primary concern of this report is to consider the merits of the step-up procedure, to seek improvement in it and to investigate rules to govern the stopping of the selection procedure.

While this and related problems are of considerable interest and pertinence in the overall trajectory problem, they should not be considered overriding.

Other approaches, where the goodness of approximation is more directly related to the cost criterion or to the equations of motion and where the mission fulfillment is more directly imposed, show at least equal promise and are being considered for subsequent study.

Objectives

1. To conduct empirical investigation of the efficacy of using the step-up procedure in the selection of a fixed number of estimation variables out of a larger number in obtaining functional approximations by the method of LS.

2. To seek modifications of the procedure for the purpose of enhancing its efficiency.

3. To develop reasonable rules which will control the process of stopping the estimation variables selection procedure and to study empirically the sensitivity of the efficiency of the estimation to variations in these rules.

4. To explore empirically the general applicability of low-degree polynomial approximation (in the sense of least squares) to representative function of several variables.

5. To develop an efficient, flexible and unified computer program which, in carrying out a least squares approximation, at least has the option of utilizing such selection procedures and stopping rules as have been developed.

Plan of Research

To accomplish the aims of this part of the study research was organized in four phases:

A. A review of the geometry, linear algebra and statistics involved in the method of least squares and the step-up procedure. This phase extended

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to include discussions of modifications to the step-up procedure and various criteria for stopping the selection process. Also included were algorithms for computer programs.

B. Development of the structure of the empirical investigations. In this phase decisions were reached on types of functions to be estimated, data patterns, size of data base, specific form of the estimation variables (as functions of independent variables), how data would be obtained and reduced to the regression format with particular regard to the important case of polynomial approximation.

C. Development of computer programs. In this phase algorithms developed in preceding phases were converted to programs, with attention to computational efficiency and cost.

D. A battery of examples with interpretations and, if possible, conclusions. In this phase a few preliminary examples were designed to test the efficiency of using the step-up procedure. Later, more sophisticated examples were used to develop the other objectives cited above.

Summary

A. Mathematical review (see the supporting study titled: "Selection of Significant Estimation Variables in a Least Squares Problem: Mathematical Review.")

The well-known method of least squares (LS) is invoked to estimate a presumed functional relationship between a dependent variable Y and a set of independent variables $X_1, \ldots, X_\pi$ on the basis of a set of observed points. According to the method a class of functions of the form,

$$a_0 + a_1 Z_1(X_1, \ldots, X_\pi) + \ldots + a_p Z_p(X_1, \ldots, X_\pi),$$

is considered for all real sets of coefficients. The Z's are specified estimation variables depending on the independent X's. For any function of the above class, corresponding to an observed vector of X's, one could compute values $z_{\mu 1}, \ldots, z_{\mu p}$ of the estimation variables and a value $\hat{y}_\mu = a_o + a_1 z_{\mu 1} + \ldots + a_p z_{\mu p}$, which could be compared with the corresponding observed value y_μ of the dependent variable Y. From this specified class of functions the method of LS selects one for which is minimized the sum of squares of the deviations of the so-called predicted values $\hat{y}_\mu$ from the observed values y_μ. Such a function is called a best estimate or best-fitting approximation (in the class) in the sense of LS.

The choice of the functions to be used as the estimation variables, $Z_1, \ldots, Z_p$, is open, giving the method great flexibility, but also making it vulnerably dependent on the choice. In the next section of this summary some discussion is devoted to the choice of Z's and the reduction of data to the form of observation vectors $(y_\mu, z_{\mu 1}, \ldots, z_{\mu p})$ on the variables $(Y, Z_1, \ldots, Z_p)$. This form is now assumed.

The least squares approach admits of an accessible geometrical interpretation. Supposing there are N observation vectors, for each estimation variable Z_i consider the N observed values (adjusted to the mean). These values constitute the i-th estimation vector z_i. Similarly, consider the mean adjusted dependent-variable vector y. The LS problem translates to finding that vector in the space spanned by the estimation vectors which lies closest to the y vector. Or it may be interpreted as finding the projection of the y vector onto the estimation space.

The cosine of the angle between the y vector and its projection in the estimation space is called the multiple correlation coefficient, R. It is a

measure of the efficiency of the estimate, attaining a maximum of unity when the y vector coincides with the projection estimate.

The difference between the y vector and its projection onto the estimation space is called the error vector. A pythagorean property holds, expressing the square of the length of the y vector as the sum of squares of the lengths of the estimate and the error. The estimate itself can be resolved into orthogonal components, and the same is true of the error vector.

If only k out of the p available estimation vectors are to be used to estimate y (corresponding to selecting k out of the p possible estimation variables), a difficult problem of deciding which k to elect arises, since trying all combinations is ordinarily computationally infeasible.

The step-up procedure is a practical, though not always perfectly optimal, way to select k estimation vectors. It evolves naturally from the geometric model described above. In this procedure the first estimation vector is chosen by finding the one on which the y vector has the longest projection (by the pythagorean property this leaves the shortest error vector). In the next step for each of the remaining vectors it is easy to determine the length of a component orthogonal to the first vector chosen, whose square added to the square of the projection on the first vector gives the square of the projection of y on the estimation space of these two vectors. Selected is the vector having the longest such component. The procedure is then repeated.

Since the y vector may lie in the plane of two vectors but possibly closer to a third vector (not in the plane), the step-up procedure is not always optimal, for it would activate the third vector first, then one of the others, but the combination would not be as efficient as the first and second.

A modification of the procedure has been incorporated to allow for the elimination of a vector from the active estimation set. It works in the follow-

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ing way. The error vector for the k selected variables is compared with the error vector when one vector is deleted from the active estimation set. The difference measures the net reduction of error due to the one vector deleted. Computationally it is easy to compare the lengths of these reductions. One may wish to eliminate a variable which contributes little net reduction. A measure of the net reduction due to each estimation vector is provided by the cosine of the dihedral angle formed by the plane containing the y vector and its projection in the reduced estimation space, on the one hand, and the plane containing the two projections on the other hand. This is called the partial or net correlation coefficient between the dependent variable y and the estimation variable in question.

It appears evident that the simple rule of selecting k of p estimation vectors will not always be a good stopping rule. From the geometrical description several other natural criteria emerge as possible stopping rules whose use may be varied according to considerations of the particular problem at hand. For example, if the multiple correlation coefficient is "very high" the addition of other variables may seem unnecessary. Again, even if R is not high, the modified step-up procedure may be making no appreciable improvement in the estimate so that further addition of variables to the active estimation set may be deemed useless. Also, depending on the criteria for continuing to bring in new variables and to eliminate old ones, some stopping rule should be available to guard against cycling.

The most difficult choices for these decision rules are those concerning whether to eliminate an active estimation vector and whether adding one or several more will make any significant reduction in the error vector. One might adopt the rule of introducing two vectors and eliminating one, until a

stopping rule stops the process. One might eliminate the vector to which

corresponds the lowest net correlation coefficient, provided that the co-

efficient reaches a certain "low" value. One might stop adding vectors if the

last r added make an average addition to R of less than some fixed amount.

However, caution should be exercised in the fixing of criteria, since certain

combinations of these rules increase the chances of cycling.

Finally, we have considered elimination-stopping rule combinations based

on F statistics. Briefly, an F statistic is a ratio of the average of certain

of the estimation components to the average of the error components. In a

statistical context, if the estimation components have on the average the

same length as the error components, they are considered insignificant and are

attributable to random error. In short these vectors are not considered of

estimative significance. From such a point of view there is some intuitive

appeal in the decision rule: Do not add if $F \leq 1$; do not drop if $F \geq 1$.

However, the rationale for using the F statistic rules is tenuous and, such as

it is, depends on hypotheses of a statistical model which are not always

appropriate. A fuller discussion of the statistical model is given in the

supporting study.

While the mathematical and statistical analysis suggested the foregoing

procedures and rules, it has also indicated considerable need for the

empirical tests subsequently made.

The mathematical analysis included a translation of the geometrical

steps described above into algorithms capable of being converted to computer

programs. These well-known algorithms also are developed in detail in the

supporting study with every effort made to retain geometrical interpretations

in the development.

B. Structure of the Empirical Investigations

The data were organized in two main phases. The purpose of empirical runs in the first phase was primarily to gain insight on the efficiency of the step-up method for activating a subset of estimation variables out of a large set of such variables. The principal aim of the runs in the second phase was to explore the relative merits of various rules for stopping the step-up procedure of adding variables to the active estimation set and rules for eliminating such variables. Auxiliary purposes of empirical runs were to test and correct pertinent computer programs and to obtain from diversified experience an idea of the general validity of the LS approach as an approximation technique.

As pointed out in the previous section, the generality of the method of LS leaves considerable latitude in the selection of test cases. In organizing test runs representing a variety of problem types some of the factors on which decisions had to be reached included:

1. The type of function to be approximated, including its form, the number of variables and the selection of a representative member.

2. The class of approximating functions, i.e. a selection of the estimation variables $Z_i = Z_i(X_1, \ldots, X_\pi)$ i $= 1, 2, \ldots, p$, where $(X_1, \ldots, X_\pi)$ presumably is in the domain of the function to be approximated.

3. The number, extent and distribution of data points.

Admittedly decisions reached during the test construction concerning these factors were somewhat arbitrary. They were made, however, with awareness of their significance.

Briefly, it was decided to construct data for a few selected functions of three variables, using a rectangular grid of data and balanced polynomials as approximating functions. In addition, a few runs were made using active

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data, which were developed in certain statistical regression analyses. Except for the actual data runs the data grids consisted of 500 or 1000 points generated from evenly spaced values of the three variables on the margins. Thus the undoubtedly important effects (on goodness of fit) of varying the distribution of data points or varying the types of estimating functions were not studied here. Indeed these factors were held more or less constant in order not to obscure the comparisons of variable-selection procedures.

These decisions led to fairly general and easy algorithms for generating data for a given test run and reducing them to the format of LS input. Thus, for a given function $F(X_1, X_2, X_3) = Y$, a given class of balanced polynomials of the form

$$\tilde{Y} = \Sigma\, a_{\ell_1 \ell_2 \ell_3} X_1^{\ell_1} X_2^{\ell_2} X_3^{\ell_3},$$

and a given rectangular grid of points,

$$(x_{1t_1}, x_{2t_2}, x_{3t_3}),$$

observation vectors $(y_\mu,\ z_{\mu 1},\ z_{\mu 2}, \ldots,\ z_{\mu p})$ were generated by the computer. Here y_μ is the value of Y at some $(x_{1t_1}, x_{2t_2}, x_{3t_3})$, and the estimation variables Z_i are the several terms of the balanced polynomial of the form

$$Z_i = X_1^{\ell_1} X_2^{\ell_2} X_3^{\ell_3},$$

while $z_{\mu i}$ is the value of Z_i when $(X_1, X_2, X_3) = (x_{1t_1}, x_{2t_2}, x_{3t_3})$. The observation vectors were then in a form to obtain LS estimates of the coefficients in the best-fitting balanced polynomial, or more specifically to manipulate in a way aimed at activating the most significant estimative terms of the balanced polynomial as described in the foregoing section.

Runs in the first phase were limited to estimating a polynomial (of higher order than the approximating ones) and estimating a rational function, while the approximating balanced polynomial class was restricted to be of second degree in X_1 and X_2 and first degree X_3, which restricted the number p of estimation variables (terms of the polynomial) to 17 or less. The test procedure for these runs was, for each $k = 1,2,\ldots,p-1$, to determine the efficiency (multiple correlation) of each of the $\binom{p}{k}$ subsets of k vectors and compare the optimal set with the set produced by the step-up procedure. Computer time was a limiting factor in these tests.

Runs in the second phase included estimating an exponential function and a few algebraic functions other than rational functions, and they included two runs using actual statistical data. Some effort was made to include poorly fitted functions as well as accurately fitted ones. Also, the form of the approximating balance polynomial was stepped up to develop 47 estimation variables. Usually, for each example, several runs were initiated in which were varied the policies of stopping the selection procedure or of eliminating a variable.

Considered, but not developed in this study, was an experimental design in which runs would be made for the various different combinations of prescribed levels of the main factors thought to influence efficient variable selection.

C. Development of Computer Programs (see the supporting study titled, "Selection of Significant Estimation Variables in a Least Squares Problem: Computer Programs.")

Corresponding to the two phases of the study mentioned in the last section, two computer programs were developed. The purpose of the first

program was to compare in a few examples the subset of k estimation vectors selected by the step-up procedure with the optimal subset of k. This first phase of programming was begun before the Burroughs 5000 was operational on contractor facilities and was programmed in the ALGOL 58 compiler language for the Burroughs 220 computer. Because of core memory limitations the program restricts the total number of estimation vectors to twenty-five. It would be a simple matter to translate the program to one for the more advanced computer. This has not yet been done, primarily because the number of comparisons to be made even with the restriction to 25 variables makes for an almost prohibitive amount of computation time.

The program depends on using (1) rectangular grid data and (2) a balanced polynomial as the general form of the approximating function. One part of the program, using as input the specified values of each of the variables and the degree of the balanced polynomial in each variable, generates internally the grid of data points and computes for each such point the value of each term of the balanced polynomial. Thus the estimation vectors are generated.

Also the program allows for a procedure to be inserted to incorporate the computation of the values of the function which is to be approximated, at each of the grid points of data. Thus the dependent variable vector y is generated.

As an intermediate calculation the program mean adjusts the above vectors and produces the intercorrelation matrix for all the vectors, including the dependent variable vector. There will be $L_1 L_2 \ldots L_\pi = p + 1$ such vectors. These are restricted in number to 25.

In the next part of the program, for each $k = 2, 3, \ldots, p-1$, each one of the $\binom{p}{k}$ subsets of k estimation vectors is manipulated to compare the estimation efficiency (multiple correlation) of those subsets. For each k the

subset of k vectors which gives maximum efficiency is printed as is also its corresponding multiple correlation coefficient.

In the final part of the program the estimation vectors are selected in the order prescribed by the step-up procedure. At each stage an index of the estimation vector introduced at that stage is printed out, as well as the multiple correlation coefficient obtained with the set of vectors selected up to that stage.

In this program checks were instituted to restrain the incorporation of vectors which were practically dependent on vectors already included in the active estimation set. Also, considerable effort was made to abbreviate the matrix-inversion type calculations in order to produce only the multiple correlation, since the number of such calculations, $2^p - p - 2$, rapidly gets large.

The purpose of the second program, to a considerable extent based on the assumption that the step-up procedure was reasonably efficient, was to make available a fairly flexible program for estimations based on the method of LS in which would be included at least options for activating subsets of the estimation variables according to the step-up procedure and other modified procedures, and also included would be options which could be exercised to stop the selection. The program was done for the Burroughs 5000 in the ALGOL 60 compiler language.

As it now stands the program has several options for obtaining the basic matrix of the dot products of the adjusted vectors (which matrix reduces to the intercorrelations matrix when the rows and columns are appropriately standardized).

(1) One of these options is the same as in the previous program, except that the admissible order of the matrix has now been increased to more than 100. This option allows for the rapid generation of data for experimental studies.

(2) Either the matrix of dot products or the intercorrelation matrix may be read in directly. This allows further study, especially of subset selection procedures, of previously studied regression problems, least squares fittings, and so forth.

(3) Observation vectors may be directly read in. This will be the way data will arise in most realistic problems, although values of the estimation variables may require preliminary transformation (e.g., if the estimation variables are terms in a balanced polynomial).

In this program, once the basic matrix has been obtained, it is retained in memory and can be used over and over, to facilitate comparisons when various procedures for selection, elimination, stopping are employed.

In case the intercorrelations matrix was not introduced directly the program gives an option for computing and printing it and using it in the remainder of the program.

In the main part of the program estimation vectors are introduced in the priority order dictated by the step-up procedure. In addition, however, the procedure carries options which allow for various rules to be set to make possible the elimination of an estimation vector and the stopping of the selection process.

At present there are two criteria either one of which may be used to eliminate an estimation variable. One option automatically eliminates an estimation variable after two have been included. Of course the one deleted

is the one of lowest net correlation with the dependent variable (see Section A preceding). In the other option the pertinent F statistic for the variable with smallest net correlation is computed (see Section A) and is tested against a preassigned threshold value. If it is below this value, the variable is deleted. It is possible to prevent any such eliminations by setting the threshold equal zero.

Currently there are four criteria which can be used to stop the process of adding estimation variables. The program effectively permits bypassing any or all of these criteria. They are:

(1) Stop if the F ratio for the next single variable to be introduced does not exceed that threshold value corresponding to a preassigned significance level. The procedure stops after that estimation variable has been added. This can be bypassed by setting the threshold at zero.

(2) Stop if the current value of the multiple correlation coefficient is sufficiently large. This can be bypassed by setting the multiple correlation threshold at unity.

(3) Stop if the number of variables chosen reaches a preassigned number. This can be bypassed by setting that number equal to the total number available.

(4) Stop when the number of computational iterations for adding or eliminating a vector has exceeded a preassigned number.

It is noteworthy that the computational procedures for eliminating and for adding a vector are the same, once the vector has been earmarked.

It should also be mentioned that the same precautions as in the earlier program were taken to prevent the introduction of almost linearly dependent vectors.

In this program of course the output includes the LS regression coefficients of the selected estimation vectors, as well as indices of the vectors selected, and the multiple correlation coefficients.

D. Test Runs on the Computer (see the supporting study titled, "Selection of Significant Estimation Variables in a Least Squares Problem: Empirial Computer Studies.")

As indicated in previous sections, these tests were broken roughly into two phases. In a very limited way the preliminary set of tests was conducted to gain a measure of confidence in the step-up procedure as a means for selecting an efficient subset of estimation variables in a least squares model. In the tests made a balanced polynomial of relatively low order was selected, the terms of which provided the full set of estimation variables. Estimation vectors, as well as a dependent-variable vector, were generated from rectangular design data. Dependent-variable data were computed as values of the function which was to be approximated. As described previously, subsets of estimation vectors selected by the step-up procedure were compared with the optimal set. Primary difficulty in test runs arose from fact that the determination of the actual optimal set of k vectors required comparisons of $\binom{p}{k}$ sets of vectors, where p was total number of estimation variables available. Computational feasibility dictates that p be severely restricted.

Nevertheless, several preliminary runs were made where p was kept to about 11, and in all cases less than 18. Several functions were approximated. These in general represented the class of rational functions. For one of the functions, which had a pole in the region of data points, only a poor approximation was obtained. Otherwise, even with low-degree polynomials, the multiple correlation coefficient was rather high.

In most of these tests the step-up procedure selected, at each stage, the optimal set of variables. There was one example, however, where the procedure did not select the optimal set of two vectors, although the correct selection of a larger number of variables was achieved. It is also noted that, when R became stable or nearly so, additional variables introduced by the step-up procedure were not always optimal. It is possible that this could have been the result of round-off error.

In general these experimental results indicated the step-up procedure is probably quite efficient, at least when a fair scatter of points is available. It was noted that, even when the method failed, the value of R was near optimal. The actual occurrence of failures, even at early stages, suggested that some means for eliminating variables would be desirable. Such techniques were introduced and used in the second phase of testing.

For the second set of test runs the Burroughs 5000 program was used. As mentioned earlier, this program allows for a larger number of estimation vectors to be handled, incorporates options of data input, variable elimination and program stops, but does not make the comparisons to determine a purely optimal subset of estimation variables. In most of the examples studied in this phase several runs were made for each example to throw light on the effects of changing the pattern of variable elimination and stopping rules. Attention was focused on varying the elimination criterion, the effects of varying other rules being discernible from the print-out, with the principal basis for elimination being an F statistic (see Section A of Summary). To observe the effect of certain stopping rules (which can be set in the program options) print-out includes for each "sweep" (where a variable is eliminated or added to the estimation set) the number of sweeps up to that stage, the number of estimation variables

being used, an index of the last one eliminated or added, the F_I value of the F statistic for a variable brought in or the F_O value of the F statistic corresponding to a variable being eliminated (if it was below the criterion level), and the square R^2 of the multiple correlation coefficient, as well as the reduced R^2 which diminishes if and only if the last variable introduced gave an F_I value less than unity.

The examples included: Approximating three non-polynomial functions, with the available variables being the 48 terms of a balanced polynomial cubic in X_1 and X_2 and quadratic in X_3 and the 500 data points generated from $X_1 = 0.25(0.25)2.50$, $X_2 = 0.25(0.25)2.50$ and $X_3 = 0.25(0.25)1.25$; approximating a dependent variable from actual data with available variables constituting a balanced polynomial in four variables, where the data are (as would usually be the case in practice) not in rectangular design; and approximating a dependent variable from actual data where the intercorrelation matrix of available estimation vectors was given, the presumption being that these could be non-polynomial terms.

In the first group of example the functions chosen to be approximated were

$$F_1(X_1,X_2,X_3) = \exp(-X_1^2 X_2 X_3)$$

$$F_2 = (X_1^4 + X_2^3 + X_3^2)|X_1 + X_2 - \tfrac{\pi}{2}X_3|^{-\frac{1}{2}}$$

$$F_3 = \sqrt{X_1^2 + X_2^2 + X_3^2} \ .$$

As in all examples the data were mean-adjusted. The functions F_1 and F_3, especially F_3, were very closely approximated (in the range of data) by the full set of 47 estimation vectors in the sense that R^2 was near unity, while R^2 for the case of F_2 was near 0.9. For each example runs were made with F_O

set over a range of values from high to low. In the case where F_0 was set very low the tendency was to eliminate few or no variables and thus to be very close to the simple step-up procedure.

The test runs for these examples show that different subsets of estimation variables will be selected when the elimination (and stopping) rules are varied. They provide concrete examples wherein the step-up procedure is bettered by a procedure modified to include an elimination criterion; where the opposite happens; where an F_I stopping criterion of 1.00 (on the last variable brought in) could stop the procedure which if continued would later introduce variables significant at this same level. These test runs suggest, but not markedly or universally, that the elimination criterion is effective in obtaining a higher R^2 for the same number of estimation variables; that a high criterion value is more effective for variables selected early but not for those selected later; that the F_I test may stop the procedure too soon unless modified; that different problems seem to need somewhat different rules; that while the set of variables selected may vary considerably R^2 has a tendency to be fairly stable for different procedures.

The examples with actual data provided experience with data more of the type expected in a realistic problem. In addition the first provided a good example in which an F stopping rule based on a single variable (last introduced) would have stopped the procedure too soon. The last example illustrates another point, viz. that out of 14 variables the last nine variables tested together are not significant at 50% level while the 6th one tested alone is significant at this level.

It should be noted that in all the examples, in terms of the multiple correlation coefficient, a few estimation variables usually accounted for most of the value of R^2.

It is recommended that further insight be obtained by examining the summary data for the various test runs, given in the supporting study referred to above.

Conclusions and Recommendations

The step-up procedure, which first activates the one estimation variable best in the sense of least squares, activates next the one which contributes the most to a further reduction in the sum of least squares, and so forth, is supported as an efficient and computationally feasible procedure for selecting priority-rated estimation variables in a least squares approximation problem.

The nonoptimality of the procedure is manifest in practice. However, the evidence is strong that even in such case the results are near-optimal, as measured by the multiple correlation coefficient, R. The empirical evidence indicates more reliability of the step-up procedure in the activation of the earlier and presumably more significant variables than in later variables. When a large number of estimation variables is involved, the optimal value of R appears to be nearly reached by several subsets of estimation vectors. Thus, although frequently in these cases the set selected by the step-up procedure is not optimal, it is very nearly so.

If it is important to restrict the number of estimation variables, there appears to be a need for a means of eliminating variables previously activated. The procedure of eliminating an active variable whose net contribution to the reduction in the sum of least squares is least (and small) is practicable and frequently effective. Examples show, however, that the elimination modification does not always improve on the simple step-up procedure. Moreover, it carries the same cost as activating an estimation variable. No fixed elimination criterion is best for any wide variety of problems. The experiments indicated an overall tendency for a large elimination criterion to be more effective when

the active estimation subset is small and a small criterion to be more effective when the number of active estimation variables has become sizable.

The use of rules to stop the activation of additional estimation variables must often depend on such factors as available computer time and rate of computer time utilization. A comprehensive set of rules, which may be used in various combinations, includes stopping when R is sufficiently large, when the activation of additional variables does not contribute significantly to the estimation, when the number of variables reaches a preassigned number or when the computational procedure begins to cycle. Examples show that the second of these can occasionally stop the process too soon, so that the contribution of the last several active variables, rather than just the last one, should probably be tested. The speed with which variables were eliminated or introduced in the examples indicates that large blocks of variables could be introduced before making any decision on which variables to keep active.

The study shows that at the current state of computer science it is still infeasible to examine all combinations of subsets of estimation variables to determine the optimal subset, unless the total number is quite small, and thus that the need remains for such a procedure as the step-up procedure. The study has also given evidence of the feasibility of the rapid selection of efficient estimation variables even from a set of several hundred, using a fairly sophisticated system of optional variable-elimination and stopping rules.

Finally, with reservation, it should be noted that in all the examples there was a marked relative efficiency of a small set of active estimation variables to the entire set of estimation variables available.

In view of the foregoing results the step-up procedure is recommended as an effective means for selecting priority-rated estimation variables in a least squares analysis. The use of the modified procedure and the various

stopping rules is also recommended with the admonition that the various settings ought insofar as possible to be adjusted to suit the experience of workers familiar with the problem area under study.

Specifically, with regard to the context of estimating optimal trajectories, i.e. with regard to the problem giving rise to this study, it is recommended that further general analysis of the method described herein, either theoretical or empirical, not be undertaken, but that the method and experience gained be applied in a series of experiments with actual trajectory data as soon as possible, where the experience of researchers in the field and the knowledge of physics pertinent to the problem will be utilized to help delimit the class of approximating functions.

Finally, using methods of design of experiments and a limited class of functions presumably pertinent to trajectory problems and including some live data, it may be feasible to study the effects (on approximation efficiency) of varying certain factors such as data distribution, type of approximation, elimination criterion, and so on.

SELECTION OF SIGNIFICANT ESTIMATION VARIABLES
IN A LEAST SQUARES PROBLEM: MATHEMATICAL REVIEW

1. Introduction. The principle of least squares (LS) can be formulated
in the following terms. Presumed to exist is some sort of functional dependence
of one variable, Y, called the _dependent_ variable, on a vector, $(X_1, \ldots, X_\pi)$, of
π other variables, called _independent_ variables. Available is a number (say N)
of _observations_, i.e. values of Y corresponding to values of the vector $(X_1, \ldots, X_\pi)$.
Next is chosen a class of _admissible_ _functions_ of the form,
$a_1 Z_1 (X_1, \ldots, X_\pi) + \ldots + a_p Z_p (X_1, \ldots, X_\pi)$, where the $Z_1, \ldots, Z_p$ are fixed functions
of the X's and the _parameters_ of the class are $a_1, a_2, \ldots, a_p$. The functions
Z_i presumably are chosen to enhance the likelihood that the unknown functional
relationship (between Y and the X's) will be nearly of the prescribed form.
Each function of the class is linear in the variables, $Z_1, \ldots, Z_p$, which we shall
call _estimation_ variables; each function is also linear in the parameters. In
any case the basic idea in the least squares approach is to approximate the
unknown functional relationship with one of the admissible functions. For any
one of the functions in the class, corresponding to each observation, $(x_{\mu 1}, \ldots, x_{\mu \pi})$,
is the value of the function, $\tilde{y}_\mu = a_1 z_{\mu 1} + \ldots + a_p z_{\mu p}$, where
$z_{\mu i} = Z_i (x_{\mu 1}, \ldots, x_{\mu \pi})$, which is comparable with the value of Y (say y_μ)
corresponding to this same observation, $(x_{\mu 1}, \ldots, x_{\mu \pi})$. The sum of squares,

$$\sum_{\mu=1}^{N} (\tilde{y}_\mu - y_\mu)^2,$$

is taken as a measure of the estimative value of the function $\tilde{Y} = a_1 Z_1 + \ldots + a_p Z_p$.
According to the principle of least squares, out of the class of admissible
functions

$$\mathcal{Y} = \{\tilde{Y} \,|\, \tilde{Y} = a_1 Z_1 + \ldots + a_p Z_p\},$$

is chosen as an estimate of Y one function which minimizes the sum of squares of deviations. Such an estimate (we shall see that one does exist) is written as $\hat{Y} = \sum_1^p b_i Z_i$; we shall call such a function a <u>best estimate</u> or <u>best-fitting approximation</u> (in the class) in the sense of least squares. The sum of squares of deviations, $\sum_1^N (\hat{y}_\mu - y_\mu)^2$, is called the <u>sum of least squares</u> or the <u>residual sum of squares due to error</u>. The procedure of obtaining a best estimate in the above sum is frequently called a <u>regression analysis</u>, or more properly a <u>linear regression analysis</u>. The b_i are often called <u>regression coefficients</u>.

The method of LS was known and used by Gauss over 150 years ago. He discovered that under certain conditions the method of least squares in a sense yields an optimal estimate. This is the famous Gauss-Markov theorem. Briefly, the principal hypothesis for this theorem is that except for random deviations the observed values of Y are values corresponding to one of the functions in the class $\mathcal{Y}$. The random deviations are assumed to be statistically uncorrelated, with a common variance and mean zero. Under the additional hypothesis of normality of the distribution of these deviations an elegant statistical theory of estimation and hypothesis testing can be constructed. The statistical model is discussed briefly in Section 5 below.

The method of LS is used widely in numerical analysis even when the support of the Gauss-Markov theorem cannot honestly be invoked. In many cases other methods perhaps are equally or more justifiable; but often the method of LS has an intuitive appeal in that it seeks an estimate which minimizes one obvious measure of error.

It is also possible to consider classes of admissible functions, from which an estimate will be chosen on the basis of the LS principle, which classes are

nonlinear in the parameters. In many instances such problems are resolved
satisfactorily by iterative techniques. The procedure of obtaining estimates
of the parameters in such a case is called a <u>nonlinear regression analysis</u>.

Excellent accounts of the statistical linear regression model are given
in GRAYBILL, SCHEFFÉ, and ZELEN. The method of LS is given space in most
numerical analysis books, and sometimes the nonlinear case is discussed.
E.g., see SCARBOROUGH. Nonlinear regression analysis is treated from a sta-
tistical point of view in WILLIAMS.

In applications of LS it is often the case that the number of estimation
variables, for which values are computable from observations on independent
variables, is very large. Certain recurring and nagging questions arise,
varying somewhat with the circumstances. If only k of p variables can be used,
which k should be chosen? Does the use of additional variables contribute
significantly to increased efficiency of estimate? The second of these
questions is not mathematically meaningful until the word "significantly" is
defined. However, in the context of a given problem, the question is one that
frequently must be raised, given meaning and acted on.

There is an obvious answer to the first question raised above, viz., to
determine by computation which of the $\binom{p}{k}$ sets of estimation variables yields
the minimum sum of least squares from the data. Unfortunately this straight-
forward procedure is computationally infeasible. A more tractable and completely
reliable method of finding the optimal set of k estimation variables remains an
open problem. However, at least as early as 1931, WHERRY proposed a procedure
for selecting a reasonably efficient subset of estimation variables. This
procedure we call -- because it has become our habit -- simply the step-up
procedure. It consists in selecting first the one estimation variable best in
the sense of LS, next the one which contributes the most to a further reduction

in the sum of LS, and so forth. In this way variables are added until some rule stops the process. The procedure is computationally very feasible and fast. However, it is easy to show it is not always optimal. The step-up procedure has recently been described without much critical analysis in papers by ANDERSON and FRUCHTER, and SCHULTZ and GOGGANS.

The aims of the present paper are: To illuminate the method of LS in linear regression analysis with geometrical arguments, giving clear interpretation of certain measures of estimation efficiency; thus to lead into a natural development of the step-up procedure where its weakness as well as its intuitive appeal are exposed; to examine the geometrical structure for a procedure for elimination of a variable previously selected, and thus mitigate the flaws in the step-up procedure; to explore the statistical model for reasonable decision rules on when to eliminate and when to keep adding variables; and finally to provide a translation of the various geometrically conceived procedures to computable algorithms.

2. <u>Geometric formulation of the principle of least squares</u>. The notion
of obtaining an estimate, $\hat{Y} = \Sigma_1^b b_i Z_i$, out of the admissible class $\mathcal{Y}$ which
minimizes the sum of squares of deviations, is one admitting of accessible
and correct geometrical descriptions. Such a formulation is helpful in under-
standing the step-up procedures for selecting significant estimation variables
(to be described in the next section) and seems to hold the only hope of devising
techniques even more defensible than the step-up procedure. We proceed now
toward such a formulation.

Assumed available are the N observation vectors, $(y_\mu, z_{\mu 1}, \ldots, z_{\mu p})$, $\mu = 1, 2, \ldots, N$,
where $z_{\mu i} = Z_i (x_{\mu 1}, \ldots, x_{\mu \pi})$, as indicated in the preceding section. Associated
with each of the p estimation variables Z_i, i = 1,2,...,p, is the vector,
lying in the euclidean N-space E^N, consisting of N values $z_{\mu i}$, $\mu = 1, 2, \ldots, N$,
observed on that variable. We shall call these vectors <u>estimation</u> vectors; we
write them, z_i (i = 1,2,...,p); and for matrix manipulations they will be thought
of as column vectors. Hence, using the letter T to indicate matrix transpose,
$z_i^T = (z_{1i}, z_{2i}, \ldots, z_{Ni})$. In this section the N x p matrix of these estimation
vectors will be denoted as z. Similarly, the symbol y represents the vector of
the observed values of the dependent variable Y. It will be assumed, without
any real loss of generality, that N > p and that the estimation vectors are
linearly independent. Thus the estimation vectors constitute a basis of a
p-dimensional vector space V_p, lying in E^N.

Consider now the sum of squares criterion. Writing the parameter vector
as a, this criterion is

$$g(a) = \sum_{\mu=1}^{N} (y_\mu - \tilde{y}_\mu)^2 = d^T d,$$

where $d = y - \tilde{y}$ is the vector of deviations. Note that $\tilde{y} = \Sigma_1^p a_i z_i$ lies in

the vector space V_p generated by the estimation vectors and that $d^T d$ is the square of the (euclidean) distance between y and $\hat{y}$. Since the aim was to determine b such that $g(b) = \min\{g(a) \mid a\}$, the least squares problem may be interpreted as finding a vector in the space spanned by the estimation vectors which lies nearest the dependent-variable vector y.

Geometrical intuition now supplies the correct solution to the least squares problem; viz., the vector in V_p lying nearest y is the projection of y onto V_p. Other important points are indicated by the geometry. Writing $\hat{y}$ as the projection of y onto V_p, $e = y - \hat{y}$, and $e^2 = e^T e$, etc., pythagorean relations are indicated. E.g., $y^2 = \hat{y}^2 + e^2$; i.e., the square of the length of the dependent-variable vector equals the sum of the squares of the lengths of the best estimate vector and the least squares residual error vector. This is often stated as, "The total sum of squares equals the sum of squares due to regression (estimation) plus the sum of squares due to error." Also, if $\tilde{y} = \Sigma a_i z_i$ is another vector lying in V_p, if $d = y - \tilde{y}$, then $d^2 = e^2 + (\hat{y} - \tilde{y})^2$. Also, the e vector will be orthogonal to V_p. Finally, the angle between y and its projection should be less than the angle between y and any other vector in V_p. Thus $\cos \theta(y, \hat{y}) > \cos \theta(y, \tilde{y})$, where $\theta(u,v)$ means the angle between vectors u and v.

In statistical terminology the cosine of the angle between two such vectors is called a _correlation_ coefficient. Recall that

$$\cos \theta(u,v) = \frac{(u \circ v)}{\sqrt{u^2 v^2}} = \frac{\Sigma u_i v_i}{\sqrt{\Sigma u_i^2 \Sigma v_i^2}}$$

In the above instance $\cos \theta(y, \hat{y}) = R$ is called the _multiple_ _correlation_ _coefficient_ between y and $\hat{y}$. Note that this should be unity if y does indeed lie in V_p, and should reduce progressively to zero when the estimation space is

less and less effective. Thus R provides a rather useful and suggestive index of the efficiency of the estimation space. The square of the length of the least squares residual error vector, $e^T e$, is another closely related measure of the efficiency of estimation.

The situation is represented schematically in the following diagram:
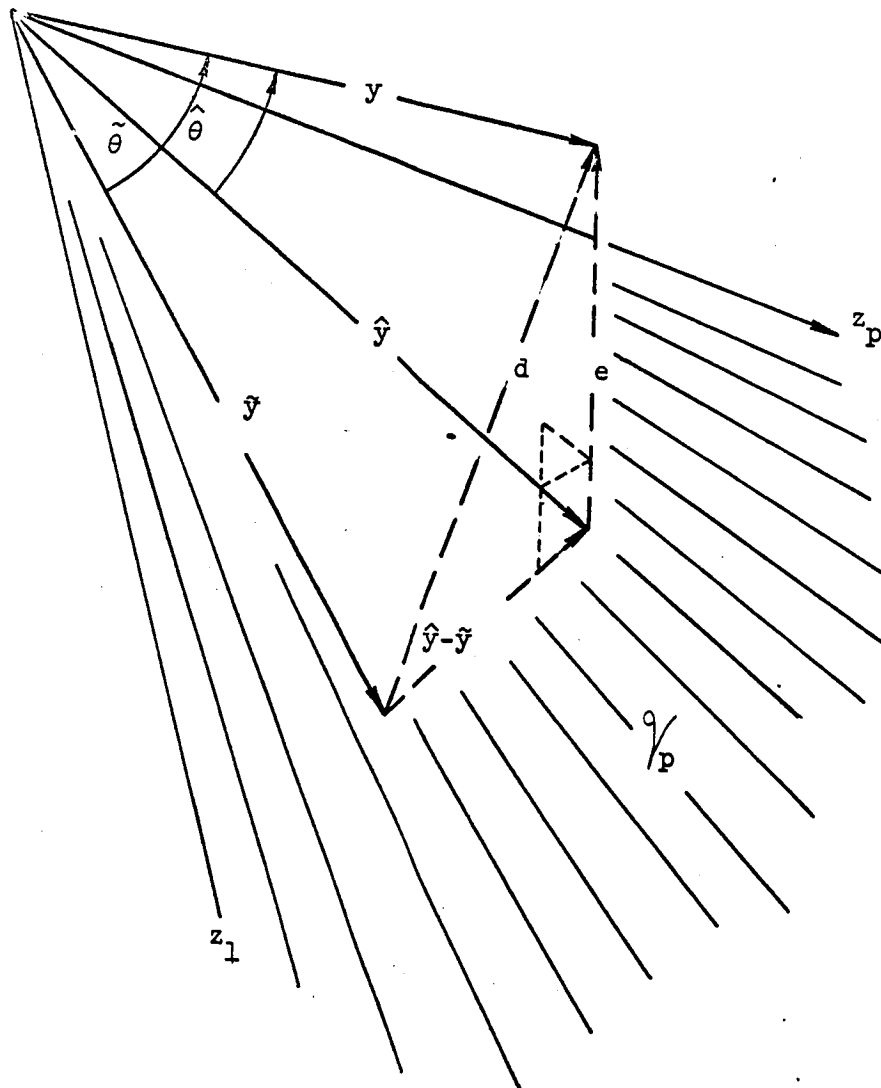
The foregoing geometrical discussion can be substantiated with a detailed algebraic development. Such substantiation is a consequence of the argument to follow, but the primary purpose of the argument is to make the geometrical entities explicit, to make essential quantities computable and to set the stage for the next section.

