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STATISTICAL DESIGN AND DATA ANALYSIS TECHNIQUES

FOR SPACE STATION APPLICATION: AN ESSAY

by

T. L. Boullion, H. L. Gray and P. L. Odell

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Department of Mathematics
Texas Tech University
Lubbock, Texas 79409

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PREFACE

"Since statisticians do not usually perform experiments, their claim to attention when they write on this subject requires some explanation. It is true that on many important aspects of experimentation the statistician has no expert knowledge. Nevertheless, in recent years, research workers have turned increasingly to statisticians for help both in planning their experiments and in drawing conclusions from the results. That this has happened is convincing evidence that statistics has something to contribute."

W. G. Cochran and G. M. Cox,
Experimental Design.

0.1. The Aim

This monograph is written primarily for the engineers who will design and plan the laboratories in the space station, and scientists, biological and physical, who in their efforts to fly their experiments need to know each others problems. They should know these problems in such detail and manner so that fruition of a truly excellent and useful multipurpose space laboratory can come about and be put into space in order that significant scientific investigations can be performed in the very near future.

During the preliminary planning and engineering analysis of equipment of a multipurpose laboratory in a manned space station, it became apparent to some engineering and scientific personnel at NASA Headquarters, Washington, D.C., and at the Marshall Space Center, Alabama, there could exist alternative ways of designing experiments as statistical procedures which in turn could induce alternatives in equipment and manpower requirements for performing those experiments.

The major aim of this monograph is to develop the concept that there do exist alternative statistical data analysis techniques which are applicable in inducing alternative equipment and manpower requirements for the laboratory of the proposed space station. We also attempt to illustrate and illuminate how alternative experimental designs and sophisticated statistical data analysis techniques can affect equipment, personnel, and data processing requirements.

0.2 On Collecting Background Data for This Study

In order to facilitate understanding we first review the aim of the space station mission. A loose general statement of this aim follows:

The Mission. To develop a multipurpose federal scientific laboratory in space by making available in a space station the best scientific equipment to support a large spectrum of scientists who will perform a large spectrum of significant experiments within projected economic and time constraints.

Since one is projecting what will be significant experiments beginning perhaps in the late seventies, it is necessary to obtain estimates from potential principal investigators, or those who will closely approximate principal investigators of the eighties vintage, of what they feel will be meaningful experiments along with their estimates of equipment requirements. When a sample of these scientists were identified and accepted by the authors as good estimates, their research papers were reviewed with respect to the types of experimental designs and data analysis techniques that they have used in the past. These designs and techniques were considered primitive models of what one might expect in space experiments in the eighties. Additional information was gleaned from a NASA-compiled source book called the "blue book", and the analysis of the experiments flown on Biosatellite II [1] were also studied as primitive models of projected biological experiments. Relevant industrial reports supplied to the authors by NASA official were also gleaned for data [2], [3], [4], [5]. Several proceedings of symposia on the role of the vestibular organs in space exploration [9], [10], [11], [12], gave some information concerning interphasing between measuring devices with primates and small animals. Several schematics of special containers and proposed instrumentation schemes for obtaining data from an animal gave insight as to type of data one would expect from such experimental modules.

Several well-known and a few relatively recent statistical data analysis techniques were selected to demonstrate and illuminate the alternatives that can be induced. We have chosen to select

general techniques in favor of considering specific ones since the development of the space station laboratory equipment requirements are at this time in an early and still relatively general phase of formulation. Some of the techniques considered here can be found in current statistical and engineering literature and are well-known to many statisticians who specialize in engineering statistics and engineering data analysis. The length of our discussion of a technique is directly proportional to our knowledge of the technique and not its relative importance of its application to the space station goals.

0.3 About This Monograph

The concept of a space station containing one or more, multi-purpose laboratories which will also have the capability of monitoring and maintaining one or more free flying modules transporting special experiments, can introduce constraints on usual laboratory techniques, laboratory equipment requirements, and on admissible experimental designs. The environmental conditions and state of the art instrumentation limitations pose problems as to whether or not specified experiments can be flown and significant data obtained.

Two extremes bound the problem immediately; a space station as the ultimate in sophistication and completeness in which all things are available to all principal investigators, or a space station as a bare frame upon which each principal investigator will "hang" his experimental module which is a complete entity

within itself in every way. The first extreme implies a relatively large initial expense followed perhaps by a large maintenance expense, while the second implies perhaps a relatively small initial expense with even a larger maintenance expense. When weight, size, power and personnel constraints are introduced for communality and economic reasons, the necessity for the usual trade-off studies become clear in order that a flexible multi-purpose laboratory results within the time profile established.

This monograph is concerned primarily with the development of the thesis that alternative ways for statistically processing data and alternative ways for statistically designing the experiments can lead to a spectrum of admissible equipment configurations from which one can select an optimal with respect to some preassigned criteria of excellence.

The monograph is divided into ten chapters in which the first, second and last are written in a self contained manner so that managers, system planners, and potential principal investigators can read easily without the tedious business of working through some mathematical analysis. This analysis is included in the remaining chapters made available there for design engineers and scientists who may wish to pursue deeper into one of the advanced statistical techniques.

We wish to acknowledge the help of various NASA planning engineers and scientists for making available to us pertinent government and industrial literature, inviting us to relevant conferences and introducing to us potential investigators whose past work and proposed work form a basis for this analysis.

0.4. References.

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CHAPTER I

The Nature of Experimental Designs.

A mighty maze! but not without a plan.

Alexander Pope, Essay on Man.

1.1. Introductory Remarks.

There will be many readers of this monograph who will find this chapter "old stuff." Those well prepared in the topics of general linear hypothesis and linear estimation theory should become familiar with the notation used and proceed to the next chapter. However, those who are not familiar with these principles should read carefully what is presented here since all the quantitative analysis in this monograph are based on the models and concepts developed in this chapter.

1.2. The Concept of a Model.

A major aim of scientific investigation is to describe and predict events in the world (and space) in which we live. A useful and popular way to do this is for the scientist to model his world, that is, to devise a formula which relates what he can observe to those parameters which he cannot or wishes not to observe, but would like to predict. How well one estimates these parameters is measured by computing or estimating a pay-off or a cost. In the case of classical statistical techniques, expected risk,

expected mean square error or variance (these are costs) are minimized to yield an optimal design or estimator.

Let the scalar functional relationship

$$y = g(x_1, x_2, \dots, x_p) \quad (1)$$

denote a formula or model of how y , a dependent variable, is related to the independent variables $x_1, x_2, \dots, x_p$. The following proposition [1] is assumed to be true.

Proposition. Suppose y is a quantity "in the real world" which we want to predict. Then there exists a finite number of variables $x_1, x_2, \dots, x_n$ and a function g such that (1) holds.

Two questions immediately arise: (i) Does the experimenter know all the independent variables $x_1, x_2, \dots, x_p$ which effect the value of y ? (ii) If the experimenter knows $x_1, x_2, \dots, x_p$, does he know the function g ? For space applications there exists at least a third question, that being; (iii) Does there exist a subset of $x_1, x_2, \dots, x_p$ say $x_1, x_2, \dots, x_q$, $q < p$ and a function g_1 such that

$$g(x_1, x_2, \dots, x_p) - g_1(x_1, x_2, \dots, x_q)$$

is not significantly different from zero? If the answer to (iii) is yes then, there exists a smaller number ($q < p$) variables from which one can predict y "well enough" using the formula

$$y = g_1(x_1, x_2, \dots, x_q) \quad (2)$$

instead of the correct model (1). Note that if one knows the variables $x_1, x_2, \dots, x_p$ but incorrectly assumes $g = g_2$, g known, i.e.

$$y = g_2(x_1, x_2, \dots, x_p) , \quad (3)$$

then one introduces an equation or modeling error given by

$$e_m = g(x_1, \dots, x_p) - g_2(x_1, x_2, \dots, x_p). \quad (4)$$

In other cases, one may know g exactly but cannot measure (in applications) the x_i 's exactly so that one introduces a measurement error in predicting y . The measurement error is given by

$$e_M = g(x_1, \dots, x_p) - g(x_1 + \Delta_1, \dots, x_p + \Delta_p)$$

where Δ_i is the error made in measuring x_i . Clearly, in other applications there are various combinations of these kinds of errors. The experience and capability of the scientist or engineer (engineering judgment) directly affects the validity of the model, while the equipment accuracy or the laboratory technique of the scientist is directly related to the size of measurement error.

In most cases one does not know the function g , and hence one assumes that g belongs to a known (up to a set of parameter $\beta_1, \beta_2, \dots, \beta_n$) family of functions. One then uses data taken during an experiment to estimate these parameters. On placing the estimates in the model g , one is able to predict statistically the value of y given values $x_1, x_2, \dots, x_p$. That is, let (the form

of h is known)

$$g \in G = \{h(x_1, x_2, \dots, x_p; \beta_1, \beta_2, \dots, \beta_n)\}.$$

Then on estimating $\beta_1, \beta_2, \dots, \beta_n$ by the estimates $\hat{\beta}_1, \hat{\beta}_2, \dots, \hat{\beta}_n$ one estimates g by

$$\hat{g} = h(x_1, x_2, \dots, x_p; \hat{\beta}_1, \hat{\beta}_2, \dots, \hat{\beta}_n) \quad (5)$$

thus y can be predicted by $\hat{y} = \hat{g}$. How well one has done depends on the magnitude of the residual function $y - \hat{g}$.

One estimates the parameters by selecting N values of $x_1, x_2, \dots, x_p$, say $x_{i1}, x_{i2}, \dots, x_{ip}$, $i = 1, 2, \dots, N$ and observing the values of y at those values of $x_1, x_2, \dots, x_p$. These values are denoted by Y_i , $i = 1, 2, \dots, N$ where

$$Y_i = y_i + e_i, \quad (6)$$

and e_i is an unobservable random error with statistical properties

$$E(e_i) = 0 \quad i = 1, 2, \dots, N \quad (7)$$

and

$$E(e_i e_j) = \delta_{ij} v_{ij} \quad (8)$$

where $E(\cdot)$ is the expectation of $(\cdot)$ and $\delta_{ij} = 1$ if $i = j$ and zero otherwise. The equality (8) can be interpreted that the errors are assumed uncorrelated and the variance of the i^{th} error is v_{ii} , $i = 1, 2, \dots, N$.

The data to estimate $\beta_1, \beta_2, \dots, \beta_n$ are $Y_1, Y_2, \dots, Y_N$ and the

values of $X_i = (x_{i1}, x_{i2}, \dots, x_{ip})$, the i th values of $x_1, x_2, \dots, x_p$ in (5), along with g gives the N errors

$$e_i = Y_i - h(x_{i1}, x_{i2}, \dots, x_{ip} ; \beta_1, \dots, \beta_n)$$

$i = 1, 2, \dots, N$. To estimate $\beta_1, \dots, \beta_n$ one selects $f_1, f_2, \dots, f_n$

$$\hat{\beta}_1 = f_1(Y_1, \dots, Y_N; X)$$

$$\hat{\beta}_2 = f_2(Y_1, \dots, Y_N; X)$$

$$\vdots$$

$$\hat{\beta}_n = f_n(Y_1, \dots, Y_N; X)$$

in such a manner that a specified cost function is minimized.

Note that the $N \times n$ values of x_{ij} are known and in most cases can be selected by the experimenter. Thus, points to be sampled can be represented by a design matrix

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & & & \\ x_{N1} & x_{N2} & \dots & x_{Nn} \end{bmatrix} . \quad (9)$$

The estimate for y is then given by $\hat{y}$ in (5).

One should note that two quantities can be chosen by the experimenter in order for his experiment to be optimal with respect to some criteria of excellence. These quantities are the

sample size N and the elements x_{ij} of the design matrix, X .

What this means in the space station application is that there may exist pairs of quantities (N_i, X^i) $i = 1, 2, \dots, M$ which are admissible to estimate y in a manner such that a cost criterion is minimized yet M different equipment, manpower, and power requirements give the same minimal cost. Clearly, if the M pairs give different costs one needs only to select that pair (equivalently then, that equipment) that minimizes the cost.

1.3. Linear Models.

Classical experimental designs are modelled by selecting a linear function for g in (1). This means that

$$y = \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p$$

is the model from which y can be predicted if one knows the values $\beta_1, \beta_2, \dots, \beta_p$ and $x_1, x_2, \dots, x_p$ are given. Note that if $\beta_1, \beta_2, \dots, \beta_p$ are not known then one estimates the function y by using the data, $Y_i = y_i + e_i$ or

$$Y_i = \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + e_i \quad (10)$$

$i = 1, 2, \dots, N$. A convenient way to write the model (10) is in matrix notation

$$Y = X\beta + e$$

where $Y = [Y_1, Y_2, \dots, Y_N]^T$, $e = [e_1, e_2, \dots, e_N]^T$ are $N \times 1$ vectors of observations and unobservable random errors, respectively;

$\beta = [\beta_1, \beta_2, \dots, \beta_p]^T$ the $p \times 1$ unknown parameter vector we wish to estimate, and

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & & & \vdots \\ x_{N1} & x_{N2} & \dots & x_{Np} \end{bmatrix}$$

is an $N \times p$ design matrix.

It is well known [1] that if $E(e) = \phi$, the null matrix, and $E(ee^T) = V$, then the minimum variance linear unbiased estimator $\hat{\beta}$ for β is given by (the elements of X are assumed non-random)

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y ,$$

the Gauss-Markov estimator [1] [2]. Thus

$$\hat{y} = \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_p x_p .$$

The covariance matrix for $\hat{\beta}$ is given by

$$V(\hat{\beta}) = (X^T V^{-1} X)^{-1} .$$

It may be true that in some applications that the elements of the design matrix X are random. There are statistical techniques for estimating the β_i 's, [6].

If one restricts the values of x_{ij} to the values zero and one, then the model is called the experimental design model. If one restricts the model to being an experimental design and assumes

that $\beta_1, \beta_2, \dots, \beta_p$ are random variables, the model is called the component of variance model. Clearly, other models can be devised by mixing the models discussed here. However, we will not discuss this further since our purpose is not to develop the theory of estimation in linear models [4] but to indicate the types of models which are fundamental to this theory and to hypothesis testing.

1.4. Fundamentals in Planning an Experiment.

The objective of an experimental design is to obtain more information for less cost by selecting a precise procedure for carrying out the experiment so that the final estimates (information) are optimal (less cost). Engineering scientists, especially design engineers, may not be as familiar with the principles we include here as those scientists who are sometimes called experimental scientists. Many experimental scientists think of an experimental research activity to be composed of three parts, the experiment, the design and the analysis.

The experiment includes a statement of the problem to be solved. It is important that one flies only those experiments in which it has been established by someone just what the experiment is intended to accomplish.

Choice must be made as to the dependent variable (y) or variables to be investigated. Are these measurable? How accurately can they be measured on the instruments available? If they are not measurable, what type of response can be expected? Are the results to be yes or no responses, or perhaps simply counting data?

Is it necessary to define independent variables or factors which may affect the value of the dependent variable? Are these factors to be held constant, to assume certain specified levels, or to be averaged out by a process of randomization? Are the factors to be varied quantitative (such as magnitudes of temperature) or qualitative (an astronaut)? All of the above considerations go into the definition of the experiment.

The design includes the determination of the number (N) of observations to be taken; the order of experimentation; if randomization is to take place, what method is to be used; and finally, what mathematical model is valid to describe the experiment.

The analysis is a term which implies the process of collecting and processing the data taken; computing the estimates for interpretation; and finally modification of the design if further experimentation is required.

The planning engineers and management engineers or their representatives for space station development and application may need formal training in such topics in order to appreciate in a general way the special problems of the experimental scientist. This is recommended to avoid his having to understand the specific details of each and every experiment and experimental design.

1.5. Concerning "Fishing Expeditions".

In the space station application due to the peculiar constraints, exploratory research may not be justified. However, there exist some biologists who feel that this type of research

may pose the greatest challenge. How one takes these kinds of experimental activities into consideration during the laboratory equipment specification phase is not at all clear.

Consider the following paragraph extracted from a paper [5] by the plant scientist, Allan Brown.

"How best to design exploratory studies requires careful judgment. It is deceptively simple to propose just to measure whatever biological properties can easily be observed in a space laboratory in the hope of finding something exciting but this naive approach, often categorized as a "fishing expedition", is hardly warranted. I believe it should be self evident that optimizing exploratory efforts may be an even greater challenge to our scientific ingenuity than designing the analytical studies which logically will follow."

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CHAPTER II

On Selecting Statistical Data

Analysis Techniques for Space Station

Applications

"The notion that experiments and other research investigations can be conducted statistically or non-statistically at the will of the investigator is firmly held by many, it is usually entirely false" D. J. Finney, Experimental Design and its Statistical Basis.

2.1. Preliminary Remarks.

The aim of this chapter is to develop the concept that there do exist alternative statistical data techniques which may in turn induce alternative equipment requirements for a laboratory on-board a proposed space station.

It is clear that if a scientist adopts the philosophy that his experiment is to be totally contained in a container which requires no support of any type from the station, except the transport support, then that scientist will accept the responsibility not only as the principal investigator but the instrument design engineer, the selector of the experimental design, etc. This in a sense eliminates the requirement of laboratory equipment being available on board the space station. One should however note that this forces a requirement that the principal investigator have many capabilities including various instrumentation and experimental design capabilities. He should be able to select optimal equipment and optimal experimental design, with all other experiments to

be flown taken in consideration, in order to assure that other experiments may not be eliminated from the flight program due to his requirements. If instead, the principal investigator relies wholly on the space station for his instrumentation needs, this implies that the design engineer must have the capability of formulating optimal experimental design.

One suspects a desirable and reasonable situation is perhaps some mixture of the two philosophies. In any event, principal investigators and design engineers need to be made aware that there do exist such entities as "optimal" experimental designs. It should be noted that criteria of optimality must be compatible with the space station requirements and applications.

To facilitate reading we note that the minimum variance linear unbiased or so-called "best estimator" for the $n \times 1$ non-random parameter vector β in the linear model

$$Y_N = X_N \beta + e_N \quad (1)$$

which includes most experimental design models, is given by

$$\beta_N = (X_N^T V_N^{-1} X_N)^{-1} X_N^T V_N^{-1} Y_N \quad (2)$$

where Y_N is an $N_p \times 1$ vector of observations whose i^{th} element Y_i denotes a $p \times 1$ vector of observations taken at time t_i , $i = 1, 2, \dots, N$; the $N_p \times n$ matrix X_N is known and is a function of t_i and the magnitude of the coordinates of the observation station taking the measurements. The covariance matrix of the $N_p \times 1$ vector of random errors e_N is denoted by

$$V_N = E(e_N e_N^T) , \quad (3)$$

since it is assumed that

$$E(e_N) = \phi . \quad (4)$$

The operator $E(\cdot)$ is the expectation of $(\cdot)$.

Since (a) the value of N is extremely large in many space-station application problems, (b) the amount of time available for performing computation can be relatively small, and (c) the storage of the computers is limited, techniques that reduce time of computation and amount of storage are pertinent to our present discussion.

The problem remains the same, that is, to estimate β in (1), but the constraint of minimizing the computing and storage requirements is added. In the early portions of this chapter, five concepts for achieving these ends are discussed. They are:

- a. The concept of an optimal design
- b. The concept of a recursive technique for estimating the parameter vector
- c. The concept of compressing the data vector
- d. The concept of redundancy removal, and
- e. The concept of selecting characteristics to measure.

The sixth portion of this chapter deals with a procedure of reducing computing times in discriminating, a useful technique associated with problems in earth survey work, and perhaps some astronomy applications. The seventh section deals with the problem of designing experiments when there exist variables that one cannot control. In classical statistical literature this is called covariance analysis involving what is popularly

called concomitant variables. The ninth section is devoted to some concluding remarks that discuss briefly the effect of the techniques for selecting equipment configurations for laboratories in the space station.

It is interesting to note the complexity of the task that has evolved for the modern applied mathematician. Not only is the mathematician required to prove the existence of a solution of a problem, but he must be able to formulate an algorithm that will converge to the true solution and establish that the algorithm is stable and realistically compatible for use on the computer available. Furthermore, he must, due to so-called "real time" requirements for the solution, be able to achieve an "optimal" approximation to the solution in a specified amount of computing time using a specified amount of computer storage space.

2.2. Inverting the Output of Data Measuring Equipment.

In order to introduce the concept of possible trade-offs in selecting data recording or measuring equipment consider the following example: Let $y(t)$ denote a scalar real valued function (an observation signal) of a real variable t (time). Let $h(t)$ denote the impulse response function of the measuring equipment recording the data, $y(t)$. The output of the equipment in many cases can be modeled as

$$\tilde{y}(t) = \int_{-\infty}^t h(t - T)y(T)dT. \quad (1)$$

Now if $h(t)$ is a Dirac delta function $\delta(t)$, then

$$\tilde{y}(t) = y(t) = \int_{-\infty}^t \delta(t - T)y(T) dT, \quad (2)$$

and one reproduces the signal $y(t)$ exactly. However, this in general cannot be done.

Suppose one is willing to partition the measuring and recording operation into two distinct parts.

- (i) receiving and measuring
- (ii) inverting the measured signal or reconstructing the received signal.

Then, the measured signal is given to some degree of approximation by

$$m(t) = \int_{-\infty}^t h_1(t - u)y(u) du.$$

Thus, when possible, one needs to select equipment whose impulse response function is $h_1(t)$ which can be optimal with criterion compatible to the space station mission constrained to the condition that there exists an impulse response function $h_2(t)$ such that

$$\hat{y}(t) = \int_{-\infty}^t h_2(t - T)m(T) dT \quad (3)$$

where for all t

$$|\hat{y}(t) - y(t)|$$

is "arbitrarily" small for t sufficiently large. The impulse response function $h_2(t)$ is the inverse response function associated with the response function $h_1(t)$. That is, ideally one would wish that

$$\delta(t) = \int_0^t h_2(t - T)h_1(T) dT$$

the Dirac delta function. Then one would reproduce the signal exactly as it arrived at the measuring equipment. However, in any case when we consider (3) in the form given by (1) we have

$$h(t) = \int_0^t h_2(t - T)h_1(T) dT .$$

What we have introduced is the concept that one can select an admissible set of measuring equipment (E_1) where

$$E_1 = \{E_{1i}, i = 1, 2, \dots, k\}$$

whose impulse response functions are

$$H_1 = \{h_{1i}(t); i = 1, 2, \dots, k\};$$

in turn whose inverse impulse response functions are

$$H_2 = \{h_{2i}(t); i = 1, 2, \dots, k\}$$

such that for all $i = 1, 2, \dots, k$

$$h(t) = \int_0^t h_{1i}(t - T)h_{2i}(T) dT .$$

Note that the set H_2 induces a set of equipment

$$E_2 = \{E_{2i}; i = 1, 2, \dots, k\}$$

which are inverse filters associated with the set E_1 .

In many applications every element of the set E_2 can be simulated by a digital computer, either on board the space station, or if a high degree of fidelity in reproducing $y(t)$ is

desirable, then one can use off-board digital equipment.

If one considers the measuring equipment defined by the impulse response function $h(t)$ to be "good enough" one can compute the costs induced by the i^{th} filter pair, (h_{1i}, h_{2i}) . Let C_i denote the cost. Hence one selects the optimal by ordering the costs. That is,

$$C_j = \min_{i=1,2,\dots,k} \{C_i\}$$

implies that the j^{th} equipment with the response pair (h_{1j}, h_{2j}) is the optimal measuring equipment with respect to impulse response $h(t)$.

In summary, all measuring devices have an impulse response $h_1(t)$. It is important that for every measuring device flown $h_1(t)$ be known, so one can if necessary invert the output of the device to reproduce with accuracy the observation signal received.

2.3. The Optimal Design.

If one notes that the covariance matrix of the estimator $\hat{\beta} = \beta_N$ in (2) is

$$V(\beta_N) = (X_N^T V_N^{-1} X_N)^{-1}, \quad (5)$$

it becomes clear that it is desirable to select the matrix X_N so that $V(\beta_N)$ is minimal in the sense defined below.

Definition 1: Two positive definite matrices A and B are said to be comparable if either A-B or B-A are positive semi-definite.

Definition 2: The positive definite matrix A is said to be less

than the positive definite matrix B if B-A is positive semi-definite.

It is assumed in Definitions 1 and 2 that a positive definite matrix is also positive semi-definite.

The elements of the matrix X_N represent values some of which can be selected by the scientist. In the orbit determination problem the elements of X_N are functions of time and the coordinates of the observation station taking the i^{th} observation. The matrix X_N , which may in some cases be predetermined, is called the design matrix. The problem then is to select X_N so that (5) is as small as possible in the sense of Definition 2. Since replacing X_N by CX_N (C is a constant) replaces $(X_N V_N^{-1} X_N)^{-1}$ by $C^{-2} (X_N V_N^{-1} X_N)^{-1}$, the covariance matrix of the latter is a decreasing function of C and in fact decreases to the null matrix. Such a selection of X_N as CX_N is generally not possible since the validity of the linear model is a local property. If C were selected large, the linearity assumptions would be violated and the model (1) invalidated.

