KULLBACK-LEIBLER INFORMATION FUNCTION AND THE SEQUENTIAL.

SELECTION OF EXPERIMENTS TO DISCRIMINATE AMONG

SEVERAL LINEAR MODELS

by

Steven Michael Sidik

NASA-CR-136615) KULLBACK-LEIBLER ² N74-15304 INFOPMATION FUNCTION AND THE SEQUENTIAL SELECTION OF EXPERIMENTS TO DISCRIMINATE AMCNG SEVERAL LINEAR MODELS *(Case Western Unclas* Unclas Reserve Univ.) 135 p HC \$8.75 CSCL 12A 63/19 27572 Reserve Univ.) $\frac{135}{135}$ **p HC** \$8.75 CSCL 12A

Submitted in partial fulfillment of the requirements for the

Degree of Doctor of Philosophy

Thesis Advisor: Shelemyahu Zacks ,

Department of Mathematics and Statistics

CASE WESTERN RESERVE UNIVERSITY

June 7, **1972**

KULLBACK-LEIBLER INFORMATION FUNCTION AND THE SEQUENTIAL SELECTION OF EXPERIMENTS TO DISCRIMINATE AMONG SEVERAL LINEAR MODELS

Abstract

by

Steven Michael Sidik

Assume that a finite sqt of potential linear models relating several controlled variables to an observed variable is postulated and that exactly one.of these models is the true model. The problem is to sequentially design most informative experiments so that the correct model can be determined with as little experimentation as possible. We assume that the error variance of the process is known. In addition, we assume the statistician possesses prior information which can be expressed as the prior probability that each of the proposed models is indeed the correct model and prior multivariate normal distributions on the parameters of each of the postulated model equations. After each stage of sampling, the prior distributions and. the observed data values are used to compute posterior probabilities of the models being the true one and posterior distributions on the parameters of the models. Then sampling is terminated if either a prespecified number of observations has been taken or if any of the posterior probabilities of the models exceeds a prespecified minimum stopping probability. Upon termination of sampling, the model with the largest posterior

ii

probability is chosen to be the correct model. If sampling is not to be terminated, the next experiment chosen is that one in the set of allowable values of the controlled variables which maximizes the expected Kullback-Leibler information function based upon the current posterior probabilities and distributions.

An analytical study of this procedure is too complex and difficult to adequately achieve. Hence a number of Monte-Carlo simulatioh experiments were performed to obtain information about the performance of this adaptive design procedure. Two basic types of Monte-Carlo experiments were performed. In the first, one of the models was chosen to be used to generate the random observations using known fixed values for the parameters. Then a large number of observations were taken using the Kullback-Leibler information functions as a criterion to choose the sequence of experiments. It was found the posterior probability of the chosen model relatively rapidly approaches the value of 1.0 and then fluctuates near 1.0. The posterior mean of the parameters of the correct model also rapidly approaches the known fixed values used to generate the observations. In the second type of experiment, one of the models was chosen to be used to generate the random observations. Then for various combinations of the maximum number of observations, stopping probability, prior .distributions of the parameters, and error variance of the process, a large number of repetitions of the sequential design procedure were executed. Then a probability of correct selection and average sample number were calculated based unon the

iii

number of times the procedure chose the correct model and the number of observations taken until termination. In general, it was found that as long as the prior mean of the correct model is not too distant from the true value with respect to the means of the other models the probability of correct selection is respectably high.

~- -- r~~-- - - - *lr-r* .--- ,--------1-7--m- , r I - - ^r- - ~rlN

ACKNOWLEDGMENTS

The author wishes to express his gratitude for the time and encouragement given him by Prof. **S.** Zacks.

Special thanks are due the National Aeronautics and Space Administration Lewis Research Center for their generous support of the author's research in terms of salary, tuition, typing, and computer time.

v

TABLE OF CONTENTS

vi,

LIST OF FIGURES

vii '

Figure Page 2014 Page

 $\frac{1}{4}$ $\overline{1}$

O

 $v:$ ii

CHAPTER 1 - INTRODUCTION AND LITERATURE SURVEY

The general linear model has become one of the most useful statistical tools available to the modern scientific experimenter. There have been many books and papers written about techniques for choosing the appropriate or "best" linear model to fit to a set of data already collected. In general, these have been methods of hypothesis testing to determine which of a set of specified terms in a model equation may be dropped from the model. Much work has also been done with regard to the problem of designing best or optimal experiments to estimate the parameters of specified model equations.-

In this dissertation we study a sequential adaptive experimental design procedure for a related problem. Assume that a finite set of potential linear models relating certain controlled variables to an observed variable is postulated and that exactly one of these models is correct. The problem is to sequentially design most informative experiments so that the correct model equation can be determined with as little experimentation as possible. We also assume that the error variance of the process is known. In addition, we assume that the statistician possesses prior information which can be expressed by the prior probability that each of the proposed models is indeed the correct model and prior multivariate normal distributions on the parameters of the various models. We then de-

rive an adaptive procedure for designing the successive experiments using the Kullback-Leibler information function to maximize the anticipated information for discriminating among the models. That is, after each stage of sampling, the prior distributions and the observed values are used to compute posterior probabilities of the postulated models being correct and posterior distributions on the parameters of the models. Then if sampling is not to be terminated, the next experiment chosen is that which maximizes the expected Kullback-Leibler information based on the current posterior probabilities and distributions. Sampling₂is terminated whenever either a prespecified number of observations is finally taken or whenever any of the posterior probabilities of the models exceeds a prespecified values Upon termination of sampling, the model with the largest posterior probability is chosen to be the correct model.

An analytical study of this procedure is too complex and difficult to adequately achieve. Hence a number of Monte-Carlo simulation experiments were performed to obtain information about the performance of this adaptive design procedure. Two basic types of Monte-Carlo experiments were performed. In the first, one of the models was chosen to be used to generate the random observations using known fixed values for the parameters. Then a large number of observations were taken using the Kullback-Leibler information as a criterion to choose the sequence of experiments. It was found the posterior probability of the chosen model relatively rapidly approaches the value of 1.0 and then fluctuates near **1.0.** The

o

 \mathcal{L}

posterior mean 'of the parameters of the correct model also rapidly approach the known fixed values used to generate the observations. In the second type of experiment, one of the models was chosen to be used to generate the random observations. 'Then for various'combinations of the maximum number of observations, stopping probability, prior distributions of the parameters, and error variance of the process, a large number of repetitions of the sequential design procedure were executed. Then a probability of correct selection and average sample number were calculated based upon the number of times the procedure chose the correct model and the number of observations taken until termination. In general, it was found that as long as the prior mean of the correct model is not too distant from the true value with respect to the means of the other models the probability of correct selection is :respectably high.

We now briefly indicate the general organization of the dissertation. In Chapter 2 the notation used is described and the structure of the linear models is derived. Chapter 3 then develops the distribution theory which will be basic to the remainder of the dissertation. In particular, the posterior probabilities of the models, the posterior distributions of the parameters, and the Markovian nature of the sampling process are developed. Some large sample results are then derived for the situation where the sequence of experiments is specified in advance of experimenting. These results do not thus formally apply to the adaptive design procedure.

We find, however, that they do appear to be true to a surprising extent and provide some help in explaining and interpreting the Monte-Carlo results.

In Chapter 4, the Kullback-Leibler information concept is introduced and the derivation of the anticipated information as a function of the current posterior probabilities of the models and the current posterior distributions of the parameters is presented. This anticipated information is the criterion function used to define the most informative experiment. Its use is discussed both from the point of view of its relation to the expected decrease in entropy and the point of view that it results in a very simple function measuring the amount by which the expected value of the observed variable under each model is separated.

The sequential experiment selection, stopping, and model selection rules are presented in Chapter 5.

In Chapter 6, the Monte-Carlo simulation experiments are described and the results presented and discussed. Chapter 7 presents an example of application. Several appendixes are also included. Of most .importance is appendix A which presents the computer program used to perform the simulation experiments.

We now turn to a discussion of works by earlier authors who have considered similar problems.

Lindley (1956) was one of.the first to consider the general idea of applying information concepts to the problems of statistical inference. He modified the concept of entropy and developed a num-

ber of interesting general results on the amount of information in an experiment about the parameters of the distribution of a random variable.

Stone (1959) was one of the first to consider information concepts as applied to designing and comparing regression experiments. He used a Bayesian framework, but the problem he considers is that of parameter estimation rather than that of model selection.

Another early and more relevant paper is that of Chernoff (1959) who applied the Kullback-Leibler information function to the sequential design of experiments when the cost of experimenting is small. His results are valid for the case of two terminal decisions and a finite number of experiments and states of nature. These results have been generalized by Albert (1961) to an infinite number of states of nature and by Bessler (1960) to an infinite number of experiments and k terminal actions. Kiefer and Sacks (1963) have also provided some extensions.

The statement of Chernoff's problem and the problem considered here are not identical and we proceed by analogizing his results to the problem at hand. In the context of the current problem, he would proceed by first assuming that at each stage of sampling the model with the largest posterior probability is the correct one. Then if A denotes the space of allowable experiments, define the Kullback-Leibler (K-L) information about model j in experiment acA when model i is true as

.5

$$
I(a,i,j) = \int \ln \left[\frac{f_i(y|a)}{f_j(y|a)}\right] f_i(y|a) dy
$$

where $f_4(y|a)$ denotes the probability density of y under model i when experiment acA is performed. Let \hat{i} denote the model with the highest current probability of being the correct one. Then in analogy to Chernoff, we define the optimal experiment as $a(i)$ where a(i) is defined by that experiment satisfying

$$
I[a(\hat{i}), \hat{i}, \hat{j}] = \sup_{a \in A} \inf_{k \neq \hat{i}} I(a, \hat{i}, k)
$$

That is, Chernoff represents the problem as a game between nature and the statistician where the statistician maximizes over A and nature minimizes over the alternative models assuming \hat{i} is the correct model. Chernoff also specifically derives a stopping rule which we do not discuss here.

Hunter and Reiner (1965).considered a sequential design procedure for discriminating between two model equations. Their procedure chooses the experimental conditions which, based upon maximum likelihood estimates of the parameters from the data already collected, separate the expected values of the observed variable under the two models by as much as possible.

Box and Hill (1967) discussed the use of the Kullback-Leibler information function, deriving it from corsiderations involving the entropy function. They consider the use of the K-L information function to sequentially discriminate among several mechanistic (nonlinear) model equations. Besides the fact that they consider

nonlinear models, their approach is different in the sense that although they do assume prior probabilities on the proposed models, and compute posterior probabilities from the observations, they assume the parameters of the model equations are known constants.

Meeter, Pirie, and Blot (1970) have done a number of computer simulations comparing the methods of Chernoff and of Box and Hill. They found that the Box-Hill procedure performed quite well on the examples in comparison to Chernoff's procedure. It is interesting to note that Chernoff seems to be the only one of these authors who defined an explicit rule for terminating sampling. Although Chernoff's procedure is known to be asymptotically optimal, it is also known to require very large sample sizes.

CHAPTER 2

STRUCTURE OF THE LINEAR MODELS

In the theory of the general linear statistical model, we are concerned with problems involving model equations relating k controlled variables $(z_j; i=1, \ldots, k)$ to an observed variable (y). The form of the model equation is required to be

$$
y = \sum_{i=1}^{I} \beta_i h_i(z_1, \ldots, z_k) + \varepsilon
$$

The known functions h_i are arbitrary except that they may not contain any unknown parameters. The equation is linear in the unknown parameters $\beta_{\mathbf{i}}$ and ϵ is assumed to be a random variable with $\mathsf{ex}\text{-}$ pectation zero and known finite variance. We may write $x_i = h_i (z_1, \ldots, z_k)$ and henceforth express the models in terms of the **x_i** variables. If n observations are made upon **y** we let $\mathbf{x}_{\mathbf{j}}$ denote the value of $\mathbf{x}_{\mathbf{i}}$ at which the \mathbf{j}^{th} observation is made. Thus for the n observations the model may conveniently be written as

$$
\vec{y} = M\vec{\beta} + \vec{\epsilon} \tag{2-1}
$$

where

$$
\ddot{y}' = (y_1, y_2, \ldots, y_n)
$$

and the ε ₁ are uncorrelated. The matrix M is called the design matrix for the experiment consisting of the *n* observations. The problem of experimental design is that of choosing the x_{j1} values in some "optimal" manner.

In certain situations in practice the experimenter can postulate several possible models involving different functions of the z. variables which correspond to several possible mechanistic or **¹** empirically based theories. These may lead to the various models containing different sets of x_i . There may be some overlapping of the x_i among the models or there may be none.

There are then two problems requiring solution. The first is that of choosing experiment designs which will enable the experimenter to decide which of the potential models is the correct one. Then, having chosen the model, the parameters must be estimated. The second problem has many solutions using a variety of standard

.9

techniques. This dissertation concerns itself primarily with a method of designing experiments to provide information for choosing the appropriate model equation.

We assume there are L different competing model equations. These models may be combined into one large possible model equation and then the L hypothetical models are equivalent to there being L hypotheses restricting certain sets of parameters of the large model to be a priori zero. For example, we might have two controlled variables x_1 and x_2 . And suppose the model equations postulated are:

> $H_1: y = \beta_1^{(1)}x_1 + \epsilon$ $H_2: y = \beta_2^{(2)}x_2 + \varepsilon$ (3) _y $+$ _R (3) $\frac{13}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

where $\beta_i^{(j)}$ denotes the coefficient of controlled variable i in model equation j. The distinction must be made because although $\beta_i^{(j)}$ and $\beta_i^{(k)}$ are coefficients of variable i, their distributions need not be the same. This notation is clumsy, however, and if we implicitly accept the fact that the distributions of the $\beta_i^{(j)}$ depend upon the model, we may more simply rewrite the models as

> H_1 **:** $y = \beta_1 x_1 + \epsilon$ $H_2: y = \beta_2 x_2 + \varepsilon$ **H₃:** $y = β_1 x_1 + β_2 x_2 + ε$

We say that models 1 and 2 are nested within model 3. This is

equivalent to writing one model as $y = \beta_1 x_1 + \beta_2 x_2 + \varepsilon = \overrightarrow{x} \cdot \overrightarrow{B} + \varepsilon$ and hypothesizing

$$
H_1: \beta_2 = 0
$$

$$
H_2: \beta_1 = 0
$$

$$
H_3: \beta_1 \neq 0, \beta_2 \neq 0
$$

In this sense it is seen that the terms model and hypothesis are interchangeable and will be used interchangeably in the remainder of this dissertation. The notation we adopt is that H_{ρ} claims

$$
\vec{y} = M_{\ell} \vec{a}_{\ell} + \vec{\epsilon}
$$

where $\vec{\alpha}_g$ is the appropriate $k_g \times 1$ vector of β 's from \vec{B} which appear in model ℓ and M_0 is the appropriate matrix of x' s.

We now precisely state the three basic distributional assumptions about.the parameters and random variables of the models:

(1) The vector $\vec{\epsilon}$ follows a multivariate normal distribution with mean $\vec{0}$ and precision matrix T. T is assumed known. (The precision matrix is the inverse of the covariance matrix of the distribution.) Since T must be positive definite symmetric, we need only consider the special case where $T = T I$ since linear transformation of the y reduces all other cases to this one. Note that we assume τ is known. Thus $\vec{\epsilon} \sim N(\vec{0}, \tau \mathbb{I})$.

(2) For each $k = 1, \ldots, L$ the prior distribution of $\vec{\hat{\alpha}}_0$ is $\vec{\alpha}_{\ell}$ - $N(\vec{\mu}_{\ell,0}, \psi_{\ell,0})$

where $\vec{\mu}_{g,0}$ and $\Psi_{g,0}$ are known.

(3) The prior probability that the ℓ^{th} model is the correct

model equation is assumed specified and denoted by $\theta_{k,0}$. We re-L quire $\sum_{\alpha=0}^{\infty}$ $\theta_{\alpha=0}$ = 1.0. In order to satisfy this requirement in a **k=l** completely precise manner, we must make the models mutually exclusive. As described so far, this need not be true. However, this is a simple problem to get around for the following reason. Each of the H_R specifies that $\vec{\alpha}_{\ell}$ is an element of a k_R dimensional subset of K-space which we denote as E_{ℓ} . For any pair H_i and H_k we have either (1) $E_j \gg E_k$, (2) $E_k \gg E_j$, or (3) neither space contains the other and $E_j \bigcap E_k$ has measure zero with respect to H_j and H_k . For case 1 define θ_j as $\theta_j = Pr{\vec{\alpha}_j \in E_j - E_k}$. But Ek has zero measure with respect.to H. and hence the distribution **k-J.** function of \vec{a} restricted to \vec{E} - \vec{E} is identical to the distribution function of \vec{u}_1 over all of E_1 . Thus for any practical purpose, the fact that $E_i \bigcirc F_k$ does not affect any probability computations. Similar arguments apply to cases two and three.

We now describe the space A of allowable experiments in more detail. If the number of elements of \vec{X} is K, then a choice of experiment acA is composed of the number J of observations to take and J vectors from some subset of Euclidean K-space. J vectors specify the values of the controlled variables x_{ij} . At the jth experiment or jth stage of experimenting the particular choice from A is denoted a..

CHAPTER 3

PREREQUISITE DISTRIBUTION THEORY

In the remainder of this dissertation, much use'will be made of the distribution of the observed variable, the posterior probabilities of the models, and the posterior distributions of the parameters of the model equations. The first part of this chapter develops these distributions. The second part derives the fact that the sampling procedure is Markovian in nature and provides a notation for describing the state of the process. The third section of this chapter discusses some results on the limiting behavior of the posterior distributions when the sequence of experiments is chosen in advance. The strong restrictions that must be made to accomplish these large sample results and the fact that they do not describe the adaptive process might lead one to believe that they are not worthwhile pursuing.

We find in chapter 6, however, that there is a close analogy between these results and the behavior of the adaptive procedure, and that these results help explain and interpret the Monte Carlo simulation results.

3.1 Posterior and Marginal Distributions

Let $f_g(\vec{y}_{i+1}|a_{i+1},\vec{a}_g)$ denote the density function of the vector \vec{y}_{i+1} under H_g when the parameter values are given by $\vec{\alpha}_0$ at stage $j + 1$ of sampling. Let the probability density function

of \vec{a}_{ℓ} after j stages of sampling be denoted $\vec{\epsilon}_{\ell,j}(\vec{\alpha})$. This is a preposterior density since it serves as the posterior density of $\vec{\alpha}_{\rho}$ after j stages of sampling and the prior density of $\vec{\alpha}_{\rho}$ before the $j + 1^{st}$ stage of sampling occurs.

Lemma 3.1: After j stages of sampling, $\vec{\alpha}_{\ell}$ follows a multivariate normal distribution with mean vector $\vec{v}_{2,i}$ and precision matrix

 $\frac{\Psi}{\sqrt{3}}$. That is, after j stages of sampling,

$$
\vec{\alpha}_{\ell} \sim N(\vec{\mu}_{\ell,j}, \Psi_{\ell,j})
$$

where

$$
\Psi_{\ell,j} = \Psi_{\ell,j-1} + M_{\ell,j}^{\dagger} \mathbf{m}_{\ell,j} \n= \Psi_{\ell,0} + \sum_{i=1}^{j} M_{\ell,i}^{\dagger} \mathbf{m}_{\ell,i}
$$
\n(3-1)

and

$$
\vec{u}_{\ell,j} = \Psi_{\ell,j}^{-1} (M_{\ell,j}^{\dagger} T_{\mathcal{Y}_{j}}^{\dagger} + \Psi_{\ell,j-1} \vec{u}_{\ell,j-1})
$$
\n
$$
= \Psi_{\ell,j}^{-1} \left[\sum_{i=1}^{j} M_{\ell,i}^{\dagger} T_{\mathcal{Y}_{i}}^{\dagger} + \Psi_{\ell,0} \vec{u}_{\ell,0} \right]
$$
\n(3-2)

and where $M_{\ell,i}$ denotes the design matrix specified by a_i under H_{ℓ} .

Proof: By Bayes theorem, if \vec{y}_j is the observed vector at stage j ϵ $\vec{\tau}$ \vec{r} $\vec{\tau}$ $\vec{\tau}$ $\vec{\tau}$

$$
\xi_{\ell,j}(\vec{\alpha}) = \frac{r_{\ell}(y_j | a_j, \alpha) \xi_{\ell,j-1}(\alpha)}{\int f_{\ell}(y_j | a_j, \vec{\alpha}^*) \xi_{\ell,j-1}(\vec{\alpha}^*) d\vec{\alpha}^*}
$$

 f_{α} **f**_{α} $\left(y_{j} | a_{j}(\vec{\alpha})\right)$ *(3-3)* (3-3)

The symbol α means "proportional to" and is used in the context of DeGroots (1970, p. 160) usage. Thus

$$
\xi_{\ell,j}(\vec{\alpha}) \propto e^{-Q/2}
$$

where (dropping subscripts)

 $Q = (M\vec{\alpha} - \vec{\vec{v}})^T (M\vec{\alpha} - \vec{\vec{v}}) + (\vec{\alpha} - \vec{u})^T \Psi(\vec{\alpha} - \vec{u})$

Since T and Y are positive definite symmetric we can write $Q = \vec{\alpha}^{\prime} (\Psi + M^{\prime}TM) \vec{\alpha} - 2(\vec{\mu}^{\prime} \Psi + \vec{y}^{\prime}TM) \vec{\alpha} + (terms not involving \vec{\alpha})$

 $= \left[\vec{\alpha} - (\Psi + M^{\dagger}TM)^{-1}(M^{\dagger}T\vec{v} + \Psi \vec{u})\right]^{\dagger} \cdot (\Psi + M^{\dagger}TM)$

 \vec{a} - (Y + M[']TM)⁻¹(M[']Ty⁺ + $\vec{v_1}$)] + (terms not involving \vec{a}) The terms not involving $\overrightarrow{\alpha}$ may be factored out through use of the proportionality device, leaving the kernel of a multivariate normal distribution with parameters as specified by the lemma. Thus \hat{a}_{θ} is distributed as claimed.