The estimation space V_p is spanned by sets of orthogonal vectors of unit length. Let z_1^*, z_2^*, ..., z_p^* be one such set. Since every vector in V_p is a unique linear combination of the estimation vectors,

$$z_1^* = q_{11} z_1 + \cdots + q_{1p} z_p$$

$$\vdots \quad \vdots \quad \vdots$$

$$z_p^* = q_{p1} z_1 + \cdots + q_{pp} z_p$$

i.e., $z^* = zQ$, where Q is a non-singular $p \times p$ matrix, and, of course, $z = z^* Q^{-1}$. Also, every vector in V_p has a unique representation either as a linear combination of $z_1, \ldots, z_p$ or of $z_1^*, \ldots, z_p^*$. If $\tilde{y}$ lies in V_p, then there exists a unique vector a such that $\tilde{y} = \sum_1^p a_i z_i = za$, and there exists a unique vector a* such that $\tilde{y} = z^* a^*$. But $z = z^* Q^{-1}$, so that $a^* = Q^{-1} a$. Thus there is a one-one correspondence between coefficient vectors a for the z basis and vectors a* for the z* basis. In particular, if b* is such that $\hat{y} = z^* b^*$ is the one vector in V_p closest to y, then $\hat{y} = zb$, where $b = Qb^*$.

With these orthogonal vectors z* in mind an orthogonal transformation is now imposed on the points in E^N in such a way that, in the transformed space $E^{N'}$, the z* become the unit vectors u_1, u_2, ..., u_p. Such a transformation is accomplished with an $N \times N$ orthogonal matrix P whose first p rows are the vectors z^{*T}. It is easily seen that distances and angles are preserved under such a transformation, so that the least squares problem is invariant under

the transformation. Note that the image V'_p of V_p is simply the linear combinations of the unit vectors, $u_1, \ldots, u_p$. Let $y' = Py$, and let $\tilde{y} = z*a*$ lie in V_p, so that $\tilde{y}' = \sum_1^p a_i^* u_i$. Then the square of the error vector is

$$d^T d = d'^T d' = (y' - \sum a_i^* u_i)^T (y' - \sum a_i^* u_i) = \sum_1^p (y_i' - a_i^*)^2 + \sum_{p+1}^N y_\mu'^2 \quad .$$

Evidently the projection of y' onto V'_p ought to be the vector whose first p components are those of y' and whose remaining components are zero. Thus the a_i^* which produce the combination of u_i ($i=1,2,\ldots,p$) constituting the projection of y' on V'_p are y_i'. In short, $b_i^* = y_i'$, $i = 1,2,\ldots,p$. That this is correct algebraically can be seen in the preceding equation, where it is obvious that these are the values of a_i^* which minimize the square of the error vector. Write $\hat{y}' = \sum_1^p b_i^* u_i = [y_1', \ldots, y_p', 0, \ldots, 0]^T$. Note that the residual error vector $[0, \ldots, 0, y_{p+1}', \ldots, y_N']^T = e'$ so that e' and $\hat{y}'$ are orthogonal. Note also that $\sum_1^p (y_i' - a_i^*)^2 = (\hat{y}' - \tilde{y}')^2$ and hence, from the foregoing equation, that

$$d'^2 = (\hat{y}' - \tilde{y}')^2 + (y' - \hat{y}')^2 = (\hat{y}' - \tilde{y}')^2 + e'^2.$$

Having seen now that, relative to an orthogonal basis of V_p, $b* = z*^T y$ (which follows from the fact that $b_i^* = y_i'$ and $y_i' = z_i^{*T} y$ for $i = 1, 2, \ldots, p$), it is now desirable to obtain $\hat{y}$ and $e^T e$ in terms of the original estimation vectors and the dependent variable vector. But $\hat{y} = z*b* = zb$, where $b = Qb* = Qz*^T y = QQ^T z^T y$. Now

$$(QQ^T)^{-1} = Q^{-1^T} Q^{-1} = Q^{-1^T} z*^T z* Q^{-1} = (z* Q^{-1})^T (z* Q^{-1}) = z^T z.$$

Thus, writing $h = z^T z$ and $g = z^T y$, in terms of original data, $b = h^{-1} g$. Also

$$e^2 = \sum_1^p y_i'^2 = b*^2 = y^T z*z*^T y = y^T zQQ^T z^T y = (z^T y)^T b = \sum_i b_i g_i.$$

Thus computationally the problem is one of solving the system of equations hb = g. In the succeeding discussion it will be important to remember the following principle which summarizes much of the preceding development and unifies the geometry and algebra of the least squares problem: Given a set of k linearly independent vectors $z_1, \ldots, z_k$ in an euclidean space and a $(k+1)$-st vector w, if $h = z^T z$ where $z = (z_1, \ldots, z_k)$ and $v = z^T w$; then the solution x of the equations hx = v is such that zx is the projection of w onto the space generated by the z_i, and the solution effectively resolves the w vector into its projection zx and a component, e = w - zx, orthogonal to the projection.

3. <u>The Step-up Procedure</u>. In this section emphasis is shifted to the selection of a subset of (say) k estimation vectors out of a total number of (say) p. An optimal set of k, by definition, will be that set of k corresponding to which the length of the error vector is least (or equivalently the multiple correlation coefficient R is most.) The plausibility of the step-up procedure, as well as its deficiencies, will be seen from the geometrical development. Computational feasibility and procedures will be evident from the corresponding algebra.

For the moment we suppose that k-1 vectors have been chosen and that our purpose is to add another one from the p-(k-1) remaining. We shall refer to estimation vectors selected as being in the <u>active estimation space</u> or as being active.

With regard to a least square problem involving y and the k-1 active estimation vectors (which of course are a basis for a vector space V_{k-1} of dimensionality k-1) everything in the preceding section is directly applicable. This succession of problems with 1,2,...,k,...,p vectors in the active estimation space is sometimes called the succession of the 1st, 2nd,..., kth,...,pth <u>fittings</u>. We shall frequently use a superscript to indicate the fitting, or dimension of the active estimation space. This notation does not specify which of the vectors are in the active estimation space, but we shall tacitly assume they have been relabeled so that the active estimation vectors are now z_1, z_2,...,z_{k-1}. According to the preceding section
$\hat{y}^{(k-1)} = \Sigma_{i=1}^{k-1} b_i^{(k-1)} z_i = z^{(k-1)} b^{(k-1)}$, where $b^{(k-1)}$ is the solution to the system of equations, $h^{(k-1)} b^{(k-1)} = g^{(k-1)}$, with
$h^{(k-1)} = z^{(k-1)^T} z^{(k-1)}$, $g^{(k-1)} = z^{(k-1)^T} y$, and $z^{(k-1)} = (z_1,...,z_{k-1})$.

Recall that $\hat{y}^{(k-1)}$ is the projection of y onto V_{k-1} and that the residual error vector $e^{(k-1)}$ has length whose square is $(b^{(k-1)} \cdot g^{(k-1)})$.

Suppose next that the kth vector to become active has been selected. Consider the system of equations $h^{(k-1)} x^{(k-1)} = v^{(k-1)}$, where $v^{(k-1)} = z^{(k-1)^T} z_k$. Recall that $\sum_{i=1}^{k-1} x_i^{(k-1)} z_i$ is the projection of z_k onto V_{k-1}, and $z_k' = z_k - \sum_{i=1}^{k-1} x_i^{(k-1)} z_i$ is the component of z_k lying orthogonal to the space spanned by the $z_1, \ldots, z_{k-1}$. The vectors $z_1' = z_1, z_2', \ldots, z_k', \ldots$, thus defined are a particular determination of <u>Gram-Schmidt orthogonal vectors</u>. In matrix form the matrix of the first k of these Gram-Schmidt vectors is

$$z'^{(k)} = z^{(k)} Q'^{(k)}, \text{ where } Q'^{(k)} = \begin{bmatrix} 1 & - x_1^{(1)} & - x_1^{(2)} & \cdots & - x_1^{(k-1)} \\ 0 & 1 & - x_2^{(2)} & \cdots & \vdots \\ \vdots & 0 & 1 & \cdots & \\ \vdots & & \ddots & \ddots & - x_{k-1}^{(k-1)} \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

from the equation above.

Normalized Gram-Schmidt vectors are obtained when the columns of $Q'^{(k)}$ are divided by $(z_i' \cdot z_i')^{\frac{1}{2}}$. Thus orthonormal Gram-Schmidt vectors are

$$z*^{(k)} = z^{(k)} Q^{(k)},$$

where $Q^{(k)}$ is upper triangular with the reciprocals of the lengths of the Gram-Schmidt vectors in the diagonal.

Recapitulating at this point, we have an orthonormal basis for the active estimation space in terms of the Gram-Schmidt orthogonal vectors, where the last Gram-Schmidt vector was the component of the last estimation vector selected orthogonal to the space of the others.

It is interesting to note that the lengths of the Gram-Schmidt vectors z_k' are readily available from the original estimation vectors. In fact, using the basis $z_1^*,\ldots,z_k^*$ derived from the Gram-Schmidt vectors as the orthonormal basis of the previous section, it follows from the results of that section that $z*^{(k)} = z^{(k)} Q^{(k)}$, where $Q^{(k)}$ is triangular with $(z_k' \cdot z_k')^{-\frac{1}{2}} = q_{kk}$, and that $h^{(k)^{-1}} = Q^{(k)} Q^{(k)^T}$, or, writing $a^{(k)} = h^{(k)^{-1}}$, that $a_{kk}^{(k)} = q_{kk}^2 = (z_k' \cdot z_k')^{-1}$.

Now, given orthonormal vectors, $z_1^*,\ldots,z_{k-1}^*$, z_k^*, from the preceding section the square of the projection of y onto V_{k-1} was $\Sigma_{i=1}^{k-1} b_i^{*2}$, where

$$b*^{(k-1)} = z*^{(k-1)^T} y;$$

while the square of the projection onto V_k is $\Sigma_{i=1}^{k} b_i^{*2}$, where

$$b*^{(k)} = z*^{(k)^T} y.$$

Thus, b_k^{*2} is the increase in the square of the projection vector obtained by activating the estimation vector z_k (whose component orthogonal to V_{k-1} is z_k'); or, equivalently, b_k^{*2} is the reduction in the square of the residual error vector obtained by activating z_k.

Now the principle of the step-up procedure becomes clear. Given the problem of augmenting by one vector an active estimation set of k-1, the answer is to choose that one for which the new projection of y in V_k has the largest component orthogonal to the old projection in V_{k-1}; i.e., choose z_k

so that relative to the augmented Gram-Schmidt orthonormal system, $z_1^*, \ldots, z_{k-1}^*, z_k^*, b_k^{*2}$ is maximum.

Again, it is important to be able to examine what values b_k^{*2} could have for the various possible vectors which could be chosen as z_k, and to do this easily in terms of the original vectors. But recall that

$$z^{*(k)} = z^{(k)} Q^{(k)}, \quad Q^{(k)} b^{*(k)} = b^{(k)} = h^{(k)^{-1}} g^{(k)},$$

so that the triangularity of $Q^{(k)}$ implies that

$$q_{kk} b_k^* = b_k^{(k)}, \quad \text{or} \quad b_k^{*2} = \frac{b_k^{(k)2}}{a_{kk}^{(k)}} .$$

It is worth noting that the residual error vector can be considered as a final Gram-Schmidt vector, since $e^{(k)} = y - \hat{y}^{(k)}$, where $\hat{y}^{(k)}$ is the projection of y onto V_k. But we have seen that the reciprocal of the square of the kth Gram-Schmidt vector is the last diagonal element of the inverse of $h^{(k)}$. Thus, if the $h^{(k)}$ matrix being used is augmented with an additional column $z^{(k)^T} y$ and a symmetric row, corresponding to the dependent-variable vector y, then the last diagonal element of the inverse of this augmented matrix will be the reciprocal of the sum of least squares.

A computation synthesis of the procedure can be envisaged as a sequence of <u>gaussian elimination tableaux</u>, where starting with

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$$
\left[
\begin{array}{ccc|c|cccc|c}
h_{11} & \cdots & h_{1p} & g_1 & 1 & 0 & \cdots & 0 & 0 \\
 & & & & 0 & \ddots & & \vdots & \vdots \\
\vdots & & \vdots & \vdots & \vdots & \ddots & & 0 & 0 \\
h_{p1} & \cdots & h_{pp} & g_p & 0 & \cdots & 0 & 1 & 0 \\
\hline
g_1 & \cdots & g_p & y^T y = G & 0 & \cdots & \cdots & 0 & 1
\end{array}
\right]
$$

after k-1 stages we have

$$
\left[
\begin{array}{cccc|cc|cc|ccc|c}
1 & & 0 \cdots & 0 & h_{1,k}^{(k-1)} & \cdots & b_1^{(k-1)} & a_{11}^{(k-1)} & \cdots & a_{1,k-1}^{(k-1)} & 0 \cdots 0 & 0 \\
0 & \ddots & & \vdots & \vdots & & \vdots & \vdots & & & \vdots & \vdots \\
\vdots & \ddots & & 0 & & & & & & & & \\
0 & \cdots & 0 & 1 & h_{k-1,k}^{(k-1)} & \cdots & b_{k-1}^{(k-1)} & a_{k-1,1}^{(k-1)} & \cdots & a_{k-1,k-1}^{(k-1)} & 0 \cdots 0 & 0 \\
\hline
0 \cdots & \cdots & & 0 & h_{kk}^{(k-1)} & \cdots & g_k^{(k-1)} & \vdots & & \vdots & 1 0 \cdots 0 & 0 \\
 & & & & & & & & & & 0 \ddots \vdots & \vdots \\
\vdots & & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots \ddots 0 & \vdots \\
0 \cdots & \cdots & & 0 & & & g_p^{(k-1)} & & & & 0 \cdots 0 1 & 0 \\
\hline
0 \cdots & \cdots & & 0 & \cdots & \cdots & G^{(k-1)} & \cdots & \cdots & \cdots & 0 \cdots 0 & 1
\end{array}
\right]
$$

Note that $\begin{bmatrix} h_{1k}^{(k-1)} \\ \vdots \\ h_{k-1,k}^{(k-1)} \end{bmatrix}$ is the solution of $h^{(k-1)} x^{(k-1)} = v^{(k-1)}$ from which the

kth Gram-Schmidt vector is obtainable. Note that $\begin{bmatrix} b_1^{(k-1)} \\ \vdots \\ b_{k-1}^{(k-1)} \end{bmatrix}$ is the solution of

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$h^{(k-1)} \, b^{(k-1)} = g^{(k-1)}$. Note that if z_k is to be the next vector activated, then to obtain solutions to $h^{(k)} x^{(k)} = v^{(k)}$ and $h^{(k)} b^{(k)} = g^{(k)}$, and to obtain $a^{(k)} = h^{(k)-1}$, requires only to operate on the above matrix with elementary (row) transformations so as to reduce the kth column to the unit vector u_k. This will produce

$$b_k^{(k)} = \frac{g_k^{(k-1)}}{h_{kk}^{(k-1)}} \quad \text{and} \quad a_{kk}^{(k)} = \frac{1}{h_{kk}^{(k-1)}} \,.$$

Thus $b_k*^2 = g_k^{(k-1)2} / h_{kk}^{(k-1)}$.

From the last equation it is easy to see that, to find the vector yielding maximum b_k*^2, one need only examine the ratios $(g_j^{(k-1)2})/h_{jj}^{(k-1)}$ for $j = k, k+1, \ldots, p$.

Note finally that, after k vectors have been chosen, the last diagonal element of the inverse of the augmented matrix would be $1/G^{(k)}$. Hence $G^{(k)} = e^{(k)2}$, the sum of squares of residual error.

Attention is called to the obvious fact that the step-up procedure of activating estimation vectors in the order of the further reduction made to sum of squares of error is not necessarily optimal in selecting say k vectors out of p. E.g. the y vector could be practically in the space of two vectors, z_1 and z_2, but lying closer to a third z_3 (not in the space) than to either of the given two. Thus the first vector selected would be vector z_3. Then regardless of which one was selected next, the pair chosen would be inferior to z_1, z_2.

One other word of caution is in order. The criterion for activating the next estimation vector is a maximum ratio. The denominator of this ratio is the square of the length of the component of the new vector in the direction orthogonal to the then current estimation space. Of course, if some of the

remaining vectors lie in the currently active estimation space (i.e., they are linearly dependent on vectors already chosen) they should not be considered as candidates. Because of roundoff errors such dependency must be defined approximately. Note that an almost dependent vector will produce a small orthogonal component which will tend to produce a large criterion ratio (which may be primarily an accident of roundoff error). To avoid spurious selections caused in this way the criterion should be compared only for those vectors whose orthogonal component exceeds a minimum value. What minimum value ought to be chosen is at this time a matter for conjecture.

4. _Criterion for eliminating insignificant variables._ From the discussion in the preceding section it evidently may happen that, in trying to activate an efficient set of k estimation vectors, the step-up procedure will select at one stage a vector which later on would be more efficiently eliminated. So far no procedure for deactivating any of the active estimation vectors has been incorporated. However, the algebraic technique for eliminating any designated active estimation vector and obtaining the regression analysis for the reduced set is well-known. It is a question of deciding whether to eliminate one and if so which one to eliminate. The purpose of this section is to provide a geometrically appealing and obvious answer to the second aspect of this question. Criteria for deciding whether to eliminate a variable will be discussed in the next section.

Therefore we suppose k estimation vectors have been activated and the corresponding analysis laid out, say in the manner of the sequence of gaussian tableaux referred to in the last section, and we suppose the decision has been made to eliminate one of the vectors. The question is: Which one shall we eliminate? Fix attention on one of the active z_i, say for definiteness the last one, z_k. Now the projection $\hat{y}^{(k)}$ of y onto V_k can be resolved into its projection $\hat{y}^{(k-1)}$ onto V_{k-1}, the space spanned by $z_1, \ldots, z_{k-1}$, and a component orthogonal to $\hat{y}^{(k-1)}$. The projection $\hat{y}^{(k-1)}$ of $\hat{y}^{(k)}$ onto V_{k-1} is indeed the same as the direct projection of y onto V_{k-1}, so that the orthogonal component mentioned above in the resolution of $\hat{y}^{(k)}$ is the net effect of the active vector z_k in the estimation of y with $\hat{y}^{(k)}$. Still keeping attention to z_k, we have already seen that the square of the length of this orthogonal component is b_k^{*2}, where in fact b_k^* is a component in the direction of the kth Gram-Schmidt vector generated according to the order in which the z_i were selected. Also,

$$b_k^{*2} = \frac{b_k^{(k)2}}{a_{kk}^{(k)}} \, ,$$

where, it will be recalled,

$$h^{(j)}b^{(j)} = g^{(j)}$$

for any $j = 1,2,\ldots,p$; with $h^{(j)} = z^{(j)^T}z^{(j)}$, $z^{(j)} = (z_1,\ldots,z_j)$, $a^{(j)} = h^{(j)-1}$.

Recall also the pythagorean relation for each $j = 1,2,\ldots,p$,

$$(y \cdot y) = y^2 = \hat{y}^{(j)2} + e^{(j)2},$$

where

$$\hat{y}^{(j)2} = \sum_{i=1}^{j} b_i^{*2} \text{ and } e^{(j)2} = \sum_{\mu=j+1}^{N} y_\mu'^2 ,$$

with $y' = Py$, the image of y under orthogonal transformation. Thus, remembering that $b_i^{*} = y_i'$,

$$y^2 = \hat{y}^{(k-1)2} + b_k^{*2} + e^{(k)2}.$$

Evidently b_k^{*2} can be interpreted as the net reduction in the square of the error vector obtained by activating z_k, or, equally as well, as the net increment (provided by activating z_k) in the square of the active estimate.

Imagine now that the gaussian elimination has proceeded to the point of obtaining a solution to $h^{(k)} b^{(k)} = g^{(k)}$ with $a^{(k)} = h^{(k)-1}$:

$1 \quad 0 \ldots 0$	$h_{1,k+1}^{(k)} \ldots h_{1p}^{(k)}$	$b_1^{(k)}$	$a_{11}^{(k)} \ldots$	$0 \ldots 0$	0
$0 \qquad 0$	$\vdots$	$b_j^{(k)}$	$\ddots \; a_{jj}^{(k)} \; \ddots$	$\vdots$	$\vdots$
$0 \ldots 0 \quad 1$	$h_{k,k+1}^{(k)} \ldots h_{kp}^{(k)}$	$b_k^{(k)}$	$\ldots \qquad a_{kk}^{(k)}$	$0 \ldots 0$	0
$0 \ldots 0$	$\ldots$	$g_{k+1}^{(k)} \ldots$		$1 \quad 0 \ldots 0$	0
$\vdots$	$\vdots$	$\vdots$		$0 \quad \ddots \quad 0$	$\vdots$
$0 \ldots 0$	$\ldots$	$g_p^{(k)} \ldots$		$0 \ldots 0 \quad 1$	0
$0 \ldots 0$	$\ldots$	$G^{(k)} \ldots$		$0 \ldots 0$	1

But now suppose $j < k$ and that the order in which z_j and z_k have been introduced is reversed. Imagine re-scheduling the calculations in the gaussian elimination for this revision. In the tableaux this would be accomplished if in the initial tableau the jth and kth rows were interchanged and the jth and kth columns (to restore the initial unit matrix on the right the (p+1+j)-th and the (p+1+k)-th columns would also have to be interchanged), and thereafter repeating the operations which produced the kth tableau laid out above. The solution vector $b^{(k)}$ in this case would be the same as before except that the order of $b_j^{(k)}$ and $b_k^{(k)}$ would be interchanged. Moreover, the inverse matrix would be the same except that the jth and kth rows and the jth and kth columns would be switched, putting $a_{jj}^{(k)}$ in the (k,k)- position and $a_{kk}^{(k)}$ in the (j,j)-position. Note now that $b_j^{(k)2}/a_{jj}^{(k)}$ plays the role of b_k^{*2}, and hence the quantity $b_j^{(k)2}/a_{jj}^{(k)}$ is the net reduction in the square of the error vector due to the z_j vector.

Now it is clear which of the k active estimation vectors should be eliminated, viz. that z_j $(j \leq k)$ for which $b_j^{(k)2}/a_{jj}^{(k)}$ is minimum. Observe that these ratios are computable from the kth gaussian tableau set out above without any re-computations.

Having decided which estimation vector is to be eliminated from the active set of k, the procedure for making the elimination and obtaining the regression analysis for the reduced set of k-1 active estimation vectors is as follows. According to the foregoing remarks no generality will be lost if we assume that the vector to be eliminated is z_k. But recall that to add z_k to the active set, $z_1, \ldots, z_{k-1}$, and to obtain the regression analysis for the augmented set it was only necessary to perform on the (k-1)-st tableau those elementary row transformations which reduce the kth column to the unit vector u_k. Therefore, to eliminate z_k it is only necessary to undo these calculations. It is not hard to verify that the reversing calculations are those elementary row transformations (on the kth tableau) which reduce the kth column of the inverse $a^{(k)}$ back to u_k.

It is of course only a notational convenience to assume that the estimation vectors activated are the first k of the p listed in the tableaux. The swapping of rows and columns, while tidying up the written portrayal of the tableaux, etc., is completely unnecessary for computer handling of the problem.

Finally we shall mention that the rule described above for deciding which vector to eliminate is equivalent to that of eliminating the active vector that has the smallest _partial correlation_ with the dependent variable vector. The partial correlation coefficient between z_k (say) and y is the cosine of the angle between $e^{(k-1)}$ and $\hat{y}^{(k)} - \hat{y}^{(k-1)}$.

From the sketch below it is clear that this correlation decreases as the length $||\hat{y}^{(k)} - \hat{y}^{(k-1)}|| = |b_k^*|$ decreases:
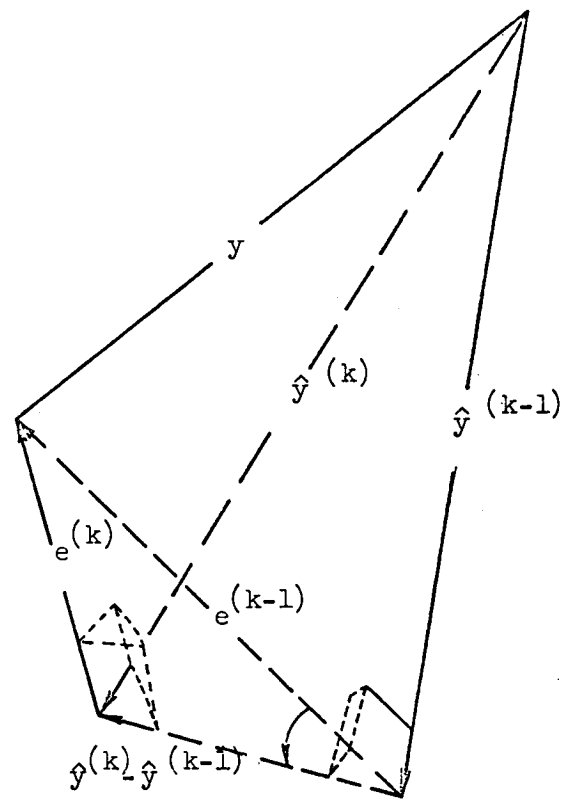
From the definition of cosine between $e^{(k)}$ and $\hat{y}^{(k)} - \hat{y}^{(k-1)}$ it is easy to show that

$$\cos^2 \theta(e^{(k-1)}, \hat{y}^{(k)} - \hat{y}^{(k-1)}) = \frac{b_k^{*2}}{(e^{(k-1)} \cdot e^{(k-1)})} = G^{(k-1)}b_k^{*2} = \frac{G^{(k-1)}b_k^{(k)2}}{a_{kk}^{(k)}}$$

5. Decision rules: the statistical model. In the last section the question answered was which active estimation variable ought to be eliminated once the decision had been made to eliminate one. The question of constructing decision rules to tell when to eliminate a variable was left for this section. Defining a sweep or iteration as a step in which either an inactive estimation vector is activated or an active one is deactivated, an obvious type of decision rule is the following: Activate two vectors according to the step-up procedure, then eliminate one by the method described in the preceding section, and continue operating under this rule until some stopping rule (see below) stops the entire procedure. It is conceivable that such a rule would have utility if it is important in the ultimate application to have no more than k vectors while the cost of the extra sweeps is relatively unimportant.

Of course if of k active estimation vectors one has a partial correlation with the dependent variable vector of practically zero, it would seem wise to eliminate it. This suggests another quite arbitrary type of elimination rule: Of the k currently active estimation vectors eliminate the one of lowest partial correlation with y if said partial correlation is less than some level $\propto(k)$, possibly a function of k.

Another decision problem must be dealt with, viz. that of constructing a stopping rule to stop the step-up procedure (with or without modification to allow for deletions). Here again, certain obvious but rather arbitrary rules come to mind. E.g., stop when k vectors have been activated (actually this was the somewhat naïve rule used to motivate the section on the step-up procedure). It seems clear that, by itself, this is not a good rule, since in a particular example a satisfactory estimate may be attainable with far fewer than k vectors

(i.e., the multiple correlation coefficient may be already very near one with fewer vectors or simply may not be improved "significantly" to warrant the inclusion of more).

We take the position at the present time of recommending a fairly comprehensive battery of stopping rules, any combination of which might be used, with a variety of sensitivity settings possible. Intuition suggests that appropriate settings will vary with the type of problem, the usage requirements and the burden of cost in time and money. Perhaps a battery of stopping rules should at least make provision for stopping when a fixed number of estimation vectors have been activated, when the estimate is of sufficiently high accuracy (multiple correlation sufficiently near one), when the number of sweeps exceeds a certain number (this acts as a safeguard against a cyclic pattern of activation and elimination of vectors), and when the last r (say) vectors activated have not produced a "significant" change in the estimate.

Again the word, "significant", requires specific interpretation before the rule can be operational. One modus operandi might be: Stop the procedure if the increase in the multiple correlation coefficient R, produced by adding the last r active estimation vectors, was less than $\beta(r,k)$.

Both in the question of whether to deactivate an active estimation vector and in the question of when to stop activating estimation vectors the notion of significant effect arises. This suggests the possibility of resorting to a statistical model where the techniques of testing hypotheses might be invoked as a basis for decisions on whether to eliminate a variable or whether to stop the activation process.

In the remainder of this section we shall sketch the outline of a statistical model perhaps sufficiently to indicate the attractiveness of such a decision mechanism as well as to indicate some of the limitations of such a model.

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Very briefly the model develops a <u>statistic</u>, or function of the observed active estimation vectors and the dependent variable vector, called an F statistic which is the decision-making instrument--large F means significance of the effects being tested and small F means nonsignificance. Under the hypothesis of the statistical model, and under the additional hypothesis that the effects of the estimation vectors being tested are only "noise" effects or effects introduced by virtue of random fluctuations, the F statistic is expected to have a value of about unity.

Actually, the F statistic is a ratio of the average of the effects of the vectors being tested to the average of some random error effects. In the terminology developed in previous sections suppose that $z_{k-r+1},\ldots,z_k$ are active estimation vectors whose combined effect is being tested. Recall that $\hat{y}^{(k)}$ is the projection of y on the space spanned by $z_1,\ldots,z_k$; and that $\hat{y}^{(k-r)}$ is the projection of $\hat{y}^{(k)}$ as well as the projection of y onto the subspace spanned by $z_1,\ldots,z_{k-r}$.
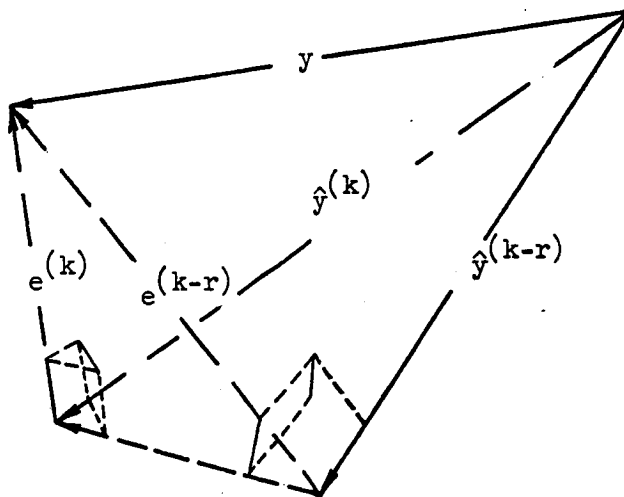
In the F ratio the average of the effects of the r vectors $z_{k-r+1}, \ldots, z_k$ is measured as $\frac{1}{r}$ times the square of the length of the vector, $\hat{y}^{(k)} - \hat{y}^{(k-r)}$; while the average of error components is measured as $\frac{1}{N-k}$ times the square of the so-called error vector, $e^{(k)}$ (recall that $e^{(k)}$ lies in a space of N-k dimensions orthogonal to the space generated by $z_1, \ldots, z_k$ in which $\hat{y}^{(k)} - \hat{y}^{(k-r)}$ lies). Obviously, values of the F statistic less than one would not tend to support significant effects of $z_{k-r+1}, \ldots, z_k$, while values greater than one presumably would. With the normal law of errors assumed in the statistical model and under the hypothesis that these supposed effects of the last r vectors are noise effects, it turns out that the chances are approximately even that F should exceed the <u>critical</u> <u>value</u> of unity. If the critical value is increased the probability that the F statistic will exceed it diminishes rapidly. These probabilities are tabulated for various critical values and various <u>degrees</u> <u>of</u> <u>freedom</u> (r and N-k in our case). One may establish a decision rule to reject the hypothesis of no systematic effect (from the estimation vectors being tested) if the value of the F statistic observed is improbably larger than one.

The decision rule is not complete until specific numbers or functions are attached to the words "improbably larger." Undoubtedly a judicious choice depends on several factors involved in the balancing of cost and return in a particular problem. This is one of the open questions we have tried to study experimentally in another supporting study.

To complete the exposition some description of the characteristics of the assumed statistical model is warranted, although as we have mentioned there are recent excellent accounts of this model.

In the statistical linear regression model it is assumed that, except for random variations, Y is a linear function of the Z_i. Thus

$$y_u = \sum_{i=1}^{p} \beta_i z_{\mu i} + \varepsilon_\mu, \quad \mu = 1, 2, \ldots, N,$$

where ε_μ are random errors. In addition it is usually assumed that the ε_μ are uncorrelated with a common variance σ^2 and a mean of zero. The β_i are parameters which may be estimated in an optimal way under the circumstances. In fact, the <u>best</u> <u>linear</u> <u>unbiased</u> <u>estimate</u> of a linear combination of the β_i, say $\eta = \sum_{i=1}^{p} \beta_i Z_i$, best in the sense of smallest variance, is $\hat{Y} = \sum b_i Z_i$, where the b_i are precisely those which produce the least squares estimate. This is the Gauss-Markov theorem. It implies that, if the true functional relationship is except for a random error $Y = \eta = \sum \beta_i Z_i$, then, faced with not knowing the exact values of the β_i, the next best thing is to use the estimation function $Y = \hat{Y} = \sum b_i Z_i$.

To see the truth of this theorem we shall need to use the <u>expected value</u> or <u>mean value operator</u> E operating on a random variable or vector or matrix, with the expected value of a matrix of random variables being the matrix of expected values. From this definition it follows directly that $E A X B = A(EX)B$, if X is a random matrix and A and B are nonrandom matrices.

Now under the statistical model above, $y = z\beta + \varepsilon$, where $y^T = (y_1, \ldots, y_N)$, $z = (z_1, \ldots, z_p)$, $z_i^T = (z_{1i}, \ldots, z_{Ni})$, $\beta^T = (\beta_1, \ldots, \beta_p)$, $\varepsilon^T = (\varepsilon_1, \ldots, \varepsilon_N)$, with ε (and hence y) being random vectors. According to the assumptions, $E\varepsilon = 0$ so that $Ey = z\beta$; and the ε_μ are uncorrelated with a common variance σ^2, so that $E\varepsilon\varepsilon^T = \sigma^2 I$, I being an identity matrix. Note that the z_i vectors are nonrandom.

First we show that $Eb = \beta$, i.e., that the b_i are <u>unbiased</u> estimates of the corresponding β_i. In fact

$$Eb = Eh^{-1}g = h^{-1}Eg = h^{-1}Ez^Ty = h^{-1}z^TEy =$$
$$h^{-1}z^Tz\beta = h^{-1}h\beta = I\beta = \beta.$$

Next we exhibit the covariance matrix of the estimates b:

$$E(b - Eb)(b - Eb)^T = E(b - \beta)(b - \beta)^T =$$
$$E(h^{-1}g - Eh^{-1}g)(h^{-1}g - Eh^{-1}g)^T =$$
$$h^{-1}E(g - Eg)(g - Eg)^T h^{-1},$$

since h and h^{-1} are symmetric. Now

$$E(g - Eg)(g - Eg)^T = E(z^Ty - Ez^Ty)(z^Ty - Ez^Ty)^T =$$
$$z^T E(y - Ey)(y - Ey)^T z = z^T E\varepsilon\varepsilon^T z = z^T \sigma^2 I z = \sigma^2 h.$$

Hence, substituting above,

$$E(b - Eb)(b - Eb)^T = h^{-1}\sigma^2 h h^{-1} = h^{-1}\sigma^2.$$

Now consider $\hat{Y} = \Sigma b_i Z_i = z^T b$ as an estimate of $\eta = \Sigma \beta_i Z_i = Z^T\beta$. Observe that

$$\hat{Y} = Z^T b = (Z^T h^{-1} z^T) y = a^T y,$$

where $a^T = Z^T h^{-1} z^T$. This is what is meant by saying that $\hat{Y}$ is a linear estimate of η; i.e. it is a linear combination of the observed values of the random dependent variable Y.

Also $E\hat{Y} = E Z^T b = Z^T Eb = Z^T\beta = \eta$. Hence $\hat{Y}$ is an unbiased estimate of η.

Finally we must show that the variance of $\hat{Y}$ is less than that of any other linear unbiased estimate of η. Suppose $\tilde{Y}$ to be another linear unbiased estimate of η, so that $\tilde{Y} = c_1 y_1 + \dots + c_N y_N = c^T y$, and $E c^T y = \eta$.

Now consider vectors in euclidean N-space. Note that $a = z(h^{-1}Z)$, a vector lying in the estimation space spanned by the vectors $z_1, \dots, z_p$. We shall see that the vector a is the projection of c onto the space spanned by $z_1, \dots, z_p$.

Since $Ea^Ty = Ec^Ty$, then $0 = E(c-a)^Ty = (c-e)^TEy = (c-a)^Tz\beta$. This identity can hold only if $(c-a)^Tz = 0$. But this implies that

$$(c - a)^Ta = (c - a)^Tz(h^{-1}z) = 0.$$

Hence a and c-a are orthogonal, and the pythagorean relation, $c^2 = a^2 + (c-a)^2$, holds.