If we are allowed to choose the rows of X_N from an unbounded region, the elements of $(X_N V_N^{-1} X_N)^{-1}$ can be made arbitrarily close to zero. Suppose, however, the columns of X_N are chosen so that (x_i is the i^{th} column of X_N).

$$x_i^T V_N^{-1} x_i = C_i^2 \quad i = 1, 2, \dots, n \quad (6)$$

where C_i is given, then Rao [1] has shown the following theorem.

Theorem 1: Let X_N be a design matrix and $\hat{\beta}$ the minimum variance

linear unbiased estimator of β . Then, under the conditions (6)
on X_N ,

$$V(\hat{\beta}_j) \geq \frac{1}{c_j^2} \quad (7)$$

and the minimum is obtained when

$$x_i^T V^{-1} x_j = c \quad (8)$$

for all $j = 1, 2, \dots, i-1, i+1, \dots, n$.

What this means is that, theoretically, one can select the position of the observation stations and the times at which the observations are to be taken so that X_N , a function of these quantities, will have the property that the covariance matrix $V(\hat{\beta}_N)$ is minimized.

It is important to note, however, that this may not be an easy task, since we are in practice usually allowed to select row elements of X_N which must yield column properties to satisfy (6) and (8). There exist technical problems due to lack of uniqueness of the optimal design matrix. Odell and Cooper have studied this problem in some detail and a portion of their results are found in Cooper's dissertation dated August 1970. In their study, they have defined criteria that gives a unique optimal design for all values of N . Their work should lead to a mathematical model that will be a basis for the scientist or engineer to determine parameters and those times at which observations can be made to gain the greatest amount of information from the observations taken. Hence, it would be possible for fewer

observations to be taken for a specified level of variation of the estimator, $\hat{\beta}_N$.

2.4. On Selecting Characteristics to Measure

In most data analysis techniques one assumes that the observations are given, that is, the characteristics that are being measured are known a priori. However, there are applications in which one has the freedom to select the characteristic one would measure in order to perform a task efficiently.

Consider the following example for illustrative purposes. In many remote sensing experiments the $p \times 1$ observation vector y is composed of amplitude measurements for p radiation wave lengths. The wave lengths are selected a priori and therefore may be selected so that a cost criterion is minimized. In this case the cost function one wishes to minimize would be the expected probability of misclassification. A second example is applicable when one determines that it is impractical to measure a large number of characteristics; hence one asks the question, is there a subset of characteristics to measure which when measured gives "almost all" the information that the total set yields. If one measures a smaller number of characteristics, clearly one would expect less equipment to be required to accomplish the experiment. Space station applications with their weight limitations make these concepts important. Unfortunately, in many cases, there exists a need to be able to predict a response given the values of observations eliminated by selecting a subset to measure.

This creates a need for the capability to be able to predict the values of the eliminated observations using those observations taken. The following well-known theorem gives this capability.

Theorem 2: Let Y_1 and Y_2 denote two random vectors such that the following moments are known:

$$E[Y_1] = \mu_1$$

$$E[Y_2] = \mu_2$$

$$E[(Y_i - \mu_i)(Y_i - \mu_i)^T] = V_{ii} \quad i = 1, 2$$

and

$$E[(Y_1 - \mu_1)(Y_2 - \mu_2)^T] = V_{12} ,$$

then the best (in sense of minimum matrix squared error) linear predictor $\hat{Y}_1$ for Y_1 is given by

$$\hat{Y}_1 = \mu_1 + V_{12}V_{22}^{-1}(Y_2 - \mu_2) .$$

Note that the value of $\hat{Y}_1$, the predictor for Y_1 , is a function of Y_2 and the moments of Y_1 and Y_2 . Hence one can predict the values of Y_1 without actually making the observations. Of course, some information will be lost. Whether or not the amount of information lost is significant will depend on the values of the moments.

It is important to note that the principal investigator should be able to perform such an analysis and provide the equipment design engineer with a minimal list of characteristics to measure. The minimal list of characteristics may not be the

optimal list, optimal with respect to equipment and cost criteria, although by definition the characteristics in the optimal list yield maximum information. The equipment engineer may wish for engineering purposes to make trade-off decisions to select characteristics that are optimal with respect to criteria imposed by the space station requirements.

Abstractly, the characteristic selection for measuring can be stated as follows: Let $T_1, T_2, \dots, T_p$ denote p characteristics to be measured to produce a sample of size N . Let Y_j be the vector

$$Y_j = [Y_{1j}, Y_{2j}, \dots, Y_{pj}]^T \quad (9)$$

where Y_{ij} denotes the measurement or observation on the j^{th} individual from the i^{th} characteristic. The $p \times N$ data matrix is then

$$Y = [Y_1, Y_2, \dots, Y_p]$$

where Y_j is given by (9). In many such experiments there exist two or more sets of characteristics, say

$$S_z = \{T_1, \dots, T_q\}$$

$$S_x = \{T_{q+1}, \dots, T_t\}$$

.

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.

$$S_k = \{T_{m+1}, \dots, T_p\}$$

which essentially yield the "same" information about the individuals possessing the characteristics. Our task is to use

the data Y and determine which of the sets $S_z, S_x, \dots, S_k$ can be used to obtain "good" predictors of the measurements in the other remaining sets and yet contain a maximal amount of information.

2.5. Data Compression and Redundancy Removal

The term "data compression" has been used to denote at least two general concepts in data handling. These are:

- (1) recording only observations and times of observations that are "significantly different" from a previous observation, and
- (2) selecting a filter which replaces a "long" vector of observations with a "short" vector and retains as large amount of the information as possible. The first technique is essentially a redundancy removal technique, or a technique to replace the original observation (signal) with a close approximating function that requires less storage capacity and in the end may be easier to use for computational purposes.

The second technique is not based on the concept eliminating redundancy. It is, however, a recently developed concept [2].

The nature of the techniques can be described as follows:

Redundancy Removal Technique: Let $y = y(t)$ be a real scalar function of the real variable t representing an observation, and let the ordinate axis be divided into non-overlapping abutting intervals $\{\dots, y_{-2}, y_{-1}, 0, y_1, y_2, \dots\}$, where $|y_j - y_{j-1}| = d$, and d is a significant change, then one wishes to replace $y(t)$, with a step function approximation y (there are other variations to this approach but our discussion here contains the flavor of those

approaches also). Thus

$$\tilde{y}(t) = y_j, \quad y_j < y(t) \leq y_j + d,$$

but one stores only t_{1j} and t_{2j} and the value y_j such that

$$\tilde{y}(t) = y_j \quad \text{for all } t_{1j} \leq t \leq t_{2j}$$

and

$$\tilde{y}(t) = y_j \quad \text{for } t_{1,j-1} \quad \text{or} \quad t_{2,j+1}.$$

Data Compression Technique: Let Y be an $N_p \times 1$ vector of $p \times 1$ observations vectors y_i , $i = 1, 2, \dots, N$ such that $EY = [\mu^T, \mu^T, \dots, \mu^T]^T$ where $\mu = E[y_i]$ for each y_i and $V(Y) = \{V_{ij} \delta_{ij}\}$. One selects an $M_p \times N_p$ matrix B such that if $Z = BY$ is the compressed vector, then

$$EZ = [\mu^T, \mu^T, \dots, \mu^T]^T$$

and the covariance matrix of X is the block diagonal matrix

$$V(Z) = \{k V_{ij} \delta_{ij}\}$$

and the scalar k is minimized ($\delta_{ij} = 0$ if $i \neq j$ and unity otherwise).

An application which may clarify problems associated with compressed data is one in which one wishes to estimate the parameter vector β in the linear model given by

$$Y = X\beta + e,$$

where

$$E(e) = 0$$

and

$$E(ee^T) = \{V_{ij} \delta_{ij}\} = V.$$

However, the $N_p \times 1$ vector is replaced by the compressed vector

$$Z = BY \quad .$$

Then the linear model is replaced by

$$Z = BY = BX\beta + Be \quad ,$$

and the best linear unbiased estimator for β after the data compression is given by

$$\hat{\beta} = [X^T B^T (BV^{-1} B^T)^{-1} B X]^{-1} X^T B^T (BV^{-1} B)^{-1} Z \quad .$$

The covariance matrix is then given by

$$V(\hat{\beta}) = [X^T B^T (BV^{-1} B^T)^{-1} B X]^{-1} \quad ,$$

which is larger than the covariance matrix of the minimum variance linear unbiased estimator, β_{MV} , given by

$$\beta_{MV} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y \quad ,$$

whose covariance matrix is

$$V_{MV} = (X^T V^{-1} X)^{-1} \quad .$$

Necessary and sufficient conditions can be established on X so that $V_{MV} = V(\hat{\beta})$, for all admissible β .

It is important to note that if it is found desirable to compress the vector Y , one might wish to select a compressing matrix B (a linear filter) to satisfy other conditions than the ones given here for optimality.

2.6. Recursive Techniques

Let the sequence $\{Y_i, i = 1, 2, \dots, N\}$ be a sequence of $p \times 1$ vectors (observations) related to a state vector x by the linear model

$$Y_i = h_i x + e_i \quad i = 1, 2, \dots, N \quad (10)$$

where h_i is a known mapping matrix and e_i an unobservable $p \times 1$ random vector such that

$$E e_i = 0$$

$$E e_i e_j^T = V_{ij} \delta_{ij}$$

$$\delta_{ij} = 1 \quad \text{if } i = j$$

$$= 0 \quad \text{if } i \neq j.$$

The model (10) can be written in matrix notation in the following manner (note this is (1)):

$$Y_N = H_N x + E_N$$

where

$$Y_N = \begin{bmatrix} Y_1 \\ \vdots \\ Y_{N-1} \\ Y_N \end{bmatrix} = \begin{bmatrix} Y_{N-1} \\ Y_N \end{bmatrix}; \quad H_N = \begin{bmatrix} h_1 \\ \vdots \\ h_{N-1} \\ h_N \end{bmatrix} = \begin{bmatrix} H_{N-1} \\ h_N \end{bmatrix}$$

and the

$$E(E_N E_N^T) = V_N = \begin{bmatrix} V_{11} & 0 & & 0 \\ 0 & V_{22} & & 0 \\ & & \ddots & \\ 0 & 0 & & V_{NN} \end{bmatrix}$$

and

$$E_N = \begin{bmatrix} e_1 \\ \vdots \\ e_{N-1} \\ e_N \end{bmatrix} = \begin{bmatrix} e_{N-1} \\ e_N \end{bmatrix}.$$

The Gauss-Markov Theorem states that the best linear unbiased estimator, say $\hat{x}_N$, is given by (2), which is again,

$$\hat{x}_N = [H_N^T V_N^{-1} H_N]^{-1} H_N^T V_N^{-1} Y_N.$$

This quantity can be written

$$\begin{aligned} \hat{x}_N &= \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1} \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} y_i \right] \\ &= \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1} \left[\sum_{i=1}^{N-1} h_i^T V_{ii}^{-1} y_i + h_N^T V_{NN}^{-1} y_N \right] \\ &= \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1} \left[(H_{N-1}^T V_{N-1}^{-1} H_N)^{-1} \hat{x}_{N-1} + h_N^T V_{NN}^{-1} y_N \right] \end{aligned}$$

$$= \hat{x}_{N-1} + [\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} h_{ii}]^{-1} h_{NN}^T V_{NN}^{-1} [y_N - h_N \hat{x}_{N-1}] .$$

Note that if we "save-up" the last k observations before making a computation, the result is the same (this is sometimes called batch processing), i.e.

$$\hat{x}_N = \left[\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} h_{ii} + \sum_{i=N-k+1}^N h_{ii}^T V_{ii}^{-1} h_{ii} \right]^{-1} \left[\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} y_i + \sum_{i=N-k+1}^N h_{ii}^T V_{ii}^{-1} y_i \right]. \quad (11)$$

But

$$\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} y_i = \left(\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} h_{ii} \right) \hat{x}_{N-k}$$

and

$$\sum_{i=N-k+1}^N h_{ii}^T V_{ii}^{-1} y_i = \left(\sum_{i=N-k+1}^N h_{ii}^T V_{ii}^{-1} h_{ii} \right) \hat{x}_k'$$

that is the best estimate based on last k observations. Also we note that if $R_{\hat{x}}$ denotes the covariance matrix for $\hat{x}$, that

$$R_{\hat{x}_{N-k}} = \left(\sum_{i=1}^{N-k} h_{ii}^T V_{ii}^{-1} h_{ii} \right)^{-1}$$

$$R_{\hat{x}_k} = \left(\sum_{i=N-k+1}^N h_{ii}^T V_{ii}^{-1} h_{ii} \right)^{-1} .$$

Then (11) is simply

$$\hat{x}_N = [R_{\hat{x}_{N-k}}^{-1} + R_{\hat{x}_k}^{-1}]^{-1} [R_{\hat{x}_{N-k}}^{-1} \hat{x}_{N-k} + R_{\hat{x}_k}^{-1} \hat{x}_k'] . \quad (12)$$

It is important to note that the formula (12) is the linear combination of the best estimate for x given $N-k$ observations and the best estimate for x given the last k observations.

Unfortunately, one must store the last k observations. Yet $\hat{x}_{N-k}$ can be computed recursively and the first $N-k$ observations can be "thrown away" since all the information needed to estimate X is contained in the first $N-k$ observations is contained in $\hat{x}_{N-k}$.

2.7. Fast Techniques for Discriminate Analysis

The application of discriminate analysis to earth surveys is well-known [3]. There are those who know of this technique through their work with remote sensing devices [4]. The problem is to classify an object as being a member of a population by using data corrupted by random error. However, in an earth survey application, if this process is performed a very large number of times, and on-board data processing is a desirable mode of operation, there may be a requirement for large data storage facilities and high speed computing capabilities on the space station.

The Problem: Let x_{α}^j , $\alpha = 1, 2, \dots, N_j$ and $j = 1, 2, \dots, k$ denote N_j $p \times 1$ sample vectors from k distinct populations $\pi_1, \pi_2, \dots, \pi_k$ whose respective probability density functions $p_1(x), \dots, p_k(x)$ are unknown. Let X be a $p \times 1$ sample vector from an individual from one of the populations. Using this data assign this individual in an optimal manner to one of the populations $\pi_1, \pi_2, \dots, \pi_k$.

A solution to this problem is well-known [3] and well studied [5], [6], [7]. However, the fact that this must be repeated a large number of times in many applications can affect the equipment requirements.

A single image to be reduced is composed of mn identifications (number of frames per image). Each identification using classical discriminant techniques involves a computation of a quadratic form

$$Q_j = x^T \hat{\Sigma}_j^{-1} x \quad j = 1, 2, \dots, k$$

where $\hat{\Sigma}_j^{-1}$ is an estimate of the covariance matrix of the observations from the j th population. Note that for each j that there will be $p^2 + p$ multiplications.

For illustrative purposes let $k = 10$, $p = 5$, $m = 2 \times 10^2$, and $n = 10^3$. This is a close approximation to what LARS [4] is performing. Then for each identification one performs 30 additions, 30 multiplications, and 1 ordering of numbers. For one, a single image, the number of operations performed is six million additions and six million multiplications, plus 2×10^5 orderings of 10 numbers per ordering.

One strategy to reduce the computational load is to select a $q \times p$ matrix P where $q < p$ and define a compressed vector

$$Y = PX \tag{4}$$

then an estimate of the j^{th} covariance matrix of Y is

$$\hat{V}_j = P \hat{\Sigma} P^T \quad (5)$$

a $q \times q$ matrix. What is gained in computation is related to the fact that now one does $q^2 + q$ additions and $q^2 + q$ multiplications.

However, the question of efficiency remains, that is what has been lost with respect to reducing the probabilities of proper classifications.

It is important to note that the classical technique for discriminate analysis is formulated on a normality assumption. One might increase the probabilities of proper classification by using the training data used to estimate $\hat{\Sigma}_j$, to estimate $P(X)$, $j = 1, 2, \dots, k$, the probability density function of the observations associated with the j th population.

Eppler [8] has considered this problem of selecting the matrix in (4) P so that the probabilities of proper classification of crop patterns has not been significantly reduced yet computing times have been reduced to the order of $1/32$ the time. Wilks [5] has given a way of selecting an optimal P . His optimality criterion is not probabilities of proper classification but is directly related to this latter criterion.

2.8. Statistical Methods for Controlling Variability

In planning a multipurpose laboratory housed in a space station, planning engineers become acutely aware of the problem of being able to control the variability of environmental factors within the space station to the level specified by principle

investigators. One can expect that there will be some experiments that cannot be performed due to the inability to control sufficiently environmental factors in the laboratory or within the experimental package in which the experiment is to be carried out.

Fortunately there exist experimental situations in which one may introduce the concept of modeling the effects of the variations in the environment on the observations to be taken in a proposed experiment. Since experimental designs are plans for direct control of variability, it seems desirable that what we will suggest here should be especially compatible with the existing classical techniques for analysis of experiments. In fact, what is being suggested is a generalization of a practice which the statistician calls covariance analysis.

There are two general methods for controlling variability due to experimental error which we will call direct and statistical. Direct control includes such methods as grouping the experimental units into homogeneous strata or blocks, to increase the accuracy of measurements. Replicated experiments, randomized block designs, split-plot designs, and other sophisticated designs use the direct control principle to increase the precision of the experiment.

Note that in a space station application, a requirement to increase the uniformity of the conditions under which the experiment is to be run and increasing the accuracy of measurements generally imply a requirement for sophistication of equipment to be included in the station. "State of the art" of measuring

equipment and environmental control devices as well as simple economics may be such that requirements of accuracy and uniformity may not be obtainable. These restrictions, at some level, will always prevent some experiments from being flown. Yet, it should be our efforts to develop alternative techniques which will allow perhaps more experiments to be acceptable to the "state of the art" laboratory finally flown.

Fortunately, there exist experimental designs which use an indirect, or statistical control (1) to increase the precision of the experiment and (2) to remove potential sources of bias in the experiment. These techniques should be introduced to the project managers, design engineers and those scientists who are potential principle investigators.

The problem of removing bias is an objective that is of particular importance in those situations where the experimenter cannot assign individuals at random to the experimental conditions. Statistical control is achieved by measuring one or more concomitant variates in addition to the variate of primary interest. Common usage suggests the term co-variate for concomitant variates. Measurements on covariates are made for the purpose of adjusting the measurements on the observed variate, the observation.

Direct control and statistical control may, of course, be used simultaneously within the same experiment. One or more variates may be under direct control while others may be under statistical control.

In the section that follows, we will present an example in

which we attempt to clarify our statements in this paragraph.

Let us consider a simple example incorporating a classical model of an experimental design, that is, a two-way classification with unequal numbers in subclasses. The model is given by the formula

$$Y_{ijk} = \mu + T_i + \beta_j + e_{ijk} ,$$

where

$$i = 1, 2, \dots, t$$

$$j = 1, 2, \dots, b$$

$$k = 1, 2, \dots, n_{ij} ;$$

and μ denotes a mean effect due to the population of experimental units involved, T_i denotes an effect due to the i^{th} treatment, β_j denotes an effect due to the j^{th} block, y_{ijk} denotes the observed value of the primary variate, and e_{ijk} an unobservable random variate usually assumed to be such that

$$E[e_{ijk}] = 0 \quad \text{for all } i, j, \text{ and } k$$

and

$$\begin{aligned} E[e_{ijk}e_{i'j'k'}] &= 0 \text{ if } i \neq i' \text{ or } j \neq j' \text{ or } k \neq k' \\ &= \sigma^2 \text{ if } i = i' \text{ and } j = j' \text{ and } k = k'. \end{aligned}$$

The inclusion of β_j in the model is a direct method for controlling variability due to some set of blocks $\{\beta_1, \beta_2, \dots, \beta_b\}$. One can think of T_1 as being a zero-gravity treatment and T_2 as a one-gravity treatment while β_1 and β_2 are the different effects due

to laboratories, one on the space station and one on the earth. Here $t = 2$ and $b = 2$.

However, suppose in the space station there exist environmental factors $X_1, X_2, \dots, X_q$ associated with the space station, and these covariates are believed or perhaps only conjectured to affect the value of Y_{ijk} . Hence, we must find a means to control the variability of experimental error due to these factors. One method is by direct means, that is, we might consider $X_1, X_2, \dots, X_q$ as block effect and extend the experimental model by adding p_i , $i = 1, 2, 3, \dots, q$ levels of each factor X_i , $i = 1, 2, 3, \dots, q$. However, if it is not possible to fix and maintain the levels of the factors X_i , $i = 1, 2, \dots, q$ there still exists the indirect technique for controlling the variability of the experimental error by adjusting for the variation in the covariates.

The indirect technique is to model the effect of the covariates. In the case discussed here, the model would be modified by adding the function g , that is,

$$Y_{ijk} = \mu + T_i + \beta_j + g(x_{ij1}, x_{ij2}, \dots, x_{ijq}) + e_{ijk}$$

where x_{ijp} , $p = 1, 2, \dots, q$ denotes the covariate for T_i and β_j . The function g denotes the manner in which Y_{ijk} varies with the values of the covariates. Of course, if g is known, that is, the form of g is known exactly then we define

$$Y_{ijk}^* = Y_{ijk} - g(x_{ij1}, \dots, x_{ijq})$$

and the model

$$y_{ijk}^* = \mu + T_i + \beta_j + e_{ijk}$$

is the classical original design, adjusted for the covariates.

Unfortunately, the form of g is generally unknown to the experimenter, and hence, must be approximated using the data taken. One can assume that the function g is a member of a class of functions, which we will denote here by G , defined by a set of parameters

$$\theta_1, \theta_2, \dots, \theta_p.$$

that is,

$$g = g(x_{ij1}, x_{ij2}, \dots, x_{ijq}; \theta_1, \dots, \theta_p),$$

where the rule for defining the set G is known. One such class could be the planes in Euclidean p -space. That is to say,

$$g = \sum_{j=1}^p \theta_j x_j$$

and one must select the estimates

$$\hat{\theta}_1, \hat{\theta}_2, \dots, \hat{\theta}_p$$

so that the true g is optimally estimated with respect to some criteria. If G is a known class of non-linear functions, then we recognize the problem as one in non-linear curve fitting or non-linear regression.

2.9. Concluding Remarks

It is clear that one can select a spectrum of data analysis techniques as well as assure that designs are optimal in order to

obtain a desirable final configuration of equipment.

What has been presented here is an expository on some rather sophisticated techniques which can lead to alternatives in equipment requirements for the space station application. Figure 1 has been included to exemplify the large number of alternatives which can be available for cost effectiveness analysis.

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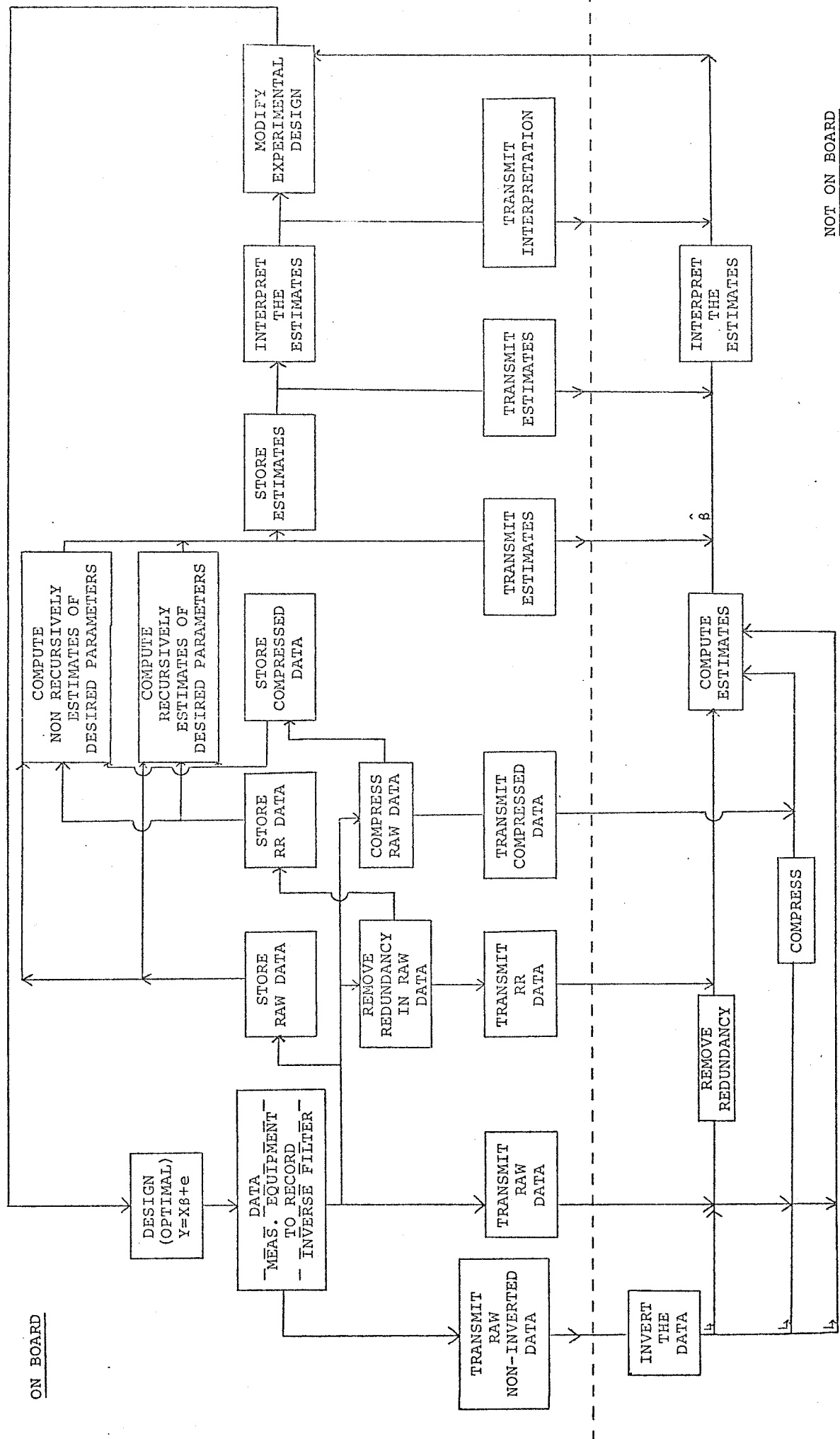


Figure 1

CHAPTER III

On Selecting an Optimal Design Matrix

"By the "design" of an experiment is meant: (i) the set of treatments selected for comparison; (ii) the specification of the units (animals, field plots, samples of blood) to which the treatments are to be applied; (iii) the rules by which the treatments are to be allocated to experimental units; (iv) the specification of the measurements or other records to be made on each unit. The relevance of an experiment to the problems under investigation and the trustworthiness of conclusions drawn from the experiment depend very largely upon these matters."