Q.E.D.

Owen (1970) has derived a result similar to Lemma 3.1 in the case of a two factor experiment where the factors are treatments and blocks.

We now turn to determining the distribution of \vec{y}_{j+1} . This is done in two stages. First we do not know which of the models is in fact the correct one. Then for any given model, we do not know the value of $\vec{\alpha}_{g}$. Let $f_{\ell}(\vec{y}_{j+1} | a_{j+1}, \vec{\alpha})$ denote the distribution of \vec{y}_{j+1} under H_{ℓ} when experiment a_{j+1} and is performed and $\vec{\alpha}_{\ell}$ is specified. Since we do not know $\stackrel{\rightarrow}{\alpha}_{\ell}$ we must average this distribution over all $\vec{\alpha}_{g}$. Let $f_{g}(\vec{y}_{i+1} | a_{i+1})$ denote the mixture of the densities $f_{\ell}(\vec{y}_{j+1} | a_{j+1}, \vec{k})$ with respect to the marginal posterior of \vec{a}_0 .

Lemma 3.2 The conditional distribution of
$$
\bar{y}
$$
, given H_{ℓ} and a_{1}
is a multivariate normal distribution with mean: vector $\vec{s}_{\ell,1}$ and
precision matrix $R_{\ell,1}$ where

$$
R_{\ell,j} = T \left[I - M_{\ell,j} (M_{\ell,j}^{\dagger} M_{\ell,j} + \Psi_{\ell,j-1})^{-1} M_{\ell,j}^{\dagger} T \right]
$$
(3-4)

$$
\vec{s}_{\ell,j} = R_{\ell,j}^{-1} T M_{\ell,j} (M_{\ell,j}^{\dagger} M_{\ell,j} + \Psi_{\ell,j-1})^{-1} \Psi_{\ell,j-1} \vec{\mu}_{\ell,j-1}
$$
(3-5)

Proof: The required mixture distribution is gi.ven by

$$
f_{\ell}(\vec{y}_j | a_j) = \int f_{\ell}(\vec{y}_j | a_j, \vec{\omega}) \epsilon_{j,j-1}(\vec{\alpha}) d\vec{\alpha}
$$

$$
= \int e^{-Q/2} d\vec{\alpha}
$$

where

$$
Q = (\vec{y}_j - M_{\ell, j}\vec{\alpha})' T(\vec{y}_j - M_{\ell, j}\vec{\alpha}) + (\vec{\alpha} - \vec{\mu}_{\ell, j-1})' \psi_{\ell, j-1}(\vec{\alpha} - \vec{\mu}_{\ell, j-1})
$$

\n
$$
= \vec{\alpha} \cdot (M'TM + \Psi)\vec{\alpha} - 2\vec{\alpha} \cdot (M'TM + \Psi)(M'TM + \Psi)^{-1}(M'T\vec{y} + \Psi\vec{\mu})
$$

\n
$$
+ \vec{y}'T\vec{y} + \vec{\mu}'\Psi\vec{\mu}
$$

\n
$$
= \vec{\alpha} \cdot (M'TM + \Psi)\vec{\alpha} - 2\vec{\alpha} \cdot (M'TM + \Psi)(M'TM + \Psi)^{-1}(M'T\vec{y} + \Psi\vec{\mu})
$$

\n
$$
+ (M'T\vec{y} + \Psi\vec{\mu})' (M'TM + \Psi)^{-1}(M'Ty + \Psi\vec{\mu})
$$

\n
$$
- (M'T\vec{y} + \Psi\vec{\mu})' (M'TM + \Psi)^{-1}(M'T\vec{y} + \Psi\vec{\mu}) + \vec{y}'T\vec{y} + \vec{\mu}'\Psi\vec{\mu}
$$

The first three terms yield the quadratic form

^f., -, . - % . **:,.** ; - : , **:C** i -Z .

$$
Q_{1} = [\vec{\alpha} - (M'TM + \Psi)^{-1}(M'T\vec{y} + \Psi\vec{\mu})]^{T} \cdot (M'TM + \Psi)
$$

$$
\cdot [\vec{\alpha} - (M'TM + \Psi)^{-1}(M'T\vec{y} + \Psi\vec{\mu})]
$$

 $C_{\rm rad}$ -Q₁/2 The remainder of Q does not involve α and e is the kernel of a multivariate normal distribution \approx 0 that when e^{-Q}1^{/2}

• . t , ,.-. **r'** " ,

。
→ Profile → Line → Line → Line → Line → Line → Line → Line → Line → Line → Line → Line → Line → Line → Line → L

is integrated over **a** we remain with

$$
f_{\ell,j-1}(\vec{y}_j|_{a_j}) = e^{-Q_2/2}
$$

where

$$
Q_2 = -(M^{\dagger}T\vec{y} + \vec{\Psi_{\mu}})^{\dagger} (M^{\dagger}TM + \vec{\Psi})^{-1} (M^{\dagger}T\vec{y} + \vec{\Psi_{\mu}}) + \vec{y}^{\dagger}T\vec{y} + \vec{\mu}^{\dagger}\vec{\Psi_{\mu}} \\
= y^{\dagger} [T - TM(M^{\dagger}TM + \vec{\Psi})^{-1}M^{\dagger}T]\vec{y} - 2\vec{y}TM(M^{\dagger}TM + \vec{\Psi})^{-1}\vec{\Psi_{\mu}}\n\end{aligned}
$$

+ (terms not involving \vec{y})

 $=$ $(\vec{y} - \vec{s})^T R(\vec{y} - \vec{s}) + ($ terms not involving \vec{y}) The terms not involving **y'** may be factored out via the proportionality device leaving

$$
f_{\hat{y}}(\vec{y}_j|a_j) \propto e^{- (\vec{y}-\vec{s}_{\hat{y}},j)^T R_{\hat{y},j} (\vec{y}-\vec{s}_{\hat{y},j}) / 2}
$$

This is the kernel of a multivariate normal distribution with mean vector $\overrightarrow{s}_{k,j}$ and precision matrix $R_{l,j}$ as claimed. Thus the density of y_j given H_g and a_j is given by

$$
f_{\ell}(\vec{y}_j | a_j) = (2\pi)^{-J/2} |R_{\ell,j}|^{1/2} \exp\left\{ -\frac{1}{2} (\vec{y}_j - \vec{s}_{\ell,j})^2 R_{\ell,j} (\vec{y}_j - \vec{s}_{\ell,j}) \right\}
$$
(3-6)

Q.E.D.

Since the true model is unknown we now compute the mixture of the distributions of Lemma 3.2 with respect to the probabilities $^{\theta}$ $_{i,j}$ as

$$
f(y_j | a_j) = \sum_{\ell=1}^{L} \theta_{\ell, j-1} f_{\ell}(\vec{y}_j | a_j)
$$
 (3-7)

To compute the posterior probability of each model being cor-

rect after the observation y_{j+1} is obtained, we apply Bayes theorem directly to get

$$
\theta_{\ell,j+1} = \frac{f_{\ell}(\vec{y}_{j+1}|a_{j+1})\theta_{\ell,j}}{\sum_{k=1}^{L} f_k(\vec{y}_{j+1}|a_{j+1})\theta_{k,j}}
$$
(3-8)

3.2 Markovian Nature of Sampling.Process

Consider a sequence of random variables W_1, W_2, \ldots which take on values in a sample space or state space **Q.** We let **C** denote the σ -field of subsets of Ω for which probabilities are defined. The sequence of random variables **W.** form a Markov Process **1** if for every $\mathbf{F} \in \mathcal{F}$ and for all w_1, \ldots, w_n in Ω , and all for n, $n = 1, 2, 3, ...$ we have

$$
\Pr\{W_{n+1}\in F|W_1 = w_1, \dots, W_n = w_n\}
$$

=
$$
\Pr\{W_{n+1}\in F|W_n = w_n\}
$$

=
$$
\int_F g_{n+1}(w|w_n) dw
$$
 (3-9)

where $g_{n+1}(w|w_n)$ denotes the generalized conditional probability density function of W_{n+1} . If the conditional probabilities in equation (3-9), equivalently the g_n , do not depend upon n the transition process is called stationary. The state space in this paper can be described by a vector containing: (1) the probabilities θ_{θ} , (2) the elements of the vectors describing the current posterior means under the various H_{ρ} , and (3) the lower triangular part of the current posterior precision matrices under the various H_{ℓ} . Thus

$$
\Omega = \left\{ \theta_1, \ldots, \theta_L, \mu_1^{(1)}, \mu_1^{(2)}, \ldots, \mu_2^{(1)}, \mu_2^{(2)}, \ldots, \mu_L^{(1)}, \ldots, \mu_L^{(1)}, \ldots, \mu_L^{(K_L)}, \mu_1^{(1)}, \ldots, \mu_L^{(K_L, K_L)} \right\}
$$
\n
$$
\Psi_{\mathbf{i}} \text{ positive definite for } \mathbf{i} = 1, \ldots, L \right\} \qquad (3-10)
$$

For any given state we Ω the transition to the next state depends only upon the state w and the experiment a A that is chosen.

This is true because a detemines the posterior precision matrices regardless of the value of y, and the posterior means $\vec{\mu}_g(y)$ and probabilities $\vec{\theta}(y)$ are determined by equations (3-1) and (3-8) which again depend only upon w, y, and a. Thus the transition process on the states is Markovian. The process is stationary, also, since for given initial g_i the successive gn **4o yot** depend upon n. The transition function may be described as follows. Define a mapping $T: \Omega \times Y \to \Omega$ and let $Q(\Omega \times Y)$ denote the Borel sets on QxY and **Q(Q)** denote the Borel sets on **Q.** Let $T^{-1}(F)$ denote the inverse image of F where $FeQ(\Omega)$ and $T^{-1}(F) \epsilon Q(\Omega \times Y)$. Then if w' denotes the state of the system after sampling,

$$
\Pr(\mathbf{w}' \in \mathbf{F} | \mathbf{w}, \mathbf{a}) = \int \sum_{\mathbf{i} = 1}^{L} \theta_{\mathbf{i}} f_{\mathbf{i}}(\mathbf{y} | \mathbf{a}, \mathbf{w}) \mathrm{d}\mathbf{y}
$$

$$
(\mathbf{w}, \mathbf{y}) \in \mathsf{T}^{-1}(\mathsf{F})
$$

$$
\frac{3 \cdot 3 \text{ Large Sample and Limiting Results}}{3 \cdot 3 \text{ large Sample and Limiting Results}}
$$

Even though this paper is concerned primarily with small sample procedures, it is interesting and informative to know the large sample or limiting behavior of the parameters and tne sampling $\mathcal{Q} \mathcal{T}$

process. Unfortunately, for the adaptive procedure this is an extremely difficult subject to study. Thus we do not study the adaptive procedure here but instead consider the experiment selection procedure under the restrictions listed below in the hope that these results will illuminate the adaptive procedure in some sense.

(1) Assume A is finite with N(A) elements, and represented as

$$
A = {a^{(1)}, a^{(2)}, \ldots, a^{[N(A)]}}
$$

(2) An infinite sequence $\{a_{i}\}\$ is specified such that as the number of experiments approaches infinity, the proportion of times that $a^{(i)}$ is performed approaches p_i with $0 \leq p_i \leq 1$ and $\Sigma p_i = 1.0$. The experiments a_i are chosen independently of each other.

(3) Assume H_{1*} is the true model and that $\overrightarrow{\mu}^*$ is the true value of the parameters in the model.

(4) Assume that only one observation is taken in each experiment $a^{(i)}$.

(5) Assume that the structure of A is such that all matrices under consideration are nonsingular.

It should be noted that the mos't restrictive of the above assumptions is the second. For in a true sequential decision procedure, the actual experiment chosen is a random variable depending upon the previous observations obtained. Since we are in fact studying a problem other than the one of most importance the remainder of the chapter will not be developed in rigorous decall and the results

obtained cannot be rigorously applied to the sequential procedure. It will be seen in Chapter 6, however, that fairly extensive Monte Carlo simulations seem to bear.up the general conclusions reached here.

Let k(j) denote the superscript of the experiment performed at stage j. Thus if $a_{10} = a^{(5)}$, then k(10) = 5. Also let $n(i,j)$ denote the number of times $a^{(i)}$ is performed in the sequence of experiments up to and including the j^{th} stage. Let $M_{\ell, i}$ denote the design matrix under H_v when $a⁽¹⁾$ is chosen. Lemma 3.3 Under the above assumptions the posterior precision matrices and mean vectors converge with probability one as $j \rightarrow \infty$ to:

$$
\frac{1}{j\tau} \Psi_{\ell,j} \to \Psi_{\ell} = \sum_{i=1}^{N(A)} p_i^M_{\ell,i}^M_{\ell,i}
$$
\n
$$
\vec{\mu}_{\ell,j} \to (\Psi_{\ell})^{-1} \left(\sum_{i=1}^{N(A)} p_i^M_{\ell,i}^M_{\ell,i}^M_{i*} \right)_{\mu}
$$

Proof: To prove the first limit, recall from equation (3-1) that

$$
\Psi_{\ell,j} = \Psi_{\ell,0} + \sum_{i=1}^{j} \tau M_{\ell,k(i)}^{N_{\ell,k(i)}}
$$

 \mathbf{r} Thus

$$
\frac{1}{j\tau} \Psi_{\ell,j} = \frac{1}{j\tau} \Psi_{\ell,0} + \sum_{i=1}^{j} \frac{1}{j} M_{\ell,k(i)}^{'} M_{\ell,k(i)}
$$

$$
= \frac{1}{j\tau} \Psi_{\ell,0} + \sum_{i=1}^{N(A)} \frac{n(i,j)}{j} M_{\ell,i}^{'} M_{\ell,i}
$$

As $j \rightarrow \infty$, the first term goes to zero and the factors $\frac{n(i,j)}{j}$ + p_j by assumption.

To prove the second part note that $y_j = M_i *_{i,k(j)} \vec{l}^* + \varepsilon_j$. where $E_i \sim N(0,\tau)$. Using the second form of equation (3-2) we get

$$
\vec{\mu}_{\ell,j} = (\Psi_{\ell,j})^{-1} \left\{ \sum_{i=1}^{j} M_{\ell,k(1)}^{i} y_i + \Psi_{\ell,0} \vec{\mu}_{\ell,0} \right\}
$$
 (3-11)

Then substituting the expression for y_j into equation (3-11) gives.

$$
\vec{\mu}_{\ell,j} = (\Psi_{\ell,j})^{-1} \left\{ \sum_{i=1}^{N(A)} n(i,j) \pi_{\ell,i}^{N} M_{i^*, i} \vec{\mu}^* \right\}
$$

$$
+ \tau \sum_{i=1}^{N(A)} M_{\ell,i}^{\dagger} \left(\sum_{m=1}^{j} \epsilon_{m} \delta_{k(m),i} \right) + \Psi_{\ell,0} \widetilde{\mu}_{\ell,0}^{\dagger}
$$

where $\delta_{i,i}$ denotes the Kronecker delta function. Thus

$$
\vec{\mu}_{\ell,j} = \left(\frac{1}{j\tau} \Psi_{\ell,j}\right)^{-1} \left\{\sum_{i=1}^{N(A)} \frac{n(i,j)}{j} M_{\ell,j}^{\dagger} M_{i}^{*}, \vec{\mu}^{*} \right\} + \sum_{i=1}^{N(A)} M_{\ell,j}^{\dagger} M_{\ell}^{\dagger}, \vec{\mu}_{\ell} \left(\frac{1}{j} \sum_{m=1}^{j} \epsilon_{m} \delta_{k(m),i}\right) + \frac{1}{j\tau} \Psi_{\ell,0} \vec{\mu}_{\ell,0} \right\}
$$

From assumption 2 we know that $n(i,j) + \infty$ as $j + \infty$ and since the

form a sequence of independent and identically distributed random variables, the strong law of large numbers may be applied to show for $i = 1, \ldots, L$

$$
\Pr\left\{\lim_{n\left(i,j\right)\to\infty}\frac{1}{n(i,j)}\sum_{m=1}^{j}\epsilon_{m}\delta_{k(m),i}=0\right\}=1.0
$$

Since $\frac{1}{j\tau} \rightarrow 0$ as $j \rightarrow \infty$ we then have

$$
\vec{\mu}_{\ell,j} = \Psi_{\ell}^{-1} \left(\sum_{j=1}^{N(A)} \frac{n(i,j)}{j} M_{\ell,j}^{'} M_{i}^*, j \right)^{**}
$$

This sequence will not have a limit unless $\lim_{i \to \infty} \frac{n(i, j)}{j} = p_i$ exists. If such a limit exists, the lemma follows immediately.

Q.E.D.

Lemma 3.4 Under the assumptions stated, $R_{\ell, i} \rightarrow \tau$ irrespective of {**a**, *j* and

$$
s_{\ell,j} = M_{\ell,k(j)} (\Psi_{\ell})^{-1} \left(\sum_{i=1}^{N(A)} p_i M_{\ell,i}^{\dagger} M_i^{\dagger} x_{,i} \right)_{\mu}^{+k}
$$

for large enough i.

Proof: From equation (3-4) and the assumptions

$$
R_{\ell,j} = \tau \left\{ 1.0 - \tau M_{\ell,k(j)} [\Psi_{\ell,j} + \tau M_{\ell,k(j)}^{\dagger} M_{\ell,k(j)}]^{-1} M_{\ell,k(j)}^{\dagger} \right\}
$$

As $j \rightarrow \infty$, $[\Psi_{\ell,j} + \tau M_{\ell,k(j)}^N A_{\ell,k(j)}] \rightarrow (\infty)$ and hence its inverse \rightarrow (0). But then $R_{\ell, j} \rightarrow \tau$ as claimed.

From equation (3-5)

$$
s_{\ell,j} = (R_{\ell,j})^{-1} \Biggl\{ \tau M_{\ell,k(j)} [M_{\ell,k(j)}^{\dagger} M_{\ell,k(j)}^{\dagger}]^T + \Psi_{\ell,j}^{\dagger} \Biggr\}^{-1} \Psi_{\ell,j} \Biggr\}
$$

For large enough j, $[M^{\dagger}_{g}{}_{k(j)}M_{g}{}_{k(j)}\tau + \Psi_{g}{}_{j}]^{-1}\Psi_{g}{}_{j}$ is asymptotically like the identity matrix, I, so that

$$
s_{\ell, j} \approx \frac{1}{\tau} \left\{ \tau M_{\ell, k(j)} \vec{v}_{\ell, j} \right\}
$$

$$
\approx M_{\ell, k(j)} (\Psi_{\ell})^{-1} \left[\sum_{i=1}^{N(A)} P_i M_{\ell, i}^{\dagger} M_i^{\dagger} \Psi_{i, j} \right] \vec{v}
$$

We note that if $\& = i^*$, then from the definition of Ψ_{ℓ} , we have $s_{i^*,j} = M_i^*, k(j)$ ¹ as expected.

Q.E,D.