The variance of $\tilde{Y}$ is

$$E(\tilde{Y} - E\tilde{Y})^2 = E(\tilde{Y} - E\tilde{Y})\ (\tilde{Y} - E\tilde{Y})^T$$

$$= E(c^Ty - Ec^Ty)\ (c^Ty - Ec^Ty)^T$$

$$= c^TE(y - Ey)\ (y - Ey)^Tc = c^TE\varepsilon\varepsilon^Tc$$

$$= \sigma^2c^Tc = \sigma^2\{a^Ta + (c - a)^T\ (c - a)\} > \sigma^2a^Ta.$$

But of course by the same reasoning the variance of $\hat{Y}$ is σ^2a^Ta. This shows that $\hat{Y}$ is of minimum variance.

To arrive at the F-statistic test for our decision rule in eliminating an estimation vector, or in stopping the activation of estimation vectors, additional assumptions are needed. Suppose that k of the estimation vectors, $z_1, \ldots, z_k$ has been activated, and it happens that $Y = \sum\limits_{i=1}^{k} \beta_i Z_i + \varepsilon$, in short that the statistical model is valid with these k variables, so that
$y_\mu = \sum\limits_{i=1}^{k} \beta_i z_{\mu i} + \varepsilon_\mu$ or $y = z^{(k)} \beta^{(k)} + \varepsilon$, when $\varepsilon^T = (\varepsilon_1, \ldots, \varepsilon_N)$.

Suppose, in addition to the conditions that $E\varepsilon = 0$ and $E\varepsilon\varepsilon^T = \sigma^2I$, we require that the ε_μ be normally distributed. Now suppose we wish to test the hypothesis (H_o) that the last r parameters $\beta_{k-r+1}, \ldots, \beta_k$ are in fact all zero. (Accepting this hypothesis implies that the activation of the last r estimation variables adds nothing to the estimate available with the first k-r variables.)

The basic idea of such a test is to divide the <u>sample space</u>, i.e. the space of possible values of the vector y, into a <u>rejection region</u> R and its complement, an <u>acceptance region</u>, the ultimate decision rule being to reject H_o in case the observed value of y falls in R. Naturally, in order to make the test a discriminating or <u>powerful</u> one the points in the rejection region ought to be chosen roughly so as to maximize the probability of rejection when H_o is not true, while at the same time the probability of rejection when H_o is true should be kept below a certain bound. Such a test is approximately obtained by putting in R those points with highest "trade-off ratio," this ratio being essentially the ratio of the maximum of the probability density functions (pdf) over the entire family of pdf's defined by the admissible values of the parameters, to the maximum of the pdf's over the subfamily where the hypothesis H_o holds. This ratio is called the <u>likelihood ratio</u> λ. Such points of highest likelihood ratio are placed in R until the set is as large as it can be and still have the desired bound or the probability of rejection when H_o is true.

The optimal character of the likelihood ratio test for the problem at hand is given excellent treatment in SCHEFFÉ.

Let Ω stand for the <u>parameter space</u> of admissible values of the parameters. In our case

$$\Omega = \{\beta^{(k)}, \sigma^2 \mid -\infty < \beta^{(k)} < \infty, \sigma^2 > 0\}.$$

Let ω stand for the subset of Ω where H_o is true; i.e.

$$\omega = \{\beta^{(k)}, \sigma^2 \mid -\infty < \beta^{(k-r)} < \infty, \beta_{k-r+1} = \ldots = \beta_k = 0, \sigma^2 > 0\}.$$

According to the hypothesis of the model the ε_μ are normally distributed, uncorrelated (and hence independent) with common variance, σ^2. Thus the joint pdf of the random vector y is (for a parameter point in Ω)

$$f(y; \beta^{(k)}, \sigma^2) = \prod_{n=1}^{N} (2\pi\sigma^2)^{-\frac{1}{2}} \exp\left\{ -\frac{1}{2\sigma^2} (y_\mu - \sum_{i=1}^{k} \beta_i z_{\mu i})^2 \right\}$$

$$= (2\pi\sigma^2)^{-N/2} \exp\left\{ -\frac{1}{2\sigma^2} (y - z^{(k)}\beta^{(k)})^T (y - z^{(k)}\beta^{(k)}) \right\}.$$

Now to determine R it is necessary to maximize f over Ω and over ω, form the ratio λ, and select values of y for which this is highest.

$$R = \left\{ y \mid \lambda(y) = \frac{\sup_\Omega f}{\sup_\omega f} \geq \lambda_\alpha \right\} ,$$

where λ_α is a critical value chosen so that

$$Pr\{y \varepsilon R \mid H_o \text{ is true }\} \leq \alpha;$$

here α is called the __significance__ or __rejection level__ of the test.

We recall now that a sum of squares of m normal independent random variables with mean zero and variance one (N(0,1)) is said to be a __Chi-square variable with m degrees of freedom__. The ratio of the average of two such sums of squares of independent N(0,1) variables, with m_1 terms in the numerator and m_2 in the denominator, is called an __F variable with m_1 and m_2 degrees of freedom__. The probability distribution of the F variable is widely tabulated. The following result is the one pertinent to our problem. For a statistical linear regression model, where the errors are $N(0,\sigma^2)$ independently distributed, the rejection region R of significance level α, provided by the likelihood ratio criterion for rejecting H_o as described above, is given by

$$R = \left\{ y \ \left| \ \frac{(\hat{y}^{(k)} - \hat{y}^{(k-r)})^2)/r}{e^{(k)^2}/(N-k)} \geq F^{(\alpha)}_{r,N-k} \right\} \right.,$$

where $F^{(\alpha)}_{r,N-k}$ is the critical value in the $F_{r,N-k}$ distribution for which $\Pr\left\{F_{r,N-k} \geq F^{(\alpha)}_{r,N-k}\right\} = \alpha$.

The proof of this important theorem, is obtained by constructing the likelihood ratio λ, in which the maximization problems are observed to be essentially the least squares problem, then reducing the inequality $\lambda(y) \geq \lambda_\alpha$ which defines the rejection set to the form given in the conclusion. Used in the proof are: The orthogonal transform of y based on the Gram-Schmidt vectors $z'_1, \ldots, z'_{k-r}, z'_{k-r+1}, \ldots, z'_k$ and the fact that orthogonal transforms of normal vectors are normal. Although the proof is available in numerous references, we sketch it here.

<u>Lemma 1.</u> Let y be a vector of $N(m_\mu, \sigma^2)$, independent, random variables, and let $y' = Py$ be an orthogonal transform of y. Then y' is a vector of $N(m'_\mu, \sigma^2)$, independent, random variables, with $m'_\mu = \sum_{\nu=1}^{N} p_{\mu\nu} m_\nu$, where $P = (p_{\mu\nu})$. Proof: Write $m^T = (m_1, \ldots, m_N)$, and let $G(\xi')$ be the distribution function of y'. Then

$$G(\xi') = \Pr[y' \leq \xi'] = \Pr[Py \leq \xi'] = \Pr[\{y | Py \leq \xi'\}]$$

$$= \int_{\{y | Py \leq \xi'\}} (2\pi\sigma^2)^{-N/2} \exp\left\{-\frac{1}{2\sigma^2}(y-m)^T(y-m)\right\}.$$

Now, making the transformation $y' = Py$ in the integal, the Jacobian of the transformation is the determinant of the orthogonal matrix P, hence in absolute value is one; the domain of integration is transformed into $\{y' | y' \leq \xi'\}$; and the integrand becomes $(2\pi\sigma^2)^{-N/2} \exp-\left\{\frac{1}{2\sigma^2}(y'-Pm)^T(y'-Pm)\right\}$.

Hence

$$G(\xi') = \prod_{\mu=1}^{N} \int_{-\infty}^{\xi'_\mu} (2\pi\sigma^2)^{-1/2} \exp\left\{-\frac{1}{2\sigma^2}(y'_\mu - m'_\mu)^2\right\} dy'_\mu \ ,$$

so that obviously the y'_μ are $N(m',\sigma^2)$, independent.

It is a corollary of <u>lemma 1</u> that, if ε is a vector of $N(0,\sigma^2)$, independent variables and $\varepsilon' = P\varepsilon$, P orthogonal, then ε' is a vector of $N(0,\sigma^2)$ independent variables.

<u>Lemma 2.</u> Let $y = z^{(k)}\beta^{(k)} + \varepsilon$ be a statistical linear regression model. Let $z*^{(k)}$ be the matrix of orthonormal vectors generated from $z_1,\ldots,z_k$ by the Gram-Schmidt process, so that $z*^{(k)} = z^{(k)}Q^{(k)}$ where $Q^{(k)}$ is upper triangular. Let $\beta*^{(k)} = Q^{(k)^{-1}}\beta^{(k)}$. Then $\beta_{k-r+1} = \ldots = \beta_k = 0$ if and only if $\beta*_{k-r+1} = \ldots = \beta*_k = 0.$

Proof: Suppose $\beta_{k-r+1} = \ldots = \beta_k = 0$; it follows from the equation $\beta*^{(k)} = Q^{(k)-1}\beta$ and the fact that $Q^{(k)^{-1}}$ is upper triangular that $\beta*_k = 0$, then $\beta*_{k-1} = 0$, etc., until $\beta*_{k-r+1} = 0$. The converse argument is the same.

<u>Proof of the main theorem:</u> By Lemma 2

$$\omega = \{\beta^{(k)}, \sigma^2 \,|\, -\infty < \beta*^{(k-r)} < \infty, \ \beta*_{k-r+1} = \ldots = \beta*_k = 0, \ \sigma^2 > 0\},$$

and of course, since $y = z^{(k)}\beta^{(k)} + \varepsilon$ and $z*^{(k)}\beta*^{(k)} = z^{(k)}Q^{(k)}Q^{(k)-1}\beta^{(k)} = z^{(k)}\beta^{(k)}$, then $y = z*^{(k)}\beta*^{(k)} + \varepsilon.$

Now

$$\lambda(y) = \frac{\sup\{f(y;\beta^{(k)},\sigma^2)\,|\,(\beta^{(k)}, \sigma^2)\varepsilon\Omega\}}{\sup\{f(y;\beta^{(k)},\sigma^2)\,|\,(\beta^{(k)}, \sigma^2)\varepsilon\omega\}}$$

where $f = (2\pi\sigma^2)^{-N/2} \exp\left\{-\frac{1}{2\sigma^2}\varepsilon^T\varepsilon\right\},$

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with $\varepsilon = y - z*^{(k)}\beta*^{(k)}$. Clearly the extremizations in both cases can be obtained by first minimizing $\varepsilon^T\varepsilon$ with respect to the β_i^*, substituting these back in, and maximizing the resulting expressions with respect to σ^2.

But minimizing $\varepsilon^T\varepsilon$ is precisely the LS problem encountered before. Using (as before) the orthogonal transform, $y' = Py$ and $\varepsilon' = P\varepsilon$ where the first k rows of P are $z*^{(k)T}$,

$$\varepsilon^T\varepsilon = \varepsilon'^T\varepsilon' = (y_1' - \beta_1^*)^2 + \ldots + (y_k' - \beta_k^*)^2 + \sum_{\mu=k+1}^{N} y_\mu'^2.$$

Obviously $\varepsilon^T\varepsilon$ over Ω is minimized when $\beta_i^* = y_i'$, $i = 1,\ldots,k$ with the value of $\varepsilon^T\varepsilon$ reducing to $\sum_{\mu=k+1}^{N} y_\mu'^2 = e^{(k)2}$; while $\varepsilon^T\varepsilon$ is minimized on ω when $\beta_i^* = y_i'$, $i = 1,\ldots,k-r$ (recall that $\beta_{k-r+1}^* = \ldots = \beta_k^* = 0$ in this case), with the value of $\varepsilon^T\varepsilon$ reducing to

$$\sum_{\mu=k-r+1}^{N} y_\mu'^2 = (\hat{y}^{(k)} - \hat{y}^{(k-r)})^2 + e^{(k)2}$$

in this case.

Substituting these extreme values back in and maximizing the numerator and denominator with respect to σ^2, gives for the numerator $\hat{\hat{\sigma}}^2 = \dfrac{e^{(k)2}}{N}$ and for the denominator $\hat{\sigma}^2 = \dfrac{\hat{y}^{(k)} - \hat{y}^{(k-r)})^2 + e^{(k)2}}{N}$.

Replacing these in the expression for $\lambda(y)$ we get

$$\lambda(y) = \left[\frac{\hat{\hat{\sigma}}^2}{\hat{\sigma}^2}\right]^{N/2} = \left[1 + \frac{(\hat{y}^{(k)} - \hat{y}^{(k-r)})^2}{e^{(k)2}}\right]^{N/2}.$$

Now

$$R = \{y| \lambda(y) \geq \lambda_\alpha\} = \{y| \left[1 + \frac{\hat{y}^{(k)} - \hat{y}^{(k-r)})^2}{e^{(k)2}}\right]^{N/2} \geq \lambda_\alpha\}$$

$$= \{y| \frac{(\hat{y}^{(k)} - \hat{y}^{(k-r)})^2/r}{e^{(k)2}/(N-k)} \geq \frac{(\lambda_\alpha^{2/N} - 1)(N - k)}{r}\}.$$

Finally, since $(\hat{y}^{(k)} - \hat{y}^{(k-r)})^2 = \sum\limits_{i=k-r+1}^{k} y_i'^2$ and $e^{(k)^2} = \sum\limits_{\mu=k+1}^{N} y_\mu'^2$, since

by Lemma 1 $y' = Py$, a vector of normal independent variables with common variance σ^2, and since under the hypothesis H_o $Ey_i' = 0$ $(i = k-r+1,\ldots,k)$, then the ratio

$$\frac{(\hat{y}^{(k)} - \hat{y}^{(k-r)})^2/r}{e^{(k)^2}/(N-k)} = \frac{\sum\limits_{i=k-r+1}^{k} (y_i'/\sigma)^2/r}{\sum\limits_{\mu=k+1}^{N} (y_\mu'/\sigma)^2/(N-k)}$$

is a ratio of averages of sums of squares of $N(0,1)$ independent random variables when H_o is true. That is, the likelihood ratio is equivalent to an F statistic when H_o is true.

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SELECTION OF SIGNIFICANT ESTIMATION VARIABLES
IN A LEAST SQUARES PROBLEM: EMPIRICAL COMPUTER STUDIES

The object of these studies was to investigate the usefulness of the step-up procedure or modifications of it, in choosing a subset of a large number of estimation variables which is good in a least squares sense. In the first phase of these studies we wished to compare the step-up procedure with the procedure of finding the best subset at each stage. Because of the large number of matrix inversions required in the last method we could handle only a very small number of terms.

The results of the first phase are summarized in the two examples which follow. In the first run we note that the step-up procedure gave two terms with $R^2 = 0.724$ whereas the best two terms give $R^2 = 0.886$.

Phase One - Run 1

In this run the dependent variable was

$$F(X_1, X_2, X_3) = 3/(1+X_1^2+2X_3) \ .$$

The polynomial model was a balanced polynomial linear in $X_1, X_2,$ and X_3, i.e., $a_1X_1+a_2X_2+a_3X_3+a_4X_1X_2+a_5X_1X_3+a_6X_2X_3+a_7X_1X_2X_3$. The 125 data points were in a rectangular design with $X_1 = .25(.25) \ 1.25$, $X_2 = .25(.25) \ 1.25$, and $X_3 = .25(.25) \ 1.25$. As will be noted in this run the function F is actually independent of X_2 and hence the estimation variables Z_2, Z_4, Z_6, Z_7 should not enter the regression equation.

Step-up Procedure		Optimum Set	
Estimation Variables	R^2	Estimation Variables	R^2
5	.569815	5	.569815
5,3	.724129	3,1	.885715
5,3,1	.957606	3,1,5	.957605
5,3,1,2	.957615	3,2,1,5	.957615
5,3,1,2,4	.957631	3,2,1,5,4	.957631
5,3,1,2,4,6	.957632	3,2,6,1,5,4	.957632
5,3,1,2,4,6,7	.957634	3,2,6,1,5,4,7	.957634

Note that the step-up procedure did not select the optimum subset of two variables.

Phase One - Run 2

In this run the dependent variable and the polynomial model were the same as in Run 1. The 500 data points were in a rectangular design with $X_1 = .25(.25)2.50$, $X_2 = .25(.25) 2.50$, and $X_3 = .25(.25) 1.25$.

Step-up Procedure		Optimal Set	
Estimation Variables	R^2	Estimation Variables	R^2
1	.702925	1	.702925
1,3	.884762	3,1	.884762
1,3,5	.963786	3,1,5	.963786
1,3,5,2	.963789	3,2,1,5	.963789
1,3,5,2,6	.963791	3,2,6,1,5	.963790
1,3,5,2,6,4	.963791	3,2,6,1,5,4	.963791
1,3,5,2,6,4,7	.963791	3,2,6,1,5,4,7	.963791

In this case, the step-up procedure gave the optimal subset in each case.

Conclusions from Phase One

These runs indicated that some modification (e.g., a throw-out rule)

might be helpful in obtaining a regression equation which would be close to the optimal. To investigate every possible regression equation even from a small set of terms is so time consuming that we did not use any example with a large number of terms in this phase.

Phase Two

In this phase we used examples with a large number of terms. We used various throw-out criteria to investigate the relative merits of each. We did not find the optimal subsets.

Summary of Phase Two

In the first 12 runs in this phase we used a balanced polynomial model to approximate the dependent variables

$$F_1(X_1,X_2,X_3) = (X_1^4+X_2^3+X_3^2)|X_1+X_2-\frac{\pi}{2}X_3|^{-\frac{1}{2}}$$

$$F_2(X_1,X_2,X_3) = \exp(-X_1^2X_2X_3)$$

$$F_3(X_1,X_2,X_3) = \sqrt{(X_1^2+X_2^2+X_3^2)}.$$

The results of these runs are tabulated below.

In the case of $F_3 = \sqrt{X_1^2+X_2^2+X_3^2}$, the 47-term polynomial fits very well with $R^2 = 0.999972$. In fact the 4 terms X_1X_2, X_2X_3, X_1^2, X_2^2 give a fit with $R^2 = 0.962$. The first 7 terms obtained by the stepwise procedure are X_1X_2, X_2X_3, X_1^2, X_2^2, $X_2^2X_3$, X_1, X_3^2, and have $R^2 = 0.992$. With a throw-out criterion $\geq$ 1.44, however, we find that X_1X_2, X_1^2, X_2^2, $X_2^2X_3$, X_1, X_3, X_2^2 fit with $R^2 = 0.996$.

Now for the case $F_2 = \exp(-X_1^2X_2X_3)$ we found that the 47-term polynomial fit with $R^2 = 0.996$. The first seven terms obtained by the step-up procedure were X_1, X_2X_3, X_1^2, X_2^2, X_3^2, $X_1^3X_2^2X_3^2$, $X_1X_2X_3$, and $X_1^2X_2X_3$ with $R^2 = 0.949$. With a throw out criterion ≥ 0.8 we find that the seven terms X_2X_3, X_1^2, $X_2^2X_3^2$, $X_1^3X_2^2X_3^2$, $X_1X_2X_3$, $X_1^2X_2X_3$, and $X_1X_2^2X_3^2$ is a better seven and fit with $R^2 = 0.965$.

With a throw-out criterion ≥ 4.9 we find that the seven terms X_1, X_2X_3, $X_1^2X_3^2$, $X_1X_2X_3$, $X_1^2X_2X_3$, $X_1X_2^2X_3^2$, $X_1^3X_2^3X_3^2$ fit with $R^2 = 0.962$ and that the seven terms X_1, $X_1X_2X_3$, $X_1^2X_2X_3$, $X_1X_2^2X_3^2$, $X_1^3X_2^3X_3^2$, $X_1^2X_2^2X_3$, and $X_1^2X_2$ fit with $R^2 = 0.978$. We also find in fact that the first five terms in the last fit have $R^2 = 0.962$. Thus the five terms x_1, $X_1X_2X_3$, $X_1^2X_2X_3$, $X_1X_2^2X_3^2$, and $X_1^3X_2^3X_3^2$ fit better than the seven terms given by the step-up procedure with no throw-out criterion.

In case $F_1 = \dfrac{X_1^4 + X_2^3 + X_3^2}{\sqrt{\left| X_1 + X_2 - \frac{\pi}{2}X_3 \right|}}$ where the denominator has zeros in the region of fitting we find that the fit is not quite as good. The 47-term polynomial gives $R^2 = 0.938$. Again, however, we find that a seven-term polynomial will do almost as well. The straight step-up procedure gives the seven terms $X_1^3X_3$, X_1^3, X_3^2, X_2^3, $X_1^2X_2X_3$, $X_1^3X_2^2X_3$, and X_2X_3 which fit with $R^2 = 0.894$. With a throw-out criterion ≥ 6.3 we find that the seven terms X_1^3, X_2^3, $X_1^2X_3^2$, $X_1X_2X_3^2$, $X_2X_3^2$, $X_1X_2^2X_3^2$, and $X_2^3X_3^2$ fit with $R^2 = 0.902$.

This example also gave rise to the situation where, while $X_1^3X_3$ is the best single term, it is not one of the best two terms. The best two terms involving $X_1^3X_3$ are $X_1^3X_3$ and X_1^3 which fit with $R^2 = 0.733$. However, the two terms X_1^3 and X_3^2 fit with $R^2 = 0.775$. Another situation which occurred on this example was that with a throw-out criterion of ≥ 4.9 we would arrive at a five-term polynomial with $R^2 = 0.876$ whereas the step-up procedure with no throw-out criterion leads to a five-term polynomial with $R^2 = 0.884$. Hence, having a throw-out criterion is not always better.

As an example of a non-balanced design with an arbitrary linear model we used a correlation matrix given in Anderson and Fruchter, "Prediction Selection Method," _Psychometrika_, Vol. 25, No. 1. The results are tabulated in Run 17. Here we found that the throw-out criterion was not used, and so

the variables were selected by the step-up procedure without this option. The overall fit using 14 variables gave $R^2 = 0.270$ and an $F(14,295) = 7.8$ which is significant at 0.005. However, an F test of the hypothesis that the last 9 variables have zero coefficients is not significant at even the 50% level. The R^2 for the first five terms of the step-up procedure is $R^2 = 0.259$.

Phase Two - Run 1

In this run, the dependent variable was $F(X_1, X_2, X_3) = (X_1^4 + X_2^3 + X_3^2) | X_1 + X_2 - \frac{\pi}{2} X_3 |^{-\frac{1}{2}}$. To fit this expression we used the polynomial model

$$\sum_{\ell_1 = 0}^{3} \sum_{\ell_2 = 0}^{3} \sum_{\ell_3 = 0}^{2} a_{\ell_1 \ell_2 \ell_3} X_1^{\ell_1} X_2^{\ell_2} X_3^{\ell_3} .$$

All the terms, including the dependent variable are first adjusted for their means. Thus we wish to find subsets of the 47 terms in this polynomial which give the best approximation to the dependent variable. The values of $F(X_1, X_2, X_3)$ and $X_1^{\ell_1} X_2^{\ell_2} X_3^{\ell_3}$ were all calculated at 500 points in a balanced design. In this run we used the points $X_1 = .25(.25) 2.50$, $X_2 = .25(.25) 2.50$, and $X_3 = .25(.25) 1.25$.

The throw-out criterion for this run was $F_0 = 1.5$. A tabulation of the terms as they were brought in follows. (Reduced R^2 is $1 - \frac{N-1}{N-m} (1-R^2)$ where R^2 is the square of the multiple correlation coefficient and N = 500, the number of observations, and m is the number of terms in the model.)

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	37	$X_1^3 X_3$	1058		.680	.680
2	2	36	X_1^3	98.96		.733	.733
3	3	2	X_3^2	99.34		.778	.777
4	4	9	X_2^3	103.15		.816	.815
5	5	28	$X_1^2 X_2 X_3$	292.59		.88447	.884

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
6	6	43	$X_1^3 X_2^2 X_3$	25.37		.890	.839
7	7	4	$X_2 X_3$	19.01		.894	.893
8	8	14	$X_1 X_3^2$	26.76		.900	.898
9	9	16	$X_1 X_2 X_3$	15.58		.903	.901
10	8	2	X_3^2		0.21	.903	.901
11	9	17	$X_1 X_2 X_3^2$	8.34		.904	.903
12	10	19	$X_1 X_2^2 X_3$	10.78		.906	.905
13	9	43	$X_1^3 X_2^2 X_3$		0.11	.906	.905
14	8	37	$X_1^3 X_3$		1.47	.906	.905
15	9	1	X_3	12.94		.909	.907
16	10	10	$X_2^3 X_3$	11.01		.911	.909
17	11	45	$X_1^3 X_2^3$	15.92		.913	.912
18	12	5	$X_2 X_3^2$	14.62		.916	.914
19	13	38	$X_1^3 X_3^2$	6.96		.917	.915
20	14	2	X_3^2	6.66		.918	.916
21	13	1	X_3		0.15	.918	.916
22	14	40	$X_1^3 X_2 X_3$	6.69		.919	.917
23	13	28	$X_1^2 X_2 X_3$		0.04	.919	.917
24	14	43	$X_1^3 X_2^2 X_3$	3.23		.920	.918
25	15	44	$X_1^3 X_2^2 X_3^2$	2.84		.920	.918
26	16	12	X_1	3.93		.921	.918
27	17	11	$X_2^3 X_3^2$	3.27		.921	.919
28	16	4	$X_2 X_3$		0.02	.921	.919
29	17	21	$X_1 X_2^3$	1.62		.922	.919

Run 2

In this run the dependent variable, the polynomial model and the data points were all the same as in Run 1. The throw-out criterion was $F_0 = 0.9$. This run should tend to throw out terms less often than Run 1. This should lead to fewer sweeps to reach k terms but perhaps the fit for these terms will not be as good as in Run 1. The tabulation through Sweep 13 is the identical with Run 1.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
13	9	43	$x_1^3 x_2^2 x_3$		0.11	.906	.905
14	10	1	x_3	11.46		.909	.907
15	9	37	$x_1^3 x_3$		0.05	.909	.907
16	10	10	$x_2^3 x_3$	11.01		.911	.909

Sweeps 16 through 29 are the same as Run 1

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
29	17	21	$x_1 x_2^3$	1.62		.922	.919
30	16	45	$x_1^3 x_2^3$		0.03	.922	.919
31	17	26	$x_1^2 x_3^2$	1.34		.922	.919
32	18	24	x_1^2	3.09		.922	.920
33	19	13	$x_1 x_2$	1.20		.923	.920
34	20	18	$x_1 x_2^2$	2.86		.923	.920
35	19	21	$x_1 x_2^3$		0.00	.923	.920
36	20	1	x_3	1.01		.923	.920
37	19	11	$x_2^3 x_3^2$		0.59	.923	.920
38	20	37	$x_1^3 x_3$	1.42		.923	.920
39	21	47	$x_1^3 x_2^3 x_3^2$	1.53		.924	.920

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
40	22	45	$X_1^3 X_2^3$	2.13		.924	.921
41	23	7	$X_2^2 X_3$	1.94		.924	.921
42	22	16	$X_1 X_2 X_3$		0.31	.924	.921
43	23	23	$X_1 X_2^3 X_3^2$	1.10		.924	.921
44	24	11	$X_2^3 X_3^2$	1.22		.925	.921
45	25	25	$X_1^2 X_3$	0.92		.925	.921

Run 3

In this run the dependent variable, the polynomial model and the data points were all the same as in Run 1. The throw-out criterion for Run 3 was $F_0 = 8.0$. This run should tend to throw out terms more often than Run 1 or Run 2. This should lead to more sweeps to reach k terms but hopefully the fit for these k terms will be better than in Run 1 or Run 2. (Compare, however, Run 3, Sweep 7, with Run 1, Sweep 5 and also Run 3, Sweep 18 with Run 1, Sweep 12). Note that in Run 3 we see that the best term No. 37 is not one of the best two terms.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	37	$X_1^3 X_3$	1058.24		.680	.680
2	2	36	X_1^3	98.96		.733	.733
3	3	2	X_3^2	99.34		.778	.777
4	2	37	$X_1^3 X_3$		4.88	.775	.775
5	3	9	X_2^3	102.13		.814	.813
6	4	15	$X_1 X_2$	219.83		.871	.870

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Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
7	5	20	$X_1 X_2^2 X_3^2$	18.48		.875710	.875
8	6	26	$X_1^2 X_3^2$	40.36		.885	.884
9	7	17	$X_1 X_2 X_3^2$	22.30		.890	.889
10	6	20	$X_1 X_2^2 X_3^2$		5.12	.889	.888
11	7	5	$X_2 X_3^2$	40.48		.897	.896
12	8	20	$X_1 X_2^2 X_3^2$	20.02		.901	.900
13	7	15	$X_1 X_2$		6.22	.900	.899
14	8	11	$X_2^3 X_3^2$	12.04		.903	.901
15	7	2	X_3^2		2.93	.902	.901
16	8	38	$X_1^3 X_3^2$	26.81		.907	.906
17	9	18	$X_1 X_2^2$	22.83		.911	.910
18	10	41	$X_1^3 X_2 X_3^2$	8.20		.912	.911

Run 4

In this run the dependent variable, the polynomial model and the data points were all the same as in Run 1. The throw-out criterion was $F_0 = 10^{-3}$. This run should not throw out variables very often, at least not until they are very insignificant. A partial tabulation of this run follows.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	37	$X_1^3 X_3$	1058.00		.680	.680
2	2	36	X_1^3	98.96		.733	.733
3	3	2	X_3^2	99.34		.778	.777
4	4	9	X_2^3	103.15		.816	.815

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Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
5	5	28	$X_1^2 X_2 X_3$	292.59		.884	.884
6	6	43	$X_1^3 X_2^2 X_3$	25.37		.890	.889
7	7	4	$X_2 X_3$	19.01		.894	.893
8	8	14	$X_1 X_3^2$	26.76		.900	.898
9	9	16	$X_1 X_2 X_3$	15.58		.903	.901
10	10	41	$X_1^3 X_2 X_3^2$	10.40		.905	.903
11	11	45	$X_1^3 X_2^3$	11.46		.907	.905
12	12	21	$X_1 X_2^3$	23.71		.911	.909
13	13	46	$X_1^3 X_2^3 X_3$	6.60		.913	.910
14	12	9	X_2^3		0.00	.913	.911
15	13	1	X_3	3.93		.913	.911
16	14	10	$X_2^3 X_3$	3.10		.914	.911
20	16	2	X_3^2		0.00	.916	.914
25	21	25	$X_1^2 X_3$	3.67		.920	.917
30	22	24	X_1^2		0.00	.923	.920
35	27	39	$X_1^3 X_2$	5.35		.927	.923
40	30	9	X_2^3		0.00	.92828	.92385
45	31	20	$X_1 X_2^2 X_3^2$	0.53		.92866	.92410
50	34	34	$X_1^2 X_2^3 X_3$	15.23		.93196	.92714
55	37	6	X_2^2		0.00	.93459	.92950
60	40	42	$X_1^3 X_2^2$	0.44		.93682	.93146
65	45	18	$X_1 X_2^2$	0.55		.93730	.93124
66	46	9	X_2^3	1.04		.93745	.93125
67	47	30	$X_1^2 X_2^2$	5.08		.938142	.931860

Run 5

In this run, the dependent variable was $F(X_1, X_2, X_3) = \exp(-X_1^2 X_2 X_3)$. We used the same balanced polynomial model as in the first four runs, cubic in X_1 and X_2, quadratic in X_3. The 500 data points were in the same balanced design, $X_1 = .25(.25)\ 2.50$, $X_2 = .25(.25)\ 2.50$, $X_3 = .25(.25)\ 1.25$. The polynomial model in this case should fit better than in the first four runs.

The throw-out criterion in the first runs in this series was $F_0 = 1.5$.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	12	X_1	836.43		.627	.627
2	2	4	$X_2 X_3$	529.77		.819	.819
3	3	24	X_1^2	212.65		.874	.873
4	4	8	$X_2^2 X_3^2$	308.40		.922	.922
5	5	44	$X_1^3 X_2^2 X_3^2$	61.94		.931	.930
6	6	16	$X_1 X_2 X_3$	103.35		.943	.942
7	7	28	$X_1^2 X_2 X_3$	62.76		.949	.949
8	8	20	$X_1 X_2^2 X_3^2$	231.18		.965	.965
9	7	12	X_1		0.79	.965	.965
10	8	23	$X_1 X_2^3 X_3^2$	27.03		.967	.967
11	9	22	$X_1 X_2^3 X_3$	138.53		.974	.974
12	10	21	$X_1 X_2^3$	411.57		.986	.986
13	11	27	$X_1^2 X_2$	8.79		.986	.986
14	12	25	$X_1^2 X_3$	97.48		.989	.988
15	13	30	$X_1^2 X_2^2$	67.45		.990	.990
16	14	38	$X_1^3 X_3^2$	73.37		.991	.991

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
17	13	24	X_1^2		0.03	.991	.991
18	14	33	$X_1^2X_2^3$	32.08		.992	.992
19	15	39	$X_1^3X_2$	23.02		.992	.992
20	16	32	$X_1^2X_2^2X_3^2$	75.84		.993	.993
25	17	42	$X_1^3X_2^2$	33.90		.99431	.99412
26	18	35	$X_1^2X_2^3X_3^2$	14.09		.99449	.99428
27	17	23	$X_1X_2^3X_3^2$		1.20	.99446	.99427
28	18	8	$X_2^2X_3^2$	11.81		.99459	.99440
29	19	14	$X_1X_3^2$	18.00		.99479	.99459
30	20	45	$X_1^3X_2^3$	5.57		.99485	.99464
35	25	21	$X_1X_2^3$	11.63		.99594	.99573
40	26	21	$X_1X_2^3$		1.12	.99604	.99583
44	26	21	$X_1X_2^3$	0.93		.99606	.99585

Run 6

This run used the same dependent variable, polynomial model and data points as in Run 5. The throw-out criterion was $F_0 = 0.9$. This will tend to throw out terms less often than in Run 5. In fact, however, the runs are identical through Sweep 26.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
25	17	42	$X_1^3X_2^2$	33.90		.99431	.99412
26	18	35	$X_1^2X_2^3X_3^2$	14.09		.99447	.99428
27	19	11	$X_2^3X_3^2$	13.66		.99462	.99492
28	18	20	$X_1X_2^2X_3^2$		0.00	.99462	.99443

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
29	19	14	$X_1 X_3^2$	16.67		.99480	.99461
30	20	45	$X_1^3 X_2^3$	6.19		.99487	.99467
35	23	42	$X_1^3 X_2^2$		0.44	.99574	.99555
40	26	11	$X_2^3 X_3^2$		0.48	.99609	.99588
41	25	38	$X_1^3 X_3^2$		0.59	.99608	.99589
42	24	14	$X_1 X_3^2$		0.61	.99608	.99589
43	25	31	$X_1^2 X_2^2 X_3$	0.79		.99608	.99589

Run 7

In this run the dependent variable, the polynomial model and the data points were all the same as in Run 5. The throw-out criterion was $F_0 = 8.0$. The variables brought in were the same as in Run 5 through Sweep 7.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
7	7	28	$X_1^2 X_2 X_3$	62.76		.94925	.94863
8	6	24	X_1^2		4.41	.94879	.94827
9	5	44	$X_1^3 X_2^2 X_3^2$		4.83	.94829	.94787
10	6	20	$X_1 X_2^2 X_3^2$	69.96		.95471	.95425
11	7	47	$X_1^3 X_2^3 X_3^2$	100.42		.96239	.96193
12	6	4	$X_2 X_3$		1.81	.96225	.96187
13	5	8	$X_2^2 X_3^2$		1.07	.96217	.96186
14	6	31	$X_1^2 X_2^2 X_3$	63.95		.96651	.96617
15	7	27	$X_1^2 X_2$	269.22		.97836	.97809
16	8	23	$X_1 X_2^3 X_3^2$	123.13		.98270	.98245

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Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
17	9	4	$X_2 X_3$	73.73		.98496	.98471
18	10	25	$X_1^2 X_3$	72.64		.98690	.98666
19	11	26	$X_1^2 X_3^2$	50.82		.98814	.98790
20	12	36	X_1^3	52.25		.98929	.98905
21	13	44	$X_1^3 X_2^2 X_3^2$	46.61		.99023	.98999
22	14	30	$X_1^2 X_2^2$	47.15		.99109	.99085
23	15	33	$X_1^2 X_2^3$	78.01		.99233	.99211
24	14	47	$X_1^3 X_2^3 X_3^2$		0.88	.99232	.99211
25	13	12	X_1		3.00	.99227	.99208
26	14	8	$X_2^2 X_3^2$	55.18		.99306	.99287
27	15	22	$X_1 X_2^3 X_3$	6.18		.99314	.99295

Run 8

In this run the dependent variable, the polynomial model and the data points were all the same as in Run 5. The throw-out criterion was $F_0 = 10^{-3}$. The variables brought in were the same as in Run 5 through Sweep 8.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
8	8	20	$X_1 X_2^2 X_3^2$	251.18		.96550	.96501
9	9	23	$X_1 X_2^3 X_3^2$	26.72		.96728	.96675
10	10	22	$X_1 X_2^3 X_3$	137.60		.97447	.97400
11	11	21	$X_1 X_2^3$	416.70		.98623	.98595
12	12	36	X_1^3	32.83		.98710	.98681
13	13	40	$X_1^3 X_2 X_3$	50.05		.98830	.98801

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
14	14	15	$X_1 X_2$	9.58		.98853	.98822
15	15	13	$X_1 X_3$	148.72		.99122	.99097
20	20	6	X_2^2	20.37		.99481	.99461
25	25	33	$X_1^2 X_2^3$	10.32		.99537	.99514
30	30	7	$X_2^2 X_3$	4.12		.99576	.99550
35	35	30	$X_1^2 X_2^2$	3.22		.99619	.99591
40	38	17	$X_1 X_2 X_3^2$	5.45		.99630	.99601
45	43	38	$X_1^3 X_3^2$	2.68		.99638	.99605
50	44	8	$X_2^2 X_3^2$	0.87		.99640	.99606
54	46	32	$X_1^2 X_2^2 X_3^2$	0.18		.996399	.996042
55	47	46	$X_1^3 X_2^3 X_3$	2.21		.996416	.996052
56	46	12	X_1		0.00	.996416	.996061
57	47	12	X_1	0.00		.996416	.996052

Run 9

In this run the dependent variable was $F(X_1, X_2, X_3) = \sqrt{X_1^2 + X_2^2 + X_3^2}$. The 47-term balanced polynomial, cubic in X_1 and X_2 and quadratic in X_3, was used as the model to fit the dependent variable over the 500 data points $X_1 = .25(.25)\ 2.50$, $X_2 = .25(.25)\ 2.50$, and $X_3 = .25(.25)\ 1.25$.

