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SOME RESULTS ON DESIGNS FOR REGRESSION EXPERIMENTS, DESIGN OF EXPERIMENTS WITH AUTOCORRELATED ERRORS PRESENT, AND DECISION THEORY APPROACH TO COMPLEX EXPERIMENTATION

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CANOGA PARK, CALIFORNIA

JUNE 1963

AERONAUTICAL RESEARCH LABORATORIES
OFFICE OF AEROSPACE RESEARCH
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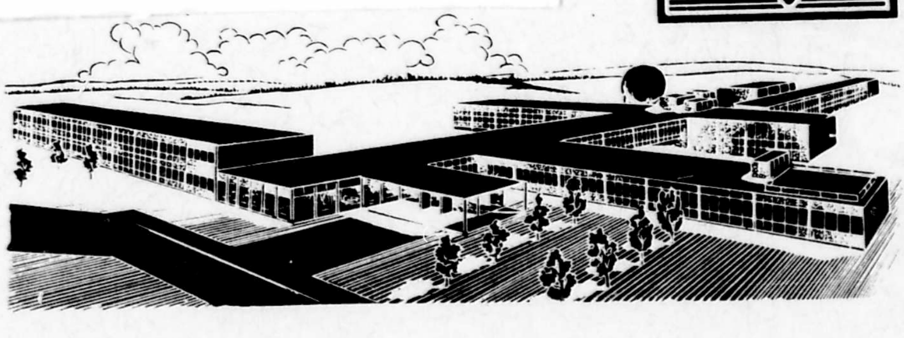

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FOREWORD

This interim technical report was prepared by Rocketdyne, A Division of North American Aviation, Inc., Canoga Park, California, for the Aeronautical Research Laboratories, Office of Aerospace Research. The research was done under Project No. 7071, Mathematical Techniques of Aeromechanics and Task No. 7071-01, Research in Mathematical Statistics and Probability Theory, on Contract No. AF33(616)-7372 entitled "Research on Statistical Design of Complex Experimental Programs", under the cognizance of Dr. H. Leon Harter of the Applied Mathematics Research Laboratory of ARL.

This report is divided into three segments. Part I is entitled "Designs for Regression Experiments" and was written by Dr. Madeline Alexander and Dr. Steve Webb. The first two sections of Part I deal with experimental designs based on regression models in which the cost of an experimental run depends on the point at which the run is made. The work is an extension of the research reported on in Ref. (1) and was done by Dr. Alexander and Dr. Webb. The third section reports on the work of Mr. Kenneth W. Last in the area of expansible-contractible designs.

Part II is the work of Dr. N. R. Goodman and is entitled "Design of Experiments with Autocorrelated Errors Present". It represents a continuation of Dr. Goodman's research reported on in Ref. (6).

The third part, entitled "The Decision Theory Approach to Complex Experimentation", is the work of Dr. Mitchell O. Locks. It is an extension of research work previously reported on in Ref. (2). Included are the results of computer simulation runs of the variable configuration model and a formulation of the associated dynamic programming problem.

ABSTRACT

Results of research conducted during the period 15 February 1962 - 14 February 1963 in the statistical design of complex experimental programs are reviewed. Included are discussions of the loss function methods for determining regression designs to minimize cost and variance (Part I), the design of experiments with autocorrelated errors (Part II), and applications of decision theory and dynamic programming to the design of reliability growth programs (Part III).

TABLE OF CONTENTS

LIST OF TABLES

LIST OF ILLUSTRATIONS

PART I

DESIGNS FOR REGRESSION EXPERIMENTS

INTRODUCTION

The loss function approach described in Ref. (1) has led to several interesting results in special cases. However, inherent mathematical difficulties have prevented obtaining satisfactory solutions in the general case of designs based on regression models with an arbitrary number of variables. Consequently, in recent months two new approaches to the problem have been taken. In place of a variance plus cost form for the loss function previously considered we have directed attention to

(1) a new form for the loss function

(2) minimization of the variance for fixed cost.

A new form of loss function which has intuitive appeal is the ratio of cost to quality of a design, or the product of the cost of an experimental design and the average variance obtained by using the design. As was done with the cost plus quality loss function in Ref. (1), it is assumed that the cost is expressible as a quadratic form in the independent variables. The variance term used here is the variance of a predicted true response averaged with respect to a (finite) measure of interest. By the use of this approach several interesting results have been obtained, among them a general necessary and sufficient condition that the optimum design be orthogonal, and explicit computations of the optimum designs for simple cost structures.

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The second approach is to minimize a variance term subject to fixed cost, i.e., to find the best design to fit a fixed budget. It can also be considered as minimizing the cost with the variance fixed, i.e., finding the least expensive design maintaining a fixed quality. The cost function that has been considered is quite general. The variance term is the variance of a predicted true response at the point of maximum interest. Under these assumptions, necessary conditions for a design to minimize the variance term have been derived in an important special case. A general proof that any design satisfying these conditions provides an absolute minimum variance has not as yet been obtained.

Finally, consideration has been given to the generation of designs which are appropriate for prematurely halted experiments. For problems of this type, a large class of designs have been derived which have the property that they may be expanded or contracted by one factor at a time.

THE PRODUCT LOSS FUNCTION APPROACH

Suppose the expected value of the response in an experiment depends on $m + 1$ unknown parameters $\beta_0, \beta_1, \ldots, \beta_m$, and is given by $y = \sum_{i=0}^{m} x_i\beta_i \equiv x'\beta$. The independent variable x_0 is usually taken to be identically equal to 1. Suppose the cost of an experiment at the point x is expressible as the positive definite quadratic form $x'Cx$, where the "cost matrix" $C = \{c_{ij}\}$ is known. An experimental design may be considered as a finite measure $\mu(x)$ over the space of possible vectors x. Let $A = \{a_{ij}\}$ be the cross-product matrix of the design, that is the matrix such that a_{ij} is given by $a_{ij} = \int x_i x_j d\mu(x)$. Suppose $\nu(x)$ is a measure of prior interest and suppose that the quality of a design is defined as the reciprocal of the variance of a predicted true response averaged with respect to ν. Using as a loss function the ratio of cost to quality, the loss for a design μ may therefore be written as the cost times the average variance, or

$$L(\mu) = \int x'Cxd\mu \cdot \int x'Bxd\nu ,$$

where $B = A^{-1}$.

Without loss of generality the independent variables may be linearly transformed by using the moments of ν so that $\int x'Bxd\nu$ reduces to trace B. By expanding the quadratic form and integrating, $\int x'Cxd\mu$ may be expressed in the form $\sum_{i=0}^{m} \sum_{j=0}^{m} c_{ij}a_{ij}$. Therefore, $L(\mu)$ depends on μ only through A, and may be written

$$L(A) = (\Sigma\, c_{ij}a_{ij})(\Sigma\, b_{ii}) .$$

In most practical regression problems the independent variables are functionally related. For example, x_3 may be x_1^2 and x_4 may be $x_1 x_2$. For our present purposes we will try to find designs to minimize L without such restrictions. If for a given regression model a solution we obtain satisfies the given restrictions, then we have indeed found the best design. If the general solution does not satisfy the restrictions, then the problem of finding the best design must be done separately for the particular situation.

The Connection Between the Product Loss Function and Minimizing Variance with Cost Fixed

If the first independent variable x_0 is identically equal to one, the parameter β_0 is called the grand mean. If an experiment has N runs, then the element a_{00} of the cross-product matrix A is equal to N.

Theorem 1. The loss L(A) can be written in a form which is independent of N. Therefore, the A which minimizes L can only be determined up to a multiplicative constant.

Proof. Write L in the form $L = K \cdot V$, where K is the cost term $\Sigma a_{ij} c_{ij}$, and V is the variance term trace B. Suppose every element of A is divided by $a_{00} = N$. Then K is also divided by N, as are the eigenvalues of A. Call these eigenvalues $\lambda_0, \ldots, \lambda_m$. But V is just the sum $\sum_{i=0}^{m} 1/\lambda_i$, so that V is multiplied by N.

The significance of this theorem is that two designs for which the moment matrices are proportional are equivalent. Therefore, an optimum experiment may be doubled and the resulting experiment is still optimum. In view of Theorem 1, we have the following corollary which shows the connection between minimizing L and minimizing the variance for fixed cost.

Theorem 2. Among the class of designs for which L is minimized is one which minimizes $\int x'Bxd\nu$ subject to the restriction that $\int x'Cxd\mu$ be fixed.

Proof. By Theorem 1 if there exists a design which minimizes L then there is a minimal solution for any value of N. If the cost K is to be fixed, it is an easy task to solve for the N which will give the optimum design with the given fixed cost. Since cost K is fixed and KV is minimized, V is minimized.

Optimum Designs for Simple Cost Structures

We turn our attention to the explicit computation of designs which minimize L. We consider the cases where the cost matrix C is diagonal and where it has one non-zero off-diagonal entry. It is a well known result that subject to the restriction that the columns of the design matrix be of fixed length, orthogonal designs minimize variances of the individual parameter estimates. An analogous result holds in the present context if C is diagonal.

Theorem 3. An orthogonal design minimizes L if and only if C is diagonal. If C is diagonal, L is minimized when $a_{ii}\sqrt{c_{ii}}$ is a constant.

Proof. We will prove that if C is diagonal the given orthogonal design minimizes L. The proof of the converse will be deferred until after the proof of Theorem 4. If C is diagonal then K does not involve the off-diagonal elements of A. It is a consequence of the fact stated before the statement of the theorem that for fixed diagonal elements of A, trace B is minimized if A is diagonal. Therefore, no matter what the values of the a_{ii} are, L can be decreased by forcing the off-diagonal terms a_{ij} to zero. If A is diagonal, L equals $(\Sigma_i a_{ii}c_{ii})(\Sigma_i 1/a_{ii})$. Let a_{jj} be one of the a_{ii} and write $L = a_{jj}c_{jj}(\Sigma_{i\neq j} 1/a_{ii}) + c_{jj} + (\Sigma_{i\neq j}a_{ii}c_{ii})/a_{jj} + (\Sigma 1/a_{ii})(\Sigma a_{ii}c_{ii})$. As a_{jj}

approaches zero or infinity L becomes infinite, and, as a function of a_{jj}, L has one minimum for positive a_{jj}. Therefore, the minimum can be found by setting equal to zero the partial derivatives of L with respect to the a_{ii}. For all i we have $c_{ii}V - K/a_{ii}^2 = 0$, or $a_{ii}\sqrt{c_{ii}} = \sqrt{K/V}$. This expression holds for any i and the right hand side is independent of i. Since by Theorem 1 we can only hope to determine the elements of A up to a multiplicative constant, we have as a solution $a_{ii}\sqrt{c_{ii}}$ equals a constant for all i.

The condition that C be diagonal implies that the point of minimum cost coincides with the point of maximum interest. This is, of course, not realistic in many practical situations. A situation which is a little more general is one in which the point of minimum cost is displaced along one axis from the point of maximum interest. This case is covered by the following theorem.

Theorem 4. If one of the off-diagonal elements of C, say c_{01}, is non-zero and the remaining off-diagonal terms are zero, then the design which minimizes L has $a_{00}(\Delta\sqrt{c_{00} + c_{11} + 2\Delta})/(c_{11} + \Delta)$, $a_{11}(\Delta\sqrt{c_{00} + c_{11} + 2\Delta})/(c_{00} + \Delta)$, $-a_{01}(\Delta\sqrt{c_{00} + c_{11} + 2\Delta})/c_{01}$, and $a_{ii}\sqrt{c_{ii}}$, for $i > 1$, equal to the same constant, where $\Delta = \sqrt{c_{00}c_{11} - c_{01}^2}$, and the remaining off-diagonal terms are zero.