Lemma 3.5 If H_{i^*} is the true hypothesis and the model of H_{i^*} is nested within the model of H_{ϱ} , then under the above assumptions and assuming the parameter vectors are rearranged appropriately

$$
\Pr\left\{\vec{\mu}_{\ell,j} \to \begin{pmatrix} \vec{\mu}^* \\ \vec{0} \end{pmatrix} \right\} = 1.0
$$

Proof: From Lemma 3.3 we have

$$
\vec{\mu}_{\ell,j} \rightarrow \Psi_{\ell}^{-1} \left(\sum_{i=1}^{N(A)} p_i M_{\ell,i}^{\dagger} M_{i}^{\dagger} \right) \vec{\mu}^*
$$

If the parameters are rearranged appropriately then $M_{\ell,i}$ may be written

$$
M_{\ell, i} = (M_{i^*, i}, M_{\ell, i}),
$$

where $\tilde{M}_{\ell, i}$ denotes the design matrix corresponding to the independent variables in H_{ℓ} but not in H_{i^*} . Thus

> $\frac{1}{M}$, $\frac{1}{M}$ $\frac{M}{2}$, $i^M i^*, i$ $\frac{M}{2}$, $i^M j$

and

$$
\Psi_{\ell} = \begin{bmatrix} \Psi_1 * & \cdot & \Psi_1 * \\ \cdot & \cdot & \Psi_1 * \\ \cdot & \cdot & \tilde{\Psi}_{\ell} \end{bmatrix}
$$

where

$$
\Psi_{i*} = \sum_{i=1}^{N(A)} p_{i}{}^{N^{i}_{i*}}, {}^{N}_{i*}, i
$$

$$
\Psi_{i*}, \ell = \sum_{i=1}^{N(A)} p_{i}{}^{N^{i}_{i*}}, i^{N} \ell, i
$$

and

$$
\tilde{\Psi}_{\ell} = \sum_{i=1}^{N(A)} p_i \tilde{M}_{\ell,i} \tilde{M}_{\ell,i}
$$

Thus from a well known identity (e.g., Graybill (1969), p. 165) **,1 1** *,)* **J** i **i** i Ψ_{g}^{-1} = -1 -

Also

$$
\sum_{i=1}^{N(A)} p_i^{M_i}, i^{M_i *}, i = \sum_{i=1}^{N(A)} \begin{pmatrix} p_i^{M_i *}, i^{M_i *}, i \\ p_i^{M_i}, i^{M_i *}, i \end{pmatrix} = \begin{pmatrix} \Psi_i * \\ \Psi_i * \\ \Psi_i * \end{pmatrix}
$$

Thus

$$
\Psi_{\ell}^{-1} \begin{pmatrix} \Psi_{\mathbf{1}^{*}} & \Psi_{\mathbf{1}^{*}}^{-1} \Psi_{\mathbf{1}^{*}} \Psi_{\mathbf{1}^{*}} \Psi_{\mathbf{1}^{*}} & \Psi_{\mathbf{1}^{*}}^{-1} \Psi_{\mathbf{1}^{*}} \Psi_{\mathbf{1}^{*}} & \Psi_{\mathbf{1}^{*}}^{-1} \Psi_{\mathbf{1}^{*}} \
$$

upon application of Lemma 3.6 which follows. Thus

$$
Q.E.D.
$$

Lemma 3.6 (Problem 2.9 of Rao (1965)) If A and D are matrices possessing inverses, then

$$
(A + BDB')^{-1} = A^{-1} - A^{-1}B(B'A^{-1}B + D^{-1})^{-1}B'A^{-1}
$$

Proof: By direct multiplication we only need show

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

\n
$$
= I - B(B'A^{-1}B + D^{-1})^{-1}B'A^{-1} + BDB'A^{-1}
$$

\n
$$
- BDB'A^{-1}B(B'A^{-1}B + D^{-1})^{-1}B'A^{-1}
$$

\n
$$
= I - B[-(B'A^{-1}B + D^{-1})^{-1} + D - DB'A^{-1}B(B'A^{-1}B + D^{-1})^{-1}]B'A^{-1}
$$

\n
$$
= I - B[D - [I + DB'A^{-1}B][B'A^{-1}B + D^{-1}]^{-1}]B'A^{-1}
$$

\n
$$
= I - B[D - D[D^{-1} + B'A^{-1}B][D^{-1} + B'A^{-1}B]^{-1}]B'A^{-1}
$$

\n
$$
= I - B[D - D[B'A^{-1}]
$$

 $= I$ Q,E,D

To apply this result to Lemma 3.5 simply set ϵ

$$
B = \Psi_{i*},
$$

$$
D = -\tilde{\Psi}_{o}^{-1}
$$

 $A = \Psi$ *

We now turn to consideration of the limiting behavior of $\theta_{k,j}$. Computer simulations for both nested and non-nested cases indicate that for any k where H_{i*} is not nested in H_k , $\theta_{k,i}$ + 0.0 fairly rapidly and steadily. If H_{i^*} is nested in H_k then it seems that $\theta_{k, j} \rightarrow 0.0$. The rate is initially rapid but then becomes very slow and it behaves in a very erratic manner. These points are discussed in some detail in Chapter 6.

It should be reiterated and these discussions have assumed the sequence $\{a_{i}\}\$ to be specified and fixed for the sequence of experiments. In a sequential decision problem the sequence $\{a_i\}$ is not fixed, but k(j) is in fact a random variable whose distribution depends upon $k(i)$ for $i < j$ and the y_i for $i < j$.

CHAPTER 4

ENTROPY FUNCTIONS AND THE KULLBACK-LEIBLER INFORMATION FUNCTION

When comparing a number of experiments to determine which is the optimal one to perform, one must define optimal. In this dissertation, that experiment which yields the largest expected K-L information is defined as the optimal experiment. In particular, let I(w,a) denote the expected K-L information as a function of the experiment a and the current state w of the process. This function will be specified explicitly later. In this chapter, we first describe how the K-L information arises from attempting to reduce the entropy of the probabilities of the models. We then develop an expression for I(w,a) and finally discuss the operational meaning of the use of I(w,a) from a heuristic point of view.

4.1 Development of the K-L Information Function

The problem under consideration here is that we must choose one of a set of postulated model equations. For each model we have the posterior probability $\theta_{\ell,i}$ that it is the correct one. We would like to choose experiments which cause the posterior probability of the correct model to increase most rapidly. An indirect method of accomplishing this is to choose experiments which most rapidly decrease the entropy of the set of probabilities $\theta_{\ell,j}$. The entropy is defined as

28

O
$$
\mathcal{E}(\mathbf{w}) = -\sum_{\ell=1}^{L} \theta_{\ell, j} \ln(\theta_{\ell, j})
$$

It can be verified that the entropy attains a maximum when all the probabilities are equal and attains a minimum when any one of the probabilities is one and the rest are zero.

Box and Hill (1967) proposed the use of the expected decrease between the entropy at the current stage of sampling and the anticipated entropy at the next stage of sampling as the criterion for selection of experiments. They found, however, that the entropy function is quite intractable analytically and applied a well-known inequality to show the expected K-L information function provides an upper bound on the reduction of entropy. Let $\theta_i(\vec{y}|\mathbf{w},\mathbf{a})$ denote the posterior probability of model i if the value \overrightarrow{y} is observed when the state was w . Let $w(\vec{y})$ denote the state of the process after observing the value \overrightarrow{y} when it was in state w. Then the anticipated entropy is given by

$$
E\left\langle \mathcal{E}[w(\vec{y}),a]\right\rangle = -\int \left\langle \sum_{\ell=1}^{L}\theta_{\ell}(\vec{y}|w,a)\ln[\theta_{\ell}(\vec{y}|w,a)]\right\rangle f(\vec{y}|w,a)d\vec{y}
$$

Thus if the current state of the sampling process is $w \in \Omega$, and the experiment atA is performed, the expected decrease in entropy, $R(w, a)$, is then defined as

o

$$
R(w, a) = \mathcal{E}(w) - E\{\mathcal{E}[w(\vec{y}), a]\}
$$

\n
$$
= -\sum_{i=1}^{L} \theta_i \ln(\theta_i) + \int \left\{\sum_{i=1}^{L} \theta_i(\vec{y}|w, a) \ln[\theta_i(\vec{y}|w, a)]\right\}.
$$

\n
$$
= -\sum_{i=1}^{L} \theta_i \ln(\theta_i) + \int \sum_{\ell=1}^{L} \theta_\ell \mathbf{f}_\ell(\vec{y}|w, a) \ln\left[\frac{\theta_\ell \mathbf{f}_\ell(\vec{y}|w, a)}{\sum_{k=1}^{L} \theta_k \mathbf{f}_k(\vec{y}|w, a)}\right] d\vec{y}
$$

\n
$$
\leq \int \sum_{\ell=1}^{L} \theta_\ell \left\{\sum_{i=1}^{L} \theta_i \mathbf{f}_\ell(\vec{y}|w, a) \ln\left[\frac{\mathbf{f}_\ell(\vec{y}|w, a)}{\sum_{k=1}^{L} \theta_k \mathbf{f}_k(\vec{y}|w, a)}\right] d\vec{y} \right\}
$$
(4-1)

by application of the following inequality (Kullback (1969), p. 15)

$$
\sum_{i=1}^{L} \theta_i f_{\ell}(\vec{y}|w, a) \ln \left[\frac{f_{\ell}(\vec{y}|w, a)}{f_i(\vec{y}|w, a)} \right] \geq f_{\ell}(\vec{y}|w, a) \ln \left[\frac{f_{\ell}(\vec{y}|w, a)}{\sum_{k=1}^{L} \theta_k f_k(\vec{y}|w, a)} \right]
$$

Let

$$
I(w,a,i,j) = \int f_1(\vec{y}|w,a) \ln \left[\frac{f_1(\vec{y}|w,a)}{f_1(\vec{y}|w,a)} \right] d\vec{y}
$$
 (4-2)

We note $I(w,a,i,j)$ is defined as the expected amount of information in the observations from experiment a for discriminating against H_j in favor of H_i. Let $\mathcal{Y}(w,a)$ denote the matrix whose **i,j** element is I(w,a,i,j). Then the inequality (4-1) may be written as

$$
R(w,a) \leq \vec{\theta} \cdot \mathcal{Q}(w,a) \vec{\theta} = I(w,a) \qquad (4-3)
$$

Meeter et al. (1970) proposed the following heuristic argument in favor of using $I(w,a)$. If one knew that H_1 were indeed the correct hypothesis and wished to maximize the information about H_k for $k \neq i$, then it would be natural to maximize

$$
\sum_{k\neq i}\theta_{k}I(w,a,i,k)
$$

But since H_i is assumed correct only with probability θ_i , it is equally natural to multiply the foregoing expression by θ_i and sum over i. But in doing this, one does end up with $I(w,a)$.

4.2 Evaluation of K-L Information Function

From equation $(3-6)$ we have $(if \vec{y}$ is $J\times1)$ that the density of \overrightarrow{y} under H_{ℓ} is given by

$$
f_{\ell}(\vec{y}|a) = (2\pi)^{-J/2} |R_{\ell}|^{1/2} e^{-1/2(\vec{y}-\vec{s}_{\ell})'R_{\ell}(\vec{y}-\vec{s}_{\ell})}
$$

Hence

$$
\frac{f_{m}(\vec{y}|a)}{f_{n}(\vec{y}|a)} = |R_{m}|^{1/2} |R_{n}|^{-1/2} \frac{e^{-1/2(\vec{y}-\vec{s}_{m})^{2}} R_{m}(\vec{y}-\vec{s}_{m})}{e^{-1/2(\vec{y}-\vec{s}_{n})^{2}} R_{n}(\vec{y}-\vec{s}_{n})}
$$

Moreover

$$
\ln\left[\frac{f_m(\vec{y}|a)}{f_n(\vec{y}|a)}\right] = \frac{1}{2} (\ln|R_m| - \ln|R_n|)
$$

$$
-\frac{1}{2}(\vec{y} - \vec{s}_m)^T R_m(\vec{y} - \vec{s}_m)
$$

$$
+\frac{1}{2} (\vec{y} - \vec{s}_n)^T R_n(\vec{y} - \vec{s}_n)
$$

(4-4)

$$
I(w, a, m, n) = \int \ln \left[\frac{f_m(\vec{y}|a)}{f_n(\vec{y}|a)} \right] f_m(\vec{y}|a) d\vec{y}
$$

$$
= E \left\{ \ln \left[\frac{f_m(\vec{y}|a)}{f_n(\vec{y}|a)} \right] \right\}
$$
(4-5)

where the expectation is taken under the assumption $\vec{y} \sim N(\vec{s}_m, R_m)$. Note that $I(w,a,m,n) = 0.0$ for $m = 1, \ldots, L$. Lemma 4.1 If $\vec{y} \sim N(\vec{c}, R)$ and R is positive definite, and A. is symmetric, then

$$
E\{\vec{y}^{\dagger}A\vec{y}\} = tr(AR^{-1}) + \vec{c}^{\dagger}A\vec{c}
$$

Proof. By theorem 10.3.2 of Graybill (1969)

$$
E\{ (\dot{y} - \dot{c}) A(\dot{y} - \dot{c}) \}
$$
\n
$$
= \frac{|R|^{1/2}}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} (\vec{y} - \vec{c}) A(\vec{y} - \vec{c}) e^{-1/2(\vec{y} - \vec{c}) R(\vec{y} - \vec{c})} d\vec{y}
$$
\n
$$
= tr (AR^{-1})
$$

But

$$
E\{\vec{y} - \vec{c}\} A\vec{y} - \vec{c}\} = E\{\vec{y}^T A\vec{y}\} - \vec{c} A\vec{c}
$$

The lemma follows immediately.

Q.E.D.

Applying the lemma to the expectations of the quadratic forms in equation (4-4) we see:

1.
$$
\vec{y} \sim N(\vec{s}_m, R_m) \Rightarrow E\{(\vec{y} - \vec{s}_m)^T R_m(\vec{y} - \vec{s}_m)\} = tr(R_m R_m^{-1}) = J
$$

\n2. $\vec{y} - \vec{s}_n \sim N(\vec{s}_m - \vec{s}_n, R_m) \Rightarrow E\{(\vec{y} - \vec{s}_n)^T R_n(\vec{y} - \vec{s}_n)\}$
\n $= tr(R_n R_m^{-1}) + (\vec{s}_m - \vec{s}_n)^T R_n(\vec{s}_m - \vec{s}_n)$

Thus

$$
I(w,a,m,n) = \frac{1}{2} \left\{ ln \left| R_m \right| - ln \left| R_n \right| \right\} - \frac{1}{2} J + \frac{1}{2} tr (R_n R_m^{-1})
$$

+ $\frac{1}{2} (\vec{s}_m - \vec{s}_n)' R_n (\vec{s}_m - \vec{s}_n)$ (4-6)

$$
I(w,a,m,n) + I(w,a,n,m) = -J + \frac{1}{2} \left[tr (R_n R_m^{-1}) + tr (R_m R_n^{-1}) \right]
$$

+ $\frac{1}{2} \left[(\vec{s}_m - \vec{s}_n)' R_n (\vec{s}_m - \vec{s}_n) + (\vec{s}_n - \vec{s}_m)' R_m (\vec{s}_n - \vec{s}_n) \right]$
= $-J + \frac{1}{2} \left[tr (R_n R_n^{-1}) + tr (R_m R_n^{-1}) \right]$
+ $\frac{1}{2} \left[\vec{s}_m - \vec{s}_n)' (R_m + R_n) (\vec{s}_m - \vec{s}_n) \right]$

$$
+ \frac{1}{2} \left[\vec{s}_m - \vec{s}_n)' (R_m + R_n) (\vec{s}_m - \vec{s}_n) \right]
$$

$$
I(w,a) = \sum_{n=1}^{L} \sum_{n=1}^{n-1} \theta_n \theta_n [I(w,a,m,n) + I(w,a,n,m)]
$$

$$
n=2 m=1
$$
\n
$$
= \sum_{n=2}^{L} \sum_{m=1}^{n-1} \theta_{n} \theta_{n} \left\{ -J + \frac{1}{2} \left[\text{tr} \left(R_{n} R_{m}^{-1} \right) + \text{tr} \left(R_{m} R_{n}^{-1} \right) \right] + \frac{1}{2} \left[\left(\vec{s}_{m} - \vec{s}_{n} \right)' \left(R_{m} + R_{n} \right) \left(\vec{s}_{m} - \vec{s}_{n} \right) \right] \right\}
$$
\n
$$
= -J \sum_{n=2}^{L} \sum_{m=1}^{n-1} \theta_{m} \theta_{n} + \frac{1}{2} \sum_{n=1}^{L} \theta_{n} \text{tr} \left[\sum_{m \neq n} \theta_{m} R_{m} \right] R_{n}^{-1} + \frac{1}{2} \sum_{n=2}^{L} \sum_{m=1}^{n-1} \theta_{n} \theta_{m} \left(\vec{s}_{m} - \vec{s}_{n} \right)' \left(R_{m} + R_{n} \right) \left(\vec{s}_{m} - \vec{s}_{n} \right) \qquad (4-8)
$$

The last form of this equation appears to be the most convenient for computing purposes.

4.3 Intuitive Analysis

Looking at the computing form of equation (4-8) it can be L n seen that there are three terms. The first term is $-J \sum_{i=1}^{\infty} \Theta_{i}^{-1} \Theta_{i}$ $n=2$ $n=1$ $n=1$ The value of this term does not depend upon a and hence has no effect upon the choice of a. From this consideration we note that computing the value of this term would not be beneficial if only one more stage of experimentation is available,

The third term of the sum is a weighted sum of the quadratic -o forms

 $(\vec{s}_m - \vec{s}_n)'$ (R_m + R_n) $(\vec{s}_m - \vec{s}_n)$

Thus this term is in effect a separating function in the sense that these quadratic forms will be maximized when the pairs of expected values of \overrightarrow{y} under the various hypotheses are as far apart as possible in comparison to the precisions of \overrightarrow{y} . If the precisions R_m and R_n are large then \overrightarrow{s}_{m} and \overrightarrow{s}_{n} do not need to be far apart to provide much information whereas if these precisions are small then the expected values \overrightarrow{s}_{m} and \overrightarrow{s}_{n} must be further apart to provide the same information. The weighting factors are the products $\theta_n \theta_m$. Thus when θ_n and θ_m are both small, $\theta_n \theta_m$ is very small and the information due to the separation of \overrightarrow{s}_n and \overrightarrow{s}_m is discounted somewhat. If θ_n and θ_m are large then the information due to separation of \overrightarrow{s} and \overrightarrow{s} is given more importance. Thus this third term causes experiments to'be chosen which separate the expected values of \vec{y} under the respective hypotheses which are still in serious contention for being chosen.

It is interesting to note that some authors (Hunt and Reiner (1965), e.g.) have proposed criteria for selection of experiments involving only distances between expected values. In a later paper, Box and Hill (1967) proposed that the distances as such are not important, but the distances weighted by some function of the variability about the expected values are important. It is seen here that the expected K-L information function does just that.

The second term in equation (4-8) is

o

 $\frac{1}{2}\sum_{n=1}^{L}\theta_n$ tr $\left(\sum_{m\neq n} \theta_m R_m\right)R_n^{-1}$. This can be thought of as a weighted sum of ratios of precisions. If only one y value is to be observed, this component becomes

$$
\frac{1}{2} \sum_{n=1}^{L} \theta_n \frac{\sum_{m \neq n} \theta_m R_m}{R_n}
$$
 (4-9)

It would be interesting to see when this term is maximized. Upon taking partial derivatives of equation (4-9), setting to zero, and simplifying, one arrives at the following set of simultaneous nonlinear equations.

$$
\sum_{k=1}^{L} \theta_i \left(\frac{R_k^2 - R_i^2}{R_i} \right) = 0 \qquad i = 1, \ldots, L
$$

It can be immediately seen that one solution to this system is $R_1 = R_2 = \ldots = R_L$. This solution implies that the experiments should tend to give the same precision for the expected value of \tilde{y}

under each hypothesis. This term is not considered any further here.

In summary, it can be seen that the expected K-L information function in this case is basically a rather simple separating function. One would be hard pressed to construct a much simpler separating function which has more intuitive appeal. If multivariate observations are permitted, then it might be possible to delete the second term of equation (4-8) to save a good deal of computing..

C

 $\mathbf{f} = \mathbf{f} \cdot \mathbf{f} + \mathbf$

CHAPTER 5

THE SEQUENTIAL DECISION PROCEDURE

Three components are required for a sequential adaptive decision procedure; (1) a rule which determines if sampling should be terminated or continued, (2) a rule which specifies the experiment to be performed given the current state of the system, and (3) a -.rule which selects the model equation which will be claimed to be true when sampling is terminated. The first part of this chapter discusses the experiment selection rule and the second section presents the stopping and model selection rules.

5.1 Experiment Selection Rule

The procedure adopted for this dissertation is^t the so-called myopic procedure. This rule simply chooses as the next experiment that one which maximizes the anticipated K-L information for the next stage only.

We assume that an upper limit, J_{MAX} , to the number of observations is specified. This number may be infinite. An allocation of the observations to the stages of sampling is described by a $J_{MAX} \times 1$ vector \overrightarrow{n} , where n_i gives the number of observations at stage i. The question arises as to how the observations should be allocated. That is, should all J_{MAX} be taken at once, strictly one-at-a-time, or in different sized groups. As the first step in answering this, let A₁ denote the set of experiments in A which

specify that j observations should be taken. For any given state weΩ, let $a_i^*(w)$ denote the element of A_i such that

$$
I[w, a_j^*(w)] = \sup_{a_j \in A_j} I(w, a_j)
$$

Lemma 5.1 For any we Ω , and i, j such that i > γ we have $I[w, a_{i}^{*}(w)] \ge I[w, a_{i}^{*}(w)].$

Proof: We introduce the following notation. Let $y_k(a_i^*)$, **k** = 1, \cdot .,i denote the random variables observed under $a_i^*(w)$ and $y_k(a_j^*)$, $k = 1, \ldots, j$ denote the random variables observed under a_i^* . Define another experiment a_i^* a_i by choosing the first j observations according to a_j^* and the remaining $i - j$ observations according to the last $i - j$ of a_{i}^{*} . This leads to the random variables

$$
\tilde{y}_{k}(\tilde{a}_{i}) = \begin{cases} y_{k}(a_{j}^{*}) & k = 1, \dots, j \\ y_{k}(a_{i}^{*}) & k = j + 1, \dots, i \end{cases}
$$

Because $I(w,a,m,n)$ is positive definite and is additive for independent observations

$$
\mathbb{I}(\mathbf{w}, \tilde{\mathbf{a}}_{i}, \mathbf{m}, \mathbf{n}) \geq \mathbb{I}(\mathbf{w}, \mathbf{a}_{j}^{\ast}, \mathbf{m}, \mathbf{n})
$$

Thus

$$
I(w, \tilde{a}_{i}) = \vec{\theta}^{t} [I(w, \tilde{a}_{i}, m, n)] \vec{\theta}
$$

\n
$$
\geq \vec{\theta}^{t} [I(w, a_{j}^{*}, m, n)] \vec{\theta} = I(w, a_{j}^{*})
$$

But by definition $I(w, a_i^*) \ge I(w, a_i)$ and hence

$$
\mathrm{I}(w,a_{i}^{*}) \geq \mathrm{I}(w,a_{j}^{*})
$$

Q.E.D.