As expected in this case, the fit is very good. Because of the symmetry involved the terms in X_1 and X_2 should be the same, at least in the complete model. The lack of symmetry in the way these terms were brought is interesting.

The throw-out criterion for this run was $F_0 = 1.5$.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	15	$X_1 X_2$	1337.01		.72861	.72861
2	2	4	$X_2 X_3$	98.19		.77338	.77293
3	3	24	X_1^2	309.02		.86037	.85981
4	4	6	X_2^2	1324.25		.96201	.96178
5	5	7	$X_2^2 X_3$	302.54		.97644	.97625
6	6	12	X_1	553.58		.98890	.98879
7	7	2	X_3^2	202.14		.99213	.99204
8	8	3	X_2	427.10		.99579	.99573
9	9	4	$X_2 X_3$		1.44	.99578	.99573
10	8	14	$X_1 X_3^2$	469.05		.99784	.99781
11	9	19	$X_1 X_2^2 X_3$	169.84		.99840	.99837
12	10	5	$X_2 X_3^2$	177.58		.99882	
13	11	9	X_2^3	144.20		.99909	
14	12	36	X_1^3	204.27		.99936	
15	13	17	$X_1 X_2 X_3^2$	171.96		.99953	
16	14	21	$X_1 X_2^3$	87.04		.99960	
17	15	39	$X_1^3 X_2$	59.18		.99964	
18	16	30	$X_1^2 X_2^2$	125.68		.99972	
19	17	1	X_3	55.81		.99975	
20	18	4	$X_2 X_3$	114.22		.99980	
25	23	16	$X_2 X_1 X_3$	107.82		.99994	
30	26	38	$X_1^3 X_3^2$	40.36		.99996	
35	27	20	$X_1 X_2^2 X_3^2$		0.09	.99996	
40	30	21	$X_1 X_2^3$		0.00	.99996	

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
45	35	45	$x_1^3 x_2^3$	9.43		.999969	
46	34	39	$x_1^3 x_2$		0.26	.999969	
47	35	21	$x_1 x_2^3$	3.23		.999969	
48	36	41	$x_1^3 x_2 x_3^2$	0.40		.999969	

Run 10

In this run the dependent variable, the polynomial model and the data points were the same as in Run 9. The throw-out criterion for this run was $F_0 = 0.9$. The tabulation of the results is identical with Run 9 through Sweep 8.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
8	8	3	x_2	427.10		.99579	
9	9	14	$x_1 x_3^2$	470.79		.997854	
10	10	16	$x_1 x_2 x_3$	174.96		.998420	
11	11	1	x_3	212.37		.998899	
12	12	9	x_2^3	156.79		.999167	
13	13	36	x_1^3	230.76		.999435	
14	14	13	$x_1 x_3$	279.64		.999642	
15	15	45	$x_1^3 x_2^3$	82.42		.999694	
16	16	35	$x_1^2 x_2^3 x_3^2$	52.71		.999724	
17	17	37	$x_1^3 x_3$	107.84		.999774	
18	18	21	$x_1 x_2^3$	47.97		.999795	
19	19	39	$x_1^3 x_2$	259.26		.999867	
20	20	31	$x_1^2 x_2^2 x_3$	202.22		.999906	

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
25	25	23	$X_1 X_2^3 X_3^2$	76.83		.999950	
30	28	29	$X_1^2 X_2 X_3^2$	3.73		.999957	
40	30	45	$X_1^3 X_2^3$	6.72		.999960	
50	32	29	$X_1^2 X_2 X_3^2$	4.50		.999963	
60	36	41	$X_1^3 X_2 X_3^2$	10.53		.999967	
65	37	32	$X_1^2 X_2^2 X_3^2$	0.86		.999968	

Run 11

In this run the dependent variable, the polynomial model and the data points were the same as in Run 9. The throw-out criterion was $F_0 = 8.0$. The variables were included in the same order as in Run 9 through Sweep 15.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2 = Reduced R^2
15	13	17	$X_1 X_2 X_3^2$	171.96		.999528
16	12	7	$X_2^2 X_3$		2.77	.999525
17	13	39	$X_1^3 X_2$	49.15		.999569
18	14	1	X_3	37.69		.999600
19	13	19	$X_1 X_2^2 X_3$		2.18	.999598
20	14	21	$X_1 X_2^3$	59.03		.999642
21	15	30	$X_1^2 X_2^2$	142.48		.999723
22	16	13	$X_1 X_3$	52.63		.999750
23	17	4	$X_2 X_3$	58.95		.999778
24	18	16	$X_1 X_2 X_3$	60.90		.999803
25	17	17	$X_1 X_2 X_3^2$		0.20	.999802

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2 = Reduced R^2
26	18	16	$x_2^3 x_3$	61.82		.999825
27	19	22	$x_1 x_2^3 x_3$	177.78		.999872
28	20	37	$x_1^3 x_3$	102.41		.999895
29	21	40	$x_1^3 x_2 x_3$	390.39		.999942
30	22	46	$x_1^3 x_2^3 x_3$	38.26		.999946
35	25	38	$x_1^3 x_3$	10.63		.999957
36	24	14	$x_1 x_3^2$		2.26	.999957
37	25	47	$x_1^3 x_2^3 x_3^2$	7.35		.999958

Run 12

In this run the dependent variable, the polynomial model, and the data points were the same as in Run 9. The throw-out criterion was $F_0 = 10^{-3}$. The variables came in the same order as in Run 10 through Sweep 28.

No throw outs were made.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2 = Reduced R^2
25	25	23	$x_1 x_2^3 x_3^2$	76.83		.999950
30	30	42	$x_1^3 x_2^2$	6.11		.999958
35	35	43	$x_1^3 x_2^2 x_3$	15.94		.999962
40	40	28	$x_1^2 x_2 x_3$	21.80		.999967
45	45	25	$x_1^2 x_3$	28.42		.999971
46	46	34	$x_1^2 x_2^3 x_3$	11.16		.999972
47	47	47	$x_1^3 x_2^3 x_3^2$	1.10		.999972

Run 13

In this run the dependent variable was $F(X_1, X_2, X_3) = \exp(-X_1^2 X_2 X_3)$ as in Run 9. The polynomial model was the same 47-term balanced polynomial cubic in X_1 and X_2, quadratic in X_3. There were 1000 data points in a rectangular design $X_1 = .25(.25)\ 2.50$, $X_2 = .25(.25)\ 2.50$, $X_3 = .25(.25)\ 2.50$.

On this run the throw-out criterion was $F_0 = 1.0$.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2
1	1	12	X_1	1277.16		.561
2	2	4	$X_2 X_3$	619.57		.729
3	3	24	X_1^2	582.22		.829
4	4	8	$X_2^2 X_3^2$	472.27		.884
5	5	28	$X_1^2 X_2 X_3$	267.53		.9088
6	6	16	$X_1 X_2 X_3$	69.37		.9147
7	7	40	$X_1^3 X_2 X_3$	225.79		.9305
8	8	36	X_1^3	27.10		.9324
9	9	11	$X_2^3 X_3^2$	27.63		.9342
10	10	10	$X_2^3 X_3$	151.95		.9430
11	11	9	X_2^3	234.89		.9539
12	12	13	$X_1 X_3$	23.34		.9550
13	13	15	$X_1 X_2$	141.45		.9606
14	14	44	$X_1^3 X_2^2 X_3^2$	84.24		.9637
15	15	20	$X_1 X_2^2 X_3^2$	257.55		.9713
16	16	14	$X_1 X_3^2$	130.45		.9746
17	15	12	X_1		0.01	.9746
18	16	18	$X_1 X_2^2$	307.20		.980673

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Sweep	m Terms in Model	Term No	Term	F in	F out	R^2
19	17	21	$X_1 X_2^3$	113.99		.982683
20	16	4	$X_2 X_3$		0.53	.982674
21	17	32	$X_1^2 X_2^2 X_3^2$	20.32		.983025
22	16	44	$X_1^3 X_2^2 X_3^2$		0.09	.983023
23	17	12	X_1	31.96		.983658
24	18	4	$X_2 X_3$	53.90		.984415
25	17	9	X_2^3		0.75	.984403
30	22	19	$X_1 X_2^2 X_3$	8.60		.986977
35	25	44	$X_1^3 X_2^2 X_3^2$	6.49		.988926
36	26	22	$X_1 X_2^3 X_3$	3.53		.988966
37	27	1	X_3	2.05		.988989

Run 14

In this run the dependent variable, the polynomial model and the data points were the same as in Run 13. The throw-out criterion was $F_0 = 10^{-3}$. The tabulation is identical with Run 13 through Sweep 16.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2
16	16	14	$X_1 X_3^2$	130.45		.9746
17	17	18	$X_1 X_2^2$	318.07		.98084
18	18	32	$X_1^2 X_2^2 X_3^2$	144.76		.98330
19	19	21	$X_1 X_2^3$	155.92		.98560
20	20	47	$X_1^3 X_2^3 X_3^2$	16.89		.98584
21	21	34		53.87		.98658

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2
22	22	19	$X_1 X_2^2 X_3$	4.65		.98664
23	23	17	$X_1 X_2 X_3^2$	25.46		.98698
24	24	33	$X_1^2 X_2^3$	89.60		.98808
25	25	23	$X_1 X_2^3 X_3^2$	15.91		.98827
30	30	2	X_3^2	10.28		.98926
35	35	38	$X_1^3 X_3^2$	4.23		.98950
40	36	22	$X_1 X_2^3 X_3$	0.91		.989603
45	37	40	$X_1^3 X_2 X_3$		0.00	.989686
50	40	26	$X_1^2 X_3^2$	2.43		.989835
55	39	21	$X_1 X_2^3$		0.00	.989862
60	42	?		4.51		.990066
65	45	?		0.05		.990040
66	46	?		0.00		.990040

Run 15

In this run, the data were taken from Bulletin 336, Agricultural Experiment Station, Auburn University, Auburn, Alabama.

The throw out was $F_0 = 10^{-3}$ but was never used.

Sweep	m Terms in Model	Term No	Term	F in	R^2	Reduced R^2
1	1	4	X_4	86.98	.696	.696
2	2	2	X_2	3.14	.720	.712
3	3	5	X_4^2	0.64	.725	.710
4	4	3	X_3	0.24	.726	.704
5	5	6	$X_1 X_4$	0.13	.728	.696
6	6	1	X_1	0.58	.732	.693

Run 16

This run used the same data as in Run 15, but the polynomial model was taken to be a balanced polynomial linear in X_1, X_2, and X_3 and quadratic in X_4. This gives 23 terms in addition to the constant term.

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
1	1	1	X_4	86.98		.69596	.69596
2	2	5	$X_3X_4^2$	3.38		.72142	.71409
3	3	3	X_3	0.41		.72453	.70964
4	4	7	X_2X_4	1.13		.73314	.71091
5	5	14	$X_1X_4^2$	1.71		.74590	.71686
6	6	12	X_1	5.75		.78361	.75179
7	7	9	X_2X_3	0.55		.78724	.74856
8	8	16	$X_1X_3X_4$	2.55		.80340	.76040
9	9	2	X_4^2	1.51		.81280	.76449
10	10	23	$X_1X_2X_3X_4^2$	3.49		.83293	.78281
11	11	4	X_3X_4	0.34		.83491	.77798
12	12	6	X_2	0.98		.840665	.778069
13	13	17	$X_1X_3X_4^2$	0.74		.845059	.776197
14	14	13	X_1X_4	2.02		.856626	.784939
15	13	23	$X_1X_2X_3X_4^2$		0.00	.856624	.792901
16	14	8	$X_2X_4^2$	0.64		.860176	.790265
17	15	15	X_1X_3	0.27		.861736	.784308
18	16	21	$X_1X_2X_3$	0.10		.862309	.776253
19	17	10	$X_2X_3X_4$	0.35		.864448	.770151

Sweep	m Terms in Model	Term No	Term	F in	F out	R^2	Reduced R^2
20	16	12	X_1		0.00	.864446	.779725
21	17	18	X_1X_2	0.50		.867472	.775279
22	18	23	$X_1X_2X_3X_4^2$	0.89		.872836	.774572
23	17	21	$X_1X_2X_3$		0.00	.872835	.784373
24	18	19	$X_1X_2X_4$	0.61		.876437	.780957
25	17	3	X_3		0.00	.876435	.790476
26	18	11	$X_2X_3X_4^2$	0.61		.879902	.787099
27	19	12	X_1	0.12		.880637	.778325
28	20	22	$X_1X_2X_3X_4$	0.19		.881802	.769515
29	21	3	X_3	0.20		.883701	.761282
30	20	19	$X_1X_2X_4$		0.00	.883697	.773210
31	21	20	$X_1X_2X_4^2$	0.13		.884550	.760023
32	22	21	$X_1X_2X_3$	0.06		.884958	.750743
33	23	19	$X_1X_2X_4$	0.01		.885035	.736256
34	22	18	X_1X_2		0.00	.885034	.750906
35	23	18	X_1X_2	0.00		.885035	.736256

Run 17

In this run the data were a correlation matrix taken from Anderson, H. E., and Fruchter, B., "Predictor Selection Methods", _Psychometrika_, Vol. 25, No. 1, March 1960. In this run the throw-out criterion of $F_0 = 10^{-3}$ was never used.

Sweep	m Terms in Model	Term No	F in	R^2	Reduced R^2
1	1	6	56.94	.156025	.156025
2	2	4	21.38	.210965	.208403

Sweep	m Terms in Model	Term No	F in	R^2	Reduced R^2
3	3	3	10.18	.236372	.231397
4	4	13	4.90	.248451	.241083
5	5	12	4.13	.258529	.248805
6	6	10	1.38	.261881	.249741
7	7	1	0.92	.264125	.249553
8	8	8	0.71	.265861	.248844
9	9	2	0.42	.266898	.247413
10	10	5	0.37	.267803	.245837
11	11	9	0.40	.268785	.244330
12	12	7	0.29	.269503	.242538
13	13	11	0.17	.269932	.240435
14	14	14	0.02	.269970	.237908

Conclusions

We feel that the step-up procedure is an effective tool in the problem of finding a regression equation with a small number of estimation variables from a model with a large number. Using the various throw-out criteria and stopping rules, the problems of interest could be explored. The throw-out criterion and stopping rule which best fit the problem could be selected and then a regression equation determined. We feel that most future investigation of this procedure should be problem-oriented. We need the data for a problem to help develop an effective way of handling the data.

SELECTION OF SIGNIFICANT ESTIMATION VARIABLES
IN A LEAST SQUARES PROBLEM: COMPUTER PROGRAMS

1. Comparison of variables selected by step-up procedure with optimal set.

This procedure was programmed in the ALGOL 58 compiler language for the Burroughs 220 computer. Because of limitations on the memory the procedure is restricted to 25 variables.

The purpose of the program is to determine whether or not the step-up procedure actually selects the best k estimation variables. This program was preliminary to a more elaborate program for the Burroughs 5000.

First, the data are generated. The estimation variables $Z_1, \ldots, Z_{n-1}$ are terms of a balanced polynomial in independent variables $X_1, \ldots, X_\pi$, i.e.,

$$Z_k = X_1^{\ell_1} \ldots X_\pi^{\ell_\pi}, \quad \ell_i = 0, 1, \ldots L_i, \quad i=1, 2, \ldots, \pi,$$

where $(\ell_1, \ldots, \ell_\pi)$ takes on all possible values in the given range except $(0, \ldots, 0)$. Certain terms of the balanced polynomial are to be used to estimate a dependent variable, which is some function of the X's. It is convenient to label this variable Z_n. Corresponding to an index, $t_i = 1, 2, \ldots, T_i, i=1, 2, \ldots, \pi$, the observed value of X_i is $x_{i t_i}$. Thus, corresponding to the set $\{(t_1, \ldots, t_\pi) | t_i = 1, 2, \ldots, T_i, i=1, 2, \ldots, \pi\}$ is a rectangular set of data-points $\{(x_{1 t_1}, \ldots, x_{\pi t_\pi}\}$ from which are calculated observed values, $(z_{\mu 1}, \ldots, z_{\mu, n-1}, z_{\mu n})$, of the vector consisting of the estimation variables and the dependent variable.

Next, regression analyses are made using all possible combinations of k estimation variables, where $k=2, \ldots, n-2$. For each k, the combinations of variables which give maximum and minimum sums of squares due to regression (and hence maximum and minimum multiple correlation) are printed along with the sums of squares.

Finally, the step-up procedure is used. At the k'th step, the variable is selected from those not already included which maximizes $S_{kn}^{(k')2}/S_{kk}^{(k')}$. The procedure then uses that variable Z_k, as the pivot variable. It makes the following calculations:

$$S_{kj}^{(k'+1)} = \frac{S_{kj}^{(k')}}{S_{kk}^{(k')}} \qquad\qquad j = 1,2,\ldots n$$

$$S_{ij}^{(k'+1)} = S_{ij}^{(k')} - \frac{S_{ik}^{(k')}S_{kj}^{(k')}}{S_{kk}^{(k')}} \qquad\qquad i = 1,\ldots k-1,k+1,\ldots n, j=1,2,\ldots n.$$

In these calculations (S_{ij}) is the augmented matrix of dot products of the estimation vectors and the dependent-variable vector. The superscript k' indicates the number of transformations on (S_{ij}) in which a column has been reduced to a unit vector. The list of variables, included in the regression, and the sum of squares due to regression are printed.

In some cases the stepwise procedure gave optimal solutions, while in others it did not. In an attempt to run the program with 18 variables the time required to calculate the regression analyses for all combinations of variables turned out to be prohibitive.

The flow chart for this program is found in Appendix A and the program listing in Appendix B.

Operating Instructions for B-220 Program

1. Load the program, with the proper procedure (FCN) inserted to calculate the independent polynomial variables and the dependent variables.

2. Load the following data card, using more than one card if necessary, with 5 punched in the first column of each card.

Card Contents	Card Format
a) Number of independent polynomial variables	Skip at least one column; punch integer
b) Number of observations of independent polynomial variable	Skip at least one column; punch integer
c) Repeat (b) for each variable	
d) Order in independent polynomial variable	Skip at least one column; punch integer
e) Repeat (d) for each variable	
f) Lower bound for diagonal element	Skip at least one column; punch floating point number
g) Lower bound for difference between 1.0 and off-diagonal correlation	Skip at least one column; punch floating point number
h) F-statistic for stopping	Skip at least one column; punch floating point number; leave rest of card blank.

3. Repeat (2) for each analysis to be made.

4. Load 2 blank cards.

2. <u>Comprehensive program for selection of variables with step-up procedure incorporating elimination rules and stopping rules</u>. This procedure attempts to select the most significant estimation variables for a least squares fitting. It has been programmed for the Burroughs 5000 computer in the ALGOL 60 compiler language.

There are four options for obtaining the n x n augmented (S_{ij}) matrix

(1) Either the (S_{ij}) matrix or the correlation matrix may be read in. (Only the diagonal and the lower triangle are read in.)

(2) Each of the M observations $(z_{\mu 1}, \ldots, z_{\mu n})$ may be read in. An estimate $(m_1, \ldots, m_n)$ of the means is available. As the data are read in, the sums

$$S_i = \sum_{\mu=1}^{M} (Z_{\mu i} - m_i)$$

$$S_{ij}' = \sum_{\mu=1}^{M} (Z_{\mu i} - m_i)(Z_{\mu j} - m_j) \qquad\qquad i = 1,2,\ldots n, \ j = 1,2,\ldots,i$$

are calculated. The adjusted (S_{ij}) matrix

$$S_{ij} = S_{ij}' - \frac{S_i S_j}{M} \qquad\qquad i = 1,2,\ldots n, \ j = 1,2,\ldots,i$$

is then computed.

(3) Each observation may be generated from balanced polynomials. A set of fixed data points $(x_{\mu 1}, \ldots x_{\mu\pi})$ is given. The estimation variables are the terms of a balanced polynomials, so that

$$z_{\mu k} = x_{\mu 1}^{\ell_1} x_{\mu 2}^{\ell_2} \ldots x_{\mu\pi}^{\ell\pi}$$

where $\ell_i = 0,1,\ldots,L_i$, $i = 1,2,\ldots\pi$. Each of these combinations of exponents (except all exponents zero) corresponds to one estimation variable. The values $x_{\mu 1}, \ldots, x_{\mu\pi}$ may be read in, or they may be part of a rectangular design, with each μ corresponding to some value of the index $(t_1,\ldots,t_\pi)$, where $t_i = 1,\ldots,T_i$, $i = 1,2,\ldots,\pi$. Values $z_{\mu n}$ of the dependent variable may be read in or they may be computed values of a specified function, corresponding to values $x_{\mu 1},\ldots,x_{\mu\pi}$. These vectors $x_{\mu 1},\ldots,x_{\mu\pi},z_{\mu n}$ are generated in a procedure which may be varied with each run. As the observations $z_{\mu 1},\ldots,z_{\mu n}$ are generated, the sum of squares matrix (S_{ij}) is calculated as above.

Once the adjusted sum of squares matrix has been obtained, it may be used for more than one analysis. The diagonal and lower triangle only are used in the analysis. Since the matrix is symmetric, the necessary values may be stored in the upper triangle (with the diagonal in a separate vector) for performing other analyses under different conditions.

If the correlation matrix was read in, it is used in the regression analysis; otherwise, there is the option of computing and using the correlation matrix. The matrix to be used shall be denoted as $\left(S_{ij}^{(0)}\right)$. The program includes the option of printing this matrix.

In a hand computation the system of normal equations would be solved for regression coefficients in a sequence of gaussian eliminations, and the inverse matrix would be built up on a unit matrix. The initial tableau $\left(R_{ij}^{(0)}\right)$ for such an elimination and matrix inversion procedure would be defined by

$$
R_{ij}^{(0)} = \begin{cases} S_{ij}^{(0)} & i = 1,2,\ldots n; \ j = 1,2,\ldots,i \\[2mm] S_{ji}^{(0)} & i = 1,2,\ldots n-1; \ j = i+1,\ldots,n \\[2mm] 1 & i = 1,2,\ldots,n; \ j = n+i \\[2mm] 0 & i = 1,2,\ldots n; \ j = n+1,\ldots,2n, \ j \neq n+i \end{cases}
$$

The original S matrix is of the form

$$
\begin{matrix}
S_{11}^{(0)} & & & \\
S_{21}^{(0)} & S_{22}^{(0)} & & \\
\vdots & \vdots & \ddots & \\
S_{n-1,1}^{(0)} & S_{n-1,2}^{(0)} & \ldots S_{n-1,n-1}^{(0)} & \\
S_{n1}^{(0)} & S_{n2}^{(0)} & \ldots S_{n,n-1}^{(0)} & S_{nn}^{(0)}
\end{matrix}
$$

while the original R matrix is of the form

$$
\begin{array}{ccccccccc}
S_{11}^{(0)} & S_{21}^{(0)} & \cdots & S_{n-1,1}^{(0)} & S_{n1}^{(0)} & 1 & 0 & \cdots & 0 \\
S_{21}^{(0)} & S_{22}^{(0)} & \cdots & S_{n-1,2}^{(0)} & S_{n2}^{(0)} & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \cdots & & \vdots & \vdots & \vdots & \cdots & \vdots \\
S_{n-1,1}^{(0)} & S_{n-1,2}^{(0)} & \cdots & S_{n-1,n-1}^{(0)} & S_{n,n-1}^{(0)} & 0 & 0 & \cdots 1 & 0 \\
S_{n1}^{(0)} & S_{n2}^{(0)} & \cdots & S_{n,n-1}^{(0)} & S_{nn}^{(0)} & 0 & 0 & \cdots 0 & 1
\end{array}
$$

Because of symmetry operations need be made only on the lower triangle of the S matrix. Hence the entire R matrix need not be stored in memory.

The stepwise procedure now begins. It is assumed that at the k'th step, k estimation variables $Z_{p_1}, \ldots, Z_{p_k}$ are included in the regression, while the n-k-1 variables $Z_{q_1}, \ldots, Z_{q_{n-k-1}}$ are excluded. The variables $Z_{p_{max}}$ and $Z_{q_{min}}$ which minimize $(S_{np_i}^{(k')2})/S_{p_i p_i}^{(k')}$ and maximize $(S_{nq_j}^{(k')2})/S_{q_j q_j}^{(k')}$, respectively, are determined. The variable $Z_{p_{min}}$ shall be considered significant if

$$
\frac{(S_{np_{min}}^{(k')})^2/S_{p_{min}p_{min}}^{(k')}}{S_{nn}^{(k')}/(M-k-1)} \geq F_0
$$

and the variable $Z_{q_{max}}$ shall be considered significant if

$$
\frac{(S_{nq_{max}}^{(k')})^2/S_{q_{max}q_{max}}^{(k')}}{[S_{nn}^{(k')} - (S_{nq_{max}}^{(k')})^2/S_{q_{max}q_{max}}^{(k')}]/(M-k-2)} > F_I
$$

where F_I and F_O are criteria based on the F-distribution. F_I should not be less than F_O; if it were, looping might occur.

The procedure now tests whether $Z_{p_{min}}$ is to be dropped from the regression. There are two options for dropping a variable:

(1) If $Z_{p_{min}}$ is not significant, it is dropped. (This may be bypassed by setting F_O equal to zero.)

(2) The procedure alternately adds two variables and drops one. If $Z_{p_{min}}$ is not to be dropped, the procedure checks whether to stop or not.

There are four criteria for stopping, the first two of which are now checked.

(1) If $Z_{p_{max}}$ is not significant, it is added and then the procedure terminates. (This may be bypassed by setting F_I to zero.)

(2) When a specified maximum number of terms have been included in the regression, the procedure terminates. Unless otherwise specified, this will be the number of estimation variables.

(3) If the square of the multiple correlation coefficient is greater than a specified amount R^2_{max}, the procedure terminates. (This may be bypassed by setting R^2_{max} to 1.)

(4) When the procedure has gone through a specified number of iterations, it terminates. If the procedure is following the option of adding two variables and dropping one, this will be three times the maximum number of terms; otherwise, it will be twice the maximum number of terms.

If $Z_{p_{min}}$ is not to be dropped, and if the procedure does not stop, $Z_{q_{max}}$ is now added to the regression.

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The jth column of the S matrix corresponds to the (j+n)-th of the R matrix if the jth variable has been included in the regression and to the jth column otherwise. (At all stages, either the jth column or the (j+n)-th column of the R matrix will be a unit vector. The S matrix will contain the column which is not. Of course the storage of the unit vector is unnecessary.)

It will be assumed that the qth variable is to be added or dropped. (The computational procedure is the same in both cases. It will also be assumed that $H_j^{(k')} = -1$ if the j-th variable is included in the regression after k' iterations and that $H_j^{(k')} = +1$ otherwise. Note that $H_n^{(k')} = +1$ throughout the analysis. $H_q^{(k')}$ depends on the status of the qth variable before, rather than after it is added or dropped.)

The following formulae determine the matrix $\left(S_{ij}^{(k'+1)} \right)$:

$$S_{qq}^{(k'+1)} = \frac{1}{S_{qq}^{(k')}}$$

$$S_{qj}^{(k'+1)} = \frac{S_{qj}^{(k')}}{S_{qq}^{(k')}} \qquad j < q$$

$$S_{iq}^{(k'+1)} = -\frac{S_{iq}^{(k')}}{S_{qq}^{(k')}} \qquad i > q$$

$$S_{ij}^{(k'+1)} = S_{ij}^{(k')} - \frac{S_{qi}^{(k')} S_{qj}^{(k')} H_i^{(k')} H_q^{(k')}}{S_{qq}^{(k')}} \qquad j \leq i < q$$

$$S_{ij}^{(k'+1)} = S_{ij}^{(k')} - \frac{S_{iq}^{(k')} S_{qj}^{(k')}}{S_{qq}^{(k')}} \qquad j < q < i$$

$$S_{ij}^{(k'+1)} = S_{ij}^{(k')} - \frac{S_{iq}^{(k')} S_{jq}^{(k')} H_j^{(k')} H_q^{(k')}}{S_{qq}^{(k')}} \qquad q < j \leq i$$

This is equivalent, on adding a variable, to

$$R_{qj}^{(k'+1)} = \frac{R_{qj}^{(k')}}{R_{qq}^{(k')}}$$

$$R_{ij}^{(k'+1)} = R_{ij}^{(k'+1)} - \frac{R_{iq}^{(k')} R_{qj}^{(k')}}{R_{qq}^{(k')}}$$

or, on dropping a variable, to

$$R_{qj}^{(k'+1)} = \frac{R_{qj}^{(k')}}{R_{q,q+n}^{(k')}}$$

$$R_{ij}^{(k'+1)} = R_{ij}^{(k')} - \frac{R_{i,q+n}^{(k')} R_{qj}^{(k')}}{R_{q,q+n}^{(k')}}$$

where the (q+n)-th column of the R matrix takes the place of the qth in the S matrix when a variable is being added.

If the first k variables were included in the regression, then the R matrix would be of the form

$$\begin{bmatrix}
1 & 0 & -S_{k+1,1}^{(k)} & \cdots & -S_{n-1,1}^{(k)} & -S_{n1}^{(k)} & S_{11}^{(k)} & \cdots S_{k1}^{(k)} & 0 & \cdots & 0 \\
\cdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \cdots \vdots & \vdots & & \vdots \\
0 & 1 & -S_{k+1,k}^{(k)} & \cdots & -S_{n-1,k}^{(k)} & -S_{nk}^{(k)} & S_{k1}^{(k)} & \cdots S_{kk}^{(k)} & 0 & \cdots & 0 \\
0 \cdots 0 & & S_{k+1,k+1}^{(k)} & \cdots & S_{n-1,k+1}^{(k)} & S_{n,k+1}^{(k)} & S_{k+1,1}^{(k)} & \cdots S_{k+1,k}^{(k)} & 1 & & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & & & \cdots \\
0 \cdots 0 & & S_{n-1,k+1}^{(k)} & & S_{n-1,n-1}^{(k)} & S_{n,n-1}^{(k)} & S_{n-1,1}^{(k)} & \cdots S_{n-1,k}^{(k)} & 0 & & 1 \\
0 \cdots 0 & & S_{n,k+1}^{(k)} & & S_{n,n-1}^{(k)} & S_{nn}^{(k)} & S_{n1}^{(k)} & \cdots S_{nk}^{(k)} & 0 & \cdots & 0
\end{bmatrix}$$

In effect the program inverts the S matrix in place, proceeding from pivot element to pivot element without rearranging rows and columns. Also, advantage is taken of the symmetry in carrying out calculations in the lower triangle only. For more details the flow chart in Appendix A and the program listing in Appendix C may be consulted.

At this point, a list of included or active variables, the mean-squares due to regression and to error, the F-ratio, and the square of the multiple correlation coefficient are printed. There are options for printing the inverse matrix, the reduced sum of squares matrix, the partial regression coefficients of the dependent variable on each of the active variables, and the regression coefficients of the dependent variable on the active variables.

Operating Instructions for B-5000 Program

1. Load the program, with the proper procedure (CALC) inserted to calculate the polynomial estimation variables and the dependent variable. (If that option is not used, a procedure must still be declared.)

2. Load the following data card:

Card Contents	Card Format
a) Upper bound to number of independent polynomial variables (at least 1)	Punch integer; punch comma; skip at least one space
b) Upper bound to number of variables in regression analysis (both estimation and dependent)	Punch integer; punch comma; leave remaining columns on card blank

3. If data are to be generated from polynomial variables, load the following data card, using more than one card if necessary:

Card Contents	Card Format
a) Number of independent polynomial variables	Punch integer; punch comma; skip at least one column
b) Number of observations of independent polynomial variable (if observations are read in, punch 1)	Punch integer; punch comma; skip at least one column

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Card Contents	Card Format
c) Repeat (b) for each variable if observations are read in, punch number of observations for last variable)	
d) Order in independent polynomial variable	Punch integer; punch comma; skip at least one column
e) Repeat (d) for each variable	
	Leave rest of card blank

4. If data are not to be generated from independent polynomial variables, load the following data card:

Card Contents	Card Format
a) 1	Punch 1; punch comma; skip at least one column
b) The number of observations	Punch integer; punch comma; skip at least one column
c) The number of estimation variables	Punch integer; punch comma; leave rest of card blank

5. Load the following card:

(a) If estimates of the means are to be read in, skip 3 columns, punch TRUE: otherwise, skip 2 columns, punch FALSE.

(b) Punch the next 14 columns according to one of the following 4 options:

   i) If data are to be generated from polynomial variables, skip 2 columns, punch FALSE, skip 2 columns, punch FALSE.

   ii) If the estimation variables are to be read in, skip 2 columns, punch FALSE, skip 3 columns, punch TRUE.

   iii) If the sum of squares or intercorrelations matrix is to be read in, skip 3 columns, punch TRUE, skip 2 columns, punch FALSE.

   iv) If the analysis to be made uses a matrix which has just been used, skip 3 columns, punch TRUE, skip 3 columns, punch TRUE.

(c) If the matrix is to be printed, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

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(d) If the intercorrelations matrix is to be used, skip 3 columns, punch

TRUE; otherwise, skip 2 columns, punch FALSE.

6. If estimates of the means are to be read in, load the following data

card, using more than one card if necessary:

	Card Contents	Card Format
a)	Number of observations	Punch integer; punch comma; skip at least one space
b)	Number of estimation variables in regression analysis (including dependent variable)	Punch integer; punch comma; skip at least one space
c)	Estimate for mean of estimation variable	Punch number; punch comma; skip at least one space
d)	Repeat (c) for each variable	
e)	Estimate for mean of dependent variable	Punch number; punch comma; leave rest of card blank

7. Load the following data card:

	Card Contents	Card Format
a)	F-statistic for stopping	Punch number; punch comma; skip at least one column
b)	F-statistic for elimination of a variable	Punch number; punch comma; skip at least one column
c)	Lower bound for diagonal element	Punch number; punch comma; skip at least one column
d)	Maximum number of terms	Punch integer; punch comma; skip at least one column
e)	Maximum value for R^2	Punch number; punch comma; leave rest of card blank

8. If the sum of squares or intercorrelations matrix is to be read in, load

the following data card(s):

Card Contents	Card Format
a) Element of matrix	Punch number; punch comma; skip at least one space
b) Repeat (a) for each element in row up through the diagonal element	
c) Repeat (a) - (b) for each row	
d) Sum of squares of dependent variable	Punch number; punch comma; leave the rest of card blank

9. If the individual observations on the estimation variables are to be read in, load the following data cards:

Card Contents	Card Format
a) Observation on estimation variable	Punch number; punch comma; skip at least one column
b) Repeat (a) for each estimation variable	
c) Observation on dependent variable	Punch number; punch comma; leave rest of card blank
d) Repeat (a) - (c) for each observation	

10. If the independent polynomial variables are to be read in, load the cards as described in (9), using polynomial variables instead of estimation variables. The procedure CALC must specify reading these variables.

11. Load the following card:

   a) If the inverse matrix is to be printed, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

   b) If the reduced sum of squares matrix is to be printed, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

   c) If the partial regression coefficients are to be printed, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

d) If the regression coefficients are to be printed, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

e) If the option of adding two variables and eliminating one is used, skip 3 columns, punch TRUE; otherwise, skip 2 columns, punch FALSE.

