SOME SEQUENTIAL DESIGN PROCEDURES

by

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INTRODUCTION

In this thesis, I will treat some of the sequential experimentation procedures that have arisen in recent years. Special emphasis will be placed upon optimization techniques.

Chapter I contains essentially descriptive material. Here the Hotelling technique [17][1], the Kiefer-Wolfowitz procedure [18], the Friedman-Savage method [14], Blum's procedure [5], and the Box-Wilson process [10] are described and compared on certain very general points set forth at the beginning of the chapter.

Chapter II contains a development of some of the operating characteristics of one of the above techniques, namely, the Kiefer-Wolfowitz stochastic approximation procedure for estimating the maximum of a regression function in the case where the true regression is quadratic. In particular, a method is suggested for determining from a preliminary experiment values for some of the arbitrary constants which appear in the recursive relation defining the Kiefer-Wolfowitz procedure. This method is studied with the aid of the Monte Carlo approach in the appendix.

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1. The figures in square brackets refer to the bibliography.

CHAPTER I

A STUDY OF SOME PROCEDURES FOR LOCATING THE OPTIMUM POINT[1]

1.1. Terminology.

Many of the standard terms and expressions of statistics will be used in a special sense in this paper. These definitions are given below.

(1.1.1) Independent Variable.

An independent variable, denoted by x_i, is any variable that is under the control of the experimenter.

(1.1.2) Response.

A response is defined to be any variable of interest that is not an independent variable. We shall denote a response by the symbol y.

(1.1.3) Response Surface.

A representation of the response in terms of the independent variables is said to be a response surface.

(1.1.4) Single Independent Variable Case.

The single independent variable situation is defined to be that where there is a single independent variable x, and we are attempting to express the response as a function of x, say $y = f(x)$.

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(1.1.5) Multiple Independent Variable Case.

The multiple independent variable case is defined to be that where there are k independent variables: $x_1, x_2, \ldots, x_k$; and we are attempting to express the response as a function of $(x_1, x_2, \ldots, x_k)$, say $y = f(x_1, x_2, \ldots, x_k)$.

(1.1.6) Observation.

An observation is defined to be a determination of the k+1 values:

$$(x_{1i}, x_{2i}, \ldots, x_{ki}, y_i).$$

(1.1.7) Experiment.

The determination of one or more observations according to some pre-arranged plan is said to be an experiment.

(1.1.8) Experimental Design.

A pre-arranged plan describing the values of the independent variables for each observation is defined to be on experimental design.

(1.1.9) Sequential Procedure.

A method of experimentation by means of which the values of the independent variables for the n-th observation are determined by a procedure laid down in advance of the experiment from the values for the response on one or more of the preceding n-1 observations is called a sequential procedure.

(1.1.10) Row Vector.

A row vector consisting of the p elements $(x_1, x_2, \ldots, x_p)$ shall be denoted by the symbol $\underline{x}$.

(1.1.11) Optimum Point.

A combination of the values of the independent variables which maximizes the response is called an optimum point and is designated by θ in the single independent variable situation and by $\underline{\theta}$ in the multiple independent variable situation. We shall consider only the problem of maximizing the response, since the minimization problem can be handled by maximizing the negative of the response.

(1.1.12) NID Notation.

A random variable w is said to be NID(u,v) if, in every sample, the w_i are identically and independently distributed with mean u and variance v.

1.2. The Purpose of Experimentation.

Although all experimentation is undertaken with the ultimate goal of increasing man's knowledge about the world in which he lives, the short-term goal of an experiment may be modified by the funds or equipment available, the extent of the experimenter's knowledge concerning the phenomena under investigation, or by the phase of the investigation. The primary objectives may be summarized as:

(1.2.1) Deciding on important independent variables;

(1.2.2) Mapping the response surface over the area of interest;

(1.2.3) Optimizing a response or a combination of responses;

(1.2.4) Obtaining an insight into the basic mechanism of the system.

The objective of any particular experiment may be one or several of these goals, but usually the experimenter will progress in his knowledge and understanding of the system by taking steps in the

order listed above.

In addition to (1.2.1) through (1.2.4) it should be the objective of every experiment to:

(1.2.5) Point out the direction in which further research should proceed.

No scientific investigation is an end in itself. It is the essence of all progress that we continue to accumulate information and to modify and, if necessary, discard our ideas and our theories as new evidence comes to light.

> The laws of science constitute a growing, ever-changing organism, but the changes are generally evolutionary in character and represent modifications, improvements, and extensions more often than drastic repudiation of the old.[2]

1.3. Deficiencies of Factorial Design.

There has been a growing realization of late that there exist many special experimental problems for which factorial designs and their modifications: the latin squares, the balanced incomplete block designs, the confounded designs, and the fractionally replicated designs may not provide a realistic or an economically feasible solution. The experimenter, for instance, may be interested in picking out the most important variables from a large group of potentially important variables; or he may be working with a number of populations with unknown means and wish to pick a group of three or four of these populations, say those with the largest means, for further study. Alternatively, he may wish

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2. E. Bright Wilson, Jr., An Introduction to Scientific Research. New York: McGraw Hill, 1952. pp. 30.

to optimize some response as a function of the independent variables under his control. We shall be concerned in this thesis primarily with the problem of optimizing a response.

The complete factorial designs have been found to be unsatisfactory for this purpose mainly because:

(1.3.1) The conclusions obtained from the analysis apply only to a discrete set of factor combinations, while in reality many of the variables are continuous.

(1.3.2) When the number of factors is large, the number of observations required even for a 2^n experiment becomes prohibitively large. Fractionally replicated designs are some help here but not the whole answer.

(1.3.3) With many factors much of the information obtained from the experiment concerns the high-order interactions. Quite often this is information of little value to the experimenter because:

i) In some fields high-order interactions have been shown to be usually small when compared with the main effects and first order interactions.

ii) Even when one of the high-order interactions is large, its physical interpretation may be difficult.

(1.3.4) These designs devote observations to regions which may be of little interest to the experimenter since, in the light of the results, these regions may be far from a maximum.

We are thus led to seek for designs which:

(1.3.5) Take into consideration the continuous nature of some of the

variables.

(1.3.6) Provide degrees of freedom for estimating the main effects and the low-order interactions but do not devote observations to determining the high order interactions.

(1.3.7) Concentrate most of the observations in the neighborhood of the maximum.

As a result of these considerations, several new experimental design and sequential experimentation techniques have come into use in recent years. It is the purpose of this chapter to list some of these techniques, to provide a list of questions which it is hoped will be of assistance in comparing these techniques, and to describe briefly some of the optimum-locating techniques and indicate the general area where each might prove useful.

1.4. The New Techniques.

In 1941, Hotelling [17] treated the problem of maximizing the response due to a single independent variable.

Friedman and Savage [14] proposed, in 1947, a sequential one-factor-at-a-time approach to the problem of approximating the maximum or mapping the area in the neighborhood of the maximum of a response based on several independent variables. Sequential plans for the single independent variable case have been devised by Robbins and Monro [22], 1951, and by Kiefer and Wolfowitz [18], 1952. Robbins and Monro considered the problem of estimating x such that

$$f(x) = \alpha \quad ,$$

where α is pre-determined, and Kiefer and Wolfowitz obtained a sequential procedure for estimating x such that $f(x)$ is a maximum. Blum [5], 1954, extended the Kiefer-Wolfowitz procedure to the multidimensional case. Dixon and Mood [13], 1948, presented a seqqential procedure for sensitivity testing.

Box and Wilson [10], 1951, introduced a method of sequential progression by the method of "steepest ascent", and have contributed a whole new class of experimental designs ranging from the first order designs to the central and non-central composite designs and the rotatable designs.

Bechhofer [3], 1954, and Bechhofer, Dunnet and Sobel [4], 1954, have given procedures for choosing from among a group of populations a sub-group with the following property: a probability p is chosen by the experimenter; then the probability that the chosen sub-group contains the population with the greatest (smallest) mean is greater than or equal to p.

Satterthwaite [23], 1956, has introduced the random balance designs. These designs are constructed to screen a large group of variables and pick out those which have a noticeable effect on the response.

1.5, Some Questions.

We list here some questions which we hope will prove helpful in determining the usefulness of and the limitations on the new techniques.

(1.5.1) Number of Observations.

What is the number of observations needed for a given result? Is this number fixed or variable? If it is variable, do we know its probability distribution or can we place bounds upon it?

(1.5.2) Reliability of Predictors.

In those cases where we obtain regression coefficients, what are the standard deviations and biases of these regression coefficients? What is $\text{var}(\hat{y})$? What is $\text{var}(\hat{\underline{\theta}})$?

(1.5.3) Is the Procedure Robust?

How sensitive is the procedure to the existence of interactions? What is the effect in the sequential procedures of changing the starting point, or in the "steepest ascent" procedure of changing the initial region? Is the procedure at the mercy of time trends? Can we adapt the design to some form of blocking when serious non-heterogeneity exists? What is the effect of using the wrong model? How about biases, non-normality, etc.? Will a large experimental error seriously damage the efficiency of the procedure?

(1.5.4) Can We Test for Goodness of fit and Change the Model if Necessary?

Can we make at least a rough test for goodness of fit? If such a test indicates another model, can we make this change? Can we add a variable during the course of the experimentation? If the first experiments indicate that we should move to a new experimental region, can we salvage the information obtained from these first experiments, i.e., can we "nest" the design?

(1.5.5) Opportunity to use Past Knowledge.

Does the technique offer the investigator opportunity to make use of his knowledge and skill?

(1.5.6) Interpretation of Results.

Can the results of the analysis be interpreted in such a way that the experimenter with little or no statistical training will clearly understand them?

(1.5.7) Computational Considerations.

What about the computational procedures involved? Will they become too cumbersome? Can they be programmed on an electronic computer? What is known about the distributions of the estimates obtained from the sequential plans? What is the effect of optional stopping in the sequential plans?

We shall discuss below some of the new designs which may be used to estimate the location of the maximum response. We shall take up separately the single independent variable designs and the multiple independent variable designs.

Single Independent Variable Designs

We shall discuss here the Hotelling procedure and the Kiefer-Wolfowitz procedure.

1.6. The Hotelling Procedure.

The Hotelling procedure is described in [17] and is summarized briefly below.

The experiment is divided into two parts: an initial experiment to determine the approximate location of the maximum response and a second experiment to determine a more precise estimate of the location of the maximum response and to map the response in the vicinity of the maximum.

For the initial experiment assume a fifth order regression model[3], i.e.,

$$(1.6.1) \qquad y = \beta_0+\beta_1 x+\beta_2 x^2+\beta_3 x^3+\beta_4 x^4+\beta_5 x^5 + \varepsilon \quad ,$$

where ε is $NID(0,\sigma^2)$. Take at least 6 equally spaced levels of x: $x_{(1)}, x_{(2)}, \ldots, x_{(p)}$, $p \geq 6$, and make n determinations of the response ($n \geq 2$) at each level of x. The total number of observations in this initial stage is then $np \geq 12$. Fit a fifth degree curve to these observations with the use of orthogonal polynomials, thus obtaining the prediction equation:

$$(1.6.2) \qquad \hat{y} = b_0 + b_1 x + b_2 x^2 + b_3 x^3 + b_4 x^4 + b_5 x^5 \quad ,$$

where b_i is the least squares estimate of β_i, for $i = 0, 1, \ldots, 5$.

