OPTIMUM-SEEKING DESIGNS FOR SIMULATION EXPERIMENTS WITH MODELS OF AGRICULTURAL SYSTEMS

by

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Research Report No. 87

December 1978

THE AGRICULTURAL ECONOMICS RESEARCH UNIT

Lincoln College, Canterbury, N.Z.

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PREFACE

Over the last decade there has been a remarkable increase in the use of systems modelling for research in farm management. This has been accompanied by substantial progress in the development of model building techniques for farming systems. Progress has been less rapid, however, in the development of procedures for testing the validity of bioeconomic models and for using them to explore the response of systems to factors under the control of management. This publication is concerned with the latter problem area. Various procedures for designing simulation experiments to determine optimal factor levels are discussed and compared.

Dr Harrison, lecturer in economics in the Department of External Studies, University of Queensland, has prepared this Report during a sabbatical period in the Department of Farm Management & Rural Valuation at Lincoln College.

The material presented is based on a series of lectures given by Dr Harrison to graduate students as part of a course in agricultural systems. Subsequent to offering these lectures a package of computer programs for optimization purposes was developed. These programs are in the form of FORTRAN subroutines which have been designed for ease of coupling to agricultural systems models. Listings of the programs and output for test functions are provided as appendices.

J. B. Dent
Director

ACKNOWLEDGEMENTS

The author expresses gratitude to

Michael Alemson, Malcolm Blackie, Barry Dent,

Gary Fick, Roger Gale, and John Longworth for

comments on earlier drafts of this Report.

CHAPTER 1

INTRODUCTION

There has been a rapid expansion in the application of the systems approach to farm management research problems in the last 15 years. Consequently there has been an increasing awareness of the need for efficient procedures for implementing systems models so that information about the real farming systems they represent can be derived. Progress has also been made in the development of experimental design procedures for identifying levels of variables which optimize the performance of systems. These design procedures, which are based on mathematical methods of numerical optimization, have not been widely exploited by agricultural systems researchers. Rather the tendency has been to conduct simulation experiments with traditional designs such as factorials and response surface designs. This report explains various optimum-seeking design procedures for simulation experiments with agricultural systems models. The practical aspects of implementing these procedures are also discussed.

The current chapter begins with a brief overview of systems research philosophy and methodology. The experimentation stage of the systems approach is then examined in some detail and differences between simulation experiments and the more traditional experiments conducted on real agricultural systems are discussed. Finally, a perspective for viewing farm-management oriented simulation is provided.

Chapter 2 reviews traditional designs for agricultural experiments with particular emphasis on factorials and central composite designs. Chapter 3 outlines methods of optimization with respect to a single controllable factor while Chapter 4 introduces "hill-climbing" or multivariate search with reference to the

method of steepest ascent. More efficient design procedures including the simplex method, alternating variable search, conjugate directions and random-search-with-learning are explained in Chapter 5. Chapter 6 examines related issues such as dealing with uncertainty in stochastic models and handling resource constraints. In addition, the application of search procedures to parameter estimation during the construction of the model is outlined. Suggestions are made concerning the choice of experimental design for particular modelling situations.

The general layout of five computer subroutines for optimum-seeking experimental designs which have been developed at Lincoln College is explained in Appendix I, and the subroutines themselves are provided as FORTRAN listings in Appendices II through to VI.

1.1 The Systems Approach

The term 'system' is used here in the context presented by Shannon: 'a group of objects united by some form of interaction or independence to perform a specified function' [Shannon, 1975:15]. In essence the 'systems approach' involves construction of a model of the particular objects of interest and their interrelationships, and manipulation of this model to gain a knowledge of how the real system would behave under a range of operating conditions and environments. Extensive development of techniques for the investigation of organized systems (henceforth referred to as systems research techniques) has taken place in engineering, aeronautics, meteorology, management science, agriculture, ecology and other disciplines. Within agriculture, many farm economists, agronomists, agrostologists, animal nutritionists and entomologists have come to embrace this approach. Agricultural systems which have been modelled include entire regions, industries, farms, pastures and crop enterprises, groups of animals and

individual animals, soil water profiles over time, plant-disease systems and many others. The form of model most frequently employed is an abstract representation of the behaviour of the system over time, expressed in symbolic language and programmed to a computer. The rationale for building such models is that the extent of manipulation which can be carried out on the system itself (real system) is severely limited. If experiments are conducted with a computer model there is the possibility of saving both cost and time; the real system (if it exists) is not altered or harmed by the experiments; and, of course, experiments can be performed on models of systems which are not yet in existence.

Most systems of interest are so complex that it is impossible to understand them completely. The model, therefore, does not contain every detail of the system it is designed to mimic, but only those of importance to the particular application for which it is to be used.