12. Repeat (3) - (11) for each analysis to be made.

13. Load the following data card:

Card Contents	Card Format
a) 0	Punch 0; punch comma; leave rest of card blank

14. Load end-of-deck card.

APPENDIX A

FLOW DIAGRAMS
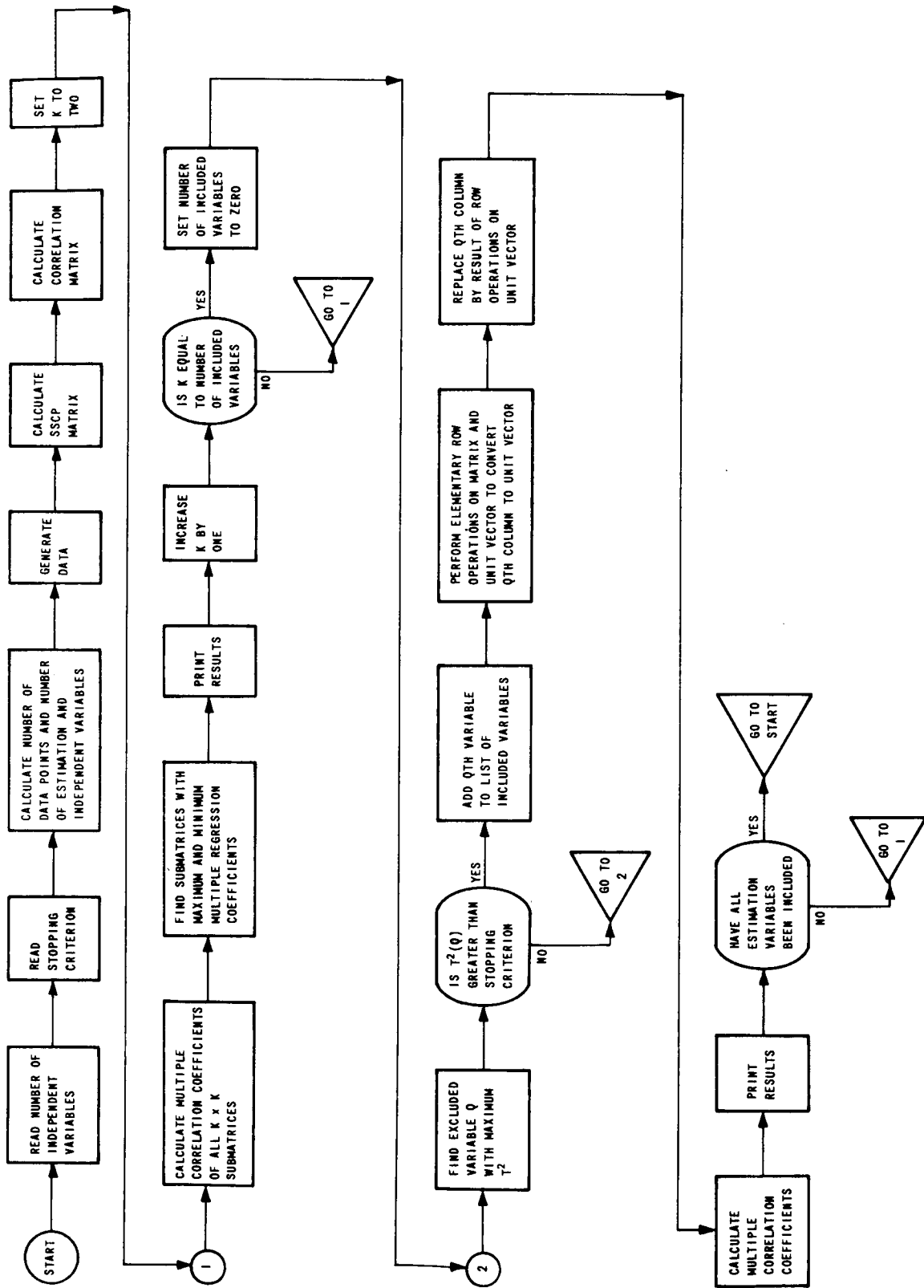
Figure 1. Flow Diagram for the Comparison Program.
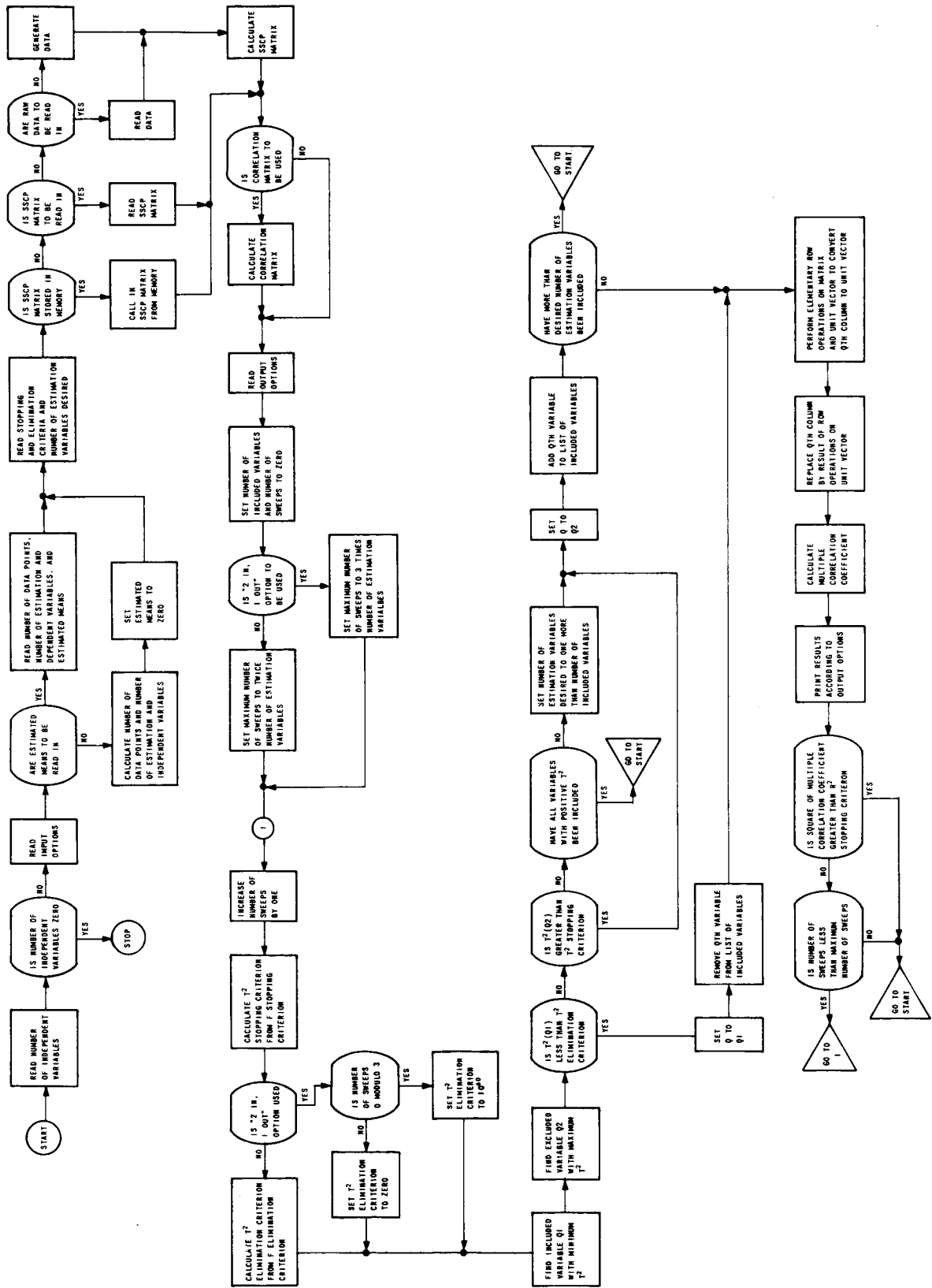
Figure 2. Flow Diagram for the Comprehensive Step-up Procedure.

APPENDIX B

PROGRAM FOR THE COMPARISON OF VARIABLES
SELECTED BY THE STEP-UP PROCEDURE
WITH THE OPTIMAL SET

```
2         COMMENT---PSEUDO-OPTIMAL PROCEDURE FOR SELECTING K VARIABLES
2                   OUT OF N FOR LEAST SQUARES FITTING  $
2  INTEGER  I,J,K,L,M,N,N1,P,PI,Q,T  $
2  INTEGER  Y,Z  $
2  ARRAY    E(4),L(3),T(3),U(3),V(25),X(25),M(3,25),R(24,24),S(25,25)  $
2           PROCEDURE FCN(P,PI,T(),U())$ANS)  $
2  BEGIN
2           COMMENT----THIS IS AN EXAMPLE OF THE PROCEDURES WHICH WERE USED
2                      TO GENERATE THE INDEPENDENT AND DEPENDENT VARIABLES.
2                      OTHER PROCEDURES WERE ALSO USED  $
2           INTEGER P,Q,T,PI  $
2           FOR Q = (P,1,PI)  $
2           U(Q) = 0.25.T(Q)  $
2           ANS = 3.0/(1.0 + U(1).U(1) + U(3) + U(3))  $
2  RETURN  $
2  END FCN()  $
2  INPUT    DATA(PI,FOR I = 1,2$FOR J = (1,1,PI)$M(I,J),E(1),E(2),E(3))  $
2  OUTPUT   ER(K,I,J)  $
2  OUTPUT   VB(K,FOR I = (1,1,K)$M(P,I))  $
2  OUTPUT   MX(A)  $
2  OUTPUT   MN(B)  $
2  FORMAT   ERF(*ERROR*,3I4,W0)  $
2  FORMAT   VBL(I4,*VARIABLES*,30I3,W4)  $
2  FORMAT   FMX(*MAX SSR*,F20.8,W0)  $
2  FORMAT   FMN(*MIN SSR*,F20.8,W0)  $
2  FORMAT   PAGE(W1)  $
2           COMMENT---INITIALIZATION OF CONDITIONS  $
2  START..
2           READ($$DATA)  $
2           N = K = 1  $
2           FOR I = (1,1,PI)  $
2  BEGIN
2           K = K.M(1,I)  $
2           N = N.(M(2,I) + 1)  $
2  END  $
2           NP = FLOAT(K)  $
2           N1 = N - 1  $
2           E(2) = 1.0 - E(2)  $
2           FOR I = (1,1,N)  $
2  BEGIN
```

```
2        V(I) = 0  $
2        FOR J = (1,1,I)  $
2        S(I,J) = 0  $
2 END  $
2        WRITE($$PAGE)  $
2        COMMENT---COMPUTATION OF INTERCORRELATIONS MATRIX  $
2        FOR P = (1,1,PI-1)  $
2        T(P) = 1  $
2        T(PI) = 0  $
2 FIXT..  P = PI  $
2        UNTIL T(P) LSS M(1,P)  $
2 BEGIN  P = P - 1  $
2        IF P EQL 0  $
2        GO TO IC  $
2 END  $  T(P) = T(P) + 1  $
2        FOR Q = (P+1,1,PI)  $
2        T(Q) = 1  $
2        FCN(P,PI,T(),U()$X(N))  $
2        K = 0  $
2        FOR P = (1,1,PI)  $
2        L(P) = 0  $
2 FIXL..  P = PI  $
2        UNTIL L(P) LSS M(2,P)  $
2 BEGIN  P = P - 1  $
2        IF P EQL 0  $
2        GO TO CP  $
2 END  $  L(P) = L(P) + 1  $
2        FOR Q = (P+1,1,PI)  $
2        L(Q) = 0  $
2        K = K + 1  $
2        TEMP = 1.0  $
2        FOR P = (1,1,PI)  $
2        FOR Q = (1,1,L(P))  $
2        TEMP = TEMP.U(P)  $
```

```
2        X(K) = TEMP   $
2        GO TO FIXL    $
2 GP..
2 BEGIN   FOR I = (1,1,N)   $
2         V(I) = V(I) + X(I)   $
2         FOR J = (1,1,I)   $
2         S(I,J) = S(I,J) + X(I)*X(J)   $
2 END  $
2        GO TO FIXT   $
2 IC..
2         FOR I = (1,1,N)   $
2         FOR J = (1,1,I)   $
2         S(I,J) = S(I,J) - V(I)*V(J)/NP   $
2         K = P = 0   $
2         FOR I = (1,1,N)   $
2 BEGIN   EITHER IF S(I,I) LSS E(1)   $
2 BEGIN   J = 1   $
2         P = 1   $
2         WRITE(SSER,ERF)   $
2 END  $
2 BEGIN   OTHERWISE   $
2         V(I) = SQRT(S(I,I))   $
2         S(I,I) = 1.0   $
2 END  $
2 END  $
2         IF P NEQ 0   $
2         GO TO START   $
2         FOR I = (2,1,N)   $
2         FOR J = (1,1,I-1)   $
2 BEGIN   S(I,J) = S(J,I) = S(I,J)/(V(I)*V(J))   $
2         IF ABS(S(I,J)) GEQ E(2)   $
2 BEGIN   P = 1   $
2         WRITE(SSER,ERF)   $
2 END  $
```

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```
2 END  $
2      IF P NEQ 0  $
2      GO TO START  $
2      COMMENT--REGRESSION OF ALL COMBINATIONS OF VARIABLES  $
2      FOR K = (2,1,N-2)  $
2 BEGIN
2      Q = K + 1  $
2      A = 0  $
2      R = 0.99999999**49  $
2      FOR P = (1,1,K-1)  $
2      M(1,P) = 1  $
2      M(1,K) = 0  $
2      M(1,Q) = N  $
2 FIXM..
2      P = K  $
2      UNTIL M(1,P) LSS (N+P-Q)  $
2 BEGIN
2      P = P - 1  $
2      IF P EQL 0  $
2      GO TO PRNT  $
2 END  $
2      M(1,P) = M(1,P) + 1  $
2      FOR I = (P+1,1,K)  $
2      M(1,I) = M(1,I-1) + 1  $
2      R(1,1) = 1.0  $
2      FOR I = (2,1,Q)  $
2 BEGIN
2      R(I,I) = 1.0  $
2      P = M(1,I)  $
2      FOR J = (1,1,I-1)  $
2      R(I,J) = R(J,I) = S(P,M(1,J))  $
2 END  $
2      FOR I = (1,1,K)  $
2 BEGIN
2      TEMP = R(I,I)  $
2      IF TEMP LSS E(1)  $
2      GO TO FIXM  $
2      FOR J = (I+1,1,Q)  $
2      R(I,J) = R(I,J)/TEMP  $
2      FOR P = (I+1,1,Q)  $
```

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```
2 BEGIN
2     TEMP = R(P,I)  $
2     FOR J = (I+1,1,Q)  $
2     R(P,J) = R(P,J) - TEMP.R(I,J)  $
2 END  $
2 END  $
2     TEMP = 1.0 - R(Q,Q)  $
2     IF TEMP GTR A  $
2 BEGIN
2     A = TEMP  $
2     FOR I = (1,1,K)  $
2     M(2,I) = M(1,I)  $
2 END  $
2     IF TEMP LSS B  $
2 BEGIN
2     B = TEMP  $
2     FOR I = (1,1,K)  $
2     M(3,I) = M(1,I)  $
2 END  $
2     GO TO FIXM  $
2 PRNT..
2     P = 2  $
2     WRITE(SSVB,VBL)  $
2     WRITE(SSMX,FMX)  $
2     P = 3  $
2     WRITE(SSVB,VBL)  $
2     WRITE(SSMN,FMN)  $
2 END  $
2     COMMENT--STEPWISE REGRESSION PROCEDURE  $
2     FOR I = (1,1,N1)  $
2     M(1,I) = 0  $
2     FOR K = (1,1,N1)  $
2 BEGIN
2     A = 0  $
2     FOR I = (1,1,N1)  $
2 BEGIN
2     IF (M(1,I) EQL 0) AND (S(I,N).S(I,N)/S(I,I) GEQ E(1))  $
2 BEGIN
2     TEMP = S(I,N).S(I,N)/S(I,I)  $
2     IF TEMP GTR A  $
```

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```
2 BEGIN
2      A = TEMP    $
2      Q = I    $
2 END $
2 END $
2 END $
2      IF A LSS E(3)    $
2      GO TO START    $
2      M(1,Q) = 1    $
2      M(2,K) = Q    $
2      TEMP = 1.0/S(Q,Q)    $
2      S(Q,Q) = 1.0    $
2      FOR J = (1,1,N)    $
2      S(Q,J) = TEMP.S(Q,J)    $
2      FOR I = (1,1,Q-1),(Q+1,1,N)    $
2 BEGIN
2      TEMP = S(I,Q)    $
2      S(I,Q) = 0    $
2      FOR J = (1,1,N)    $
2      S(I,J) = S(I,J) - TEMP.S(Q,J)    $
2 END $
2      P = 2    $
2      A = 1.0 - S(N,N)    $
2      WRITE($$VB,VBL)    $
2      WRITE($$MX,FMX)    $
2 END $
2      GO TO START    $
2      FINISH $
```

APPENDIX C

PROGRAM FOR THE SELECTION OF
VARIABLES WITH THE STEP-UP PROCEDURE
INCORPORATING ELIMINATION RULES AND STOPPING RULES

```
BEGIN
COMMENT----THIS IS A STEPWISE PROCEDURE FOR SELECTING K VARIABLES OUT
          OF N FOR A LEAST SQUARES FITTING;
INTEGER I, J, K, M, N, P, Q, Y, Z, PMAX, NMAX, PI, M1, N1, Q1, NT,
        MNT, AG, MODAG, MAXAG;
REAL A, B, FI, FO, TI, TX, ROF, SQM, SSY, SSE, SUE, RSQ, RSQMX, TIM,
     TEMP1, TEMP2;
BOOLEAN OP1, OP2, OP3, OP4, OPP, CORR;
FILE IN FILE2 (2,10);
READ(FILE2, /, PMAX, NMAX);
BEGIN
LABEL START, STPWSE, EXIT;
REAL ARRAY S[1:NMAX,1:NMAX], DIAG[1:NMAX];
FILE OUT FILE1 1 (2,15);
FORMAT OUT LINE(8E15.6),
           TIMER(X20, "TIME FOR RUN WAS", F9.2, "SECONDS"),
           ADJSS(X20, "ADJUSTED SUM OF SQUARES MATRIX");
START: BEGIN
COMMENT----INITIALIZATION OF CONDITIONS;
LABEL DATA, POINT, VAR, FORM, SQUARE, PRINT;
BOOLEAN CORR;
INTEGER ARRAY T[1:PMAX], L1[1:PMAX], T[1:PMAX], L[1:PMAX];
REAL ARRAY X[1:PMAX], DAT[1:NMAX], TOT[1:NMAX], MN[1:NMAX],
           STDEV[1:NMAX];
FORMAT IN OP(5(X2, L5));
FORMAT OUT MNST(X20, "MEANS AND STANDARD DEVIATIONS");
PROCEDURE CALC;
BEGIN
COMMENT----THIS IS AN EXAMPLE OF THE PROCEDURES WHICH WERE USED TO
          GENERATE THE INDEPENDENT AND DEPENDENT VARIABLES.
          OTHER PROCEDURES WERE ALSO USED;
FOR I:=1 STEP 1 UNTIL PI DO
X[I] := 0.25 × T[I];
TEMP1 := X[I] + X[2] - 1.5707963268 × X[3];
DAT[N] := (X[I]↑4 + X[2]↑3 + X[3] × X[3])/SQRT(ABS(TEMP1));
END CALC;
TIM := TIME(1);
READ(FILE2, /, PI, FOR P:=1 STEP 1 UNTIL PI DO T1[P], FOR P:=1 STEP 1
           UNTIL PI DO L1[P]);
IF PI = 0 THEN GO TO EXIT;
```

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```
READ(FILE2, OP, OP1, OP2, OP3, OP4, CORR);
IF NOT OP2 OR NOT OP3 THEN
BEGIN
IF OP1 THEN
READ(FILE2, /, M, N, FOR I:=1 STEP 1 UNTIL N DO MN[I]) ELSE
BEGIN
M := N := 1;
FOR P:=1 STEP 1 UNTIL PI DO
BEGIN
M := M x T1[P];
N := N x (L1[P] + 1);
END;
FOR I:=1 STEP 1 UNTIL N DO
MN[I] := 0.0;
END;
M1 := M - 1;
N1 := N - 1;
SQM := SQRT(M1);
END;
READ(FILE2, /, FI, FO, ROF, MNT, RSQMX);
FOR I:=1 STEP 1 UNTIL N DO
BEGIN
TOT[I] := 0.0;
FOR K:=1 STEP 1 UNTIL I DO
S[I,K] := 0.0;
END;
IF OP2 THEN
BEGIN
IF OP3 THEN
BEGIN
FOR I:=1 STEP 1 UNTIL N DO
BEGIN
S[I,I] := DIAG[I];
FOR K:=I+1 STEP 1 UNTIL N DO
S[K,I] := S[I,K];
END;
END ELSE
READ(FILE2, /, FOR I:=1 STEP 1 UNTIL N DO FOR K:=1 STEP 1 UNTIL I DO
GO TO SQUARE;
S[I,K], SSY);
```

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```
END;
SSY := 0.0;
FOR P:=1 STEP 1 UNTIL PT-1 DO
T[P] := 1;
T[P]] := 0;
J := 0;
DATA:
IF OP3 THEN
BEGIN
  READ(FILE2, /, FOR I:=1 STEP 1 UNTIL N DO DAT[I]);
  GO TO FORM;
END;
P := PT;
POINT:
IF T[P] ≥ T1[P] THEN
BEGIN
  T[P] := 1;
  P := P - 1;
  GO TO POINT;
END;
T[P] := T[P] + 1;
CALC;
K := 0;
FOR P:=1 STEP 1 UNTIL PT DO
L[P] := 0;
P := PT;
VAR:
IF L[P] ≥ L1[P] THEN
BEGIN
  L[P] := 0;
  P := P - 1;
  GO TO VAR;
END;
L[P] := L[P] + 1;
K := K + 1;
TEMP1 := 1.0;
FOR P:=1 STEP 1 UNTIL PT DO
FOR I:=1 STEP 1 UNTIL L[P] DO
TEMP1 := TEMP1 × X[P];
DAT[K] := TEMP1;
```

```
IF K < N1 THEN
BEGIN
   P := PI;
   GO TO VAR;
END;
FORM:
J := J + 1;
FOR K:=1 STEP 1 UNTIL N DO
BEGIN
   TEMP1 := DAT[K] := DAT[K] - MN[K];
   TOT[K] := TOT[K] + TEMP1;
   FOR I:=1 STEP 1 UNTIL K DO
   S[K,I] := S[K,I] + TEMP1 × DAT[I];
END;
IF J < M THEN GO TO DATA;
SQUARE:
FOR K:=1 STEP 1 UNTIL N DO
BEGIN
   TEMP1 := TOT[K]/M;
   MN[K] := MN[K] + TEMP1;
   FOR I:=1 STEP 1 UNTIL K DO
   S[K,I] := S[K,I] - TOT[I] × TEMP1;
END;
IF NOT OP2 OR NOT OP3 THEN
BEGIN
   FOR I:=1 STEP 1 UNTIL N DO
   BEGIN
      DIAG[I] := S[I,I];
      FOR K:=I+1 STEP 1 UNTIL N DO
      S[I,K] := S[K,I];
   END;
END;
IF SSY = 0.0 THEN
SSY := S[N,N];
FOR K:=1 STEP 1 UNTIL N DO
BEGIN
   TEMP1 := S[K,K];
   IF TEMP1 < ROF THEN
   BEGIN
      CORR := FALSE;
```

```
            OP4 := TRUE;
            STDEV[K] := 0.0
        END ELSE
            STDEV[K] := SQRT(TEMP1);
    END;
    IF CORR THEN
    BEGIN
        FOR K:=1 STEP 1 UNTIL N DO
        BEGIN
            TEMP1 := STDEV[K];
            S[K,K] := 1.0;
            FOR I:=K+1 STEP 1 UNTIL N DO
            S[I,K] := S[I,K]/(STDEV[I] x TEMP1);
            STDEV[K] := TEMP1/SQM;
        END;
        SUE := SSY;
    END ELSE
    BEGIN
        FOR K:=1 STEP 1 UNTIL N DO
        STDEV[K] := STDEV[K]/SQM;
        SUE := 1.0;
    END;
    PRINT:
    IF NOT OP2 OR NOT OP3 THEN
    BEGIN
        WRITE(FILE1, MNST);
        WRITE(FILE1, LINE, FOR K:=1 STEP 1 UNTIL N DO MN[K]);
        WRITE(FILE1, LINE, FOR K:=1 STEP 1 UNTIL N DO STDEV[K]);
    END;
    IF OP4 THEN
    BEGIN
        WRITE(FILE1, ADJSS);
        FOR K:=1 STEP 1 UNTIL N DO
        WRITE(FILE1, LINE, FOR I:=1 STEP 1 UNTIL K DO S[K,I]);
    END ADJUSTED SUM OF SQUARES MATRIX;
    READ(FILE2, OP, OP1, OP2, OP3, OP4, OPP);
    GO TO STPWSE;
END OF START BLOCK;
STPWSE: BEGIN
COMMENT---STEPWISE PROCEDURE;
```

```
LABEL AGAIN, COMPARE, SWEEP, OUTSTEP;
INTEGER ARRAY INL[1:N], ORL[1:N], OUTL[1:N];
REAL ARRAY S1[1,N], S2[1,N];
FORMAT OUT EDINT("DF FOR E", I5, X4, "DF FOR R", I5, X4, "OMITTED DF",
                 I5, X4, "SWEEPS", I4),
           INCV("INCLUDED VARIABLES"),
           FXCV("EXCLUDED VARIABLES"),
           VBL(30I4),
           RDF( "FI AND FO REDUCED" ),
           ALWA("MSE", F14.6, X5, "MSR", E14.6, X5, "F", F10.2, X5,
                "R X R", F10.6, X5, "AR X AR", F10.6),
           OINV(X20, "INVERSE MATRIX"),
           ALRG(X20, "PARTIAL REGRESSION COEFFICIENTS"),
           RG(X20, "REGRESSION COEFFICIENTS");

FOR K:=1 STEP 1 UNTIL N DO
BEGIN
    INL[K] := 0;
    ORL[K] := 0;
END;
NT := AG := MODAG := 0;
IF MNT = 0 THEN
MNT := N1;
MAXAG := N1 + N1;
IF OPP THEN
MAXAG := N1 + MAXAG;
AGAIN:
A := 0;
B := 1.0@60;
TI := (FIXS[N,N])/((M1-NT-1)+FI);
AG := AG + 1;
IF OPP THEN
BEGIN
    MODAG := MODAG + 1;
    IF MODAG = 3 THEN
    BEGIN
        MODAG := 0;
        TX := 1.0@60;
    END ELSE
    TX := 0.0;
END ELSE
```

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```
TX := (FO×S[N,N])/(M1-NT);
FOR K:=1 STEP 1 UNTIL N1 DO
BEGIN
  TEMP2 := S[K,K];
  IF TEMP2 > ROF THEN
  BEGIN
    TEMP1 + S[N,K];
    TEMP1 := (TEMP1 × TEMP1)/TEMP2;
    IF INL[K] = 0 THEN
    BEGIN
      IF TEMP1 > A THEN
      BEGIN
        A := TEMP1;
        Y := K;
      END;
    END ELSE
    BEGIN
      IF TEMP1 < B THEN
      BEGIN
        B := TEMP1;
        Z := K;
      END;
    END;
  END;
END;
COMPARE:
IF B < TX THEN
BEGIN
  NT := NT - 1;
  FOR K:=INL[Z] STEP 1 UNTIL NT DO
  BEGIN
    ORL[K] := ORL[K+1];
    INL[ORL[K]] := INL[ORL[K]] - 1;
  END;
  INL[Z] := 0;
  ORL[NT+1] := 0;
  Q := Z;
  GO TO SWEEP;
END;
IF A > TI THEN
```

```
BEGIN
  B := A;
  NT := NT + 1;
  IF NT > MNT THEN GO TO OUTSTEP;
  INL[Y] := NT;
  ORL[NT] := Q := Y;
  GO TO SWEEP;
END;
IF A = 0 THEN GO TO OUTSTEP;
MNT := NT + 1;
TI := FI := FO := 0;
WRITE( FILE1, RDF );
GO TO COMPARE;
SWEEP:
Q1 := Q - 1;
S1[Q] := S[Q,Q] := TEMP1 := 1.0/S[Q,Q];
FOR K:=1 STEP 1 UNTIL Q1 DO
BEGIN
  S2[K] := S[Q,K];
  S1[K] := S[Q,K] := S2[K] x TEMP1;
END;
FOR K:=Q+1 STEP 1 UNTIL N DO
BEGIN
  S2[K] := S[K,Q];
  S1[K] := S2[K] x TEMP1;
  S[K,Q] :=0.0;
END;
IF INL[Q] ≠ 0 THEN
BEGIN
  FOR K:=1 STEP 1 UNTIL Q1 DO
  IF INL[K] ≠ 0 THEN
    S2[K] := -S2[K];
  FOR K:=Q+1 STEP 1 UNTIL N1 DO
  IF INL[K] ≠ 0 THEN
    S1[K] := -S1[K];
END ELSE BEGIN
  FOR K:=1 STEP 1 UNTIL Q1 DO
  IF INL[K] = 0 THEN
    S2[K] := -S2[K];
  FOR K:=Q+1 STEP 1 UNTIL N DO
```

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```
    IF INL[K] = 0 THEN
    S1[K] := -S1[K];
    END;
    FOR I:=1 STEP 1 UNTIL Q1, Q+1 STEP 1 UNTIL N DO
    BEGIN
    TEMP1 := S2[I];
    FOR J:=1 STEP 1 UNTIL I DO
    S[I,J] := S[I,J] - S1[J] x TEMP1;
    END;
    IF AG = 1 THEN
    WRITE(FILE1[PAGE]) ELSE
    WRITE(FILE1[DBL]);
    WRITE(FILE1, EDINT, M1-NT, NT, N1-NT, AG);
    WRITE(FILE1, INCV);
    WRITE(FILE1, VBL, FOR I:=1 STEP 1 UNTIL NT DO ORL[I]);
    SSE := SUE x S[N,N];
    RSQ := 1.0 - SSE/SSY;
    IF SSE > ROF THEN
    WRITE(FILE1,ALWA, SSE/(M1-NT), (SSY-SSE)/NT, ((M1-NT)xB)/S[N,N], RSQ,
                        1.0 - (M1/(M-NT))x(SSE/SSY) );

    IF OP1 THEN
    BEGIN
    WRITE(FILE1, OINV);
    FOR K:=1 STEP 1 UNTIL NT DO
    BEGIN
    Q := ORL[K];
    FOR I:=1 STEP 1 UNTIL Q DO
    S[I] := S[Q,I];
    FOR I:=Q+1 STEP 1 UNTIL N1 DO
    S[I] := S[I,Q];
    WRITE(FILE1, LINE, FOR I:=1 STEP 1 UNTIL K DO S[ORL[I]]);
    END;
    END INVERSE MATRIX;
    IF OP2 OR OP3 THEN
    BEGIN
    J := 0;
    FOR K:=1 STEP 1 UNTIL N DO
    IF INL[K] = 0 THEN
    BEGIN
    J := J+1;
```

```
        OUTL[J] := K;
        END;
    WRITE(FILE1, EXCV);
    WRITE(FILE1, VBL, FOR I:=1 STEP 1 UNTIL J DO OUTL[I]);
    IF OP2 THEN
    BEGIN
        WRITE(FILE1, ADJSS);
        FOR K:=1 STEP 1 UNTIL J DO
        BEGIN
            Q := OUTL[K];
            FOR I:=1 STEP 1 UNTIL Q DO
            S[I] := S[Q,I];
            WRITE(FILE1, LINE, FOR I:=1 STEP 1 UNTIL K DO S[OUTL[I]]);
        END;
    END ADJUSTED SUM OF SQUARES MATRIX;
    IF OP3 THEN
    BEGIN
        WRITE(FILE1, ALRG);
        FOR K:=1 STEP 1 UNTIL NT DO
        BEGIN
            Q := ORL[K];
            Q1 := Q - 1;
            FOR I:=1 STEP 1 UNTIL Q1 DO
            S[I] := S[Q,I];
            FOR I:=Q+1 STEP 1 UNTIL N DO
            S[I] := -S[I,Q];
            WRITE(FILE1, LINE, FOR I:=1 STEP 1 UNTIL J DO S[OUTL[I]]);
        END;
    END PARTIAL REGRESSION COEFFICIENTS;
    IF OP4 THEN
    BEGIN
        WRITE(FILE1, RG);
        FOR K:=1 STEP 1 UNTIL NT DO
        S[K] := -S[N,ORL[K]];
        WRITE(FILE1, LINE, FOR K:=1 STEP 1 UNTIL NT DO S[K]);
    END REGRESSION COEFFICIENTS;
    IF AG < MAXAG AND RSQ < RSQMX THEN GO TO AGAIN;
OUTSTEP:
    WRITE(FILE1[PAGE], TIMER, (TIME(1)-TIM)/60);
```

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```
GO TO START;
END OF STEPWISE BLOCK;
EXIT: END;
END.
```

APPENDIX 3

FITTING GUIDANCE FUNCTIONS BY STEPWISE REGRESSION

I. INTRODUCTION

In a plumbline coordinate system x represents the distance, in meters, parallel to the launch azimuth; y represents the distance in meters, parallel to the gravity gradient passing through the launch site with the radius of the earth subtracted; and z represents the distance, in meters, in a direction which with x and y form a right-hand coordinate system.

The state variables for a trajectory of the flight of a powered space vehicle consist of the three space coordinates x, y, z; the three velocity components $\dot{x}$, $\dot{y}$, $\dot{z}$, measured in meters per second; the thrust per unit mass $\frac{F}{m}$ measured in meters per second per second; the time from lift off T measured in seconds; and the rate of change of mass per unit mass $\frac{\dot{m}}{m}$, measured per second.

The three guidance functions under consideration are the pitch steering angle X_p, measured in degrees; the yaw steering angle X_y, measured in degrees; and the time remaining to cutoff of power TR, measured in seconds.

The three guidance functions

$$X_p = X_p \left(x,\ y,\ z,\ \dot{x},\ \dot{y},\ \dot{z},\ \frac{F}{m},\ T,\ \frac{\dot{m}}{m} \right),$$

$$X_y = X_y \left(x,\ y,\ z,\ \dot{x},\ \dot{y},\ \dot{z},\ \frac{F}{m},\ T,\ \frac{\dot{m}}{m} \right),$$

and

$$TR = TR \left(x,\ y,\ z,\ \dot{x},\ \dot{y},\ \dot{z},\ \frac{F}{m},\ T,\ \frac{\dot{m}}{m} \right)$$

are approximated by third degree polynomials in the nine variables. With this approximation there are 219 estimation variables (220 with a constant term included). However, since it is difficult to measure $\frac{\dot{m}}{m}$, this variable might

be eliminated. In this case there would be 164 estimation variables (165 with a constant term included).

The objective of this study was to find an optimal (or near optimal) polynomial approximating the guidance functions by employing the stepwise regression procedure.

The data were taken from 75 calculus of variations trajectories generated by the Marshall Space Flight Center at Huntsville, Alabama, to simulate actual flight. The trajectories were between 600 and 700 seconds in length with data sampled at five second intervals from 140 seconds to cutoff. Two data bases were used consisting of subsets of the total sampled data. The first data base consisted of data taken at five second intervals from 140 seconds to 300 seconds, at 20 second intervals from 300 seconds to 540 seconds, and at 40 second intervals from 540 seconds to cutoff. The second data base, a subset of the first, consisted of data samples at 140 seconds, at 260 seconds, at 500 seconds, and at 60 second intervals from 300 seconds to 540 seconds together with data in either or both of two groups sampled at 15 second and 50 second intervals from 540 seconds to cutoff. The second data base is weighted more heavily near the end of the trajectory, since the guidance functions are more critical in that region. The two data bases consist of 2605 and 1219 data points respectively.

Several of the variables were scaled to get the elements of the sum of squares matrix to approximately the same order of magnitude. The variables x, y, and z are multiplied by 10^{-6}, $\dot{x}$, $\dot{y}$, and $\dot{z}$ by 0.001, T by 0.01, and $\frac{\dot{m}}{m}$ by 100.

Several B-5500 runs were made using the stepwise regression procedure. In ten of the eighteen runs X_p was the dependent variable, while in four runs

each X_y and TR was the dependent variable. The terms involving $\frac{\dot{m}}{m}$ were excluded from all but two of the runs. A detailed description of the individual runs is given in the next section.

II. DESCRIPTION OF RUNS

Run 1

The matrix used in this analysis was the NASA supplied single precision sum of squares matrix adjusted for the mean with X_p as the dependent variable. There were 164 terms in the polynomial model in addition to the constant term. The matrix was accurate to approximately eight digits before mean adjustment.

This run stopped due to accumulation of roundoff error after picking up eleven terms. The results are shown in Table I. The column labelled "No. of

TABLE I

RESULTS OF RUN 1

No of Terms	Term	F	R^2
1	$y^2\dot{z}$	278716.35	.9900
2	$y^2\dot{x}$	129.50	.9905
3	$y^2\dot{y}$	1092.25	.9932
4	$\frac{F}{m}t^2$	663.46	.9945
5	$y\dot{z}^2$	666.72	.9955
6	$\dot{y}t^2$	875.77	.9966
7	$y\dot{x}$	282.43	.9969
8	xz^2	1105.93	.9978
9	$z\dot{x}$	3227.71	.9990
10	$z^2\dot{z}$	913.12	.9992
11	$yz\dot{x}$	---	---

Terms" contains the number of estimation variables (excluding the mean) included in the regression model at the end of that step. The column "Term" is the estimation variable added to the model in that step. The column "F" is the F-statistic,

$$F = \frac{\displaystyle\sum_{\mu=1}^{N}\left(\sum_{i=1}^{M} b_i z_{\mu i}\right)^2 \Big/ m-1}{\displaystyle\sum_{\mu=1}^{N}\left(y_\mu - \sum_{i=1}^{m} b_i z_{\mu i}\right)^2 \Big/ N-m} ,$$

where m is the number of estimation variables in the model; N is the number of observations; b_1, b_2, ..., b_m are the regression coefficients at a stage; y_1, y_2, ..., y_N are observations (mean adjusted) on the dependent variable; and z_{11}, z_{21}, ..., z_{N1}, ..., z_{1m}, ..., z_{Nm} are observations (mean adjusted) on the estimation variables. The column "R^2" is the square of the multiple correlation coefficient,

$$R^2 = \frac{\displaystyle\sum_{\mu=1}^{N}\left(\sum_{i=1}^{m} b_i z_{\mu i}\right)^2}{\displaystyle\sum_{\mu=1}^{N} y_\mu^2}$$

The values of F and R^2 are meaningless for the last term added to the model, since the sum of squares of error went negative due to excessive roundoff.

It was hoped that this run would duplicate the results obtained at NASA, but such was not the case. It was discovered that the difference was due to the fact that the matrix used in the NASA run was not mean-adjusted, while that

used in this run was mean-adjusted. A significant conclusion from this run was that the very high multiple correlation for a small number of terms made confirmation to pick out the best forty terms unnecessary.

Run 2

The matrix used in this analysis was a part of that used in run 1. It was mean-adjusted and in addition to the mean had fifty-two terms in the model. These terms were those which had been selected in run 1 together with those selected by NASA. No throwout criterion was used.

This run stopped due to accumulation of roundoff error after sixteen terms were selected. The results are shown in Table II. The first four columns have the same significance as in Table I. The additional column "R^2 (Run 1)" gives, for comparison purposes, the value of R^2 for the same number of terms in Run 1. The higher correlation is considered better.

The object of this run was to determine why run 1 failed to duplicate the NASA run. The adjusted sum of squares matrix was printed at each step for further study. It was concluded that more precision was needed in the original matrix. However, it was later found that this was not a serious problem.

This run should have had the same terms enter as in run 1. However, inadvertently the variable yz^2 was omitted from the model. Even though this term was left out the multiple correlation was better than in run 1.