Determine the value of x which maximizes (1.6.2). Call this value t. This can be determined graphically or by differentiating (1.6.2) with respect to x, solving the resulting quartic equation, and taking the root which maximizes $\hat{y}$. Now conduct a second experiment in

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3. We assume a fifth order regression model in order to obtain estimates of β_2, β_3, β_4, and β_5 which are used in obtaining the design points for the second stage of the experiment.

the neighborhood of t taking n_1 [4] observations. The experimental designs for this phase of the investigation are given in [17]. Designs specifying three levels of x are given for both equal and unequal frequencies in the cells corresponding to the levels of x. Since we will limit ourselves to a small neighborhood of t, a quadratic model should adequately describe the response in this region. Thus we assume the model

$$(1.6.3) \qquad y = \beta_0' + B_1'(x-t) + \beta_2'(x-t)^2 + \varepsilon' \quad ,$$

where ε' is NID$(0,\sigma'^2)$, and obtain the least squares estimates b_i' of the β_i'. The equation of prediction becomes,

$$(1.6.4) \qquad \hat{y} = b_0' + b_1'(x-t) + b_2'(x-t)^2 \quad .$$

Differentiating (1.6.4) with respect to $(x-t)$ and setting equal to zero, we obtain

$$(1.6.5) \qquad \hat{y}' = b_1' + 2b_2'(x-t) = 0 \quad ,$$

and thus,

$$(1.6.6) \qquad \widehat{x-t} = \hat{\theta}_1 = -\frac{b_1'}{2b_2'} \quad ,$$

so that $\hat{\theta} = \hat{\theta}_1 + t$ is the best estimate of the abscica at the maximum response.

Discussion.

Note that the total number of observations is fixed, being

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4. n_1 is for all practical purposes arbitrary.

$np + n_1$. The estimates of the regression coefficients, both in the first and second phases of experimentation, are minimum variance estimates and the variance matrix for these regression coefficients is obtained in the standard manner. Furthermore, the designs in phase two are constructed so that the cubic bias in the regression coefficients is zero and the quartic bias is minimized. Also, the expectation of the square of the total error in $\hat{\theta}$, up to and including terms of fourth order in the bias, is minimized by a proper balance between the sampling variance and the quartic bias.

The variance of $\hat{y}$ for any x, say x', is estimated by

$$\text{(1.6.7)} \qquad \operatorname{Var}(\hat{y}\,|\,x') = \sum_{i=0}^{2} \sum_{j=0}^{2} c_{ij}(x')^{i+j} s^2 \quad ,$$

where s^2 is the estimate of σ^2, and where c_{ij} is the appropriate term from the inverse normal matrix C.

$$C = \begin{array}{c} \begin{array}{ccc} x^0 & x^1 & x^2 \end{array} \\ \begin{pmatrix} c_{00} & c_{01} & c_{02} \\ c_{10} & c_{11} & c_{12} \\ c_{20} & c_{21} & c_{22} \end{pmatrix} \end{array} \begin{array}{c} x^0 \\ x^1 \\ x^2 \end{array}$$

We can obtain confidence limits for θ by a device due to Fieller. See [15]. Let $(x-t) = z$. Then from (1.6.5)

$$\hat{y}' = b_1' + 2b_2'z = \delta, \text{ say} \quad .$$

The variance of this quantity can be estimated by

(1.6.8) $\quad \mathrm{Var}(\delta)=(c_{11}+4z^2c_{22}+4zc_{12})s^2=v$, say .

Thus,

$$(1.6.9) \qquad \frac{(b_1'+2b_2'z)^2}{v} = t^2_{\alpha,n_1-3} \ ,$$

where t_{α,n_1-3} is the α percentage point for the Student's t distribution with n_1-3 degrees of freedom. Substituting from (1.6.8),

$$(1.6.10) \qquad \frac{(b_1'+2b_2'z)^2}{(c_{11}+4z^2c_{22}+4zc_{12})s^2} = t^2_{\alpha,n_1-3} \ ,$$

that is,

$$(1.6.11) \quad (b_2'^2-s^2t^2c_{22})4z^2+(b_1'b_2'-s^2t^2c_{12})4z+b_1'^2-s^2t^2c_{11}=0 \ ,$$

where

$$t^2 = t^2_{\alpha,n_1-3} \ .$$

Thus, by solving (1.6.11) for z, we can obtain confidence limits for z with confidence coefficient $(1-\alpha)$. Since $x = z + t$, we can then get confidence limits for x, i.e., for θ. These confidence limits will be correct, however, only if the true regression is quadratic. If the true regression is not quadratic, the confidence band for θ will be wider than that indicated by the computed limits due to the presence of bias effects.

Another advantage of the Hotelling technique is that the order of the experimental runs for either or both phases of the investigation can be randomized so that a time trend will not seriously bias the esti-

mate of θ.

The Hotelling approach probably does not offer as much opportunity for the employment of the knowledge and skill of the experimenter as do some of the experimental techniques discussed below. About the only contribution that the experimenter can make towards designing the experiment is in deciding what range to cover and how to space the x's. A check on the adequacy of the model may be obtained by running 2 or 3 confirmatory observations, at points slightly displaced from the estimated maximum and comparing the observed with the predicted response for these points. This idea of taking confirmatory observations is a very important one and can be carried out with all of the experimental techniques discussed in this section.

The main results of interest to the experimenter will be the estimate of θ, the regression equation for predicting y in the neighborhood of θ, and the residual variance, with perhaps an indication of how the response behaves in a region distant from θ. All of these concepts are capable of simple interpretation by a man with the bare minimum of statistical training.

Finally, most of the computation involved is the standard least squares type of computation which should present no difficulty to the statistician. Orthogonal polynomials can be employed in the initial phase of the experiment, and, if a lot of this work is going to be done, it might prove useful to compute a set of orthogonal polynomials for the designs involving unequally spaced x-intervals in phase two.

In summary, the Hotelling procedure is a fixed sample size procedure well-suited to estimating the maximum of a response based on a single independent variable and to mapping the function in the neighborhood of the maximum response. It is also a procedure for which the mathematical properties of the estimates obtained are well-known and in many senses optimum.[5]

1.7. The Kiefer-Wolfowitz Procedure.

The Kiefer-Wolfowitz procedure [18] for the stochastic estimation of the maximum of a regression function may be described as follows:

Select two sequences of positive terms: $\{a_n\}$ and $\{c_n\}$. See (2.1) for the rules governing the choice of these sequences. Let z_1 be the best advance estimate of θ. Then at each stage of the sequentiel procedure obtain the experimental points (z_n-c_n, y_{2n-1}) and (z_n+c_n, y_{2n}), and let z_{n+1} be determined by the rule:

$$z_{n+1} = z_n + \frac{a_n}{c_n}(y_{2n}-y_{2n-1}) \quad . \tag{1.7.1}$$

At the n-th stage of the sequential procedure let z_{n+1} be the best estimate of θ. Kiefer and Wolfowitz have shown [18] that, under very general conditions, the most important being that the function possess a unique maximum in the region of interest, that z_n will

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5. Many of the optimum properties of this technique are based upon large sample approximations. The estimates obtained may be far from optimum when the sample is small.

converge in probability to θ.

In Chapter II of this thesis a number of the properties of the sequential procedure for the case when the regression function is a quadratic function are investigated. I shall state here what appear to be the very general properties of the procedure, and shall refer to Chapter II for a more detailed description of these properties for the special case considered there.

Discussion.

N, the number of observations, is unknown, of course, in advance of the experiment, and, in fact, there is no well-known procedure for terminating the sequence of experimentation (see (2.43) for suggestions), let alone any knowledge of the probability distribution of N. This fact seems to be the main deterrent to widespread use of the procedure. If at least bounds for N can be determined for a given situation, then the sequential procedure gives promise of being more efficient than a fixed sample size experiment to accomplish the same objective. Perhaps the Monte Carlo method might be used to generate stochastic sequences and thus study various stopping procedures and their operating characteristics.

In addition to merely estimating θ, we can, of course, map the response in the neighborhood of the maximum by assuming, say, a quadratic model and computing the least squares regression coefficients. This procedure can also give us another estimate of θ since, as in (1.6.6),

(1.7.2) $$\hat{\theta} = - b_1/2b_2 \quad .$$

Exact statements about the biases and variances of the regression coefficients so obtained cannot be made in advance of the experiment, but their properties should in general be good since it is the tendency of the stochastic procedure to concentrate observations in the neighborhood of the maximum response. Thus the function should be well-mapped in this neighborhood.

Some possible disadvantages of the procedure are that the rate of convergence of z_n to θ may depend heavily upon the choice of z_1 and that the process may be quite vulnerable to time-trends. An advantage is that we do not have to worry about experimenting in the wrong region. The sequential procedure will, in due time, usually[6] lead us to the right region.

The chance for the utilization of the skill of the investigator is somewhat limited to the choice of z_1 and the choice of the sequences $\{a_n\}$ and $\{c_n\}$ which are essentially scale factors. The proper choice of these two sequences is essential in order that z_n converge to θ rapidly. See (2.48) and (2.49).

In the case where the regression coefficients are estimated, it is easy to check upon the adequacy of the model. Since x will, in general, not be limited to three levels as in phase two of the Hotelling scheme, we can compute the additional sums of squares due to cubic, quartic, ... effects and test these for significance in the

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6. The procedure may not lead to the region of the maximum response if there is more than one maximum. In such a case we may be led to a local maximum smaller than the absolute maximum. This is true of nearly all of the sequential optimization techniques.

standard manner. Alternatively confirmatory observations may be taken.

The computational work and its interpretation are, in the case where we are merely estimating θ, extremely simple, making the procedure admirably suited to wide-scale application by non-statisticians.

In summary, the Kiefer-Wolfowitz procedure shows promise for the purpose of locating the position of the maximum response and for describing the response in the vicinity of the maximum. Its principal advantages are: simplicity of use, a well-defined procedure for progressing to the region of the maximum response, concentration of the observations in the neighborhood of the maximum response, the presence of a check for goodness of fit, and possibly an increase in efficiency over the fixed sample size experiments. The principal disadvantages of the Kiefer-Wolfowitz procedure are: the absence of a general stopping rule, lack of knowledge concerning the probability distribution of N, dependence of the rate of convergence upon the choice of the starting point, and sensitivity of the procedure to time trends and other forms of non-heterogeneity.

Multiple Independent Variable Situation

We shall now consider three techniques that may be used in the multiple independent variable situation. These techniques are: the Friedman-Savage procedure, the Blum procedure, and the Box-Wilson procedure. Many of the ideas and arguments used here are identical with those used in the single independent variable situation. The com-

plexity of the problem is, of course, increased over that of the single independent variable case due to the multiplicity of factors and due to two added functions of the experiment:

i) to separate out important independent variables;

ii) to detect interactions.