D. J. Finney,
Experimental Design

3.1 Introduction [1] [2]

In this chapter we consider the problem of estimating the coefficients in a full-rank linear model

$$Y = Hx + u \quad . \quad (1)$$

We let Y be an $N \times 1$ observable random vector, H an $N \times (p + 1)$ design matrix of rank $p + 1$ whose rows are the points at which observations are made, x a $(p + 1) \times 1$ parameter vector to be estimated, and U an $N \times 1$ random error vector such that

$$E(U) = 0$$

$$E(UU^T) = V \quad ,$$

where V is a known positive definite $N \times N$ matrix.

It is well known (Gauss-Markov theorem) that the best linear unbiased estimator $\hat{X}$ of x is given by

$$\hat{X} = (H^T V^{-1} H)^{-1} H^T V^{-1} Y$$

with covariance

$$\text{Cov}(\hat{X}) = (H^T V^{-1} H)^{-1} \quad .$$

Note that the covariance of $\hat{X}$ is a function of the design matrix H . It is desirable, then, to select the design matrix H in such a manner as to minimize the diagonal elements of the matrix $(H^T V^{-1} H)^{-1}$. Thus the corresponding estimator $\hat{X}$

has been improved in the sense of minimizing the variances of the elements of $\hat{X}$.

To define what we mean by an optimum design matrix H so that the diagonal elements of $(H^T V^{-1} H)^{-1}$ are minimized we make the following definition. In the discussion to follow, we shall make $V = \sigma^2 I$ since there will be no loss in generality.

Definition 3-1.1. A matrix H is said to be as good as a matrix Z , written $H \leq Z$, if $(Z^T Z)^{-1} - (H^T H)^{-1}$ is positive (semidefinite).

Definition 3-1.2. A matrix H is said to be better than a matrix Z , written $H < Z$, if $(Z^T Z)^{-1} - (H^T H)^{-1}$ is positive semidefinite and not null.

Definition 3-1.3. A matrix H is said to be equivalent to a matrix Z , written $H \approx Z$, if $(H^T H)^{-1} = (Z^T Z)^{-1}$.

Lemma 3-1.1. The relation $\leq$ defined above satisfies the following three properties of a partial ordering:

1. For any matrix H , $H \leq H$.
2. If $H \leq Z$ and $Z \leq W$, then $H \leq W$.
3. If $H \leq Z$ and $Z \leq H$, then $H \approx Z$.

Example 3-1.1 shows why the following property, $H \leq Z$

and $Z \leq H$ implies $H = Z$, does not hold here. It should be noted, however, that the two matrices in Example 3-1.1 are somewhat related in that they are both "optimal" designs.

Example 3-1.1. Let

$$H = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix} \quad \text{and} \quad Z = \begin{bmatrix} 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

Then it follows that

$$(H^T H)^{-1} = (Z^T Z)^{-1} = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}.$$

The standard definitions for comparability for partial ordering follow.

Definition 3-1.4. Two matrices H and Z are said to be comparable if either $H \leq Z$ or $Z \leq H$.

It is easy to show that all matrices are not comparable;
for suppose

$$(H^T H)^{-1} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

and

$$(Z^T Z)^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

It then follows that neither

$$(H^T H)^{-1} - (Z^T Z)^{-1}$$

nor

$$(Z^T Z)^{-1} - (H^T H)^{-1}$$

are positive semidefinite. Since all matrices are not comparable under Definition 3-1.3 and 3-1.4 we add Definitions 3-1.5 and 3-1.6.

Definition 3-1.5. The matrix H is said to be weakly better

than the matrix Z , written $H \leq_w Z$, if

$$\max\{a_{ii}\} \leq \max\{b_{ii}\} ,$$

where

$$(H^T H)^{-1} = (a_{ij}) \quad \text{and} \quad (Z^T Z)^{-1} = (b_{ij}) .$$

Definition 3-1.6. The matrix H is said to be weakly better than the matrix S , written $H <_w Z$, if

$$\max\{a_{ii}\} < \max\{b_{ii}\} .$$

Lemma 3-1.2. The following properties hold:

1. For any matrix H , then $H \leq_w H$.
2. If $H \leq_w Z$ and $Z \leq_w W$, then $H \leq_w W$.
3. For any two matrices, then either $H \leq_w Z$ or $Z \leq_w H$.

Proof: To prove property 1, let H be any matrix, then

$$(H^T H)^{-1} = (H^T H)^{-1}, \text{ which implies } \max\{a_{ii}\} = \max\{a_{ii}\}. \text{ Thus}$$

$$H \leq_w H.$$

To prove property 2, let $H \leq_w Z$ and $Z \leq_w W$; then

$$\max\{a_{ii}\} \leq \max\{b_{ii}\} \text{ and } \max\{b_{ii}\} \leq \max\{c_{ii}\}, \text{ where}$$

$(H^T H)^{-1} = (a_{ij})$, $(Z^T Z)^{-1} = (b_{ij})$, and $(W^T W) = (c_{ij})$. Hence $\max\{a_{ij}\} \leq \max\{b_{ii}\} \leq \max\{c_{ii}\}$ implies $\max\{a_{ii}\} \leq \max\{c_{ii}\}$ and consequently, $H \underset{W}{\leq} W$.

To prove property 3, let H and Z be any two matrices, where $(H^T H)^{-1} = (a_{ij})$ and $(Z^T Z)^{-1} = (b_{ij})$. Let $a = \max\{a_{ii}\}$ and $b = \max\{b_{ii}\}$; then since a and b are real numbers we either have $a \leq b$ or $b \leq a$. Therefore, $H \underset{W}{\leq} Z$ or $Z \underset{W}{\leq} H$.

Notice that the relation $\underset{W}{\leq}$ satisfies all of the properties for a total ordering except for the antisymmetric property defined above. However, we do have the property that any two matrices are comparable under the definition.

The relationship between the inequalities $\leq$ and $\underset{W}{\leq}$ is demonstrated by Lemma 3-1.3.

Lemma 3-1.3. If $H \leq Z$, then $H \underset{W}{\leq} Z$.

Proof: Let $(H^T H)^{-1} = (a_{ij})$ and $(Z^T Z)^{-1} = (b_{ij})$. Then $H \leq Z$ implies that $(Z^T Z)^{-1} - (H^T H)^{-1}$ is positive semidefinite or that $(b_{ij}) - (a_{ij})$ is positive semidefinite. But each diagonal element $b_{ii} - a_{ii}$ is a principal submatrix of $(Z^T Z)^{-1} - (H^T H)^{-1}$ and has a non-negative determinant. Therefore, $b_{ii} - a_{ii} \leq 0$ or $a_{ii} \leq b_{ii}$ for all i . Thus $\max\{a_{ii}\} \leq \max\{b_{ii}\}$ and $H \underset{W}{\leq} Z$.

The following additional properties of the relation $\leq$ will help to demonstrate our interest in it with respect to the present problem of minimizing $\text{Var}(\hat{\beta})$ by selecting the design matrix H . The first of these properties could have been chosen as the basic definition and since matrix inversion in practice is at best tedious or inexact, Property 3-1.1 will be used extensively.

Property 3-1.1. $H \leq Z$ if and only if $H^T H - Z^T Z$ is positive semidefinite.

Proof: Let $A_1 = (H^T H)$, $A_2 = (Z^T Z)$, and $A = A_1 - A_2$.

Suppose A is positive semidefinite. Then $A_1 = A_2 + A$ or $A_1^{-1} = (A_2 + A)^{-1} = (A_2 + C^T C)^{-1} = A_2^{-1} - A_2^{-1} C^T (I + C A_2^{-1} C^T)^{-1} C A_2^{-1}$, where $A = C^T C$. Therefore, $A_2^{-1} - A_1^{-1} = A_2^{-1} C^T (I + C A_2^{-1} C^T)^{-1} C A_2^{-1}$ is positive semidefinite since A_2^{-1} and $C^T (I + C A_2^{-1} C^T)^{-1} C$ are positive semidefinite. Thus $(Z^T Z)^{-1} - (H^T H)^{-1}$ is positive semidefinite and hence $H \leq Z$.

The converse can be similarly shown.

Property 3-1.2. If $H = (J, H_1, \dots, H_p)$, $Z = (J, Z_1, \dots, Z_p)$,

and $T = (\emptyset, t_1 J, \dots, t_p J)$, where the t_i 's are known constants,

then $H \leq Z$ implies that $(H + T) \leq (Z + T)$.

Proof: From the definition of H , Z , and T we see that

$$(H + T) = (J, H_1 + t_1 J, \dots, H_p + t_p J) \quad \text{and}$$

$(Z + T) = (J, Z_1 + t_1 J, \dots, Z_p + t_p J)$. Therefore, by multiplication we have

$$\begin{aligned} (H + T)^T (H + T) &= \\ &= \begin{bmatrix} J^T J & J^T (H_1 + t_1 J) & \dots & J^T (H_p + t_p J) \\ (H_1 + t_1 J)^T J & (H_1 + t_1 J)^T (H_1 + t_1 J) & \dots & (H_1 + t_1 J)^T (H_p + t_p J) \\ \vdots & \vdots & & \vdots \\ (H_p + t_p J)^T J & (H_p + t_p J)^T (H_1 + t_1 J) & \dots & (H_p + t_p J)^T (H_p + t_p J) \end{bmatrix} \\ &= \begin{bmatrix} J^T J & J^T H_1 + t_1 J^T J & \dots & J^T H_p + t_p J^T J \\ H_1^T J + t_1 J^T J & H_1^T H_1 + t_1 H_1^T J & & H_1^T H_p + t_p H_1^T J \\ & + t_1 J^T H_1 + t_1 t_1 J^T J & \dots & + t_1 J^T H_p + t_1 t_p J^T J \\ \vdots & \vdots & & \vdots \\ H_p^T J + t_p J^T J & H_p^T H_1 + t_1 H_p^T J & \dots & H_p^T H_p + t_p H_p^T J \\ & + t_p J^T H_1 + t_p t_1 J^T J & & + t_p J^T H_p + t_p t_p J^T J \end{bmatrix}. \end{aligned}$$

Consider the nonsingular matrix of elementary operations:

$$E = \begin{bmatrix} 1 & -t_1 & -t_2 & \dots & -t_p \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

Then by multiplication, $E^T(H + T)^T(H + T)E$ is

$$\begin{bmatrix} J^T J & J^T H_1 & \dots & J^T H_p \\ H_1^T J & H_1^T H_1 & \dots & H_1^T H_p \\ \vdots & \vdots & & \vdots \\ H_p^T J & H_p^T H_1 & \dots & H_p^T H_p \end{bmatrix}$$

which is $H^T H$. That is, $(H + T)^T(H + T) = E^{-T} H^T H E^{-1}$, where $E^{-T} = (E^{-1})^T$.

Similarly we see that $E^T(Z + T)^T(Z + T)E = Z^T Z$ or $(Z + T)^T(Z + T) = E^{-T} Z^T Z E^{-1}$. But by Property 3-1.1, $H \leq Z$ implies that $H^T H - Z^T Z$ is positive semidefinite. The difference $(H + T)^T(H + T) - (Z + T)^T(Z + T) = E^{-T} H^T H E^{-1} - E^{-T} Z^T Z E^{-1} = E^{-T} (H^T H - Z^T Z) E^{-1}$ is positive semidefinite since $H^T H - Z^T Z$ is positive semidefinite. Hence, by Property 3-1.1, $(H + T) \leq (Z + T)$.

Property 3-1.3. If R is a nonsingular matrix, then $H \leq Z$

implies that $HR \leq ZR$.

Proof: $(HR)^T(HR) - (ZR)^T(ZR) = R^T H^T H R - R^T Z^T Z R = R^T (H^T H - Z^T Z) R$.

But $H^T H - Z^T Z$ is positive semidefinite since $H \leq Z$. Thus $R^T (H^T H - Z^T Z) R$ is positive semidefinite and $HR \leq ZR$.

Property 3-1.4. If R is an orthogonal matrix, then $H \leq Z$ implies that $RH \leq RZ$.

Proof: $(RH)^T(RH) - (RZ)^T(RZ) = H^T R^T R H - Z^T R^T R Z = H^T I H - Z^T I Z = H^T H - Z^T Z$. But $H \leq Z$; hence $H^T H - Z^T Z$ is positive semidefinite and $(RH)^T(RH) - (RZ)^T(RZ)$ is positive semidefinite, and therefore, $RH \leq RZ$.

Property 3-1.5. If $H \leq Z$, then $|H^T H| \geq |Z^T Z|$.

Proof: Let $A_1 = H^T H$ and $A_2 = Z^T Z$. Then by Property 3-1.1 we have $H \leq Z$ implying that $A = A_1 - A_2 = H^T H - Z^T Z$ is positive semidefinite. Hence $A_1 = A + A_2$ and

$|A_1| = |A + A_2| \geq |A| + |A_2| \geq |A_2|$ by Minkowski's determinant theorem. Thus $|H^T H| \geq |Z^T Z|$.

Property 3-1.6. If $H \leq Z$, then $\text{tr}(H^T H) \leq \text{tr}(Z^T Z)$.

Proof: Let $H^T H = (a_{ij})$ and $Z^T Z = (b_{ij})$. Then $H \leq Z$ implies by Property 3-1.1 that $H^T H - Z^T Z$ is positive semidefinite. Therefore, each diagonal element $a_{ii} - b_{ii}$ is a

principal submatrix of $H^T H - Z^T Z$, and has a nonnegative determinant. Thus $a_{ii} - b_{ii} \geq 0$ for all i and hence

$$\text{tr}(H^T H) = \sum_{i=1}^{p+1} a_{ii} - \sum_{i=1}^{p+1} b_{ii} = \text{tr}(Z^T Z).$$

3.2 Rectangular and Ellipsoidal Regions

We now consider $\text{Cov}(\hat{X}) = \sigma^2 (H^T H)^{-1}$ to see if there are any natural restrictions placed on the selection of H . Theorem 3-2.1 by Rao [3] is of interest.

Theorem 3-2.1. Let $\text{Cov}(\hat{X}) = \sigma^2 (H^T H)^{-1}$ be the covariance matrix of the best linear unbiased estimate for x in the linear model $Y = Hx + u$. Then if one can select the columns of $H = (H_0, H_1, \dots, H_p)$ such that the scalar $H_i^T H_i$ is maximal and $H_i^T H_j = 0$ for $i \neq j$, the $\text{Cov}(\hat{X})$ is minimal.

Proof: Let

$$\text{Cov}(\hat{X})/\sigma^2 = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}^{-1}.$$

Then $V_{11} = (R_{11} - R_{12} R_{22}^{-1} R_{21})^{-1} = R_{11}^{-1} + R_{11}^{-1} R_{12} V_{22} R_{21} R_{11}^{-1}$. To

minimize V_{11} we certainly want to choose R_{12} such that

$R_{11}^{-1} R_{12} V_{22} R_{21} R_{11}^{-1} = 0$. But since $(H^T H)^{-1}$ is positive definite,

then V_{22} is positive definite. Hence $R_{21}R_{11}^{-1} = R_{11}^{-1}R_{12} = 0$ or $R_{12} = R_{21} = 0$. But by definition R_{12} is a matrix whose elements are of the form $H_i^T H_j$ for $i \neq j$. Thus $H_i^T H_j = 0$ for all $i \neq j$. If R_{11} is a scalar then $R_{11} = H_1^T H_1$ and consequently $v_{11} = (H_1^T H_1)^{-1}$. Thus, to minimize v_{11} we must maximize $H_1^T H_1$, by selecting H_1 as far away from the $N \times 1$ zero vector as possible in the L_2 norm sense. This will be true for any of the diagonal elements v_{ii} of V since multiplication on the left by the elementary matrix E interchanges rows 1 and i and on the left by E^T interchanges v_{ii} and v_{11} . Hence v_{ii} is minimized when $H_i^T H_i$ is maximized, that is, when H_i is selected as far from the $N \times 1$ zero vector as possible.

Theorem 3-2.1 indicates that if one selects H_i at the $N \times 1$ "infinity" vector, then $\text{Cov}(\hat{X}) = 1/\sigma^2 (v_{ij}) = 0$.

This is not practical for two reasons.

1. The linearity assumptions on which the model is based are valid in only a bounded region R in E_{p+1} and/or
2. The physical limitations on sampling restrict our attention to a bounded region R in E_{p+1} .

Thus $R = \{(h_0, h_1, \dots, h_p) : \sum_{i=0}^p h_i^2 \leq c\}$, for some positive

real number c .

We shall consider two special regions, rectangular and ellipsoidal, given by

$$R_1 = \{(1, h_1, \dots, h_p) : (a_1, \dots, a_p) \leq (h_1, \dots, h_p) \leq (b_1, \dots, b_p)\}$$

and

$$R_2 = \{(1, h_1, \dots, h_p) : (h_1, \dots, h_p) A (h_1, \dots, h_p)^T \leq 1\} \quad ,$$

where A is a $p \times p$ positive definite matrix.)

Using Theorems 3-2.2 through 3-2.4 we see that we shall need to consider only those rectangular and ellipsoidal regions whose centers are at the origin and whose axes are parallel to the coordinate axes.

Definition 3-2.1. A translation matrix T is an $N \times (p + 1)$ matrix of the form $T = (\emptyset, t_1 J, \dots, t_p J)$, where $\emptyset$ is the $N \times 1$ vector of zeros, J is the $N \times 1$ vector of ones, and the constants t_i are known.

It should be noted that for the regions described above the design matrix H of the regression linear model [2] can be written in the form

$$H = (J, H_1, \dots, H_p) \quad .$$

Theorem 3-2.2. (Translation). Let H and Z be any two design matrices of the form above and let T be a translation matrix. Then $H + T \leq Z + T$ if and only if $H \leq Z$.

Proof: It is clear that the design and translation described here are precisely the matrices of Property 3-1.2; hence Theorem 3-2.2 is proved.

Theorem 3-2.3. If H is a design matrix and T is a translation matrix then $\det((H + T)^T(H + T)) = \det(H^TH)$.

Proof: In Property 3-1.2 we described a matrix E such that $(H + T)^T(H + T) = E^{-T}H^TH E^{-1}$. But E is a product of elementary column operations matrices each of which has determinant 1. Thus E has determinant 1, and $\det[(H + T)^T(H + T)] = \det(E^{-T}H^TH E^{-1}) = \det(E^{-T}) \cdot \det(H^TH) \det(E^{-1}) = [\det(E^{-1})]^2 \det(H^TH) = \det(H^TH)$.

Definition 3-2.4. A rotation matrix is a $(p + 1) \times (p + 1)$ orthogonal matrix.

Theorem 3-2.4. (Rotation). Let H and Z be any two design matrices of the form above and let R be a rotation matrix. Then $HR \leq ZR$ if and only if $H \leq Z$.

Proof: Since R is orthogonal, $R^T = R^{-1}$ and by Property 3-1.3, $HR \leq ZR$ if $H \leq Z$.

Theorem 3-2.5. Let R be a $(p+1) \times (p+1)$ nonsingular matrix; then for any design matrix H $\det[(HR)^T(HR)] = \det(R)^2 \det(H^T H)$.

Proof: $\det[(HR)^T(HR)] = \det(R^T H^T H R) = \det(R^T) \det(H^T H) \det(R)$
 $= \det(R) \det(R^T) \det(H^T H) = \det(RR^T) \det(H^T H) = [\det(R)]^2 \det(H^T H)$.

Corollary 3-2.1. If H is a design matrix and R is a rotation matrix then $\det[(HR)^T(HR)] = \det(H^T H)$.

Proof: In Theorem 3-2.5 we have that $\det[(HR)^T(HR)] = \det(RR^T) \det(H^T H)$. But $RR^T = I$ and thus $\det(RR^T) = 1$. Hence $\det[(HR)^T(HR)] = \det(H^T H)$.

Definition 3-2.3. A scaling matrix is a $(p+1) \times (p+1)$ diagonal matrix with all diagonal elements positive constants.

Theorem 3-2.6. Let H and Z be any two design matrices and let S be a scaling matrix. Then $HS \leq ZS$ if and only if $H \leq Z$.

Proof: Since S is a diagonal matrix with all diagonal elements positive constants, then S is nonsingular. Thus H and S are the matrices of Property 3-1.3 and $HS \leq ZS$ if $H \leq Z$.

Since the relation $\leq$ is less than a partial ordering and not all designs are comparable, there may not be an optimal

design. Consequently, we define a minimal class of designs from which a best design may be selected.

Definition 3-2.4. A design H is said to be admissible if there is no design Z better than H .

Definition 3-2.5. A class of admissible designs A is said to be complete if for every design Z not in A there is a design H in A that is better.

Definition 3-2.6. A class of admissible designs A is said to be minimal complete if A has no complete subsets.

Definition 3-2.7. A class of admissible designs A is said to be essentially complete if for every design H not in A there is a design in A that is at least as good.

Definition 3-2.8. A class of admissible designs A is said to be minimally essentially complete if A has no essentially complete subsets.

3.3 Potential Application for Space Station

In many cases the elements of the design matrix are a function of time or the position of the space station, and hence may be chosen by the experimenter. If one can select location and time for making an observation, then one can conceptually select an optimal design matrix.

In other applications certain stars are used for orientation of instruments and navigation equipment. Selecting sets of stars from an admissible set may in these applications be equivalent to selecting the optimal design matrix H from an admissible set of matrices induced by the admissible set of stars available.

The concepts presented here are early results and only few applications have been formulated [4], [5].

3.4. References.

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CHAPTER IV

Statistically Redundant Characteristics

"I'm afraid we have been a little too sure that the Stoat turns white to make itself invisible against its background of snow, in accordance with the theory of protective coloration. That explanation is very pretty and snug, but it looks silly sometimes, especially when there is no snow within miles. Perhaps we need more data on whether the Stoat was expecting snow when it turned white."

From, "How to Become Extinct", by Will Cuppy

4.1. Introduction.

There are occasions in some research activities where a large number of characteristics have been measured on an individual or experimental unit and one wonders if the information in the data vector perhaps is redundant. Furthermore, one wonders if there may be a subset of the total set of characteristics that would yield all or perhaps more realistically a large portion of the information in the total set of tests.

Principle component and factor analysis have been used to describe the variation in the data vector. Each method in some sense has a desirable feature of possibly discarding redundant information. However in principle components one has little control over which elements that will be discarded. For example an element of small variance and high correlation with other elements of the data vector could be discarded. Quite often these are the elements that one would like to retain. Likewise factor analysis has drawbacks of a similar nature.

The purpose of the chapter is to formulate a technique that is intuitive, logical, and relatively easy to compute in order to identify redundant characteristics. Also, a format is included from which the technique can be simulated and perhaps evaluated using Monte Carlo techniques.

To facilitate reading we restate the problem first stated in Chapter 2. The problem can be stated as follows: Let $T_1, T_2, \dots, T_p$ denote p characteristics of an experimental unit to be measured on a sample of size N . Let X_j be the vector

$$X_j = [X_{1j}, X_{2j}, \dots, X_{pj}]^T \quad (1)$$

where X_{ij} denotes the measurement or observation on the j th individual from the i th characteristic. The $p \times N$ data matrix is then $X = [X_1, X_2, \dots, X_p]$ where X_j is given by (1). It is our contention that in many such experiments there exists two or more subsets of characteristics, say

$$\begin{aligned} S_Z &= \{T_1, \dots, T_q\} \\ S_Y &= \{T_{q+1}, \dots, T_t\} \\ &\vdots \\ S_K &= \{T_{m+1}, \dots, T_p\} \end{aligned}$$

which yield essentially the "same information" about the individuals. Our task is to use the data in X and determine which of the sets $S_Z, S_Y, \dots, S_K$ can be used to obtain "good" predictors of the measurement in the remaining sets.