Proof. Since K does not involve any of the off-diagonal entries except a_{01}, we may conclude that the remaining off-diagonal elements of A are zero by an argument analogous to that used in the proof of Theorem 3. Setting the partial derivatives of L equal to zero we have

$$K = (a_{00}c_{00} + a_{11}c_{11} + 2a_{01}c_{01} + \Sigma_{i=2}^{m} a_{ii}c_{ii})$$

$$V = \frac{a_{00} + a_{11}}{a_{00}a_{11} - a_{01}^2} + \frac{1}{a_{22}} + \cdots + \frac{1}{a_{mm}}$$

$$\frac{\partial KV}{\partial a_{00}} = c_{00}V - K\frac{a_{01}^2 + a_{11}^2}{(a_{00}a_{11} - a_{01}^2)^2} = 0$$

$$\frac{\partial KV}{\partial a_{11}} = c_{11}V - K\frac{a_{00}^2 + a_{01}^2}{(a_{00}a_{11} - a_{01}^2)^2} = 0$$

$$\frac{\partial KV}{\partial a_{01}} = 2c_{01}V + 2K\frac{a_{01}(a_{00} + a_{11})}{(a_{00}a_{11} - a_{01}^2)^2} = 0$$

$$\frac{\partial KV}{\partial a_{ii}} = c_{ii}V - K/a_{ii}^2 = 0, \quad i > 1 .$$

Letting K/V be constant, we have

$$a_{ii}\sqrt{c_{ii}} = \sqrt{K/V}, \quad i > 1,$$

$$c_{00}D^2 = (K/V)(a_{11}^2 + a_{01}^2)$$

$$c_{11}D^2 = (K/V)(a_{00}^2 + a_{01}^2)$$

$$-c_{01}D^2 = (K/V)(a_{00} + a_{11})a_{01},$$

where $D = a_{00}a_{11} - a_{01}^2$. Eliminating D and K/V from the last three equations, we obtain

$$a_{01}^2 = \frac{-c_{00}a_{00}^2 + c_{11}a_{11}^2}{c_{00} - c_{11}} \quad \text{and}$$

$$c_{01}a_{01}^2 + c_{00}(a_{00} + a_{11})a_{01} + c_{01}a_{11}^2 = 0.$$

Substituting for a_{01} in the latter equation and squaring, we have

$$c_{00}^2(a_{00} + a_{11})^2\left(\frac{c_{11}a_{11}^2 - c_{00}a_{00}^2}{c_{00} - c_{11}}\right) = c_{01}^2\left(\frac{c_{11}a_{11}^2 - c_{00}a_{00}^2}{c_{00} - c_{11}} + a_{11}^2\right)^2 ,$$

which becomes $c_{00}^2(a_{00} + a_{11})^2(c_{11}a_{11}^2 - c_{00}a_{00}^2)(c_{00} - c_{11}) = c_{01}^2c_{00}^2(a_{11}^2 - a_{00}^2)^2$.

The solution $a_{00} + a_{11} = 0$ is not acceptable and may be discarded, yielding $(c_{11}a_{11}^2 - c_{00}a_{00}^2)(c_{00} - c_{11}) = c_{01}^2(a_{11} - a_{00})^2$. Rearranging terms and solving for a_{00} we obtain

$$a_{00} = \frac{c_{01}^2 \pm \Delta(c_{00} - c_{11})}{c_{00}^2 - \Delta^2} \cdot a_{11},$$

where $\Delta = +\sqrt{c_{00}c_{11} - c_{01}^2}$. Taking first the positive and then the negative sign, we have $a_{00}^{(1)} = a_{11}(c_{11} + \Delta)/(c_{00} + \Delta)$ and $a_{00}^{(2)} = a_{11}(c_{11} - \Delta)/(c_{00} - \Delta)$. To these two solutions correspond two values of a_{01}^2, namely $a_{01}^2 = a_{11}^2 c_{01}^2/(c_{00} \pm \Delta)^2$, with the plus and minus signs being associated with $a_{00}^{(1)}$ and $a_{11}^{(2)}$, respectively. Substituting back into the equation $c_{00}D^2 = (K/V)(a_{01}^2 + a_{11}^2)$, we obtain the equation

$$c_{00}a_{11}^4\left(\frac{c_{11} \pm \Delta}{c_{00} \pm \Delta} - \frac{c_{01}^2}{(c_{00} \pm \Delta)^2}\right)^2 = (K/V)a_{11}^2\left(1 + \frac{c_{01}^2}{(c_{00} \pm \Delta)^2}\right) .$$

The solution $a_{11} = 0$ is not acceptable and may be discarded, yielding $a_{11}^2\Delta^2(c_{00} + c_{11} \pm 2\Delta) = (K/V)(c_{00} \pm \Delta)^2$. We must now find out (i) whether the plus or the minus sign should be associated with Δ, (ii) whether the positive or the negative square root should be taken in the expression for a_{11}, and (iii) whether the positive or the negative square root should be taken in the expression for a_{01}. The determinant D must be positive; it is given by

$$D = \frac{\pm \Delta(c_{00} + c_{11} \pm 2\Delta)}{(c_{00} \pm \Delta)^2} \cdot a_{11}^2 = \frac{\pm \Delta\, (K/V)}{\Delta^2} .$$

Therefore, the plus sign must be associated with Δ. Since a_{11} must be positive, the positive square root must be taken in the solution for a_{11}. Finally, in order to satisfy the equation $-c_{01}D^2 = (K/V)(a_{00} + a_{11})a_{01}$, the negative square root must be taken in the expression for a_{01}. Therefore, we have

$$a_{11} = \frac{\sqrt{K/V}(c_{00} + \Delta)}{\Delta\sqrt{c_{00} + c_{11} + 2\Delta}} ,$$

$$a_{00} = \frac{\sqrt{K/V}(c_{11} + \Delta)}{\Delta\sqrt{c_{00} + c_{11} + 2\Delta}} , \text{ and}$$

$$a_{01} = \frac{-\sqrt{K/V}\, c_{01}}{\Delta\sqrt{c_{00} + c_{11} + 2\Delta}} .$$

This is the only permissible extremum. Since L becomes infinite as any of the a_{ij} become infinite it cannot be a maximum; hence this design yields the unique minimum for L.

In view of Theorem 4, which did not depend on Theorem 3, we can now easily prove the converse of Theorem 3.

Proof of Converse of Theorem 3. Suppose C is not diagonal. By rearranging the rows and columns of C we may let c_{01} be one of the non-zero off-diagonal entries. Then by Theorem 4, the design mentioned in the statement of Theorem 4 has a lower value for L than the best orthogonal design.

Recommendations and Conclusions

This approach appears to have promise. The results obtained thus far have been obtained with a great deal of computational difficulty, but appear interesting and capable of generalization. The two cases considered in detail, where the cost matrix C is diagonal and where it contains a single non-zero off-diagonal entry, should cover a fair number of practical situations. Therefore, it would appear to be advisable to continue the present line of attack.

THE GENERALIZED FIXED-COST APPROACH

Introduction

In our previous work, only cost functions which are quadratic forms in the independent variables have been considered. This may not be realistic in some situations, and in this section we will develop an approach for a wider class of cost functions.

The goal will be to find those designs which minimize the variance of the predicted true response at a point of maximum interest, subject to the condition that the total cost of the experiment be fixed. One may derive necessary conditions for such designs in the most general case, but the resulting expressions are complex and hard to interpret.

Instead, we shall consider the important special case in which the possible levels of the variables are specified in advance, and it is desired to determine the optimum number of replications of each treatment combination for minimization of the variance under fixed cost. In this case, interesting necessary conditions are obtained and an example of an optimum design is given.

Additional studies of this type are planned for future work.

Formulation of the Problem

We consider again experimental designs based on a linear regression model with m independent variables. To avoid double subscripts we denote these variables by $x, y, z, \ldots$, so that the response Y is represented by the model

$$Y = \beta_0 + \beta_1 x + \beta_2 y + \cdots + \epsilon, \qquad (1)$$

where ϵ is a normal, zero-mean random variable with variance σ^2.

Given an experiment with tests at the points $(x_1, y_1, \dots)$; $(x_2, y_2, \dots), \dots, (x_N, y_N, \dots)$, the variance of the predicted true response at the point $\underline{x} = (1, x, y, \dots)'$ is given by

$$V = \underline{x}'(X'X)^{-1}\underline{x}\,\sigma^2 , \tag{2}$$

where $X'X$ is the information matrix of the design. It is convenient for subsequent calculations to write the variance in the form

$$V = \sigma^2\{c_0 + x_0 x + y_0 y + \dots\} , \tag{3}$$

where the $m + 1$ quantities $c_0, x_0, y_0, \dots$ are determined from the $m + 1$ equations

$$\begin{aligned} Nc_0 + S_x x_0 + S_y y_0 + \dots &= 1 \\ S_x c_0 + S_{xx} x_0 + S_{xy} y_0 + \dots &= x \\ S_y c_0 + S_{xy} x_0 + S_{yy} y_0 + \dots &= y \\ \vdots \qquad\qquad &\quad \vdots \end{aligned} \tag{3'}$$

and $S_x = \sum_{i,j\dots} n_{ij\dots} x_i$, $S_{xy} = \sum_{i,j\dots} n_{ij\dots} x_i y_j$, etc.

We suppose that experiments are to be performed at t levels of each of the variables $x, y, \dots$ and consider the cost function in the form

$$C = \sum_{i,j,\dots=1}^{t} n_{ijk\dots} f(x_i, y_j, \dots) \tag{4}$$

where $f(x_i, y_j, \dots) \geq 0$ in the region of interest, and $n_{ijk\dots}$ represents the number of tests at treatment combination $(x_i, y_j, z_k, \dots)$. The $n_{ijk\dots}$ to minimize (2) are to be found.

Since C is fixed Eq. (4) determines one of the $n_{ijk...}$, say $n_{111...}$, in terms of C and the remaining $n_{ijk...}$. For simplicity we will consider here the case $m = 2$; the procedure in the general case is completely analogous.

From the cost equation (4) we have

$$- n_{11} f(x_1, y_1) = \sum_{i,j}{}' n_{ij} f(x_i, y_j) - C , \tag{5}$$

where the sum Σ' omits the combination $i = j = 1$. But since n_{11} is a function of the remaining n_{ij} and C, we have

$$f(x_i, y_j) = - f(x_1, y_1) \frac{\partial n_{11}}{\partial n_{ij}}$$

or

$$\frac{\partial n_{11}}{\partial n_{ij}} = - \frac{f(x_i, y_j)}{f(x_1, y_1)} \tag{6}$$

for all i, j except $i = j = 1$.