1.8. The Friedman-Savage Procedure.

The procedure of Friedman and Savage is treated in [14]. A description of the Friedman Savage procedure is as follows:

(1.8.1) Choose an initial factor combination. Presumably this will be the best advance estimate of the optimal factor combination.

(1.8.2) Order the independent variables. One suggestion is to rank them in their estimated order of importance.

(1.8.3) Holding all other independent variables constant, vary the levels of the first until an approximate optimum is achieved. Either the Hotelling or the Kiefer-Wolfowitz ideas might be employed here.

(1.8.4) Using the optimal level of the first independent variable and holding all other independent variables but the second at their initial levels, find an approximate optimal level for the second. Continue in this manner until all independent variables have been investigated. Call this process a round of experimentation.

(1.8.5) Continue experimenting in this fashion until the changes in response become small by some standard. Use for the initial

factor combination of each round the estimate of those levels of the independent variables maximizing the response for the previous round.

Discussion.

As in the case of the Kiefer-Wolfowitz procedure, the sample size N is a random variable about which little is known. Friedman and Savage suggest that the procedure may be more efficient than a factorial design when there are no interactions and when experimental error is small. Since the tendency of the procedure is to concentrate observations in the neighborhood of the maximum response, it may be possible to map the response surface fairly well in the vicinity of the maximum, but because of the possibly restricted approach to the maximum, this mapping may not be so complete as that of some of the other sequential procedures.

It appears that the procedure may be very sensitive to the choice of the starting factor combination and that it may be quite inefficient in the presence of large interactions or large experimental error. It is also evident that we are quite at the mercy of time trends. On the positive side, as in the case of many sequential procedures, the model that we choose is a very general one, and the procedure may be relatively insensitive to non-normality, etc.

This technique more than any of the others resembles the pre-analysis of variance technique of classical experimentation. It thus should be easy for the experimenter to understand and offers consider-

able scope for the use of his knowledge and ingenuity. Another advantage is that we can easily add new variables which come to mind or drop those of the original variables which in the initial stages of experimentation prove to be unimportant. The addition of a new variable in many of the designs is accomplished by repeating the whole experiment with the new factor at a different level, possibly doubling the cost of the experiment. With the Friedman-Savage procedure we may add a new variable, even in the final stages of the experiment, simply by holding all the old variables at their estimated optimum levels and varying the new factor over its set of levels, i.e., perhaps by as few as five or six additional observations.

The computational burden is not heavy. It is suggested that at least in the early rounds the optimization procedure may be done graphically.

In summary, the advantages of the Friedman-Savage procedure are: it is easily understood by the experimenter since it probably conforms to his ideas on experimentation; we can add or drop variables during the course of the experiment with ease; the model is very general; the procedure concentrates observations in the neighborhood of the maximum response; and the procedure is possibly more efficient[7] than the corresponding factorial experiment when interactions and experimental error are small. The disadvantages of the technique are that not much

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7. When there are no interactions and no experimental error the Friedman-Savage process will converge to the maximum response in one round of experimentation.

is known about the probability distribution of N; the procedure may be quite sensitive to the choice of the starting factor combination and may be inefficient in the presence of large interactions or large experimental error and is quite vulnerable to time-trends.

It appears that this procedure may be effective in the early stages of an investigation as follows: in separating the important independent variables from the unimportant independent variables, in obtaining an estimate of the location of the maximum response, and in mapping the response surface fairly well in the immediate vicinity of the maximum and roughly elsewhere.

1.9. The Blum Procedure.

The Kiefer-Wolfowitz procedure for stochastic estimation of the maximum of a regression function with one independent variable has been extended to the multiple independent variable case by Blum [5], 1954. His procedure is described below.

Choose $\{a_n\}$ and $\{c_n\}$ as two infinite sequences of positive numbers satisfying (2.1) and let U be the matrix:

(1.9.1)
$$\begin{pmatrix} u_1 & & 0 \\ & u_2 & \\ & & \ddots \\ 0 & & u_k \end{pmatrix}$$

composed of the row vectors

$$\underline{u}_1 = (u_1, 0, 0, \ldots, 0) \quad ,$$

$$\underline{u}_2 = (0, u_2, 0, \ldots, 0) \quad ,$$

$$\ldots \ldots \ldots \ldots \ldots \ldots \ldots$$

$$\underline{u}_k = (0, 0, 0, \ldots, u_k) \quad .$$

Let $\underline{x}_i$ be the row vector $(x_{1i}, x_{2i}, \ldots, x_{ki})$ and let $Y_{\underline{x}_i}$ be the measured response for the factor combination $\underline{x}_i$. Let $\underline{Y}_n^*$ be the vector

$$(1.9.2) \quad \left((Y_{\underline{x}_n+c_n\underline{u}_1} - Y_{\underline{x}_n}), (Y_{\underline{x}_n+c_n\underline{u}_2} - Y_{\underline{x}_n}), \ldots, (Y_{\underline{x}_n+c_n\underline{u}_k} - Y_{\underline{x}_n}) \right) ,$$

and define a recursive sequence of random vectors by choosing $\underline{x}_1$ arbitrarily and letting

$$(1.9.3) \quad \underline{x}_{n+1} = \underline{x}_n + \frac{a_n}{c_n} \underline{Y}_n^* \quad .$$

Very general conditions for convergence of $\underline{x}_n$ to $\underline{\theta}$ are given in [5].

The operating characteristics of the Blum procedure appear to be very similar to those given for the Kiefer-Wolfowitz procedure and will not be restated here. Note that the term $Y_{\underline{x}_n}$ appears in each component of $\underline{Y}_n^*$ which means that if the experimental error is large the procedure may be very slow to converge. Perhaps the designs of Plackett and Burnam [19] could be used to advantage here. They present a sequence of designs for use when the sample size is of the type $4n$ where

the estimate of each main effect is orthogonal to the estimate of all other main effects. Thus, for example, if there are eight independent variables, the procedure outlined in (1.9.3) requires nine observations per round and the component of the change in factor x_p ($p=1,2,\ldots,8$) is determined from two observations. Using one of the Plackett and Burnam designs, we could take, say, 12 observations and the component of the change in factor x_p would be determined with the use of all 12 observations. Thus by increasing the number of experiments by one third we have increased the efficiency of the experiment by a factor of six, and furthermore with three degrees of freedom left for error, we can obtain some idea concerning the significance of the various factors. Perhaps the confounding of interactions with main effects which occurs in the Plackett and Burnam designs will prevent their use in this context, but I can see no reason why this confounding should be any more serious than that which would occur with the use of (1.9.3).

As an extension of the results given in (2.48) it appears that the proper choice of the sequences $\{a_n\}$ and $\{c_n\}$ and the matrix U are essential for reasonably rapid convergence of $\underline{x}_n$ to $\underline{\theta}$. Possibly a preliminary experiment to yield rough estimates of the second degree regression coefficients would be helpful in the choice of these factors. Again, this is a field where the Monte Carlo method might be used to study the properties of a procedure based upon such a choice.

(1.10) The Box-Wilson Procedure.

The Box-Wilson technique is described in [10] and is outlined in steps (1.10.4) to (1.10.9) below.

We will first introduce a coding of the independent variables which will simplify the presentation of the designs. Suppose that there are k independent variables: $x_1, x_2, \ldots, x_k$. Further, suppose that N observations are to be taken. Then we introduce a new set of variables: $z_1, z_2, \ldots, z_k$ where

$$(1.10.1) \qquad z_{iu} = \frac{x_{iu} - \bar{x}_{iu}}{\sqrt{\sum_{u=1}^{N} (x_{iu} - \bar{x}_{iu})^2 / N}} \quad \text{for } i = 1,2 \ldots,k \quad ,$$

and such that the z_i obey the relations:

$$(1.10.2) \qquad \sum_{u=1}^{N} z_{iu} = 0 \ ,$$

and

$$(1.10.3) \qquad \sum_{u=1}^{N} z_{iu}^2 = N \ , \quad \text{where } i=1,2,\ldots,k \quad .$$

Box and Wilson then proceed as follows:

(1.10.4) An initial experiment is conducted somewhere in the region of interest (persumably in the neighborhood of the best estimate of the optimum factor combination). The initial experiment is often a factorial or fractional factorial experiment with all independent variables at two levels. The design is called a first-order design and the model adopted is:

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i z_{iu} + \sum_{i<j}^{k} \beta_{ij} z_{iu} z_{ju} + \varepsilon_u \quad ,$$

where the ε_u are NID(0, σ^2).

(1.10.5) Compute the regression coefficients corresponding to the main effects and two-factor interactions in (1.10.4). If the main effects are large compared with the two-factor interactions, conduct a second experiment (again using a first order design) in which the factor levels are changed in the direction of largest response in the initial experiments. This is called the path of steepest ascent. Continue this process until the first order effects are small in comparison with the two-factor interactions. Box calls such a region a near-stationary region.

(1.10.6) Take additional observations to determine the quadratic components of the main effects. A whole series of designs has been developed for this purpose, and these designs are discussed briefly in (1.10.10). The model becomes:

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i z_{iu} + \sum_{i=1}^{k} \beta_{ii} z_{iu}^2 + \sum_{i<j}^{k} \beta_{ij} z_{iu} z_{ju} + \varepsilon_u \quad ,$$

where the ε_u are NID(0, σ^2) .

(1.10.7) Compute the least squares estimates of the β_p. Denote these by b_p. The equation of prediction becomes

$$\hat{y}_u = b_0 + \sum_{i=1}^{k} b_i z_{iu} + \sum_{i=1}^{k} b_{ii} z_{iu}^2 + \sum_{i<j}^{k} b_{ij} z_{iu} z_{ju} \quad .$$

By differentiating this expression with respect to $z_1, z_2, \ldots, z_k$, setting equal to zero and then solving the resulting system of k simultaneous equations in k unknowns, the estimates $z_1^0, z_2^0, \ldots, z_k^0$

which maximize the response can be found. The estimated maximum response is

$$\hat{y}_m = b_0 + \sum_{i=1}^{k} b_i z_i^0 + = \sum_{i=1}^{k} b_{ii} z_i^{0^2} + \sum_{i<j}^{k} b_{ij} z_i^0 z_j^0 \quad .$$

(1.10.8) The expression (1.10.7) is reduced to the canonical form,

$$\hat{y}_u - \hat{y}_m = \sum_{i=1}^{k} B_i \bar{z}_{iu}^2 \quad ,$$

where

$$\bar{z}_i = a_{i1} z_1 + a_{i2} z_2 + \ldots + a_{ik} z_k \quad ,$$

that is a linear function in the z_i.

(1.10.9) Confirmatory observations are taken.

(1.10.10) The Designs.

The Box-Wilson designs, which we shall consider, are of two types: the first order designs, which are used to locate the direction of steepest ascent, and the second order designs, which are used to estimate the regression coefficients in a near-stationary region. (Gardiner, Grandage, and Hader present an excellent discussion of third order designs in [16]).