4.2. The Theory.

We first assume the observation vector X can be written in the following partitioned way:

$$X = \begin{bmatrix} Z \\ Y \end{bmatrix} .$$

The following theorem gives a method for selecting those characteristics S_Z and S_Y such that the information in S_Y can be used to predict the measurement of S_Z .

Theorem 1. Let Z and Y be real valued random vectors such that

$$\begin{array}{lll} E(Z) = 0 & E(ZZ^T) = V_{ZZ} & E(ZY^T) = V_{ZY} \\ E(Y) = 0 & E(YY^T) = V_{YY} & = V_{YZ}^T \end{array}$$

then the linear predictor of Z in terms of Y which minimizes the matrix value squared error loss function

$$Q_Z^{\hat{Z}} = E[(\hat{Z} - Z)(\hat{Z} - Z)^T] \quad (2)$$

is

$$\hat{Z} = V_{ZY} V_{YY}^{-1} Y \quad (3)$$

We say that $\hat{Z}$ is the best linear predictor for Z in terms of Y .

Proof: Since $\hat{Z}$ is restricted to be a linear predictor for Z in terms of Y , Z can be written as

$$\hat{Z} = BY \quad (4)$$

and our problem is to select the matrix B so that Z is minimized. On substituting (4) into (2),

$$\begin{aligned} Q_Z^{\wedge}(B) &= E[(BY - Z)(BY - Z)^T] \\ &= E[BYY^TB^T - BYZ^T - ZY^TB^T + ZZ^T] \\ &= BV_{YY}B^T - BV_{YZ} - V_{ZY}B^T + V_{ZZ} \end{aligned} \quad (5)$$

A necessary condition for $Q_Z^{\wedge}(B)$ to be minimal is for the first variation in $Q_Z^{\wedge}(B)$ with respect to a variation in B to be the zero matrix, that is

$$\delta Q_Z^{\wedge}(B) = \delta B[V_{YY}B^T - V_{YZ}] + [BV_{YY} - V_{ZY}] \delta B^T$$

is the zero matrix, $\emptyset$. The notation $\delta(.)$ denotes the first variation in $(.)$. The fact $Q_Z^{\wedge}(B) \equiv \emptyset$ for all B implies that

$$BV_{YY} - V_{ZY} \equiv \emptyset$$

or

$$B = V_{ZY}V_{YY}^{-1} \quad (6)$$

On substituting (6) into (4), one obtains (3) the desired result.

The value for $Q_Z^{\wedge}$, when (6) holds, is given by (5) and (6), that is

$$Q_Z^{\wedge}(V_{ZY}V_{ZZ}^{-1}) = V_{ZZ} - V_{ZY}V_{YY}^{-1}V_{YZ}$$

One can show that $Q_Z^{\wedge}(V_{ZY}V_{ZZ}^{-1})$ is indeed minimal by selecting an arbitrary matrix say B_1 and show that

$$Q_Z^{\wedge}(V_{ZY}V_{ZZ}^{-1}) - Q(B_1)$$

is negative definite.

Corollary 1. If Z and Y are random vectors such that

$$E(Z) = \mu_Z \quad E[(Z - \mu_Z)(Z - \mu_Z)^T] = V_{ZZ}$$

$$E(Y) = \mu_Y \quad E[(Y - \mu_Y)(Y - \mu_Y)^T] = V_{YY}$$

and

$$V_{ZY} = E[(Z - \mu_Z)(Y - \mu_Y)^T] = V_{YZ}^T,$$

Then the best linear predictor for Z is given by

$$\hat{Z} = \mu_Z + V_{ZY}V_{YY}^{-1}(Y - \mu_Y) \quad (7)$$

and the minimal $Q_Z^{\wedge}$ is given by

$$Q_Z^{\wedge} = V_{ZZ} - V_{ZY}V_{YY}^{-1}V_{YZ} \quad (8)$$

Let us now assume the observation vector X can be rearranged so that

$$X = \begin{bmatrix} Z \\ Y \\ W \end{bmatrix}$$

where Z, Y, and W are subvectors associated with the three sets

$S_1 = \{T_1, \dots, T_q\}$, $S_2 = \{T_{q+1}, \dots, T_{q+r}\}$ and $S_3 = \{T_{q+r+1}, \dots, T_p\}$.

By an analysis similar to the one above, we can identify which

characteristics can be used to predict the other characteristics.

For example, suppose we assign to the set S_3 those characteristics which are uncorrelated with Z and Y. That is, let the covariance of X be:

$$V_{XX} = \begin{bmatrix} V_{ZZ} & V_{ZY} & \emptyset \\ V_{YZ} & V_{YY} & \emptyset \\ \emptyset & \emptyset & V_{WW} \end{bmatrix} . \quad (9)$$

Then the best predictor for Z and Y in terms of W is

$$\begin{pmatrix} \hat{Z} \\ \hat{Y} \end{pmatrix} = \begin{pmatrix} \mu_Z \\ \mu_Y \end{pmatrix} + (V_{WZ}, V_{WY})^T V_{WW}^{-1} (W - \mu_W) .$$

Since

$$(V_{WZ}, V_{WY})^T = \begin{pmatrix} \emptyset \\ \emptyset \end{pmatrix} ,$$

then

$$\begin{pmatrix} \hat{Z} \\ \hat{Y} \end{pmatrix} = \begin{pmatrix} \mu_Z \\ \mu_Y \end{pmatrix}$$

which does not depend on the observation W. Note that Z can be predicted in terms of Y and vice-versa. However if the covariance matrix of X is

$$V_{XX} = \begin{bmatrix} V_{ZZ} & V_{ZY} & \emptyset \\ V_{YZ} & V_{YY} & V_{YW} \\ \emptyset & V_{WY} & V_{WW} \end{bmatrix} , \quad (10)$$

or

$$V_{XX} = \begin{bmatrix} V_{ZZ} & V_{ZY} & V_{ZW} \\ V_{YZ} & V_{YY} & \emptyset \\ V_{WZ} & \emptyset & V_{WW} \end{bmatrix} , \quad (11)$$

then in case of (1) (similar results hold for (11))

$$\begin{aligned} \begin{pmatrix} \hat{Z} \\ \hat{Y} \end{pmatrix} &= \begin{pmatrix} \mu_Z \\ \mu_Y \end{pmatrix} + \begin{pmatrix} V_{ZW} \\ V_{YW} \end{pmatrix} V_{WW}^{-1} (W - \mu_W) \\ &= \begin{pmatrix} \mu_Z \\ \mu_Y \end{pmatrix} + \begin{pmatrix} 0 \\ V_{YW} \end{pmatrix} V_{WW}^{-1} (W - \mu_W) . \end{aligned}$$

Therefore we gain no information concerning Z from observing W, but we do gain information about Y. On the other hand,

$$\begin{pmatrix} \hat{Z} \\ \hat{W} \end{pmatrix} = \begin{pmatrix} \mu_Z \\ \mu_W \end{pmatrix} + \begin{pmatrix} V_{ZY} \\ V_{WY} \end{pmatrix} V_{YY}^{-1} (Y - \mu_Y) \quad (12)$$

implies that Y gives us information about values of Z and W.

The corresponding minimized matrix value squared error loss function Q of $(\hat{Z}^T, \hat{W}^T)^T$ is

$$Q = \begin{bmatrix} V_{ZZ} - V_{ZY} V_{YY}^{-1} V_{YZ} & -V_{ZY} V_{YY}^{-1} V_{YW} \\ -V_{WY} V_{YY}^{-1} V_{YZ} & V_{WW} - V_{WY} V_{YY}^{-1} V_{YW} \end{bmatrix} . \quad (13)$$

A question that naturally arises is does Y contain all the information that is in Z and W. To answer this we assume without loss of generality that W is included in the vector Z. Hence

$$X = \begin{bmatrix} Z \\ Y \end{bmatrix} \quad V = \begin{bmatrix} V_{ZZ} & V_{ZY} \\ V_{YZ} & V_{YY} \end{bmatrix}$$

where $V_{ZY} \neq \emptyset$.

Note that Q in (8) is zero if and only if

$$V_{ZZ} - V_{ZY}V_{YY}^{-1}V_{YZ}$$

Definition 1. We say that the characteristic set S_Z is equivalent to S_Y if and only if

$$V_{ZZ} - V_{ZY}V_{YY}^{-1}V_{YZ} \equiv \emptyset.$$

That is $Q \equiv 0$, and one can predict exactly the Z scores from the Y scores.

Theorem 2. S_Y is equivalent to S_Z if and only if there exists a matrix L such that for every sample Y , $Z = LY$.

Proof: Let $Z = LY$, the $V_{ZZ} = LV_{YY}L^T$ and $V_{ZY} = LV_{YY} = V_{YZ}^T$.

Then

$$\begin{aligned} Q &= LV_{YY}L^T - LV_{YY}V_{YY}^{-1}V_{YY}L^T \\ &= \emptyset. \end{aligned}$$

Suppose $V_{ZZ} - V_{ZY}V_{YY}^{-1}V_{YZ} = 0$, then

$$V = \begin{bmatrix} V_{ZY}V_{YY}^{-1}V_{YZ} & V_{ZY} \\ V_{YZ} & V_{YY} \end{bmatrix}.$$

But

$$\begin{bmatrix} I & -V_{ZY} \\ \phi & I \end{bmatrix} \begin{bmatrix} I & \phi \\ \phi & V_{YY}^{-1} \end{bmatrix} \begin{bmatrix} V_{ZY}V_{YY}^{-1}V_{YZ} & V_{ZY} \\ V_{YZ} & V_{YY} \end{bmatrix} \begin{bmatrix} I & \phi \\ \phi & V_{YY}^{-1} \end{bmatrix} \begin{bmatrix} I & \phi \\ -V_{YZ} & I \end{bmatrix} \\ = \begin{bmatrix} \phi & \phi \\ \phi & V_{YY}^{-1} \end{bmatrix}.$$

That is to say, the elements of the vector Z are simple linear combinations of the elements of the vector Y , or there exists a matrix L such that $Z = LY$.

The problem then is to select the characteristic set S_Z and S_Y so that Q is zero. Of course, for every covariance matrix V , one may not in general select sets S_Z and S_Y so that Q is zero. If this is the case (this is the usual case), then one selects sets S'_Z and S'_Y so that $Q(Z')$ is minimal. Clearly, one can enumerate all possible cases. Note that enumeration leads to a large number of cases to check. For the case $p = 10$, the number of enumerations is 1022. Thus, it is clear that for $p > 10$ computing time will become a factor.

For cases in which $p \leq 10$ it is suggested that complete enumeration be the strategy with the aid of high speed computing

equipment. For cases greater than $p = 10$, each problem of complete enumeration must be determined computationally feasible.

4.3. Some Illuminating Examples.

In this section we will discuss briefly four examples that heuristically lead one naturally to the algorithm formulated in section 4 of this paper. The matrix $V = \{\sigma_{ij}\}$ is a $p \times p$ covariance matrix of the data vector.

Example 3.1: Let $p = 3$ and

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{21} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}.$$

The possible enumerations are as follows:

$$\begin{bmatrix} x_1 \\ \dots \\ x_2 \\ x_3 \end{bmatrix}; \begin{bmatrix} x_2 \\ \dots \\ x_1 \\ x_3 \end{bmatrix}; \begin{bmatrix} x_3 \\ \dots \\ x_1 \\ x_2 \end{bmatrix}; \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_3 \end{bmatrix}; \begin{bmatrix} x_1 \\ x_3 \\ \dots \\ x_2 \end{bmatrix}; \begin{bmatrix} x_2 \\ x_3 \\ \dots \\ x_1 \end{bmatrix},$$

where the dots are used to indicate the manner in which the vector is partitioned. The first three enumerations give respectively the best linear predictors

$$\hat{x}_1 = \mu_1 + \sigma_{12} \sigma_{22}^{-1} (x_2 - \mu_2),$$

$$\hat{x}_2 = \mu_2 + \sigma_{21} \sigma_{11}^{-1} (x_1 - \mu_1).$$

and

$$\hat{X}_3 = \mu_3 .$$

Note that $\hat{X}_3$ is the constant μ_3 and not a function of X_1 and/or X_2 .

The second three enumerations give the following best linear predictors,

$$\begin{bmatrix} \hat{X}_1 \\ \hat{X}_2 \end{bmatrix} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

$$\begin{bmatrix} \hat{X}_1 \\ \hat{X}_3 \end{bmatrix} = \begin{bmatrix} \mu_1 + \sigma_{12} \sigma_{22}^{-1} (X_2 - \mu_2) \\ \mu_3 \end{bmatrix}$$

$$\begin{bmatrix} \hat{X}_2 \\ \hat{X}_3 \end{bmatrix} = \begin{bmatrix} \mu_2 + \sigma_{21} \sigma_{11}^{-1} (X_1 - \mu_1) \\ \mu_3 \end{bmatrix}$$

Again we note that $\hat{X}_3$ in the best linear predictors do not depend on either X_1 and X_2 .

Example 3.2: Let $p = 3$ and

$$V = \begin{bmatrix} 11 & 12 & \vdots & 13 \\ 21 & 22 & \vdots & 0 \\ \dots & \dots & \vdots & \dots \\ 31 & 0 & \vdots & 33 \end{bmatrix}$$

Since X_1 is correlated with X_2 and X_3 , it is natural to conjecture that one might predict successfully X_1 using the scores X_2 and X_3 . The linear predictor of X_1 in terms of X_2 and X_3 is

$$\hat{X}_1 = \mu_1 + \sigma_{12} \sigma_{22}^{-1} (X_2 - \mu_2) + \sigma_{13} \sigma_{33}^{-1} (X_3 - \mu_3)$$

The value of Q is given by

$$Q_{\hat{X}_1} = \sigma_{11} - \sigma_{12} \sigma_{22}^{-1} \sigma_{21} - \sigma_{13} \sigma_{33}^{-1} \sigma_{31}$$

Note that if we wish to predict X_3 using the scores X_1 and X_2 that

$$\begin{aligned} X_3 &= \mu_3 + (\sigma_{31}, 0) \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{bmatrix}^{-1} \begin{bmatrix} X_1 - \mu_1 \\ X_2 - \mu_2 \end{bmatrix} \\ &= \sigma_{31} \sigma_{12} (\sigma_{11} \sigma_{22} - \sigma_{21} \sigma_{12})^{-1} (X_2 - \mu_2) \end{aligned}$$

Note that even though X_3 is uncorrelated with X_2 , that X_3 is a function of X_2 . This was not the case in Example 3.1, however it is easy to see that there exists a relationship of X_3 and X_2

through the relationship of X_3 to X_1 since σ_{13} and σ_{12} are both non-zero.

Example 3.3. Let $p = 5$ and

$$V = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \vdots & \sigma_{13} & \sigma_{14} & \sigma_{15} \\ \sigma_{21} & \sigma_{22} & \vdots & \sigma_{23} & \sigma_{24} & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \sigma_{31} & \sigma_{32} & \vdots & \sigma_{33} & 0 & 0 \\ \sigma_{41} & \sigma_{42} & \vdots & 0 & \sigma_{44} & 0 \\ \sigma_{51} & 0 & \vdots & 0 & 0 & \sigma_{55} \end{bmatrix}$$

On studying the covariance matrix V it is conjectured that X_1 and X_2 might be predicted by using X_3 , X_4 , and X_5 . If one partitions the observation vector X in the following manner

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \cdots \\ X_3 \\ X_4 \\ X_5 \end{bmatrix},$$

then

$$\begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} \mu_1 + \sigma_{13} \sigma_{33}^{-1} (x_3 - \mu_3) + \sigma_{14} \sigma_{44} (x_4 - \mu_4) + \sigma_{15} \sigma_{55}^{-1} (x_5 - \mu_5) \\ \mu_2 + \sigma_{23} \sigma_{33} (x_3 - \mu_3) + \sigma_{24} \sigma_{44}^{-1} (x_4 - \mu_4) \end{bmatrix}.$$

If one partitions the observation vector in the following manner

$$X = \begin{bmatrix} x_5 \\ \dots \\ x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

that the linear predictor for x_5 is a function of x_1 , x_2 , x_3 , and x_4 , since each are related to x_2 through x_1 . This is the same effect that we observed in Example 3.2.

Example 3.4. This example is included to illustrate the fact that random variables that are uncorrelated cannot be used to predict each other. Let $p = 5$ and

$$V = \begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 & 0 & 0 \\ \sigma_{21} & \sigma_{22} & 0 & 0 & 0 \\ 0 & 0 & \sigma_{33} & \sigma_{34} & \sigma_{35} \\ 0 & 0 & \sigma_{43} & \sigma_{44} & \sigma_{45} \\ 0 & 0 & \sigma_{53} & \sigma_{54} & \sigma_{55} \end{bmatrix}.$$

It is true that if we partition the observation vector as follows:

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \dots \\ X_3 \\ X_4 \\ X_5 \end{bmatrix}$$

then

$$\begin{bmatrix} \hat{X}_1 \\ \hat{X}_2 \end{bmatrix} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

is not a function of X_3 , X_4 , and X_5 . However, one can perhaps predict X_1 using data from X_2 by the formula

$$\hat{X}_1 = \mu_1 + \sigma_{12}\sigma_{22}^{-1}(X_2 - \mu_2)$$

Note that

$$Q_{\hat{X}_1} = \sigma_{11} - \sigma_{12}\sigma_{22}^{-1}\sigma_{21}$$

which implies that if σ_{22} is small and σ_{21} is large, then $Q_{\hat{X}_1}$ could be forced to zero. Also X_2 can be predicted by

$$\hat{X}_2 = \mu_2 + \sigma_{21}\sigma_{11}^{-1}(X_1 - \mu_1)$$

and

$$Q_{\hat{X}_2} = \sigma_{22} - \sigma_{21}\sigma_{11}^{-1}\sigma_{12}$$

One must now determine whether one should measure the characteristic T_1 and predict X_2 using X_1 , or measure T_2 and predict X_1 using X_2 .

4.4. Predictor Pairs.

In order to determine a best strategy for eliminating the redundancy in a set of characteristics the following definitions are helpful. The first two definitions will be given for $p = 2$ and $X = (X_1, X_2)^T$.

Definition 1: We say that the linear predictor $\hat{X}_1 = \mu_1 + \sigma_{12}\sigma_{22}^{-1}(X_2 - \mu_2)$ is at least as good as the linear predictor $\hat{X}_2 = \mu_2 + \sigma_{21}\sigma_{11}^{-1}(X_1 - \mu_1)$ if $\max\{\sigma_{11} - \sigma_{12}\sigma_{22}^{-1}\sigma_{21}, \sigma_{22}\} \leq \max\{\sigma_{11}, \sigma_{22} - \sigma_{21}\sigma_{11}^{-1}\sigma_{12}\}$.

Definition 2: The linear predictor X_1 is better than the linear predictor $\hat{X}_2$ if strict inequality holds in Definition 1.

Here we have introduced the concept of predictor pairs, that is $(\hat{X}_1, X_2)^T$ and $(X_1, \hat{X}_2)^T$ where

$$\hat{X}_1 = \mu_1 + \sigma_{12}\sigma_{22}^{-1}(X_2 - \mu_2)$$

$$\hat{X}_2 = \mu_2 + \sigma_{21}\sigma_{11}^{-1}(X_1 - \mu_1).$$

In practice one replaces the measurements (X_1, X_2) with one of the pairs $(\hat{X}_1, X_2)$ or $(X_1, \hat{X}_2)$, depending on which is the better predictor, X_1 or X_2 .

Now we extend the concept to the case involving more than two elements. Let the $p \times 1$ observation vector X be partitioned into a $q \times 1$ vector $X^{(1)}$ and the $(p - q) \times 1$ vector $X^{(2)}$ whose covariance

matrix

$$V = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$$

is partitioned compatibly so that the $q \times q$ matrix V_{11} is the covariance matrix of $X^{(1)}$, V_{22} is the covariance matrix of $X^{(2)}$, and $V_{12} = V_{21}^T$ is the covariance matrix of $X^{(1)}$ and $X^{(2)}$.

Hence the observation vector X and the mean vector μ are partitioned as

$$X = \begin{bmatrix} X^{(1)} \\ X^{(2)} \end{bmatrix} \quad \text{and} \quad \mu = \begin{bmatrix} \mu^{(1)} \\ \mu^{(2)} \end{bmatrix} \quad \text{respectively.}$$

Then the predictor pairs are the vectors

$$\hat{X}^{(1)} = \mu^{(1)} + V_{12}V_{22}^{-1}[X^{(2)} - \mu^{(2)}].$$

$$\hat{X}^{(2)} = \mu^{(2)} + V_{21}V_{11}^{-1}[X^{(1)} - \mu^{(1)}].$$

If q and $p - q$ are not equal, one may optimistically hope that $\hat{X}^{(1)}$ is the better predictor whenever $q > p - q$. However in practice this may not be the case.

Definition 3: The predictor pair $(\hat{X}_1, \hat{X}_2)^T$ is said to be better than the predictor pair $(X_1, X_2)^T$ if

$$\max_{i=1, \dots, p} \{a_{ii}\} \leq \max_{i=1, \dots, p} \{b_{ii}\}$$

where

$$\{a_{ij}\} = \begin{bmatrix} v_{11} - v_{12}v_{22}^{-1}v_{21} & \phi \\ \phi & v_{22} \end{bmatrix}$$

and

$$\{b_{ij}\} = \begin{bmatrix} v_{11} & \phi \\ \phi & v_{22} - v_{21}v_{11}^{-1}v_{12} \end{bmatrix}$$

Note that there is no clue as to the value of q . In example 3.3 we selected $q = 2$, which from the covariance matrix seemed to be the thing to do. Unfortunately, complete enumeration seems to be the only accurate way of selecting best predictor pairs.

Also, one would not expect to know exactly the covariance matrix V , but only an estimate of the matrix. This in itself presents a problem in informing predictor pairs. We denote the estimate by $\hat{V}$. Hence we introduce an additional problem in selecting the best predictor pairs.

It is important to note that what we are proposing here is not a function of statistical inference; but a logical and straight forward technique for eliminating redundant or nearly redundant characteristics to measure. Assuming normality of observations, one may be able to develop a sequence of characteristics which could have meaning in terms of precise inference. However, it has been our experience that verifying the basic assumptions is a task of

great magnitude and is seldom done even if one could verify them.

CHAPTER V

Compression and Redundancy Removal

"Statistical thinking will one day be as necessary for efficient citizenship as the ability to read and write."

H. G. Wells

5.1 Introductory Remarks.

The term "data compression" has been used to denote at least two general concepts in data handling. These are:

(1) selecting a filter which replaces a "long" vector of observations with a "short" vector and retains as large an amount of the information as possible; (2) recording only observations and times of observations that are "significantly different" from a previous observation.

The first technique is generally known as data compression and the second as redundancy removal.

5.2 On Compressing the Data

We now consider the problem of compressing the data vector Y_N . What we mean by "compressing" is that we wish to replace the $N_p \times 1$ data vector by an $M_p \times 1$ vector Z_M where $M < N$, and if

$$E[Y_N] = J_N \mu \quad (2.1)$$

then

$$E[Z_M] = J_M \mu, \quad (2.2)$$

where μ is a $p \times 1$ parameter vector, and the covariance matrix of Z_M is given by

$$V(Z_M) = \text{Dia}\{V_Z, V_Z, V_Z, \dots, V_Z\} \quad (2.3)$$

and is minimal. We say that we have linearly compressed Y_N if

$$Z_M = B Y_N \quad (2.4)$$

where B is an $M_p \times N_p$ matrix selected so that (2.2) and (2.3) are true. The vectors J_N and J_M in (2.1) and (2.2) are $N_p \times p$ and $M_p \times p$ matrices whose every elements are $p \times p$ identity matrices. The condition (2.2) on the vector Z_M assures that the $p \times 1$ subvectors are uncorrelated. This appears to be desirable property and, of course, independence will follow if Y_N is normal.

From (2.1), (2.2), and (2.4) we deduce that

$$J_M \mu = E[Z_M] = E[B Y_N] = B J_N \mu,$$

which in turn implies for all μ that

$$BJ_N = J_M \quad (2.5)$$

Solving (2.5) for B , we find that

$$B = J_M J_N^+ + U[I - J_N J_N^+] \quad (2.6)$$

where U is an $M_p \times N_p$ arbitrariness matrix to be assigned later and J_N^+ is the pseudo-inverse of J_N . In this case

$$J_N^+ = J_N^T / N \quad (2.7)$$

and

$$J_N J_N^+ = \frac{J_N J_N^T}{N} = \frac{1}{N} \{I\} \quad (2.8)$$

an $N_p \times N_p$ matrix made up of $p \times p$ identity submatrices.

Also we note that

$$J_N^T J_N = NI \quad (2.9)$$

a $p \times p$ diagonal matrix, and

$$J_M^T B J_N = J_M^T J_M = MI \quad (2.10)$$

We now wish to select U so that (2.3) is true and $V(Z_M)$ is minimal. However, this is difficult so we modify the problem slightly to achieve our aim.