Since V is to be minimized, we must have $\frac{\partial V}{\partial n_{ij}} = 0$

or, from Eq. (3)

$$\frac{\partial V}{\partial n_{ij}} = \left[\frac{\partial c_0}{\partial n_{ij}} + x \frac{\partial x_0}{\partial n_{ij}} + y \frac{\partial y_0}{\partial n_{ij}} \right] \sigma^2 = 0 . \tag{7}$$

Then replacing n_{11} in Eq. (3') by means of Eq. (5) and differentiating, one obtains

$$N \frac{\partial c_0}{\partial n_{ij}} + S_x \frac{\partial x_0}{\partial n_{ij}} + S_y \frac{\partial y_0}{\partial n_{ij}} = - c_0 - x_0 x_i - y_0 y_j - (c_0 + x_0 x_1 + y_0 y_1) \frac{\partial n_{11}}{\partial n_{ij}}$$

$$S_x \frac{\partial c_0}{\partial n_{ij}} + S_{xx} \frac{\partial x_0}{\partial n_{ij}} + S_{xy} \frac{\partial y_0}{\partial n_{ij}} = -c_0 x_i - x_0 x_i^2 - y_0 y_j x_i - (c_0 x_1 + x_0 x_1^2 + y_0 y_1 x_1) \frac{\partial n_{11}}{\partial n_{ij}}$$

$$S_y \frac{\partial c_0}{\partial n_{ij}} + S_{xy} \frac{\partial x_0}{\partial n_{ij}} + S_{yy} \frac{\partial y_0}{\partial n_{ij}} = -c_0 y_j - x_0 x_i y_j - y_0 y_j^2 - (c_0 y_1 + x_0 x_1 y_1 + y_0 y_1^2) \frac{\partial n}{\partial n_{ij}} \quad . \tag{8}$$

In equations (7) and (8) there are four equations in the three unknowns $\frac{\partial c_0}{\partial n_{ij}}, \frac{\partial x_0}{\partial n_{ij}}, \frac{\partial y_0}{\partial n_{ij}}$; therefore the 4×4 determinant of coefficients must be zero; i.e.,

$$\begin{vmatrix} 1 & x & y & 0 \\ N & S_x & S_y & (c_0+x_0x_i+y_0y_j) + (c_0+x_0x_1+y_0y_1)\, \partial n_{11}/\partial n_{ij} \\ S_x & S_{xx} & S_{xy} & (c_0x_i+x_0x_i^2+y_0x_iy_j) + (c_0x_1+x_0x_1^2+y_0x_1y_1)\, \partial n_{11}/\partial n_{ij} \\ S_y & S_{xy} & S_{yy} & (c_0y_j+x_0x_iy_j+y_0y_j^2) + (c_0y_1+x_0y_1x_1+y_0y_1^2)\, \partial n_{11}/\partial n_{ij} \end{vmatrix} = 0$$

The determinant can be expanded in terms of the last column. If this is done, and the solution of the system (3') is written in determinant form (e.g. using Cramer's rule) one obtains

$$c_0(c_0 + x_0 x_i + y_0 y_j) + c_0(c_0 + x_0 x_1 + y_0 y_1) \frac{\partial n_{11}}{\partial n_{ij}} +$$

$$x_0(c_0 x_i + x_0 x_i^2 + y_0 x_i y_j) + x_0(c_0 x_1 + x_0 x_1^2 + y_0 x_1 y_1) \frac{\partial n_{11}}{\partial n_{ij}} + \tag{9}$$

$$y_0(c_0 y_j + x_0 x_i y_j + y_0 y_j^2) + y_0(c_0 y_1 + x_0 x_1 y_1 + y_0 y_1^2) \frac{\partial n_{11}}{\partial n_{ij}} = 0 \ .$$

On simplification, Eq. (9) yields

$$(c_0 + x_0x_i + y_0y_j)^2 = -(c_0 + x_0x_1 + y_0y_1)^2 \frac{\partial n_{11}}{\partial n_{ij}} . \tag{10}$$

Substituting from Eq. (6) for $\frac{\partial n_{11}}{\partial n_{ij}}$ gives

$$(c_0 + x_0x_i + y_0y_j)^2 = (c_0 + x_0x_1 + y_0y_1)^2 \frac{f(x_i,y_j)}{f(x_1,y_1)} \tag{11}$$

or

$$c_0 + x_0x_i + y_0y_j = (c_0 + x_0x_1 + y_0y_1) \sqrt{\frac{f(x_i,y_j)}{f(x_1,y_1)}} . \tag{12}$$

We see therefore that the variance at a treatment combination is proportional to the square root of the cost. For each pair of indices (i, j) an equation similar to (11) results. (Equation (12) for $i = j = 1$ is an immediate identity.) Multiplying each by n_{ij} and summing over the t levels of x and y we find

$$c_0N + x_0S_x + y_0S_y = \frac{c_0 + x_0x_1 + y_0y_1}{\sqrt{f(x_1,y_1)}} \sum_{j=1}^{t} \sum_{i=1}^{t} n_{ij} \sqrt{f(x_i,y_j)} . \tag{13}$$

Equation (12) can also be multiplied by $n_{ij}x_i$ or $n_{ij}y_j$ and summed, yielding

$$\begin{aligned} c_0S_x + x_0S_{xx} + y_0S_{xy} &= \frac{c_0 + x_0x_1 + y_0y_1}{\sqrt{f(x_1,y_1)}} \sum_{j=1}^{t} \sum_{i=1}^{t} n_{ij}x_i \sqrt{f(x_i,y_j)} \\ c_0S_y + x_0S_{xy} + y_0S_{yy} &= \frac{c_0 + x_0x_1 + y_0y_1}{\sqrt{f(x_1,y_1)}} \sum_{j=1}^{t} \sum_{i=1}^{t} n_{ij}y_j \sqrt{f(x_i,y_j)} . \end{aligned} \tag{14}$$

Using Eq. (3') and eliminating the factor $\frac{c_0 + x_0x_1 + y_0y_1}{\sqrt{f(x_1,y_1)}}$, we have finally

$$x\sum_{i,j} n_{ij} \sqrt{f(x_i,y_j)} = \sum_{i,j} n_{ij}x_i \sqrt{f(x_i,y_j)}$$

$$y\sum_{i,j} n_{ij} \sqrt{f(x_i,y_j)} = \sum_{i,j} n_{ij}y_j \sqrt{f(x_i,y_j)} \tag{15}$$

which are necessary conditions for a minimum.

We now construct a simple design which satisfies these necessary conditions. Suppose $n_{ij} \sqrt{f(x_i,y_j)} = K$, a constant, and consider design levels satisfying $\sum_1^t x_i = tx$, $\sum_1^t y_j = ty$, where (x,y) is the point of maximum interest. Then conditions (12) are satisfied. Indeed,

$$x\sum_{i=1}^{t}\sum_{j=1}^{t} n_{ij} \sqrt{f(x_i,y_j)} = x\sum_1^t\sum_1^t K = Kxt^2$$

$$\sum_{i=1}^{t}\sum_{j=1}^{t} n_{ij}x_i \sqrt{f(x_i,y_j)} = \sum_{i=1}^{t} x_i \cdot \sum_{j=1}^{t} K = Kt \cdot \sum_{i=1}^{t} x_i$$

and since

$$\sum_{i=1}^{t} x_i = xt,$$

$$x\sum_{i,j} n_{ij} \sqrt{f(x_i,y_j)} = \sum_{i,j} n_{ij}x_i \sqrt{f(x_i,y_j)} .$$

In a similar way it is easily seen that the second condition is satisfied.

A proof that the design specified above actually provides an absolute minimum (say by consideration of the second derivatives of the function V) has not as yet been completed. When this is accomplished, one will be able to conclude that when the mean of the design levels is the point of maximum interest, the optimum number of replications at each treatment combination is inversely proportional to the square root of the cost at that combination.

EXPANSIBLE AND CONTRACTIBLE DESIGNS

A design which can be expanded or contracted one factor at a time has two important areas of application:

(1) Suppose there is a high probability that a design may be prematurely stopped due to running out of time or money, or breakdown of equipment. If a contractible design is run, the most important main effects and interactions can still be estimated, conditionally on less important variables being fixed.

(2) Suppose that after an experiment has been carried out it is decided that a factor which was previously held fixed should be studied. If an expansible design was run for the initial experiment, the new factor can be introduced with a minimum of additional experimentation.

A wide class of expansible-contractible designs for factors at two levels can be derived from the Pascal triangle. The rows of the triangle represent the number of factors which are varied, with the $(n + 1)$-st row representing n factors. The entries in each row, from left to right, are the numbers of treatment combinations with exactly zero, one, two, ..., n factors at their high level. Consider such a triangle extended through seven rows:

$n = 0$	1							
$n = 1$	1	1						
$n = 2$	1	2	1					
$n = 3$	1	3	3	1				
$n = 4$	1	4	6	4	1			
$n = 5$	1	5	10	10	5	1		
$n = 6$	1	6	15	20	15	6	1	
$n = 7$	1	7	21	35	35	21	7	1

A selection of a set of columns, for example the first, second, and fourth, corresponds to a series of expansible-contractible designs. For one factor, the design consists of the treatment combinations 0 and 1. If a new factor is added which was at its low level in the previous experiment, the design consists of treatment combinations 00, 10, and 01, of which the first two have already been run. If a third factor is added, the design consists of runs at treatment combinations 000, 100, and 010, which have already been run, plus the new combinations 001 and 111. If a fourth factor is added, the runs 0000, 1000, 0100, 0010, and 1110 have been done and 0001, 1101, 1011, and 0111 remain to be done, and so forth.

These expansible-contractible designs form a subclass of the general class of permutation invariant designs introduced by Webb in Ref. (3). Designs of this latter general type need not be expansible-contractible in the sense described above. Webb, in Ref. (4), proposed several of the Pascal-triangle-based designs and showed that their efficiency with respect to orthogonal designs is often very high. In particular, Webb examined the design corresponding to the first, third, and sixth columns for $n = 6$ and the design corresponding to the first, third, and seventh columns for $n = 7$.

From the fact that the Pascal-triangle-based designs are permutation invariant it follows that the cross-product matrices are very easy to invert when they are non-singular. If only main effects are to be estimated only five constants must be evaluated to determine the inverse, no matter how many factors are included in the design. If main effects and two-factor interactions are to be estimated, the inverse involves the evaluation of at most ten constants, no matter how many factors are included. This feature of permutation invariant designs makes this particular class of expansible-contractible designs particularly appealing, and further study of their properties is planned.

PART II

DESIGN OF EXPERIMENTS WITH AUTOCORRELATED ERRORS PRESENT

INTRODUCTION

This part of the present interim report is a continuation of work done by Goodman, Ref. (6), and the reader is requested to refer to Ref. (6) for definitions and previous results. The problem stated in Ref. (6) was the following: Given the model

$$X(t) = \sum_{j=1}^{J} a_j S_j(t) + n(t) \tag{1}$$

where the observed record $X(t)$, $-T \leq t \leq T$, is a linear combination of known signals $S_j(t)$, $j = 1, \ldots, J$, (with the constants a_j, $j = 1, \ldots, J$ unknown) plus a zero-mean weakly stationary noise $n(t)$ (with the spectral density $s(\omega)$ of the noise $n(t)$ unknown), simultaneously "measure" (statistically estimate) the unknown constants a_j, $j = 1, \ldots, J$ and the spectral density $s(\omega)$ from the finite length $X(t)$, $-T \leq t \leq T$, of observed record.

In regard to the problem of the design of experiments with correlated errors, the design feature of the problem stated above enters by choosing (when a choice is possible) the known signals $S_j(t)$, $j = 1, \ldots, J$, in a rational or desirable manner. There exist practical problems where the experimenter does possess the opportunity of choosing (before an experiment is conducted) the known signals $S_j(t)$ from a set of permissible signals with the aim of simultaneously "measuring" (after the experiment is conducted) the unknown constants a_j and the unknown spectral density $s(\omega)$ of the noise $n(t)$. For example, in several practical problems the set of permissible signals $S_j(t)$ may be restricted to the trigonometric functions $[\cos\omega_j t, \sin\omega_j t]$ with the frequencies ω_j more or less arbitrary.

There also exist problems where the experimenter, or mathematical statistician, is confronted (after an experiment is conducted) with an observed record $X(t), \ -T \leq t \leq T$, with $X(t)$ satisfying the model stated in Eq. (1), where no a priori choice of the $S_j(t)$ was made or where no such choice was possible. In such problems one is in reality confronted with the problem of measuring the <u>signal component</u> $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. If the problem stated above is taken literally the $S_j(t)$, $j = 1, \ldots, J$, are known or given, and the problem of measuring the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ reduces to the problem of measuring the unknown constants a_j, $j = 1, \ldots, J$. A method for solving the problem under such ideal conditions is outlined in Ref. (6). However, in some problems of this type the $S_j(t)$, $j = 1, \ldots, J$, are rarely known exactly and in fact may be entirely unknown. In such situations measuring the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ is the real problem and we now turn our attention to this case. In order to utilize the method described in Ref. (6), it is necessary to make a choice (either explicitly or implicitly) of the appropriate $S_j(t)$ to use and in this way the design feature of the problem then enters. The present interim report is limited to a discussion of such design problems.