Let us here introduce another notational device:

Let

$$z_0 = z_0 \quad ,$$

$$z_1 = z_1 \quad ,$$

.....

$$z_k = z_k \quad ,$$

$$z_1 z_2 = z_{k+1} \quad ,$$

$$z_1 z_3 = z_{k+2} \quad ,$$

$$\cdots\cdots\cdots$$

$$z_{k-1} z_k = z_\ell \quad ,$$

$$z_1^2 = z_{\ell+1} \quad ,$$

$$z_2^2 = z_{\ell+2} \quad ,$$

$$\cdots\cdots\cdots$$

$$z_k^2 = z_m \quad ,$$

where

$$\ell = k + \frac{k(k-1)}{2} = \frac{k(k+1)}{2} \quad ,$$

and

$$m = k + \frac{k(k-1)}{2} + k = \frac{k(k+3)}{3} \quad .$$

Optimum first order designs, in the sense that the variances of the regression coefficients become smallest, are achieved by the use of factorial designs with all factors at two levels. These designs also have the property that

$$\text{cov}\,(b_i, b_j) = 0 \quad ,$$

where

$$i = 1, 2, \ldots, \ell \; ;$$

$$j = 1, 2, \ldots, \ell \; ;$$

$$i \neq j \quad .$$

When the number of independent variables is five or more, fractional factorials may be used in this phase of the investigation.

One criterion for the choice of good second-order designs is the criterion of rotatability. With a rotatable design, the response surface is determined with equal precision at points equi-distant from the experimental center. With two independent variables, the regular figures, i.e., points equally spaced on a circle, with the addition of one or more center points, will give rotatable designs providing that the number of points on the circle is five or more.

Box and Wilson propose the central composite designs which may be constructed as follows. Suppose that the last first-order experiment performed was a $1/2^p$ replicate of a 2^k factorial. Designate the k factor levels at the center of the $1/2^p \times 2^k$ design as $(0, 0, \ldots, 0)$, and add $2k+1$ additional observations to the set of 2^{k-p} observations by taking the factor combinations:

$$(0,0,\ldots,0),(\pm\alpha,0,\ldots,0),(0,\pm\alpha,\ldots,0),\ldots,(0,0,\ldots,\pm\alpha) .$$

This portion of the design is known as the cross-polytrope. By a proper adjustment between α and the radius of the hypercube, the central composite designs become rotatable designs.

While rotatability is a desired property in these designs it is not the sole criterion for the choice of good second-order designs. It is possible to choose α, for instance, so that $\mathrm{cov}(b_i, b_j) = 0$, where $i = 1, 2, \ldots, m$; $j = 1, 2, \ldots, m$; $i \neq j$. These are called orthogonal designs. Box and Wilson also give [6] non-central composite designs.

These are designs which concentrate the observations taken during the second-order phase of the experiment in a particular corner of the last first-order design.

Discussion.

The Box-Wilson procedure is, like the other procedures we have been discussing, a sequential procedure. It is not a formal sequential procedure in the sense of the Kiefer-Wolfowitz procedure because, although the direction of steepest ascent is determined by earlier observations, the magnitude of the step taken in this direction must be chosen by the experimenter. The number of observations, N, is clearly a random variable, but one on which, it seems, plausibility, if not probability, bounds can be placed. Let us consider the central composite designs. If the first-order experiments cover a sufficiently wide experimental region and successive first-order designs are spaced far enough apart, it seems to this writer unlikely that more than three of these will be necessary to reach a near-stationary region. Thus, if each of the first order designs is a $1/2^p$ replicate of a 2^k factorial, and if the second order design is a central composite design, lower and uppper bounds for N, call them N_ℓ and N_h can be computed and are shown in Table 1.10 for k = 2, 3, ..., 6. The number of experiments in a 3^k factorial design is shown for comparative purposes.

TABLE 1.10

NUMBER OF OBSERVATIONS[8]

k	Design	N_ℓ	N_h	3^k
2	2^2 + cp.	9	17	9
3	2^3 + cp.	15	31	27
4	2^4 + cp.	25	57	81
5	2^5 + cp.	43	107	243
5	$\frac{1}{2} \times 2^5$ + cp.	27	59	243
6	$\frac{1}{2} \times 2^6$ + cp.	45	109	729

The central composite designs may be used, of course, as designs in their own right -- without the preliminary use of first-order designs. If there are several responses, for example, we cannot carry out the first-order experimentation sequence on all of them simultaneously. In that case our primary concern may be in mapping each response over the area of interest. The sample size for this type of experiment is that given in the N_ℓ column of Table 1.10.

The variances and covariances of the estimated regression coefficients can, of course, be obtained from:

---

8. The abbreviation cp. is used to indicate cross-polytrope.

(1.10.11) $\quad \text{Var}\,(b_i) = c_{ii}s^2, \quad \text{for } i = 0, 1, 2, \ldots, m \ ,$

and

$$\text{cov}\,(b_i, b_j) = c_{ij}s^2 \ ,$$

where

$$i = 0, 1, 2, \ldots, m \ ,$$
$$j = 0, 1, 2, \ldots, m \ ,$$
$$i \neq j \ ,$$

where c_{ij} is the element in the i-th row and j-th column of the inverse normal matrix C, and

$$s^2 = \frac{\sum_{u=1}^{N} (y_u - \hat{y}_u)^2}{N-m-1} \ .$$

The variance of the estimated response at any point $\underline{z}' = (z_1', z_2', \ldots, z_k')$ may be estimated from

$$v(\hat{y} \mid \underline{z}') = \left\{ \sum_{i=0}^{k} \sum_{j=0}^{k} c_{ij} z_i' z_j' \right\} s^2 \ .$$

The Box-Wilson designs lend themselves to blocking [9] and thus can be used when real non-heterogeneity or a time trend is anticipated. Interactions can be detected with the first-order designs and the direction of steepest ascent determined with the aid of these interactions. On the other hand, the Blum and Friedman-Savage procedures assume in each round of experimentation that the effects are additive and for this reason may require more experiments when large

interactions do exist.

(1.10.12) The goodness of fit can be checked in one of several ways.

i) If the design permits, we may add cubic or higher order terms to the model and test whether or not the increase in the regression sum of squares is significant.

ii) We may know or have an idea of the magnitude of the experimental error variance and compare the obtained residual variance with this estimate, or we may replicate some of the experimental points and divide the error variance into two parts: that due to replication and a remainder, and compare these two variances.

iii) We may plot $\Delta y = (y - \hat{y})$ against y and examine for indications of correlation.

iv) We may take confirmatory observations. These are perhaps best taken along the canonical axes.

(1.10.13) If one of the procedures suggested in (1.10.12) indicates that we have chosen the wrong model we can either:

i) In those cases where the model permits, write a new regression equation including the cubic or higher order terms determined in (1.10.12, i), if by doing so we find that the fit is sufficiently improved; or,

ii) Add points to the experimental design. The Box-Wilson designs adapt themselves very nicely to "nesting", for instance. Gardiner, Grandage and Hader [16] give

procedures for nesting a second-order design into a third-order design.

The third degree regression coefficients calculated from the second-order design in (i) may be biased. If unbiased estimates of these coefficients are desired, or if the second-order design does not furnish sufficient degrees of freedom to estimate all the relevant third-degree regression coefficients, then additional observations as in (ii) are required. Note that the cost of (i) may be quite small when compared with that of (ii). Perhaps the procedure (i) may be used to indicate whether additional points should be taken or not.

An important use of the canonical equations is as follows. Quite often one of the canonical coefficients, i.e., the B_i, will be very large when compared with all the others. Suppose that this is B_p. What this often means is that $\bar{z}_p$, which itself is a linear combination of the z_i, is the fundamental variable of the system. We give two examples to illustrate this point.

Example 1.

Suppose that in a chemical experiment x_1 and x_2 represent the logarithms of the concentrations of ingredients one and two, respectively. Suppose further that $B_1 >> B_2$ and that $B_1 \approx K(x_1-x_2)$ with K some constant. This then would indicate that the absolute concentration of neither ingredient is the controlling factor, but rather that the ratio of their concentrations is the important variable.

Example 2.

Secondly, a type of response surface frequently encountered is that of the ridge system. See [6] for a representation of some possible response surfaces. Again suppose that there are two independent variables x_1 and x_2, but that their product x_1x_2 is really the fundamental variable of the system, and that the equation of prediction is

$$y = -(x_1x_2)^2 + 3(x_1x_2) \quad . \tag{1.10.14}$$

Then there will be a wide variety of pairs (x_1,x_2) for which the response is at a maximum. Upon differentiating (1.10.14) with respect to x_1x_2 and setting equal to zero we obtain,

$$-2(x_1x_2) + 3 = 0, \text{ i. e., } x_1x_2 = 3/2 \quad . \tag{1.10.15}$$

Thus y is maximized for all points (x_1,x_2) lying on the hyperbola $x_1x_2 = 3/2$, i.e., $(1, \frac{3}{2})$, $(\frac{3}{2}, 1)$, $(3, \frac{1}{2})$, ...

Hence, we can often with multiple responses obtain the locus of the maximum response for, say, the first response and then move along this locus to a point where the second response is also maximized.

These designs do offer the experimenter an opportunity for the use of his knowledge in choosing the position of the first-order design, the levels of the independent variables, the probable degree of the actual response surface, and in estimating which variables are likely to have quadratic effects and which pairs of variables are likely to interact.

The interpretation of the results, while more complex than that for any of the other designs discussed here, is still within the experimenter's grasp. When there are only two independent variables, or perhaps only two that turn out to be important, and with somewhat more difficulty when there are three independent variables, the response surface can be represented in the form of a contour drawing [6] which displays the significant features of the surface. These contour representations are perhaps most easily obtained from the canonical equations.

The computational procedures involved are none other than those of multiple regression made somewhat easier by the presence of several zeros in the matrix of the normal equations. If electronic computing facilities are available, the uncoded independent variables may be used and all of the computational work, including the inversion of large matrices, should proceed with little difficulty.

In summary, the Box-Wilson procedure is useful in all phases of experimental work: in separating out the important independent variables, in mapping the response surface, in locating the position of the maximum response, in gaining understanding about the mechanism of the system, and in pointing out the direction in which further experimentation should proceed. The properties of the regression coefficients so obtained are well-known and, in many respects, optimum. Goodness of fit may be tested by a number of procedures, and if the fit is shown to be bad, a new model may be set up or the design augmented by additional points to correct this difficulty. The designs themselves are extremely versatile

and can be set up in different ways according to the immediate objective of the experiment. The designs offer the experimenter an opportunity to use his skill and knowledge and the contour representation of the response surface is easily understood by him.

1.11. Summary.

This chapter has discussed briefly some of the inadequacies of factorial design in the response surface problem and has attempted to outline a few of the procedures recently developed for this purpose. The treatment given these procedures has been by no means complete and many of the arguments presented are clearly heuristic. I will have served my purpose if I have managed to indicate at least some of the problems that will be met in the application of these designs.

CHAPTER II

APPLICATION OF THE KIEFER-WOLFOWITZ STOCHASTIC APPROXIMATION PROCEDURE TO A SECOND DEGREE REGRESSION FUNCTION

We are interested in applying the Kiefer-Wolfowitz procedure for estimating a maximum to a quadratic function and in determining the operating characteristics of the procedure in this case. The general method is given by Kiefer and Wolfowitz [18] and is described briefly below.