Define $p \times Np$ matrix C by

$$C = J_M^T B . \quad (2.11)$$

Then by (2.10)

$$CJ_N = MI$$

or

$$\sum_{i=1}^N C_i = MI . \quad (2.12)$$

Now we compute the covariance matrix of Z_M from (2.4) and obtain

$$\begin{aligned} V(Z_M) &= V(BY_N) \\ &= BV(Y_N)B^T . \end{aligned} \quad (2.13)$$

Since y_i , $i = 1, 2, \dots, N$ are sample values we assume that they have been obtained so that y_i is independent of y_j for all $i \neq j$ and have the same $p \times p$ covariance matrix V_Y for

all i . Hence,

$$V(Y_N) = \text{Dia}\{V_Y, V_Y, \dots, V_Y\} \quad (2.14)$$

We note also that (2.14) and (2.11) imply

$$J_M V(Z_M) J_M^T = J_M B V(Y) B^T J_M^T$$

$$= C V(Y) C^T$$

$$= \sum_{i=1}^N C_i V_Y C_i^T$$

Instead of selecting the matrix B judiciously, we select C so that the following constrained payoff function is minimized.

$$Q = \sum_{i=1}^N C_i V_Y C_i^T + (MI - \sum_{i=1}^N C_i) \lambda + \lambda^T (MI - \sum C_i^T), \quad (2.15)$$

where λ is a matrix Lagrange multiplier.

Let $(SQ)_i$ be the variation in Q with respect to a variation SC_i in C_i , then

$$(SQ)_i = [C_i V_Y - \lambda^T I] SC_i^T + SC_i [V_Y C_i^T - \lambda]$$

A necessary condition for Q to be minimal is for all $i = 1, 2, \dots, N$

$$C_i V_Y - \lambda^T = \phi ,$$

the null matrix, or for all $i = 1, 2, \dots, N$

$$C_i = \lambda^T V_Y^{-1} . \quad (2.16)$$

However, from (2.12) and (2.16) we know that

$$\sum C_i = N \lambda^T V_Y^{-1} = M I$$

or

$$\lambda^T = \frac{M}{N} V_Y . \quad (2.17)$$

Note also that (2.16) and (2.17) imply that for all i

$$C_i = \frac{M}{N} I \quad (2.18)$$

for Q to be minimal. From (2.18) we see that

$$C = \frac{M}{N} J_N^T$$

or if substituted into (2.11)

$$J_M^T B = \frac{M}{N} J_N^T \quad . \quad (2.19)$$

From definition of $V(Z_M)$ and

$$J_M^T V(Z_M) J_M = J_M^T B V(Y_N) B^T J_M$$

$$= C V(Y_N) C^T$$

$$= \left(\frac{M}{N}\right)^2 J_N^T V(Y) J_N$$

$$= N \left(\frac{M}{N}\right)^2 V_Y \quad .$$

But

$$J_M^T V(Z_M) J_M = M V_Z$$

if

$$V(x) = \text{Dia}\{V_Z, \dots, V_Z\} \quad , \quad \text{or}$$

$$V_Z = \frac{M}{N} V_Y \quad . \quad (2.20)$$

Consider (2.6), (2.13), and (2.20)

$$\text{Dia}\{\frac{M}{N} V_Y, \dots, \frac{M}{N} V_Y\} = B[\text{Dia}\{V_Y, \dots, V_Y\}]B^T$$

and select U in (2.6) so that the above relation is true.

The following identities are helpful:

$$J_N^T V(Y) = N V_Y \quad (2.21)$$

$$V(Y) J_N = J_N V_Y \quad (2.22)$$

$$[I - \frac{J_N J_N^T}{M}] J_M = \phi \quad (2.23)$$

If

$$U = (\frac{M}{N})^{1/2} [\phi : I - \frac{J_M J_M^T}{M}] \quad (2.24)$$

then

$$U [I - \frac{J_N J_N^T}{N}] = U \quad (2.25)$$

It is straightforward but tedious to show that U is a matrix (not unique) which gives a desired B , that is

$$B = \left[\frac{J_M J_N^T}{N} : \left(\frac{M}{N}\right)^{1/2} I - \frac{1}{(MN)^{1/2}} J_M J_M^T \right]$$

is an optimal compression matrix satisfying our criteria. It is easy to show that if $M = p$, then

$$B = \frac{1}{N} [I : I : \dots : I] = \frac{1}{N} J_N$$

and if $M = N$, then $M/N = 1$ and $B = I$.

It is important to note, however, that compressing the data vector implies an increase in the covariance matrix of $\hat{x}$.

Suppose that the data vector Y_N is compressed in the classical linear model $Y_N = H_N x + E_N$, then

$$BY_N = BH_N x + BE_N \quad (2.26)$$

and

$$\tilde{x}_N = (H_N^T B^T (BV^{-1} (Y_N) B^T)^{-1} BH_N)^{-1} H_N^T B^T (BV^{-1} (Y_N) B)^{-1} BY_N$$

The covariance matrix

$$V(x_N) = [H_N^T B^T (BV^{-1} (Y_N) B^T)^{-1} BH_N]^{-1}$$

should then be compared with the covariance matrix of the best linear unbiased estimate $\hat{X}_N = (H_N^T V_N^{-1} H_N)^{-1} H_N^T V_N^{-1} Y_N$ to determine the loss of information. Since H_N differs from problem to problem, this comparison must be done for each problem. Note that one may select B in any manner he wishes, yet (2.25) produces an unbiased estimator for the parameter x . The penalty for this problem is measured by the increase in variance given by

$$\Delta = V(\hat{X}) - V(\tilde{X})$$

An interesting case would be to select $p = N$ and $M = 1$ and let B be given by

$$B = \frac{1}{N} [I : I : \dots : I] ,$$

that is we simply average the N data values. This procedure is easy to accomplish on the computer and the question remains to the amount of variance lost. For example, let $V(Y_N) = I$, then

$$V(\tilde{X}) = \left[\left(\sum_{i=1}^N H_i \right)^T \left(\sum_{i=1}^N H_i \right) \right]^{-1}$$

and

$$V(\hat{X}) = \left[\sum_{i=1}^N H_i^T H_i \right]^{-1}.$$

Note that $V(\tilde{X}) = V(\hat{X})$ if and only if

$$\sum_{i \neq j}^N H_i^T H_i = \phi$$

This can be accomplished if the design matrix H_N is selected so that $H_i^T H_j = \phi$ for all $i \neq j$. Here H_i is $p \times n$ matrix, yet one observes the resemblance to the requirements of Theorem 1 for optimal designs. Also, note that the matrix U in this section is not unique, and hence one can place further desirable constraints and theoretically compute a U that will not only satisfy the old constraints but those added.

5.3 Redundancy Removal Techniques.

The necessity for removal of redundant data after encoding but prior to transmission is evident upon analyzing the power density spectrum of normal pulse code modulation data. If the power density is uniform from 0 to f_c , sampling theory dictates that an adequate sampling rate is $1/2f_c$. However, for realistic data a precise sampling rate is difficult to establish, hence, the tendency is to over-sample, which produces a high

redundancy content in most transmitted messages.

Let $y_i = y(t_i)$, $i = 1, 2, \dots$ be a real scalar function defined on a sequence of real variables $\{t_i, i = 1, 2, \dots\}$ representing observations taken at different times. One usually assumes that $|t_i - t_{i+1}| = \Delta t$ for all i . Let the y -axis be divided into non-overlapping abutting intervals whose end points are $\{\dots, y_{-2}, y_{-1}, y_0, y_1, y_2, \dots\}$, where $|y_j - y_{j-1}| = \Delta y$ and Δy is a significant change defined by the application.

Suppose that $y = y(t_i)$ is a "slow changing" process so that in many instances

$$|y(t_i) - y_j| \leq \Delta y$$

for $i = k, k+1, \dots, k+n$ where n is "large". Also, assume that

$$|y(t_{k-1}) - y_j| > \Delta y$$

and

$$|y(t_{k+n}) - y_j| > \Delta y \quad .$$

If recording and storing data is desired we have immediately two simple alternatives

- (i) store the $n + 1$ pairs $(t_k, y(t_k)), (t_{k+1}, y(t_{k+1})), \dots, (t_{k+n}, y(t_{k+n}))$, or
- (ii) store only the following (y_j, t_k, t_{k+n}) ,

thereby reducing storage requirements perhaps significantly and maintaining approximately the same information as the original sample.

One notes that we are replacing the discrete function $y(t_i)$ with an approximating discrete step function. Other techniques for approximating the data sequence $\{y(t_i)\}$ are given by Gabriel R. Wallace [1] and still others and discussed by J. W. Stumpe [2].

It is important to note that one should evaluate the desirability of redundancy removal techniques by evaluating the estimates computed from the approximation to the data measured.

In order to discuss redundancy removal algorithms, we first define some of the terminology involved.

Definition 1. Redundant data is defined to be data which is not significantly different from previously obtained data.

To remove redundant data, some parameter of the data which is proportional to the change is usually monitored. This could be a moving average, a particular derivative, or some other statistic which would reflect a significant change in adjacent samples.

Definition 2. A corridor is the region in which subsequent samples must fall in order to be classified as redundant.

Redundancy removal methods also differ in the choice of the sample that is transmitted when a nonredundant sample is detected. One may choose to transmit the nonredundant sample, the sample preceding the nonredundant sample, or the predicted value of the sample preceding the nonredundant sample.

We now present several redundancy removal algorithms.

1. Zero order, Fixed corridor, Nonredundant sample transmitted.

For this algorithm, the occurrence of a nonredundant sample requires that a new corridor be established. Lines of zero slope are drawn through the end points of the tolerance range placed around the nonredundant sample. If a subsequent sample lies inside the corridor, it is a redundant sample and is discarded. If a subsequent sample lies outside the corridor, it is a nonredundant sample and is transmitted.

To reconstruct the data we connect adjacent nonredundant sample points. If there are intermediate omitted samples, a straight line of zero slope is drawn from the first transmitted sample to the time of occurrence of the sample preceding the second transmitted sample. The end of this line is then connected to the second transmitted sample with a second line.

2. Zero order, Variable corridor, Preceding sample transmitted.

In this algorithm, the occurrence of a nonredundant sample requires that a new corridor be established. Lines of zero slope are drawn through the end points of the tolerance range placed around the nonredundant sample. Whenever a subsequent sample lies inside the corridor, it is considered redundant and discarded once it is used to establish a new corridor. The new corridor consists of that part of the previous corridor which is overlapped by the tolerance range placed about the redundant sample. If a subsequent sample lies outside the corridor, it is nonredundant, but not transmitted.

The data reconstruction procedure is the same as for method (1) except that when there are intermediate omitted samples, a straight line of zero slope is drawn from the second transmitted sample back to the time of occurrence of the first sample following the first transmitted sample. The end of this line is then connected to the first transmitted sample with a second line.

The maximum peak error between raw data and reconstructed, reduced data is plus or minus one-half the tolerance range.

3. Zero order, Variable corridor, Artificial preceding sample transmitted.

The occurrence of a nonredundant sample requires that a new corridor be established. Lines of zero slope are drawn through the end points of the tolerance range placed around the non-

redundant sample. A subsequent sample is redundant and can be discarded when one end of the tolerance range placed about the sample falls within the corridor. The sample itself is not required to be within the corridor. For a redundant sample, the new corridor consists of that part of the previous corridor that is overlapped by the tolerance range placed about the redundant sample. If the tolerance range placed about a sample does not overlap the corridor, the sample is nonredundant, but not transmitted. Rather, the midpoint of the corridor used to analyze this sample, actually the predicted value of the sample, is transmitted for the preceding sample.

The reconstruction procedure is the same as for method (2) above.

4. First order, Fixed corridor, nonredundant sample transmitted.

The occurrence of a nonredundant sample requires that a new corridor be established. Tolerance ranges are placed around the nonredundant sample and the previous sample, and two straight lines are drawn, one through the upper ends of the tolerance ranges and the other through the lower ends. If a subsequent sample lies inside this corridor, it is a redundant sample, otherwise it is nonredundant and transmitted.

To reconstruct the data, transmitted samples are connected by straight lines.

5. First order, Fixed corridor, Preceding sample transmitted.

The occurrence of a nonredundant sample requires that a new corridor be established. Tolerance ranges are placed around the nonredundant sample and the previous sample, and two straight lines are drawn, one through the upper ends of the tolerance ranges and the other line through the lower ends. If a subsequent sample lies inside this corridor, it is redundant, otherwise it is nonredundant but not transmitted. Instead, the preceding sample is transmitted.

The reconstruction process is the same as for (4).

6. First order, Fixed corridor, Artificial preceding sample transmitted.

The occurrence of a nonredundant sample requires that a new corridor be established. Tolerance ranges are placed around the nonredundant sample and the artificial preceding sample that is transmitted. Two straight lines are drawn, one line through the upper ends of the tolerance ranges and the other through the lower ends. If a subsequent sample lies inside this corridor, it is redundant and thus discarded. If not, it is nonredundant but not transmitted. Rather, an artificial value for the previous sample is transmitted. This is the midpoint of the corridor for the previous sample, which is the predicted value for that sample.

The reconstruction process is the same as for (4) and (5).

7. First order, Variable corridor, Preceding sample transmitted.

Whenever nonredundant samples occur a new corridor has to be established. A tolerance range is placed around the nonredundant sample and two straight lines are drawn; one through the previous sample and the upper end of the tolerance range; the second through the same sample and the lower end of the tolerance range. If a subsequent sample lies inside this corridor, it is redundant and discarded. Each redundant sample modifies the corridor for the next sample as follows: If a boundary line of the corridor does not pass through the tolerance range placed around the redundant sample, a new boundary is established that passes through the nearest end point of the tolerance range. Either or both boundary lines can be affected. A sample outside the corridor is nonredundant but the preceding sample is transmitted.

Transmitted samples are connected by straight lines to reconstruct the data.

8. First order, Variable corridor, Artificial preceding sample transmitted.

A tolerance range is placed around a nonredundant sample and two straight lines are drawn. The first through the artificial preceding sample, which is transmitted, and the upper end of the tolerance range; the second through the same sample and the lower end of the tolerance range. A subsequent sample

is redundant and can be discarded when one end of the tolerance range placed around the sample falls within the corridor. The sample itself is not required to be within the corridor. For a redundant sample the corridor is modified for the next sample. If a boundary line of the corridor does not pass through the tolerance range placed around the redundant sample, a new boundary is established that passes through the nearest end point of the tolerance range.

If the tolerance range placed about a sample does not overlap the corridor, the sample is nonredundant, but not transmitted. Rather, an artificial value for the preceding sample is transmitted, which is simply the predicted value of the previous sample. This value is the midpoint of the corridor at the time corresponding to the previous sample, and the corridor is the one used for the analysis of the nonredundant sample. The reconstruction is accomplished by simply connecting transmitted samples by straight lines.

It is clear that all of the above algorithms differ in the order, corridor used, and sample transmitted. Thus, many other redundancy removal algorithms could be constructed from those discussed by combinations of the order, corridor and selection of sample to be transmitted.

5.4 References.

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CHAPTER VI
Best Linear Recursive
Estimation

"There is no more common error than to assume that, because prolonged and accurate mathematical calculations have been made, the application of the result to some fact of nature is absolutely certain." A. N. Whitehead.

6.1. Introductory Remarks.

Real time estimation requirements, along with limited storage space constraints in onboard computers for estimating parameters in spacecraft orbit determination problems, have stimulated interest in recursive estimation techniques [1], [2], [7], [8], [11], [13], and [15]. For these reasons the techniques are especially applicable to various space station applications. The problem is to write the best linear unbiased estimator for the parameter vector x in a recursive form in the sense that the estimator after N observations (an observation may be a vector) is the estimator after $N-1$ observations plus a correction which is a linear function of the N^{th} observation and the estimator based on $N-1$ observations.

Kalman and Bucy [8] and Shumway and Dean [14] have given recursive forms of the best linear unbiased estimator of the parameter vector $X(t)$ in the linear model $Y(t) = H(t)X(t) + U(t)$ for continuous data. Blum [3], [4], [5], and [6] studied a

similar problem when the linear model was for discrete data. His results formulated the scalar form of the problem discussed in this paper. That is, we give a matrix formulation of the same problem allowing the vector of observations taken at each epoch of time to be correlated. The matrix notation leads to a multi-dimension extension of the technique proposed by Blum and induces a clearer understanding of the technique.

In the discussion to follow lower case letters will be used for nonrandom vectors. Upper case Roman letters will be used for random vectors. Both lower and upper case Roman letters will be used to denote nonvector matrices, which will always be considered nonrandom.

6.2. Linear Model.

In many problems of estimation, computational difficulties arise because of large amounts of data or because of having to perform on-line or real-time parameter estimations. Attempts to lighten this computation difficulty have led to recursive schemes such that it is not necessary to store all the previous data but only previous estimates and current data. This section presents a practical technique for obtaining a best linear unbiased estimator for the parameter vector x in equation (1) defined below.

Let Y_i be a $p \times 1$ random vector which is observed at time t_i , $i = 1, 2, \dots, N$. Let

$$Y_i = h_i x + U_i, \quad i = 1, 2, \dots, N \quad (1)$$

be a linear model relating the random vector Y_i of observations

with the $n \times 1$ unknown parameter vector x . The $p \times n$ matrix h_i , $i = 1, 2, \dots, N$, is assumed known and the $p \times 1$ error vector U_i , $i = 1, 2, \dots, N$, is such that

$$E[U_i] = 0 \quad (2)$$

and

$$E[U_i U_j^T] = V_{ij} \quad i = 1, 2, \dots, N, \quad j = 1, 2, \dots, N \quad (3)$$

where V_{ij} is a known $p \times p$ covariance matrix.

A problem in which the linear model defined by (1) has been used with success is to estimate the initial or insertion location and velocity of a spacecraft in orbit. The parameter vector to be estimated a 6×1 vector defined by $(x, y, z, \dot{x}, \dot{y}, \dot{z})^T$ where x , y , and z are the location coordinates of the spacecraft in space and $\dot{x}$, $\dot{y}$, and $\dot{z}$ are the corresponding velocity components evaluated at the initial time, say t_0 . The observations taken are range, range rate, and azimuth, which we denote by $r(t)$, $\dot{r}(t)$, and $\theta(t)$ respectively. These yield a 3×1 observation vector $Y_t = (r(t), \dot{r}(t), \theta(t))^T$. The elements of the observation vector are related to the elements of the parameter vector by three non-linear equations of motion. The matrix h_t is obtained by linearizing these equations about a "nominal" trajectory yielding the linear model (1).

The model (1) can be written in matrix notation as

$$T_N = H_N x + E_N \quad (4)$$

where

$$T_N = \begin{bmatrix} Y_1 \\ \vdots \\ Y_{N-1} \\ Y_N \end{bmatrix} = \begin{bmatrix} T_{N-1} \\ Y_N \end{bmatrix}$$

is an $Np \times 1$ vector of $p \times 1$ observation vectors Y_i , $i = 1, 2, \dots, N$,

$$H_N = \begin{bmatrix} h_1 \\ \vdots \\ h_{N-1} \\ h_N \end{bmatrix} = \begin{bmatrix} H_{N-1} \\ h_N \end{bmatrix}$$

is an $Np \times n$ matrix of $p \times n$ submatrices h_i , $i = 1, 2, \dots, N$, and

$$E_N = \begin{bmatrix} U_1 \\ \vdots \\ U_{N-1} \\ U_N \end{bmatrix} = \begin{bmatrix} E_{N-1} \\ U_N \end{bmatrix}$$

is an $Np \times 1$ vector of $p \times 1$ random error vectors U_i , $i = 1, 2, \dots, N$.

The covariance of E_N is

$$E[E_N E_N^T] = V_N = \begin{bmatrix} V_{1,1} & \dots & V_{1,N-1} & V_{1,N} \\ \vdots & & \vdots & \vdots \\ V_{N-1,1} & \dots & V_{N-1,N-1} & V_{N-1,N} \\ V_{N,1} & \dots & V_{N,N-1} & V_{N,N} \end{bmatrix}. \quad (5)$$

Each V_{ii} , $i = 1, \dots, N$ will be assumed to be positive definite and each H_n will be assumed to be of full column rank.

The Gauss-Markov Theorem [10] states that the best linear unbiased estimator, say $\hat{X}_N$, for the nonrandom parameter vector x is given by

$$\hat{X}_N = [H_N^T V_N^{-1} H_N]^{-1} H_N^T V_N^{-1} T_N. \quad (6)$$

However, if the restriction that V_{ij} in (3) is such that

$$V_{ij} = V_{ij} \delta_{ij}$$

where

$$\delta_{ij} = 1 \text{ if } i = j$$

$$= 0 \text{ if } i \neq j,$$

then V_N in (5) can be written as

$$V_N = \begin{bmatrix} V_{N-1} & 0 \\ 0 & V_{NN} \end{bmatrix}. \quad (7)$$

Hence (6) can be written as

$$\begin{aligned} \hat{X}_N &= \left[(H_{N-1}^T, h_N^T) \begin{pmatrix} V_{N-1}^{-1} & 0 \\ 0 & V_{NN}^{-1} \end{pmatrix} \begin{pmatrix} H_{N-1} \\ h_N \end{pmatrix} \right]^{-1} (H_{N-1}^T, h_N^T) \begin{pmatrix} V_{N-1}^{-1} & 0 \\ 0 & V_{NN}^{-1} \end{pmatrix} \begin{pmatrix} T_{N-1} \\ Y_N \end{pmatrix} \\ &= [H_{N-1}^T V_{N-1}^{-1} H_{N-1} + h_N^T V_{NN}^{-1} h_N]^{-1} [H_{N-1}^T V_{N-1}^{-1} T_{N-1} + h_N^T V_{NN}^{-1} Y_N]. \end{aligned}$$

By letting

$$A = H_{N-1}^T V_{N-1}^{-1} H_{N-1}$$

and

$$B = h_N^T V_{NN}^{-1} h_N$$

then

$$\hat{X}_N = (A+B)^{-1} (H_{N-1}^T V_{N-1}^{-1} Y_{N-1} + h_N^T V_{NN}^{-1} Y_N)$$

Noting that

$$\hat{X}_{N-1} = A^{-1} H_{N-1}^T V_{N-1}^{-1} T_{N-1}$$

then it follows that

$$\hat{X}_N = (A+B)^{-1} (A \hat{X}_{N-1} + h_N^T V_{NN}^{-1} Y_N)$$

Since

$$(A+B)^{-1} A = I - (A+B)^{-1} B$$

then

$$\hat{X}_N = \hat{X}_{N-1} + (A+B)^{-1} (h_N^T V_{NN}^{-1} Y_N - B \hat{X}_{N-1})$$

or

$$\hat{X}_N = \hat{X}_{N-1} + (H_{N-1}^T V_{N-1}^{-1} H_{N-1} + h_N^T V_{NN}^{-1} h_N)^{-1} h_N^T V_{NN}^{-1} (Y_N - h_N^T \hat{X}_{N-1}). \quad (8)$$

It is well known [12, page 29, problem 2.9] that $[H_N^T V_N^{-1} H_N]^{-1}$ can be written as

$$\begin{aligned} [H_N^T V_N^{-1} H_N]^{-1} &= [H_{N-1}^T V_{N-1}^{-1} H_{N-1} + h_N^T V_{NN}^{-1} h_N]^{-1} \\ &= (H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1} - (H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1} h_N^T [V_{NN} \\ &+ h_N (H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1} h_N]^{-1} h_N (H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1} \end{aligned} \quad (9)$$

The storage space required to compute (6) is $\frac{(N-1)p}{2} (p + 2n + 3)$ elements of past data plus present data, while the storage space required to compute (8) is $n + \frac{p^2+p}{2}$ elements of past data plus present data. If N is large then a considerable amount of storage space could be saved by using equation (8). It is also important to note that (9) allows one to compute the covariance matrix of $\hat{X}_N$ by inverting the $p \times p$ matrix

$$V_{NN} + h_N (H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1} h_N^T$$

resulting in some computational advantage if N is large. Note that $(H_{N-1}^T V_{N-1}^{-1} H_{N-1})^{-1}$ has already been computed and is available in storage.

Another useful form of $\hat{X}_N$ when (7) is true is

$$\begin{aligned} \hat{X}_N &= \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1} \left[\sum_{i=1}^N h_i^T V_{ii}^{-1} Y_i \right] \\ &= \left[\sum_{i=1}^{N-K} h_i^T V_{ii}^{-1} h_i + \sum_{i=N-K+1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1} \left[\sum_{i=1}^{N-K} h_i^T V_{ii}^{-1} Y_i + \sum_{i=N-K+1}^N h_i^T V_{ii}^{-1} Y_i \right] \\ &= [P_{1,N-K}^{-1} + P_{N-K+1,N}^{-1}]^{-1} [P_{1,N-K}^{-1} \hat{X}_{N-K} + P_{N-K+1,N}^{-1} X_N^*] \end{aligned}$$

where

$$P_{1,N-K} = \left[\sum_{i=1}^{N-K} h_i^T V_{ii}^{-1} h_i \right]^{-1}$$

and

$$P_{N-K+1,N} = \left[\sum_{i=N-K+1}^N h_i^T V_{ii}^{-1} h_i \right]^{-1}.$$

$P_{1,N-K}$ and $P_{N-K+1,N}$ are the covariance matrices of $\hat{x}_{N-K}$ and x_N^* , the best linear unbiased estimators for x using the first $N-K$ observations and the last K observations, respectively.