Any application of systems research proceeds through a number of more or less clearly defined stages. Various classifications of these research steps have been advanced; the following list is an adaption of that by Anderson [1974], and is explained more fully therein:

1. Formulation of the problem;
2. Analysis of the system;
3. Synthesis of the model;
4. Programming the model to a computer;
5. Testing the model;
6. Implementation of the model; and
7. Interpretation of the results and reporting to the relevant authority.

These steps are performed in the sequence in which they are listed, although there may be some cycling between them.

For instance, validation tests (step 5) may reveal a need for refinement to model structure (step 3) which would be followed by further testing (step 5).

There has been a tendency in agricultural systems studies for most of the researcher's time to be devoted to model construction (steps 2 to 4), with inadequate attention being given to testing (step 5) and experimentation with the model (step 6). This imbalance of research effort has been attributed to the exhaustive demands of constructing models and getting them to operate on the computer [Wright, 1971]. Increasing attention is now being paid to validation tests.[1] On the other hand, although highly efficient designs have recently become available for simulation experiments, their rate of adoption by agricultural systems researchers has been slow.

1.2 The Experimentation Phase

As already indicated, construction and validation of a model is only a part of the systems research effort. Once a satisfactory model is available the researcher can set about to answer some of the questions originally posed. Careful planning prior to the execution of these experiments is essential if the potential usefulness of the model is to be fully realised.

Before examining the special features of computer simulation experiments it is necessary to consider briefly agricultural experimentation in general. Regardless of whether an experiment is carried out in the field, glasshouse, laboratory or on a computer model, there will be certain variables which we wish to adjust, or set at a number of levels, and these are known as experimental factors. The factors may be qualitative, such as

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[1] For example, see Hermann [1967], Mihram [1972] and Harrison and Fick [1978].

crop variety, strain of animal, spray versus no-spray decisions. They may be quantitative and measurable in whole units only (e.g. number of cultivations throughout the crop growing season) or they may be quantitative and adjustable on a continuous scale (e.g. fertilizer application rates, animal feeding levels). Often we wish to vary more than one factor at a time, and a single combination of levels of all factors is known as a treatment. For example, nitrogen and phosphorus application rates of 30 and 10 kg per ha respectively would constitute a treatment, 30 and 20 kg would be another, 40 and 30 kg yet another. An experiment consists of the evaluation of two or more treatments in terms of some measure of response. For example, the response variable in a crop fertilizer trial is usually crop yield, expressed on a per hectare basis.

In a field experiment such as a fertilizer trial a small plot of land is allocated to each treatment. Plots for the various treatments may be laid out in a completely randomized fashion or perhaps randomized within blocks or groupings of treatments. An attempt is made when carrying out the experiment to control as fully as possible those factors which are not being purposefully adjusted. Thus soil type, slope, seed quality etc. are made as uniform as possible, pest and disease incidence is strictly limited, each plot is given the same number of cultivations, and so on. But even under the best of management the response from a given treatment will depend not only on the levels of the experimental factors but also on other factors beyond the control of the experimenter. In other words, if the same treatment is applied to two or more plots then different responses will be obtained from each. For this reason it is usual to include a number of repetitions or replicates of each treatment, and to average the response over these replicates when determining the effects of the factors.

The choice of experimental design, and subsequent analysis of the response observations, will depend on the purpose for carrying

out the experiment. Generally, agricultural experiments fall into two broad classes: (a) "where next" or "yes/no" experiments, and (b) "how much" experiments [Dillon, 1966:64]. Those in the former group are designed to explore certain points on the response pattern or surface; the latter seek to determine the combination of factor levels which is consistent with optimal response (e.g. maximal yield or most profitable yield). On the above basis, Hunter and Naylor [1970] distinguish between exploratory and optimization experiments. This report is concerned primarily with the latter class.

A wide variety of experimental designs are used for agricultural experiments, including complete and incomplete factorials, response surface designs, incomplete block designs, lattice and latin squares and many others. These designs are explained in a number of standard reference works.[2]

Field experiments normally take considerable time to carry out, even though the treatments are managed and evaluated simultaneously (i.e., each plot is planted on or about the same day, cultural operations are carried out at the same times, and the plots are harvested together). Time and resource limitations usually restrict the experimenter to examine responses with respect to at most two or three factors, particularly with experiments involving crops, pastures or large animals.

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[2] See, for example, Cochran and Cox [1957], Dillon [1977], Heady and Dillon [1961], Johnson and Leone [1964], Mendenhall [1968], Myers [1971] and Snedecor and Cochran [1967].

Since the experiment is carried out at a given location, in a given season, the results are only strictly applicable to that particular environment, and great caution must be exercised in drawing implications for other sites and seasons. Of course, the experiment may be repeated in space or time, but only at a substantial increase in research costs. These problems associated with field experiments also apply to glasshouse and laboratory experiments, though perhaps to a lesser extent in that the cost of materials and time span may not be as great.