The sequences $\{a_n\}$ and $\{c_n\}$ are chosen subject to the restrictions (2.1).

(2.1.1) $$c_n \longrightarrow 0 \quad ,$$

(2.1.2) $$\sum_{n=1}^{\infty} a_n = \infty \quad ,$$

(2.1.3) $$\sum_{n=1}^{\infty} a_n c_n < \infty \quad ,$$

(2.1.4) $$\sum_{n=1}^{\infty} \left(\frac{a_n}{c_n}\right)^2 < \infty \quad .$$

One choice for these sequences and the one which we shall consider in this paper is (2.2).

(2.2.1) $$\{a_n\} = \frac{R}{n} \quad ,$$

(2.2.2) $$\{c_n\} = \frac{S}{n^k} \quad ,$$

where R and S are arbitrary positive constants and $0 < k < \frac{1}{2}$. It is easily seen that (2.1.1) and (2.1.2) are verified, and since

$$\sum_{n=1}^{\infty} a_n c_n = \sum_{n=1}^{\infty} \frac{RS}{n^{k+1}} ,$$

and

$$\sum_{n=1}^{\infty} \left(\frac{a_n}{c_n}\right)^2 = \sum_{n=1}^{\infty} \left(\frac{R}{S}\right)^2 \frac{1}{n^{2(1-k)}} ,$$

and since the well known series $\sum_{n=1}^{\infty} \frac{1}{n^p}$ converges for $P > 1$, it is seen that all of the conditions of (2.1) are satisfied by (2.2).

The sequential procedure is then described as follows. Let θ be the value of x for which $y = f(x)$ is a maximum and let z_1 be the best advance estimate of θ. At each stage of the experiment two experimental points are obtained: (x_{2n-1}, y_{2n-1}) and (x_{2n}, y_{2n}), where $x_{2n-1} = z_n - c_n$ and $x_{2n} = z_n + c_n$, and where y_i is the measured response at x_i. z_{n+1} is then given by

$$z_{n+1} = z_n + \frac{a_n}{c_n}(y_{2n} - y_{2n-1}) . \tag{2.3}$$

Conditions on $f(x)$ which are necessary for the convergence of z_n to θ are given in [18].

Now suppose that the true regression is quadratic, i.e., $f(x)$ is given by

(2.4) $$y_u = f(x_u) = ax_u^2 + bx_u + c + \varepsilon_u \quad ,$$

where the errors of measurement, i.e., the ε_u, are $NID(0,\sigma_\varepsilon^2)$. Then from (2.4)

(2.5.1) $$y_{2n-1} = a(z_n-c_n)^2 + b(z_n-c_n) + c + \varepsilon_{2n-1}$$

$$= a(z_n^2-2c_nz_n+c_n^2)+b(z_n-c_n)+c+\varepsilon_{2n-1} \quad ,$$

and

(2.5.2) $$y_{2n} = a(z_n+c_n)^2+b(z_n+c_n)+c+\varepsilon_{2n}$$

$$= a(z_n^2+2c_nz_n+c_n^2)+b(z_n+c_n)+c+\varepsilon_{2n} \quad .$$

Employing (2.3) we obtain

(2.6.1) $$z_{n+1} = z_n + \frac{a_n}{c_n}\left\{4ac_nz_n + 2bc_n + \varepsilon_{2n} - \varepsilon_{2n-1}\right\}$$

$$= z_n + 4aa_nz_n + 2ba_n + \frac{a_n}{c_n}(\varepsilon_{2n} - \varepsilon_{2n-1})$$

$$=(1 + 4aa_n)z_n + 2ba_n + \frac{a_n}{c_n}(\varepsilon_{2n} - \varepsilon_{2n-1}) \quad .$$

Remembering that $\theta = -\frac{b}{2a}$, we can rewrite (2.6.1) free of the parameter b as

(2.6.2) $$z_{n+1} = z_n(1+4aa_n) - 4aa_n\theta + \frac{a_n}{c_n}(\varepsilon_{2n} - \varepsilon_{2n-1}) \quad .$$

Since $E(\varepsilon_{2n} - \varepsilon_{2n-1}) = 0$, we have

(2.7.1) $$E(z_{n+1} \mid z_n) = z_n(1 + 4aa_n) + 2ba_n \quad ,$$

or

$$E(z_{n+1} \mid z_n) = z_n(1+4aa_n) - 4aa_n\theta \quad . \tag{2.7.2}$$

Also,

$$\text{var}\,(z_{n+1} \mid z_n) = \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \quad . \tag{2.8}$$

Rewriting (2.7.2) slightly, we see that

$$E(z_{n+1} - z_n \mid z_n) = 4aa_n(z_n - \theta) \quad . \tag{2.9}$$

We are now led to

THEOREM 2.1.

$$E(z_{n+1} \mid z_1) = \left\{(z_1-\theta) \prod_{i=1}^{n} (1+4aa_i)\right\} + \theta \quad .$$

PROOF BY MATHEMATICAL INDUCTION.

(i) Take the case $n = 1$. Then from (2.7.2), we obtain

$$E(z_2 \mid z_1) = z_1(1+4aa_1) - 4aa_1\theta \tag{2.10}$$

$$= (z_1-\theta)(1+4aa_1) + \theta \quad .$$

So the theorem holds for $n = 1$.

(ii) Assume that the theorem is true for $n = k$, i.e., that

$$E(z_{k+1} \mid z_1) = \left\{(z_1-\theta) \prod_{i=1}^{k} (1+4aa_i)\right\} + \theta \quad . \tag{2.11.1}$$

Then we wish to show that the theorem is true for $n = k + 1$, i.e., that

$$E(z_{k+2} \mid z_1) = \left\{(z_1-\theta) \prod_{i=1}^{k+1} (1+4aa_i)\right\} + \theta \quad . \tag{2.11.2}$$

However, from (2.7.2), it is seen that

$$(2.12) \qquad E(z_{k+2} \mid z_{k+1}) = (1+4aa_{k+1})\, E(z_{k+1} \mid z_1) - 4aa_{k+1}\theta \ .$$

Substituting (2.11.1) into (2.12), we obtain

$$(2.13) \qquad E(z_{k+2} \mid z_1) = (z_1-\theta) \prod_{i=1}^{k+1} (1+4aa_i)$$

$$+ (1+4aa_{k+1})\,\theta - 4aa_{k+1}\,\theta$$

$$= \left\{ (z_1-\theta) \prod_{i=1}^{k+1} (1+4aa_i) \right\} + \theta \ .$$

But this is the form (2.11.2). Thus we have proved Theorem 2.1.

THEOREM 2.2.

$$E(z_{n+1} \mid z_1) \longrightarrow \theta \text{ as } n \longrightarrow \infty \ .$$

Proof.

Since $f(x)$ is a quadratic function possessing a maximum, the sign of a will be negative, and if the sequence $\{a_n\}$ is chosen to be R/n, $R > 0$, as indicated in (2.2), then we may write

$$(2.14) \qquad E(z_{n+1} \mid z_1) = \left\{ (z_1 - \theta) \prod_{m=1}^{n} \left(1 - \frac{K}{m}\right) \right\} + \theta \ ,$$

where

$$K = -4aR > 0 \ .$$

Now $(z_1 - \theta)$ is finite and $\leq Q$ say. The infinite product

$\prod_{m=1}^{\infty} (1 - \frac{K}{m})$ vanishes by a well-known theorem; hence, given any $\varepsilon/Q > 0$,

there exists an N such that

$$(2.15.1) \qquad \left| \prod_{m=1}^{N} (1 - \frac{K}{m}) \right| \leq \frac{\varepsilon}{Q} ,$$

and hence

$$(2.15.2) \qquad \left| (z_1 - \theta) \prod_{m=1}^{N} (1 - \frac{K}{m}) \right| \leq \varepsilon .$$

Therefore,

$$\left| E(z_{n+1} \mid z_1) - \theta \right| \leq \varepsilon ,$$

but ε is arbitrarily small. Hence,

$$E(z_{n+1} \mid z_1) \longrightarrow \theta \text{ as } n \longrightarrow \infty .$$

Let us make the following notation: Let

$$(2.16.1) \qquad (1 + 4aa_i) = P_i ,$$

and let

$$(2.16.2) \qquad P_{\ell}^2 P_{\ell-1}^2 \cdots P_{\ell-t+1}^2 \left(\frac{a_{\ell-t}}{c_{\ell-t}}\right)^2 = R_{\ell,t}^2$$

for $t \geq 1$, and let

$$(2.16.3) \qquad \left(\frac{a_{\ell}}{c_{\ell}}\right)^2 = R_{\ell,0}^2 .$$

Then we may state

THEOREM 2.3.

$$\text{var}(z_{n+1} \mid z_1) = \left\{ \sum_{t=0}^{n-1} R_{n,t}^2 \right\} 2\sigma_\varepsilon^2 \quad .$$

PROOF BY MATHEMATICAL INDUCTION.

(i) Take the case $n = 1$. We see from (2.8) that $\text{var}(z_2 \mid z_1) = 2(\frac{a_1}{c_1})^2 \sigma_\varepsilon^2$. The theorem states that $\text{var}(z_2 \mid z_1)$ is $(R_{1,0}^2)2\sigma_\varepsilon^2$, which, using definition (2.16.3), is also $2(\frac{a_1}{c_1})^2 \sigma_\varepsilon^2$.

Hence, the theorem is true for $n = 1$.

(ii) Assume that the theorem is true for $n = k$, i.e.,

$$\text{var}(z_{k+1} \mid z_1) = \left\{ \sum_{t=0}^{k-1} R_{k,t}^2 \right\} 2\sigma_\varepsilon^2 \quad . \tag{2.17.1}$$

We attempt to show

$$\text{var}(z_{k+2} \mid z_1) = \left\{ \sum_{t=0}^{k} R_{k+1,t}^2 \right\} 2\sigma_\varepsilon^2 \quad . \tag{2.17.2}$$

From (2.6.1), we see that

$$\text{var}(z_{k+2} \mid z_1) = (1+4aa_{k+1})^2 \text{ var } (z_{k+1} \mid z_1) + (\frac{a_{k+1}}{c_{k+1}})^2 2\sigma_\varepsilon^2 \quad . \tag{2.18}$$

Making use of the induction assumption (2.17.1) and the notation (2.16), we obtain

$$(2.19)\quad \operatorname{var}(z_{k+2} \mid z_n) = P_{k+1}^2 \left\{ \sum_{t=0}^{k-1} R_{k,t}^2 \right\} 2\sigma_\varepsilon^2$$

$$+ \left(\frac{a_{k+1}}{c_{k+1}}\right)^2 2\sigma_\varepsilon^2$$

$$= \left\{ P_{k+1}^2 \sum_{t=0}^{k-1} R_{k,t}^2 + \left(\frac{a_{k+1}}{c_{k+1}}\right)^2 \right\} 2\sigma_\varepsilon^2$$

$$= \left\{ \sum_{t=0}^{k} R_{k+1,t}^2 \right\} 2\sigma_\varepsilon^2 \quad .$$

But this is expression (2.17.2). Hence, Theorem 2.3 is proved. Note that, as a corollary, we have obtained the recursive relation

$$(2.20)\qquad \operatorname{var}(z_{n+1} \mid z_1) = P_n^2 \left\{ \operatorname{var}(z_n \mid z_1) \right\} + \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \quad .$$

We may also calculate at this point $E(z_{n+1}-\theta)^2$. Making use of the relation

$$(2.21)\qquad E(z_{n+1}-\theta)^2 = \operatorname{var}(z_{n+1}-\theta) + \left\{E(z_{n+1}-\theta)\right\}^2$$

$$= \operatorname{var}(z_{n+1}) + \left\{E(z_{n+1}-\theta)\right\}^2 \quad ,$$

we see that

$$(2.22)\qquad E\left\{(z_{n+1}-\theta)^2 \mid z_1\right\} = \left\{ \sum_{t=0}^{n-1} R_{n,t}^2 \right\} 2\sigma_\varepsilon^2$$

$$+ (z_1-\theta)^2 \prod_{i=1}^{n} P_i^2 \quad .$$

THEOREM 2.4.

$$\left\{\operatorname{var}(z_{n+1} \mid z_1)\right\} \text{ is a null sequence in } n.$$

PROOF.