6.3. A Useful Generalization.

We will consider in this section a more general case in which V_{ij} need not be null for all $i \neq j$.

Suppose that

$$E(E_N E_N^T) = \{V_{ij}\}, \quad i = j = 1, 2, \dots, N,$$

and let

$$V_N = \{V_{ij}\}$$

be the covariance matrix of E_N where V_{ij} is a $p \times p$ matrix not necessarily null for $i \neq j$. Again the minimum variance linear unbiased estimator for x is given by (6). In order for (6) to be useful V_N is assumed to be known or equivalently V_N^{-1} is known. Since V_N^{-1} is positive definite, it can be written as a result of the square root method [12] to be

$$V_N^{-1} = Q_N Q_N^T \quad (10)$$

where Q_N can be generated recursively with respect to the subscript N . We mean by the statement that Q_N is generated recursively that the $(N-1)p^{\text{th}}$ row of Q_N does not depend on the Np^{th} row of V_N for all N ; that is, the elements of Q_{N-1} do not depend on the Np^{th} row of V_N . The matrix Q_N is a lower triangular matrix with positive elements along the principal diagonal. Substituting the right side of (10) into (6) one can rewrite (6)

$$\hat{X}_N = (G_N^T G_N)^{-1} G_N^T Z_N \quad (11)$$

where

$$G_N = Q_N^T H_N \quad (12)$$

$$Z_N = Q_N^T T_N \quad (13)$$

Consider the following partitioning of

$$Q_N = \begin{bmatrix} Q_{N-1} & 0 \\ q_N & q_{NN} \end{bmatrix} \quad (14)$$

where the $(N-1)p \times (N-1)p$ matrix Q_{N-1} is such that

$$V_{N-1}^{-1} = Q_{N-1} Q_{N-1}^T$$

q_N is a $p \times (N-1)p$ matrix and q_{NN} is a $p \times p$ lower triangular matrix.

It follows from (12) and (14) that

$$G_N = \begin{bmatrix} Q_{N-1}^T & q_N^T \\ 0 & q_{NN}^T \end{bmatrix} \begin{bmatrix} H_{N-1} \\ h_N \end{bmatrix} = \begin{bmatrix} G_{N-1} + q_N^T h_N \\ q_{NN}^T h_N \end{bmatrix}$$

and similarly from (13) and (14) that

$$Z_N = \begin{bmatrix} Z_{N-1} + q_N^T Y_N \\ q_{NN}^T Y_N \end{bmatrix}.$$

Note that the dimensions of G_N and Z_N are $N_p \times n$ and $N_p \times 1$, respectively. It follows that

$$G_N^T G_N = G_{N-1}^T G_{N-1} + G_{N-1}^T q_N^T h_N + h_N^T q_N G_{N-1} + h_N^T q_N q_N^T h_N + h_N^T q_{NN} q_{NN}^T h_N \quad (15)$$

and

$$G_N^T Z_N = G_{N-1}^T Z_{N-1} + h_N^T q_N Z_{N-1} + G_{N-1}^T q_N^T Y_N + h_N^T q_N q_N^T Y_N + h_N^T q_{NN} q_{NN}^T Y_N. \quad (16)$$

Neither of these quantities can be generated recursively since

$$h_N^T q_N Z_{N-1}, \quad G_{N-1}^T q_N^T Y_N \quad (17)$$

and

$$h_N^T q_N G_{N-1} \quad (18)$$

require every element of Z_{N-1} and G_{N-1} to compute these quantities.

Hence, we believe that unless further assumptions can be made concerning the form of the covariance matrix V_N a recursive form of the estimator $\hat{X}_N$ cannot be formulated from the approach that we have taken. A realistic assumption that yields a recursive estimator, yet requires one to retain for computing several latter elements of Z_{N-1} and G_{N-1} is the assumption that

$$V_{ij} = 0$$

for all i and j such that $|i - j| > c$. For example, if we suppose that $c = 2$, then V_N is of the following form:

$$V_N = \begin{bmatrix} V_{11} & V_{12} & V_{13} & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ V_{21} & V_{22} & V_{23} & V_{24} & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ V_{31} & V_{32} & V_{33} & V_{34} & V_{35} & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & V_{42} & V_{43} & V_{44} & V_{45} & V_{46} & \dots & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & V_{N,N-2} & V_{N,N-1} & V_{NN} \end{bmatrix}$$

It can be shown that if $V_{ij} = 0$ for $|i - j| > c$ then $Q_N = \{e_{ij}\}$ is such that

$$e_{ij} = 0$$

for $|i - j| > c$. This is fortunate indeed since this implies that if $c > 0$, then q_N can be written in the form

$$q_N = [\phi_N : \bar{q}_N] \quad (19)$$

where ϕ is a $p \times Np - (cp + p)$ null matrix and $\bar{q}_N$ is a $p \times cp$ non-null matrix. If $c = 0$, then $q_N = \phi_N$ where ϕ_N is a $p \times Np - p$ null matrix. Substituting the right side of (19) into (15) and (16) one obtains

$$(G_N^T G_N) = (G_{N-1}^T G_{N-1}) + \bar{G}_{N-1}^T \bar{q}_N^T h_N + h_N^T \bar{q}_N \bar{G}_{N-1} + h_N^T \bar{q}_N \bar{q}_N^T h_N + h_N^T q_{NN} q_{NN}^T h_N \quad (20)$$

and

$$G_N^T Z_N = (G_{N-1}^T G_{N-1}) \hat{X}_{N-1} + h_N^T \bar{q}_N \bar{Z}_{N-1} + \bar{G}_{N-1}^T \bar{q}_N^T Y_N + h_N^T \bar{q}_N \bar{q}_N^T Y_N + h_N^T q_{NN} q_{NN}^T Y_N \quad (21)$$

where

$$\hat{X}_{N-1} = (G_{N-1}^T G_{N-1})^{-1} G_{N-1}^T Z_{N-1}.$$

$\bar{G}_{N-1}$ and $\bar{Z}_{N-1}$ are the last cp rows of G_{N-1} and Z_{N-1} , respectively.

Finally

$$\begin{aligned} \hat{X}_N = [G_{N-1}^T G_{N-1} + (\bar{G}_{N-1}^T h_N^T) K_N \begin{pmatrix} G_{N-1} \\ h_N \end{pmatrix}]^{-1} [G_{N-1}^T G_{N-1} \hat{X}_{N-1} \\ + (\bar{G}_{N-1}^T h_N^T) K_N \begin{pmatrix} Z_{N-1} \\ Y_N \end{pmatrix}] \end{aligned} \quad (22)$$

where

$$K_N = \begin{bmatrix} 0 & \bar{q}_N^T \\ \bar{q}_N & \bar{q}_N \bar{q}_N^T + q_{NN} q_{NN}^T \end{bmatrix}, \quad (230)$$

and

$$G_{N-1}^T G_{N-1} + (\bar{G}_{N-1}^T h_N^T) K_N \begin{pmatrix} \bar{G}_{N-1} \\ h_N \end{pmatrix}$$

can be inverted recursively as a function of $(G_{N-1}^T G_{N-1})^{-1}$ by applying the inside-out rule defined by (9) to obtain the covariance matrix of X_N . Note that if $c = 0$, then (22) reduces to (8). The storage space required to compute (22) is $\frac{n}{2}(n + 3 + 2cp) + cp$ elements of past data plus present data

6.4. An Example

In order to clarify the partitioning of the matrices in the

previous section consider the following example where $p = 2$, $c = 2$, and $N = 4$. Let

$$Q_4 = \left[\begin{array}{cccccc|cc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \end{array} \right]$$

hence

$$Q_3 = \left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{array} \right]$$

$$q_4 = \left[\begin{array}{cc|cc} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{array} \right] ;$$

$$q_{44} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} ; \quad \bar{q}_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} ; \quad \phi_4 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} ;$$

$$V^{-1} = Q_4 Q_4^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 2 & 2 & 2 & 2 & 2 & 0 & 0 \\ 1 & 2 & 3 & 3 & 3 & 3 & 1 & 1 \\ 1 & 2 & 3 & 4 & 4 & 4 & 2 & 2 \\ 1 & 2 & 3 & 4 & 5 & 5 & 3 & 3 \\ 1 & 2 & 3 & 4 & 5 & 6 & 4 & 4 \\ 0 & 0 & 1 & 2 & 3 & 4 & 5 & 5 \\ 0 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix}$$

and finally K_4 in (23) is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 5 & 5 \\ 1 & 1 & 1 & 1 & 5 & 6 \end{bmatrix}$$

6.5. An Autoregressive Model.

There are many problems [9], [16] where the observation vectors Y_i , $i = 1, 2, \dots, N$ in (1) are related by an autoregressive series [6]. In this section we will define a matrix analog of the univariate autoregressive series and indicate how one can use (8) to estimate the corresponding x in (1). The autoregressive series is defined as follows. Let the errors U_i , $i=1, 2, \dots, N$ be such that

$$U_1 = Z_1$$

$$U_2 = AZ_1 + Z_2$$

$$U_3 = AU_2 + BU_1 + Z_3$$

⋮

$$U_k = AU_{k-1} + BU_{k-2} + \cdots + JU_1 + Z_k$$

⋮

$$U_j = AU_{j-1} + BU_{j-2} + \cdots + JU_{j-(k-1)} + KU_{j-k} + Z_j$$

for all $j > k$, (k , a positive integer)

$$E_1[Z_i] = \phi$$

$$E[Z_i Z_j^T] = V_{ij} \delta_{ij}, \quad i, j = 1, 2, \dots, N. \quad (24)$$

The $A, B, C, \dots, K$ are $p \times p$ matrices. We can rewrite the above equations in matrix form by letting

$$U = RZ \quad (25)$$

where

$$U = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_n \end{bmatrix}, \quad Z = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_n \end{bmatrix}$$

and the elements of R are the coefficient matrices of the z_i 's.

It is computational to show that

$$R^{-1} = \begin{bmatrix} I & \Phi & . & . & . & \Phi & \Phi \\ -A & I & & & & \Phi & \Phi \\ -B & -A & & & & \Phi & \Phi \\ \vdots & \vdots & & & & \vdots & \vdots \\ -K & -L & & & & \Phi & \Phi \\ \Phi & -K & & & & \Phi & \Phi \\ \vdots & \vdots & & & & \vdots & \vdots \\ \Phi & \Phi & & & & I & \Phi \\ \Phi & \Phi & & & & -A & I \end{bmatrix}$$

is a lower triangular band diagonal matrix. It is clear from (24) and (25) that the covariance matrix of U is given by

$$RV_N R^T.$$

By substituting (26) into (6) and noting that R^{-1} exists, it follows that

$$\hat{x}_N = (H_N^T R^{-T} V_N^{-1} R^{-1} H_N)^{-1} H_N^T R^{-T} V_N^{-1} R^{-1} T_N.$$

If we let

$$H_N^* = R^{-1} H_N = \begin{bmatrix} h_1 \\ h_1 - Ah_2 \\ h_3 - Ah_2 - Bh_1 \\ \vdots \\ h_{k+1} - Ah_k - Bh_{k-1} - \dots - Kh_1 \\ h_{k+2} - Ah_{k+1} - Bh_k - \dots - Kh_2 \\ \vdots \\ h_N - Ah_{N-1} - Bh_{N-2} - \dots - Kh_{N-k} \end{bmatrix} = \begin{bmatrix} h_1^* \\ h_2^* \\ h_3^* \\ \vdots \\ h_{k+1}^* \\ h_{k+2}^* \\ \vdots \\ h_N^* \end{bmatrix}$$

and

$$T_N^* = \begin{bmatrix} Y_1 \\ Y_2 - AY_1 \\ Y_3 - AY_2 - BY_3 \\ \vdots \\ Y_{k+1} - AY_k - BY_{k-1} - \dots - KY_1 \\ Y_{k+2} - AY_{k+1} - BY_{k-1} - \dots - KY_1 \\ \vdots \\ Y_N - AY_{N-1} - BY_{N-2} - \dots - KY_{N-K} \end{bmatrix} = \begin{bmatrix} Y_1^* \\ Y_2^* \\ Y_3^* \\ \vdots \\ Y_{k+1}^* \\ Y_{k+2}^* \\ \vdots \\ Y_N^* \end{bmatrix}$$

then $\hat{X}_N$ can be written as

$$\hat{X}_N = (H_N^{*T} V_N^{-1} H_N^*)^{-1} H_N^{*T} V_N^{-1} T_N^* .$$

Since V_N is block diagonal, then by (8)

$$\hat{X}_N = \hat{X}_{N-1} + (H_{N-1}^* V_{N-1}^{-1} H_{N-1}^* + h_N^{*T} V_{NN}^{-1} h_N)^{-1} h_N^{*T} V_{NN}^{-1} (Y_N^* - h_N^{*T} \hat{X}_{N-1}).$$

Note however, one must retain $Y_{N-1}, Y_{N-2}, \dots, Y_{N-k}$ in order to compute Y_N^* , and hence, we still must require k_p additional memory spaces. The elements of the matrix H_N^* can be computed prior to the estimation.

6.6. Concluding Remarks.

There are other forms of V_N which admit recursive estimators of x . The total family of V_N 's for which various forms of recursive estimators exist still needs to be characterized.

It is natural to formulate a recursive estimator for x in the linear model when the unknown covariance matrix is block diagonal and the block matrices are all equal. The estimator is essentially (6) with V_N replaced by an estimator for V_N and then written in a recursive form similar to (8). Unfortunately, the expectation of this estimator or its variance cannot be computed easily and at best one can only say the estimator is effective in the cases studied using Monte Carlo methods.

6.7. References.

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CHAPTER VII

Inverse Kalman Filtering In Data Evaluation

Only on things uncertain I rely

I have no doubt except in certainty

And from blind chance for knowledge I inquire.

-Francois Villon, the 15th-century French Poet.

7.1. Introduction.

In section 2 of Chapter II we discussed the concept of inverse filtering. In this chapter we review the notions which suggest the need for such estimation procedures and discuss a particular method referred to as inverse Kalman filtering.

In almost all experiments data will be collected by means of a specified measuring instrument. In essentially every one of these cases instrument specifications have been determined, usually at great expense, so as to insure the credibility of the data. Two basic questions however, should be considered in this light. That is, even on good equipment what statistical techniques should be employed to enhance the signal (or data) quality and secondly can these techniques be used to reduce the required quality of the measuring equipment necessary for various experiments? Both of these questions can be partially answered by the discussion which follows. As is well known, when large amounts of data are available in the measurement of a particular parameter,

accuracy requirements on the data can be loose. We will not however, discuss this aspect of data collection since for the present we assume the original specifications were made with that in mind. The aspect of data collection which we wish to discuss here relative to the present question is inverse filtering. We outline the subject below since present investigation of NASA's available literature on planned experiments (as well as previous ones) shows no indication that proper, if any, use of this technique has been made in current experimental designs.

7.2. Inverse Filtering.

In the use of electronic equipment for data collection a common problem has arisen which is referred to as inverse filtering or signal restoration, see [2], [4], or [5]. The problem arises because of the fact that few, if any, measuring devices record the actual received signal. Schematically the measuring system can be described as follows:

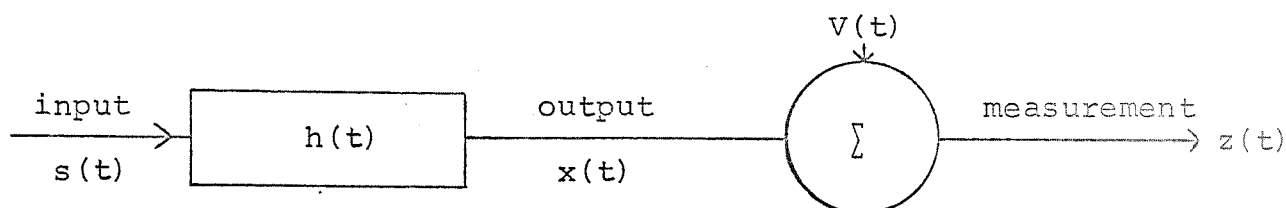


Figure 1

In figure 1, $s(t)$ is an input signal; $h(t)$ represents a measuring instrument, and $x(t)$ represents the resulting measurement, which may be "smeared" by the instrument. Since this measurement may be observed in presences of noise (random interference) a noise vector $v(t)$ is added in and the recorded result

is $z(t)$. Various versions of the above such as $\text{input} = s(t) + n(t)$, $n(t)$ an additional noise vector, can easily be given, but we shall not discuss them here.

From figure 1 above, it is clear that the problem of inverse filtering is one of constructing a filter such that when $z(t)$ is the input $s(t)$, i.e., the restored signal, is the output.

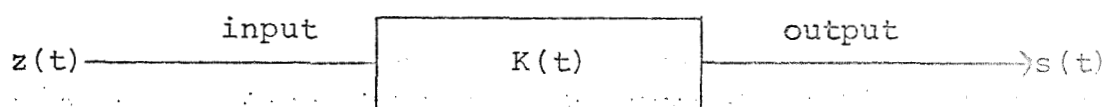


Figure 2

Since the original signal has been corrupted by random noise and it is physically impossible to remove all instrument measurement effects, it is not possible to construct the filter $K(t)$. A satisfactory solution to the problem when the noise is not too excessive does, however, often exist. That is, for many cases it is possible to construct a filter $\hat{K}(t)$ such that when $z(t)$ is input, the output is $\hat{s}(t)$, where $\hat{s}(t)$ is the best linear unbiased estimate of $s(t)$. A number of different approaches to this problem have been and still are being considered in the literature.

A method referred to as inverse Kalman filtering [2] appears, at least theoretically, to offer the best solution to the problem. It can be described as follows:

Let

$$s(t) = n \times 1 \quad \text{input data vector}$$

$$x_1(t) = m \times 1 \quad \text{output vector}$$

$$A_1(t) = m \times m \text{ matrix}$$

$$G_1(t) = m \times n \text{ matrix}$$

$$Y(t) = H_1(t)X_1(t), H_1(t) \text{ a } p \times m \text{ matrix}$$

$$Z(t) = Y(t) + V(t).$$

Then assume the dynamic system of figure 1 can be described by the system of differential equations

$$\dot{X}_1(t) = A_1(t) X_1(t) + G_1(t) s(t)$$

$$Z(t) = Y(t) + V(t) = H_1(t)X_1(t) + V(t) . \quad (1)$$

Now up to second order moments the original signal $s(t)$ can also be described by the dynamic system

$$\dot{X}_2(t) = A_2(t) X_2(t) + G_2(t) u(t)$$

$$s(t) = H_2(t) X_2(t) , \quad (2)$$

where $u(t)$ is a white noise vector and $A_2(t)$, $G_2(t)$ and hence $X_2(t)$ are matrices which are completely determined by the covariance matrix of $u(t)$. Thus from (1) we can write

$$\dot{X}(t) = F(t) X(t) + G(t) u(t)$$

$$z(t) = H(t) X(t) + V(t) , \quad (3)$$

where

$$X(t) = \begin{pmatrix} X_1(t) \\ X_2(t) \end{pmatrix}$$

$$F(t) = \begin{bmatrix} A_1(t) & G_1(t) & H_2(t) \\ 0 & A_2(t) & \end{bmatrix}$$

$$G(t) = \begin{bmatrix} 0 \\ G_2(t) \end{bmatrix} \text{ and } H(t) = [H_1(t), 0] \quad (4)$$

But from (3) it is well known that the best linear unbiased estimate of $X(t)$ and hence $s(t)$ is $\hat{X}(t)$, where $\hat{X}(t)$ is the output of the corresponding Kalman filter. Thus when the dynamics of the receiving system can be described by a linear system (not necessarily time invariant) and the covariance of $u(t)$ is known, $\hat{s}(t)$ is the output of a Kalman filter which can theoretically be determined. Practically speaking a number of difficulties still remain in applying the above in particular situations and the details of particular inverse filters will have to be worked out. However, the method has been used with good restoration results. The following graph gives a pictorial description of inverse filtering.

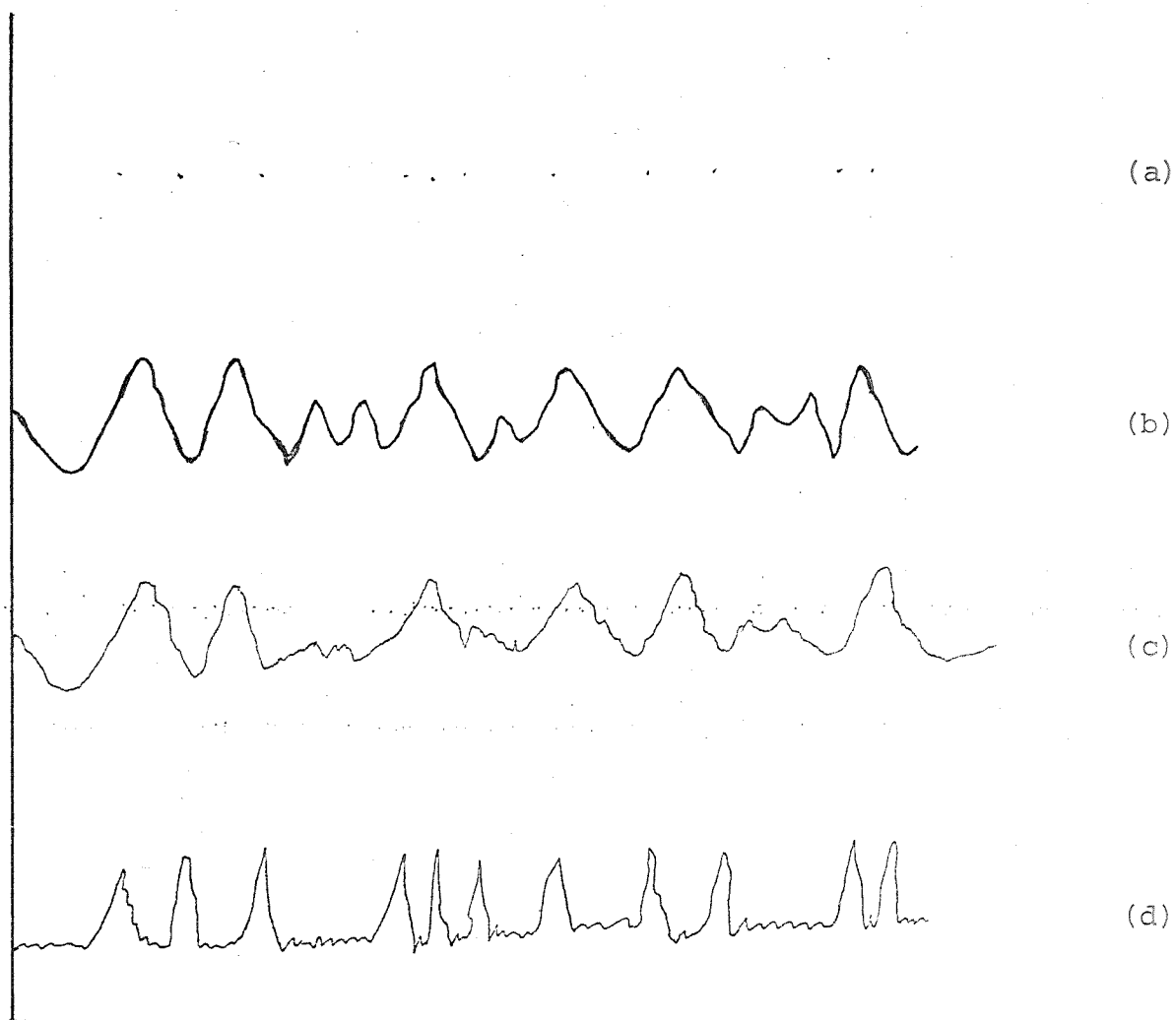


Figure 3

Analog computer simulation of application of inverse Kalman filter to a seismic filter problem. a) actual signal; b) superimposed wavelet; c) wavelet plus noise; d) estimated impulse through inverse filtering.

7.3. Concluding Remarks.

From figure 3, and the previous discussion it is clear the inverse filtering is a useful tool in signal restoration. These restoration effects have the following impact on experimental design whenever electronic measuring (or other) equipment is

employed. Namely, selection of all measuring equipment should be done with due consideration to the inverse filter problem. From a cost effectiveness point of view this means that the cost of the following trade off must be considered; cost of highly efficient equipment versus cost of development of inverse filters for less efficient equipment.

From a mission requirements standpoint, inverse filtering should be considered to improve measurement capabilities of first line equipment. We now give a simple example.

Example: Consider the analysis which produced figure 3. That is, let

$$u(t) = \sum_{i=1}^{\infty} \delta(t - t_i) - Q$$

be a sequence of Poisson impulses where Q is the occurrence rate in the associated Poisson process. Then $E[u(t)] = 0$ and $u(t)$ is clearly white noise. Now let $s(t)$ be the input signal which is to be recovered and assume $s(t)$ is generated from $u(t)$ as shown below.