DESIGN PROBLEMS

In this section we consider the problem of measuring the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$.

<u>The Case where Little is Known about the $S_j(t)$, $j = 1, \ldots, J$</u>.

When little or perhaps no a priori knowledge about the $S_j(t)$ is available, one must in some sense measure (statistically estimate) the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ from the available finite observed record

$X(t)$, $-T \leq t \leq T$. Two methods will be discussed. In the first method the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ is described in the time domain and in the second method it is described in the frequency domain. For both cases, however, the measurement or statistical estimation procedures are carried out in the frequency domain utilizing the method summarized in Ref. (6). The reasons for conducting the measurement procedures in the frequency domain are discussed in Ref. (6).

Finally, a combined time domain and frequency domain description of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ is discussed. Again, the measurement or statistical estimation procedure is conducted in the frequency domain.

Time Domain Description of the Signal Component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. Let $T_0 = -T$, $T_J = T$, and select times $T_1, T_2, \ldots, T_{J-1}$ such that $T_0 < T_1 < T_2 < \ldots < T_{J-1} < T_J$. The time interval $-T \leq t \leq T$ is then partitioned into the J sub-intervals $T_0 \leq t < T_1$, ..., $T_{j-1} \leq t < T_j$, ..., $T_{J-1} \leq t \leq T_J$. The sub-intervals $T_{j-1} \leq t < T_j$, $j = 1, \ldots, J$ need not be of equal length.

The Case of Locally Constant Signals in the Time Domain. Perhaps the simplest description of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ to presuppose at the start of an investigation is that of a piecewise constant function. Thus, for the partition of the time interval $-T \leq t \leq T$ given above, we take in Eq. (1) $S_j(t) = 1$ for $T_{j-1} \leq t < T_j$ and $S_j(t) = 0$ elsewhere. The constants a_j, $j = 1, \ldots, J$, in Eq. (1) then are the piecewise constant values of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. The procedure to be used in measuring the constants a_j, $j = 1, \ldots, J$ is that described in Ref. (6). One notes that with the above choice, $S_j(t)$ is the characteristic function of the jth time interval, $j = 1, \ldots, J$, and one may expect (with the frequency domain statistical procedures indicated in Ref. (6)) to have the constants a_j, $j = 1, \ldots, J$, estimable from more than one or even from all the local frequency bands $\omega^{(1')} \leq \omega < \omega^{(2')}$ (see Ref. (6)). In this regard much depends on the time domain and frequency domain partitions employed. For the method just described to be reasonably effective in measuring the true signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ one needs (1) the true signal component essentially constant over the local time intervals of the partition of $-T \leq t \leq T$, and (2) the spectral density $s(\omega)$ of $n(t)$ essentially constant over the local frequency bands employed in the statistical estimation procedure.

The Case of Locally Linear Signals in the Time Domain. When the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ is not adequately described by a piecewise constant function, a next reasonable description is that of a piecewise linear function. Thus, for the partition of the time interval $-T \leq t \leq T$ given above, we take in Eq. (1) $a_j S_j(t) = a_{j0} + a_{j1} t$ for $T_{j-1} \leq t < T_j$ and $a_j S_j(t) = 0$ elsewhere $(j = 1, \ldots, J)$. The constants to be measured in order to describe the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ are now (a_{j0}, a_{j1}), $j = 1, \ldots, J$. The time domain partition used need not be the same one used above. For example, the number of local time intervals used may be fewer than employed in the previous case, although the number of constants (a_{j0}, a_{j1}), $j = 1, \ldots, J$, to be estimated may be the same.

The procedure to be used in measuring the constants (a_{j0}, a_{j1}), $j = 1, \ldots, J$, is that described in Ref. (6). With the choice of $a_j S_j(t)$, $j = 1, \ldots, J$, given above one may again expect to have the constants (a_{j0}, a_{j1}), $j = 1, \ldots, J$, estimable from more than one or even from all the local frequency bands $\omega^{(1')} \leq \omega \leq \omega^{(2')}$. For the method just described to be reasonably effective in measuring the true signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ one needs (1) true signal component essentially <u>linear</u> over the local time intervals of the partition of $-T \leq t \leq T$, and (2) the spectral density $s(\omega)$ of $n(t)$ essentially constant over the local frequency bands employed in the statistical estimation procedure.

<u>The Case of Locally Polynomial-Like Signals in the Time Domain</u>. Continuing along these lines one might more generally consider the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ to be a piecewise polynomial function of time t and proceed in an analogous fashion. In such cases, one need not use the same degree polynomial for each local time interval of the partition of $-T \leq t \leq T$.

More generally, one may introduce in any particular local time interval functions other than polynomials. For example, one may take $a_j S_j(t) = a_{j0}\phi_{j0}(t) + a_{j1}\phi_{j1}(t) + \ldots + a_{jp}\phi_{jp}(t)$ for $T_{j-1} \leq t < T_j$ and $a_j S_j(t) = 0$ elsewhere $(j = 1, \ldots, J)$ where the functions $[\phi_{j0}(t), \ldots, \phi_{jp}(t)]$, $j = 1, \ldots, J$, are appropriately chosen. Pilot studies or slight a priori knowledge of the phenomena being investigated will guide the selection of such alternative functions.

<u>Frequency Domain Description of the Signal Component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$.</u>

Using the notation of Ref. (6) let the total effective frequency band $0 \leq \omega \leq \omega_{max}$ be partitioned into sub-bands, and consider a particular sub-band denoted by $\omega^{(1)} \leq \omega < \omega^{(2)}$. From Ref. (6) one has

$$\Delta U_x(\omega_k) = \sum_{j=1}^{J} a_j \Delta U_j(\omega_k) + \Delta U_n(\omega_k) ,$$
$$\Delta V_x(\omega_k) = \sum_{j=1}^{J} a_j \Delta V_j(\omega_k) + \Delta V_n(\omega_k) , \quad k = 1, \ldots, K ; \qquad (2)$$

where the frequencies ω_k, $k = 1, \ldots, K$, $(\omega^{(1)} \leq \omega_1 < \omega_2 < \ldots < \omega_k < \ldots < \omega_K \leq \omega^{(2)})$ are equally spaced a frequency interval B apart. The spectral density $s(\omega)$ of $n(t)$ is taken to be essentially constant in the frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$. The random variables $\Delta U_n(\omega_k)$, $\Delta V_n(\omega_k)$, $k = 1, \ldots, K$ in Eq. (2) are then approximately uncorrelated and possess approximately the same variance. Furthermore, in Eq. (2) $\Sigma_{j=1}^{J} a_j \Delta U_j(\omega_k)$ is the real part of a finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ evaluated at the frequency $\omega = \omega_k$, and $\Sigma_{j=1}^{J} a_j \Delta V_j(\omega_k)$ is the imaginary part of a finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ evaluated at the frequency $\omega = \omega_k$. We now describe $\Sigma_{j=1}^{J} a_j S_j(t)$ by the real and imaginary parts of a finite Fourier transform of this signal component and direct attention to measuring (statistically estimating) such descriptions.

The Case of Locally Constant Finite Fourier Transforms of Signals. For the frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$ take in Eq. (2) the real and imaginary parts, respectively, of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ to be

$$\sum_{j=1}^{J} a_j \Delta U_j(\omega_k) = a_{U0} ,$$

$$\sum_{j=1}^{J} a_j \Delta V_j(\omega_k) = a_{V0} , \quad k = 1, \ldots, K ; \tag{3}$$

i.e., take the finite Fourier transform to be constant in the frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$. Standard methods of the analysis of variance may be used in conjunction with Eqs. (2) and (3) to estimate simultaneously the constants a_{U0}, a_{V0}, and the common variance of the random variables $\Delta U_n(\omega_k)$, $\Delta V_n(\omega_k)$, $k = 1, \ldots, K$. A similar method is used for other sub-bands $\omega^{(1')} \leq \omega < \omega^{(2')}$ of the partition of the total effective frequency band $0 \leq \omega \leq \omega_{max}$.

With this choice of the finite Fourier transform, one has the constants a_{UO}, a_{VO} pertaining to a given frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$ estimable only from that particular frequency band. Thus, in comparison with the analogous time domain description of the signal component the frequency domain description of the signal component may be said to give rise to disconnected designs. For the statistical estimation method just described to be reasonably effective one needs (1) the true real and imaginary parts of the finite Fourier transform of the signal component of $X(t)$ essentially constant over the frequency bands of the partition of $0 \leq \omega \leq \omega_{max}$, and (2) the spectral density $s(\omega)$ of $n(t)$ also essentially constant over these frequency bands.

This frequency method requires that only two constants be measured from each sub-band $\omega^{(1')} \leq \omega < \omega^{(2')}$, whereas the analogous time domain description of the signal component generally requires that more than two (usually many more) constants be measured from each sub-band $\omega^{(1')} \leq \omega < \omega^{(2')}$. Thus, with the frequency domain description of the signal component the band-width $\omega^{(2')} - \omega^{(1')}$ of each sub-band $\omega^{(1')} \leq \omega < \omega^{(2')}$ may be taken smaller than the band-width required with the analogous time domain description of the signal component. When the observed record $X(t)$, $-T \leq t \leq T$, is of moderately long duration, small band-widths B (see Ref. (6)) are attainable; consequently small band-widths $\omega^{(2')} - \omega^{(1')}$ may be employed in the frequency domain statistical estimation procedure. The condition (1) above that the true real and imaginary parts of the finite Fourier transform of the signal component of $X(t)$ be essentially constant over such frequency band-widths $\omega^{(2')} - \omega^{(1')}$ is then not too stringent a condition to impose.

<u>The Case of Locally Linear Finite Fourier Transforms of Signals</u>. When the real and imaginary parts of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ are not adequately described by piecewise constant functions of frequency, a next reasonable description is that of piecewise linear functions of frequency. In this case, we have in place of Eq. (3)

$$\sum_{j=1}^{J} a_j \Delta U_j(\omega_k) = a_{U0} + a_{U1}\omega_k ,$$

$$\sum_{j=1}^{J} a_j \Delta V_j(\omega_k) = a_{V0} + a_{V1}\omega_k ; \quad k = 1, \ldots, K , \qquad (4)$$

where we now have four constants $(a_{U0}, a_{U1}; a_{V0}, a_{V1})$ to be measured. The frequency domain partition used here need not be the same one used previously; for example, with more constants to be measured one might quite reasonably have the band-width $\omega^{(2)} - \omega^{(1)}$ here larger than that of the one in the locally constant case. Standard methods of the analysis of variance may be used with Eqs. (2), (4) to estimate simultaneously the constants $(a_{U0}, a_{U1}; a_{V0}, a_{V1})$, and the common variance of the random variables $\Delta U_n(\omega_k)$, $\Delta V_n(\omega_k)$, $k = 1, \ldots, K$. The method is similarly used for other sub-bands $\omega^{(1')} \leq \omega < \omega^{(2')}$ of the partition of the total effective frequency band $0 \leq \omega \leq \omega_{max}$. With this choice of the finite Fourier transform of the signal component, one has the constants $(a_{U0}, a_{U1}; a_{V0}, a_{V1})$ pertaining to a given frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$ estimable <u>only</u> from that particular frequency band. Thus, in comparison with the analogous time domain description of the signal component the frequency domain description of the signal component may be said to give rise again to <u>disconnected designs</u>. Comments concerning the applicability of this method can be made in a manner completely analogous to the previous discussion of the locally constant case. Finally, our methods may be extended as before to the case where the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ is taken to be a piecewise polynomial or even a more general function of frequency.