From (2.20), we see that

$$\operatorname{var}(z_{n+1} \mid z_1) = P_n^2 \operatorname{var}(z_n \mid Z_1) + \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \quad , \tag{2.23}$$

$$\operatorname{var}(z_{n+2} \mid z_1) = P_{n+1}^2 \left\{ P_n^2 \left[\operatorname{var}(z_n \mid z_1) \right] + \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \right\}$$

$$+ \left(\frac{a_{n+1}}{c_{n+1}}\right)^2 2\sigma_\varepsilon^2 \quad ,$$

and, in fact,

$$\operatorname{var}(z_{n+k} \mid z_1) = P_{n+k-1}^2 P_{n+k-2}^2 \cdots P_n^2 \operatorname{var}(z_n \mid z_1)$$

$$+ \left\{ P_{n+k-1}^2 P_{n+k-2}^2 \cdots P_{n+1}^2 \left(\frac{a_n}{c_n}\right)^2 + \cdots + P_{n+k-1}^2 \left(\frac{a_{n+k-2}}{c_{n+k-2}}\right)^2 \right.$$

$$\left. + \left(\frac{a_{n+k-1}}{c_{n+k-1}}\right)^2 \right\} 2c_\varepsilon^2 \quad .$$

Now, there exists an M such that for all $n \geq M$, $P_n^2 \leq 1$. Thus, for all $n \geq M$,

$$\operatorname{var}(z_{n+k} \mid z_1) \leq P_{n+k-1}^2 P_{n+k-2}^2 \cdots P_n^2 \operatorname{var}(z_n \mid z_1) \tag{2.24}$$

$$+\left\{\left(\frac{a_n}{c_n}\right)^2+\left(\frac{a_{n+1}}{c_{n+1}}\right)^2+\ldots+\left(\frac{a_{n+k-1}}{c_{n+k-1}}\right)^2\right\}2\sigma_\varepsilon^2 \quad .$$

Thus,

$$(2.25)\qquad \lim_{\substack{n\to\infty\\ k\to\infty\\ k-n\to\infty}} \operatorname{var}(z_{n+k}\,|\,z_1) = \lim_{\substack{n\to\infty\\ k\to\infty\\ k-n\to\infty}} P_{n+k-1}^2 P_{n+k-2}^2 \cdots P_n^2 \operatorname{var}(z_n\,|\,z_1)$$

$$+\lim_{\substack{n\to\infty\\ k\to\infty\\ k-n\to\infty}} 2\sigma_\varepsilon^2\left\{\sum_{m=n}^{n+k-1}\left(\frac{a_m}{c_m}\right)^2\right\} .$$

Consider the second term on the right-hand side. From (2.2), we see that this expression may be written as

$$(2.26)\qquad \lim_{\substack{n\to\infty\\ k\to\infty\\ k-n\to\infty}} \frac{2R^2\sigma_\varepsilon^2}{s^2}\sum_{m=n}^{n+k-1}\frac{1}{m^P} \quad ,$$

where $1 < P < 2$. Consider the sequence $\left\{\sum_{m=n}^{n+k-1}\frac{1}{m^P}\right\}$, every term of which is less than the corresponding term of $\left\{\sum_{m=n}^{\infty}\frac{1}{m^P}\right\}$.

But this latter sequence is a null sequence in n and hence, by comparison, $\left\{\sum_{m=n}^{n+k-1}\frac{1}{m^P}\right\}$ and $\left\{2\sigma_\varepsilon^2\sum_{m=n}^{n+k-1}\left(\frac{a_m}{c_m}\right)^2\right\}$ is a null sequence in n.

The first term on the right-hand side of (2.25) may be written using the notation of (2.14) as

$$(2.27) \qquad \lim_{\substack{n \to \infty \\ k \to \infty \\ k-n \to \infty}} \prod_{m=n}^{n+k-1} \left(1 - \frac{K}{m}\right)^2 \operatorname{var}\left(z_n \,\middle|\, z_1\right) \quad ,$$

where $K > 0$. It has been shown in (2.14) that, given any $\varepsilon > 0$, there exists an N such that

$$\left| \prod_{m=1}^{N} \left(1 - \frac{K}{m}\right) \right| \leq \varepsilon \quad ,$$

and, if we take ε such that $0 < \varepsilon \leq 1$,

$$(2.28) \qquad \left| \prod_{m=1}^{N} \left(1 - \frac{K}{m}\right)^2 \right| \leq \varepsilon^2 \leq \varepsilon \quad .$$

Thus, $\left\{ \prod_{m=n}^{n+k-1} \left(1 - \frac{K}{m}\right)^2 \right\}$ is a null sequence in n.

Now we shall show that for large enough n, $\left\{\operatorname{var}\left(z_n \,\middle|\, z_1\right)\right\}$ is a monotone decreasing sequence in n. Again, from (2.20),

$$\operatorname{var}\left(z_{n+1} \,\middle|\, z_1\right) = \left(1 + 4aa_n\right)^2 \operatorname{var}\left(z_n \,\middle|\, z_1\right) + \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \quad .$$

Using the notation of (2.14), this may be written as

$$(2.29) \qquad \left(1 - \frac{K}{n}\right)^2 \operatorname{var}\left(z_n \,\middle|\, z_1\right) + \left(\frac{a_n}{c_n}\right)^2 2\sigma_\varepsilon^2 \quad ,$$

Thus,

$$(2.30) \qquad \operatorname{var}\left(z_{n+1} \,\middle|\, z_1\right) = \left\{1 - \frac{2K}{n} + \frac{K^2}{n^2}\right\} \operatorname{var}\left(z_n \,\middle|\, z_1\right) + \left(\frac{R^2}{s^2 n^2}\right) 2\sigma_\varepsilon^2 \quad ,$$

where

$$1 < P < 2 \quad \text{and} \quad K > 0,$$

and

$$(2.31) \qquad \lim_{n \longrightarrow \infty} \operatorname{var}(z_{n+1} \mid z_1) = \left(1 - \frac{2K}{n}\right) \operatorname{var}(z_n \mid z_1) \quad .$$

Thus, $\operatorname{var}(z_n \mid z_1)$ is for large enough n, monotone decreasing in n.

Hence, since $\prod_{m=n}^{n+k-1} \left(1 - \frac{K}{m}\right)^2$ is a null sequence in n, so is $\prod_{m=n}^{n+k-1} \left(1 - \frac{K}{m}\right)^2 \operatorname{var}(z_n \mid z_1)$. But this means that $\operatorname{var}(z_{n+k} \mid z_1)$ may be written as the sum of two null sequences, and hence is itself a null sequence. Thus, $\operatorname{var}(z_n \mid z_1)$ is a null sequence.

COROLLARY.

$E(z_{n+1} - \theta)^2$ is a null sequence in n.

PROOF.

$$E(z_{n+1}-\theta)^2 = \operatorname{var}(z_{n+1}) + \left\{E(z_{n+1}-\theta)\right\}^2 \quad .$$

The first term on the right-hand side, we have just shown to be a null sequence; the second term on the right-hand side can be shown, with the aid of (2.28), to be a null sequence. Thus, $E(z_{n+1}-\theta)^2$ is the sum of two null sequences and hence is itself a null sequence.

We now seek $\operatorname{cov}(z_{n+1}, z_n \mid z_1)$. We shall prove Theorem 2.5.

THEOREM 2.5.

$$\operatorname{cov}(z_{n+1}, z_n \mid z_1) = P_n \operatorname{var}(z_n \mid z_1) \, .$$

PROOF.

$$(2.32) \qquad \operatorname{cov}(z_{n+1}, z_n \mid z_1) = E\left\{\left[z_{n+1} - E(z_{n+1})\right]\left[z_n - E(z_n)\right]\right\}$$

$$= E(z_{n+1}z_n \mid z_1) - E(z_{n+1} \mid z_1)E(z_n \mid z_1) \quad .$$

We shall work first with the left-hand term in the last expression. Employing (2.6.2),

$$(2.33) \quad (z_{n+1})(z_n) = z_n \left\{ z_n(1+4aa_n) - 4aa_n\theta + \frac{a_n}{c_n}(\varepsilon_{2n} - \varepsilon_{2n-1}) \right\}$$

$$= z_n^2(1 + 4aa_n) - 4aa_n\theta z_n + \frac{a_n}{c_n} z_n(\varepsilon_{2n} - \varepsilon_{2n-1}) \quad ,$$

and

$$E\left\{ (z_{n+1})(z_n) \mid z_1 \right\} = (1+4aa_n)E(z_n^2) - 4aa_n\theta\, E(z_n) \quad ,$$

but

$$E(z_n^2) = \mathrm{var}(z_n) + \left\{ E(z_n) \right\}^2 \quad .$$

Thus,

$$E\left\{ (z_{n+1})(z_n) \mid z_1 \right\} = (1+4aa_n)\left\{ \mathrm{var}(z_n \mid z_1) + \left\{ E(z_n) \right\}^2 \right\}$$

$$- 4aa_n\, \theta E(z_n)$$

$$= P_n \left\{ \left\{ \sum_{t=0}^{n-2} R_{n-1,t}^2 \right\} 2\sigma_\varepsilon^2 + \left\{ (z_1-\theta) \prod_{i=1}^{n-1} P_i \right\}^2 \right\}$$

$$-4aa_n\theta \left\{ (z_1-\theta) \prod_{i=1}^{n-1} P_i \right\} + \theta^2$$

$$= P_n \left\{ \left\{ \sum_{t=0}^{n-2} R_{n-1,t}^2 \right\} 2\sigma_\varepsilon^2 + (z_1-\theta)^2 \prod_{i=1}^{n-1} P_i^2 \right.$$

$$\left. +2\theta(z_1-\theta) \prod_{i=1}^{n-1} P_i + \theta^2 \right\}$$

$$- 4aa_n\theta \left[(z_1-\theta) \prod_{i=1}^{n-1} P_i + \theta \right].$$

The second of the expressions in (2.32) may be written as

(2.35)
$$E(z_{n+1} \mid z_1)\, E(z_n \mid z_1)$$

$$= \left\{(z_1-\theta) \prod_{i=1}^{n} P_i + \theta\right\} \left\{(z_1-\theta) \prod_{i=1}^{n-1} P_i + \theta\right\}$$