The lemma simply proves that an experiment with more observations will be expected to provide more information than one with' fewer observations. In determining an allocation one'should also consider the cost of experimenting. In particular, if we assume that each observation has'a constant cost associated with it, then it is reasonable to choose the experiment which maximizes

$$
\frac{1}{j} I(w, a_j) \qquad j = 1, \ldots, J_{MAX}
$$

k-1 Thus prior to stage k let $m = \sum_{i=1}^{n} n_i$ and assume $m < J_{MAX}$. The $i=1$ optimal experiment is the element a^*eA which for the current state w_{k-1} yields

$$
j = 1, \ldots, J_{MAX} - m \begin{pmatrix} \text{MAX} & \frac{1}{j} & I(w_{k-1}, a) \\ a \in A_j & J \end{pmatrix}
$$

If sampling has not been terminated by the rules developed in Chapter 5.2, then we stop when $\sum n_i = J_{MAX}$ and select the model according to the rules in Chapter 5.2.

5.2 Stopping and Model Selection Rules

We now discuss the problems of determining which of the postulated models is the true one and determining when the results of the experiments are sufficiently informative to stop sampling and make the choice.

Box and Hill (1967) suggested that for their procedure, experimenting be terminated whenever one model is clearly superior to

39.

the others. This is obviously a reasonable statement but it is in need of formal definition before it can be used as a stopping and selection rule. We propose general stopping and selection rules and a modified version which might be used in certain instances involving nested models.

(1) Stopping rule: Let θ_m be some specified value $1/L < \theta_m \leq 1.0$. Let J_{MAX} denote the maximum number of observations permitted, Then terminate sampling whenever either $S_{i,j,L}$ $\{ \theta_j \} \ge \theta_m$ or J_{MAX} observations have been taken, whichever occurs first.

(2) Model selection rule: Upon termination choose the correct model to be H_i^* where $\theta_{i^*} = \frac{MAX}{i=1, L} \{ \theta_i \}$

We now present a modified stopping and selection procedure for use with nested models which may be of some value when θ_m is very near 1.0 and/or when J_{MAX} is relatively large. The reason for presenting a modified procedure arises from the large sample results of Chapter 3 and the Monte-Carlo results of Chapter 6. First, if H_{i^*} denotes the unknown true model, it is not known whether $\theta_{i^*,j} \rightarrow 1.0$ or not. From the Monte-Carlo results it seems that the typical behavior of θ_{i^*} for nested models is to fairly rapidly increase to something near 1.0 and then fluctuate, possibly slowly approaching 1.0. Thus, if θ_m is very near 1.0 it may be that extremely large samples would be required. Thus we would like to reduce the average sample size without seriously detracting from the probability of choosing the correct model.

، 40°

To introduce the modified procedure consider the following example:

$$
H_1
$$
: $y = \beta_1 x_1 + \epsilon$
 H_2 : $y = \beta_1 x_1 + \beta_2 x_2 + \epsilon$

If **H1** is actually the true.model, then the posterior distribution of (β_1, β_2) under H_2 should approach a point distribution with **.(2= 0** and **PM** equal to the unknown value of the parameter. How-2 **1** ever, $\theta_{1,j}$ may not approach 1.0 . Assume some small positive constant γ is specified. Then after each stage of sampling, test if

$$
d = \left[\mu_1^{(1)} - \mu_1^{(2)} \right]^2 + \left[\mu_2^{(2)} \right]^2 \le \gamma
$$

If $d \leq \gamma$ then drop model 2 from contention and replace θ_1 by θ_1 + θ_2 . Then apply the previously described stopping and selection rules. In this simple example, the dropping of model 2 would automatically cause sampling to be terminated. This would of course not necessarily be true in more general situations.

To generalize the procedure some additional notation and concepts must be introduced. We use the symbol \supseteq to denote inclusion. Thus $H_i \supset H_i$ means that the model of H_i is nested within the model of H_i . The set of models $\{H_i\}$ is a partially ordered set under the partial ordering relation \mathfrak{D} . In the theory of partially ordered sets a chain is defined to be a partially ordered set such that for any two elements $(H_1$ and H_2 say) of the set either $H_1 \supset H_2$ or $H_2 \supset H_1$. For the purposes of this dissertation we define a string of elements from the partially ordered set as a sub-

set of elements such that the subset forms a chain. A maximal string is constructed from any string by adding all the elements of ${H_i}$ to the string which can be added without causing the enlarged set to lose the property of being a chain.

To formulate the modified stopping and selection procedure we first construct all of the maximal strings that can be constructed from the set $\{H_i\}$ and order the elements of the strings using the relation $\mathbf{D}.$

For example, suppose $L = 5$ and the five models are as specified below:

The maximal strings are easily verified as being

$(H_1 \subset H_3 \subset H_5)$ $(H_1 \subset H_4 \subset H_5)$ $(H_2 \subset H_4 \subset H_5)$

In each of these strings the maximal element is H_5 .

The modified procedure consists of computing for the first

maximal string the squared distance of the posterior mean vector of the maximal element from the posterior mean vector of the submaximal or next largest submodel of the string. If this quantity is less than some prespecified value γ , the maximal model is dropped from the set $\{H_{\overline{A}}\}$. The posterior probability of the maximal element is added to the probability of the next element of the string until either only one model remains or there is no need to drop models. Before considering the next maximal string, all models which have .been dropped must also be deleted from the remaining strings. The above procedure is then repeated for each maximal string in turn.

Once this has been completed and all models which can be dropped because they reduce to models with fewer parameters have been dropped, the same stopping and selection rules proposed for the non-nested case are applied.

Note: The procedure just described is not necessarily the best or the most natural one to use for combining models. For example, an alternative to the distance of the means might be to combine models when the probability distribution of the maximal element is sufficiently concentrated about the mean of the submaximal element. This would have the advantage of using the information contained in the precisions of the distributions also.

43°

CHAPTER 6

COMPUTER SIMULATION RESULTS

The purpose of this chapter is to report and discuss the results of a number of Monte-Carlo simulation studies of the sequential procedure proposed in Chapter 5. The chapter is divided into four major sections. The first section describes the general simu- ..lation procedure and presents a brief description of the algorithm used. A computer program based on this algorithm is described in further detail in appendix **A.** The second section presents and discusses the results of a number of simulations performed to gain further information about the large sample behavior first discussed in Chapter 3. The primary concern is with the posterior probabilities and the posterior means of the parameter distributions after a large number of observations. The third section presents and discusses the results of some simulation studies -of the proposed sequential procedure when the number of observations is limited and when the stopping rule of Chapter 5 is used. The primary concern is with the probability of the procedure actually selecting the correct model and the average sample size required until termination. The last section of the chapter presents an overall discussion of the results.

6.1 General Simulation Procedure

The sequential procedure proposed in Chapter 5 consisted of

(1) an experiment termination rule, (2) an experiment selection rule, and (3) a model selection rule. Because of the mathematical complexity of the posterior distributions involved it was not feasible to analytically examine how well these rules work. The general procedure by which the Monte Carlo simulation technique was used to study performance is outlined in the following algorithm.

1. Input:

 $\vec{\mu}_{\nu,\Omega}$ the prior means of the parameters of the models $\Psi_{\ell=0}$ the prior precision matrices of the parameters of the models

 $\theta_{k,0}$ the prior probabilities of the models being correct

N the number of simulations

0m stopping probability

J_{MAX} maximum number of observations

i^{*} the model chosen to generate the observed variable $\frac{1}{2}$ **values of the parameters of the true model**

3. PCS ***** 0

2. n **- 0**

- 4. \overline{N}_{i} + 0 (for i = 1, J_{MAX})
- 5. $j + 0$
- $6. j + j + 1$

7. Determine optimal acA as described in Chapter 4. Denote as a^{*} and let M_{a^*} denote design matrix for model i^{*} when a is chosen. (All simulations in this dissertation

consider strictly one-at-a-time sampling for simplicity.) $8. y_j + M_a * \mu^*$ 9. Generate a pseudo-random observation ϵ _i from a $N(0, \tau)$ distribution, (Described in detail in appendix A) 10. $y_i^2 + y_i^2 + \varepsilon_i^2$ 11. For $k = 1, \ldots, L$ compute $\theta_{\ell, j}$, $\Psi_{\ell, j}$, and $\Pi_{\ell, j}$ from y_j and $\theta_{k,j-1}$, ψ_{j-1} , and ψ_{j-1} as described in Chapter 3. 12. Find **k** such that $\theta_{k,j} = \text{MAX}\{\theta_{i,j}\}\$ 13. If $j \geq J_{MAX}$ or $\theta_{k,j} \geq \theta_{m}$ go to 14. Otherwise go to 6. 14. $N_j + N_j + 1$ 15. If $k = i^*$; PCS + PCS + 1 $16. n + n + 1$ 17. If $n \geq N$ go to 18. Otherwise go to 5. 18. PCS \div PCS/N 19. ASN $\left(\sum_{i=1}^{J_{\text{MAX}}} i \overline{N}_i\right)$

20. Stop

Upon stopping, the value of PCS is the observed probability of correctly choosing i^* as the true model for the prior distributions specified when in fact the true value of the parameters is given by μ^* . ASN gives the average sample number upon termination.

The above algorithm can be easily used for either large sample or small sample studies. For example, for large sample studies set $\theta_m = 1.0$, $N = 1$, and J_{MAX} to some large number, say 100 or 500.

For small sample studies set $\theta_{\rm m}$ < 1.0, ${\rm J}_{\rm MAX}$ to some small number, and N to some larger number, say 500 or 1000.

6.2 Large Sample Studies

In this section we examine the large sample properties of the posterior probabilities of the models and the posterior means of the parameter distributions. Three sets of problems are studied. First, two sets of nested polynomial models are studied. The posterior probabilities of each model, the posterior means of the parameter distributions, and the proportion of times each of the allowable values of the independent variable isochosen as optimal are tabulated for simulations of 100 and 500 observations. Second, one set of nested factorial models is studied for three different prior distributions' on the models. And third, one set of non-nested factorial models is simulated. For the last two, the posterior probabilities and means of the parameter distributions are tabulated.

6.2.1 Polynomial Model Studies

Two sets of nested polynomial models are considered which have the following general form:

$$
H_{\ell}: y = \sum_{j=0}^{\ell-1} \beta_j x^j + \epsilon, \ell = 1, L
$$

Two values of L are studied, and for each of these choices, two choices of H_{i^*} are made. The values of τ , $\theta_{\ell,0}$, and $\Psi_{\ell,0}$ are specified as

t = **100.0**

$$
\Psi_{\chi,0} = T
$$

for all simulations. The values of **P-,0** are tabulated at the tops of figures 1 and 2 and the resulting functions are graphed on the interval $x [-1, +1]$ at the bottoms of the respective figures. For $L = 4$, the two choices of H_{1*} are H_{2} and H_{3} . For $L = 6$, the two choices of H_{i*} are H_{3} and H_{5*} For simplicity, the actual values of the parameters used to generate the data were chosen to be $\overline{\mu}_{i^*0}$ for each of the four cases.

For these simulations, the definition of A was arbitrarily taken to be

$$
A = \{a^{(1)}: 1 = 0, \ldots, 9\}
$$

where

 $a^{(1)}$: $x = -1 + \frac{2}{9}$

Note that sampling is strictly one observation per stage.

The simulation results are summarized in table 1 and given in further detail in tables 2 through 9. For each choice of L and i , five simulations of 100 observations and five simulations of 500 observations were performed. For these simulations, the sample paths of the $\theta_{k,j}$ were printed out and the choice of $a^{(1)}$ at each stage were printed. The posterior means of the parameter distributions were printed only after the last stage. Tables 2, 4, 6, and 8 give the posterior probabilities after 100 observations and the first 100 out of 500 observations. The proportions p_i of using $a^{(i)}$ are also given. Tables 3, 5, 7, and 9 give the same informa-

48

<u>لم</u>

Z,0 L

Figure 1. - Tabulations of the prior means of the parameters and graphs of the resulting functions over the interval $\left[-1, +1\right]$ for large sample polynomial study one.

Figure 2. - Tabulations of the prior means.of the parameters and graphs of the resulting functions over the interval $\begin{bmatrix} -1, & +1 \end{bmatrix}$ for large sample polynomial study t'WAo.

tion for the 500 observation simulations.

Figures 3 and 4 present typical sample paths for the posterior probability of the correct model. In figure 3, the value of $\theta_{2,1}$ is plotted for the first 250 observations of the third simulation for $L = 4$ and $i^* = 2$. In figure 4, the value of $\theta_{3,j}$ is plotted for the first 250 observations of the first simulation for $L = 4$ and $i^* = 3$. These figures illustrate the typical behavior of $\theta_{i^*,j}$. It fairly rapidly rises to a value of about 0.85 to 0.95 and then slowly and erratically oscillates. This is suspected to be because of the nested nature of the model equations. It was because of this behavior that the modified selection rule of Chapter 5 was first introduced. Consideration of the posterior means of the parameter distributions will also provide some information concerning this modified rule.

For $L = 4$, consideration of tables 2, 3, 4, and 5 show that as j increases, $\vec{\mu}_{i,j} \rightarrow {\begin{bmatrix} 1 & , & j \\ 0 & 1 & j \end{bmatrix}}$ for $i > i$. This is in accord with the conclusions of Chapter 3. For $L = 6$ and $i^* = 3$ we again see the same close agreement with Chapter 3 as evidenced by tables 6 and 7. However, for $i^* = 5$, an entirely different situation arises. To understand this we should note that the model used to generate the sequential observations is

 $y = 0.5 x + 0.1 x⁴ + \varepsilon$

This function can be very closely approximated by a model of the

form

 $y = ax + bx^2 + \epsilon$

over the range of x values considered. And in fact we note that there is a marked preference for choosing the lower degree model as indicated by $\Theta_{3,i}$ becoming close to 1.0. It is also interesting to note the behavior of $\overrightarrow{\mu}_{i,j}$ for $i > 3$. We do <u>not</u> see that $\begin{pmatrix} \vec{\mu} \\ \vec{\mu}_1, \vec{j} \end{pmatrix}$ as might be expected when H_3 is so close to being true, except for the case of $i = 4$. For μ_{5} we note that the average posterior mean of the coefficient of $\begin{array}{ccc} \texttt{3} & \texttt{is quite close to} \end{array}$ zero and the <u>sum</u> of the posterior means of the coefficients of x^2 and x^4 is quite close to 0.1. For $\overrightarrow{\mu}_6$ we note that the sums of the posterior means of the coefficients of x^2 and x^4 is close to 0.1 and the sum of the posterior means of the coefficients of x, x^3 , and x^5 is close to 0.5. From these simulation studies it is not clear whether this behavior is simply because 500 observations is not.a sufficiently large number to discriminate well between such nearly equivalent functions or if this behavior will persist no matter how large the number of observations

We now turn to a discussion of the observed proportions of times the $a^{(i)}$ were chosen as the optimal experiments. From tables 2 and 3 which present the results of $L = 4$ and $i^* = 2$ we see that the largest p_i are for p_0 , p_4 , p_5 , and p_9 . These correspond to $x = -1$, $x = -1/9$, $x = +1/9$, and $x = +1$. Because of the discretization of the interval $(-1,+1)$ we might assume that the asymptotically most informative experiments were $x = -1$, $x = 0$, and $x = +1$. From tables 4 and 5 we see the largest p_i are p_0 , P₂, P₇, and **p_g** corresponding to $x = -1$, $x = -5/9$, $x = +5/9$, and

 $x = +1$. The relationship of these proportions and x points to the experimental designs which are optimal from other considerations might be interesting. For example, Kiefer and Wolfowitz (1959) consider optimal designs for regression problems of a somewhat different nature. The comparison of the current results with such other works is currently being pursued but will not be reported in this dissertation

6.2.2 Nested Factorial Models

A second set of simulation studies were made using the following models

$$
H_1: y = \beta_0 + \epsilon
$$

\n
$$
H_2: y = \beta_0 + \beta_1 x_1 + \epsilon
$$

\n
$$
H_3: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon
$$

\n
$$
H_4: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon
$$

with $\tau = 2.0$, $\Psi_{\ell,0} = I$, and $i^* = 3$. The prior means $\vec{\mu}_{\ell,0}$ were chosen as

$$
\begin{aligned}\n\vec{\mu}_{1,0}^{t} &= (0) \\
\vec{\mu}_{2,0}^{t} &= (0,1) \\
\vec{\mu}_{3,0}^{t} &= (0,1,-1) = \begin{pmatrix} +1 \\ 1 \end{pmatrix} \\
\vec{\mu}_{4,0}^{t} &= (0,1,-1,0)\n\end{aligned}
$$

Three sets of $\theta_{\ell,0}$ were chosen:

1. $\theta_{1,0} = 0.1$ $\theta_{2,0} = 0.2$ $\theta_{3.0} = 0.3$ $\theta_{4,0} = 0.4$ 2. $\theta_{\ell_5 0} = 0.25$ $\ell = 1, 4$ 3. $\theta_{1,0} = 0.4$ $\theta_{2,0} = 0.3$ $\theta_{3,0} = 0.2$ $\theta_{4,0} = 0.1$

The experiment space A is defined as $A = \{(x_1, x_2): x_1 = \pm 1\}.$ Note that experimenting is strictly one-at-a-time. ^cThe sequential selection procedure of Chapter 5 was used for five simulations of 500 observations each. The results are presented in table 10. We note.that the posterior values are again in close agreement with Chapter 3 and the results of the polynomial models. There does not seem to be a pronounced effect upon the posterior probabilities of the models from changing the prior distribution although there does appear to be slightly higher posterior values of $\theta_{3,500}$ when the $\theta_{\ell,0}$ distribution is skewed toward the lower values. A possible explanation for this is that when this distribution is skewed toward the high values, the procedure is choosing experiments primarily to discriminate between H_3 and H_4 . Since H_3 is true, the model of

C

55°

 H_d will rapidly become close to that of H_3 and the resulting experiments will not be very informative. When the prior probabilities are larger for the lower degree polynomials, however, the procedure chooses experiments primarily to discriminate between H_1 and H_2 . These experiments should then more rapidly tend to prove H_1 and H_2 to be inadequate.

6.2.3 Non-Nested Factorial Models

In this study, the following non-nested models were studfed.

o $H_1: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 +$ $H_2: y = \beta_0 + \beta_1 x_1 + \beta_3 x_3 + \epsilon$ $H_3: y = \beta_0 + \beta_2x_2 + \beta_3x_3 + \epsilon$

The values of the parameters are chosen as

 $i^* = 1$ $\left\{\n \begin{aligned}\n \overrightarrow{\mu}_{\ell,0} &= (1,1,1)^{\mathsf{T}} \\
 \overrightarrow{\mu}_{\ell,0} &= 1\n \end{aligned}\n \right.\n \qquad\n \left.\n \begin{aligned}\n \overrightarrow{\mu}_{\ell,0} &= (1,1,1)^{\mathsf{T}} \\
 \overrightarrow{\mu}_{\ell,0} &= (1,1,1)^{\mathsf{T}}\n \end{aligned}\n \right\}$ $\int_{0}^{\infty} \theta_{\ell, 0} = \frac{1}{3}$ $\tau = 0.0$ *f*, 1,100 \overrightarrow{u} = $(1,1,1)^{9}$

The experiment space A was assumed to allow only one observation at a time with $x_i = \pm 1$. Five simulations were performed for each value of τ . For $\tau = 100$ it took only three observations for θ_3 to become 1.0 (within the accuracy of the computer). For $\tau = 1.0$ the number of observations required for the final posterior probabilities to reach 1.0 are tabulated in table 11. For $\tau = 0.01$,

1000 observations were taken and the resulting posterior probabilities are given in table 11. Again the results are in general agreement with Chapter 3.