TABLE II

RESULTS OF RUN 2

No of Terms	Term	F	R^2	R^2 (Run 1)
1	$y^2\dot{z}$	278716.35	.9900	.9900
2	$y^2\dot{x}$	129.50	.9905	.9905
3	$y^2\dot{y}$	1092.25	.9932	.9932
4	$\frac{F}{m}t^2$	663.46	.9945	.9945
5	$y\dot{x}$	622.07	.9955	.9955
6	xz^2	1480.22	.9970	.9966
7	y	3794.25	.9987	.9969
8	$y^2\frac{F}{m}$	606.17	.9990	.9978
9	$z\dot{x}$	391.55	.9991	.9990
10	$\frac{F}{m}t$	723.06	.9993	.9992
11	xyt	833.33	.9994	---
12	$yz\dot{x}$	---	---	---
13	x	---	---	---
14	$y\dot{x}\dot{z}$	---	---	---
15	z	---	---	---
16	$\dot{x}$	---	---	---

<u>Run 3</u>

The matrix used for this run was the same as that in run 2, except that it was accurate to twelve significant figures (B-5500 single precision) before mean-adjustment. No throwout criterion was used.

This run stopped after selecting thirteen terms. The results are shown in Table III. The columns have the same significance as in run 1.

TABLE III

RESULTS OF RUN 3

No of Terms	Term	F	R^2
1	$y^2\dot{z}$	278715.24	.9900
2	$y^2\dot{x}$	129.53	.9905
3	$y^2\dot{y}$	1092.35	.9932
4	$\frac{F}{m}t^2$	663.43	.9945
5	$y\dot{x}$	622.40	.9955
6	xz^2	1472.72	.9970
7	$yz\dot{x}$	3554.06	.9987
8	yt	823.00	.9990
9	x	332.94	.9991
10	y^3	122.67	.9991
11	$z\dot{x}$	3728.64	.9996
12	$(\frac{F}{m})^2t$	---	---
13	$x\dot{y}^2$	---	---

The object of this run was to show that the NASA run could be duplicated
if precision were increased. Again this failed, because the matrix was mean-
adjusted. A comparison of regression coefficients obtained in run 2 and run 3
is shown in Table IV. The column "No. of Terms" contains the number of esti-
mation variables in the regression model at that step. The column "Term" con-
tains each variable in the model at that step. The columns "Coefficients"
with the names of the two runs contain the regression coefficients at that
stage.

Discrepancies occurred, because of the slightly different sum of squares
matrix. This run confirmed the suspicion that the difference in the results
obtained here and at NASA was due to the mean-adjustment of the matrix.

TABLE IV

COMPARISON OF REGRESSION COEFFICIENTS FOR X_p - ORIGINAL MATRIX IN
SINGLE PRECISION (RUN 2) vs. DOUBLE PRECISION (RUN 3)

No of Terms	Term	Coefficients	
		Run 2	Run 3
1	y^2_z	- .8234568	- .8234567
2	y^2_z	- .4853059	- .4852689
	y^2_x	.1805880	.1806077
3	y^2_z	- .3400263	- .3399650
	y^2_x	.7191974	.7192526
	y^2_y	.4772935	.4773168

(Continued)

TABLE IV (Concluded)

No of Terms	Term	Coefficients Run 2	Coefficients Run 3
4	$y^2\dot{z}$	− .6921609	− .6920876
	$y^2\dot{x}$	.6865594	.6866178
	$y^2\dot{y}$	.7106122	.7106299
	$\frac{F}{m}t^2$	.01106846	.01106811
5	$y^2\dot{z}$	− .5068506	− .5068816
	$y^2\dot{x}$	1.989755	1.989662
	$y^2\dot{y}$	.7014382	.7014511
	$\frac{F}{m}t^2$	.003688024	.003687849
	$y\dot{x}$	− 8.378824	− 8.378211
6	$y^2\dot{z}$	− .5587895	− .5592727
	$y^2\dot{x}$	6.607538	6.589411
	$y^2\dot{y}$	.9721991	.9712973
	$\frac{F}{m}t^2$	.002051094	.002051780
	$y\dot{x}$	−38.13662	−38.02102
	xz^2	39.95789	39.82414

Run 4

The matrix used on this run was the same as that used in run 3, except that it was not mean adjusted. The mean was not considered as a variable in the model. No throwout criterion was used.

This run stopped due to accumulation of roundoff error after selecting twenty terms. The results are shown in Table V. The columns have the same significance as in Table I, except that the variables used in calculating F and R^2 were not mean adjusted.

TABLE V

RESULTS OF RUN 4

No of Terms	Term	F	R^2
1	$y^2\dot{z}$	5385402.59	.99948
2	$y^2\dot{y}$	302.80	.99953
3	z	535.37	.99961
4	x	204.50	.99963
5	y	116.17	.99965
6	$y^2\dot{x}$	597.52	.99971
7	$(\frac{F}{m})^3$	115.97	.99972
8	y^3	849.62	.99979
9	$y\dot{y}t$	2748.11	.99989
10	$\dot{y}^3$	491.29	.99991
11	yt	1882.93	.99994
12	xyt	189.91	.99995
13	$\dot{z}t^2$	111.16	.99995
14	$x\dot{y}^2$	554.16	.99996
15	$y\dot{x}$	1108.53	.99997
16	$\frac{F}{m}t$	3802.84	.99999
17	z^2	---	---

(Continued)

TABLE V (Concluded)

No of Terms	Term	F	R^2
18	$\ddot{y}\dot{z}^2$	---	---
19	$y^2\frac{F}{m}$	---	---
20	$z\left(\frac{F}{m}\right)^2$	---	---

The object of this run was to duplicate the NASA run. The first fourteen terms were the same in the two runs. This agreement is very good considering the high correlation involved.

The coefficients obtained on this run agree with those on the NASA run to three significant digits through the first eight terms. An additional comparison was made by inverting the sum of squares submatrices in double precision. These results and those of run 4 were more in agreement with each other than with the NASA run. Some comparisons of coefficients are shown in Table VI.

TABLE VI

COMPARISON OF REGRESSION COEFFICIENTS FOR X_p, NOT MEAN ADJUSTED - NASA, STEPWISE PROCEDURE (RUN 5), DOUBLE PRECISION

No of Terms	Term	Coefficients		
		NASA	Stepwise	DP
1	$y^2\dot{z}$	- .8484887	- .8484887	- .8484887
3	$y^2\dot{z}$	- .5550050	- .5550408	- .5550408
	$y^2\dot{y}$	.3300267	.3299901	.3299901
	z	- 68.26085	- 68.25281	- 68.25281

(Continued)

TABLE VI (Continued)

No of Terms	Term	Coefficients		
		NASA	Stepwise	DP
5	$y^2\dot{z}$	- .8622132	- .8620839	- .8620839
	$y^2\dot{y}$	.4707735	.4706966	.4706966
	z	-168.8408	-168.7116	-168.7116
	x	57.08999	- 57.02029	- 57.02030
	y	- 2.828727	- 2.827894	- 2.827895
8	$y^2\dot{z}$	- .5177044	- .5170714	- .5170715
	$y^2\dot{y}$	.9110512	.9110047	.9110048
	z	-136.2729	-136.0928	-136.0930
	x	- 41.52626	- 41.45290	- 41.45297
	y	- 26.72016	- 26.71975	- 26.71976
	$y^2\dot{x}$	.6128534	.6134570	.6134570
	$(\frac{F}{m})^3$	.00071270	.00071228	.00071228
	y^3	.3381630	.3380557	.3380558
10	$y^2\dot{z}$	- .4573042	- .4563642	- .4563643
	$y^2\dot{y}$	1.546414	1.535040	1.535043
	z	- 99.03508	- 98.42050	- 98.42082
	x	- 10.74897	- 10.76470	- 10.76480
	y	-114.4591	-113.1464	-113.1468
	$y^2\dot{x}$	.4089275	.4129437	.4129428
	$(\frac{F}{m})^3$	.00016815	.00017921	.00017921

(Continued)

TABLE VI (Continued)

No of Terms	Term	Coefficients		
		NASA	Stepwise	DP
10	y^3	2.470939	2.439340	2.439349
	$y\dot{y}t$	- 1.407387	- 1.387498	- 1.387504
	$\dot{y}^3$	.6043025	.6001786	.6001800
13	$y^2\dot{z}$	- .3357826	- .3344632	- .3344556
	$y^2\dot{y}$	1.071897	1.078982	1.078989
	z	-125.2351	-124.0098	-124.0111
	x	20.85913	20.43924	20.44013
	y	-155.2974	-151.3697	-151.3699
	$y^2\dot{x}$	.02238136	.04456476	.04456466
	$(\frac{F}{m})^3$	.00177447	.00172243	.00172242
	y^3	3.807856	3.698213	3.698219
	$y\dot{y}t$	- .7860138	- .7902662	- .7902785
	$\dot{y}^3$	1.321196	1.298609	1.298624
	yt	- 4.607292	- 4.406400	- 4.406398
	xyt	2.278608	2.131351	2.131290
	$\dot{z}t^2$	.3072210	.2824692	.2824499
14	$y^2\dot{z}$	- .6586389	- .6833111	- .6832994
	y^2y	.2644380	.2103839	.2104183
	z	- 88.77506	- 84.89537	- 84.89571
	x	- 74.89652	- 82.89925	- 82.89576

(Continued)

TABLE VI (Concluded)

No of Terms	Term	Coefficients		
		NASA	Stepwise	DP
14	y	-144.9732	-140.6013	-140.6016
	$y^2\dot{x}$	.1242356	.1526890	.1526897
	$(\frac{F}{m})^3$	.00212057	.00209391	.00209388
	y^3	3.525092	3.403921	3.403924
	$y\dot{y}t$	.5923321	.6921863	.6921283
	$\dot{y}^3$	6.345729	6.642542	6.642404
	yt	- 3.677377	- 3.435859	- 3.435833
	xyt	4.989600	5.077270	5.077138
	$\dot{z}t^2$	.9154489	.9405285	.9405001
	$x\dot{y}^2$	10.38705	11.07432	11.07403

The columns "No. of Terms" and "Term" have the same significance as in Table IV. The columns of coefficients are labelled "NASA," those in the NASA run; "Stepwise," those in Run 5; and "DP," those obtained by the double precision inversion procedure.

This run confirmed the method used in the NASA run and indicated more strongly that because of the high correlations all terms beyond the first few were probably not needed. A great deal of accuracy was lost due to the high correlation.

Run 5

The matrix used in this run was the NASA sum of squares matrix, accurate to sixteen significant digits (NASA double precision). The mean and most significant variable $(y^2\dot{z})$ were eliminated in double precision, leaving about twelve digits after the adjustment. This gives a model with 163 terms and a fairly accurate sum of squares matrix. No throwout criterion was used.

This run stopped after selecting twelve terms. The results are shown in Table VII. The columns have the same significance as in Table I, except that the

TABLE VII

RESULTS OF RUN 5

No of Terms	Term	F	R^2
1	$y^2\dot{x}$	129.57	.0442
2	$y^2\dot{y}$	1092.74	.3124
3	$\frac{F}{m}t^2$	663.67	.4441
4	$y\dot{z}^2$	666.82	.5510
5	$\dot{y}t^2$	875.31	.6580
6	$y\dot{x}$	284.12	.6895
7	xz^2	1096.91	.7770
8	$yz\dot{x}$	2930.59	.8911
9	$\dot{x}\dot{z}t$	639.18	.9114
10	$z^2\dot{z}$	340.26	.9210
11	$z\dot{x}$	---	---
12	x^2t	---	---

variables used to calculate F and R^2 are adjusted for the most significant variable as well as for the mean. The column "No. of Terms" excludes the previously eliminated variable. The object of this run was to choose the most accurate fit by the straight step-up procedure to compare with subsequent runs using a throwout criterion. Mean-adjustment was used because it seems more reasonable to eliminate the constant term since it is so easy to evaluate in a polynomial model.

A comparison of this run with Run 1 shows that the first eight terms were selected in the same order. This indicates that these terms are not sensitive to slight matrix errors.

Run 6

The matrix used in this run was the NASA sum of squares matrix, accurate to about 12 significant digits after adjustment for the mean and most significant variable $(y^2\dot{z})_N$ in double precision with the terms in the model consisting of the terms selected in run 5 together with all terms containing $\dot{m}/m$. (The $\dot{m}/m$ terms had been omitted in all previous runs.) This gave a model with 66 terms. No throwout criterion was used.

This run stopped after obtaining 11 additional terms. The third term brought in was $yt\frac{\dot{m}}{m}$ with an F of 757. The corresponding terms in run 5 was $\frac{F}{m}t^2$, brought in with an F of 664. The results are shown in Table VIII.

The columns have the same meaning as in Table I. Due to an error in the program R^2 was not found. F was based on variables adjusted for $y^2\dot{z}$ as well as the mean.

The object of this run was to see if the $\frac{\dot{m}}{m}$ terms would greatly improve the fit of the model. A slight programming error prevented a complete analysis of

TABLE VIII

RESULTS OF RUN 6

No of Terms	Term	F
1	$y^2\dot{x}$	129.57
2	$y^2\dot{y}$	1092.74
3	$yt\frac{\dot{m}}{m}$	756.89
4	x^2t	326.96
5	$\dot{y}t^2$	1163.19
6	$y\dot{x}$	274.36
7	xz^2	1122.50
8	$z\dot{x}$	2770.60
9	$z^2\dot{z}$	362.31
10	$t\frac{\dot{m}}{m}$	7305.95
11	$\dot{y}\frac{F}{m}\frac{\dot{m}}{m}$	---

this study but it seems clear that the $\frac{\dot{m}}{m}$ terms do not make a radical improvement in the least squares fit.

Run 7

In this run the matrix described in run 5 was used, with the mean and most significant variable ($y^2\dot{z}$) eliminated in double precision. A throwout criterion was used. This criterion consisted of throwing out any variable which had an F of less than F_c and then admitting the "best" variable if it had an F greater than F_c. If the best variable did not have an F greater than F_c then F_c was

halved and the process repeated. The process started with F_c = 1000 and selected the first variable with an F of 130. The entire run was made with an F_c of 125. There was no provision for throwing out the mean or $y^2\dot{z}$. The run stopped after selecting nineteen terms. The results are shown in Table IX.

TABLE IX

RESULTS OF RUN 7

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 5)
1	1	$y^2\dot{x}$	129.57		.0442	.0442
2	2	$y^2\dot{y}$	1092.74		.3124	.3124
3	3	$\frac{F}{m}t^2$	663.67		.4441	.4441
4	4	$y\dot{z}^2$	666.82		.5510	.5510
5	5	$\dot{y}t^2$	875.31		.6580	.6580
6	4	$\frac{F}{m}t^2$		3.50	.6575	.5510
7	5	$y\dot{x}$	269.15		.6876	.6580
8	6	xz^2	1120.15		.7769	.6895
9	7	$z\dot{x}$	2747.50		.8875	.7770
10	6	$y\dot{z}^2$		1.50	.8874	.6895
11	7	$\dot{y}$	128.17		.8923	.7770
12	6	$y^2\dot{y}$		20.90	.8915	.6895
13	7	$\frac{F}{m}$	434.29		.9061	.7770
14	8	$\frac{F}{m}t$	328.81		.9160	.8911
15	9	xz	300.53		.9241	.9114
16	10	xyz	2602.78		.9607	.9210

(Continued)

TABLE IX (Concluded)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 5)
17	9	xz^2		3.04	.9607	.9114
18	10	$z^2\dot{y}$	---		---	.9210
19	11	$\dot{x}^2\dot{y}$	---		---	---

The column "Sweep" contains the number of steps in which a variable was either added or dropped. The column "No. of Terms" contains the number of estimation variables in the regression model after the step. The column "Term" contains the estimation variable added or dropped from the model at this step. The column "F in" contains the value of F after the step if a variable was added. The column "F out" contains the value of F before the step if a variable was dropped. The column "R^2" has the same meaning as in Table I. The column "R^2 (Run 5)" contains the value of R^2 for the same number of terms in the model in Run 5. Again in this case, F and R^2 were calculated from variables which were adjusted from the most significant variable as well as the mean.

As a sample comparison, the best seven-term polynomial obtained on this run had R^2 = .906 while the seven-term polynomial obtained in run 5 without a throw-out criterion had R^2 = .777. This indicates that the throwout criterion is of significant value in this model.

Run 8

In this run a sub-sample of the data used in the previous runs was selected. A matrix with 164 terms in the model was generated and adjusted for the mean. No throw-out criterion was used.

This run stopped after 27 terms due to accumulation of roundoff error. The results are shown in Table X. The columns have the same meaning as in Table I.

TABLE X

RESULTS OF RUN 8

No of Terms	Term	F	R^2
1	$y^2\dot{z}$	126238.18	.9905
2	$y^2\dot{x}$	59.66	.9909
3	$y^2\dot{y}$	437.03	.9933
4	$y\frac{F}{m}t$	294.10	.9946
5	$y\dot{z}^2$	174.95	.9953
6	$\dot{y}t^2$	471.52	.9966
7	$y\dot{x}$	113.75	.9969
8	x^2z	440.91	.9977
9	$yz\dot{x}$	1096.30	.9988
10	$\dot{x}\dot{z}t$	302.20	.9990
11	z	54.60	.9991
12	$z^2\dot{z}$	39.65	.9991
13	$y(\frac{F}{m})^2$	39.29	.9991
14	$\dot{y}^3$	188.69	.9993
15	$\dot{z}\frac{F}{m}t$	182.28	.9994
16	$z^2\frac{F}{m}$	102.94	.9994
17	$z\dot{z}\frac{F}{m}$	72.72	.9994

(Continued)

TABLE X (Concluded)

No of Terms	Term	F	R^2
18	$y\dot{y}$	26.71	.9995
19	$\dot{y}t$	43.04	.9995
20	$y\dot{y}\frac{F}{m}$	55.37	.9995
21	$\dot{y}\frac{F}{m}$	34.41	.9995
22	$\dot{y}$	40.25	.9995
23	$xz\dot{x}$	3770.59	.9999
24	$x\frac{F}{m}t$	---	---
25	$(\frac{F}{m})^2 t$	---	---
26	$\dot{x}(\frac{F}{m})^2$	---	---
27	$x\dot{x}y$	---	---

The object of this run was to see if the order in which the terms were chosen was data dependent. A comparison of the terms in this run with those in run 5 shows that in this run term 4 ($y\frac{F}{m}t$) and Term 8 ($x^2 z$) were substituted for $\frac{F}{m}t^2$ and xz^2, obtained in run 5. With these two exceptions the two runs agreed through 10 terms.

The comparison of regression coefficients for the two runs are shown in Table XI. The column "No. of Terms" contains the number of terms in the model, including the one previously eliminated in Run 5. The column "Term" contains the individual estimation variables in the model at each step. The coefficient of the previously eliminated variable was not available in Run 5. Blank spaces occur in the table where the two runs selected different variables.

TABLE XI

COMPARISON OF REGRESSION COEFFICIENTS FOR X_p

FOR TWO DATA BASES - RUN 5 VS. RUN 8

No of Terms	Term	Coefficients	
		Run 5	Run 8
2	$y^2\dot{z}$	---	- .48438
	$y^2\dot{x}$	.18061	.18088
3	$y^2\dot{z}$	---	- .34662
	$y^2\dot{x}$	.71925	.69356
	$y^2\dot{y}$	.47732	.45339
4	$y^2\dot{z}$	---	- .68870
	$y^2\dot{x}$	.68662	.64266
	$y^2\dot{y}$	.71063	.68497
	$\frac{F}{m}t^2$	.01107	
	$y\frac{F}{m}t$		.01581
5	$y^2\dot{z}$	---	- .82913
	$y^2\dot{x}$	.70617	.65162
	$y^2\dot{y}$	.73218	.70280
	$\frac{F}{m}t^2$	.03333	
	$y\frac{F}{m}t$		.03885
	$y\dot{z}^2$	.66818	- .48003

(Continued)

TABLE XI (Continued)

No of Terms	Term	Coefficients	
		Run 5	Run 8
6	$y^2\dot{z}$	---	- 2.1083
	$y^2\dot{x}$	.65638	.65002
	$y^2\dot{y}$	.93360	.91354
	$\frac{F}{m}t^2$	.00249	
	$y\frac{F}{m}t$		.00355
	$y\dot{z}^2$	- 2.2942	- 2.2808
	$\dot{y}t^2$	- .65313	- .64631
7	$y^2\ddot{z}$	---	- 1.5468
	$y^2\dot{x}$	3.4174	3.3683
	$y^2\dot{y}$	.92357	.91387
	$\frac{F}{m}t^2$	.00531	
	$y\frac{F}{m}t$		.00579
	$y\dot{z}^2$	- 1.3794	- 1.4387
	$\dot{y}t^2$	- .82546	- .84240
	$y\dot{x}$	-18.090	-17.870
8	$y^2\dot{z}$	---	- 1.0858
	$y^2\dot{x}$	7.2391	7.1517
	$y^2\dot{y}$	1.0728	1.0729
	$\frac{F}{m}t^2$	.01009	
	$y\frac{F}{m}t$		.00299

(Continued)

TABLE XI (Continued)

No of Terms	Term	Coefficients	
		Run 5	Run 8
8	$y\dot{z}^2$	$-$ .78559	$-$ .75808
	$\dot{y}t^2$	$-$ .63313	$-$ .61376
	$y\dot{x}$	-42.643	-41.972
	xz^2	31.507	
	x^2z		-16.355
9	$y^2\dot{z}$	$---$	$-$ .28089
	$y^2\dot{x}$	13.768	13.743
	$y^2\dot{y}$	1.1878	1.2002
	$\frac{F}{m}t^2$	$.01048$	
	$y\frac{F}{m}t$		$.01222$
	$y\dot{z}^2$	$.25766$	$.19476$
	$\dot{y}t^2$	$-$ .29513	$-$ .31085
	$y\dot{x}$	$-$ .88929	$-$ .88587
	xz^2	52.455	
	x^2z		-28.255
	$yz\dot{x}$	$-$ 3.7618	$-$ 3.6822
10	$y^2\dot{z}$	$---$	$.22053$
	$y^2\dot{x}$	13.746	13.776
	$y^2\dot{y}$	1.1367	1.1958

(Continued)

TABLE XI (Concluded)

No of Terms	Term	Coefficients	
		Run 5	Run 8
10	$\frac{F}{m}t^2$	.06048	
	$y\frac{F}{m}t$		.07341
	$y\dot{z}^2$	1.9980	1.9416
	$\dot{y}t^2$	- .39379	- .56781
	$y\dot{x}$	-88.146	-88.150
	xz^2	58.915	
	x^2z		-33.479
	$yz\dot{x}$	- 4.8790	- 4.6496
	$\dot{x}\dot{z}t$	1.5577	1.7201

The comparison indicates that the two terms $y\frac{F}{m}t$ and $\frac{F}{m}t^2$ are very nearly linearly related. In any case, a look at run 5 shows that $\frac{F}{m}t^2$ is eliminated with a very small F and that eventually xz^2 is also eliminated. The coefficients for the other terms agree remarkably well.

From this run, it seems that only about 6 terms are valid predictors but the fit is so good that it is hard to draw a firm conclusion.

Run 9

The matrix used in run 8, with the most significant variable $(y^2\dot{z})$ omitted from the model was used in this run. There were 163 terms in the model. No throwout criterion was used.

The run stopped after selecting 31 variables. The results are shown in Table XII. The columns have the same significance as in Table I. A comparison of R^2 with that of Run 8 with the same number of terms is included.

TABLE XII

RESULTS OF RUN 9

No of Terms	Term	F	R^2	R^2 (Run 8)
1	$y^2\dot{x}$	120293.22	.9900	.9905
2	$y^2\dot{y}$	487.82	.9929	.9909
3	$y\dot{z}$	200.71	.9939	.9933
4	z	83.50	.9943	.9946
5	y^3	35.10	.9943	.9953
6	$y\dot{y}t$	1479.98	.9975	.9966
7	$\dot{y}^3$	348.10	.9980	.9969
8	y^2t	134.71	.9982	.9977
9	$z\dot{y}\frac{F}{m}$	450.26	.9987	.9988
10	$\dot{y}\dot{z}\frac{F}{m}$	332.33	.9990	.9990
11	$\dot{y}\frac{F}{m}t$	187.36	.9991	.9991
12	$y\dot{z}t$	281.19	.9993	.9991
13	$\dot{z}(\frac{F}{m})^2$	158.81	.9994	.9991
14	t^3	43.47	.9994	.9993
15	$(\frac{F}{m})^2t$	32.86	.9994	.9994
16	$x\dot{y}\frac{F}{m}$	66.93	.9994	.9994

(Continued)

TABLE XII (Concluded)

No of Terms	Term	F	R^2	R^2 (Run 8)
17	$\frac{F}{m}t^2$	21.73	.9995	.9994
18	$\dot{z}^2\frac{F}{m}$	52.20	.9995	.9995
19	$\dot{x}\frac{F}{m}t$	32.81	.9995	.9995
20	t^2	12.62	.9995	.9995
21	$\frac{F}{m}t$	30.43	.9995	.9995
22	$y\frac{F}{m}t$	65.75	.9995	.9995
23	xyt	27.20	.9995	.9999
24	$xy\frac{F}{m}$	29.95	.9996	---
25	xt	23.05	.9996	---
26	$z\dot{y}\dot{z}$	23.76	.9996	---
27	$\dot{y}t$	54.20	.9996	---
28	$yz\dot{z}$	93.46	.9996	---
29	$\dot{y}\dot{z}t$	---	---	---
30	$\dot{y}$	---	---	---
31	$\dot{x}t^2$	---	---	---

The purpose of this run was to see if $y^2\dot{z}$ was really important or if some other variables would serve just as well. This run showed that not only was $y^2\dot{z}$ not necessary but that overall the results were better without it. In particular it was not one of the best two variables since $y^2\dot{x}$ and $y^2\dot{y}$, with $R^2 = .993$, were better than $y^2\dot{z}$ and $y^2\dot{x}$, with $R^2 = .991$.

This would indicate that there are a lot of different collections of terms all of which can be made to fit very well. There is no need, therefore, to pick the "best" model if there are many models which are essentially as good.

Run 10

The matrix used in this run was the same as that used in run 8 with the throwout criterion described for run 7. The first term was selected with an F of 126,000. Fc started at 1000 and was eventually reduced to 0.9765625.

The run stopped after selecting 32 terms. The results, including a comparison with run 8, are shown in Table XIII. The results for the first six terms are the same as in run 8. The columns have the same meaning as those in Table VII (except, of course, that no variables except the mean were previously eliminated). Hence, F and R^2 are calculated with respect to variables adjusted for the mean only. The conclusion drawn from this run was that there is no reason for including more than 10 terms in the model.

TABLE XIII

RESULTS OF RUN 10

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 8)
1	1	$y^2\dot{z}$	126238.18		.9905	.9905
2	2	$y^2\dot{x}$	59.66		.9909	.9909
3	3	$y^2\dot{y}$	437.03		.9933	.9933
4	4	$y\frac{F}{m}t$	294.10		.9946	.9946
5	5	$y\dot{z}^2$	174.95		.9953	.9953

(Continued)

TABLE XIII (Continued)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 8)
6	6	$\dot{y}t^2$	471.52		.9966	.9966
7	5	$y\frac{F}{m}t$		2.34	.9966	.9953
8	6	$y\dot{x}$	109.01		.9969	.9966
9	7	x^2z	447.16		.9977	.9969
10	8	$yz\dot{x}$	966.98		.9987	.9977
11	7	$y\dot{z}^2$		0.89	.9987	.9969
12	8	$y(\frac{F}{m})^2$	128.66		.9989	.9977
13	9	$\dot{x}\frac{F}{m}t$	245.89		.9990	.9988
14	10	$\dot{y}^3$	151.85		.9992	.9990
15	11	$yz\frac{F}{m}$	126.88		.9992	.9991
16	12	$y\dot{x}\dot{z}$	156.42		.9993	.9991
17	13	$x^2\dot{y}$	72.56		.9994	.9991
18	12	$\dot{y}t^2$		7.07	.9994	.9991
19	13	$z\dot{x}\dot{y}$	37.24		.9994	.9991
20	14	$z\dot{y}^2$	22.14		.9994	.9993
21	13	$\dot{y}^3$		6.49	.9994	.9991
22	12	x^2z		6.01	.9994	.9991
23	13	z	38.31		.9994	.9991
24	14	$\dot{y}^2\dot{z}$	30.91		.9994	.9993
25	13	$z\dot{x}\dot{y}$		0.00	.9994	.9991
26	14	yz^2	4.45		.9994	.9993

(Continued)

TABLE XIII (Continued)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 8)
27	15	$\dot{z}^2$	7.79		.9994	.9994
28	14	$yz\dot{x}$		0.25	.9994	.9993
29	15	$(\frac{F}{m})^2$	5.76		.9994	.9994
30	16	$\dot{z}^2 t$	31.70		.9994	.9994
31	15	yz^2		3.11	.9994	.9994
32	16	x^3	19.25		.9994	.9994
33	17	$z\dot{x}\dot{y}$	14.72		.9995	.9994
34	18	$\dot{y}^2 t$	26.41		.9995	.9995
35	19	$z\frac{F}{m}$	58.46		.9995	.9995
40	16	z		1.02	.9995	.9994
45	17	$y^2\dot{y}$		0.20	.9995	.9994
50	18	$x^2\dot{y}$	4.47		.9995	.9995
55	21	$y^2\dot{y}\frac{F}{m}$	1.82		.9995	.9995
60	24	$\dot{z}(\frac{F}{m})^2$	8.31		.9995	---
65	23	$y\dot{x}t$	4.60		.9995	.9999
70	24	$\dot{y}^2\frac{F}{m}$	8.15		.9996	---
75	23	$x\dot{z}t$	3.55		.9996	.9999
80	24	$z\dot{z}^2$		0.06	.9996	---
85	25	xt^2	34.84		.9996	---
90	26	$y^2\frac{F}{m}$		0.97	.9996	---
91	27	$z\dot{y}t$	55.83		.9996	---
92	28	$z\dot{x}\frac{F}{m}$	151.28		.9997	---

(Continued)

TABLE XIII (Concluded)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 8)
93	27	$\dot{z}^2 \frac{F}{m}$		0.01	.9997	---
94	26	$\dot{y}^3$		0.27	.9997	---
95	27	$xy\dot{y}$	7003.83		.9999	---
96	28	$x^2 \dot{y}$	---		---	---
97	29	$\dot{y}^2 \frac{F}{m}$	---		---	---
98	30	$y\dot{z} \frac{F}{m}$	---		---	---
99	31	$y\dot{z}^2$	---		---	---
100	32	$\dot{y}^3$	---		---	---

Run 11

The matrix used in this run was the same as that used in run 5, except that the dependent variable was X_y and the most significant variable (which was eliminated in double precision, together with the mean) was y. No throwout criterion was used.

The run stopped after 12 variables were selected. The results are shown in Table XIV. The columns have the same meaning as those in Table VII.

It was not necessary to eliminate the variable y in double precision. However, the mean should be eliminated in double precision, since it accounted for most of the sum of squares.

TABLE XIV

RESULTS OF RUN 11

No of Terms	Term	F	R^2
1	$y^2\dot{x}$	2864.86	.5055
2	$y\dot{z}$	635.48	.5969
3	$yz\dot{x}$	69.47	.6066
4	$xy\dot{x}$	4461.35	.8483
5	$\dot{y}$	476.88	.8704
6	$\dot{z}^2t$	456.58	.8886
7	$\dot{x}t$	181.31	.8954
8	y^2	228.32	.9033
9	yz	224.59	.9110
10	xy	1188.58	.9376
11	$x\dot{x}$	---	---
12	xz^2	---	---

Run 12

The matrix used in this run was the NASA sum of squares matrix, accurate to about 12 places after adjustment for the mean and most significant variable (y) in double precision, with X_y as the dependent variable, the terms in the model consisting of the terms selected in run 11 together with all terms containing $\dot{m}/m$ (which had been omitted in run 11). This gave a model with 65 terms. No throwout criterion was used.

No $\frac{\dot{m}}{m}$ terms were selected for the regression equation. Hence, the results were exactly the same as in run 11. This again indicates that the $\frac{\dot{m}}{m}$ terms do not significantly improve the least squares fit.

Run 13

The matrix used in this run was the same as that used in run 8, except that the dependent variable was X_y. No throw-out criterion was used.

The run stopped after 38 terms were selected. The results are shown in Table XV. The columns have the same significance as in Table I.

<div align="center">

TABLE XV

RESULTS OF RUN 13

</div>

No of Terms	Term	F	R^2
1	y	168.62	.1217
2	$y^2\dot{x}$	1355.14	.5846
3	$y\dot{z}$	315.24	.6702
4	$y^2\dot{y}$	40.63	.6809
5	x	52.63	.6941
6	z	1781.79	.8762
7	$y\dot{y}^2$	51.75	.8812
8	$z\dot{z}^2$	328.52	.9066
9	$x\dot{z}^2$	111.34	.9145
10	$xy\dot{x}$	169.59	.9250
11	$(\frac{F}{m})^3$	76.39	.9295

(Continued)

TABLE XV (Continued)

No of Terms	Term	F	R^2
12	$\dot{x}(\frac{F}{m})^2$	51.33	.9324
13	$\dot{x}\dot{y}t$	19.45	.9334
14	$z\dot{z}\frac{F}{m}$	38.82	.9355
15	z^2	47.88	.9380
16	$\dot{x}\dot{z}\frac{F}{m}$	22.42	.9391
17	$x\dot{z}\frac{F}{m}$	75.40	.9427
18	$\dot{y}\frac{F}{m}t$	17.97	.9435
19	$\dot{y}(\frac{F}{m})^2$	10.51	.9440
20	$x\dot{z}$	18.87	.9449
21	$z\dot{x}^2$	8.76	.9453
22	$z(\frac{F}{m})^2$	10.35	.9458
23	$\dot{x}^2\dot{y}$	7.59	.9461
24	$\dot{y}\dot{z}\frac{F}{m}$	7.10	.9464
25	$\dot{x}\dot{z}^2$	3.45	.9466
26	$\dot{y}\dot{z}^2$	6.49	.9469
27	$\dot{x}\frac{F}{m}$	5.95	.9471
28	$x\dot{x}\dot{y}$	5.56	.9474
29	$x\dot{y}\dot{z}$	3.73	.9476
30	$y\dot{z}\frac{F}{m}$	1.39	.9476
31	xz	3.52	.9478
32	$y(\frac{F}{m})^2$	2.49	.9479
33	$\dot{y}\dot{z}t$	3.72	.9480

(Continued)

TABLE XV (Concluded)

No of Terms	Term	F	R^2
34	$z\dot{x}\dot{z}$	11.54	.9486
35	$x\dot{x}^2$	31.23	.9499
36	$z\dot{x}\frac{F}{m}$	1646.63	.9791
37	$\dot{y}$	---	---
38	$z\dot{z}t$	---	---

The object of this run was to find if the order in which the terms were chosen was data dependent for the variable Xy. In this case only the first three terms agree. However, a comparison of coefficients for these terms seems to indicate that they are not heavily data dependent. These comparisons are shown in Table XVI. The columns have the same significance as in Table XI.

TABLE XVI

COMPARISON OF REGRESSION COEFFICIENTS FOR Xy

FOR TWO DATA BASIS (RUN 11 VS. RUN 13)

No of Terms	Term	Coefficients	
		Run 11	Run 13
2	y	---	22.173
	$y^2 x$	.045396	.044057
3	y	---	19.031
	$y^2 x$	.30472	.31863
	$y\dot{z}$	3.0249	3.1979

Run 14

The matrix used in run 13 was used in this run with the throwout criterion described for run 7. The first variable was selected with an F of 168 (and hence with an Fc of 125). Fc was eventually reduced to 3.90625.

The procedure stopped after selection of 27 terms. The results including a comparison with run 13 is shown in Table XVII. It is seen that the results

TABLE XVII

RESULTS OF RUN 14

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 13)
1	1	y	168.62		.1217	.1217
2	2	$y^2\dot{x}$	1355.14		.5846	.5846
3	3	$y\dot{z}$	315.24		.6702	.6702
4	4	$y^2\dot{y}$	40.63		.6809	.6809
5	5	x	52.63		.6941	.6941
6	6	z	1781.79		.8762	.8762
7	7	$y\dot{y}^2$	51.75		.8812	.8812
8	8	$z\dot{z}^2$	328.52		.9066	.9066
9	9	$x\dot{z}^2$	111.34		.9145	.9145
10	8	z		27.11	.9125	.9066
11	9	$yz\dot{x}$	195.63		.9247	.9145
12	8	x		8.58	.9242	.9066
13	9	$y\dot{y}\frac{F}{m}$	50.34		.9272	.9145
14	10	$\dot{y}^2 t$	43.75		.9297	.9250

(Continued)

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TABLE XVII (Continued)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 13)
15	9	$y\dot{y}^2$		26.93	.9281	.9145
16	10	z^3	57.07		.9314	.9250
17	11	$\frac{F}{m}$	28.31		.9330	.9295
18	12	xz^2	22.21		.9342	.9324
19	13	$z\dot{z}$	25.66		.9355	.9334
20	14	$\dot{x}^2\dot{z}$	19.01		.9365	.9355
21	13	$z\dot{z}^2$		3.76	.9364	.9334
22	14	$y^2\dot{z}$	12.43		.9370	.9355
23	13	$y\dot{z}$		5.53	.9367	.9334
24	14	x^2	6.95		.9371	.9355
25	15	$z^2\frac{F}{m}$	12.49		.9377	.9380
26	16	$\dot{x}^2\frac{F}{m}$	23.05		.9389	.9391
27	15	$\frac{F}{m}$		0.39	.9389	.9380
28	14	y		0.69	.9388	.9355
29	15	$z\dot{z}\frac{F}{m}$	15.19		.9396	.9380
30	14	$y\dot{y}\frac{F}{m}$		0.01	.9396	.9355
31	13	$z^2\frac{F}{m}$		3.64	.9394	.9334
32	14	$\dot{z}(\frac{F}{m})^2$	10.37		.9399	.9355
33	15	$\dot{x}(\frac{F}{m})^2$	13.78		.9406	.9380
34	14	$y^2\dot{z}$		3.49	.9404	.9355
35	15	$\dot{y}(\frac{F}{m})^2$	15.43		.9412	.9380

(Continued)

TABLE XVII (Concluded)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 13)
40	16	$\dot{y}^2 z$	14.33		.9426	.9321
45	19	$z^2 \dot{y}$	12.60		.9446	.9440
50	18	$\dot{y}^2 z$		2.22	.9452	.9435
55	19	$\dot{z}^2 \frac{F}{m}$	4.96		.9460	.9440
60	22	$y^2 z$	14.37		.9479	.9458
61	23	$\dot{x}\dot{z}$	14.85		.9486	.9461
62	24	$xz\dot{y}$	45.16		.9504	.9464
63	25	$x^2 \dot{y}$	389.12		.9626	.9466
64	26	$y\frac{F}{m}t$	---		---	.9469
65	27	$z\frac{F}{m}$	---		---	.9471

for the first nine terms are the same as in run 3. The columns have the same meaning as the run 7. F and R^2 were calculated with respect to mean-adjusted variables.