$$= (z_1-\theta)^2 \prod_{i=1}^{n-1} P_i^2 P_n + \theta(z_1-\theta) \prod_{i=1}^{n} P_i$$

$$+ \theta(z_1-\theta) \prod_{i=1}^{n-1} P_i + \theta^2 ,$$

and (2.32) becomes

(2.36)
$$\operatorname{cov}(z_{n+1}, z_n \mid z_1) = \left\{P_n \sum_{t=0}^{n-2} R_{n-1,t}^2\right\} 2\sigma_\varepsilon^2$$

$$+(z_1-\theta)^2 \prod_{i=1}^{n-1} P_i^2 P_n + (1+4aa_n)(2\theta)(z_1-\theta) \prod_{i=1}^{n-1} P_i$$

$$+ \theta^2(1+4aa_n) - 4aa_n\theta \left[(z_1-\theta) \prod_{i=1}^{n-1} P_i \right]$$

$$- 4aa_n\theta^2 - (z_1-\theta)^2 \prod_{i=1}^{n-1} P_i^2 P_n$$

$$- \theta(z_1-\theta) \prod_{i=1}^{n-1} P_i(2+4aa_n) - \theta^2$$

$$= \left\{P_n \sum_{t=0}^{n-2} R_{n-1,t}^2\right\} 2\sigma_\varepsilon^2$$

$$+ \theta(z_1-\theta) \prod_{i=1}^{n-1} P_i \left\{ 2(1+4aa_n)-4aa_n - 2 - 4aa_n \right\} .$$

The term in brackets vanishes leaving

$$\operatorname{cov}(z_{n+1}, z_n \mid z_1) = \left\{ P_n \sum_{t=0}^{n-2} R^2_{n-1,t} \right\} 2\sigma_\varepsilon^2$$

$$= P_n \operatorname{var}(z_n \mid z_1) .$$

It now becomes a simple matter to calculate the correlation between z_n and z_{n+1}. We shall make use of

$$(2.37) \quad \operatorname{cor}(z_n, z_{n+1} \mid z_1) = \frac{\operatorname{cov}(z_n, z_{n+1} \mid z_1)}{\sqrt{\operatorname{var}(z_n \mid z_1) \operatorname{var}(z_{n+1} \mid z_1)}} .$$

On substituting into (2.37) the expressions that have been obtained for variances and covariances, we obtain

$$(2.38) \quad \operatorname{cor}(z_n, z_{n+1} \mid z_1) = \frac{\left\{ P_n \sum_{t=0}^{n-2} R^2_{n-1,t} \right\}}{\sqrt{\left\{ \sum_{t=0}^{n-1} R^2_{n,t} \right\} \left\{ \sum_{t=0}^{n-2} R^2_{n-1,t} \right\}}}$$

$$= P_n \sqrt{\frac{\sum_{t=0}^{n-2} R^2_{n-1,t}}{\sum_{t=0}^{n-1} R^2_{n,t}}}$$

$$= P_n \sqrt{\frac{\operatorname{var}(z_n \mid z_1)}{\operatorname{var}(z_{n+1} \mid z_1)}} .$$

Thus,

$$(2.39) \qquad \rho^2(z_n, z_{n+1} \mid z_1) = P_n^2 \frac{\sum_{t=0}^{n-2} R_{n-1,t}^2}{\sum_{t=0}^{n-1} R_{n,t}^2} \quad ,$$

and, using the recursive relation given in (2.20), this becomes

$$(2.40) \qquad \rho^2(z_n, z_{n+1} \mid z_1) = \frac{P_n^2 \sum_{t=0}^{n-2} R_{n-1,t}^2}{P_n^2 \sum_{t=0}^{n-2} R_{n-1,t}^2 + \left(\frac{a_n}{c_n}\right)^2} \quad .$$

Thus, we may write

$$(2.41) \qquad \frac{1}{\rho^2}(z_n, z_{n+1} \mid z_1) = 1 + \Delta \quad ,$$

where Δ is given by

$$\left(\frac{a_n}{c_n}\right)^2 \Big/ P_n^2 \sum_{t=0}^{n-2} R_{n-1,t}^2 \quad .$$

Now, from (2.2),

$$\left(\frac{a_n}{c_n}\right)^2 = \left(\frac{R}{S}\right)^2 \frac{1}{n^{2(1-k)}} \quad .$$

For very large n we may regard $\left(\frac{a_n}{c_n}\right)$, $\left(\frac{a_{n-1}}{c_{n-1}}\right)$, $\left(\frac{a_{n-2}}{c_{n-2}}\right)$, ... as being of the same magnitude. Taking this and remembering the definitions of P_n^2 and $R_{n-1,t}^2$, we have

$$(2.42) \qquad \Delta \leq \frac{\left(\frac{R}{S}\right)^2 \frac{1}{n^{2(1-k)}}}{\left(1-\frac{K}{n}\right)^2 \left(\frac{R}{S}\right)^2 \frac{1}{n^{2(1-k)}} + \left(1-\frac{K}{n}\right)^4 \left(\frac{R}{S}\right)^2 \frac{1}{n^{2(1-k)}} + \cdots}$$

$$= \frac{1}{\left(1-\frac{K}{n}\right)^2 + \left(1-\frac{K}{n}\right)^4 + \left(1-\frac{K}{n}\right)^6 + \cdots} \quad .$$

Thus as $n \longrightarrow \infty$, $\Delta \longrightarrow \frac{1}{1+1+1+\ldots} = 0$. We have used the fact that $\left(1-\frac{K}{n}\right) = \left(1+\frac{4aR}{n}\right)$ approaches unity as n approaches infinity. Thus, $\rho^2(z_n, z_{n+1} \mid z_1) \longrightarrow 1$ as $n \longrightarrow \infty$. But there always exists an N such that for all $n \geq N$, P_n is positive. Furthermore, the square root in expression (2.38) is conventionally taken to be positive. Thus, we have proved

THEOREM 2.6.

$$\text{cor}\,(z_n, z_{n+1} \mid z_1) \longrightarrow +1 \text{ as } n \longrightarrow \infty \quad .$$

(2.43) Let us now consider the problem of optional stopping. We desire some procedure whereby the information obtained from the observations is utilized to terminate the sequential procedure whenever the location of the maximum has been estimated with suitable precision. We shall mention two procedures which might be considered for this position and shall elaborate upon the second.

(2.43.1) Consider the sign of $(y_{2n}-y_{2n-1})$. Record this sign for each successive pair of observations and terminate the experiment after q changes in sign where q is an integer specified in advance of the experiment.

(2.43.2) Consider a group of s successive z's where s is an integer. Let $z_m = \max(z_{n-s+2}, z_{n-s+3}, \cdots, z_{n+1})$, and let $z_\ell = \min(z_{n-s+2}, z_{n-s+3}, \cdots, z_{n+1})$. Then terminate the experiment when $|z_m - z_\ell| \leq k$, where k is pre-designated.

Let us consider the case for $s = 2$. Then we will terminate the experiment when $|z_{n+1} - z_n| \leq k$. Since z_n, and hence $(z_{n+1} - z_n)$, is normally distributed, $\text{pr}\{|z_{n+1} - z_n| \leq k\}$ can be computed from the cumulative normal distribution function and is seen to be

$$(2.44) \qquad \Phi\left(\frac{k-u}{v}\right) - \Phi\left(\frac{-k-u}{v}\right) ,$$

where $u = E(z_{n+1} - z_n \mid z_1)$ and $v = +\sqrt{v^2}$, where $v^2 = \text{var}(z_{n+1} - z_n \mid z_1)$. We now proceed to determine u and v. Using Theorem 2.1, it is seen that

$$(2.45) \qquad E(z_{n+1} - z_n \mid z_1) = E(z_{n+1} \mid z_1) - E(z_n \mid z_1)$$

$$= \left\{ (z_1-\theta) \prod_{i=1}^{n} (1+4aa_i) + \theta \right\}$$

$$-\left\{(z_1 - \theta) \prod_{i=1}^{n-1}(1+4aa_i) + \theta\right\}$$

$$= (z_1 - \theta) \prod_{i=1}^{n-1}(1+4aa_i)(1+4aa_n-1)$$

$$= (z_1 - \theta) \prod_{i=1}^{n-1} P_i(4aa_n) \quad .$$

We obtain $\mathrm{var}(z_{n+1} - z_n \mid z_1)$ from the expression

$$\mathrm{var}(z_{n+1} - z_n \mid z_1) = \mathrm{var}(z_{n+1} \mid z_1) + \mathrm{var}(z_n \mid z_1) - 2\,\mathrm{cov}(z_{n+1}, z_n \mid z_1) \tag{2.46}$$

$$= \left\{\sum_{t=0}^{n-1} R^2_{n,t} + \sum_{t=0}^{n-2} R^2_{n-1,t} - 2P_n \sum_{t=0}^{n-2} R^2_{n-1,t}\right\} 2\sigma_\varepsilon^2 \quad .$$

Using recursive relation (2.20),

$$\mathrm{var}(z_{n+1} - z_n \mid z_1) = \left[\sum_{t=0}^{n-2} R^2_{n-1,t}\right]\left\{P_n^2 - 2P_n + 1\right\} + \left(\frac{a_n}{\sigma_n}\right)^2 \Big] 2\sigma_\varepsilon^2 \tag{2.47}$$

$$= (4aa_n)^2 \mathrm{var}(z_n \mid z_1) + \left(\frac{a_n}{\sigma_n}\right)^2 2\sigma_\varepsilon^2 \quad .$$

Substituting expressions (2.45) and (2.47) into (2.44), we obtain the

probability that the experiment terminates on or before the $(n+1)$-th trial ($2n+2$ observations). This probability will be expressed in terms of the two known sequences $\{a_n\}$ and $\{c_n\}$ and the unknown parameter a. Call this probability r_{n+1}. Then the probability that the experiment terminates on the k-th trial is $(r_k - r_{k-1})$. This probability depends upon the unknown parameter a in a complex way. Thus, in a given situation, it would seem difficult to specify k in advance and attach meaningful confidence limits to the estimate of θ obtained from the process. Perhaps a preliminary experiment to obtain an estimate of a would be helpful in this context. See (2.49) below for a discussion of how an estimate of a from a preliminary experiment might be used to determine the sequences $\{a_n\}$ and $\{c_n\}$ in order that z_n converge to θ fairly rapidly.

(2.48) The proper choice of sequences $\{a_n\}$ and $\{c_n\}$ is necessary in order to insure efficient convergence of z_n to θ. We will here, as in (2.2), confine ourselves to sequences of the type,

$$\{a_n\} = \frac{R}{n} \quad , \quad \{c_n\} = \frac{S}{n^k} \quad ,$$

(2.48.1)

where $R > 0$, $S > 0$, and $0 < k < \frac{1}{2}$. Recalling (2.9),

$$E(z_{n+1} - z_n \mid z_n) = 4aa_n(z_n - \theta) \quad ,$$

(2.48.2)

we see that there are two types of behavior against which we must guard.