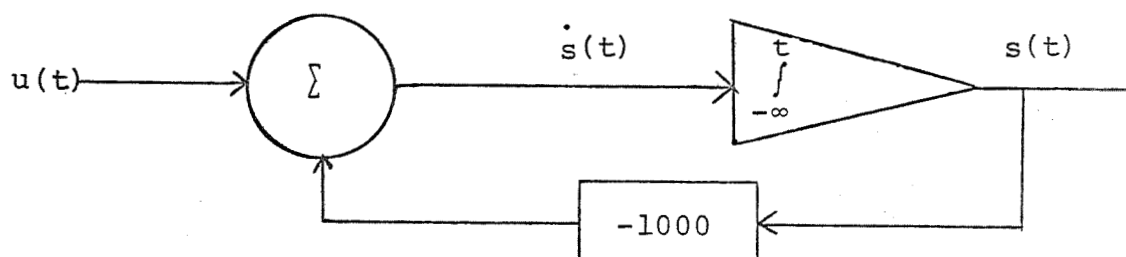


Figure 4

Then we have

$$\dot{s}(t) - 1000 s(t) = u(t)$$

so that

$$s(t) = \sum_{i=1} u(t - t_i) e^{-1000(t-t_i)} - \frac{Q}{1000} ,$$

where

$$u(t - t_i) = \begin{cases} 0 & t < t_i \\ 1 & t \geq t_i \end{cases} .$$

Further suppose the signal $s(t)$ is passed into the system shown by figure 5.

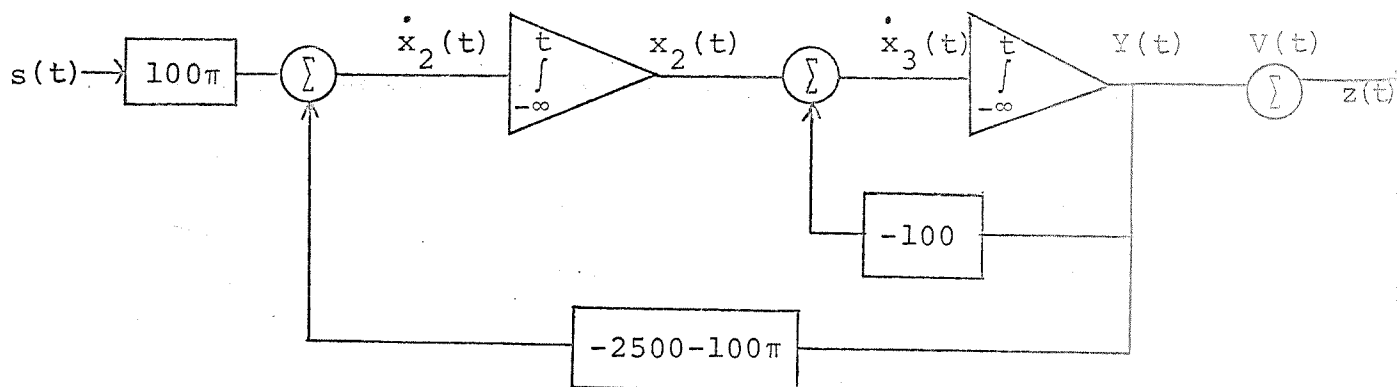


Figure 5

Then it is clear that $x_3(t)$ satisfies the differential equation

$$\ddot{x}_3 + 100\dot{x}_3 + (2500 + 100\pi)x_3 = 100\pi s ,$$

so that $V(t)$ is a sequence of superimposed equal amplitude wavelets of the form $e^{-50t} \sin \sqrt{100\pi} t$, with random time of occurrence, as shown in figure 3b. Thus the problem is to recover $s(t)$ when $Z(t) = Y(t) + V(t)$ is the output signal, where $V(t)$ is a corrupting independent identically distributed noise source with variance V .

However from figures 4 and 5 we can write

$$\frac{d}{dt} \begin{bmatrix} s(t) \\ x_2(t) \\ x_3(t) \end{bmatrix} = \begin{bmatrix} 1000 & 0 & 0 \\ 100 & 0 & -2500 - 100 \\ 0 & 1 & -100 \end{bmatrix} \begin{bmatrix} s(t) \\ x_2(t) \\ x_3(t) \end{bmatrix}$$

$$+ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} u(t).$$

Consequently we have the system in the form given by equation (3) and the best estimate for $s(t)$ is then the Kalman filter, $\hat{s}(t)$, which is completely determined by the above. Figure 3d shows graphically the estimator $\hat{s}(t)$.

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CHAPTER VIII

Fast Techniques for Discriminating

Patterns in Earth Surveys

Whenever we take a sample, we do so with the idea of learning something about the population from which the sample is drawn. Provided that the sample is drawn in an unbiased manner, we believe that it may be taken as representative of the parent population. However representatives are not all equally authoritative. Spokesmen - even official spokesmen - do not always tell a reliable tale, and it is very necessary in retelling a story from such a source that we indicate the degree of confidence which may be placed in what the spokesman has said. Just as the journalist tries to emphasize for his readers the difference between rumour and 'usually well informed sources', so too the statistician has to attempt a similar thing.

8.1. Introduction.

A problem that conceptually can be considered a multivariate discriminate analysis problem in which one must estimate the multivariate probability density functions of various populations using previously obtained data (training data) has been applied with reasonable success by the Laboratory for Agriculture Remote Sensing (LARS) at Purdue University [1] to recognize agricultural crops using remote sensing devices. Their solution is the classical statistics solution discussed in [2], and is

well-known. Unfortunately, the classical solution does not lend itself to "rapid" computation in this application, and hence it has been conjectured that the method is [3] limited in usefulness if one cannot re-formulate the problem in a manner which will lend itself to faster computing or if faster computers do not become available in the near future. Apparent need to gain a real time capability to make decisions using remote sensing data requires that faster techniques be formulated, especially if one requires onboard computing in the space station application.

The purpose of this chapter is to discuss the problem of reducing remote sensing data and to review a conjectured faster algorithm formulated and made computationally realistic by Eppler [4]. Also, we will suggest a modification of Eppler's algorithm, based upon the concepts of scatter analysis formulated by Wilks [5].

The following problem statement will establish the notation and definitions; also this will aid the reader to obtain a brief review of the problem of statistical discriminant analysis:

Problem. Let $\pi_1, \pi_2, \dots, \pi_k$ denote k populations. Associated with each individual in the population is the set of characteristics $c_1, c_2, \dots, c_p$ which can be measured. Let $x^{(i)} = (x_1^{(i)}, x_2^{(i)}, \dots, x_p^{(i)})$ denote a vector of measurements one from each characteristic on an individual from the i^{th} population. Suppose further that the a priori probability that an individual is selected from the i^{th} population is q_i , $i = 1, 2, \dots, k$ and that the multivariate probability density function of the measurement vector $x^{(i)}$ is $p_i(x)$.

Let $C(i|j)$ denote the cost of classifying an individual from the j^{th} population as a member of the i^{th} population. The problem is to devise a decision rule such that given an observation $x = (x_1, \dots, x_p)$ one can assign the individual to one of the k populations in such a manner that the expected cost of misclassification is minimized.

The solution is well-known and is given in [2]. Unfortunately, it depends on the $C(i|j)$ and the quantities $q_1, q_2, \dots, q_n$, all of which are seldom known. Also, it is difficult in some applications to defend one's choice of the multivariate probability density functions $p_1(x), p_2(x), \dots, p_k(x)$.

A popular solution is to assume that $q_i = q_j$, $C(i|i) = 0$; $C(i|j) = C(i'|j')$ for all $i' \neq j'$, and $p_i(x)$ is a normal probability density function. That is,

$$p_i(x) = N(\mu^{(i)}, \Sigma^{(i)})$$

with

$$\Sigma^{(i)} = \Sigma^{(j)} = \Sigma$$

for all i and j . These assumptions along with the assumption that Σ is known, lead to linear discriminant functions [2] which are indeed mathematically "tidy,". However, they are relatively impractical in most applications since $p_i(x)$ are usually unknown, and if normal $\Sigma^{(i)} \neq \Sigma^{(j)}$ for some or all $i \neq j$. Hence, one must estimate $p_i(x)$ using data previously taken from individuals known to come from the i^{th} population.

Suppose $\hat{p}_i(x)$ denotes the estimate of the density function $p_i(x)$ based on N_i "training" samples. Let $q_i = q_j$ and $C(i|j) = \text{constant}$ for all $i \neq j$. Then we say that an individual yielding the measurement vector $X = x_0$ comes from the j^{th} population, π_j if

$$\max \hat{p}_i(x_0) = \hat{p}_j(x_0), \quad i = 1, 2, \dots, k.$$

It is suggested by Anderson [2] (and used by many [4]), that $p_i(x)$ is a p -variate normal probability density function. That is

$$p_i(x) = (2\pi)^{-1/2} |\Sigma_i|^{-1/2} \exp\left\{-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)\right\}$$

for $i = 1, 2, \dots, k$. If $x_1^{(i)}, x_2^{(i)}, \dots, x_{N_i}^{(i)}$ denotes a random sample of N_i $p \times 1$ vectors, then one can estimate the mean vector μ_i by

$$\hat{\mu}_i = \sum_{j=1}^{N_i} x_j^{(i)} / N_i,$$

and the covariance matrix Σ_i

$$\hat{\Sigma}_i = \sum_{j=1}^{N_i} (x_j^{(i)} - \hat{\mu}_i)(x_j^{(i)} - \hat{\mu}_i)^T / (N_i - 1).$$

Then we can estimate $p_i(x) = p_i(x; \mu_i, \Sigma_i)$ by

$$\hat{p}_i(x) = p_i(x; \hat{\mu}_i, \hat{\Sigma}_i)$$

or

$$\hat{p}_i(x) = (2\pi)^{-1/2} |\hat{\Sigma}_i|^{-1/2} \exp\left\{-\frac{1}{2}(x-\hat{\mu}_i)^T \hat{\Sigma}_i^{-1}(x-\hat{\mu}_i)\right\} \quad (1)$$

One should note that this implies that normal assumptions are valid or approximately valid when one uses $\hat{p}_i(x)$.

A particular application selected for illustrative purposes that concerns us here is to recognize statistically different patterns of land uses from data obtained by sensing equipment on a reconnaissance airplane. The vegetation or lack of vegetation compose the populations; that is, corn, wheat, oats, bare land, etc., make up the populations. Six channels of data are taken, that is $p = 6$ and $X = (x_1, x_2, \dots, x_6)^T$. Each element represents a measurement of spectral radiance for a specified small interval or band of wavelengths.

Training samples of size N_i are taken composing the data

$$\begin{array}{lll}
 x_1^{(1)} , & x_2^{(1)} , & \dots , & x_{N_1}^{(1)} & \text{from } \pi_1 \\
 x_1^{(2)} , & x_2^{(2)} , & \dots , & x_{N_2}^{(2)} & \text{from } \pi_2 \\
 \vdots & \vdots & & \vdots & \\
 x_1^{(K)} , & x_2^{(K)} , & \dots , & x_{N_K}^{(K)} & \text{from } \pi_K
 \end{array}$$

from which the estimates

$$\hat{\mu}_1, \hat{\mu}_2, \dots, \hat{\mu}_K$$

and

$$\hat{\Sigma}_1, \hat{\Sigma}_2, \dots, \hat{\Sigma}_K$$

are computed. These in turn yield the estimates

$$\hat{p}_1(x), \hat{p}_2(x), \dots, \hat{p}_K(x)$$

of the probability density functions $p_1(x), p_2(x), \dots, p_K(x)$,

respectively. The Purdue system is to assume normality, hence these estimates are of the form:

$$\hat{p}_i(x) = (2\pi)^{-1/2} |\hat{\Sigma}_i|^{-1/2} \exp\left\{-\frac{1}{2}(x-\hat{\mu}_i)^T \hat{\Sigma}_i^{-1}(x-\hat{\mu}_i)\right\}.$$

A simplification is obtained by taking the logarithm of both sides.

Then

$$\ln \hat{p}_i(x) = K_i - \frac{1}{2}(x-\hat{\mu}_i)^T \hat{\Sigma}_i^{-1}(x-\hat{\mu}_i)$$

$$\text{where } K_i = -\frac{1}{2} \ln(2\pi) - \frac{1}{2} \ln|\hat{\Sigma}_i|.$$

Suppose $X = x$ denotes a measurement from which we are to classify an individual. In order to determine

$$\max_i \{\hat{p}_i(x)\}$$

we determine for some j

$$\ln \hat{p}_j(x) = \max_i \{\ln \hat{p}_i(x)\}$$

and assign or classify the individual from which the measurement came to π_j . In order to do this, we must compute

$$(x - \hat{\mu}_i)^T \hat{\Sigma}_i^{-1}(x - \hat{\mu}_i)$$

for $i = 1, 2, \dots, k$. Since $\hat{\Sigma}_i$ is computed using random data, $\hat{\Sigma}_i^{-1}$ almost surely (theoretically) contains no zero elements and is therefore not diagonal; hence, the computation will require for each $(x - \hat{\mu}_i) \hat{\Sigma}_i^{-1}$, p^2 multiplications, and p^2 additions performed k times. Then multiplying

$$[(x - \hat{\mu}_i)^T \hat{\Sigma}_i^{-1}] (x - \hat{\mu}_i)$$

requires an additional p multiplications and p additions. Thus, one must perform $p^2 + p$ multiplications and $p^2 + p$ additions to compute a single $\ln \hat{p}_i(x)$. This must be done K times, once for each population. If $\hat{\Sigma}_i^{-1}$ is diagonal, then $\ln \hat{p}_i(x)$ can be computed in $2p$ multiplications and $2p$ additions. Since it is assumed that $\hat{\mu}_i$ and $\hat{\Sigma}_i$ is computed prior to the classifying, the time and operations to compute $\ln \hat{p}_i(x)$ is an important criterion to judge an algorithm.

An image is composed of N lines of n data squares; each square yields an observation vector x to use to statistically classify that square as a member of one of the populations $\pi_1, \pi_2, \dots, \pi_k$.

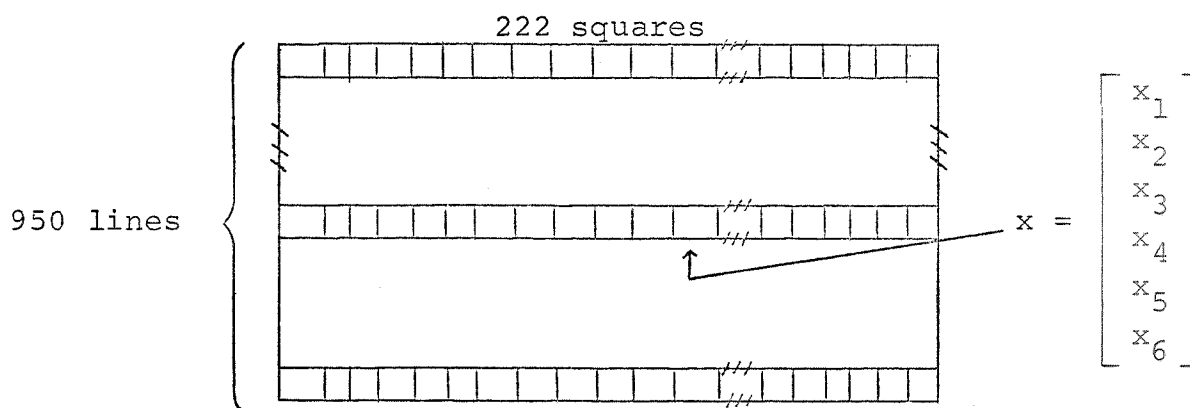


Figure 1. The Image of 950 lines with 222 squares per line and 6 channels of measurements for each square.

That is to say, one must make $k(p^2 + p)$ multiplications and $k(p^2 + p)$ additions for each square. Then for each image one must make

$Nnk(p^2+p)$ multiplications and $Nnk(p^2+p)$ additions per image. To gain some insight into realism, consider $N = 950$, $n = 222$, $k = 9$, and $p = 6$. Then

$$Nnk(p^2+p) = 79,720,200.$$

Note also, one must rank nine numbers at each data square. That is, for each image one must perform

$$Nn = 210,900$$

ranking operations on nine numbers ($\ln \hat{p}_i(x)$, $i = 1, 2, \dots, 9$).

Eppler's algorithm was formulated to reduce the computing time to analyze an image. This he has done by incorporating table lookup operations thereby reducing the number of multiplications.

8.2. The Eppler Algorithm.

Besides being "slow" the classical solution as applied by LARS tacitly involves a normality modeling assumption. Eppler has developed a non-parametric procedure to estimate marginal probability densities associated with $p_i(x)$, that is, one which does not assume a specified form for $p_i(x)$; for example, the normal form. Eppler's present algorithm also assumes that $q_i = q_j$ and $C(i|j) = \text{constant}$ for all $i \neq j$. A major disadvantage is that the decision criterion is based on the two dimensional probability density functions

$$p_i(x_i, x_j) = \int \dots \int p_k(x_1, \dots, x_p) dx_1 \dots dx_{i-1} dx_{i+1} \dots dx_{j-1} dx_{j+1} \dots dx_p$$

$i \neq j = 1, 2, \dots, p$. There are $\binom{p}{2}$ such density functions. It is these probability density functions that the Eppler Algorithm estimates. Hence, instead of estimating a single probability density function as the LARS program does Eppler must estimate

$$f_{1i} = p_i(x_1, x_2)$$

$$f_{2i} = p_i(x_1, x_3)$$

$$f_{3i} = p_i(x_1, x_4)$$

$$f_{4i} = p_i(x_1, x_5)$$

$$f_{5i} = p_i(x_1, x_6)$$

$$f_{6i} = p_i(x_2, x_3)$$

$$\vdots$$

$$f_{15i} = p_i(x_5, x_6)$$

for $i = 1, 2, \dots, 9$.

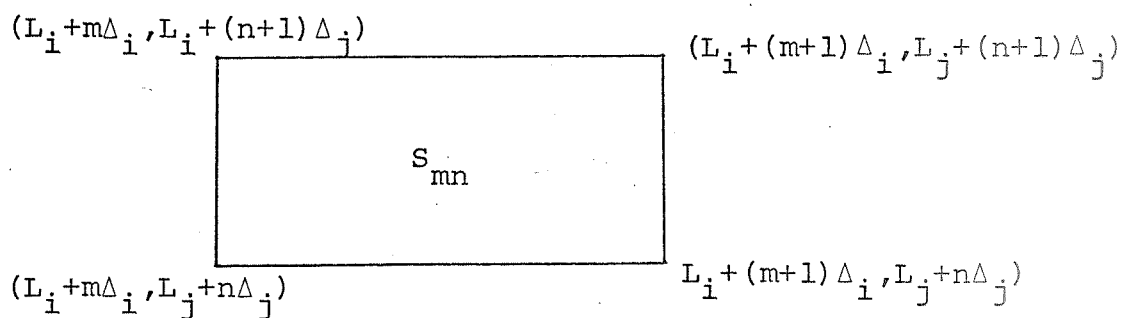
For the time being, let us suppose each f_{ij} is estimated by $\hat{f}_{ij}$ using the training samples previously defined. It is assumed that for each i and j

$$L_i \leq x_i \leq L_i + 256\Delta_i$$

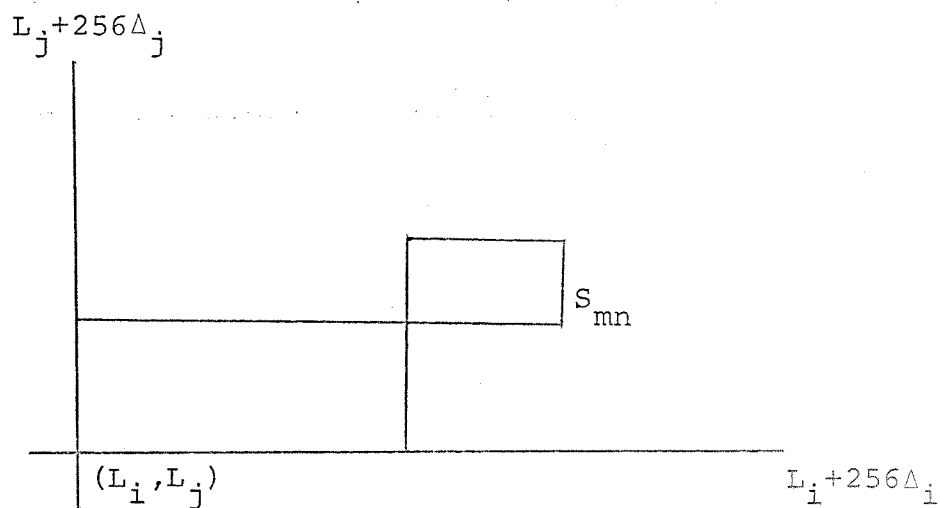
and

$$L_j \leq x_j \leq L_j + 256\Delta_j$$

where L_i and L_j denote the lower limits that x_i and x_j can take on for a specified population. The increments Δ_i and Δ_j denote the grid size one chooses so that $S_{m,n}$ is the ij^{th} rectangle



Let $\hat{f}_{ij}(S_{mn})$ be the proportion of samples with (x_i, x_j) contained in S_{mn} .



Since $\hat{f}_{ij}(S_{mn})$ is a very "rough" estimate for f_{ij} , the Eppler algorithm performs a smoothing operation by averaging over a 5×5 grid, say G , with S_{mn} as the center element. That is,

$$\hat{f}_{ij}(S_{mn}) = \frac{1}{25} \left[\sum_{m,n \in G} \hat{f}_{ij}(S_{mn}) \right]$$

If $f_{ij}(S_{mn}) \leq \varepsilon$ where ε is a previously chosen (empirically) positive number, then $\hat{f}_{ij}(S_{mn})$ is given the value zero.

It should be noted the Eppler's algorithm has replaced the

LARS decision rule which is "approximately" optimal, in the sense that if the normality assumptions hold, their rule is the classical one along with a new rule that depends only on the two-dimensional marginal probability density function. The LARS rule is to assign the individual to π_j if

$$\max_{i=1, \dots, k} \hat{p}_i(x) = \hat{p}_j(x) ,$$

while the Eppler algorithm assigns the individual to $\pi_{j'}$ if

$$\max_{i'=1, \dots, k} \{\hat{p}_{i'}(x_i, x_j)\} = \hat{p}_{j'}(x_i, x_j)$$

where i and j are selected judiciously according to an empirical rule. The symbol $\hat{p}_i(x_i, x_j)$ is an estimate of the marginal probability density function of (x_i, x_j) for the i^{th} population.

Let

$$R_j = \{(x_1, x_2, \dots, x_p); \hat{p}_j(x) = \max_{i=1, 2, \dots, k} \hat{p}_i(x)\}$$

and

$$R_j^* = \{(x_1, x_2, \dots, x_p); \hat{p}_j(x_i, x_j) = \max \hat{p}(x_i, x_j)\} .$$

Note that examples can be constructed so that $R_j \subset R_j^*$; $R_j \supset R_j^*$, and $R_j \cap R_j^* \neq \emptyset$, the null set. Hence little can be said analytically concerning the comparing of the techniques except through simulation. One compares the probabilities of proper classification by computing

$$p(\pi_j | \pi_j) = \int_{R_i} p_j(x_1, \dots, x_p) dx_1, \dots, dx_p$$

and

$$p_E(\pi_j | \pi_j) = \int_{R_i^*} p_j(x_1, \dots, x_p) dx_1, \dots, dx_p$$

$$j = 1, 2, \dots, p.$$

The Eppler algorithm lends to fast computing by replacing multiplication and addition operations by table look-up operations. If x_1 and x_2 are the data channels selected for decision making, then one forms a qualitative data vector such that for each population $\pi_1, \pi_2, \dots, \pi_k$ and data square S_{mn} , with $(x_1, x_2) \in S_{mn}$,

$$d_{mn} = [\delta_{ij}^{(1)}, \delta_{ij}^{(2)}, \dots, \delta_{ij}^{(k)}]$$

$$\delta_{ij}^{(k)} = \begin{cases} 1 & \text{if } \hat{f}_{ij}^{(k)}(x_i, x_j) > 0 \\ 0 & \text{if } \hat{f}_{ij}^{(k)}(x_i, x_j) = 0 \end{cases}$$

However, if more than two (can be changed to an arbitrary number less than or equal to k) populations produce one's in the relevant position, then one orders the set $\hat{f}_{ij}^{(k)}(x_i, x_j)$ in magnitude and assigns unity to the data element associated with the two largest values of $\hat{f}_{ij}^{(k)}(x_i, x_j)$. That is, if

$$\hat{f}^{(3)} > \hat{f}^{(5)} > \dots > \hat{f}^{(k-1)} > \hat{f}^{(k-2)}$$

then

$$d_{mn}^{(i,j)} = [0, 0, 1, 0, 1, 0, \dots, 0].$$

This decision can be coded by the number

$$N_{mn} = \delta_{ij}^{(1)} 2^0 + \delta_{ij}^{(2)} 2^1 + \delta_{ij}^{(3)} 2^2 + \dots + \delta_{ij}^{(k)} 2^{k-1}.$$

Note that the value of N_{mn} is such that if $k = 9$, then

$$N_{mn} \leq 512 .$$

However, since we allow only those data locations with only two 1's, the total number of elements in the set $\{N_{mn}\}$ is given by listing the possible entries. Note that we code the pairs of elements of the vector X . That is

$$\begin{array}{ll} (x_1, x_2) = 1 & (x_2, x_3) = p \\ (x_1, x_3) = 2 & (x_2, x_4) = p+1 \\ (x_1, x_4) = 3 & \\ \vdots & \vdots \\ (x_1, x_p) = p-1 & (x_p, x_{p-1}) = p!/2!(p-2)! \end{array}$$

In Eppler's language these will be called the set of decision pairs, while the values of N_{mn} are said to be decision locations. Note that for every data square S_{mn} there is a decision code $d_{mn}^{(ij)}$ for each decision pair. Using the r^{th} data pair one immediately has a listing of (256×256) reduced arbitrarily in Eppler's application to (64×64) decision codes for computational efficiency.