<u>A Combined Time Domain and Frequency Domain Description of the Signal Component.</u>

In the methods described above one works with the real and imaginary parts, respectively, $\Sigma_{j=1}^{J} a_j \Delta U_j(\omega_k)$, $\Sigma_{j=1}^{J} a_j \Delta V_j(\omega_k)$, $k = 1, \ldots, K$, of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. With the time domain description, the above $\Delta U_j(\omega_k)$, $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$, are computed from a chosen description of $S_j(t)$; with the frequency domain description, the above $\Sigma_{j=1}^{J} a_j \Delta U_j(\omega_k)$, $\Sigma_{j=1}^{J} a_j \Delta V_j(\omega_k)$, $k = 1, \ldots, K$, are described directly. The signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ is <u>linear</u> in the functions $S_j(t)$, $j = 1, \ldots, J$, and the finite Fourier transform is a <u>linear operator</u> on $X(t)$. One may therefore elect to use a combined time domain and frequency domain description of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. For example, in the frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$ one may take the real and imaginary parts, respectively, of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ to be

$$\sum_{j=1}^{J} a_j \Delta U_j(\omega_k) = \sum_{j'=1}^{J'} a_{j'} \Delta U_{j'}(\omega_k) + a_{U0} + a_{U1}\omega_k + \cdots + a_{Up}\omega_k^p ,$$

$$\sum_{j=1}^{J} a_j \Delta V_j(\omega_k) = \sum_{j'=1}^{J'} a_{j'} \Delta V_{j'}(\omega_k) + a_{V0} + a_{V1}\omega_k + \cdots + a_{Vp}\omega_k^p ; \quad (5)$$

$$J' < J ; \ k = 1, \ldots, K .$$

Here $\Delta U_{j'}(\omega_k)$, $\Delta V_{j'}(\omega_k)$ are, respectively, the real and imaginary parts of the finite Fourier transform of $S_{j'}(t)$ evaluated at $\omega = \omega_k$. The functions $S_{j'}(t)$, $j' = 1, \ldots, J'$, are prescribed in the time domain. In Eq. (5) the polynomial terms in ω_k are frequency domain descriptions of additional contributions to the real and imaginary parts, respectively, of the finite Fourier transform of the signal component. For a combined time domain and frequency domain method to be reasonably effective in measuring the true real and imaginary parts $\Sigma_{j=1}^{J} a_j \Delta_j(\omega_k)$, $\Sigma_{j=1}^{J} a_j \Delta V_j(\omega_k)$ of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ one needs: (1) the true finite Fourier transform adequately described (for example, by an expression such as Eq. (5)) over the frequency bands of the partition of $0 \leq \omega \leq \omega_{max}$, and (2) the spectral density $s(\omega)$ of $n(t)$ essentially constant over those frequency bands. With a choice, for example, such as Eq. (5), one may expect in most cases to have the constants $(a_{U0}, a_{U1}, \ldots, a_{Up}; a_{V0}, a_{V1}, \ldots, a_{Vp})$ pertaining to a given frequency band $\omega^{(1)} \leq \omega < \omega^{(2)}$ estimable <u>only</u> from that particular frequency band, and the constants $a_{j'}$, $j' = 1, \ldots, J'$, estimable from more than one or even from all the frequency bands of the partition of the entire effective frequency band $0 \leq \omega \leq \omega_{max}$. In regard to estimability of constants much depends on the choice of the functions $S_{j'}(t)$, $j' = 1, \ldots, J'$. In most cases then, the combined time domain and frequency domain description of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ may be said to give rise to <u>partially disconnected designs</u>.

One notes that with all the three methods [(1) time domain, (2) frequency domain, and (3) combined time domain and frequency domain] described above one always in effect measures the real and imaginary parts of the finite Fourier transform of the signal component on a set of discrete frequencies. In many practical problems such a frequency domain description of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ may be all that is required. In other situations the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$, expressed as a function of time, may be desired. In the latter case one is confronted with the necessity of (1) transforming the measured finite Fourier transform of the signal component to the time domain, and (2) determining or evaluating the statistical variability of the transform. The first problem arises when the frequency domain or combined time and frequency domain approach is taken. For the present we limit our discussion of such questions to the following situation. Suppose the observed record $X(t)$, $-T \leq t \leq T$, is of moderately long duration $2T$, so that small frequency band-widths B (see Ref. (6)) are attainable. Thus, the measured real and imaginary parts of the finite Fourier transform at a particular frequency $\omega = \omega_k$ pertain to a small frequency band at $\omega = \omega_k$. Call these estimates $\hat{A}_{\omega_k}$ and $\hat{B}_{\omega_k}$, respectively. Since the observed record $X(t)$, $-T \leq t \leq T$, is of moderately long duration $2T$, one may then reasonably take $\Sigma_{\omega_k}[\hat{A}_{\omega_k} \cos\omega_k t + \hat{B}_{\omega_k} \sin\omega_k t]$ to be a statistical estimate of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$. Here the summation on ω_k extends over all the frequencies ω_k in the total effective frequency band $0 \leq \omega \leq \omega_{max}$. Following the procedure of Ref. (6), the frequencies ω_k will be equally spaced a frequency interval B apart.

The Case in which there is Knowledge about the $S_j(t)$, $j = 1, \ldots, J$

Attention is now directed to the problem of measuring the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ in the case in which there is knowledge about the $S_j(t)$. Such knowledge is summarized by taking a certain number J' $(J' < J)$ of the $S_j(t)$ say $S_j(t)$, $j = 1, \ldots, J'$, to be known a priori. In order to measure the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ utilizing the method given in Ref. (6), one must make a choice (either explicitly or implicitly) of appropriate augmented $S_j(t)$, $j = J' + 1, \ldots, J$, to use and in this way the design of experiments feature of the problem enters. Four methods for treating design problems will now be discussed. These are reduction of the problem to that considered above, time domain approach, frequency domain approach, and finally a combined time and frequency domain treatment.

The Augmented Design Problem and Methods Previously Discussed. The signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ is linear in the functions $S_j(t)$, and the finite Fourier transform is a linear operator on $X(t)$. Thus, one may elect to describe the augmented signal component $\Sigma_{j=J'+1}^{J} a_j S_j(t)$ of $X(t)$ by any of the methods discussed in the previous sections. The statistical estimation procedure is always conducted in the frequency domain using the method given in Ref. (6). The estimability of constants from the various frequency sub-bands depends on the particular $S_j(t)$, $j = 1, \ldots, J'$, prescribed a priori and the particular description of the augmented signal component $\Sigma_{j=J'+1}^{J} a_j S_j(t)$ employed.

Time Domain Description and Choice of the Augmented Signal Component. Functions $S_j(t)$, $j = 1, \ldots, J'$ $(J' < J)$, are prescribed initially and the problem now is to determine desirable augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$. The augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$, ought in some sense to be "some distance away from" or "somewhat distinguishable from" the initially prescribed functions $S_j(t)$, $j = 1, \ldots, J'$, and also from each other. One approach is to consider augmented functions which are orthogonal (in the time interval $-T \leq t \leq T$) to the linear manifold spanned by the initially prescribed functions $S_{j'}(t)$, $j' = 1, \ldots, J'$, and in addition are orthogonal to each other.

That is with respect to a <u>chosen weighting kernel</u> $K(t)$, $-T \le t \le T$, an <u>orthogonal augmented function</u> $S_j(t)$ fulfills the conditions:

<u>Orthogonality to Initially Prescribed Functions</u>

$$\int_{-T}^{T} K(t)S_{j'}(t)S_j(t)dt = 0; \quad j' = 1, \ldots, J', \ j = J' + 1, \ldots, J \ . \qquad (6)$$

<u>Self-Orthogonality</u>

$$\int_{-T}^{T} K(t)S_j(t)S_{j*}(t)dt = 0; \quad j \neq j*, \ j, \ j* = J' + 1, \ldots, J \ . \qquad (7)$$

There is no loss in generality in normalizing the augmented functions by the following:

<u>Unit Norm</u>

$$\int_{-T}^{T} K(t)S_j^2(t)dt = 1; \quad j = J' + 1, \ldots, J \ . \qquad (8)$$

The choice of an appropriate weighting kernel $K(t)$ and a set of augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$, satisfying Eqs. (6), (7), and (8) depends to a certain extent on the particular phenomena being studied, and further study of this problem is required. The statistical estimation procedure is always conducted in the frequency domain using the method summarized in Ref. (6). The estimability of constants from the various frequency sub-bands depends on the particular functions $S_j(t)$, $j = 1, \ldots, J'$, prescribed a priori, and the particular augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$, chosen.

<u>Frequency Domain Description and Choice of the Augmented Signal Component</u>. In this section the augmented functions are described in the frequency domain and the choice of desirable augmented functions is made on the basis of frequency

domain criteria. Let the total effective frequency band $0 \leq \omega \leq \omega_{max}$ be partitioned into sub-bands, and consider a particular sub-band denoted by $\omega^{(1)} \leq \omega < \omega^{(2)}$ (see Ref. (6)). One has the real and imaginary parts of the finite Fourier transform of the signal component $\Sigma_{j=1}^{J} a_j S_j(t)$ of $X(t)$ evaluated at the frequency $\omega = \omega_k$ given by <u>$\Sigma_{j=1}^{J} a_j \Delta U_j(\omega_k)$</u> and <u>$\Sigma_{j=1}^{J} a_j \Delta V_j(\omega_k)$</u>, respectively. The frequencies ω_k, $k = 1, \ldots, K$, satisfy $\omega^{(1)} \leq \omega_1 < \omega_2 < \ldots < \omega_k < \ldots < \omega_K \leq \omega^{(2)}$ and are equally spaced a frequency interval B apart. One may write

$$\sum_{j=1}^{J} a_j \Delta U_j(\omega_k) = \sum_{j=1}^{J'} a_j \Delta U_j(\omega_k) + \sum_{j=J'+1}^{J} a_j \Delta U_j(\omega_k) ,$$

$$\sum_{j=1}^{J} a_j \Delta V_j(\omega_k) = \sum_{j=1}^{J'} a_j \Delta V_j(\omega_k) + \sum_{j=J'+1}^{J} a_j \Delta V_j(\omega_k) ; \; k = 1, \ldots, K , \tag{9}$$

where $\Sigma_{j=1}^{J'} a_j \Delta U_j(\omega_k)$ and $\Sigma_{j=1}^{J'} a_j \Delta V_j(\omega_k)$ are, respectively, the real and imaginary parts of the finite Fourier transform of the <u>prescribed signal component</u> $\Sigma_{j=1}^{J'} a_j S_j(t)$ evaluated at the frequencies $\omega = \omega_k$, $k = 1, \ldots, K$, and $\Sigma_{j=J'+1}^{J} a_j \Delta U_j(\omega_k)$ and $\Sigma_{j=J'+1}^{J} a_j \Delta V_j(\omega_k)$ are, respectively, the real and imaginary parts of the finite Fourier transform of the <u>augmented signal component</u> $\Sigma_{j=J'+1}^{J} a_j S_j(t)$ evaluated at the same frequencies. For the frequencies $\omega = \omega_k$, $k = 1, \ldots, K$, in the frequency sub-band $\omega^{(1)} \leq \omega < \omega^{(2)}$ the real and imaginary parts, respectively, of the initially prescribed functions $S_j(t)$, $j = 1, \ldots, J'$, are described by the <u>finite sequences</u> $\Delta U_j(\omega_k)$, $k = 1, \ldots, K$ and $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$, with $j = 1, \ldots, J'$. Similarly, for the same frequencies the real and imaginary parts, respectively, of the augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$, are described by the finite sequences $\Delta U_j(\omega_k)$, $k = 1, \ldots, K$ and $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$, for $j = J' + 1, \ldots, J$.