(2.48.3) First, if $4aa_n >> 1$, then

$E(z_{n+1} \mid z_1)$ will oscillate back and forth over θ in steps of increasing magnitude until we reach N such that $|4aa_N| \leq 2$, after which point, $E(z_n)$ will begin to converge to θ.

(2.48.4) Second, if $4aa_n << 1$, convergence to θ may be very slow indeed.

(2.48.5) Thus, we see that careful selection of the sequence $\{a_n\}$ is necessary in order that z_n converge rapidly to θ. We will now show that the selection of the sequence $\{c_n\}$ is not so critical. An inspection of the expansion of the expression given in Theorem 2.3 for $var(z_{n+1} \mid z_1)$ will reveal that the c_n terms appear only in the denominator. Thus, increasing the size of c_n can only reduce $var(z_{n+1} \mid z_1)$. Furthermore, this reduction will occur in the well-known proportional manner; if we take $\{c_n'\} = \{kc_n\}$, and leave $\{a_n\}$ fixed, then $var(z'_{n+1} \mid z'_1) = \frac{1}{k^2} var(z_n \mid z_1)$. Also note that $E(z_{n+1} - z_n \mid z_1)$ is free of c_n; hence, by changing $\{c_n\}$, we do not harm the convergence properties of the procedure. Thus, it is recommended that we take c_n to be as large as possible subject to the restriction that we do not take it so large that the procedure is yielding z_n values outside of the "range of interest" of the experiment. See [18] on this point.

(2.49) We present here a method by which the sequences $\{a_n\}$ and

$\{c_n\}$ may be chosen from a preliminary experiment.

(2.49.1) Choose 5 equi-spaced x-points over the area of interest. Let us call these x-points $P-2\Delta$, $P-\Delta$, P, $P+\Delta$, and $P+2\Delta$.

(2.49.2) Make one observation of the response at each x-point. Call these responses y_1, y_2, y_3, y_4, and y_5 where y_1 is the response at $(P-2\Delta)$, y_2 is the response at $(P-\Delta)$, etc.

Now, estimate a and θ by the method of least squares. It is seen that

$$(2.49.3) \qquad \hat{a} = \frac{2y_1-y_2-2y_3-y_4+2y_5}{14\Delta^2} ,$$

and that

$$(2.49.4) \qquad \hat{\theta} = \frac{7\Delta}{10}\left\{\frac{2y_1+y_2 \quad -y_4-2y_5}{2y_1-y_2-2y_3-y_4+2y_5}\right\} + P .$$

(2.49.5) Then choose $z_1 = \hat{\theta}$, $R = \cdot\frac{-1}{4\hat{a}}$, and $S = P$ and proceed as outlined in (2.3). We explain briefly these choices. $\hat{\theta}$ is, of course, the estimate of the location of the maximum obtained from the preliminary experiment and is the logical choice for z_1. Furthermore, if $\frac{-1}{4\hat{a}} \approx \frac{-1}{4a}$, then, from (2.9), we see that

$$(2.49.6) \qquad E(z_2-z_1 \mid z_1) = 4a\left(\frac{-1}{4\hat{a}}\right)(z_1 - \theta) \approx (\theta - z_1), \text{ i.e.,}$$

$$E(z_2) \approx \theta .$$

Perhaps, by choosing the sequence $\{a_n\}$ in this manner, some measure of protection against the behavior mentioned in (2.48.3) and (2.48.4) may be obtained. This seems an area where research through the use of the Monte Carlo method might prove very useful. Finally, we have chosen S equal to P in line with the considerations of (2.48.5).

At this point we might mention that there are two distinct ways in which the sequential procedure might be used to estimate θ. We may terminate the experiment after 2t observations have been taken and take

$$\hat{\theta} = z_{t+1} \quad , \tag{2.50}$$

or we may use all of the experimental points, (x_i, y_i), $i = 1,2,\ldots,$ 2t, or those of the experimental points that are in the vicinity of the maximum to estimate θ from a least squares regression equation of suitable degree. Note that in this case the sequential procedure serves to concentrate the experimental points in the vicinity of the maximum. How the standard errors and biases of the regression coefficients so obtained compare with those of regression coefficients obtained from a fixed sample size experiment using equally-spaced x-increments or with those obtained from an experiment employing the Hotelling procedure is a very important question which should be further pursued.

If the experimental error is large the sequential procedure may be slow to converge. A device that may be of assistance in this situation is that of replication, i. e., we can make k determinations

of y at each level of x and take

$$z_{n+1} = z_n + \frac{a_n}{c_n} (\bar{y}_{2n} - \bar{y}_{2n-1}) \quad , \tag{2.51.1}$$

where

$$\bar{y}_i = \sum_{s=1}^{k} y_{is} / k \quad , \tag{2.51.2}$$

and $i = 1,2,\ldots$.

(2.52) Summary.

I have in this chapter discussed briefly some of the operating characteristics of the Kiefer-Wolfowitz stochastic approximation procedure when the true regression is quadratic, and have attempted to indicate some of the consideration s that must be taken even in this simple situation. The treatment has been by no means rigorous or complete, and there is no justification for believing that the procedures suggested here will work at all well if the true regression is other than quadratic.

APPENDIX

The Monte Carlo method has been used to generate stochastic sequences with the IBM 650 computer for the purpose of evaluating the procedure suggested in Section (2.49) for determining the sequences $\{a_n\}$ and $\{c_n\}$ appearing in the application of the Kiefer-Wolfowitz procedure. The physical situation simulated in this study is described below.

Suppose that x and y are functionally related by means of the equation

$$y = -x^2/400 \quad ,$$

but there is an experimental error involved in measuring y so that actually

$$y_u = -x_u^2/400 + \delta_u \quad ,$$

where the δ_u are NID$(0, \sigma_\varepsilon^2)$[1]. Suppose that one observation on y is taken for each of the following x-points: $x = -200$, $x = 0$, $x = 200$, $x = 400$, and $x = 600$. (i.e., in the notation of (2.49) $\Delta = P = 200$.) Now the true maximum value for y occurs at $x = 0$, so we assume that the initial ignorance of the location of the optimum point

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1. δ_u was determined as follows. Let v_{iu} assume each of the values from 0 to 99 with probability 1/100, where i=1, 2, ..., 10 and u=1,2.... . Then $\delta_u = \frac{\sqrt{2}}{2}\left(\sum_{i=1}^{10} v_{iu} - 495\right)$. σ_ε^2 has been estimated from 125 of the δ_u generated by the machine and was found to be approximately 5400.

is such that the true optimum point is located half-way between the experimental center and the boundary of the experimental region. Now, on the basis of these five experimental points, suppose that a quadratic regression is fitted by the method of least squares so that

$$\hat{y}_u = b_0 + b_1 x_u + b_2 x_u^2 ,$$

and that the location of the absicca of the maximum ordinate is estimated from

$$z_1 = - b_1/2b_2 \quad .$$

Then set $R = \div \frac{1}{4b_2}$, $S = 200$, $k = \frac{1}{4}$, and apply the Kiefer-Wolfowitz procedure to obtain $z_2, z_3, \ldots, z_{26}$. Call this an experimental sequence. An experimental sequence then consists of 55 observations, i.e., five preliminary observations and 25 pairs of sequential observations.

The IBM 650 computer has been utilized to compound 111 such experimental sequences. Some of the results are summarized below.

Three examples of these experimental sequences are given in Table (3.1).

TABLE 3.1

EXPERIMENTAL SEQUENCES

	Example 1	Example 2	Example 3
z_1	32.3	160.8	38.9
z_2	- 3.5	-167.3	56.1
z_3	0.8	- 14.6	31.2
z_4	6.6	- 15.3	25.7
z_5	- 2.7	- 0.8	22.9
z_6	- 1.7	20.8	22.8
z_7	-14.0	26.5	35.0
z_8	-12.5	26.0	39.3
z_9	- 8.5	5.7	37.5
z_{10}	2.3	3.6	25.9
z_{11}	- 1.1	-16.0	27.8
z_{12}	- 8.8	- 8.4	28.2
z_{13}	-17.2	0.0	24.9
z_{14}	- 9.0	16.1	23.8
z_{15}	- 0.8	8.6	20.2
z_{16}	5.8	0.5	17.4
z_{17}	6.7	-8.7	19.7
z_{18}	7.7	10.0	17.7
z_{19}	8.5	4.2	17.3
z_{20}	11.5	12.4	20.6
z_{21}	10.8	8.8	22.4
z_{22}	9.7	17.2	23.6
z_{23}	13.8	14.0	20.2
z_{24}	13.9	20.9	16.4
z_{25}	9.4	9.3	15.7
z_{26}	5.4	- 1.6	15.1

Note that in Example 2, z_n converges quite rapidly to zero after over-correcting for an unusually poor first estimate, and that, in Example 3, z_n remains positive throughout the entire sequence.

The means and variances of z_n for selected n have been computed and appear in Table (3.2) below. All of the variances are based on 110 degrees of freedom.

TABLE 3.2

n	Number of Experiments	$\bar{z}_n$	$Var(z_n)$	Estimated $Var(z_n)^2$
1	5	8.64	3038	2707
2	7	9.07	2480	1937
3	9	4.45	1266	1505
5	13	2.34	853	1040
8	19	2.80	577	713
11	25	0.04	485	542
16	35	0.31	346	387
21	45	1.16	368	301
26	55	1.48	263	246

---

2. The estimated variance of z_n has been computed assuming that $var(z_n)$ decreases as the reciprocal of the number of experiments. Let $var(z_n) = V_n$ and let N_n be the total number of experiments performed following the determination of z_n. Then assume that $\frac{N_n}{5} V_n$ is an estimate of σ_1^2, where σ_1^2 is the estimated variance of z_1; and let $s_1^2 = \frac{1}{45} \Sigma N_n V_n$, where the summation is over the nine values of n appearing in Table 3.2. Then the estimated variance of z_n is obtained from $\frac{N_n}{5} s_1^2$.

Note that the means are all positive. This may perhaps be attributed to the fact that the mean for z_1 was rather large (but not significantly different from zero at the .05 level) and that the other means are correlated with the first. Of special interest is the behavior of $var(z_n)$ for increasing n. It appears that over the range of values of n appearing in the study that $var(z_n)$ decreases roughly as the reciprocal of the number of experiments. Following this assumption, a least squares curve has been fitted to the data of Table 3.2. The predicted values for $var(z_n)$ are shown in the last column of that table, and are seen to agree well with the experimentally obtained variances.

There remain several points of interest that could be investigated with the aid of the Monte Carlo method. A few of these are indicated below.

(i) The influence of k on $var(z_n)$ could be studied.

(ii) Various stopping rules could be evaluated.

(iii) The influence of the choice of the initial region might be investigated.

(iv) The operating characteristics of the estimation procedure in the case where the true regression is not quadratic might be studied.

(v) Various modifications of the estimation procedure could be investigated. For example, we might take three observations at each stage of the sequential procedure, say, z_n-c_n, z_n, and z_n+c_n, and let z_{n+1} be the estimate of the location

of the maximum found by fitting a quadratic regression to these three points.

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