These results seem to reaffirm the conclusion that there are many sets of variables which would serve equally well in fitting.

Run 15

The matrix used in this run was the same as that used in run 5, except that the dependent variable was TR and the most significant variable (which was eliminated in double precision, along with the mean) was t. (The most significant variable in the NASA run was y^3; however, it is logical that t

would be most significant after mean adjustment, since TR is approximately a

linear function of t.) No throwout criterion was used.

The procedure stopped after selecting 14 variables. The results are shown

in Table XVIII. The columns have the same significance as in Table I. Due to

TABLE XVIII

RESULTS OF RUN 15

No of Terms	Term	F
1	$y^2\dot{z}$	1401.83
2	t^2	5327.97
3	$y^2\dot{x}$	3837.12
4	$y^2\dot{y}$	581.56
5	x	228.87
6	$y\dot{y}^2$	27.66
7	$\dot{x}\dot{y}\dot{z}$	564.32
8	$y^2\frac{F}{m}$	574.61
9	$y\dot{x}\frac{F}{m}$	1708.72
10	$y\dot{z}^2$	2263.60
11	$\dot{x}\frac{F}{m}$	294.55
12	$\dot{y}^2 z$	354.02
13	$\dot{z}^2$	492.33
14	$x\dot{x}\dot{z}$	---

a slight programming error, the correlations were not found. F was calculated

with respect to variables adjusted for the mean and t.

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In this case, it was best to eliminate the most significant variable in double precision, since TR is almost linear in t.

Run 16

The matrix used in this run was the same as that used in run 8, except that the dependent variable was TR. No throwout criterion was used.

The run stopped after selecting 41 terms. The results are shown in Table XIX. The columns have the same significance as in Table I.

TABLE XIX

RESULTS OF RUN 16

No of Terms	Term	F	R^2
1	t	545817.58	.99778
2	$y^2\dot{z}$	477.86	.99840
3	t^2	2275.89	.99944
4	$y^2\dot{x}$	1499.67	.99975
5	$y^2\dot{y}$	308.29	.99980
6	x	118.39	.99982
7	$y\dot{y}^2$	10.91	.99982
8	$\dot{x}\dot{y}\dot{z}$	259.11	.99985
9	$y^2 \frac{F}{m}$	208.50	.99987
10	$y\dot{x} \frac{F}{m}$	700.18	.99992
11	$y\dot{z}^2$	851.81	.99995
12	$\dot{x}^2 \frac{F}{m}$	117.69	.99996

(Continued)

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TABLE XIX (Continued)

No of Terms	Term	F	R^2
13	$y\dot{y}t$	327.53	.99997
14	$y\dot{z}t$	135.75	.99997
15	$z\dot{y}$	52.09	.99997
16	$x\dot{y}$	103.71	.99997
17	xyz	86.59	.99998
18	$y\dot{y}$	40.34	.99998
19	$x\dot{x}\dot{z}$	33.38	.99998
20	xt	20.25	.99998
21	$x^2\dot{x}$	8.92	.99998
22	$\dot{x}\dot{z}^2$	5.97	.99998
23	$\dot{x}\dot{y}^2$	7.02	.99998
24	$y\dot{y}\dot{z}$	4.72	.99998
25	xt^2	9.95	.99998
26	zt^2	6.71	.99998
27	t^3	13.08	.99998
28	$\dot{y}(\frac{F}{m})^2$	18.18	.99998
29	$y\frac{F}{m}t$	5.67	.99998
30	$\dot{y}^2z$	6.32	.99998
31	$z\dot{x}\dot{y}$	3.72	.99998
32	$\dot{y}\dot{z}$	11.48	.99998
33	$xy\dot{y}$	7.21	.99998
34	x^2t	18.04	.99998

(Continued)

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TABLE XIX (Concluded)

No of Terms	Term	F	R^2
35	$x^2\dot{y}$	279.06	.99998
36	$z\dot{y}t$	---	---
37	$\dot{y}\dot{z}\,\frac{F}{m}$	---	---
38	$\dot{x}^3$	---	---
39	$z\dot{z}$	---	---
40	$\dot{z}\,\frac{F}{m}\,t$	---	---
41	$z^2\,\frac{F}{m}$	---	---

The first eleven terms were the same as in run 14. A comparison of

coefficients is shown in Table XX. The columns have the same significance as

TABLE XX

COMPARISON OF REGRESSION COEFFICIENTS FOR TWO
FOR 2 DATA BASES (RUN 15 VS. RUN 16)

No of Terms	Term	Coefficients	
		Run 15	Run 16
2	t	---	-77.506
	$y^2\dot{z}$	1.4816	1.3034

(Continued)

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TABLE XX (Continued)

No of Terms	Term	Coefficients	
		Run 15	Run 16
5	t	---	-78.477
	$y^2\dot{z}$	1.0214	1.0420
	t^2	4.6587	4.5754
	$y^2\dot{x}$	- 1.7560	- 1.7783
	$y^2\dot{y}$	- .44484	- .49051
10	t	---	-98.162
	$y^2\dot{z}$	.41178	.45415
	t^2	8.9760	8.7679
	$y^2\dot{x}$	- 1.9945	- 1.9869
	$y^2\dot{y}$	- 1.1146	- 1.1007
	x	-60.945	-56.506
	$y\dot{y}^2$	- 2.1574	- 2.1189
	$\dot{x}\dot{y}\dot{z}$	- .83500	- .88217
	$y^2 \frac{F}{m}$	- .60183	- .59466
	$y\dot{x} \frac{F}{m}$	.54114	.53880
11	t	---	-37.637
	$y^2\dot{z}$	3.4763	3.2592
	t^2	4.0752	4.5254
	$y^2\dot{x}$	- 2.0768	- 2.0941
	$y^2\dot{y}$	- 1.7610	- 1.7378
	x	- 1.4068	- 1.3353

(Continued)

TABLE XX (Concluded)

No of Terms	Term	Coefficients	
		Run 15	Run 16
11	$y\dot{y}^2$	.69807	.39229
	$\dot{x}\dot{y}\dot{z}$	- 6.7264	- 6.2677
	$y^2 \frac{F}{m}$	- 1.0021	- .97826
	$y\dot{x} \frac{F}{m}$	.94838	.92314
	$y\dot{z}^2$	5.6141	5.2330

in Table XI. This again indicates that the choice of terms is not data dependent. However, as for the other dependent variables, more terms were selected with the smaller data base.

Run 17

The matrix used in run 16, with the most significant varable (t) omitted from the model, was used in this run. No throwout criterion was used.

The procedure stopped after selecting 23 terms. The results are shown in Table XXI. The columns have the same significance as in Table II.

TABLE XXI

RESULTS OF RUN 17

No of Terms	Term	F	R^2	R^2 (Run 16)
1	yt	298484.13	.99594	.99778
2	$y^2\dot{z}$	4077.81	.99907	.99840

(Continued)

TABLE XXI (Concluded)

No of Terms	Term	F	R^2	R^2 (Run 16)
3	yt^2	628.71	.99938	.99944
4	$y^2\dot{x}$	2057.76	.99977	.99975
5	$y^2\dot{y}$	46.73	.99978	.99980
6	x	255.81	.99982	.99982
7	$y\dot{y}^2$	65.20	.99983	.99982
8	$\dot{y}z\frac{F}{m}$	171.67	.99985	.99985
9	$y^2\frac{F}{m}$	261.31	.99988	.99987
10	$y\dot{x}\frac{F}{m}$	973.93	.99993	.99992
11	$\dot{x}\frac{F}{m}$	539.56	.99995	.99995
12	$\dot{x}^2\frac{F}{m}$	159.08	.99996	.99996
13	t^2	341.00	.99997	.99997
14	$\dot{x}\dot{y}$	111.82	.99997	.99997
15	z	118.78	.99997	.99997
16	$\frac{F}{m}$	20.56	.99997	.99997
17	$\dot{x}\dot{y}t$	61.33	.99998	.99998
18	z^2t	29.19	.99998	.99998
19	xt	62.99	.99998	.99998
20	$\dot{x}^2$	27.57	.99998	.99998
21	$y\frac{F}{m}$	467.60	.99998	.99998
22	$xy\frac{F}{m}$	---	---	.99998
23	$x^2\dot{z}$	---	---	.99998

Again, as more variables were added the results seem to be better without the most significant variable.

Run 18

In this run the matrix of run 16 was used with the throwout criterion of run 7. The first term was selected with an F of 545818. During the run, F_c was reduced from 1000 to 7.8125.

The run failed due to a machine error after selecting 21 terms. The results are shown in Table XXII. The columns have the same significance as in Table XI. The results for the first twelve terms are the same as for run 16.

TABLE XXII

RESULTS OF RUN 18

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 16)
1	1	t	545817.58		.99778	.99778
2	2	$y^2\dot{z}$	477.86		.99840	.99840
3	3	t^2	2275.89		.99944	.99944
4	4	y^2x	1499.67		.99975	.99975
5	5	$y^2\dot{y}$	308.29		.99980	.99980
6	6	x	118.39		.99982	.99982
7	7	$y\dot{y}^2$	10.91		.99982	.99982
8	8	$\dot{x}\dot{y}\dot{z}$	259.11		.99985	.99985
9	9	$y^2\frac{F}{m}$	208.50		.99987	.99987
10	10	$y\dot{x}\frac{F}{m}$	700.18		.99992	.99992

(Continued)

TABLE XXII (Continued)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 16)
11	11	$y\dot{z}^2$	851.81		.99995	.99995
12	12	$\dot{x}^2\,\frac{F}{m}$	117.69		.99996	.99996
13	11	$y\dot{y}^2$		0.11	.99996	.99995
14	12	$\ddot{x}\dot{y}t$	271.77		.99996	.99996
15	11	$\ddot{x}\dot{y}\dot{z}$		0.65	.99996	.99995
16	12	$\dot{y}^3$	117.04		.99997	.99996
17	13	$y\,\frac{F}{m}$	78.44		.99997	.99997
18	14	$\frac{F}{m}$	61.02		.99997	.99997
19	15	$z\dot{z}\,\frac{F}{m}$	99.04		.99998	.99997
20	16	xyt	79.07		.99998	.99997
21	15	t^2		0.13	.99998	.99997
22	16	$z\,\frac{F}{m}$	16.95		.99998	.99997
23	17	$\ddot{x}\dot{y}$	10.75		.99998	.99998
24	16	$z\dot{z}\,\frac{F}{m}$		1.84	.99998	.99997
25	15	t		2.03	.99998	.99997
26	16	$xy\dot{z}$	8.09		.99998	.99997
27	15	$y^2\dot{z}$		1.56	.99998	.99997
28	16	$\dot{x}\,\frac{F}{m}$	18.44		.99998	.99997
29	15	$\ddot{x}\dot{y}$		0.07	.99998	.99997
30	16	$\dot{y}$	69.36		.99998	.99997
31	17	$y\frac{F}{m}t$	---		---	.99998

(Continued)

TABLE XXII (Concluded)

Sweep	No of Terms	Term	F in	F out	R^2	R^2 (Run 16)
32	18	$xz\dot{y}$	---		---	.99998
33	19	$z\frac{F}{m}t$	---		---	.99998
34	20	$\ddot{x}\ddot{y}\dot{z}$	---		---	.99998
35	21	x^2	---		---	.99998

III. SUMMARY

A summary of the runs made is given in Table XXIII. The column "Run" gives

TABLE XXIII

SUMMARY OF RUNS

Run	Guidance Function	Data Base	Adjustment	Throwout Criterion	Max No of Terms	Max R^2	Min R^2
1	Xp	1	Mean	No	10 - 11	.9992	.9900
2	Xp	1	Mean	No	11 - 16	.9994	.9900
3	Xp	1	Mean	No	11 - 13	.9996	.9900
4	Xp	1	None	No	16 - 20	.99999	.99948
5	Xp	1	Mean, $y^2\dot{z}$	No	10 - 12	.9210	.0442
6	Xp	1	Mean, $y^2\dot{z}$	No	10 - 11	---	---
7	Xp	1	Mean, $y^2\dot{z}$	Yes	10 - 11	.9607	.0442
8	Xp	2	Mean	No	23 - 27	.9999	.9905
9	Xp	2	Mean	No	28 - 31	.9996	.9900
10	Xp	2	Mean	Yes	28 - 32	.9999	.9905
11	Xy	1	Mean, y	No	10 - 12	.9376	.5055
12	Xy	1	Mean, y	No	10 - 12	.9376	.5055
13	Xy	2	Mean	No	36 - 38	.9791	.1217
14	Xy	2	Mean	Yes	25 - 27	.9626	.1217
15	TR	1	Mean, t	No	13 - 14	---	---
16	TR	2	Mean	No	35 - 41	.99998	.99778
17	TR	2	Mean	No	21 - 23	.99998	.99594
18	TR	2	Mean	Yes	17 - 21	.99998	.99778

the run number as used in this study. These runs are ordered first by dependent variable and then chronologically for each variable. The column "Guidance Function" contains the guidance function (X_p, X_y, or TR) used as the dependent variable in the run. The column "Data Base" specifies which of the two data bases was used in the run. The larger data base is represented by 1 and the smaller by 2. The column "Adjustment" indicates for which variables, if any, the sum of squares matrix was adjusted before entering the stepwise procedure. If any variable is given in addition to the mean, that variable was most significant after mean adjustment. The values of F and R^2 in the preceding tables were calculated with respect to the variables after adjustment. The column "Throwout Criterion" indicates whether a throwout criterion was used.

The first number in the column "Max. No. of Terms" is the largest number of terms in the model for which the sum of squares of error remained positive. The second is the largest number of terms found. This excludes terms for which the matrix was previously adjusted. It was found that consistently more terms were selected on runs using the smaller data base.

The column "Max. R^2" contains the largest value of R^2, as defined for Table I, found. This information was not available for Run 6 or Run 15. With the exception of run 10, this R^2 occurred with the number of terms given first in the preceding column. In Run 10, which used a throwout criterion 27 terms gave $R^2 = .9999$, as compared to $R^2 = .9997$ previously given by 28 terms. Comparisons of R^2 are valid only where the same guidance function and type of adjustment were used. The column "Min R^2" gives the value of R^2 for the best single term.

Some runs were made under the same conditions for different dependent variables. These combinations are: Runs 5, 11, and 15; Runs 6 and 12; Runs 18, 13, and 16; Runs 9 and 17; and Runs 10, 14, and 18. These could be used for comparisons.

IV. CONCLUSIONS AND RECOMMENDATIONS

The step-up procedure seems to be an effective method for selecting variables to estimate a guidance function. There were several questions which arose in this study, some of which are still unresolved. These questions included whether the data should be mean-adjusted, whether some roundoff criterion should be used, whether a throwout criterion is worthwhile, whether extra precision would be worthwhile, whether the resulting model would be data dependent, and whether the model would actually accomplish the mission. The following conclusions may be drawn from the present study:

1. Mean-adjustment

There is no evidence to indicate whether or not this should be done in this problem. In general, the computation of the sum of squares and cross products matrix should be done about some pseudo-means. Otherwise, a great deal of accuracy could be lost in the elimination of the first term. From a physical point of view it would seem advisable to include a constant term in the model.

2. Roundoff Criterion

Because of the way in which variables are introduced into this model, there is the danger that the roundoff error could cause terms which should not be included in the model to enter. This would happen, if one of the vectors in the model was itself dependent on the ones previously included. To avoid this situation, there should be some sort of lower limit on the length (diagonal terms of adjusted sums of squares matrix) of vectors to be included in the regression equation. This situation has not been investigated.

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In order to develop a roundoff criterion one could, for example, run a problem in which some of the independent variables are dependent or almost dependent on other independent variables. Then one would see what kind of roundoff criteria serve best to prevent the pick-up of these terms. One would then see if any really important terms might be omitted because of this criterion.

3. Throwout Criterion

In general, it seems that the best throwout criterion is based on the F statistic. One starts by setting this F_c at a large number like 1000. Then one proceeds to admit the best term if it can be admitted with an F greater than F_c. One then examines all included terms and eliminates those which may be eliminated with an F less than F_c. When the best term does not have an F greater than F_c then one replaces F_c by $Fc/2$ and proceeds as before.

In this problem in which there are many groups of about 10 terms which are extremely good, in the least squares sense, the throwout criterion does not make significant improvement. However, the results of run 7 show an example of some fairly good improvement resulting from the throwout criterion. In that case the straight step-up procedure gave a six term model with an R^2 of .6895, while the throwout criterion described above gave a six term model with $R^2 =$ .8915.

The throwout criterion should be used, because it very rarely will hurt the least squares fit, and most often will improve it.

4. Extra Precision

In any problem in which the first 2 variables explain 99% of the variation, these variables should be eliminated in double precision. Other than this, multiple precision is not needed. Great precision is needed in the matrix

inversion only if the matrix is relatively ill conditioned. Ill conditioned matrices can be avoided by adjustment of the roundoff criterion. Thus if the inclusion of a certain term in the model will make the matrix near singular, then that term is nearly in the space of the previously included vectors. Thus its residual length will be in some sense small. The proper roundoff criterion will then prevent the inclusion of this term.

5. Data Base

The present experiments regarding data base variations have been very limited. In some of the runs, a data set which was a subset of the original data set was used. For example, in run 8 it can be seen that the coefficients of about the first eight terms in the model were stable. This is about all one could expect in this situation.

It may be concluded that for this problem there may be some merit in searching for a good least squares fit which has stable coefficient over various different data sets rather than in searching for the best least squares fit.

6. Comparison of Models

The only reasonable way to compare models is to simulate flights using each. If the mission is not accomplished, then the model is not acceptable. If two models both accomplish the mission (from a large class of initial points), then the one with the shorter time of powered flight is better.

It is recommended that further studies in the application of the stepwise regression procedure be made. Additional experience is needed to develop efficient roundoff and throwout criteria. Further study is needed to determine the sensitivity of the model to the data base selected.

Since the least square fit is only one aspect of the overall problem (performance as far as mission requirements are concerned is the other) it is necessary to evaluate the various estimators in simulated flights employing each of these estimators. For this evaluation it is best that a simpler problem be selected. Control over the data base would be much easier with a simpler problem and a greater variety of data bases could be investigated.

APPENDIX 4

OPTIMAL CONTROL IN A FLAT EARTH PROBLEM

1. Introduction

This report is a study in some detail of a well-known and fairly uncompli-
cated problem of optimal control in a hypothetical missile trajectory.

Still, the study serves several purposes. First of all the problem lends
itself to a complete but certainly nontrivial solution. A more complex model
can to some extent be viewed as a perturbation of this simpler one, and its
solution might be attained by corresponding methods or possibly even by itera-
tions begun with the solution to the simple problem.

Secondly, the simple model and its solution are a means for generating data
in the laboratory; i.e., optimal "flights" can be readily simulated. The
ability to generate optimal-trajectory data in a somewhat controlled manner is
essential for further fruitful studies of approximating optimal trajectories.

2. The Problem Studied

The problem analyzed is one of the so-called "flat-earth" problems.
Generally speaking, a missile is launched on a trajectory which is restricted
to a plane. It takes off from a certain point with prescribed velocity com-
ponents, during powered flight maintains constant thrust, and after cutoff the
missile free-falls to a target point with prescribed velocity. During powered
flight the angle of thrust is controllable. The force of gravity is assumed
to be constant. The problem is to determine the thrust angle so as to minimize
the time until cutoff (presumably this would realistically be related to mini-
mizing fuel requirements). The plane in which the trajectory lies is thought
of as being perpendicular to a plane which is called the "flat earth" for
obvious reasons.

Ordinarily, thinking of the entire trajectory, the optimal thrust angle evolves as a function of elapsed time (as well as of the initial launch and terminal conditions). It is perhaps more pertinent to obtain the optimal thrust angle in terms of current position and velocity; i.e., to <u>synthesize</u> the optimal control function. From this point of view the problem becomes one of determining the optimal current thrust angle as a function of current state conditions. Thus synthesizing the optimal trajectory is tantamount to finding the optimal "initial" thrust angle at various new "launch" points along the optimal trajectory under new "initial" conditions.

The synthesized solution of course could be automated to respond to sensors of state conditions, and this could be done with on-board equipment, provided the computation is not too complex. (One of the aims in using approximate methods, such as polynomial functions of the state variables, is to facilitate the rapid computation of synthesized control parameters with small simple equipment.)

It should be noted that in reality the time lag between sensing the state conditions and actuating an adjustment in control causes some deviation from the theoretically optimal trajectory. Such error, however, does not accumulate, since the next adjustment will be (nearly) optimal for whatever state conditions obtain at that time.

3. Detailed Discussion of the Analysis

The equations of motion are based on Newton's second law, $F = ma$, where F is a force vector and a is the acceleration vector, within the mass.

During free-fall, after cutoff of power, the force acting on the missile is assumed to be only a constant gravitational force, $-mg$. Hence, the equations

of motion during the free-fall portion of flight are

$$\ddot{x}(t) = 0, \quad \ddot{y}(t) = -g,$$

where $\ddot{x}(t)$, $\ddot{y}(t)$ are second derivatives of the components of the position vector $(x(t), y(t))$ and make up the acceleration vector a. It will be assumed that the terminal conditions to be made at the target point at time t_T are specified:

$$x(t_T) = x_T, \; y(t_T) = y_T, \; \dot{x}(t_T) = \dot{x}_T, \; \dot{y}(t_T) = \dot{y}_T.$$

During the powered phase of flight, writing F equal to the magnitude of the force vector at $(x(t), y(t))$ and $u(t)$ the controlled angle of thrust, the force vector is resolved into

$$m\ddot{x}(t) = F \sin u(t), \; m\ddot{y}(t) = F \cos u(t) - mg,$$

where the convention is made to measure $u(t)$ positively in a clockwise turning from the upward axis (positive y-axis). Thus the differential equations governing the powered flight are

$$\ddot{x}(t) = \frac{F}{m} \sin u(t), \; \ddot{y}(t) = \frac{F}{m} \cos u(t) - g,$$

with initial conditions at time t_I given as

$$x(t_I) = x_I, \; y(t_I) = y_I, \; \dot{x}(t_I) = \dot{x}_I, \; \dot{y}(t_I) = \dot{y}_I.$$

Note that $\frac{F}{m}$ is constant by virtue of the assumption of constant thrust.

The situation is summarized in the figure below:
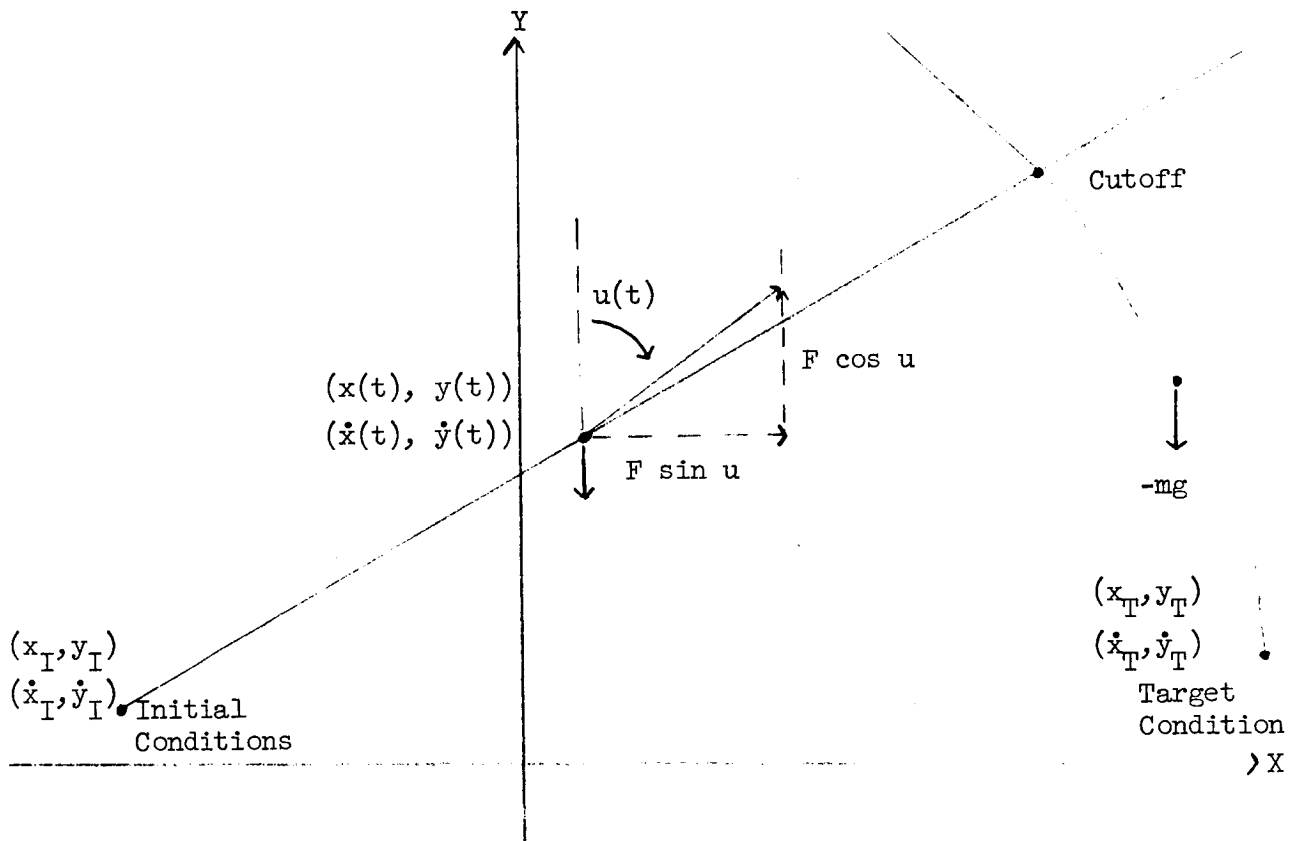
The time to cutoff is $t_c - t_I$. The synthesis problem is to determine $u(t_I)$, the initial control angle (for any t_I of course) so as to maintain an optimal trajectory (one for which $t_c - t_I$ is minimum), subject to the equations of motion and the prescribed initial and terminal condition.

Note that at cutoff time t_c both sets of differential equations will be satisfied.

The problem is simplified mathematically and conceptually if a relative coordinate system is adopted. Relative to the original coordinate system the new coordinate system has a motion due to the effect of gravity. Within the new system the complicating effect of the gravitational field is not in evidence.

Mathematically the tranformation is accomplished in order to eliminate the constant g from the differential equations. At the same time the terminal conditions can be shifted to the origin in the relative coordinate system.

The appropriate transformation is determined by integrating the free-fall equations so that the terminal conditions are met. Thus, during free-fall, in the original coordinate system,

$$\dot{x}(t) = \dot{x}_T, \quad \dot{y}(t) = -g(t-t_T) + \dot{y}_T$$

$$x(t) = \dot{x}(t-t_T) + x_T, \quad y(t) = -\frac{g}{2}(t-t_T)^2 + \dot{y}_T(t-t_T) + y_T.$$

Let

$$x_1(t) = x(t) - \dot{x}_T(t-t_T) - x_T$$

$$y_1(t) = y(t) + \frac{g}{2}(t-t_T)^2 - \dot{y}_T(t-t_T) - y_T.$$

Then

$$\dot{x}_1(t) = \dot{x}(t) - \dot{x}_T, \quad \dot{y}_1(t) = \dot{y}(t) + g(t-t_T) - \dot{y}_T.$$

For given $t > 0$ (x_1, y_1) and $(\dot{x}_1, \dot{y}_1)$ are coordinates in the relative phase space.

Theorem. A necessary and sufficient condition for the missile trajectory in the original phase space to satisfy the given equations and conditions is that in the relative phase space the following equations and conditions will be satisfied:

During free-fall

$$\ddot{x}_1(t) = 0, \quad \ddot{y}_1(t) = 0$$

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with terminal conditions

$$x_1(t_T) = y_1(t_T) = \dot{x}_1(t_T) = \dot{y}_1(t_T) = 0$$

and during powered flight

$$\ddot{x}_1(t) = \frac{F}{m} \sin u(t), \quad \ddot{y}_1(t) = \frac{F}{m} \cos u(t)$$

with initial conditions

$$x_1(t_I) = x_{1T}, \quad y_1(t_I) = y_{1T}, \quad \dot{x}_1(t_I) = \dot{x}_{1T}, \quad \dot{y}_1(t_I) = \dot{y}_{1T},$$

where x_{1T}, y_{1T}, $\dot{x}_{1T}$, $\dot{y}_{1T}$ are given in terms of x_T, y_T, $\dot{x}_T$, $\dot{y}_T$,

t_I, t_T by the transformation equations above.

Moreover, the free-fall conditions in the relative space are met if and only if

$$x(t) = y(t) = \dot{x}(t) = \dot{y}(t) = 0$$

for $t \geq t_c$.

The proof of the theorem is straightforward. Thus, e.g., in the powered flight, by differentiating the transformation equations,

$$\ddot{x}_1(t) = \ddot{x}(t) = \frac{F}{m} \sin u(t)$$

$$\ddot{y}_1(t) = \ddot{y}(t) + g = \frac{F}{m} \cos u(t) - g + g.$$

Also, during free-fall

$$\ddot{x}_1(t) = \ddot{x}(t) = 0 \text{ and } \ddot{y}_1(t) = \ddot{y}_1(t) + g = -g + g = 0.$$

And

$$x_1(t_T) = y_1(t_T) = \dot{x}_1(t_T) = \dot{y}_1(t_T) = 0,$$

as can be seen from the transformation equations and the original terminal condition. But $\ddot{x}_1 = 0$ implies that $\dot{x}_1(t)$ is constant and since $\dot{x}_1(t_T) = 0$, this constant is zero. Thus $\dot{x}_1(t) = 0$. Similarly, so is $\dot{y}_1(t)$. And, by the same reasoning, so also are $x_1(t)$ and $y_1(t)$ equal zero during free-fall.

As was indicated the problem is conceptually simpler in the relative system. It reduces to that of flying to the origin under power, having no (relative) velocity there, cutting power, subject to the initial conditions, all in minimum time $t_c - t_I$.

The problem in the relative coordinate system is thus analogous to that of steering a jet-propelled iceboat on a frictionless ice rink to some target point so that when the power is cut at the target point the boat will remain on target and to accomplish this in minimal time and subject to the initial conditions of position and velocity and the condition of operating at constant thrust.

The speculation is that the human nervous system could learn to "solve" such a problem very nearly optimally, even perhaps with variable thrust capability. Whether actual "space driving" simulations of this type would be useful, either in studying methods for approximating optimal trajectories or in personnel training, is perhaps an interesting question but well beyond the scope of this project.

By virtue of the foregoing theorem it is sufficient to be concerned with the solution to the equivalent problem in the relative coordinate system.

With this understanding the subscript indicated the transformed variables are dropped. It will also be convenient to choose force units so that $\frac{F}{m} = 1$, since $\frac{F}{m}$ was prescribed as constant. The remaining synthesis problem in the relative coordinate system is investigated by means of the Pontryagin maximality principle.

In order to minimize time to cutoff, $t_c - t_I$, while adhering to the conditions

$$\ddot{x}(t) = \sin u(t), \quad \ddot{y}(t) = \cos u(t)$$

$$x(t_I) = x_I, \quad y(t_I) = y_I, \quad \dot{x}(t_I) = \dot{x}_I, \quad \dot{y}(t_I) = \dot{y}_I$$

$$x(t_c) = y(t_c) = \dot{x}(t_c) = \dot{y}(t_c) = 0,$$

This principle imposes certain necessary conditions on $u(t)$, $t_I \leq t \leq t_c$. Let $z_1 = \dot{x}$, $z_2 = \dot{y}$, $z_3 = x$, $z_4 = y$, $z = (z_1, z_2, z_3, z_4)^T$. Then the system of two 2nd-order differential equations above is equivalent to the system of four first-order equations

$$\dot{z}_3 = z_1, \quad \dot{z}_4 = z_2, \quad \dot{z}_1 = \sin u(t), \quad \dot{z}_2 = \cos u(t).$$

with corresponding initial and terminal conditions. Or, more tersely, $\dot{z} = f(z,t)$, where $\dot{z} = (\dot{z}_1, \dot{z}_2, \dot{z}_3, \dot{z}_4)^T$ and $f(z,t) = (f_1, f_2, f_3, f_4)^T$, with

$$f_1(z,t) = \sin u(t), \quad f_2(z,t) = \cos u(t), \quad f_3(z,t) = z_1, \quad f_4(z,t) = z_2.$$

The condition imposed on $u(t)$ in the maximality principle is that, in order for control $u(t)$ to transfer a missile optimally from the given initial point to the terminal point, there must exist auxiliary forms. $\psi(t) = (\psi_1, \psi_2, \psi_3, \psi_4)^T$

such that the Hamiltonian

$$H(\psi, z, t, u(t)) = \psi \cdot f = \sum_{i=1}^{4} \psi_i f_i$$

attains a maximum on the admissible set of controls. Here ψ is a solution to the auxiliary system

$$\dot{\psi} = -f_z \psi,$$

with

$$f_z = \begin{bmatrix} \dfrac{\partial f_1}{\partial z_1} & \cdots & \dfrac{\partial f_4}{\partial z_1} \\ \vdots & & \vdots \\ \dfrac{\partial f_1}{\partial z_4} & & \dfrac{\partial f_4}{\partial z_4} \end{bmatrix}$$

Note that if $\dot{z} = f(z,t)$ and $\dot{\psi} = -f_z \psi$, then

$$H_\psi = \left(\frac{\partial H}{\partial \psi_i}\right) = f = \dot{z}$$

and

$$H_z = \left(\frac{\partial H}{\partial z_i}\right) = \left(\sum \psi_\alpha \frac{\partial f_\alpha}{\partial z_i}\right) = -\dot{\psi};$$

and, conversely, if $H_\psi = \dot{z}$ and $H_z = -\dot{\psi}$, then $z(t)$ and $\psi(t)$ satisfy the systems $\dot{z} = f(z,t)$ and $\dot{\psi} = -f_z \psi$.

Applying the principle to the system at hand,

$$H(\psi, z, t, u(t)) = f \cdot \psi = \psi_1 \sin u + \psi_2 \cos u + \psi_3 z_1 + \psi_4 z_2$$

$$= \psi_1 \sin u + \psi_2 \cos u + \psi_3 \dot{x} + \psi_4 \dot{y}.$$

Then

$$\frac{\partial H}{\partial z_1} = \psi_3 = -\dot{\psi}_1, \quad \frac{\partial H}{\partial z_3} = 0 = -\dot{\psi}_3,$$

$$\frac{\partial H}{\partial z_2} = \psi_4 = -\dot{\psi}_2, \quad \frac{\partial H}{\partial z_4} = 0 = -\dot{\psi}_4.$$

Whereupon $\psi_3 = -a$, a constant, $\psi_4 = -a'$, a constant

and

$$\psi_1 = a(t - t_I) + b, \quad \psi_2 = a'(t - t_I) + b'.$$

Thus

$$H = [a(t - t_I) + b] \sin u + [a'(t - t_I) + b'] \cos u - a\dot{x} - a'\dot{y}.$$

For fixed t, H is maximum when

$$\psi_1 \sin u + \psi_2 \cos u = \sqrt{\psi_1^2 + \psi_2^2} \cos(u - \omega)$$

is maximum, where ω is such that

$$\sin \omega = \frac{\psi_1}{\sqrt{\psi_1^2 + \psi_2^2}}, \quad \cos u = \frac{\psi_2}{\sqrt{\psi_1^2 + \psi_2^2}}$$

But this last is obviously a maximum when $\cos(u-\omega) = 1$, i.e., when $u-\omega = 2k\pi$ or when $\sin u = \sin \omega$ and $\cos u = \cos \omega$; i.e.,

$$\sin u = \sin \omega = \frac{\psi_1}{\sqrt{\psi_1^2 + \psi_2^2}} = \frac{a(t-t_I)}{\sqrt{[a(t-t_I) + b]^2 + [a'(t-t_I) + b']^2}}$$

$$\cos u = \cos \omega = \frac{\psi_2}{\sqrt{\psi_1^2 + \psi_2^2}} = \frac{a'(t-t_I)}{\sqrt{[a(t-t_I) + b]^2 + [a'(t-t_I) + b']^2}} .$$

Finally, this relation can be written in the form

$$\sin u = \frac{\tau \sin \phi + \sin \psi}{\sqrt{\tau^2 + 2\tau \cos(\psi-\phi) + 1}} \; , \quad \cos u = \frac{\tau \cos \phi + \cos \psi}{\sqrt{\tau^2 + 2\tau \cos(\psi-\phi) + 1}} \; ,$$

where $A\tau = (t-t_I)$, with $\dfrac{1}{A} = \sqrt{\dfrac{a^2 + b^2}{a'^2 + b'^2}} \geq 0$,

and $\sin \phi = \dfrac{a}{\sqrt{a^2 + a'^2}}$, $\cos \phi = \dfrac{a'}{\sqrt{a^2 + a'^2}}$

$\sin \psi = \dfrac{b}{\sqrt{b^2 + b'^2}}$, $\cos \psi = \dfrac{b'}{\sqrt{b^2 + b'^2}}$.

Substituting back in the equations of motion for relative coordinate system, evidently in order to fly an optimal trajectory it is necessary that

$$\ddot{x}(t) = \frac{\tau \sin \phi + \sin \psi}{\sqrt{\tau^2 + 2\tau \cos(\psi-\phi) + 1}} \; , \quad \ddot{y}(t) = \frac{\tau \cos \phi + \cos \psi}{\sqrt{\tau^2 + 2\tau \cos(\psi-\phi) + 1}} \; ,$$

with the initial and terminal conditions holding.