6.3 Small Sample Performance Studies

In this section we examine the performance of the proposed sequential procedure as measured by the PCS and ASN values. First, two studies are presented of the problem of discriminating among the three models

$$
H_1: y = \beta_1 x_1 + \epsilon
$$

\n
$$
H_2: y = \beta_2 x_2 + \epsilon
$$

\n
$$
H_3: y = \beta_1 x_1 + \beta_2 x_2 + \epsilon
$$

The first study assumes H_3 is true and the second study assumes H_2 is true. The experiment space A is defined as

$$
A = \{ (x_1, x_2) : x_1 = \pm 1; \text{ one-at-a-time sampling} \}
$$

Then we consider the problem of choosing among the four nested models.

$$
H_1: y = \beta_0 + \hat{e}
$$

\n
$$
H_2: y = \beta_0 + \beta_1 x_1 + \varepsilon
$$

\n
$$
H_3: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon
$$

\n
$$
H_4: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \varepsilon
$$

where A is as in the first two studies.

The primary reasons for concentrating on these simple models are-that the parameter spaces are of a low enough dimension that

they can be visualized and they are small enough that extensive simulation studies would not require inordinate amounts of computer time. The fact that the parameter spaces can be visualized allows the effect of varying prior means upon PCS and ASN to be more easily grasped. Note that the modified stopping and selection rule was not used.

 $6.3.1$ Study One $-$ H₃ Assumed True

We study discriminating among

$$
H_1: y = \beta_1 x_1 + \epsilon
$$

$$
H_2: y = \beta_2 x_2 + \epsilon
$$

$$
H_3: y = \beta_1 x_1 + \beta_2 x_2 + \epsilon
$$

A = $\{(x_1, x_2): x_1 = \pm 1; \text{ one-at-a-time sampling}\}$

c.

where.

 $\Psi_{\ell,0} = I$ $\qquad \theta_{\ell,0} = \frac{1}{3}$ $\vec{u}_{1,0} = (1.0)$ $\vec{u}_{2,0} = (1.0)$

and

$$
\overrightarrow{\mu}^* = \begin{pmatrix} 1.0 \\ 1.0 \end{pmatrix}
$$

Then a number of simulation experiments were performed for

each combination of:

 $T = 0.50, 1.0, 2.0$ $\theta_m = 0.70, 0.80, 0.90$ $J_{\text{MAX}} = 8, 16$

$$
\vec{u}_{3,0} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix}, \begin{pmatrix} 0.50 \\ 0.50 \end{pmatrix}, \begin{pmatrix} 1.0 \\ 1.0 \end{pmatrix}, \begin{pmatrix} 1.5 \\ 1.5 \end{pmatrix}
$$

The experiments for $J_{MAX} = 8$ used 1500 simulations and for J_{MAX} = 16 used 1000 simulations.

The choice of prior means deserves some comment. Figure 5 illustrates the points in (β_1, β_2) coordinate space corresponding to the prior means. The points corresponding to $\overrightarrow{\mu}_{1,0}$ and $\overrightarrow{\mu}_{2,0}$ are as close to $\overrightarrow{\mu}$ as possible since $\overrightarrow{\mu}_{1,0}$ is restricted to the horizontal axis and $\overrightarrow{\mu}_{2,0}$ to the vertical. The four choices for $\overrightarrow{\mu}_{3,0}$ then span a range about μ and hence the resulting PCS and ASN values will indicate the importance of mis-specified prior means.

Tables 12 and 13 present the observed PCS and ASN values for the combinations of θ_m , τ , and $\overrightarrow{\mu}_{3,0}$. These results are also plotted as parametric surfaces in figures 6 through 9.

In general, the results are about what should be expected. The PCS increases with τ and ASN decreases with τ . PCS increases as $\overrightarrow{\mu}_{3,0}$ gets closer to $\overrightarrow{\mu}$. We also note that in most cases, PCS increases with θ_m for fixed τ and $\overrightarrow{v}_{3,0}$. There is, however, a distinct dropping off of PCS with θ_m along the peaks of the surfaces. There does not seem to be any ready explanation for this.

-59

Figure **5. -** Illustration of prior means for performance simulation experiment one.

Figure **8.** - Probability of correct selection **(PCS)** as a function of **m,, T, P3 0** for Jmax *=* **16** and **H3** true. Small sample performance simulation expe6iment one.

Figure 9. - Average sample number (ASN) as a function of 0m, **T, P3,** 0 for Jmax **=** 16 and H3 true. Small sample performance simulation experiment one.

64

o
6,3.2 H2 Assumed True

A much less extensive study of this case was made than the case of H_3 assumed true. The same model equations were postulated and we assume

$$
\Psi_{\ell,0} = I
$$
\n
$$
\Theta_{\ell,0} = \frac{1}{3}
$$
\n
$$
\Psi_{1,0} = (0.0)
$$
\n
$$
\Psi_{3,0} = (0.0, 1.0)
$$
\n
$$
\Psi_{3,0} = (0.0, 1.0)
$$

The values of τ , θ_m , and $\tilde{\mu}_{2,0}$ which were simulated are tabulated in table 14 along with the simulation results. Figure 10 illustrates the prior means. Only one level of J_{MAX} (=8) was considered. Also, only 500 simulations were performed for each of these cases. The PCS results are also graphed as a parametric surface in figure 11. The results are generally the same as for H_3 true.

Figure 11. - Probability of correct selection (PCS) as a function of θ_{m} , τ , $\vec{\mu}_2$ of or J_{max} = 8 and H₂ true. Small sample performance simulation experi-
ment two.

6.3.3 A Four Model Problem

In this section we study the ability of the sequential procedure to choose the correct model from the following set of completely nested model equations.

$$
H_1: y = B_0 + \epsilon
$$

\n
$$
H_2: y = B_0 + \beta_1 x_1 + \epsilon
$$

\n
$$
H_3: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon
$$

\n
$$
H_4: y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon
$$

The prior distributions are defined by

$$
\theta_{\ell,0} = \frac{1}{4}
$$

\n
$$
\Psi_{\ell,0} = I
$$

\n
$$
\vec{\mu}_{1,0} = (0), \vec{\mu}_{2,0} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \vec{\mu}_{4,0} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}
$$

 ϵ

And

-*?--,-- --

$$
\vec{\mu}_{3,0} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0.5 \end{pmatrix}
$$

The equation used to generate the observations was that of H_3 with values of the parameters given by

 $\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$

The value of τ used was 1.0.

For fixed values of β_3 , the values of the prior parameter means for H_1 and H_2 and the four prior means for H_3 can be plotted in 3-space as in figure 12. For each of the four choices of $\vec{p}_{3,0}$, three values of θ_m (=0.7, 0.8, 0.9) for $J_{MAX} = 8$ were used and the resulting PCS and ASN values for the 12 combinations در السوال 1990 بنا التي في الله الأنبوة الأمر التي تارة الصحيح العام الأمر التي تعليم العام العام ا
التي تعدد المركز التي تعدد الت cases, 1000 simulations of the procedure were performed.

Figure 12. - Illustration of the prior means when **3** is held $\mathop{\mathrm{constant}}$. Small sample performance simulation experimen th ree.

6.4 Discussion of Results

We now make some general observations concerning the results of the simulation experiments.

First, consider the large sample results. In the context of the fact that sequential procedures are primarily developed in the hope that reliable decisions can be made with small samples rather than large samples, these results are not of primary importance. It is interesting and informative to know, however, that the procedures are consistent. Since the study of limiting posterior distributions resulting from.sequentially chosen experiments is known to be an extremely difficult and delicate problem, simulation experiments may be helpful by indicating to researchers what large sample behavior is likely to be true. In the problems studied in this paper it seems quite likely that when non-nested models are encountered, the posterior probability of the true hypothesis has a limiting value of unity. It also seems most likely that the limiting posterior mean of the true hypothesis does indeed equal the values of the unknown parameters generating the data.

When nested models are encountered, however, the results are not as enlightening. It appears that if the posterior probability of the correct hypothesis does not achieve a limit of unity, it at least attains a large value and then randomly fluctuates about that value. There is indication that the conjecture of Box and Hill that for these nested models there is a distinct preference by the

sequential procedure to choose the model with the smaller number of parameters as true. For instance, the polynomial study $L = 6$, $i^* = 5$ indicates that if a model with more parameters is true but can be approximated closely by one with fewer parameters, there is a preference for the smaller model.

In examining the small sample performance simulation experiments, it is seen that PCS drops off fairly rapidly as the distapce of the prior mean of the correct model from the true values of the parameters increases. This supports the conjecture of Chernoff and Meeter et al. that there may often be "initial bungling." It should be noted, however, that in all cases.studied, the prior means of the competing models were all set to be as close to the true model parameter values as could be done. Thus, in a sense, these experiments can be considered to be presenting the most unfavorable situation possible to the sequential procedure. In actual application it might be more reasonable to assume that the prior distributions of all the models are mis-specified to the same extent. This problem of "initial bungling" should also indicate that the statistician should have the prior precision matrices of the parameter distributions be as vague as the prior information permits.

One approach studied by Kiefer and Sacks (1963) was to plan small initial experiments as a basis for gaining information to plan a large second experiment. An alternative not studied in this dissertation, but which seems worthy of investigation, would be to set

a lower limit, say J_{MIN} , as the minimum number of observations taken before a stopping rule is applied. The sequential procedure would use the same rule as developed for selection of experiments but large posterior probabilities on the models would be ignored until a sufficient number of observations are taken to avoid the consequences of initial bungling. This also makes sense from the point of view of obtaining parameter estimates. Surely an experienter would not be content to terminate sampling with two or three observations even if the resulting probabilities are overwhelmingly in favor of one hypothesis unless he had extremely good prior information.

The last topic to discuss is the modified stopping and selection procedure introduced in Chapter 5. This was not applied to any of the simulation experiments performed in this dissertation. The large sample simulation results indicate that when θ_{m} and/or J_{MAX} are large, then this modified procedure may be of value. For the problems considered here, it is seen that even for nested models, the unmodified procedure performs quite well when J_{MAX} is small.

CHAPTER 7

EXAMPLE OF APPLICATION

This chapter first presents a general outline of the situations in which the results of this paper may be applied. Following this an example from the literature is presented. The purpose of this example is to illustrate how the information available from previous experimentation can be translated to the information required for the application of the sequential procedure developed herein.

A Bayesian framework is used in this paper because in a great many applications there does exist some prior information which can be incorporated. The Bayesian approach to statistical inference is the most natural and satisfying method of incorporating prior knowledge. This prior knowledge may arise in several ways.

For example, when expensive or large experiments are contemplated, there is often available data from pilot studies, the literature of the field, or poorly designed prior experiments. Typically, some type of regression analysis is performed on this data but there is so little data that practically no conclusions can be drawn, only recommendations for further experimentation. The resulting equations, however, provide a very convenient starting point for the application of Bayesian methods.

In other situations, an experimenter has a great deal of ex-

perience in experiments that are similar and involve factors with which he has some previous experience. In these cases it may be safe to extrapolate his acquired knowledge from the similar but differant experiments to the current experiment. If so, this may indicate some characteristics of the model equation.

A third possibility might arise for example in the carrying over of laboratory results to a production process or out-oflaboratory process. In the laboratory greater control can be exerted on many variables and typically only a small number of variables may be investigated. Often one or more mechanistic models are available. When the process is taken out of the laboratory, there will be less control over other variables and they must be accounted for by adding them to the model. Thus the experimenter is faced with the situation of having a partly mechanistic model and a partly empirical model.. If the mechanistic model is sufficiently smooth in the region of interest, factorial or polynomial models can be applied in these cases and prior information might indicate which interactions or terms are most likely to exist.

The example we consider is studied in Lloyd and Lipow (1962) and Draper and Smith (1966). In these books the data presented in table 16 is used to illustrate some topics in the design of experiments and multiple linear regression analysis. The dependent variable y is the chamber pressure in rocket engines put on test. The four controlled variables are

 z_1 = temperature of cycle (starting) z_2 = vibration level z_3 = shock by dropping (temperature) z_{Δ} = static fire temperature

We first postulate the model equation given by equation $(7-1)$.

$$
y = \beta_0 + \beta_1 z_1 + \beta_2 z_1^2 + \beta_3 z_2 + \beta_4 z_2^2 + \beta_5 z_3 + \beta_6 z_3^2 + \beta_7 z_4 + \beta_8 z_1 z_2
$$

+
$$
\beta_9 z_1 z_3 + \beta_{10} z_1 z_4 + \beta_{11} z_2 z_3 + \beta_{12} z_2 z_4 + \beta_{13} z_3 z_4 + \epsilon
$$
 (7-1)

The results of a multiple linear regression analysis of the model are summarized in table 17. The terms of the model are ordered in table 17 in decreasing order of descriptive significance level. The experiment is highly saturated with respect to equation (7-1) in the sense that 14 parameters are estimated from the data from 18 distinct combinations of levels of the independent variables. There are also quite a few high correlations among the terms of equation (7-1) and hence high correlations among the estimated parameters. The power of the resulting t-tests may be somewhat low under these circumstances., From examination of the various descriptive significance levels, the model equations tabulated in table 18a can be considered reasonable. The prior means of the distributions are also given in table 18b. The prior precision matrices may be derived by multiplying τ times the submatrices of order 3, 6, 9, and 15 of the matrix given in table 18c. How these prior distributions were determined is now described.

In multiple linear regression, under the usual normality

assumptions, the parameter estimates from the model

$$
\vec{y} = M\vec{\beta} + \vec{\epsilon}
$$

are given by

$$
\hat{\vec{B}} = (M'M)^{-1}M'\vec{y}
$$

and we know

$$
\hat{\vec{\beta}} - N(\vec{\beta}, \frac{1}{\sigma^2} N'N)
$$

Thus, for the first three models of table 18, the prior means and precision matrices would reasonably be the β and $\frac{1}{2}$ M'M derived **-by** least squares analysis using the appropriate subset of data from table 16. This is how the values of $\vec{\mu}_{\ell,0}$, $\Psi_{\ell,0}$ for $k = 1,2,3$ were derived. For $k = 4$ and the data of table 16, the full equation is not estimable because there are not three levels of z_4 to estimate a coefficient of z_{Λ}^2 . Thus least squares estimates were computed and M'M computed for the first 14 terms of model 4. Then an essentially diffuse prior was specified with respect to β_{14} by setting the prior mean to zero and adding the last row of the matrix in table 18c to M'M. The diagonal term was arbitrarily chosen to make the matrix nonsingular yet not comparable to any of the other diagonal elements in magnitude.

To complete the information required, τ must be specified and $^\theta \hspace{0.5pt}$ chosen. From the data of table 17 an unbiased estimate of $\,$ o 2 is 1.85 as computed from the replicated points. Thus we may use $\tau = \frac{1}{1.85} = 0.541$. To determine the $\theta_{\ell,0}$ it will be helpful to examine the F-ratios for lack-of-fit for the first three models in

table 18. These are $F = 5.295$, $F = 2.038$, and $F = 1.871$. These statistics are significantly large at about the 0.90, 0,80, and 0.75 levels, respectively. Based upon this, the following values of **⁶**£,0 seem reasonable

$$
\theta_{1,0} = 0.10
$$

\n
$$
\theta_{2,0} = 0.30
$$

\n
$$
\theta_{3,0} = 0.30
$$

\n
$$
\theta_{4,0} = 0.30
$$

REFERENCES

- Albert, A. E. (1961): The sequential design of experiments for infinitely many states of nature. Ann. Math. Statist. 32: 774-799.
- Bessler, **S.** (1960): Theory and Application of the Sequential Design of Experiments, k-actions and Infinitely Many Experiments. Part I - Theory. Part II - Applications. Technical reports No. 55 and No. 56. Applied Mathematics and Statistics Laboratories, Stanford University.
- Box, **G.** E. P. and Hill, W. J. (1967): Discrimination Among Mechanistic Models. Technometrics 9: 57-72.
- Chernoff, H. (1959): Sequential Design of Experiments. Annals Math. Statist. 30: 755-770.
- Coveyou, R. R, and Macpherson, R. **D.** (1967): Fourier Analysis of Uniform Random Number Generators. J. Assoc, Computing Mach. 14: 100-119.
- DeGroot, M. H. (1970): Optimal Statistical Decisions. McGraw-Hill N.Y.
- Draper, **N.** R. and Smith, H. (1966): Applied Regression Analysis. John Wiley & Scns.
- Fisz, M. (1963): Probability Theory and Mathematical Statistics. John Wiley & Sons.
- Graybill, F. (1969): Introduction to Matrices with Applications in Statistics. Wadsworth Publ. Co.
- Hunter, W. **G.** and Reiner, **A.** M. (1965): Designs for Discriminating Between Two Rival Models. Technometrics 7: 307-324.
- Kiefer, J. and Sacks, J. (1963): Asymptotically Optimum Sequential Inference and Design. Ann. Math. Statist. 36: 705-750.
- Kiefer, J. and Wolfowitz, J.: Optimum Designs in Regression Problems. Ann. Math. Statist. 30: 271-294.
- Kullback, S. (1968): Information Theory and Statistics. Dover Pub-
ligations. (Replace of 1959 Wiley edition)

Lindley, D. V. (1956): On the Measure of the Information Provided by an Experiment. Ann. Math. Statist. **27:** 986-1005.

- Lloyd, D. K. and Lipow, M. (1962): Reliability: Management, Methods, and Mathematics. Prentice-Hall.
- Meeter, D., Pirie, W. and Blot, W. (1970): A Comparison of Two Model-Discriminating Criteria. Technometrics, 12: 457-470.
- Owen, R. J. (1970): The Optimum Design of a Two-Factor Experiment Using Prior Information. Ann. Math. Statist. 41: 1917-1934.
- Rao, C. R. (1965): Linear Statistical Inference and Its Applications. Wiley & Sons.
- Sidik, S. M. and Holms, A. G. (1971): Optimal Design Procedures for Two-Level Fractional Factorial Experiments Given Prior Information About Parameters. NASA TN D-6527,
- Stone, M. (1959): Application of a Measure of Information to the Design and Comparison of Regression Experiments. Ann, Math. Statist. 30: 55-70.
- Taussky, **0.** and Todd, J. (1956): Generating and Testing of Pseudo-Random Numbers. Publ. in Symposium on Monte-Carlo Methods. Wiley **,&** Sons,

APPENDIX A

COMPUTER PROGRAM FOR SIMULATION STUDIES

The general flow of operations and computations performed by the program is described by the algorithm given in Chapter 6.1. The input required to perform these computations is first described. How these computations are achieved is described briefly by giving the major functions of the subprograms constituting the complete program. A complete FORTRAN listing is given.

INPUT

The program, as presented here, can only accommodate polynomial models over the interval [-l,+1] and two-level factorial models. This can be changed by writing one new subroutine (MFORM) to handle more general models. The program identifies the parameters by their integer subscripts and computes the $x_{j,i}$ values for the M-matrices according to the following convention:

1. For polynomial models, the subscript i indicates the parameter which is the coefficient of $\mathbf{x}^{\mathbf{i}}$.

2. For factorial models, the coefficients are assumed ordered in the standard order according to the description in Sidik and Holms (1971). The treatment combinations are also assumed to be in standard order and the independent variable values are constructed as described in Sidik and Holms (1971).

3. The order of the models as specified for irput are written

such that the parameter subscripts are in increasing order.

The specific input cards are now described below and illustrated by the input for a case run in Chapter **6,3.1.** The problem input is specified by the models and parameter values:

$$
H_1: y = \beta_1 x_1 + \epsilon
$$

\n
$$
H_2: y = \beta_2 x_2 + \epsilon
$$

\n
$$
H_3: y = \beta_1 x_1 + \beta_2 x_2 + \epsilon
$$

\n
$$
\Psi_{\ell,0} = I
$$

\n
$$
\theta_{\ell,0} = \frac{1}{3} \qquad \qquad \theta_m = 0.70
$$

\n
$$
\theta_{\ell,0} = \frac{1}{3} \qquad J_{\text{MAX}} = 8
$$

1500 simulations

$$
\vec{v}_{1,0} = (1,0)
$$
\n
$$
\vec{v}_{2,0} = (1,0)
$$
\n
$$
\vec{v}_{3,0} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} \qquad \vec{v}^* = \begin{pmatrix} 1.0 \\ 1.0 \end{pmatrix}
$$

Start random number generator with 041 574 **501** 221.

1. IDENTIFICATION **(13A6)**

One card for Hollerith input description of the problem.

2. NAMELIST **INPUT (\$NAML)**

Most of the control parameters are included in a NAMELIST input set. The list of parameters and their purpose fol**lows:**

number sequence. Set F if sequence is to start with initialization value. (See description of subroutines RAND and SAND for further information.) $\mathbf{e}^{(i)}_{\mathbf{q},\mathbf{q},\mathbf{q},\mathbf{q}}$

RESTRT Is this problem a restart of a case.terminated by exceeded time? T or F.

NX For polynomial models, the x space is restricted to the interval **-1** to **+1.** NX specifies the number of points used to discretize the interval into equal increments.

3. FORMAT FOR PRECISION MATRICES (13A6, A2)

For each set of model equations supply one set of 4A, 4B, 4C, 4D, and 4E.

4A. NUMBER OF PARAMETERS IN MODEL, PRIOR PROBABILITY OF MODEL (16, F12.6)

4B. PARAMETER SUBSCRIPTS (1316)

4C. PRIOR MEANS (12F6.0)

4D. TRUE VALUE OF PARAMETERS (12F6.0).

This card should be supplied only for the set corresponding to the correct model.