1.3 Computer Simulation Experiments

Following this brief review of agricultural experimentation in general, we may now examine more closely experiments carried out with a computer model rather than with the real system. These are referred to as simulation (or simular) experiments. Since this is indeed a form of experimentation, the vast literature on design layouts is entirely relevant, and in fact traditional designs such as factorials are normally employed. However, those fail to take advantage of the special features of simulation experiments with regard to the determination of optimal factor levels; these special features are:

(i) substantially lower cost per treatment;
(ii) compression of time; and
(iii) control over experimental variability.

Typically, the lion's share of the cost in a systems study is incurred in developing and perhaps testing the model. The cost of evaluating each treatment is usually small hence experiments with numbers of treatments running into the hundreds, become possible.

Since the digital computer is a sequential processor, treatments must be evaluated sequentially rather than simultaneously as in the case of experiments on a real system. This presents no serious problems because simulation of performance under each

treatment takes so little time. In fact, sequential experimentation has a major advantage in that it allows the experimenter to know the outcome under each treatment before deciding on the factor levels of the next treatment and to take advantage of information generated early in the experiment to guide its later stages. Wasted treatments are therefore eliminated and the investigation is concentrated on promising regions of the experimental factors or controllable variables. The result is that designs can be employed which will locate optimal factor combinations with a fraction of the number of treatments that would be needed in real experiments to determine optima with the same degree of precision.

Agricultural systems typically operate in a highly uncertain environment. Climatic and biological uncertainty are incorporated in systems models by generating random values of weather variables and by including random components in relationships describing plant and animal performance. As well, uncertainty in the economic environment can be built into the model by way of random price and cost variables. In multi-period (as distinct from static) models, sequences of these stochastic variables are generated for each encounter with the model, i.e., for each replicate of each treatment. Control over experimental variability lies in the method by which computer routines for generating these environmental variables or sequences of variables are initialized or <u>seeded</u>. In particular, use of identical seeds for corresponding replicates under alternative treatments leads to reproduction of identical sequences of values of the uncertain variables. This procedure eliminates response differences between treatments due to the replicate effect, and hence allows differences between treatments to be detected with a smaller sample size (fewer environmental sequences or replicates).

The combined effect of the above features - ability to include more treatments, more effective use of treatments, and minimal replication even when many uncertain environmental variables are included - is to allow larger experiments to be carried

out taking account of temporal and spatial factors. The advantage is most marked when the objective is to determine levels of several factors (say four or more) which are simultaneously optimal. However, this advantage can only be realized fully if one of a group of design procedures known as 'optimum-seeking' or 'hill-climbing' designs is used. Development of optimum-seeking experimental designs has taken place in disciplines such as mathematics and engineering. Agricultural scientists and systems researchers are not generally familiar with these designs and as yet relatively few applications have been made in bioeconomic systems research. A number of such designs are presented in Chapters 3 to 5.

1.4 Terminology of Systems Research

At this stage it is necessary to introduce a symbolic framework for viewing the experimental design problem. Just as the systems model is made up of a number of algebraic expressions, so is it useful to represent the response/factor relationship in symbolic form:

$$Z = f(X, Y)$$

where Z is the response variable;

X is a vector of factors the levels of which are adjusted during the experiment; and

Y is a vector of non-controllable or environmental factors.

For example, in a fertilizer trial Z would represent yield, X could contain elements x_1 (amount of nitrogen) and x_2 (amount of phosphorus) while Y would include factors such as rainfall, temperature, initial soil fertility, insect damage and so on.

The letter 'f' represents the relationship between response and the causal factors, i.e., it represents the systems model. From the point of view of experimentation the model is simply a procedure for predicting or estimating the response of the real system to any combination of factor levels under any environment. If the model is

deterministic then only one performance prediction is needed for each treatment. On the other hand, a number of replicates will be needed in the case of a stochastic model. The sequential nature of a simulation experiment is illustrated by Figure 1.1. In this diagram a performance prediction (or encounter with the model) takes place for each replicate of each treatment.

The placement of each successive treatment in an optimum-seeking design is controlled by a set of rules which operates on the responses from previous treatments. These rules are normally written into a subroutine which is called upon after each treatment has been evaluated. In contrast, if a traditional experimental design is used for an experiment with a simulation model on a computer then this design can be fully specified in advance. It can be incorporated as either input data or written into the main program of the systems model.