It is noted next that, when $\tau = 0$ $(t=t_I)$, then $\sin u$ $(t_I) = \sin \psi$, $\cos u$ $(t_I) = \cos \psi$. Thus the parameter ψ in the equations is identified as the optimal thrust angle at initial time t_I, or, as it will be called, the optimal initial thrust angle. Recalling that the principal aim is to synthesize the solution, the problem reduces to finding ψ as a function of the initial (current) state. Optimal powered flight time is also of interest.

It happens that the differential equations above governing the optimal powered flight, are solvable in closed form. It will be seen that the problem can be reduced directly then to that of solving for the parameters in the differential equations in terms of the initial values of the state variables. The remainder of this discussion concerns the special particulars of this solution. In a more general problem, say with nonconstant gravitational field or a three-dimensional problem, integration in closed form cannot be expected; however, the principle of solution is much the same, and the simpler problem may provide a starting point for approximations.

The integration is simplified by a rigid rotation (an orthogonal transformation) of the state variable axes. Thus, let

$$
\begin{bmatrix} \dot{x}_2 \\ \dot{y}_2 \\ \hline x_2 \\ y_2 \end{bmatrix} = \left[\begin{array}{cc|cc} \cos \psi & -\sin \psi & & \\ \sin \psi & \cos \psi & & 0 \\ \hline & & \cos \psi & -\sin \psi \\ & 0 & \sin \psi & \cos \psi \end{array} \right] \cdot \begin{bmatrix} \dot{x} \\ \dot{y} \\ \hline x \\ y \end{bmatrix} .
$$

Geometrically, the effect of this transformation is to move to a space where the optimal initial angle ψ is zero; i.e., optimal initial thrust is vertical.

Under such a transformation the zero terminal conditions are not altered, but the initial conditions in the new space are functionally dependent on ψ, not known. It is true nonetheless, and easily verified, that x, y, $\dot{x}$, $\dot{y}$ satisfy the differential equations above if and only if x_2, y_2, $\dot{x}_2$, $\dot{y}_2$ satisfy the following:

$$\ddot{x}_2(t) = \tau \sin(\phi-\psi)\Big/\sqrt{\tau^2 + 2\tau \cos(\psi-\phi) + 1}$$

$$\ddot{y}_2(t) = [\tau \cos(\phi-\psi) + 1]\Big/\sqrt{\tau^2 + \tau \cos(\psi-\phi) + 1} \quad ,$$

with corresponding modifications in the initial conditions.

It can be verified directly that

$$\frac{1}{2} \int_0^\tau \frac{2x + 2\cos\theta}{\sqrt{x^2 + 2x\cos\theta + 1}}\, dx = \sqrt{\tau^2 + 2\tau \cos\theta + 1} - 1 = q(\tau,\theta),$$

$$\int_0^\tau \frac{dx}{\sqrt{x^2 + 2x\cos\theta + 1}} = \ln\left[1 + \frac{\tau + q(\tau)}{1 + \cos\theta}\right] = \ell\,(\tau,\theta),$$

$$\int_0^\tau q(x,\theta)\, dx = \frac{1}{2}[\tau(q-1) + \ell + p\cos\theta], \quad p(\tau,\theta) = q - \ell\cos\theta,$$

$$\int_0^\tau \ell(x,\theta)\, dx = \tau\ell - p.$$

From the last differential equations, upon integrating and using the formulas above, for example

$$\dot{x}_2 = A \sin \theta \int_0^\tau \frac{x}{\sqrt{x^2 + 2x \cos \theta + 1}} \, dx + \dot{x}_{2_I}$$

$$= A \sin \theta \left\{ \frac{1}{2} \int_0^\tau \frac{2x + 2 \cos \theta}{\sqrt{x^2 + 2x \cos \theta + 1}} \, dx - \cos \theta \int_0^\tau \frac{dx}{\sqrt{x^2 + 2x \cos \theta + 1}} \right.$$

$$\left. + \dot{x}_{2_I} \right.,$$

or,

$$\dot{x}_2 - \dot{x}_{2_I} = A \sin \theta \, (q - \ell \cos \theta) = Ap(\tau, \theta) \cdot \sin \theta, \quad \theta = \emptyset - \psi.$$

Similar derivations yield the following system of equations:

$$\dot{x}_2(t) - \dot{x}_{2_I} = A \, p \sin \theta$$

$$\dot{y}_2(t) - \dot{y}_{2_I} = A \, [p \cos \theta + \ell]$$

$$x_2(t) - x_{2_I} = A \, \tau \, \dot{x}_{2_I} + A^2 \frac{\sin \theta}{2} [3p \cos \theta + \tau(2p - q - 1) + \ell]$$

$$y_2(t) - y_{2_I} = A \, \tau \, \dot{y}_{2_I} + A^2 \frac{\cos \theta}{2} [3p \cos \theta + \tau(2p - q - 1) + \ell] + A^2(\tau \ell - p).$$

It is of course easy to recover the solutions to the original equations (prior to the orthogonal transformation) by applying the inverse transformation. These are:

$$\dot{x}(t) - \dot{x}_I = A \, (p \sin \emptyset + \ell \sin \psi)$$

$$\dot{y}(t) = \dot{y}_I = A \ (p \cos \emptyset + \ell \cos \psi)$$

$$x(t) - x_I = A \ \tau \ \dot{x}_I + \frac{A^2}{2} \sin \emptyset \ [3p \cos (\emptyset - \psi) + \tau(2p-q-1) + \ell] + A^2 \sin \psi (\tau \ell - p)$$

$$y(t) - y_I = A \ \tau \ \dot{y}_I + \frac{A^2}{2} \cos \emptyset \ [3p \cos (\emptyset - \psi) + \tau(2p-q-1) + \ell] + A^2 \cos \psi (\tau \ell - p)$$

Now at cutoff time, t_c, $\dot{x}(t_c) = \dot{y}(t_c) = x(t_c) = y(t_c) = 0$, and, writing $A\tau_c = (t_c - t_I)$, $q_c = q(\tau_c, \theta)$, etc., the final system of equations to be solved is obtained:

$$\dot{x}_I = -A(p_c \sin \emptyset + \ell_c \sin \psi)$$

$$\dot{y}_I = -A(p_c \cos \emptyset + \ell_c \cos \psi)$$

$$x_I = \frac{A^2}{2} \left\{ p_c \ [2 \sin \psi - 3 \sin \emptyset \cos (\emptyset - \psi)] + \tau_c (q_c + 1) \sin \emptyset - \ell_c \sin \emptyset \right\}$$

$$y_I = \frac{A^2}{2} \left\{ p_c \ [2 \cos \psi - 3 \cos \emptyset \cos (\emptyset - \psi)] + \tau_c (q_c + 1) \cos \emptyset - \ell_c \cos \emptyset \right\} \ .$$

The numerical procedure for solving these equations, is described and illustrated in the subsequent paragraphs. Basically it is a ingenious nomograph-table which is constructed by calculating values of the state variables for various sets of ψ, τ_c, A, $\emptyset$, taking advantage of the fact that A essentially enters only as a scaling factor and of the geometry of the angles.

First consider the transformed system

$$
\begin{bmatrix} \dot{u} \\ \dot{v} \\ \text{---} \\ u \\ v \end{bmatrix}
=
\left[
\begin{array}{c|c}
\dfrac{1}{A}\begin{matrix} \cos\psi - \sin\psi \\ \sin\psi \quad \cos\psi \end{matrix} & 0 \\
\hline
0 & \dfrac{1}{A^2}\begin{matrix} \cos\psi - \sin\psi \\ \sin\psi \quad \cos\psi \end{matrix}
\end{array}
\right]
\begin{bmatrix} \dot{x}_I \\ \dot{y}_I \\ \text{---} \\ x_I \\ y_I \end{bmatrix}
$$

$$
=
\begin{bmatrix}
- p_c \sin\theta \\[4pt]
- (p_c \cos\theta + \ell_c) \\[4pt]
\hline \\[-4pt]
- \dfrac{\sin\theta}{2}\,[3p_c \cos\theta - \tau_c(q_c+1) + \ell_c] \\[6pt]
- \dfrac{\cos\theta}{2}\,[3p_c \cos\theta - \tau_c(q_c+1) + \ell_c] + p_c
\end{bmatrix}
.
$$

Note that $\dot{u}$, $\dot{v}$, u, v are functions only of τ_c and θ. Also, $\dot{u}$ and u are odd functions in θ and $\dot{v}$ and v are even.

It is thus sufficient to vary θ between 0 and τ_c in the sense that values of (u,v) and $(\dot{u},\dot{v})$ for $-\pi \leq \theta \leq 0$ can be obtained from the values corresonding to $0 \leq \theta \leq \pi$ by a reflection across the v-or $\dot{v}$-axis. Of course the functions are also periodic of period 2 , so that altogether the domain of θ may without loss be restricted to $[0,\pi]$.

From the foregoing equations a table of values, $(\dot{u},\ \dot{v},\ u,\ v)$, corresponding to values of τ_c, θ, with $\tau_c > 0$ and $0 \leq \theta \leq \pi$, is conceived. Actually tabulated, however, is a somewhat different array. Let $(\dot{u},\ \dot{v},\ u,\ v)$ correspond to some fixed $(\tau_c,\ \theta)$ in the prescribed domain. Let Υ be between $-\pi$ and τ_c and

such that

$$\sin \Upsilon = \frac{u}{\sqrt{u^2+v^2}}, \quad \cos \Upsilon = \frac{v}{\sqrt{u^2+v^2}};$$

and let $A^* = \sqrt[4]{u^2+v^2}$. Then rotate and scale the (u,v) and $(\dot{u},\dot{v})$ axes so that

$$
\begin{bmatrix} \dot{u}_1 \\ \dot{v}_1 \\ \hline 0 \\ 1 \end{bmatrix}
=
\left[
\begin{array}{c|c}
\dfrac{1}{A^*}\begin{bmatrix} \cos \Upsilon & - \sin \Upsilon \\ \sin \Upsilon & \cos \Upsilon \end{bmatrix} & 0 \\
\hline
0 & \dfrac{1}{A^{*2}}\begin{bmatrix} \cos \Upsilon & - \sin \Upsilon \\ \sin \Upsilon & \cos \Upsilon \end{bmatrix}
\end{array}
\right]
\begin{bmatrix} \dot{u} \\ \dot{v} \\ \hline u \\ v \end{bmatrix}
$$

Table I is compiled so that corresponding to each of various values of (τ_c, θ) in the domain is a quadruple $(\dot{u}_1, \dot{v}_1, \Upsilon, A^*)$. The angles θ and Υ are in degrees and the other quantities are dimensionless. Corresponding to the point $(\tau_c, \theta, \dot{u}_1, \dot{v}_1, \Upsilon, A^*)$ the point $(\tau_c, -\theta, -\dot{u}_1, \dot{v}_1, -\Upsilon, A^*)$ would also be in the table. Thus the table contains only $\tau_c > 0$ and $\theta \in [0, \pi]$.

It is also feasible to construct a graph displaying curves $(\dot{u}_1, \dot{v}_1)$ as functions of (τ_c, θ). Such a graph is exhibited in Figure 1. This graph is a plot of the level curves for τ_c and θ as functions of $\dot{u}_1$ and $\dot{v}_1$. It may be used to find τ_c and θ corresponding to a given $(\dot{u}_1, \dot{v}_1)$ and then by recourse to Table I we may also find Υ and A^*.

Putting the successive of transformations together gives

TABLE I

OPTIMAL STARTING VALUES

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.00	177.0	0.1469	-1.3969	14.5	0.688
1.00	178.0	0.1146	-1.4038	11.0	0.693
1.00	178.8	0.0802	-1.4092	7.5	0.697
1.00	179.0	0.0721	-1.4102	6.7	0.698
1.00	179.6	0.0380	-1.4130	3.5	0.703
1.00	180.0	0.0000	-1.414	0.0	1.000
1.10	178.0	0.2652	-1.3760	21.7	0.654
1.10	178.8	0.2046	-1.4001	16.0	0.642
1.10	179.6	0.1100	-1.4236	7.9	0.632
1.10	180.0	0.0000	-1.43	0.0	0.63
1.20	177.0	0.5155	-1.2752	39.6	0.615
1.20	178.0	0.4722	-1.3322	33.4	0.586
1.20	178.8	0.3836	-1.4045	25.0	0.559
1.20	179.0	0.3555	-1.4215	22.8	0.553
1.20	179.6	0.2045	-1.4834	12.3	0.536
1.20	180.0	0.0000	-1.51	0.0	0.529
1.25	178.0	0.6265	-1.2786	41.5	0.550
1.25	178.8	0.5418	-1.3946	32.0	0.512
1.25	179.6	0.3078	-1.5441	16.3	0.478
1.25	180.0	0.0000	-1.60	0.0	0.469
1.30	177.0	0.7976	-1.0831	58.0	0.568
1.30	178.0	0.8227	-1.1680	52.2	0.516
1.30	178.8	0.7864	-1.3342	42.3	0.463
1.30	179.0	0.7599	-1.3856	39.4	0.452
1.30	179.6	0.5136	-1.6294	23.0	0.411

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.30	180.0	0.0000	-1.777	0.0	0.394
1.35	177.0	0.9377	-0.9088	69.8	0.554
1.35	178.0	1.0362	-0.9587	66.0	0.491
1.35	178.8	1.1327	-1.1223	58.4	0.420
1.35	179.0	1.1453	-1.1891	55.7	0.403
1.35	179.6	1.0025	-1.6682	35.6	0.336
1.35	180.0	0.0000	-2.167	0.0	0.300
1.40	177.0	1.0330	-0.6854	82.7	0.551
1.40	178.0	1.1900	-0.6365	82.6	0.480
1.40	178.4	1.2882	-0.6216	82.2	0.444
1.40	178.6	1.3510	-0.6178	81.9	0.424
1.40	178.8	1.4274	-0.6190	81.3	0.401
1.40	179.0	1.5226	-0.6290	80.6	0.375
1.40	179.2	1.6487	-0.6569	79.3	0.345
1.40	179.4	1.8219	-0.7237	77.2	0.310
1.40	179.6	2.0788	-0.8959	73.2	0.267
1.40	179.8	2.4589	-1.4850	62.6	0.209
1.40	180.0	0.0000	-4.24	0.0	0.141
1.42	178.0	1.2136	-0.4902	89.6	0.482
1.42	178.4	1.3158	-0.4358	90.4	0.445
1.42	178.6	1.3818	-0.4029	90.9	0.424
1.42	178.8	1.4628	-0.3644	91.4	0.401
1.42	179.0	1.5659	-0.3174	92.1	0.375
1.42	179.2	1.7034	-0.2566	92.9	0.344
1.42	179.4	1.9006	-0.1696	94.2	0.308
1.42	179.6	2.2201	-0.0190	96.3	0.263
1.42	179.8	2.8791	0.3882	101.5	0.200
1.42	180.0	0.0000	4.53	180.0	0.128

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.44	178.0	1.2108	-0.3469	96.5	0.487
1.44	178.4	1.3044	-0.2547	98.5	0.451
1.44	178.6	1.3630	-0.1943	99.7	0.430
1.44	178.8	1.4327	-0.1192	101.3	0.407
1.44	179.0	1.5171	-0.0206	103.3	0.382
1.44	179.2	1.6210	0.1173	106.1	0.353
1.44	179.4	1.7486	0.3291	110.3	0.320
1.44	179.6	1.8900	0.7037	117.5	0.280
1.44	179.8	1.8860	1.5134	132.1	0.232
1.44	180.0	0.0000	2.92	180.0	0.192
1.46	178.0	1.1839	-0.2151	103.1	0.495
1.46	178.4	1.2586	-0.0929	105.9	0.460
1.46	178.6	1.3020	-0.0126	108.1	0.441
1.46	178.8	1.3493	0.0876	110.5	0.419
1.46	179.0	1.3993	0.2174	113.6	0.396
1.46	179.2	1.4470	0.3931	117.7	0.370
1.46	179.4	1.4761	0.6441	123.7	0.341
1.46	179.6	1.4332	1.0227	132.9	0.309
1.46	179.8	1.1351	1.5909	148.7	0.277
1.46	180.0	0.0000	2.12	180.0	0.255
1.5	177.0	1.0036	-0.2506	107.8	0.584
1.5	178.0	1.0790	-0.0078	115.0	0.520
1.5	178.8	1.1096	0.3666	126.8	0.452
1.5	179.0	1.0968	0.4777	129.6	0.437
1.5	179.6	0.8270	1.1162	149.7	0.380
1.5	180.0	0.0000	1.41	180.0	0.354
1.6	177.0	0.8080	-0.0321	126.6	0.658
1.6	178.0	0.7580	0.1928	135.1	0.612

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.6	178.8	0.6261	0.4397	147.7	0.571
1.6	179.0	0.5811	0.4939	150.2	0.563
1.6	179.6	0.3301	0.6792	164.6	0.538
1.6	180.0	0.0000	0.755	180.0	0.530
1.8	177.0	0.4962	-0.0196	146.7	0.844
1.8	178.0	0.4039	0.0887	154.6	0.820
1.8	178.8	0.2871	0.1761	162.8	0.802
1.8	179.0	0.2580	0.1918	164.7	0.799
1.8	179.6	0.1317	0.2379	172.4	0.789
1.8	180.0	0.0000	0.254	180.0	0.788
2.0	177.0	0.3443	-0.1349	156.0	1.032
2.0	178.0	0.2669	-0.0769	162.3	1.018
2.0	179.0	0.1624	-0.0272	169.6	1.006
2.0	180.0	0.0000	0.0000	180.0	1.0
2.6	177.0	0.1869	-0.4286	166.6	1.553
2.6	178.0	0.1397	-0.4104	170.3	1.548
2.6	179.0	0.0822	-0.3961	174.6	1.545
2.6	180.0	0.0000	-0.389	180.0	1.54
4.0	177.0	0.1607	-0.7665	172.6	2.648
4.0	178.0	0.0790	-0.7615	174.8	2.647
4.0	179.0	0.0461	-0.7577	177.2	2.646
4.0	180.0	0.0000	-0.755	180.0	2.646
10.0	180.0	0.0000	-1.141	180.0	7.00
100.0	180.0	0.0000	-1.385	180.0	70.6
0.8	20.0	0.0353	-1.4130	8.4	0.566
0.8	40.0	0.0707	-1.4085	13.3	0.565

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
0.8	60.0	0.1061	-1.4013	19.5	0.564
0.8	80.0	0.1412	-1.3916	25.0	0.563
0.8	100.0	0.1747	-1.3802	29.6	0.562
0.8	120.0	0.2032	-1.3695	32.3	0.559
0.8	140.0	0.2165	-1.3659	31.5	0.557
0.8	150.0	0.2088	-1.3708	28.8	0.557
0.8	160.0	0.1802	-1.3831	23.4	0.559
0.8	165.0	0.1531	-1.3922	19.3	0.560
0.8	170.0	0.1143	-1.4022	14.0	0.562
0.8	175.0	0.0619	-1.4107	7.5	0.565
0.8	178.0	0.0254	-1.4136	3.0	0.566
0.8	180.0	0.0000	-1.414	0.0	0.566
1.0	20.0	0.0393	-1.4124	7.7	0.707
1.0	40.0	0.0790	-1.4069	15.3	0.706
1.0	60.0	0.1196	-1.3975	22.6	0.705
1.0	80.0	0.1615	-1.3840	29.6	0.703
1.0	100.0	0.2048	-1.3662	35.7	0.700
1.0	120.0	0.2488	-1.3451	40.5	0.696
1.0	140.0	0.2896	-1.3250	42.6	0.689
1.0	150.0	0.3038	-1.3201	41.6	0.684
1.0	160.0	0.3038	-1.3257	38.0	0.679
1.0	165.0	0.2916	-1.3360	34.4	0.678
1.0	170.0	0.2616	-1.3544	28.9	0.678
1.0	175.0	0.1945	-1.3831	19.9	0.683
1.0	178.0	0.1146	-1.4038	11.0	0.693
1.0	180.0	0.0000	-1.414	0.0	0.707
1.2	20.0	0.0423	-1.4121	8.6	0.848
1.2	40.0	0.0853	-1.4055	17.0	0.847

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.2	60.0	0.1300	-1.3941	25.4	0.846
1.2	80.0	0.1771	-1.3769	33.5	0.843
1.2	100.0	0.2282	-1.3528	41.1	0.838
1.2	120.0	0.2852	-1.3197	48.0	0.831
1.2	140.0	0.3521	-1.2753	53.4	0.816
1.2	150.0	0.3919	-1.2483	55.1	0.803
1.2	160.0	0.4394	-1.2187	55.5	0.780
1.2	165.0	0.4681	-1.2046	54.9	0.760
1.2	170.0	0.5020	-1.1955	52.9	0.727
1.2	175.0	0.5328	-1.2202	46.4	0.661
1.2	178.0	0.4722	-1.3322	33.4	0.586
1.2	180.0	0.0000	-1.51	0.0	0.529
1.4	20.0	0.0446	-1.4118	9.3	0.990
1.4	40.0	0.0902	-1.4043	18.5	0.986
1.4	60.0	0.1379	-1.3911	27.8	0.986
1.4	80.0	0.1890	-1.3707	36.9	0.983
1.4	100.0	0.2459	-1.3406	45.9	0.977
1.4	120.0	0.3123	-1.2959	54.7	0.966
1.4	140.0	0.3976	-1.2249	65.6	0.943
1.4	150.0	0.4551	-1.1698	67.8	0.920
1.4	160.0	0.5361	-1.0860	72.6	0.877
1.4	165.0	0.5958	-1.0224	75.3	0.838
1.4	170.0	0.6858	-0.9296	78.4	0.773
1.4	175.0	0.8677	-0.7762	81.8	0.645
1.4	178.0	1.1900	-0.6365	97.6	0.480
1.4	180.0	0.0000	-4.24	0.0	0.141
1.6	20.0	0.0464	-1.4116	9.9	1.131
1.6	40.0	0.0940	-1.4033	19.9	1.130

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
1.6	60.0	0.1439	-1.3885	29.8	1.127
1.6	80.0	0.1980	-1.3653	39.9	1.123
1.6	100.0	0.2588	-1.3301	50.0	1.115
1.6	120.0	0.3312	-1.2750	60.6	1.101
1.6	140.0	0.4257	-1.1800	72.1	1.071
1.6	150.0	0.4896	-1.0996	78.9	1.040
1.6	160.0	0.5762	-0.9660	87.4	0.984
1.6	165.0	0.6347	-0.8564	93.1	0.936
1.6	170.0	0.7106	-0.6807	101.1	0.862
1.6	175.0	0.8027	-0.3237	115.2	0.735
1.6	178.0	0.7580	+0.1928	135.3	0.612
1.6	180.0	0.0000	0.755	180.0	0.530
1.8	20.0	0.0478	-1.4114	10.5	1.272
1.8	40.0	0.0968	-1.4024	21.0	1.271
1.8	60.0	0.1485	-1.3863	31.7	1.268
1.8	80.0	0.2046	-1.3608	42.5	1.263
1.8	100.0	0.2680	-1.3212	53.7	1.254
1.8	120.0	0.3434	-1.2576	65.7	1.237
1.8	140.0	0.4400	-1.1438	79.5	1.201
1.8	150.0	0.5012	-1.0451	88.1	1.162
1.8	160.0	0.5736	-0.8810	99.4	1.105
1.8	165.0	0.6110	-0.7492	107.1	1.057
1.8	170.0	0.6370	-0.5500	117.6	0.989
1.8	175.0	0.5921	-0.2142	135.2	0.891
1.8	178.0	0.4039	0.0887	154.5	0.820
1.8	180.0	0.0000	0.254	180.0	0.788
2.0	20.0	0.0489	-1.4112	11.0	1.414
2.0	40.0	0.0990	-1.4017	22.1	1.412

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
2.0	60.0	0.1519	-1.3845	33.3	1.408
2.0	80.0	0.2095	-1.3570	44.8	1.403
2.0	100.0	0.2743	-1.3138	56.9	1.392
2.0	120.0	0.3507	-1.2436	70.1	1.373
2.0	140.0	0.4443	-1.1166	85.8	1.340
2.0	150.0	0.4983	-1.0072	95.8	1.297
2.0	160.0	0.5495	-0.8313	108.8	1.237
2.0	165.0	0.5638	-0.6981	117.4	1.192
2.0	170.0	0.5496	-0.5137	128.9	1.135
2.0	175.0	0.4471	-0.2549	146.1	1.062
2.0	178.0	0.2669	-0.0769	162.2	1.018
2.0	180.0	0.0000	0.0000	180.0	1.000
2.4	20.0	0.0503	-1.4109	11.9	1.696
2.4	40.0	0.1019	-1.4006	23.8	1.694
2.4	60.0	0.1563	-1.3817	36.0	1.690
2.4	80.0	0.2152	-1.3513	48.7	1.683
2.4	100.0	0.2807	-1.3032	62.2	1.671
2.4	120.0	0.3550	-1.2246	77.3	1.649
2.4	140.0	0.4363	-1.0848	95.7	1.606
2.4	150.0	0.4722	-0.9705	107.2	1.570
2.4	160.0	0.4862	-0.8028	121.7	1.517
2.4	165.0	0.4705	-0.6903	130.9	1.482
2.4	170.0	0.4205	-0.5553	142.2	1.443
2.4	175.0	0.3006	-0.4034	156.9	1.401
2.4	178.0	0.1636	-0.3216	168.7	1.380
2.4	180.0	0.0000	-0.291	180.0	1.373
3.0	170.0	0.3161	-0.6682	151.8	1.91
3.0	175.0	0.2118	-0.5862	163.8	1.884

(Continued)

TABLE I (CONTINUED)

τ_c	θ	$\dot{u}_1$	$\dot{v}_1$	Υ	A^*
3.0	178.0	0.1110	-0.5474	172.4	1.874
3.0	180.0	0.0000	-0.534	180.0	1.872
5.0	170.0	0.1945	-0.9241	162.0	3.399
5.0	175.0	0.1247	-0.8983	170.4	3.394
5.0	178.0	0.0641	-0.8878	175.8	3.392
5.0	180.0	0.0000	-0.885	180.0	3.39
10.0	20.0	0.0432	-1.4109	16.0	7.070
10.0	40.0	0.0861	-1.4009	34.2	7.065
10.0	60.0	0.1277	-1.3835	51.8	7.058
10.0	80.0	0.1666	-1.3577	70.0	7.048
10.0	100.0	0.1994	-1.3226	89.2	7.035
10.0	120.0	0.2201	-1.2778	109.5	7.021
10.0	140.0	0.2173	-1.2254	131.2	7.008
10.0	150.0	0.2011	-1.1985	142.7	7.003
10.0	160.0	0.1697	-1.1735	154.6	7.000
10.0	170.0	0.1148	-1.1531	166.9	7.000
10.0	180.0	0.0000	-1.141	180.0	7.00
20.0	20.0	0.0331	-1.419	18.3	14.141
20.0	40.0	0.0653	-1.4048	36.8	14.137
20.0	60.0	0.0951	-1.3929	55.6	14.130
20.0	80.0	0.1209	-1.3763	74.7	14.122
20.0	100.0	0.1400	-1.3555	94.4	14.114
20.0	120.0	0.1482	-1.3316	114.8	14.107
20.0	140.0	0.1394	-1.3071	135.9	14.103
20.0	150.0	0.1257	-1.2958	146.7	14.103
20.0	160.0	0.1032	-1.2862	157.6	14.104
20.0	170.0	0.0678	-1.2791	168.7	14.105
20.0	180.0	0.0000	-1.275	180.0	14.10

TABLE I (CONCLUDED)

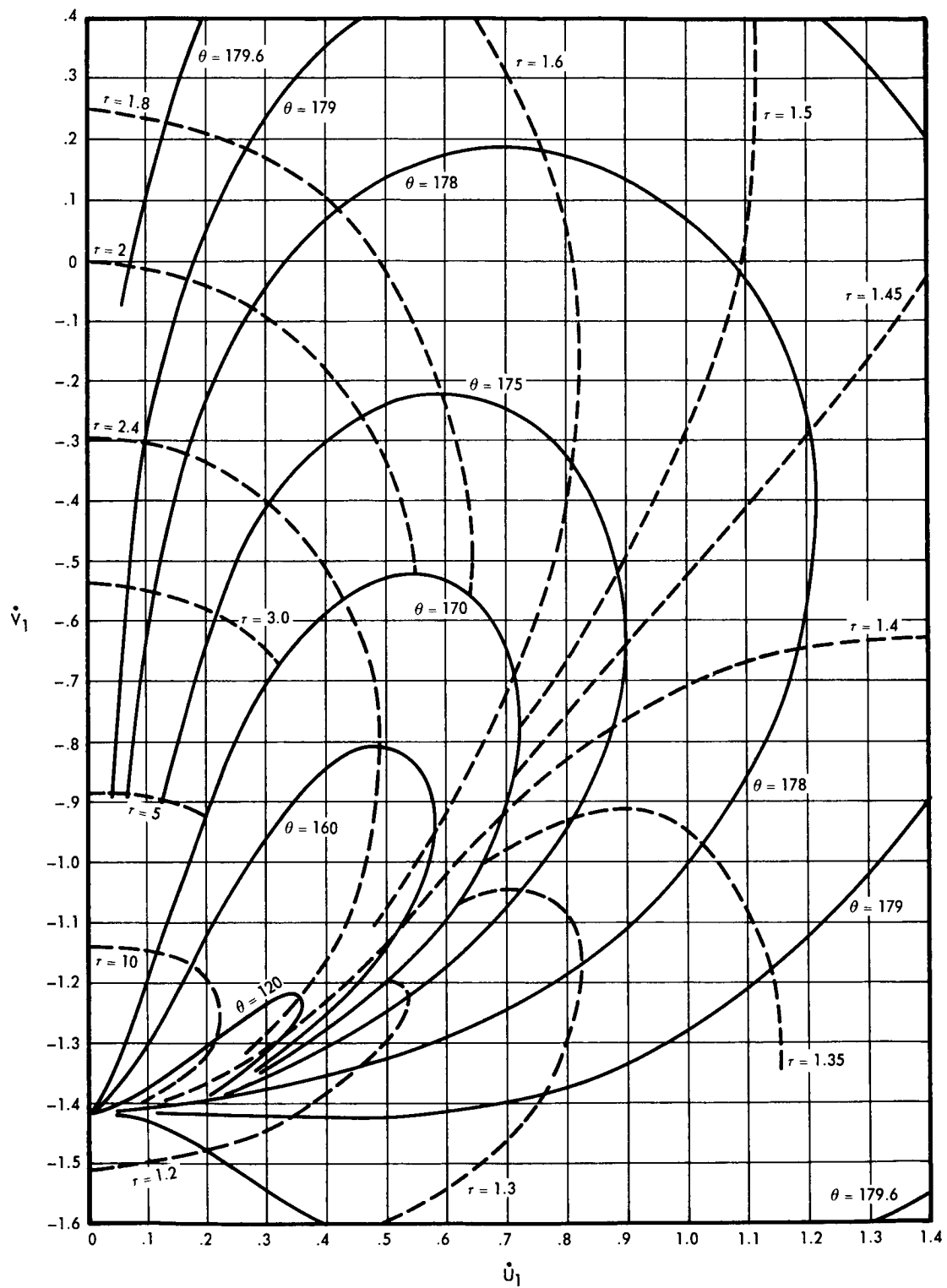| τ_c	θ	$\hat{u}_1$	$\hat{v}_1$	Υ	A^*
60.0	20.0	0.0183	-1.4131	19.4	42.425
60.0	40.0	0.0357	-1.4099	38.8	42.423
60.0	60.0	0.0509	-1.4048	58.4	42.419
60.0	80.0	0.0629	-1.3981	78.1	42.415
60.0	100.0	0.0701	-1.3903	98.1	42.411
60.0	120.0	0.0701	-1.3823	118.3	42.409
60.0	140.0	0.0635	-1.3750	138.7	42.401
60.0	150.0	0.0556	-1.3720	149.0	42.411
60.0	160.0	0.0442	-1.3696	159.3	42.412
60.0	170.0	0.0279	-1.3681	169.6	42.414
60.0	180.0	0.0000	-1.37	180.0	42.414

Figure 1. Graph of starting values versus initial conditions.

$$\begin{bmatrix} \dfrac{1}{AA^*}\begin{bmatrix} \cos\,(\psi+\Upsilon), & -\sin\,(\psi+\Upsilon) \\ \sin\,(\psi+\Upsilon), & \cos\,(\psi+\Upsilon) \end{bmatrix} & 0 \\ 0 & \dfrac{1}{(AA^{*2})}\begin{bmatrix} \cos\,(\psi+\Upsilon), & -\sin\,(\psi+\Upsilon) \\ \sin\,(\psi+\Upsilon), & \cos\,(\psi+\Upsilon) \end{bmatrix} \end{bmatrix} \begin{bmatrix} \dot{x}_I \\ \dot{y}_I \\ -- \\ x_I \\ y_I \end{bmatrix} = \begin{bmatrix} \dot{u}_1 \\ \dot{v}_1 \\ -- \\ 0 \\ 1 \end{bmatrix}$$

But, beginning with the initial conditions, it is easy to determine $\psi+\Upsilon=\delta$ and $A' = AA^*$ such that

$$\frac{1}{A'^2}\begin{bmatrix} \cos\,\delta & -\sin\,\delta \\ \sin\,\delta & \cos\,\delta \end{bmatrix}\begin{bmatrix} x_I \\ y_I \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

In fact, δ is such that

$$\sin\,\delta = \frac{x_I}{\sqrt{x_I^2 + y_I^2}}, \quad \cos\,\delta = \frac{y_I}{\sqrt{x_I^2 + y_I^2}}$$

and $A'^2 = \sqrt{x_I^2 + y_I^2}$.

Then, applying the transformation

$$\frac{1}{A'}\begin{bmatrix} \cos\,\delta & -\sin\,\delta \\ \sin\,\delta & \cos\,\delta \end{bmatrix}$$

to $\begin{bmatrix} \dot{x}_I \\ \dot{y}_I \end{bmatrix}$ yields $(\dot{u}_1, \dot{v}_1)$.

From the graph corresponding to $(\dot{u}_1, \dot{v}_1)$ is read a pair (τ_c, θ); and then from the table is read, corresponding to (τ_c, θ), values of Υ and A^*.

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But,

$$\psi = \delta - \Upsilon, \quad A = \frac{A'}{A^*}, \quad t_c - t_I = A\,\tau_c.$$

By way of illustration consider the following example. What is the optimal current thrust angle and time to freefall, given that current state relative to the origin in the relative coordinate system is $x_I = 300$ meters, $y_I = -400$ meters, $\dot{x}_I = 0$ m/sec, $\dot{y}_I = -50$ m/sec with constant thrust $F/m = 4\text{m}/\text{sec}^2$.

First, in units of thrust the state vector is $(\dot{x}_I, \dot{y}_I, x_I, y_I) =$ (0, -1 .5, 75, -100).

Second,

$$\sin \delta = \frac{75}{\sqrt{75^2 + 100^2}} = 0.6, \quad \cos \delta = \frac{-100}{\sqrt{75^2 + 100^2}} = -0.8,$$

so that $\delta \doteq 143.1°$. Also, $A'^2 = \sqrt{75^2 + 100^2} = 125$, and $A' = 5\sqrt{5} \doteq 11.18$.

Third,

$$\begin{bmatrix} \dot{u}_1 \\ \dot{v}_1 \end{bmatrix} = \frac{1}{A'} \begin{bmatrix} \cos \delta & -\sin \delta \\ \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} \dot{x}_I \\ \dot{y}_I \end{bmatrix} = \frac{1}{11.18} \begin{bmatrix} -0.8 & -0.6 \\ 0.6 & -0.8 \end{bmatrix} \begin{bmatrix} 0 \\ -12.5 \end{bmatrix} = \begin{bmatrix} 0.621 \\ 0.894 \end{bmatrix} .$$

Fourth, from the preceding graph,

$$\tau_c = 1.525, \quad \emptyset = 179.5°.$$

Fifth, from the preceding table,

$$\Upsilon = 151.1° , \quad A^* = 0.425 .$$

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Finally,

$$\Psi = \delta - \Upsilon = 143.1° - 151.1° = -8°,$$

$$A = \frac{A'}{A^*} = 26.3$$

and

$$t_c - t_I = (26.3)\ 1.525 = 40 \text{ seconds.}$$

Thus, the optimal steering angle at current time is -8° (measured from the vertical axis in the relative coordinate system), and the time to cutoff along an optimal trajectory is 40 seconds.

4. Summary and Recommendations

Equations of motion governing the two phases of flight are immediate consequences of Newton's second law. The control function (angle of thrust) enters into the equations for the powered phase of the flight.

Putting the problem in a relative coordinate system, which has a motion with respect to the old due to the gravitational field, effects a considerable simplification in the analysis both computationally and conceptually.

The Pontryagin maximum principle is applied to restrict the control function in the differential equation to a form which is necessary to make the optimal flight (i.e., to reach engine cutoff time in minimum time), while still reaching the target from the initial state.

It happens that the resulting differential equations, presumably describing the optimal flight, can be integrated in closed form to yield a system of algebraic equations which must be solved for time to cutoff and initial thrust angle

in terms of the initial state conditions. This final result is a synthesis of the control function, the current optimal thrust angle always being calculable from an input of current state conditions into the system of algebraic equations.

A numerical procedure for solving these equations is presented. It is based in part on simplification through rotation and scaling transformations.

Natural extensions of this problem abound, and it is recommended that some of these be explored. E.g., it is believed that almost exactly the same mode of solution, although somewhat more complicated, can be developed if the gravitational field is nonconstant. Also, it is recommended that the same approach, including numerical schemes, be attempted for the three-dimensional analogue.

It is recommended that further study be given to computerizing the scheme for solving the system of equations, and that these procedures be made independent of the fact that the integration was in the present case performed in closed form.

It is further recommended that the current flat-earth model be used in conjunction with a computer to generate a controlled but representative spectrum of data to be used as a benchmark for evaluating various methods of approximating an optimal trajectory, such as, for example, a best fit polynomial or a piecewise linearization of the control function.