4E. PRIOR PRECISION MATRIX

Only the upper triangular half of ψ is specified with the order being

$$
\Psi_{11}, \Psi_{12}, \Psi_{22}, \Psi_{13}, \text{etc.}
$$

5. STARTING VALUE FOR PSEUDO-RANDOM SEQUENCE (012)

A graphical illustration of a data deck is given in figure Al and a FORTRAN sheet giving the sample input is given in table Al.

 $\label{eq:2} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^{2} \left(\frac{1}{\sqrt{2}}\right)^{2} \left(\frac{1}{\sqrt{2}}\right)^{2}$

SUBPROGRAMS AND THEIR **MAJOR** FUNCTIONS

1. SEQDES. This is the main program. It reads the input cards, exercises general control over the other subroutines. It also outputs the final results.

2. ACOMB. Called once by SEQDES at the beginning of each case. This subroutine scans the lists of parameter subscripts for each model and constructs from them a new list of subscripts in ascending order which contains the parameters appearing in at least one model.

3. SVSTRT (GTSTRT). A double entry subprogram, The entry SVSTRT is used once at the beginning of each case to save the prior probabilities, means, and precision matrices. Then after each simulation, entry GTSTRT is used to re-initialize the working probability, mean, and precision vectors to the original values.

4. MFORM. There are two versions, MFORMX and MPOLY. The first is for factorial runs and the second for polynomial models. These subroutines construct the M-matrices required for each model when given the experiment choice (a level of x for polynomials, a treatment combination for factorials). It is called by INFX and YGEN.

5. INFX (UPDATE), Entry INFX accepts the current state of sampling as defined by $\{\theta_{\ell,i}, \tilde{\mu}_{\ell,i}, \Psi_{\ell,i}\}$, $k = 1, L\}$ and determines the expected K-L information for a specified experiment, Repeated calls then are made by SEQDES to determine the optimal experiment.Enery UPDATE is called by 1623 and accepts the current state Values

and an observed random response to compute the posterior distributions.

6. RANDUM. Called once for each random observation taken. Generates a random observation, ε , from $N(0, \tau)$.

7. YGEN. Called once for each random observation. This routine accepts the $N(0, \tau)$ variate generated by RANDUM and calls MFORM to compute M, where M is the design matrix appropriate for the correct model and the experiment chosen as optimal. Then

$$
y = M\mu^* + \varepsilon
$$

is computed. After generating y, posterior values for θ_{ℓ} are computed. Sampling for that simulation trial is then terminated if any. θ_g exceeds θ_m . If sampling is not terminated, YGEN calls UPDATE to compute the posterior $\hat{u}_k(y)$ and $\Psi_{\hat{y}}(y)$, and the sampling procedure is continued.

8. COUNTX. This subroutine is called by YGEN whenever a $\theta_{\ell} \geq \theta_{\rm m}$ or by SEQDES whenever J_{MAX} observations have been taken. It counts the number of times each model is chosen and records the distribution of sample sizes. These are then output after all simulations have been computed.

9. INVXTX. Inverts a symmetric matrix stored in the lower symmetric storage mode.

10. TRIOUX. Outputs a lower triangular matrix.

11. MTVEC. Computes the product vector resulting from the multiplication of a vector and a symmetric matrix.

12. RAND (SAND). This pair of entries provide the pseudorandom sequence of uniform random variates. SAND is an initializing entry which must be called before any calls to RAND. When RAND is called, it computes the next value in the random sequence from the current value. The return argument of RAND is the floating point uniform random variate. The input and return argument of SAND is an argument which saves the integer value of the random variate. The generator is the multiplicative-congruential type .obtained by taking the low order 36 bits of the product $r_{r-1} \times k$ where

 r_{r-1} is the previous random number r_0 is 1 and k is 5^{15} .

The properties of this generator are discussed by Taussky and Todd (1956) and Coveyou and Macpherson (1967).

13. BCREAD (Xl,X2). BCDUMP (X1,X2). These routines, respectively, read and punch cards in absolute binary at the rate of 22 words per card. The data read or punched begins at the location in core of the variable X1 and ends at the location in core of the variable X2.

COMMONZUNITSZ TUNIN+TUNOUT.HASK.LEVOUT.PPMT(4) 0000100 COMMON/XRAND/Y, EPS, UNIF, U 0000200 0000300 COMMON/ERR/TAU, SIGMA COMMON/ALPH/IALPH(10001,fiALPH(5121,ALPHMU(1000),REALMU(512) 0000400 ,NPARAM(10),MUD(11),PMU(1000) 0000500 х 0000600 COMMON/PS/PINDEX(11), PREC(2000) 0000700 INTEGER PINDEX COMMON/CNTRLS/NHYP.NALL.NFAC.NFULL.NEULM1.TRTMNT.NTREND.NORS.LTRUE 0000800 INTEGER TRIMNT 0000900 COMMON/PREMNC/NAVG(1000), PCS, XMSE, XMST, INITAL , IHCNT(101, MSOFAR 0001000 COMMON/INF/XINF 0001100 COMMON/PROBS/THETA(10),CSTOP 0001200 0001300 C 0001400 C 0001500 C 0001600 COMMON/MM/OESM(1000) COMMON/YDIST/S(10),R(10),SV(10),RV(10) 0001700 COMMON/XTRA/AAI10001,BIZ0001,CIZ0001,DI101 0001800 0001900 C 0002000 C** 0002100 C 0002200 DATA ENDCRD/4HENDCRD/ REAL IDENT 0002300 EQUIVALENCE (X1, EX), (KS, SK) 0002400 DIMENSION IOENT(14) 0002500 Ċ. DIMENSION INPENT(14) 0002600 LOGICAL IFSTRT, RESTRT 0002700 LOGICAL KPGEN 0002800 0002900 LOGICAL POLY NAMELIST/NAML/NFAC, NHYP, NSYM, MXTRTS, NTREND, LEVOUT, LTRUE, TAU, 0003000 0003100 X CSTOP, IMAX, JESTRI, RESTRI 0003200 X , POLY, NX 0003400 C 0003500 C****** 0003600 C 0003700 KPGEN= FALSE. 0003800 $16010 = 1$ CALL TIMELITSTRT! 0003900 1 READ(IUNIN, 5040) IDENT 0004000 0004100 IF(IDENT(I), EQ.ENDCRD) STOP 0004200 WRITELIUNOUT,6010) IDENT 0004300 C 0004400 READ CIUNTN, NAME 1 0004500 **WRITE(TUNOUT, NAML)** 0004600 NFULL=2**NFAC 0004700 NFULMI=NFULL-1 0004800 IF(POLY) NEULL=NX SIGMA= 1.0/SQRT(TAU) 0004900 READ(TUNIN, 5040) INPENT 0005000 0005100 $MUD(I1=1$ 0005200 PINDEX(1)=1 DO 190 N= 1, NHYP 0005300 $HICNT(H)=0$ 0005350 WRITE(IUNOUT.6365) 0005400 READ(TUNIN, 5020) NPARAMIN), THETAIN)
MUNIN-1)=MUDIN)+ NPARAMIN) 0005500 0005700 PINDEX(N+11=PINDEX(N)+ (NPARAM(N)+(NPARAM(N)+1))/2 0005800 0005900 $MUCO = MIO(0)$ $MUHI = MU0IN+1I-1$ 0006000

IPLO= PINDEX(N) 0006100 $IPHF = PINOEXIN+11-1$ 0006200 READ(IUNIN, 5010) (LALPH(L), L=MULO, MUHI) 9006300 0006400 READ(IUNIN, 5050) (ALPHMU(L), L=MULD, MUHI) IF (N.NE.LIRUE) GO TO 100 9006500 0066600 **KR = NPARAMER)** \mathbb{Z}^n . 9006700 WR1TE(TUNNUT,6360) 0006800 READ(IUNIN, 5050) (REALMUIL), L=1, NRI WRITE (IUNOUT,6355) (REALMUILI,L=1.NR) 0006900 0007000 WRITE (IUNOUT,6360) 0007100 **100 CONTINUE** READ(IUNIN, INPENT) (PRECILI, L= IPLO, IPHI) 0007900 \bullet WRITELLUNDUT, 60501 N, NPARAMINI, THETAINI **OOCROON** WRITE(IUNDUT,6060)(IALPH(L),ALPHMU(L),L=MULO,MUHI) 0008200 WRETE(TUNOUT,6090) 0008300 0008400 CALE TRIANGEPRECEIPLOIANPARAMENIAB, PEMT, IALPHEMULOII 0008500 C CALL MTVEC(PREC(IPEO), ALPHMU(MULO), NPARAM(N), PMU(MULO)) 0008600 0008700 IFfLEVOUT.GE.5)WRITE(IUNOUT,6060){IALPH(L), PMU(L),L=MULD, MUHI) **DOCABOO** 190 CONTINUE 00CR900 C 0009000 C 0009100 C M = NPARAMILTRUEY 0009200 0009300 $JJ = MUD[LTRUE] - I$ $XMSE=0.0$ 0009400 DO 195 J=1.K 0009500 0009600 $JJ = JJ + I$ 195 XMSE = XMSE + {ALPHMU(JJ)-REALMU(J)) == 2 0009700 0009800 XMST = SORT(XMSE*TAU) 0 C C 9 9 0 0 $XMSF = SQRT(XMSE)$ 0010000 WRITE (IUNOUT, 6100) XMSE, XMST 0010100 $XMSE = 0.0$
 $XMSE = 0.0$ 0010200 0010300 DO 197 I=1, MXTRTS 0010400 197 NAVG(I) = 0 $PCS = 0.0$ 0010500 CALL SANDEINITALI 0010600 0010700 IF(KPGEN) INITAL=NTLSV 0010800 IF(IFSTRT) READ(IUNIN, 5090) INITAL IF(.NOT.RESTRT) GO TO 200 0010900 WRITE(IUNOUT,6425) 0011000 0011100 CALL BCREAD(NAVG(1), MSOFAR) 0011200 C 0011300 C 0011400 C 0011500 C** ******************** 0011600 C 0011700 200 CONTINUE 0011800 WRITECLUNOUT, 65001 INITAL 0011900 6500 FORMAT(26H STARTING VALUE FOR RAND= 012) 0012000 CALL ACOMB 0012100 CALL SYSTRT 0012200 C 0012300 C******************************* 0012400 C 0012500 $PMA = 1$ TE(PESTRT) MMM=MSOFAR+1 0012600 0012700 DO 800 M=MMM, NSYM

WSOFAREM 0012800 CALL GISTRI 0012900 00 700 NTR=1, MXTRIS 0013000 0013100 NURS= NTR 0013200 $SINE = 0.0$ DO 600 ITRT=1, NEULL
TRIMNT= ITRT+1 0013300 0013400 0013500 CALL MEDRM CALL INFINITY 0013600 IFIXINFLLE-SINFI GO TO 600 0013700 0013800 $SME = XINE$ 1.SV= TRTMNT 0013900 DD 590 N=1, NHYP 0014000 $SV(N) = SV(N)$ 0014100 0014200 $P.V(N) = R(N)$ 590 CONTINUE 0014300 600 CONTINUE 0014400 TRIMMT= ISV 0014500 IF (LEVOUT.GE.3) WRITE(IUNDUT,6210) ISV,SINE 0014,600 CALL RNOW 0014700 0014800 700 CONTINUE 0014900 750 CALL COUNT 0015000 CALL TIMEL(TNOW) 0015100 0015200 TPRNT=(TNOW-TSTRT)/3600. 0015300 IFITPRNT.LT.TMAX1 GO TO 800 0015400 16010=2 GO TO 510 0015500 **BOO CONTINUE** 0015600 0015700 C 0015800 C 0015900 C 810 CONTINUE 0016000 WRITE(IUNOUT,6240) TPRNT 0016100 0016200 XXMSF=XMSE/FLOAT(MSOFAR) 0016300 XXMST=XXMSE*SORT(TAU) $A SN = 0.0$ 0016400 0016500 DO 850 T=1, MXTRTS 850 ASN=ASN+FLOAT(NAVG(I)*I) 0016600 ASN=ASN/FLUAT(MSOFAR) 0016700 WRITELLUNOUT.6400) (NAVG(1), I=1.MX1RTS) 0016800 WRITELLUNDUT,66001 (IHCNTTI),1=1,NHYP1 0016810 0016820 6600 **FORMAT(1H 10[10)** 6400 FORMATC1H 101121 0016900 0017000 PPCS=PCS/FLOAT(MSOFAR) WRITELLUNOUT,6300) ASN, PPCS, XXMSE, XXMST, INITAL 0017100 0017200 NTESV=INITAL 0017300 KPGEN=, TRUE. 0017400 GO TO (1,1000), 1GOTO 1000 CALL RCOUMPINAVGILI, MSOFAR, 01 0017500 WRITEITUNOUT, 64501 MSOFAR 0017600 **STOP** 0017700 0017800 C 0.017999 Carobacerterenesertrerenenen 0018000 C 0018100 5010 FORMAT(1316) 0018200 5020 FORMAT(16,3F12.6,10I1) 0018300 5040 FORMAT113A6, A21 0019400 5050 FORMAT112F6.01

5080 FORMATI616, 366, 0, 2L1) 0018500 0018600 5090 FORMATIOL21 0018700 C ** ** ** ** ** \rightarrow 0019800 C** 6010 FORMATI1H1+13A6+1421 0018900 6050 FORMATCLEHKFOR MODEL E3716R NO. PARAMETERS IS/13H PRIOR PROB. GIA.-0019000 0019100 $X \subseteq Y$ 6060 FORMATISINKTHE PARAMETERS IN THE MUDEL AND THEIR MEANS ARE-- // 0019300 0019400 x ((110,614.5))) 6090 FORMATI44HKTHE PRECISION MATRIX OF THE PARAMETERS IS--1 0019500 6100 FORMATE 49HKINETIAL DISTANCE OF PRIOR MEAN FROM TRUE VALUE 614.5%-0019600 18X.16HOIVIDED BY SIGMA.15X.G14.51 0019700 \mathbf{x} 0019800 6210 FORMAT(1H 5G18.8) 6240 FORMAT(24H CURRENT EXECUTION TIME F10.3) 0019900 6300 FORMATI6HKASN= 614.2/6H PCS= 614.6/12H AVG.DIST.= 614.6/ 0020000 14H NORMALIZED = G14.6/211* 0121 0020100 \mathbf{x} 6355 FORMAT(1H 8G16.8) 0020200 0020300 6360 FORMAT[1H 40(2H +)) 0020400 6365 FORMATI1H 80(1H*1) 6425 FORMATE 37H THIS IS A RESTART OF A PREVIOUS CASE)
6450 FORMATESSH THIS CASE WAS TERMINATED BY CLOCK. DUMPING FOR RESTART/-0020500 0020500 X , 29H NO. SIMULATIONS COMPLETED = 16) 0020700 END 0020800

"SUBROUTINE ACOMB 0000100 COMMONZUNITSZ IUNIN, IUNOUT, MASK, LEVOUT, PEMT (4) 0000200 COMMON/ALPH/IALPH(1000), JIALPH(512), ALPHMU(1000), REALMU(512) 0000300 ,NPARAM(101,MUD(111,PMU(1000) 0000400 **Y** COMMON/CNTRLS/NHYP.NALL.NFAC.NFULL.NFULMI.TRTMNT.NTREND.NOBS.LTRUE 0000500 0000600 C 0000900 C 0000900 NALL = NPARAM(1)-NTREND 0001000 IFINALL.LE.01 GO TO 110 0001100 DO 100 K =1, NALL 9001200 IIALPHIKI= IALPHIKI 100 CONTINUE 0001300 110 JF(NHYP.LE.1) RETURN 0001400 0001500 C DO 800 N=2, NHYP 0001600 MAXI= MUDIN+11-1-NTREND 0001700 $KK = 0$ 0001800 $K = MUD(N) - 1$ 9061900 150 KK=KK+1 0002000 0002100 $200 K=K+1$ IF(KK.GT.NALL) GO TO 420
IF(K.GT.MAXII GO TO 800 0002200 0002300 250 IF(IALPH(K)-IIALPH(KK)1300,150,400 0002400 0002500 300 KS=NALL+2 0002600 DO 350 J=KK, NALL 0002700 K S= K S-1 350 TTALPHEKSI=TIALPHEKS-11 0002800 0002900 IIALPHEKKI=IALPHEK) NALL=NALL+1 0003000

ł

¢

Ç Ċ

THIS IS FOR TWO-LEVEL FACTORIALS ONLY 0000100 C SUBROUTINE MEDRM 0000150 COMMON/UNITS/ TUNIN, TUNDUT, MASK, LEVOUT, PEMT (4)
COMMON/ALPH/TALPH(1000), TTALPH(512), ALPHMU(10001, REALMU(512) 0000200 0000300 0000400 $\mathbf x$.NPARAM(101.MUD(111.PMU(1000) 0000500 INTEGER TRIMNT COMMON/CNTRES/NHYP.NALE.NFAC.NFULL.NFUEMI.TRTMNT.NTREND.NOBS.ETRUE 0000600 COMMONZNMZOESME10001 0000700 0000800 C 0000900.0** 0001000 C DIMENSION LASTA(10) 0001100 EQUIVALENCE (KS.SKI, LIX, XI) 0001200 0001300 0.5 ************************** ************** 0001400 C \bullet 0001500 DO 5 N=1,NHYP LASTA(N)=0 0001690 0001700 -5 CONTINUE 0001800 C 0001900 DO 1009 I=1, NALL 0002000 IPARAM = ITALPH(I) 0002100 IFIIPARAM.NE.01 GD TO 40 $A = -1.0$ 0002200. GO TO 500 0002300 0002400 C 40 CONTINUE 0002500 0002600 **ITR=TRIMNT** $DX = 1.0$ 0002700 $J = 1$, NFAC 0002800 DO 150 **XI=ANDIMASK, [PARAM]** 0002900 0003000 $1x = 1x+1$ 60 TO (130,100), IX 0003100 0003200 100 SK=AND(MASK, ITR) 0003300 $KS = KS + 1$ 0003400 50 TO (110,130), KS 0003500 110 $DX = -DX$ 0003600 130 IPARAM= IPARAM/2 $11R = 11R/2$ 0003700 0003800 150 CONTINUE 0003900 $A = 0X_{\frac{1}{2}}$ 0004000 € 0004100 C 500 CONTINUE 0004200 IFILEVOUT.GE.7) WRITE(IUNOUT.6000) ITALPH(I), A 0004300 0004400 C 0004500 DO 950 K=1, NHYP IFILASTA(KI-NPARAMIKI + NTRENDI 520,950,950 0004600 520 TX= MUDERI+LASTAERI 0004700 IF(ITALPHIT) - IALPHITX11 950,550,9999 0004800 0004900 550 CONTINUE 0005000 LASTA(K) = LASTA(K) +1 0005100 DESM(IX)= A 0005200 950 CONTINUE 0005300 1000 CONTINUE 0065400 IF(NTREND.LE.01 GO TO 1060 0005500 $A = NOBS$ 3005600 $P = 1.050$ 0005700 00 1050 $J = 1$, NTRENO 0005800 $B = B \cdot \Delta$

0000100 C THIS IS FOR POLYNOMIALS ONLY 0000150 SUBRITUTINE MEDRM COMMON/UNITS/ IUNIN, IUNOUT, MASK, LEVOUT, PEMT(4)
COMMON/UNITS/ IUNIN, IUNOUT, MASK, LEVOUT, PEMT(4)
COMMON/ALPH/TALPH(1000), ITALPH(512), ALPHMU(1000), REALMU(512) 0000200 0000300 0000400 χ ,NPARAM(10),MUD(11),PMU(1000) 0000500 INTEGER TRIMNT COMMON/GNTRLS/NHYR, NALL, NFAC+NFULL, NFULML, TRIMNT, NTREND, NOBS, LTRUE 0000600 0000700 COMMON/MM/DESM(1000) 0000800 C α 0000900 E** \star + \pm \pm 66 自由 0001000 C 0001100 DIMENSION LASTA(10) EQUEVALENCE (KS, SK), (IX, XI) 0001200 0001400 C UX=2.0/FLOATINFULL-11 0001500 $x=-1.0+FLOATITRTMNTI*DX$ 0001600 IF(ABS(X).LF.1.0E-4) X=0.0 0001650 0001700 DO 5 N=1, NHYP 0001800 LASTAINI=0 0001900 5 CONTINUE 0062000 C DO 1000 $I = I + NALL$
 $I PARRAM = IIALPH(I)$ 0002100 0002200 $A = X$ **1PARAM 0002300 0002400 C 0002500 C 500 CONTINUE 0002600 IF(LEVOUT.GE.7) WRITE(IUNOUT,6000) IIALPH(I),A 0002700 0002800 C DO 950 K=1,NHYP
TELLASTA(K)-NPAPAM(K) + NTREND) 520,950,950 0002900 0003000 520 IX= MUDIK)+LASTAIKI 0003100 0003200 IFIIIALPHII) - IALPHIIXII 950,550,9999 0003300 550 CONTENUE LASTA(K)= LASTA(K) +1 0003400