The finite sequences described above provide the frequency domain descriptions of the functions $S_j(t)$, $j = 1, \ldots, J$, since one may restrict attention to a particular frequency sub-band $\omega^{(1)} \leq \omega < \omega^{(2)}$ of the partition of the total effective frequency band $0 \leq \omega \leq \omega_{max}$. The total frequency domain description of a function $S_j(t)$ is the collection of sequences $\Delta U_j(\omega_k)$, $k = 1, \ldots, K$, and $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$, obtained from all such frequency sub-bands of the partition of the total effective frequency band $0 \leq \omega \leq \omega_{max}$. Now, the augmented functions $S_j(t)$, $j = J' + 1, \ldots, J$, will be chosen implicitly by selecting the <u>augmented finite sequences</u> $\Delta U_j(\omega_k)$, $k = 1, \ldots, K$, and $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$ for $j = J' + 1, \ldots, J$.

In a manner analogous to the previous section we choose the set of augmented sequences $\Delta U_j(\omega_k)$, $k = 1, \ldots, K$, with $j = J' + 1, \ldots, J$ and $\Delta V_j(\omega_k)$, $k = 1, \ldots, K$, with $j = J' + 1, \ldots, J$ so that with respect to selected <u>finite weighting</u> sequences u_k, v_k, $k = 1, 2, \ldots, K$, the following conditions are fulfilled:

<u>Orthogonality to Initially Prescribed Sequences</u>

$$\sum_{k=1}^{K} u_k \Delta U_{j'}(\omega_k) \Delta U_j(\omega_k) = 0 \,,$$

$$\sum_{k=1}^{K} v_k \Delta V_{j'}(\omega_k) \Delta V_j(\omega_k) = 0 \;; \quad j' = 1, \ldots, J', \; j = J' + 1, \ldots, J \,. \tag{10}$$

<u>Self-Orthogonality</u>

$$\sum_{k=1}^{K} u_k \Delta U_j(\omega_k) \Delta U_{j*}(\omega_k) = 0 \,,$$

$$\sum_{k=1}^{K} v_k \Delta V_j(\omega_k) \Delta V_{j*}(\omega_k) = 0 \;; \; j \neq j^*, \; j, \; j^* = J' + 1, \ldots, J \,. \tag{11}$$

Unit Norm

$$\sum_{k=1}^{K} u_k(\Delta U_j(\omega_k))^2 = 1 ,$$

$$\sum_{k=1}^{K} v_k(\Delta V_j(\omega_k))^2 = 1 ; \quad j = J' + 1, \ldots, J . \tag{12}$$

Comments analogous to those of the previous section can be made here with regard to the choice of the finite weighting sequences and the statistical estimation procedure.

Combined Time Domain and Frequency Domain Description and Choice of the Augmented Signal Component. The time and frequency domain methods described above may be combined in a straightforward manner. First, by use of the time domain method augmented functions $S_j(t)$, $j = J' + 1, \ldots, J''$ $(J' < J'' < J)$, are chosen. Then, considering the functions $S_j(t)$, $j = 1, \ldots, J''$, to be prescribed functions, the frequency domain method is used to provide an implicit description and choice of the remaining augmented functions $S_j(t)$, $j = J'' + 1, \ldots, J$.

CONCLUSIONS

To a great extent the effectiveness of the various design methods discussed above will be determined by results achieved with actual experimental data. Such results may be available in the near future. In addition to determining the effectiveness of the various design methods suggested, the experience gained may also serve to guide future studies.

PART III

THE DECISION THEORY APPROACH

INTRODUCTION

The work performed on decision theory has centered on the development and use of a Bayesian model for simulating the reliability growth process of a complex system during its development and testing phases. This model has been programmed for the IBM 7090 Computer and several runs for a hypothetical reliability development program were performed under different conditions, but with a fixed utility function and set of prior probability distributions.

The discussion below is in three sections, the first two of which are based on the decision theory model described in previous reports (see Refs. (2) and (5)). In the first of these sections we discuss the formulation of the data for the hypothetical development program and the prior probability distributions. In the second, the results of the computations are presented and analyzed. In the final section a modification of the decision model which makes use of the methods of dynamic programming is presented. The explicit functional equation is formulated and a proof is given that the solution leads to maximum expected reliability at the terminal completion date.

CONSTRUCTION OF THE DATA CASES

Introduction

The purpose of this discussion is to describe the procedure for constructing the hypothetical program for evaluating the general variable configuration model described in Ref. (5). This includes selecting the sample space Z and parameter space $\boldsymbol{\Theta}$; the prior probability distributions $P_0(Z|A)$ and prior conditional distributions $P_0(\boldsymbol{\Theta}|Z)$; and the table of utility values $U(A,\boldsymbol{\Theta})$. The model and terminology are the same as they were in Ref. (5); however, certain simplifications were made, particularly in the definition of Z in order that the prior probability distributions could be based upon the binomial and Beta laws.

The Sample Space Z and the Prior Distributions $P_0(Z|A)$

We assume that the block of tests performed after each redesign of the system under development consists of n Bernoulli trials, each trial having a probability of a successful result, or reliability $\theta \epsilon \boldsymbol{\Theta} \equiv \{\theta_1, \theta_2, \ldots, \theta_I\}$, $0 < \theta < 1$, where θ is a random variable and a function of the particular system configuration being tested. The number of successes $r \epsilon \{0, 1, 2, \ldots, n\}$ in any of these blocks is governed by the binomial law with mass function

$$P(r|\theta,n) = \binom{n}{r} \theta^r (1 - \theta)^{n-r} .$$

The sample description space is denoted by the random variable $z \epsilon Z \equiv \{z_1, z_2, \ldots, z_J\}$ with z_1 the most favorable result, and z_J the least favorable. Accordingly, the set Z is defined as follows

$$\begin{aligned} z_1 &\equiv \text{no failures in } n \text{ tests} \\ z_2 &\equiv \text{one failure in } n \text{ tests} \\ &\vdots \\ z_r &\equiv (r - 1) \text{ failures in } n \text{ tests} \\ &\vdots \\ z_J &\equiv (J - 1) \text{ or more failures in } n \text{ tests} . \end{aligned}$$

Suppose (as is often the case in current programs) equipment of very high reliability is being tested so that the probability that there will be more than very few failures after the first few improvements is close to zero. Therefore, it is possible to assign a reasonably small fraction of n as a practical upper limit J (this also saves a great deal of computer time). In the cases described, with $n = 25$, J equals 6. When the reliability is greater than .9, the probability of 5 or more failures is less than .1.

During the period of development, the system undergoes a series of modifications, with each successive configuration representing the result of a greater cumulative level of reliability improvement effort. The action space $A = \{a_1 =$ accept initial configuration; $a_2 =$ retest initial configuration; $a_3, \ldots, a_L$ an ordered set of redesign actions$\}$ includes the totality of all L "configurations" that will ever be adopted or considered at any time during the program. It seems intuitively appealing to assign a different prior reliability estimate p_0 to each a, and obtain the prior probabilities for Z from the binomial tables. Here we deliberately employ the notation p_0 for a single value of reliability for a particular configuration in order to avoid confusion with θ, which is a random variable representing the set of possible values of the reliability for any configuration.

Thirty-five values of p_0 were assigned, one to each a, and for each p_0 the prior distribution of Z was obtained either from the binomial tables, Ref. (7), or by calculation. Table I gives the complete set of prior estimates of reliability, p_0, which were used to initiate simulation runs by providing a basis for calculating the initial probability distributions $P_0(Z|A)$. However, once the hypothetical development program is begun, the calculation of the probability distributions $P_n(Z|A)$ and $P_n(\Theta|A)$ at each subsequent stage n is dependent upon the sequence of test results and past actions, and no further use of these preliminary distributions is made during the sequential process.

TABLE I

PRIOR DISTRIBUTIONS $P_0(Z|A)$

L = 36   J = 6
(Based upon the Binomial Distribution)

Prior Reliability p_0	z_1	z_2	z_3	z_4	z_5	z_6	A
.6	.0	.0	.0	.002	.007	.991	a_2
.63	.0	.0	.001	.005	.015	.979	a_3
.66	.0	.0	.002	.010	.027	.961	a_4
.69	.0	.001	.006	.020	.048	.925	a_5
.72	.0	.003	.012	.037	.078	.870	a_6
.75	.0	.006	.025	.064	.117	.788	a_7
.78	.002	.014	.048	.104	.161	.671	a_8
.81	.005	.030	.085	.153	.197	.530	a_9
.84	.013	.061	.139	.203	.213	.371	a_{10}
.86	.023	.094	.183	.229	.205	.266	a_{11}
.88	.041	.140	.228	.239	.179	.173	a_{12}
.90	.072	.199	.266	.226	.138	.099	a_{13}
.91	.095	.234	.278	.211	.114	.068	a_{14}
.92	.124	.270	.282	.188	.090	.046	a_{15}
.93	.163	.307	.277	.160	.066	.027	a_{16}
.94	.213	.340	.260	.127	.045	.015	a_{17}
.95	.277	.365	.231	.093	.027	.007	a_{18}
.96	.360	.375	.188	.060	.014	.003	a_{19}
.965	.410	.372	.162	.045	.009	.002	a_{20}
.97	.467	.361	.134	.032	.005	.001	a_{21}
.975	.531	.340	.105	.021	.003	.0	a_{22}
.98	.603	.308	.075	.013	.001	.0	a_{23}
.985	.685	.261	.048	.006	.0	.0	a_{24}
.99	.778	.196	.024	.002	.0	.0	a_{25}
.992	.818	.165	.016	.001	.0	.0	a_{26}
.994	.861	.130	.009	.0	.0	.0	a_{27}
.995	.882	.111	.007	.0	.0	.0	a_{28}
.996	.905	.091	.004	.0	.0	.0	a_{29}
.997	.928	.070	.002	.0	.0	.0	a_{30}
.998	.951	.048	.001	.0	.0	.0	a_{31}
.999	.975	.024	.001	.0	.0	.0	a_{32}
.9992	.980	.020	.0	.0	.0	.0	a_{33}
.9994	.985	.015	.0	.0	.0	.0	a_{34}
.9996	.990	.010	.0	.0	.0	.0	a_{35}
.9998	.995	.005	.0	.0	.0	.0	a_{36}

The Parameter Space θ and the Prior Conditional Distributions $P_0(\theta|Z)$

Because the sample space Z we have chosen is discrete, the computation of the joint probability elements $P(Z,\theta)$ is simplified if θ is also made discrete. This has been done by breaking θ up into a set of interval values of reliability. Nine intervals were used, and their midpoints in descending order are .99625, .99, .975, .95, .90, .85, .80, .75, .3625. Note that the highest of these represents all reliabilities above .9925, and the lowest all reliabilities below .725.