One code is associated with each data square. If (x_i, x_j) belongs to S_{mn} , then d_{mn} gives the decision in the following way: If there is a single 1 in the j^{th} element of the decision vector and zeros elsewhere, assign the individual to the j^{th} population π_j . However, if there are two nonzero elements in d_{mn} , then one selects another decision pair to make

the decision. That is, if a is in both the r and q elements of d_{mn} , we must analyze the data further before making the decision between assigning the individual to π_r or π_q . This new decision pair leads to the most likely population for classification if one of the two candidate populations is repeated with a higher frequency. The use of an "and" operation gives automatic classification where d_{mn} and d_{mn} yields a vector with a single one in the classifying position.

A table is constructed with the code for decision pairs as one marginal entry and the coded decision location N_{mn} as the second marginal entry. The entry to the table gives the frequency (proportion) that a second stage decision process must be made if a particular decision pair is used and a particular decision code is observed based on the training data. To select the initial decision pair one selects that decision pair that minimizes the frequency of multiple decisions. If a pair and a decision code gives a multiple decision, then fixing the code, one selects that decision pair that minimizes the frequency of multiple decision given the observed decision code.

Unfortunately, Eppler's Algorithm is difficult to analytically formulate so that error analysis can be made. The non-parametric features as well as the reported fast computing times make it attractive. However, the two stage technique may not make up for the fact that marginal densities are used instead of the multi-variate probability density function used in the slower LARS program. It should be noted that the LARS program is also an approximation to the optimal and depends on perhaps unrealistic

normality assumptions. A Monte-Carlo simulation would be useful in comparing as well as testing on actual data.

8.3. Various Modifications to Reduce Dimension.

The single major disadvantage of the Eppler algorithm is that it bases decisions on marginal probability density instead of upon the full vector of data. Let P be a (2×6) matrix and X the (6×1) observation vector. Define

$$Y = PX$$

a two dimensional vector which is a linear combination of the values of X . Eppler selects P to be of the following form

$$P_{12}X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$P_{13}X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

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

$$P_{56}X = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} x_5 \\ x_6 \end{bmatrix}$$

where $P = \begin{bmatrix} P_{12} \\ \vdots \\ P_{56} \end{bmatrix}$

It is clear that the matrices $P_{12}, P_{13}, \dots, P_{56}$ belong to a much larger class of matrices which might be selected in such a manner as to be beneficial to correct classification.

For example, it is possible to select P so that

$$E[Y|\pi_1] = v_1$$

$$E[Y|\pi_2] = v_2$$

$$\vdots$$

$$E[Y|\pi_k] = v_k$$

where the 2×1 mean vectors $v_1, v_2, \dots, v_k$ are preassigned values.

Specifically, if $E[X_i] = \mu_i$, then select P such that

$$P[\mu_1 : \mu_2 : \dots : \mu_k] = [v_1 : v_2 : \dots : v_k]$$

or

$$P\mu = v.$$

Therefore,

$$P = v\mu^+$$

or

$$P = v\mu^T(\mu\mu^T)^{-1}.$$

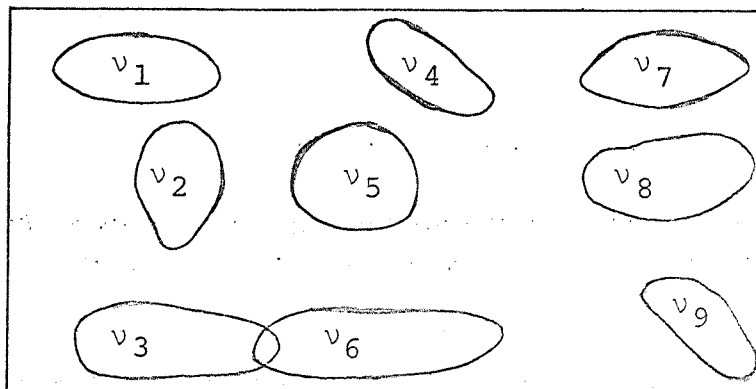
Of course, one must check and see if the covariance matrices

$$W_i = PV_iP^T$$

are small, so that classifying using the new transformed observation $Y = PX$ is practical. This would introduce twelve multiplications and twelve additions but would eliminate all second order operations. It would indeed be fortunate if one could establish the family of transformations P such that if

$$p_i(x) < p_j(x) \text{ then } p_i(x) \frac{dx}{dy} < p_j(x) \frac{dx}{dy}.$$

A basic important question arises naturally. If we classify using the Y observation, do we classify as we would if we had used the X observation? To give a partial answer, consider the following argument.



Transformed Observation Space $Y = PX$

Let the set A_{ij} be defined as follows.

$$A_{ij}(x) = \{x; p_i(x)/p_j(x) \geq 1\}$$

and

$$A_{ij}(y) = \{y; p_i(y)/p_j(y) \geq 1\}$$

where $p_i(\cdot)$ is the probability density of $(\cdot)$ given that $(\cdot)$ is from the i^{th} population.

Let $p_i(x)$ be normal, such that $E(X) = \mu^{(i)}$ and $\text{Cov}(X) = \Sigma^{(i)}$ $i = 1, 2, \dots$. Then $Y = CX$ is distributed normally with mean $C\mu^{(i)}$ and covariance matrix $C\Sigma^{(i)}C^T$. Now suppose that $p_i(x)/p_j(x) = 1$. Then

$$p_i(y)/p_j(y) = \frac{|C\Sigma^{(j)}C^T|}{|C\Sigma^{(i)}C^T|} e^{-\frac{1}{2}[(x-\mu^{(i)})^T C^T (C\Sigma^{(i)}C^T)^{-1} C(x-\mu^{(i)}) - (x-\mu^{(j)})^T C^T (C\Sigma^{(j)}C^T)^{-1} C(x-\mu^{(j)})]}$$

But we know that

$$\alpha^T C^T (C \Sigma^{(i)} C^T)^{-1} C \alpha \leq \alpha^T \Sigma^{(i)} \alpha$$

for every vector α .

Let $\Sigma^{(1)} = \Sigma^{(2)} = I$. Then

$$\frac{p_i(y)}{p_j(y)} = e^{-\frac{1}{2}[(x-\mu^{(i)})^T (C C^T)^{-1} C (x-\mu^{(i)}) - (x-\mu^{(j)})^T (C C^T)^{-1} C (x-\mu^{(j)})]}$$

which implies that in general one cannot be sure that if

$$\frac{p_i(x)}{p_j(x)} = 1$$

then

$$\frac{p_i(y)}{p_j(y)} \neq 1.$$

Clearly if $C^T (C C^T)^{-1} C = I$ when $\Sigma^{(1)} = \Sigma^{(2)} = I$, then these conditions would hold. But rank considerations force $C^T (C C^T)^{-1} C$ to be of rank r although $C^T (C C^T)^{-1} C$ is a $p \times p$ matrix.

In his text [5] Wilks discusses a concept of multi-dimensional scatter and implies that the concept can lead to ways for reducing the dimension of some statistical discriminate problems. Sebestyan [6], in developing a technique for recognizing patterns, has developed a theory similar to the theory of scatter developed by Wilks and apparently has had some effect on engineering applica-

tions [6], [7].

We define the i^{th} sample scatter matrix defined by

$$S_i = \sum_{j=1}^{N_i} (x_j^{(i)} - \bar{x}^{(i)}) (x_j^{(i)} - \bar{x}^{(i)})^T \quad (2)$$

where

$$\bar{x}^{(i)} = \sum_{j=1}^{N_i} x_j^{(i)} / N_i .$$

The determinate of the matrix

$$S_w = \sum_{i=1}^m S_i \quad (3)$$

is called the within scatter of the m samples. The determinate of the matrix

$$S_p = \sum_{i=1}^m \sum_{j=1}^{N_i} (x_j^{(i)} - \bar{x}) (x_j^{(i)} - \bar{x})^T \quad (4)$$

where

$$\bar{x} = \sum_{i=1}^m \sum_{j=1}^{N_i} x_j^{(i)} / (N_1 + N_2 + \dots + N_m) \quad (5)$$

is called the pooled scatter. It is easy to show that

$$S_p = S_w + S_B \quad (6)$$

where the determinate of the matrix

$$S_B = \sum_{i=1}^m N_i (\bar{x}^{(i)} - \bar{x}) (\bar{x}^{(i)} - \bar{x})^T \quad (7)$$

is called the between scatter. It is important to note that the rank of the matrix S_B is the maximal value of p and m (almost surely). We select the rows of C in such a manner so that $S_B(Z)$ is minimal and $S_W(Z)$ remains constant in such a way that

$$\frac{|S_W|}{|S_p|} = \frac{|S_W|}{|S_W + S_B|} = \frac{|S_W(Z)|}{|S_W(Z) + S_B(Z)|} = \frac{|S_W(Z)|}{|S_p(Z)|} \quad (8)$$

where $S_{(.)}(Z)$ denotes $S_{(.)}$ with the X 's replaced by the Z 's as defined by (8). That is, one selects C in such a manner that

$$Q = |S_B(Z)| + [K - |S_W(Z)|]\lambda \quad (9)$$

is maximum where $K = |S_W(Z)|$ is a constant. Let $r = 1$, then C is a $1 \times p$ matrix. Then (9) reduces to

$$Q = CS_B C^T + [K - CS_W C^T]\lambda$$

since

$$|S_B(Z)| = CS_B C^T \quad (10)$$

$$|S_W(Z)| = CS_W C^T \quad (11)$$

Taking the derivative of Q with respect to the elements of C^T and equating with the $p \times 1$ zero vector $\emptyset$ yields necessary conditions for a maximum, namely,

$$(S_B - \lambda S_W) C^T = 0 \quad (12)$$

and

$$K - C X_W C^T = 0 . \quad (13)$$

It is well-known that (13) has a nonzero solution only if

$$|S_B - \lambda S_W| = 0 . \quad (14)$$

Let P be a non-singular matrix (P exists) such that

$$P^T S_W P = I , \quad (15)$$

the $p \times p$ identity matrix, and

$$P^T S_B P = \begin{bmatrix} v_1 & & & & & & \emptyset \\ & v_2 & & & & & \\ & & \ddots & & & & \\ & & & \ddots & & & \\ & & & & v_r & & \\ & & & & & 0 & \\ & & & & & & \ddots \\ \emptyset & & & & & & & 0 \end{bmatrix} \quad (16)$$

where

$$v_1 > v_2 > \dots > v_r > 0 \quad (17)$$

are the characteristic roots in (15). Note that S_B is almost surely positive semi-definite and S_W is almost surely positive definite. One should note that

$$\begin{aligned}
 |P^T(S_B - \lambda S_w)P| &= |P^T S_B P - \lambda P^T S_w P| \\
 &= |L - \lambda I| .
 \end{aligned}$$

From (13) and (14) it follows that

$$\begin{aligned}
 C_j S_B C_j^T &= \lambda_j C_j S_w C_j^T \\
 &= \lambda_j K .
 \end{aligned} \tag{18}$$

Also if $C_i \neq C_j$, then from (13)

$$C_i S_B C_j^T - \lambda_j C_i S_w C_j^T = 0,$$

and

$$C_j S_B C_i^T - \lambda_i C_j S_w C_i^T = 0 .$$

From this we subtract and note that $C_i S_w C_j^T = C_j S_w C_i^T$. We find that

$$(\lambda_j - \lambda_i) C_i S_w C_j^T = 0$$

which implies that

$$C_i S_w C_j^T = 0 \tag{19}$$

since $\lambda_j \neq \lambda_i$, which in turn implies

$$C_i S_B C_j^T = 0 . \tag{20}$$

Also

$$S_w(Z) = C S_w C^T \tag{21}$$

$$\begin{aligned}
 &= \begin{bmatrix} K & 0 & 0 \\ 0 & K & 0 \\ 0 & 0 & K \end{bmatrix} \\
 &= \text{Diag } \{K\}
 \end{aligned}$$

is an $r \times r$ diagonal matrix with the constant K as the common diagonal element. The statements (20), (21), (22) and (23) lead to the result that

$$\begin{aligned} S_p(Z) &= S_w(Z) + S_B(Z) \\ &= \text{Diag } \{K\} + \text{Diag } \{\lambda_j K\} \end{aligned}$$

or

$$|S(Z)| = K^r (1 + \lambda_1)(1 + \lambda_2) \cdots (1 + \lambda_r)$$

$$|S_w(Z)| = K^r$$

Hence

$$\frac{|S_w(Z)|}{|S_p(Z)|} = \frac{1}{(1+\lambda_1)(1+\lambda_2) \cdots (1+\lambda_r)}$$

Finally we note that (16) implies that

$$|S_w| = 1/|P|^2$$

and

$$\begin{aligned} |P^T S_w P + P^T S_B P| &= |I + L| \\ &= (1+\lambda_1)(1+\lambda_2) \cdots (1+\lambda_r) \end{aligned}$$

Consequently,

$$|S_w + S_B| = \frac{(1+\lambda_1)(1+\lambda_2) \cdots (1+\lambda_r)}{|P|^2}$$

which results in

$$\frac{|S_w|}{|S_p|} = \frac{1}{(1+\lambda_1)(1+\lambda_2) \cdots (1+\lambda_r)} = \frac{S_w(Z)}{S_p(Z)} \quad (22)$$

In summary, we selected C so that the between scatter for Z 's are maximum yet (24) holds. Note that we can force the dimension from p to 1 by selecting λ_1 the largest characteristic root.

8.4. Concluding Remarks.

It is true that so-called optimal techniques exist when specific assumptions are valid. Unfortunately in most applications these assumptions are not valid nor if valid hardly ever verified. Hence, "optimal" techniques must be "verified" as useful using Monte Carlo simulation or by using real data. The only valid evaluation should be based on estimates of probabilities of misclassification performed on data from cases in which true application is experienced; all other evaluations are suspect.

It is possible to develop a systems approach in which analog equipment and digital equipment are interphased with the remote sensing equipment so that computational times are realistic and such that the amount of information lost due to dimension reduction schemes is minimal. Essentially, this means that studies will need to be performed using hybrid analog and digital equipment. Also investigation of the characteristics measured must be performed compatible with how they are measured by the remote sensing equipment.

8.5. References.

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CHAPTER IX

Statistical Methods for Controlling Variability Due to Experimental Error in Space Stations

"You have only to take in what you please and leave out what you please; to select your own conditions of time and place; to multiply and divide at discretion; and you can pay the National Debt in half an hour. Calculation is nothing but cookery." Lord Brougham, 1849

9.1. Introduction.

In section 8 of Chapter II we discussed the problem of controlling variability by statistical modeling. It was noted that this was equivalent to what the statistician calls Covariance Analysis. In this chapter we present in detail the mathematical techniques necessary to accomplish this technique of controlling variability due to random errors in the environment.

Consider the analysis of covariance model

$$Y_i = \sum_{j=1}^m a_{ij} \theta_j + g_i(x_{i1}, x_{i2}, \dots, x_{ip}; \beta_1, \dots, \beta_p) + e_i \quad (1)$$
$$i = 1, 2, \dots, N,$$

where $\sum_{j=1}^m a_{ij} \theta_j$ is determined by a given experimental design and g_i is a general regression function, not necessarily a linear function of the unknown parameters $\beta_1, \beta_2, \dots, \beta_p$.

Generally, it is assumed that the form of g_i is the same for all i , however, this is not a necessary assumption in our analysis. To facilitate discussion, assume that (1) is expressed in matrix notation as

$$Y = A\theta + G(X; \beta) + E \quad (2)$$

where $Y = (y_1, y_2, \dots, y_n)^T$ is an $N \times 1$ vector of observable random variables; $A = (a_{ij})$ is an $N \times M$ experimental design matrix; $G = (g_1, g_2, \dots, g_n)^T$ is an $N \times 1$ vector of functions g_i and E is an $N \times 1$ vector of non observable uncorrelated random errors each with zero mean and variance σ^2 . The (non-random) parameter vectors $\theta = (\theta_1, \theta_2, \dots, \theta_M)^T$ and $\beta = (\beta_1, \dots, \beta_p)^T$ are to be estimated or tested using the observed data vector Y . The general practice is to test hypotheses concerning θ once an estimate of β is obtained. Also, G is generally assumed to be linear.

9.2. The Main Result.

The analysis of covariance with A an experimental design matrix as in (2) is equivalent to estimating the parameter θ in (2) along with the regression vector β in $G(X; \beta)$ subject to the constraint

$$T\theta = C \quad (3)$$

where T is a known $q \times m$ matrix of full row rank and C is a known $q \times 1$ vector of constants. In practice C is usually a vector of zeros and T is selected so that (3) induces constraints about various sums of treatment and/or block effects being zero.

All the solutions for θ in (3) can be written as

$$\theta_s = T^+C + (I - T^+T)W \quad (4)$$

where $(\cdot)^+$ denotes the Moore-Penrose pseudoinverse of the matrix $(\cdot)$ and W is an arbitrary $m \times 1$ vector.

Substituting (4) into (2) and rewriting one obtains

$$Y - G(X; \beta) - AT^+C = A(I - T^+T)W + E. \quad (5)$$

It is important to note that if β is known, then (5) is a linear model with unknown parameter vector W . However, the matrix $A(I - T^+T)$ is in general less than full rank, hence using a result by Lewis and Odell [1], the best estimator $\hat{W}_\beta$ for W is given by

$$\hat{W}_\beta = [(I - T^+T)A^T A(I - T^+T)]^+ (I - T^+T)A^T [Y - G(X; \beta) - AT^+C],$$

which reduces to

$$\hat{W}_\beta = [A(I - T^+T)]^+ [Y - G(X; \beta) - AT^+C] \quad (6)$$

for each β , $\{(z^T z)^+ z^T = z^+\}$ is an identity [2].

It follows from (4) that the admissible set from which θ_{LS} must be selected is defined by

$$\theta(\beta) = \{\hat{\theta} : \hat{\theta} = T^+C + (I - T^+T)\hat{W}_\beta\}, \quad (7)$$

where on substituting (6) into (7) we have

$$\hat{\theta}_{\beta} = T^+C + (I - T^+T)[A(I - T^+T)]^+[Y - G(X;\beta) - AT^+C] \quad (8)$$

9.3. Computing Techniques.

In general, obtaining a least squares estimate for β , and thus for θ from (8) is a difficult computational task. Several approaches can be found in the literature [8] and we will list here three that arise naturally.

Direct search techniques [8] have been used with success. One simply searches judiciously for the value of $\beta = \beta_{LS}$ which minimizes.

$$Q = [Y - A\theta(\beta) - G(X;\beta)]^T [Y - A\theta(\beta) - G(X;\beta)]$$

by approximating β_{LS} with an a priori value, say β_k , and then iteratively computing β_{k+1} so that Q approaches a minimum.

Hartley [3] suggests a method in which he solves for β_{LS} by solving the p non-linear equations in p unknowns $\partial Q / \partial \beta = 0$ which are necessary conditions for Q to be minimal. By selecting β_k a priori and letting $G^*(X;\beta) = A\theta(\beta_k) + G(X;\beta)$ be approximately

$$G^*(X;\beta) \cong G^*(X;\beta_k) + \left[\frac{\partial G^*}{\partial \beta} \right]_{\beta=\beta_k} (\beta_{k+1} - \beta_k)$$

$$\frac{\partial G}{\partial \beta}(X;\beta) \cong \left[\frac{\partial G}{\partial \beta} \right]_{\beta=\beta_k}$$

one can solve for β_{k+1} , and on iterating the sequence $\{\beta_k\}$ converges in many cases to β_{LS} .

Walling [5] and Nelson [6] have developed techniques which take advantage of the linearity in the non-linear function $G^*(X;\beta)$. Instead of approximating $G^*(X;\beta)$ in a truncated Taylor's expansion, they approximate $G(X;\beta)$ by

$$G(X;\beta) = G(X;\beta_k) + \frac{\partial G}{\partial \beta} \bigg|_{\beta=\beta_k} (\beta_{k+1} - \beta_k)$$

$$\frac{\partial G(X;\beta)}{\partial \beta} \bigg|_{\beta=\beta_k} = \frac{\partial G}{\partial \beta} \bigg|_{\beta=\beta_k}$$

$$\theta(\beta) = \theta(\beta_k).$$

Then an a priori estimate β_k leads to β_{k+1} which when iterated gives a sequence $\{\beta_k\}$ which converges in many cases more rapidly to β_{LS} .

Comparison of Hartley's technique, Walling's technique, and Nelson's technique can be found in [6] and [7].

9.4. References.

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CHAPTER X

Concerning Preflight Review and Evaluation of Candidate Experiments

"The word statistics has two somewhat different meanings. In familiar usage, to be sure, statistics does mean simply numerical information, usually arranged in tables or graphs. It is in this sense that we say The World Almanac contains a great deal of useful statistics. But more broadly, and more technically, statistics is the name for that science and art which deals with uncertain inference--which uses numbers to find out something about nature and experience." Warren Weaver, Scientific American, January 1952.

10.1 Introductory Remarks.

The apparent complexity of the subjects discussed in this monograph and the relevancy of the subjects to the space station objectives indicate that it may be desirable to make preflight review and evaluation of each candidate experiment for purpose of optimization with respect to design and data analysis techniques. It is important that one does not confuse the two distinct functions (a) selecting an experiment as a significant research activity, and (b) determining an optimal design and data analysis techniques to assure compatibility and efficiency when the total set of experimental designs are also considered. The first function is performed prior to the second, and by persons

whose knowledge is state-of-the-art in the field from which the questions yielding the experiment originate. The second function can and, in most instances, should be developed, or at least monitored, by a group of specialists reporting directly to a key decision-making manager in the NASA organization. This decision-maker should have the responsibility for judging whether or not the experiment is "flyable" with respect to optimal design and data analysis criteria. In no way should he make any decision concerning the significance of the research. Clearly such a decision maker would require staff for providing technical assistance for not only determining whether or not an experiment is flyable, but for providing a consulting service to principle investigators to assure that their proposed experiments will be judged flyable.

It is the aim of this chapter to present recommendations concerning how one might bring about the adoption optimal design techniques compatible with the aims of the space station by the principle investigators.

10.2. Basis for Our Recommendations.

There exist several factors that may affect, through introducing bias or increasing variances, the results of an experiment. Some of these are effects introduced by different techniques of launching and transporting the experiments. These stresses and any secondary factor related to these stresses which might affect the assumptions made by the principal investigator prior to the flight must be recorded. Once the magnitude of all such factors are recorded and known, the final data can in many

cases be adjusted for them.

The space station environment in which the laboratory is contained must be known to a degree that, if deemed necessary, concomitant variables can be defined and measured. This can assure the validity of the experimental data. Clearly, the laboratory environment within the space station must also be known to a degree that additional concomitant variables can be defined.

Impulse response functions of measuring equipment must be made known and be invariant with time, to assure valid data. Knowledge of how on-board personnel might affect the observations must be known in order that valid experimental designs can be selected.

The selection of designs affect the amount and manner one computes the desired estimates; hence coordination with the available computing facilities is required. The experimental design selected can affect scheduling of other experimental activities, hence coordination with scheduling personnel is necessary.

10.3. Staffing for Pre-flight Evaluation.

In the preceding section we have listed some of the factors which could affect the usefulness of the data taken on a space station. The types of evaluation personnel are clearly indicated. The list should include launch, space transportation, space station and laboratory environmental engineers to give expertise and analysis on aspects of the environment in which the experiment is to be transported and performed. Several instrumentation engineers as well as computer scientists would provide essential

expertise which could affect the evaluation of the data. Statistical expertise needs to be made available to assure the selection of the optimal design, and in some cases one may later wish to adjust data for unexpected bias arising from the environment during the performance of the experiment.

During evaluation of each candidate experiment, the principal investigator or his representative as well as a knowledgeable representative of NASA should monitor and jointly approve the final design to be flown.

A second responsibility (perhaps the most important one) for such a group would be a service consultant responsibility for existing or potential principal investigators so that their experiments can be made flyable with minimal effort. The purpose remains to fly in a optimal way, as many significant research activities as possible without degrading the final data.

10.4. Concluding Remarks.

Due to our limited knowledge of the management structure of NASA Space Station project it is difficult for us to recommend with confidence specific lines of command for the evaluation group discussed in the early portions of this chapter.