DO 1040 K=1, NHYP 0006000 KS=KS+NPARAM(K) 0006100 $DESM(KS) = B$ 0006200 1040 CONTINUE 0006300 1050 CONTINUE 0006400 1069 CONTINUE 0006500 $ITR = MUD(NHYP+1)-1$ 0006600 IF (LEVOUT.GE.71 WRITE(IUNCUT,6010) (DESMIII,1=1,1TR) 0006700 006800 **RETURN** 0006900 C 0007000 9999 CALL EXIT 0007100 RETURN 0007200 6000 FORMAT(1H 16+F6.0) 6010 FORMAT(6H DESM= /(6X,15F8.0)) 0007300 0007400 C 0.062500 END

 $KS = J - NTREDND$

SUBROUTINE INFATN 0000100 COMMON/UNITS/ LUNIN, LUNOUT, MASK, LEVOUT, PEMT(4) 0000200 COMMON/CNTRES/NHYP, NALL, NFAC, NFULL, NFULM1, TRIMNT, NTREND, NOBS, LTRUE 0000300 INTEGER TRIMNT 0000400 COMMON/XRAND/Y, EPS, UNIF, U 0000500 COMMON/ERR/TAU, SIGMA 0000600 COMMON/ALPH/IALPHET0001,11ALPHE5121,ALPHMUE10001,REALMUE5121 0000700 .NPARAMELOI.MUDELLI.PMUEL0001 0000800 COMMON/PS/PINDEX(111, PREC(2000) 0000900 INTEGER PINDEX 0001000 0001100 COMMON / INF/XINF COMMON/PROBS/THETALLOJ,CSTOP 0001200 COMMONZMMZDESM(1000) 0001300 COMMON/YDIST/ S(101+R(101+SV(10)+RV(10) 0001400 COMMON/XTRA/AA(1000), B(2000), C(2000), D(10) 0001500 DIMENSION DESMULIOI TRACELIOI 0001600 LOGICAL UPDY 0001700 00C1800 C 0001900 0******************* 0002000 C GO 10 5 0002100 ENTRY UPDATE 0002200 UPDT=.TRUE. 0002300 0002400 GO TO 6 5 UPDT=.FALSE. 0002500 0002600 **CONTINUE** 6. DO 10 K=1, NHYP
DESMU(K)=0.0 0002700 0002800

DESMITXI= A 0003500 950 CONTENUE 0003600 1000 CONTINUE 0003700 1F(NTREND.LE.01 GD TO 1060 0003800 $A = NOBS$ 0003900 $B = 1.050$ 0004000 DO 1050 $J = 1, N$ FREND 0004100 $B = B \star A$ 0004200 $KS = J - NIREND$ 0004300 DO 1040 K=1, NHYP 0004400 K S=KS+NPARAM(K) 0004500 $DESM(K5) = R$ 0004600 1040 CONTINUE 0004700 1050 CONTINUE 0004800 1060 CONTINUE 0004900 $ITR = MUD(NHYP+11-1)$ 0005000 IF (LEVOUT.GE.7) WRITE(IUNOUT,6010) (DESM(I), E=1,ITR) 0005100 RETURN 0005200 0005300 C 9999 CALL EXIT 0005400 RETURN 0005500 6000 FORMAT (1H 16, F6.0) 0005600 6010 FORMATION DESM= /(6X,15F8.0)) 0005700 0005800 C

0005900

END

10 CONTINUE 0002900 0003000 C 0003100 C******************************* **************** 0003200 C DO 520 N=1, NHYP 0003300 IFILEVOUT.CE.5) WRITE(IUNOUT.6005) N.NOBS 0003400 0003500 $MS = MUD(N)$ 0003600 JE= NPARAM(N) 0003700 C 0003800 C 0003900 $IR = 0$ 0004000 DO 100 J=1, JE $KSI=MS+J-1$ 0004100 TECUPDI) GD TO 25 0004200 DESMUINI=DESMUINI+DESM(KS1)#ALPHMU(KS1) 0004300 25 CONTINUE 0004400 \bullet 0004500 $00100 J=1, J$ $18 = 18 + 1$
 $KS2 = MS + JJ - 1$ 0004600 0004700 0004800 BITB1= DESM(KS1)*DESM(KS2) 0004900 100 CONTINUE 0005000 C 0005200 C IFILEVOUT.GE.6) CALL TRIANGIB, JE.B, PENT, IALPHINSII 0005300 $KSI = PINDEX(N+1)-PINDEX(N)$ 0005400 KS2= PINDEX(N) 0005500 00 120 K=1, KS1 0005600 BIKI= TAUFBIKI+PRECIKS21 0005700 $C(K)=B(K)$ 0005800 $K52 = K52+1$ 0005900 120 CONTINUE 0006000 CALL INVXTX(B, JE1 0006100 IFILEVOUT.GE.6) CALL TRIANG(R, JE, 8, PEMT, IALPHIMS)) 0006200 0006300 C ** ** \bullet 0006400 C** $\bullet \bullet$ \pm \pm ± 1 IF(.NOT.UPDT) GO TO 199 0006500 $KS1 = PINDEX(N+1)$ 0006600 0006700 $IPLO = PINDEXIN$ KS1=KSI-IPLO 0006800 $MUH1 = MUD(M+1)-1$ 0006900 K S2=IPLO 0007000 nn 130 J=1,KSI 0007100 PRECIKS21=CIJI 0007200 $K52=K52+1$ 0007300 130 CONTINUE 0007400 $KSI = MS - 1$ 0007500 **NO 150** $J=1+JE$ 0007600 $KSI = KSI+1$ 0007700 AA(J)= Y*DESM(KSI)*TAU + PMU(KSI) 0007800 0007900 150 CONTINUE CALL MIVECEB, AA, JE, ALPHMUEMS))
CALL MIVECEPRECEPLOI, ALPHMUEMS), JE, PMUEMSI) 0008000 0008100 IF(LEVOUT.LT.3) GO TO 520
IF(LEVOUT.LT.3) GO TO 520 0009200 0008300 WRITE(IUNOUT,6020)(ALPHMU(L),L=MS,MUHI) 0009400 IFILEVOUT.LT.41 GD TO 520 0008500 WRITE(IUNDUT.6090) 0008600 CALL TRIANG(PREC(IPLO), JE, B, PEMT, IALPHIMSIT 0008700

GO TO 520 0008800 **160 CONTINUE** 0008900 WRITE(IUNGUT,6060)(IALPH(L),ALPHNU(L),PMU(L),L=MS,MUHT) 009900 0009100 WRITE(IUNOUT,6090) CALL TRIANG(PREC(IPLO), JF, 8, PFMT, IALPHINS)) 0009200 0009300 GO 18 520 0009400 C ************************************ 0009500 C ********** 0009600 C 0009700 C 199 CALL MTVEC(B, DESM(MS), JE, AA) 0009800 DO 300 KS2=1, JE
"280 AA(KS2)= TAU*AA(KS2) 0009900 0010000 300 CONTINUE 0010100 IFILEVOUT.GE.51 HRITE(IUNOUT,6010)(AA(J),J=1,JE) 0010200 0010300 C 0010400 C**. ** \pm \pm 0010500 C 0010600 $R[N] = 0.0$ $MNS = MS - 1$ 0010700 0010800 DO 360 J=1, JE 0010900 $MMS = MMS + 1$ 0011000 P(N)= R(N) + AA(J)*DESM(MMS) 360 CONTINUE 0011100 $R(N) = TAU* (1.0 - R(N))$ 0011200 0011300 C 0011400 C** \pm \pm 0011500 C **MMS=MS** 0011600 0041700 $\sqrt{C} = 0 + 0$ 00 500 $\mathsf{J} \circ \mathsf{I}$, $\mathsf{J} \mathsf{E}$ 0011800 C=C+AA(J)*PMU(MMS) 0011900 $MMS = MMS + 1$ 0012000 500 CONTINUE 0012100 $S(N) = C/R(N)$ 0012200 IFILEVOUT.GE.5) WRITEIIUNNUT,6020) RINF,SINE 9012300 0012400 520 CONTINUE 0012500 C 0012600 IFIUPDTI RETURN 0012700 C** ** ** ** ** $+ +$ 0012800 C 0012900 DO 1000 N=1, NHYP 0013000 $C = 0.0$ $J=1$, NHYP \Rightarrow 0013100 DO 580 IF(N.EQ.J) GO TO 580 0013200 0013300 C=C+THETAEJI *P(J) 0013400 580 CONTINUE TRACE(N)=C/R(N) 0013500 IF(LEVOUT.GE.5) WRITE(IUNOUT,6035) TRACE(N) 0013600 0013700 1000 CONTINUE 0013800 C ************************** 0014000 C 0014100 XINE = THETA(1) * TRACE(1) 0014200 DO 1500 N=2, NHYP $JE = N-1$ 0014300 0014400 $XINF = XINF + THETAINF + TRACE(N)$ 00 1450 J=1, JE
C= S(M) – S(J) 0014500 $\epsilon \rightarrow$ 0.014600

 \ddot{z}

SUBROUTINE RNDM
COMMON/XRAND/ Y₁EPS,UNIF,U
COMMON/UNITS/ IUNIN,IUNOUT,MASK,LEVOUT
COMMON/ERR/TAU,SIGMA
DATA AO/2,515517/,A1/.802851/,A2/.01132_{95/s}/
X BI/1.432788/_TR2/.189269/(N3/.00132_{95/s}/
X UMIN/.0000001/

r-availler
EPS=T-{AO+Al*T+A2*T2}/11.0+Ml*T+R2*T2+4\\\r=T2}
IF (LFVDUT.GE.7) WRITE{{UNINt\\6000} W_qT+T2+FPS
EF{UNIF.LT..50} EPS==EPS
CFTIDM
PETIDM

 $\overline{\mathcal{L}}$

71H 5G16+R1

0000100
0000200
0000300

0000400 0000500

0000600 0000700

0000800

0000900

0001000

0001100

0001200

0001300

0001900

0002000

0002100

0002200

0002300

0002400

 $\pmb{\mathsf{x}}$

 \mathbf{x} ับ=บ∣

CALL RANDIUNIFI

IF(UNIF.GT..50) U=1.0-UNIF

IFIU.LT.UMINI GO TO 100

IF(UNIF.GT..50) EPS=-EPS

T2=ALOG(1.0/(U*U))

U=UNIF

RETURN

RETURN

FND

6000 FORMATION RAND

100 FPS = - 1.0E15

 $\ddot{}$

÷

 $\ddot{\circ}$

99

 ϵ

SUBROUTINE YGEN(*) 0000100 COMMONZUNTTSZTUNIN, JUNOUT, MASK, LEVOUT, PEMT(4) 0000200 0000300 CONNONZAL PHZ1AL PHC10001, EEAL PHC5121, ALPHNU(10001, REALMUC512) 0000400 ,NPARAM(10),MUD(111,PMU(1000) COMMON/CNTRLS/NHYP, NALL, NFAC, NFULL, NFULMI, TRTMNT, NTREND, NOBS, LTRUF 0000500 INTEGER TRIMNT 0000600 COMMON/MM/DESM(1000) 0000700 COMMON/XRAND/Y, EPS, UNIF, U 0000800 COMMON/YOIST/S(10)+R(10)+SV(10)+RV(10) 0000900 COMMON/PROBS/THETA(10), CSTOP 0001000 COMMON/PREMNC/NAVG(1000), PCS, XMSE, XMST, INITAL, IHCNT(10), MSOFAR 0001100 EQUIVALENCE (SK, KS1, [IX, XI) 0001400 0001600 C 0001700 C CALL MFORM 0001800 0001900 $Y = E PS$ $M = NPARAM(LTRUE)$ 0002000 $JJ = MUDLLTRUEI-1$ 0002100 DO 550 J=1.M 0002200 0002300 $JJ = JJ + 1$ 0002400 Y = Y + DESM(JJ) *REALMU{J) 0002500 550 CONTINUE SUM = 0.0 0002600 DO 700 N=1, NHYP 0002700 $C = Y - SV(M)$ 0002800 Q=RVINI*C*C 0002900 $S(N) = SV(N)$ 0003000 $R(N) = RV(N)$ 0003100 $0 = -0.50 * 0$ 0003200 IF(ABS(Q)-60.0) 660,670,670
660 IF(THETA(N)-1.0E-18) 670,670,680 0003300 0003400 ó 0003500 670 THETAIN) = 0.0 0003600 GN 10 700 0003700 680 A = ALOGITHETAIN) + Q IF(ABS(A1.GE.70.0) GDTD 670 0003800 690 THETAINI = THETAINI * SORTIRINII * EXPIOI 0003900 0004000 $SUM = SUM + THETA(N)$ 0004100 700 CUNTINUE 0004200 $I = 0$ 0004300 DO 710 N=1, NHYP 710 THETA(N1=THETA(N1/SUM 0004400 DO 920 II=1, NHYP 0006100 IF(THETACLI)-CSTOP) 920,910,910 0006200 0006300 $910 t = 1$ GO TO 1000 0006400 920 CONTINUE 0006500 1000 CONTINUE 0006600 IF(LEVOUT.GE.2) WRITE(IUNOUT,6010) TRIMNT, (THETA(N), N=1, NHYP) 0006700 0006800 6010 FORMAT(1H I10,10F10.4) IF(LEVOUT-GE-5) WRITE(IUNOUT,6000) Y,EPS.(S(N),R(N),THETA(N),C(N),-0006900 X N = 1, NHYP)
6000 FORMAT(3H Y=G12.5,5H EPS=G12.5, 12H S,R,THETA,C / 0007000 0007100 0007200 X (2X,4G16.61) CALL UPDATE 0007300 TE(1.EQ.1) RETURN 1 0007400 RETURN 0007500 0007600 FND.
SUBROUTINE COUNT 0000100 COMMONZUNITSZ TUNTN, TUNOUT, MASK, LEVOUT 0000200 COMMON/ALPH/IALPHI10001,11ALPH(512), ALPHNUI10001, REALMUI5121 0000300 .NPARAM(101, MUDIII), PMU[1000) 0000400 x COMMON/CNTRLS/NHYP, NALL, NFAC, NFULL, NFULMI, TRTMNT, NTREND, NORS, LTRUE 0000500 COMMON/PROBS/THETA(10),CSTOP 0000600 COMMON/PREMNC/NAVG(10001,PCS,XMSE,XMST,INITAL ,IHCNT(10),MSOFAR 0001000 COMMONZERRZTAU, SIGMA 0001100 $X = 0.0$ 0001300 0001400 NAVG(NOBS) = NAVG(NOBS) +1 0001500 M = NPARAM(ETRUE) 0001600 $JJ = MUD(LIRUE) - I$ 0001700 $00.5 - J = 1.4$ 0001800 $JJ = JJ + 1$ 0001900 YM = XM+EALPHMUEJJ)-REALMUEJJJ**2 0002000 5 CONTINUE 0002100 $xMSE = SORT(XM) + XMSE$ XMST = SORTEXM*TAUE 0002200 XM = SORT(XM) 0002300 IF (LEVOUT.GT.1) WRITE(TUNOUT.6000) NOBS.XM.XMST 0002400 $IMIN = 0$ 0002500 0004200 $CMAX=0.0$ 00 910 1=1, NHYP
IF(THETA(I)-CMAX) 910, 910, 905 0004300 ż 0004400 905 CMAX=THETA(I) 0004500 0004600 $I \cup I \cup I$ 0004700 910 CONTINUE 0004800 945 CONTINUE 0004900 IF (IMIN.EO.LTRUE) PCS = PCS+ 1.0 INCNT(IMIN)=IHCNT(IMIN)+1 0004950 TF (LEVOUT LT.2) RETURN 0005000 00 950 N=1, NHYP 0005100 $MULO = MUD(N)$ 0005200 0005300 $MUHI = MUD(N+1)-1$ 0005400 WRITE (IUNOUT,6010) THETA(N) , (ALPHMU(L), L=MULD, MUHI) 0005500 950 CONTINUE 0005600 RETHRN 6000 FORMAT(22H ******OBSERVATION NO. 14,7H XMSE= G11.3,7H XMST= G11.3 -0005700 +6H******) 0005800 \mathbf{r} 0005900 6010 FORMATCIH F10.6 , 10512.4/C27X10G12.411 0006000 **END**

0000100 SUBROUTINE INVXTX(A,NN) SUBSUUTINE THE MATRIX ANNIS
ASSUMES THE MATRIX A IS SYMMETPIC AND POSITIVE DEFINITE, AND ONLY
THE UPPER TRIANGLE IS STORED AS A ONE-DIMENSIONAL ARRAY IN THE
ORDER ALL, IJ, ALL, 21, AL2, 21, AL1, 31, AL2, 31, AL3, 31, ..., 0000200 C 0000300 C 0000400 C 0000500 C 0000700 C 0000800 DIMENSION A(1) 0001500 $D=1.0$ 0001600 $k = NN$ $ITRI = 0$ 0001700 0001900 DO 145 K=1,N 0002000 C 0002100 $ITR1 = ITR1+K-1$

ś

0002200 $KP1 = K+1$ $KMI = K-1$ 0002300 $KK = 1TK1+K$ 0002400 $PV = 1.000/41KK$ 0002600 0002700 C $IIRZ = 0$ 0002800 IF (K-11 150+80+50 0002900 0003000 C REDUCE TOP PART OF TRIANGLE, LEFT OF PIVOTAL COLUMN 0003100 C 50 DB 60 J=1, KM1 0003200 0003300 $1TR2 = 1TR2+J-1$ $KJ = IIR1+J$ 0003400 \bullet 0003500 $F = A(KJ*PV)$ $00601=1.1$
 $1J = 1TR2+1$ 0003600 0003700 $1K = 11R1 + 1$ 0003800 60 A(IJ) = A(IJ) + A(IK)*F 0003900 0004000 C IF (K-N) 70,120,150 0004100 0004200 C REDUCE REST OF TRIANGLE, RIGHT OF PIVOTAL COLUMN 0004300 C 0004400 70 ITR2 = ITR1 0004500 80 DD 110 J=KP1,N 0004600 $ITR3 = ITR1$ $ITR2 = ITR2+J-1$ 00 C4 7 00 $KJ = ITR2+K$ 0004800 0004900 $F = A(KJ)*PV$ 0005000 $001001=1, J$ IF (1-K1 90,100,95) 0005100 90 $1J = ITR2+I$
IK = ITR1 + I 0005200 0005300 0005400 $A(1J) = A(1J) - A(IK)*F$ GO TO 100 0005500 0005600 95 $IJ = ITR2 + I$ $1TR3 = TTR3 + I - 1$ 0005700 $IK = ITR3 + K$ 0005800 $A([J]) = A([J]) - A([K]*F$ 0005900 100 CONTINUE 0006000 0006100 110 CONTINUE 0006200 C DIVIDE PIVOTAL ROW-COLUMN BY PIVOT, INCLUDING APPROPRIATE SIGNS 0006300 C 120 $[TR2 = ITR1]$ 0006400 00 140 1=1.N
1F (1-K) 125.130.135 $^{\circ}$ 0006500 0006600 125 IK = ITRI+I 0006700 A (IK) = $-AL1K1*PV$ 0064390 0006900 GO TO 140 (REPLACE PIVOT BY RECIPROCAL) 0007000 C 130 $A(KK) = PV$ 0007100 0007200 0007300 0007400 A(KI) *PV $A(KI) =$ 0007500 0007600 140 CONTINUE 0007700 C 0067800 145 CONTINUE 0067900 C 0008000 150 RETURN 0008100 FND

0000100 SUBROUTINE TRIANGIA, NN, NKOL, FORMAT, IDOUTI 0000200 DIMENSION A(1), FORMAT(1), IDOUT(1) 0000300 COMMON/UNITS/TUNIN, JUNOUT 1 FORMAT (1HK) 0000400 $N = NN$ 0000500 $NCOL = NKOL$ 0000600 KLUMPS = N/NCOL 9000700 0000800 C. $KEEPIR = 0$ 0000900 0001000 $K1 = 1$ $K2 = NCOL - 1$ 0001100 0001200 $K3 = NCOL$ 0001300 TF (KLUMPS JEG. 01 GO TO 120 0001400 C 0001509 DO 90 KLUMP=1, KLUMPS ITR1 = KEEPTR 0001600 0001700 $1 = -1$ $110 = (KLUMP-1)*NCDI + ITRI + 1$ 0001800 $1 = 1 + 1$
 $1 = 1 + 1$
 $1 = 1 + 1$
 $1(0) = 3(0) + 1(0) + 1(0)$
 $1(1) = 1(0) +$ 0001900 0002000 0002100 00.02200 0002300 30 WRITEFIUNDUT, FORMAT) IDOUT (K), (A(J), J=ILO, IHI) 0002400 0002500 $KEEPTR = [TR1 + K2]$ 00.60 K=K3, N 0002600 $\begin{array}{rcl} \text{ITR1} & = & \text{ITR1} + K - 1 \\ \text{ILO} & = & \text{ILO} + K - 1 \\ \text{IHI} & = & \text{ILO} + \text{NCOL} - 1 \end{array}$ 0002700 0002800 0002900 0003000 60 WRITE(IUNOUT, FORMAT)IDOUT(KI, (A(J), J=ILO, IHI) $K1 = K1 + NCOL$ 0003100 $K2 = K2 + NCDL$ 0003200 0003300 $K3 = K3 + NCOL$ 90 WRITELIUNOUT, 11 0003400 0003500 C 120 TTR1 = KEFPTR 0063600 IF (K) .GT. N) GO TO 180 0003700 $I = -1$ 0003800 11.0 = KLUMPS*NCOL + IJRI + 1 0003900 0004000 DO 150 K=K1,N $I = [+ 1$
 $I = 1 + 10 + 1$
 $I = 1 + 10 + 1$ 0004100 0004200 0004300 0004400 0004500 150 WRITE(TUNDUI, FORMAT) IDOUT(K), (A(J), J=ILO, IHI) 0004600 C 0004700 180 PETURN 0004800 **FND**

103

0000109 0000200
0000300 $N \times NN$ $0.500 J=1, N$
C(1) = 0.0
C(1) = 0.0
KADD = ((1-1) * 1) / 2
D(0) 200 K=1, 1 0000400 0000500 0000600 $\ddot{\circ}$ 0000900 KADD=KADD+1 0000900 C(J)=C(J) +A(KADD)*B(K) $C(1)=C(1)+A(KADD)*B(K)$

200 CONTINUE
 $K1=J+1$
 $E\{K1=J+1$
 $K1=K1-N1$

250,250,500

250 DO 300 K=K1,N
 $KAD0= KADD+K-1$
 $C(J)= C(J)+ A(KADD)*B(K)$

300 CONTINUE

86 CONTINUE

86 CONTINUE

86 CONTINUE

86 CONTINUE

86 CONTINUE

86 CONTINU $\begin{array}{l} 0.000000 \\ 0.001000 \\ 0.011000 \\ 0.01200 \\ 0.001300 \\ 0.001300 \\ 0.001800 \\ 0.001800 \\ 0.001800 \\ 0.001800 \\ 0.001800 \\ \end{array}$ 0001900 END

÷.

b

SUBROUTINE MTVECIA: R.ANN.CI

 $104\,$

 \overline{z}

 $\tilde{\mathcal{Z}}$

 ϵ

 $\bar{\mathbb{C}}$

 $\ddot{}$

 ϵ

105

 106°

 $\begin{array}{c} \begin{array}{c} \begin{array}{c} \end{array} \\ \begin{array}{c} \end{array} \end{array} \end{array}$

 $\ddot{}$

 $i07$

 $\label{eq:2} \frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^n\frac{1}{j!}\sum_{j=1}^$

 $\frac{1}{2}$

 \bar{z}

APPENDIX C

TABLES

OFFAN ORCHUTE DRESSWEED BY TARLES 2 TREASCH &

The column headings give the auters of L and i^{*} and the number of observations. The rew headings present the parameters whose average posterior values are gly experiment in probabilities listed for 100 observations are t

Not recorded.