The construction of the prior conditional distributions $P_0(\theta|Z)$ is based upon the well known conjugate relationship between the binomial and the Beta functions. Starting with the incomplete sum of binomial probabilities,

$$P(k \geq r|\theta,n) = \sum_{k=r}^{n} \binom{n}{k} \theta^k (1-\theta)^{n-k} .$$

We differentiate this sum with respect to θ to obtain the probability density

$$\frac{dP}{d\theta} = \frac{n!}{(n-r)!\,(r-1)!} \theta^{r-1} (1-\theta)^{n-r} . \tag{1}$$

Integrating both sides we get the identity:

$$\sum_{k=r}^{n} \binom{n}{k} \theta^k (1-\theta)^{n-k} = \frac{n!}{(n-r)!\,(r-1)!} \int_0^\theta x^{r-1} (1-x)^{n-r} dx . \tag{2}$$

Equation (2) states that the incomplete sum of binomial probabilities $P[k \geq r|\theta,n]$ is equal to the incomplete integral of the normalized Beta function $P[x \leq \theta|r,n]$. Accordingly, it becomes possible to make probability statements about θ from observation of the result of a series of Bernoulli trials. For example, if in n tests r or more successes are observed

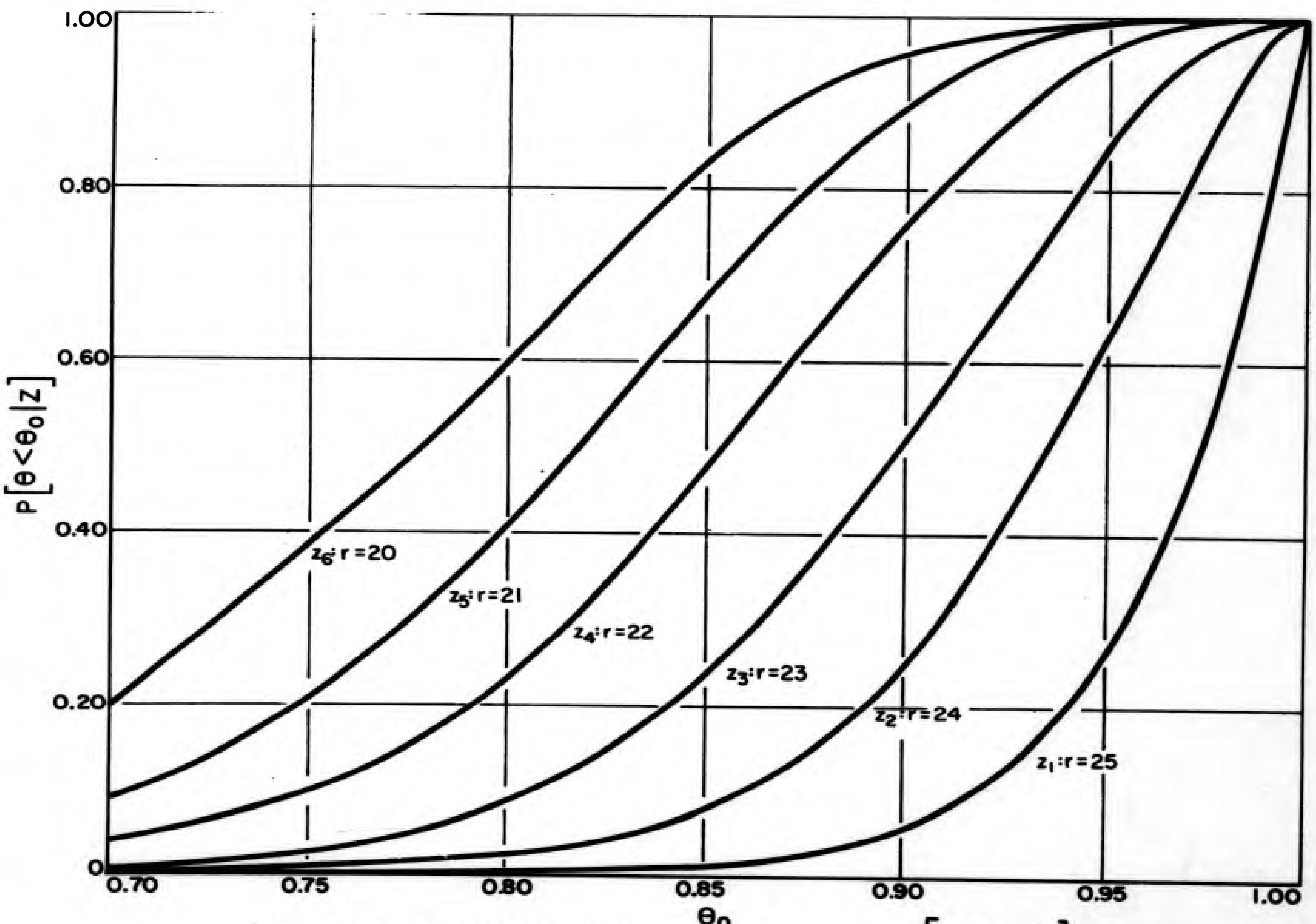

Figure 1. Conditional Distribution Functions $P\left[\theta < \theta_0 | Z\right]$, n = 25

(actually, only r successes can be observed), the probability that $\theta < \theta_0$ is given by the percentage point $I_{\theta_0}(r, n-r+1)$ of the incomplete normalized Beta function. For purposes of this data case, n is fixed at 25, and the appropriate index of z is substituted for $n-r+1$.

For every $z_j \epsilon Z$, the prior conditional distribution function $P[\theta < \theta_0 | z_j]$ is obtained from the entry $I_{\theta_0}(26-j, j)$ in the table of percentage points of the incomplete Beta function. In Fig. 1 below these distribution functions are given for $z \epsilon \{z_1, z_2, \ldots, z_6\}$; the values for plotting were obtained from a useful short table in Ref. (8) and are consistent with graphical accuracy.

The probability masses of the intervals of θ were obtained by taking differences between percentage points in this figure and are reproduced in Table II below.

TABLE II

PRIOR CONDITIONAL DENSITIES OF INTERVALS OF θ

$P_0(\theta | Z)$

θ	Reliability (Midpoint)	z_1	z_2	z_3	z_4	z_5	z_6
θ_1	.99625*	.170	.017	-	-	-	-
θ_2	.99	.180	.073	.015	-	-	-
θ_3	.975	.260	.180	.075	.020	.005	-
θ_4	.95	.230	.290	.220	.120	.045	.020
θ_5	.9	.123	.270	.310	.220	.150	.080
θ_6	.85	.028	.120	.210	.290	.250	.180
θ_7	.8	.009	.035	.110	.190	.250	.240
θ_8	.75	-	.011	.040	.090	.150	.200
θ_9	.3625$^{\Delta}$	-	.004	.020	.070	.150	.280

* Reliability $\geq$ .9925

Δ Reliability $\leq$ .725

These prior conditional distributions of the reliability were used (as was explained in Ref. (5)) to initiate the sequential process. Once a run begins, the marginal distributions $P_n(\theta|Z,A)$ at each stage n depend entirely upon the sequence of past events and actions, and there is no further reference to the initial conditional distribution except in very unusual circumstances (see below).

The Utility Table, $U(A,\theta)$

At the conclusion of a block of tests on a particular configuration, one is faced with a choice of a "best" action $a_k \epsilon \{a_1 \equiv$ accept; $a_2 \equiv$ retest; $a_3, \ldots, a_K$ an ordered set of redesign actions$\}$, $K \leq L$, for the next stage of the development program. If a_k is a redesign $(k \geq 3)$, the index 2 is reassigned to the configuration associated with that action, and correspondingly the indices for all remaining actions in the set A are reduced by $k - 2$. In principle, reliability growth is achieved by climbing up a ladder of configurations a variable number of rungs at a time, but in no case more than $k - 2$.

The choice of a best action at each stage is governed by several factors, including time and cost, present reliability status, and anticipated reliability improvement resulting from that action. It was our original intention to develop a single comprehensive utility function which incorporated all of these factors into possibly one equation, although this has not been accomplished as yet. However, for purposes of the work in "dynamic programming", we have a much simpler approach to this type of utility function, one which is based only upon reliability growth.

For purposes of the present model, time, cost, and growth factors can be combined to a reasonable degree if utility units are assigned to each couple, (a,θ), $a \in \{a_1, a_2, \ldots, a_K\}$, $\theta \in \{\theta_1, \theta_2, \ldots, \theta_I\}$. It is difficult to avoid a certain degree of arbitrariness in such an assignment because of the complexity of the process being studied. However, a simple realistic utility table can be formulated by limiting consideration to the current reliability status of the configuration under test.

For example, it is sometimes required of current modern rocket engine systems and components that there be at least a 0.5 probability that their reliability is at least 0.99. Accordingly, the utility units can be so assigned that acceptance is not the best action unless that is the case. It is also readily apparent that if the reliability is low it is more likely that a major improvement will be required than would be the case if the reliability were high.

The following utility table was used for the simulations described in this report (for $K = 5$ and $I = 9$).

TABLE III

TABLE OF UTILITY VALUES $U(A,\theta)$

(Arbitrary Units)

Rel	.99625	.99	.975	.95	.9	.85	.8	.75	.3625
Actions	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9
a_1	400	100	50	0	0	0	-60	-100	-200
a_2	90	210	160	100	50	10	0	-20	-100
a_3	10	90	110	160	140	80	30	0	0
a_4	0	50	80	90	90	100	100	100	100
a_5	0	0	0	0	20	60	130	170	300

To show how the utility function affects the course of action, we give below some typical probability distributions for θ under which each of the actions $\hat{a} \epsilon \{a_1, a_2, \ldots, a_K\}$ may be optimum if the utility units are assigned as in Table III.

TABLE IV

$P(\theta|\hat{a})$

(Typical Values)

$\hat{a}$ \ θ	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9
a_1	.25	.25	.30	.16	.03	.01	-	-	-
a_2	.16	.34	.34	.14	.02	-	-	-	-
a_3	.02	.07	.18	.29	.27	.12	.035	.011	.004
a_4	-	.02	.07	.22	.31	.21	.11	.04	.02
a_5	-	-	.01	.04	.15	.25	.25	.15	.15

In other words, each line of Table IV gives a sample probability distribution for θ for the current configuration that will result in the indicated $\hat{a}$ being chosen as the action. A comparison of the first line of Table IV to the second, particularly the entries in the first two columns, shows that acceptance (a_1) can result if $P_r\{\theta = \theta_1 \text{ or } \theta = \theta_2\} = .5$ (i.e. the reliability is greater than .99 with probability .5) but only if $P\{\theta = \theta_1\}$ is large enough. However, if $P\{\theta = \theta_2\}$ is substantially greater than $P_r\{\theta = \theta_1\}$, the continuation of testing is a better action.

We also note from Table IV that a minor redesign a_3 will be attempted if there is a possibility that the reliability is high, but the dispersion of θ is wide.

Table III was based entirely upon heuristic and intuitive considerations and was constructed only after a great deal of experimentation with different combinations of values of entries in the cells. Although it works satisfactorily for the program, a great deal more work is necessary before we can be confident that it represents a reasonable set of criteria for governing actions.

VARIABLES, ANALYSIS, AND RESULTS

Introduction

Results were obtained by performing the simulation 198 times under 99 different sets of initiating conditions for the independent variables, each set of conditions being replicated once. The purpose of this section is to describe the variables and the results and to summarize the findings with respect to the reliability growth process. A lemma is proved describing the relationship under certain conditions between the posterior conditional distributions $P_n(\theta|Z,a)$ and the prior conditional distribution $P_0(\theta|Z)$. This lemma is used to establish limitations upon the extent to which initial conditions are weighted in computing the prior probability distribution of the reliability for each configuration.

Analysis of the results of the simulation runs is performed in part by means of a regression model.

Variables

Independent Variables. Two different independent variables were considered, starting reliability p_0 (see discussion above) and the "weighting factor", α. Intuitively, one would expect the higher the reliability of the first configuration tested, the less time and the fewer the improvements required to bring the system to an acceptable reliability level. This is exactly what the results of the simulation runs indicate.

In order to define the weighting factor α we first note that there are two potential prior sources of information concerning the reliability of a configuration. One of these is the initial prior probability distribution $P_0(\theta|a)$ calculated for that configuration before the program begins, and depending on the initial distribution $P_0(Z|a)$ and the set of prior conditional distributions $P_0(\theta|Z)$. The other source of information is the results of past tests on older configurations of the same system which have a lower reliability. The factor α, $0 \leq \alpha \leq 1$ assigns the proportion of each of these sources of information that is to be used in a given development program.

If all weight is assigned to past tests $(\alpha = 0)$ as was done in the earlier version of this model, (see Ref. (5)), only in very rare circumstances is it possible to attain an acceptable reliability (say $\theta \geq .99$). The defects of the earlier designs invariably result in a sufficient number of failures in testing that zero probability is assigned to the higher reliability values both for the configuration being tested and for all future configurations. This type of weighting is unduly pessimistic and makes no allowances for the possibility of significant technological improvements being achieved by redesigns.