 \overline{z}

 ϵ

The values of the posterior probabilities and parameter means after ten simulations, of 100 observations each, of the sequential selection procedure. The last five columns arc
data from the first 100 observations of the 500 observation simulations tabulated in
table 3. The posterior means were not fecorded fo proportions p_i of the times each $a^{(i)}$ was chosen as the optimal experiment.

Model	Param		After 500 observations						
$\mathbf 1$ $\begin{array}{c} 2 \\ 3 \\ 4 \end{array}$	θ_{\perp} θ_2 \mathbf{e}_3 $\hat{\theta_4}$	$\mathbf{0}_{\perp}$.991 .009 0	0 .985 .015 0	0 .990 .009 0	0 .991 .009 0	0 .957 .040 .003			
$\mathbf{1}$	\upbeta_0	0.0875	0.0599	0.0905	0.0757	0.1317			
$\overline{2}$	β_0 $\frac{3}{2}$	0.0921 .4964	0.0984 .5010	0,0999 .5028	0.0942 .5014	0.0909 .5108			
3	$\frac{\beta}{20}$ $\frac{\beta_1}{\beta_2}$	0.0923 .4964. $-.0005$	0.1032 .5010 $-.0096$	0.0984 -5028 .0029	0.0937 .5014 .0012	0.0827 .5108 .0163			
4	β_0 $\frac{\beta_1}{\beta_2}$ β_3	0.0923 .4948 $-.0004$.0016	0.1022 .4886 -0.0086 .0126	0.0985 .5043 .0028 $-.0017$	0.0935 .4882 .0014 .0141	0.0850 .4817 .0139 .0293			
	P_{0} P ₁ P ₂ P_3 P_4 P_5 P_6 P ₇ \therefore P8 P9	0.234 0. .050 .008 .280 .110 .018 .072 0 .228	0.264 0 .010 0 .422 .060 Ω .010 0 .226	0.236 0 .056 .004 .302 .070 .026 .088 0 .218	0.236 0 .044 .008 .306 .088 .076 .038 0 .204	0.228 .002 0 0 .076 .418 .006 .002 $\mathbf 0$.268			

TABLE 3. - L = 4, i^* = 2

The values of the posterior probabilities and parameter means after 5 simulations, of 500 observations each, of the sequential selection procedure. Also listed are the proportions p_i of the times each $a^{(i)}$ was chosen as the optimal experiment.

TABLE 4. - L = 4, i^{*} = 3

The values of the posterior probabilities and parameter means after 10 simulations, of 100 observations each, of the sequential selection procedure. The last 5 columns are data from the first 100 observations of the 500 o

TABLE 5. - L = 4, 1^* = 3

The values of the posterior probabilities and parameter means after 5 simulations, of 500 observations each, of the sequential selection procedure. Also listed are the proportions $\mathbf{p_{i}}$ of the times each $\mathbf{a^{(i)}}$ was chosen as the optimal experiment.

۰.

TABLE 6. - L = 6, $i^* = 3$

*
Not recorded.

Ŵ

The values of the posterior probabilities and parameter means after 10 simulations, of 100 obser-
vations each, of the sequential selection procedure. The last 5 columns are data from the first
100 observations.of the 500 chosen as the optimal experiment.

114

Model	Param	After 500 observations						
ı \overline{c} 3 4 5 6	0 ₁ \mathbf{e}_2 $\frac{\theta_3}{\theta_4}$ $\frac{\partial_5}{\partial_6}$	0 0 .6046 .3388 .0425 .0141	0 0 .9812 .0175 .0009 .0003	0 0 .9722 .0257 .0018 .0003	0 0 .9746 .0230 .0021 .0003	\mbox{O} 0 .8526 .1316 , 0125 .0032		
1	β_0	0.1321	0.1378	0.1325	0.1349	0.1413		
$\overline{2}$	B_{0} β_1	0.1356 .2434	0.1278 . 2616	0.1247 .2541	0.1168 .2549	0.1383 .2581		
3	$\frac{\beta}{2}0$ \mathbf{s}_1 $\overline{B_2}$	-0.0026 .2446 .2542	0.0067 .2556 .2336	-0.0066 .2486 .2605	-0.0021 .2466 .2615	-0.0029 .2571 .2622		
4	$\mathbf{B}_{\mathbf{O}}$ $\beta_{\rm L}$ $\frac{6}{3}$	-0.0027 -2076 .2544 .0491	0.0067 .2515 .2335 .0055	-0.0067 .2340 .2608 .0194	-0.0017 .2341 .2609 .9167	-0.0030 .2872 .2623 $-.0399$		
5	$\frac{80}{81}$ $\frac{82}{83}$ $\frac{3}{4}$ 5	-0.0113 .2081 .2926 .0486 $-.0300$	0.0077 .2518 .2279 .0052 .0049	0.0111 .2332 .2845 .0203 -.0200	0.0063 . 2394 .2061 .0101 .0496	-0.0062 .2873 .2774 $-.0401$ -.0121		
6	$\beta_{\rm O}$ β_1 β_2 β_3 βŽ B_{5}	-0.0118 .2164 .2949 .0130 - 0317 .0270	0.0047 .3128 .2455 $-.2307$ $-.0098$.1773	-0.0100 .2432 .2801 $-.0225$ $-.0168$.0328	0.0061 .2386 .2070 .0134 .0490 $-.0026$	-0.0073 .2682 .2819 .0405 $-.0155$ $-.0618$		
	PO P_1 P2 P ₃ P4 P ₅ P_6 P ₇ Pя Pg	0.178 .004 .314 .004 .010 0 .022 .296 0 .172	0.136 .064 .206 .036 .014 .092 .004 .190 .104 . 154	0.148 .028 .198 .092 .038 .014 .012 .280 .026 .164	0.116 .070 .086 .112 .110 .024 .022 . 288 .014 .158	0.168 .012 .282 .018 .014 .016 .002 .304 .010 .174		

TABLE 7. - L = 6, i^{*} = 3

The values of the posterior probabilities and parameter means after five simulations, of 500 observations each, of the sequential selection procedure. Also listed are the proportions of the times each a⁽ⁱ⁾ was chosen as the optimal experiment.

÷.

t,

Nodel	Param	After 100 observations						After first 100 of 500 observations				
ı \bar{z} $\overline{\mathbf{3}}$ 4 $\mathsf S$ 6 ₁	$\frac{6}{3}$ $\frac{1}{8}$ $\frac{2}{3}$ $\frac{3}{4}$ $\frac{6}{9}$ 5 $\frac{5}{6}$	0 0 .945 .043 .007 .004	$\mathbf{0}$ 0 .942 .043 .012 .003	0 $\mathbf{0}$.956 .038 .005 .001	Ω .021 .895 .063 .015 .006	Ω .042 .848 .042 .033 .035	\mathbf{O} Ω .943 .048 .007 .002	0 Ω .877 .106 .013 .004	0 .011 .852 .089 .035 .013	$\mathbf{0}$.003 .904 .070 .018 .006	0 .026 .857 .076 .028 .013	
$\mathbf{1}$	Åŋ.	0.1502	-0.0299	0.0231	-0.0079	0.0034	\mathbf{r}_f	*	\mathbf{r}	\star	\star	
$\overline{2}$	$\frac{\beta}{2}$ 0 s_1	0.0356 .5159	0.0189 .5101	0.0288 .5123	0.0316 .5079	0.0431 .5106	\star	\star	\star	\star	\star	
$\overline{3}$	B_0 $\frac{61}{62}$	-0.0348 .5040 .1457	-0.0413 .5077 .1265	-0.0412 .509 _o .1478	-0.0098 .5084 .0837	0.0026 .5133 $.0850$ \circ	\star	\star	\star	$\pmb{\star}$	¥	
$\ddot{4}$	$\frac{60}{61}$ $\frac{61}{62}$ $\frac{3}{3}$	-0.0333 .4874 ,1450 .0217	-0.0396 .5288 .1252 $-.0261$	-0.0414 .5019 .1478 .0099	-0.0070 .5513 .0810 $-.0456$	0.0026 .5146 .0849 $-.0016$	¥,	¥ õ	\mathbf{r}_c	\mathbf{k}	\ast	
$\overline{5}$	$\frac{6}{2}0$ $\frac{81}{62}$ $\frac{83}{64}$	-0.0232 .4985 .0642 .0101 .0774	-0.0242 .5201 $-.0063$ -0185 .1223	-0.0431 .5039 .1616 -0074 $-.0131$	-0.0041 .5516 .0184 $-.0463$.0605	0.0161 .4861 $-.1260$.0235 -2068	\star	\star	\star	\star	\star	
6	8018183 883345	-0.0298 .6005 .1187 $-.3836$.0292 .3037	-0.0234 .5398 $-.0120$ $-.1048$.1270 .0673	-0.0435 .5233 .1655 $-.0708$ $-.0167$.0599	-0.0067 .5143 .0517 .1797 .0301 $-.1893$	0.0135 .3504 $-.0226$.6034 .1071 $-.4432$	\star	$\pmb{\star}$	\mathbf{r}	\mathbf{k}	\star	
	P ₀ P ₁ P_2 $\frac{p_3}{p_4}$ $\frac{P_5}{P_6}$ Ρž P_8 p ₉	0.10 .05 .08 .04 .08 .08 .08 . \mathfrak{U} .22 .16	0.16 .06 -20 .05 .13 .08 .04 .10 .02 .16	0.14 .07 .15 .07 .08 .10 .06 .09 .10 .14	0.24 .02 .03 .07 .26 $.12\,$.02 .03 ٥ .21	0.18 -13 -03 .02 .18 -19 .03 .05 .01 .18	0.18 .25 .06 .01 .16 .07 -03 -09 .06 .09	0.14 .04 -17 .06 .06 .17 0 .19 .03 .14	0.17 .02 .04 .01 .10 .25 o .19 .01 -21	0.18 .01 .25 .03 .10 .06 .14 .05 .01 .17	0.22 .01 .02 O. .05 .41 .01 .02 0 .26	

TABLE 8. - L = 6, i^{*} $= 5$

 k Not recorded.

The values of the posterior probabilities and parameter means after 10 simulations, of 100 observations each, of the sequential selection procedure. The last 5 columns are data from the first 100 observations of the 500 o

TABLE 9. - L = 6, $i^* = 5$

The values of the posterior probabilities and parameter means after five simulations, of 500 observations each, of the sequential selection procedure. Also listed are the proportions of the times each $\,$ a⁽ⁱ⁾ was chosen as the optimal experiment.

117

TABLE 10. - LARGE SAMPLE **STUDY** TWO

 $^{\circ}$

The values of the posterior probabilities and parameter means after five simulations, of 500 observations each, of the sequential selection procedure with three different
pri_{st} distributions on the models.

 $\bar{\mathcal{A}}$

 \bullet

TABLE 11. - LARGE SAMPLE STUDY THREE

The posterior probabilities and posterior parameter means after five simulations of the sequential selection procedure for three different values of the $i \neq 100.0$ and $t = 1.0$ the number of trials until $\theta_{1,j} = 1.0$ (

 $\mathcal{A}_{\mathcal{A}}$

TABLE 12. - SMALL SAMPLE STUDY ONE (H₃ TRUE)

*Not recorded.

Resulting-PCS and ASN values for **JMAX** ⁼**8.** and the combinations of $\theta_{\sf m}$, $\sf r$, and $\widehat{\mathfrak{u}}_{3,0}$. Results are based upon 1500 simulations of the procedure for each combination.

120

TABLE 13. - SMALL SAMPLE STUDY ONE $(H_3$ TRUE)

"MAX ∸∾⊥									
$\uptheta_{\rm m}$	T	$\overline{\overline{P}}$ ₃ ,0	PCS	ASN	Starting value for random seq.				
0.70	0.5	(0, 0)	0.354	9.48	272	036	225	461	
.70	\cdot 5	(0.5, 0.5)	.665	10.7	057	343	345	741	
.70	$\ddot{\textbf{5}}$	(1.0, 1.0)	.723	9.63	073	144	502	151	
.70	\cdot 5	(1, 5, 1.5)	-555	7.38	231	500	657	525	
.80	\cdot 5	(0, 0)	.508	13.6	033	254	034	051	
.80	\cdot 5	(0.5, 0.5)	.761	13.3	225	553	740	341	
.80	\cdot 5	(1.0, 1.0)	.806	12.3	134	537	257	651	
.80	\cdot 5	(1.5, 1.5)	.661	11.8	251	356	646	745	
.90	\cdot 5	(0, 0)	.574	15.5	056	537	424	615	
.90	\cdot 5	(0.5, 0.5)	.752	14.6	246	632	674	651	
.90	.5	(1.0, 1.0)	.800	13.9	140	077	157	311	
.90	\cdot 5	(1.5, 1.5)	.710	13.8	044	035	362	005	
.70	1.0	(0, 0)	.548	6.53	173	052	463	251	
.70	1.0	(0.5, 0.5)	.821	6.82	063	364	104	441	
.70	1.0	(1.0, 1.0)	.825	6.09	233	034	770	255	
.70	1.0	(1.5, 1.5)	.637	5.36	$\hat{\mathbb{D}}$ 017	237	125	325	
.80	1.0	(0, 0)	.808	9.48	275	264	535	015	
.80	$1.\dot{0}$	(0.5, 0.5)	.971	9.30	015	352	360	531	
-80	1.0	(1.0, 1.0)	.961	-8.16	017	142	770	505	
.80	1.0	(1.5, 1.5)	.865	7.86	004	724	275	765	
.90	1.0	(0, 0)	.927	12.1	161	027	043	101	
.90	1.0	(0.5, 0.5)	.973	10.8	101	732	737	651	
.90	1.0	(1.0, 1.0)	.964	10.1	016	351	614	135	
.90	1.0	(1.5, 1.5)	.958	10.6	171	716	572	235	
.70	2.0	(0, 0)	.700	4.25	073	021	660	321	
.70	2.0	(0.5, 0.5)	.878	4.17	003	466	340	375	
.70	2.0	(1.0, 1.0)	.855	3.59	337	170	131	645	
.70	2.0	(1.5, 1.5)	.714	3.51	055	666	256	215	
.80	2.0	(0, 0)	.911	5.67	037	537	412	725	
.80	2.0	(0.5, 0.5)	.990	5.12	111	525	350	761	
80	2.0	(1.0, 1.0)	.988	.4.84	003	413	673	201	
.80	2.0	(1.5, 1.5)	.894	4.71	055	643	644	455	
.90	2.0	(0, 0)	.996	7.13	374	543	153	375	
.90	2.0	(0.5, 0.5)	1.00	6.25	133	225	727	441	
.90	2.0	(1.0, 1.0)	1.00	5.94	332	405	117	171	
.90	2.0	(1.5, 1.5)	.995	6.20	010	312	536	461	

 $[J_1 = 16]$

Resulting PCS and ASN values for $J_{MAX} = 16$ and the combinations of **6m,** T, and **.3,0.** Results based upon 1000 simulations.

-

 τ $\begin{array}{|c|c|c|c|c|} \hline \tau&\vec{\mu}_{2,0} &\text{PCS} &\text{ASN} &\text{Starting value} \ \text{for random seq} \end{array}$ **m 2,0** for random seq. 0.70 0.5 (1.0) 0.760 7.86 052 516 237 355 .80 .5 (1.0) .734 7.98 016 160 602 721 .90 .5 (1.0) .740 7.98 245 577 171 655 .70 **1.0** (.5) .828 7.63 321 722 414 631 .70 1.0 **(1.0)** .882 7.20 340 **321** 470 071 .70 1.0 (1.5) .800 6.86 360 415 546 645 .80 **1.0** (1.0) .872 7.98 273 760 237 431 .90 **1.0** (.5) .880 7.97 006 761 404 325 .90 1.0 (1.0) .898 7.98 331 151 347 271 .90 **1.0** (1.5) ,832 7.99 372 024 174 011 .70 2.0 (1.0) .900 5.13 004 415 604 245 .80 2,0 (1.0) .936 7.89 063 456 575 211 .90 2.0 (1.0) .934 7.98 065 654 616 225

TABLE 14. - SMALL SAMPLE STUDY TWO $(H_2$ TRUE)

122

sequential procedure for each of the tabulated combinations of θ_m , τ , and $\tilde{\mu}_{2,0}$.

The PCS and ASN values resulting from 50Q simulations of the

 $[J_{MAX} = 8]$

TABLE 15. - SMALL SAMPLE STUDY THREE (FOUR MODEL PROBLEM)

 $[J,... = 8]$

Not recorded.

PCS and ASN values resulting from 1000 simulations performed for the indicated combinations of θ_m , τ , and $\tilde{\vec{p}}_3$ o

(DATA TAKEN FROM DRAPER AND SMITH)

 $\overline{}$

TABLE 17. - SUMMERY OF ANALYSIS OF EQUATION (7-1)

CETWE DATA OF TABLE 16

Replication menn square R,

TABLE 18a. - THE MODELS FOR EXAMPLE 1 $H_1: y = \beta_0 + \beta_1 z_4 + \beta_2 z_3 z_4 + \varepsilon$ H_2 : $y = \beta_0 + \beta_1 z_4 + \beta_2 z_3 z_4$ + $\beta_3 z_1$ + $\beta_4 z_2$ + $\beta_5 z_3$ + ε H_3 : $y = \beta_0 + \beta_1 z_4 + \beta_2 z_3 z_4$ + $\beta_3 \bar{z}_1$ + $\beta_4 \bar{z}_2$ + $\beta_5 \bar{z}_3$ + $\beta_6 z_2^2$ + $\beta_7 z_3^2$ + $\beta_8 z_1 z_4$ + ϵ H_4 : $y = \beta_0 + \beta_1 z_4 + \beta_2 z_3 z_4$ + $\beta_3 z_1 + \beta_4 z_2 + \beta_5 z_3$ + $\beta_6 z_2^2$ + $\beta_7 z_3^2$ + $\beta_8 z_1 z_4$ + $\beta_9 z_1^2$ + $\beta_{10} z_1 z_2$ + $\beta_{11} z_1 z_3$ + $\beta_1 z_2 z_3$ + $\beta_{13}z_2z_4$ + $\beta_{14}z_4^2$ + ε

TABLE **18b.** - THE PRIOR **MEANS** FOR EMAMPLE 1

TABLE 18c. **-** THE MATRIX FROM WHICH $\Psi_{\hat{\mathbf{x}},0}$ MAY BE TAKEN

. ,