On the other hand, one might suppose that the prior probability distribution of the reliability of a configuration is always the same until that configuration is adopted and tested $(\alpha = 1)$, regardless of the results of past tests. However, this is almost certainly too optimistic a viewpoint. The results of past tests are valuable, but not perfect indicators of the probability of success on future trials, even with a redesigned system.

In fact, when $\alpha = 1$ the prior distribution for θ for each configuration a would always be the initial prior distribution $P_0(\theta|a)$. Consequently, the result of the first test on this configuration would always be one of the prior conditional distributions $P_0(\theta|Z)$ (an undue restriction). This fact is proven in the following.

<u>Lemma</u>. If $P_n(\theta|A) = P_0(\theta|A)$,

then $P_n(\theta|Z,a) = P_0(\theta|Z)$ for the first test of any configuration a.

<u>Proof</u>. Recall that in the model, the initial joint probabilities are defined

$$P_0(Z,\theta|a) = P_0(\theta|Z) \cdot P_0(Z|a) .$$

Hence, the initial marginal distribution is

$$P_0(\theta|a) = \sum_Z P_0(Z,\theta|a),$$

and the initial conditional distribution is

$$P_0(Z|\theta,a) = P_0(Z,\theta|a) \Big/ P_0(\theta|a) .$$

The joint probabilities at stage n are defined in the model by

$$P_n(Z,\theta|a) = P_n(\theta|a) \cdot P_0(Z|\theta,a) .$$

Then, by substituting

$$P_n(Z,\theta|a) = P_0(\theta|a) \cdot P_0(Z|\theta,a) = P_0(Z,\theta|a) .$$

Hence, $P_n(Z|a) = \sum_\theta P_n(Z,\theta|a) = \sum_\theta P_0(Z,\theta|a) = P_0(Z|a)$,

and

$$P_n(\theta|Z,a) = \frac{P_n(Z,\theta|a)}{P_n(Z|a)} = \frac{P_0(Z,\theta|a)}{P_0(Z|a)} = P_0(\theta|Z).$$

Clearly, the actual situation lies between these two extremes, that is, $0 < \alpha < 1$. The reliability of a configuration is a function both of past tests and of the improvement effects of significant modifications. Accordingly, the weighting factor α may be thought of as the anticipated degree of confidence in the average effectiveness of all redesigns.

The values of α were varied from 0 to 1.0 in steps of 0.1 with a unique value assigned for each run. The program originally written (see Ref. (5)) was altered so that the weight α was assigned to $P_0(\theta|a)$, and $(1 - \alpha)$ to $P_{n-1}(\theta|a)$ as it is modified according to the results of the latest series of tests on the current configuration a_2 for all a above a_2 in computing $P_n(\theta|a)$. The formula is

$$P_n(\theta|A) = \frac{\alpha P_{n-1}(\theta|A) + (1-\alpha)\ P_0(\theta|A)}{\sum_{\theta} [\alpha P_{n-1}(\theta|A) + (1-\alpha)\ P_0(\theta|A)]} \quad .$$

The values of p_0 were varied from 0.6 to 0.84 in steps of 0.03. In order to perform this variation, it was only necessary to advance the initial configuration to the next line of Table I, and treat the remainder of that table as the set of prior distributions $P_0(Z|A)$ for all future configurations.

Dependent Variables. The dependent variable, or response, is simply the number of improvements performed before either acceptance or completion of the program. It is obtained by subtracting the index of the initial configuration from that of the final configuration. For example (see Table I), if the final configuration was a_{20} and the initial configuration a_2, 18 improvements have been performed. Repeated simulation runs using usual Monte Carlo procedures under identical conditions exhibited wide variability of results. Therefore, the number of improvements required for each pair of replicates was averaged.

<u>Data</u>

The results of all 198 runs are given below in Table V.

TABLE V

SUMMARY OF SIMULATION RUNS

Entries Give Average Number of Improvements per Run
for Given Set of Initiating Conditions

Initial Reliability \ α	α = 0	α = .1	α = .2	α = .3	α = .4	α = .5	α = .6	α = .7	α = .8	α = .9	α = 1.0
p_0 = .6	34	34	25.5	25	24	22.5	17	21	19	18	16.5
p_0 = .63	33	28.5	21	18.5	27.5	25.5	17	18.5	17.5	16.5	12.5
p_0 = .66	32	23.5	20.5	24.5	21	24.5	12.5	15.5	18.5	16.5	9
p_0 = .69	31	22.5	23	28.5	22	16.5	16.5	17	17.5	13.5	13
p_0 = .72	30	23.5	19.5	19	22	18.5	14	19	16.5	15.5	10.5
p_0 = .75	29	16	23.5	24	16.5	23.5	13	12	13	14.5	11
p_0 = .78	21	24.5	13	17.5	19	13	10.5	14.5	12.5	14	8
p_0 = .81	27	17	14.5	15.5	17.5	7	16	13.5	10	8	10
p_0 = .84	26	24.5	16.5	19.5	17	15.5	11.5	7.5	12.5	9.5	11

A cursory examination of this table shows a decided tendency for the required number of improvements to decrease with increases in both p_0 and α. One should also note the significant variability exhibited, particularly for larger α. Additional replicates of each set of initiating conditions would be required to obtain smoother results.

To structure this analysis further, a linear fit was made of the improvements (I) to α and p_0. For this purpose, the first column ($\alpha = 0$) was deleted because in all cases except one (p_0 = .78), satisfactory convergence of the sequential process was not obtained.

Three effects were considered: linear effect α, linear effect p_0, and the interaction term $p_0\alpha$. The interaction term was found to be nonsignificant in the regression, and therefore it was deleted from the subsequent analysis. The following was found to be the most reasonable fit of the data in Table V.

$$I = 49.5 - 12.3\alpha - 35.2p_0 .$$

The standard deviations of the three coefficients are respectively; 3.03, 1.11, and 4.11, and over 2/3 of the variance in I is explained by the regression. Therefore, it is clear that both α and p_0 are significant variables in explaining the number of improvements required to bring the system to an acceptable reliability level.

Conclusions

From these data it is clear that reliability growth can be simulated. The rapidity of this growth is a function of three variables: the reliability of the initial configuration, the weight assigned to the results of tests on earlier configurations $(1 - \alpha)$, and the weight assigned to anticipated breakthroughs (α). The process is very much influenced by the nature of the utility function.

THE DYNAMIC PROGRAMMING FORMULATION AND
A PROOF OF TERMINAL CONTROL OF RELIABILITY GROWTH

Introduction

In connection with the previous efforts (described above and in Ref. (2)) in applying decision theory methods to the large scale designing of complex experimental programs, it appeared desirable to use the formalism of dynamic programming in order to obtain a more concise solution to the question of optimum reliability growth. Towards this end, a criterion function based on the maximum reliability at the scheduled completion date was selected and a functional equation formulated. In the following sections we prove under appropriate assumptions that the solution to this functional equation yields the maximum expected value of terminal reliability. It is planned in the future to find methods for explicitly solving this functional equation which will not require an excessive amount of computer time. One of the techniques that will be considered is successive approximations.

Formulation of the Problem

A complex system is designed, tested, and modified with the aim of achieving a certain reliability growth in a fixed time period. We assume that the initial design and each subsequent redesign are each followed by a test, that the actions which can be taken include both redesigns and test replications without redesign and that a total of T actions can be taken in the time allotted. Let W be the collection of all "paths" or sequences of actions. Each path $w \epsilon W$ that can be taken to ultimate acceptance or rejection of the system consists of a sequence of $T - 1$ actions $a \epsilon A = \{a_1, a_2, \ldots, a_K\}$ and $T - 1$ test results

$z \in Z = \{z_1, z_2, \ldots, z_J\}$, with the a's and z's alternating, as follows:

$$w = (a^1, z^2, a^2, z^3 \ldots a^{n-1}, z^n \ldots a^{T-1}, z^T) .$$

Here the superscript n refers to the action taken or result obtained at a particular stage or point of time. We treat the set Z as a discrete-valued random variable with the values $z_1, z_2, \ldots, z_J$ and let θ denote reliability, a discrete-valued random variable with the possible values $\theta_1, \theta_2, \ldots, \theta_I$, $0 \leq \theta_1 < \theta_2 \ldots < \theta_{I-1} < \theta_I \leq 1$. Z and θ are subject to the joint probability distribution $P_{Z,\Theta}(z,\theta)$. Finally, let $E(\theta_T|w)$ denote the conditional expected value of the terminal reliability, given sequence w, where E is the expected value operator.

The Functional Equation

At stage $n < T$, a partial sequence $x_n = (a^1, z^2, a^2, \ldots, a^{n-1}, z^n)$ has been observed. The functional equation whose solution determines the next action to be taken is defined by the recurrence relationship

$$\begin{aligned} f_n(x_n) &= \underset{a^n}{\text{MAX}} \underset{z^{n+1}}{E} f_{n+1}(x_{n+1}) \\ &= \underset{a^n}{\text{MAX}} \underset{z^{n+1}}{E} f_{n+1}(x_n, a^n, z^{n+1}) , \end{aligned} \tag{3}$$

where $\underset{z^{n+1}}{E} \{ \}$ is the expected value of $\{ \}$ over Z at the n+1-st step. The functional f is initialized at the next-to-last stage as follows

$$f_{T-1}(x_{T-1}) = f_{T-1}(a^1, z^2, \ldots, a^{T-2}, z^{T-1}) = \underset{a^{T-1}}{\text{MAX}} \underset{z^T}{E} f_T(x_{T-1}, a^{T-1}, z^T) . \tag{4}$$

In order to justify Eq. (3), it is necessary to demonstrate that its solution leads to the highest expected value of the terminal reliability. Denote by w_n the set of all sequences $\{x_n \ldots\}$ whose initial subsequence is x_n. We can then state the following.

<u>Lemma</u>. $$f_n(x_n) = \underset{w \epsilon w_n}{\text{MAX}} \; E(\theta_T | w), \; n = 1, 2, \ldots, T - 1.$$

This lemma is a statement that $f_n(x_n)$ is the maximum expected value of the terminal reliability for all sequences which include x_n as the initial subsequence.

<u>Proof</u>. At the next to last stage the entire sequence w is determined by the solution to Eq. (4) and we write

$$f_{T-1}(x_{T-1}) = \underset{a^{T-1}}{\text{MAX}} \sum_{\theta} \sum_{Z} \theta p(z^T, \theta | a^{T-1}) = \underset{w \epsilon w_{T-1}}{\text{MAX}} \; E(\theta_T | w). \qquad (5)$$

Moving back one stage we find

$$\begin{aligned} f_{T-2}(x_{T-2}) &= \underset{a^{T-2}}{\text{MAX}} \; \underset{z^{T-1}}{E} \; f_{T-1}(x_{T-1}) \\ &= \underset{a^{T-2}}{\text{MAX}} \; \underset{z^{T-1}}{E} \; \underset{w \epsilon w_{T-1}}{\text{MAX}} \; E(\theta_T | w) \\ &= \underset{w \epsilon w_{T-2}}{\text{MAX}} \; E(\theta_T | w) \end{aligned}$$

and so forth. The remainder of the proof follows by induction for $n \geq 2$.

For the special case $n = 1$ it is only necessary to note that x_1 is a degenerate sequence consisting of no actions or test results, and preceded only by the initial design and the first test result z^1. But by the same reasoning employed above

$$f_1(x_1) = \max_{a^1} \mathop{E}_{z^2} \max_{w \in w_2} E(\theta_T | w)$$

$$f_1(x_1) = \max_{w \in w_1} E(\theta_T | w) ,$$

and w_1 is included in all sequences $w \in W$.

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