1.5 Management Oriented Simulation

So far the discussion on simulation experiments has been intentionally general. In this section attention will be focused on a major application of optimum-seeking experiments, viz. management-oriented research aimed at improving the efficiency of resource allocation on individual farms. Farm management research is often described as conditional normative in outlook, meaning that prescriptions are sought as to what the farmer ought to do, conditional upon him holding certain assumed goals. It is appropriate, therefore, to review briefly the nature of management decisions and the goals of farm operators which the decisions seek to achieve. The relevant goals or objectives will depend on the level of aggregation of the system being modelled. Suppose initially that this is a whole farm business. Management policies of the farm-firm may be classed as structural, strategic or tactical depending on the circumstances under which decisions are made and on the frequency of the decisions [Chudleigh, 1971]. Structural

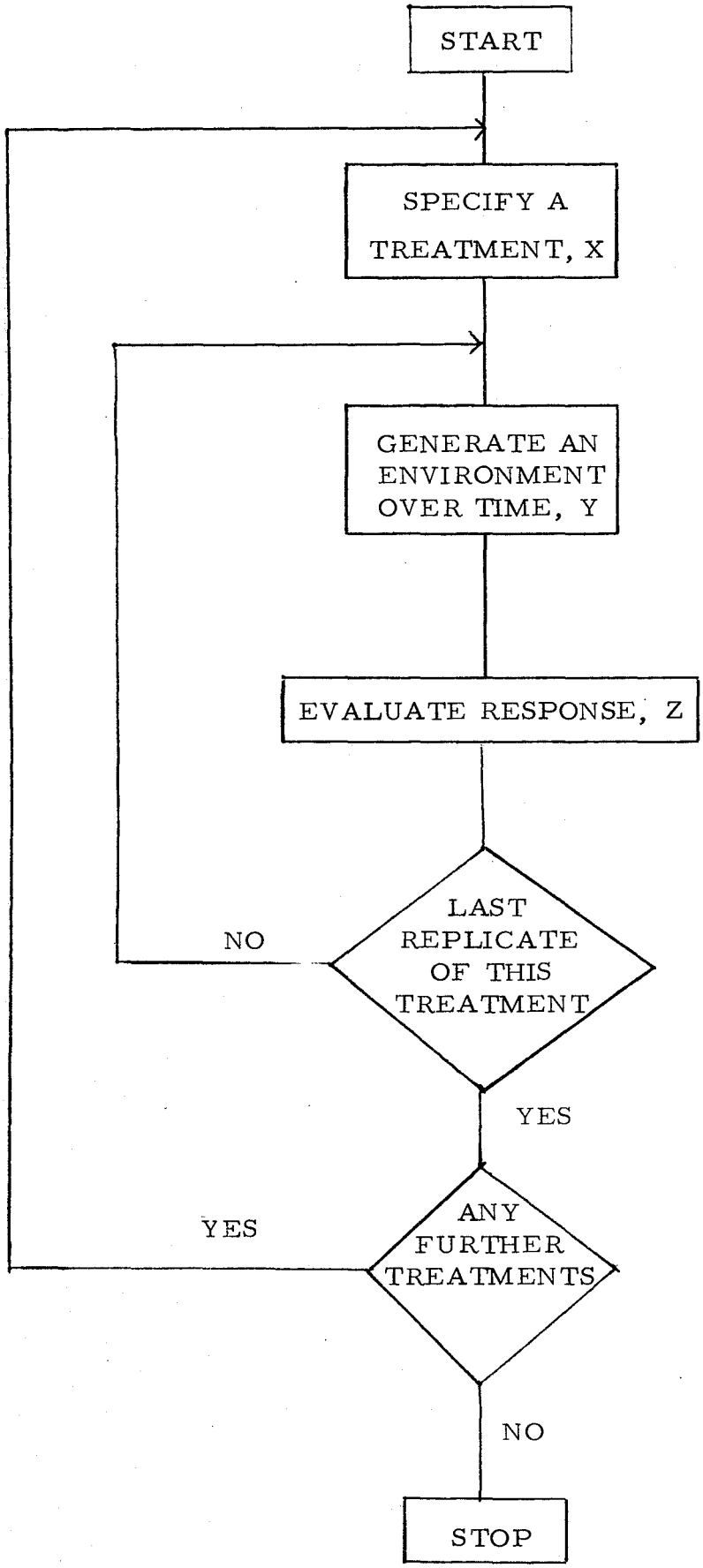

FIGURE 1.1

Flowchart of Sequential Experimentation with a Computer Model

policies concern the long-run organization of the farm business (e.g., whether to raise sheep or cattle, to grow generalist or specialist crops, or to border dyke or spray irrigate). Strategic policies are also long-term but are subject to annual revision (e.g., crop rotations, land development and machinery replacement strategies). Tactical policies are short-term and concern the response to a particular environmental situation (e.g., whether to purchase feed or sell stock during drought, when to use chemicals on insect pests). Systems models may be used to generate information which assists decision making at each of these three levels.

The decisions made by a farmer at each of the above policy levels will depend on his short-run and long-run goals. In the short term (typically represented by annual models) the literature suggests a dominant goal of profit maximization or maximization of utility as a function of income level and income variance. In the long term it is appropriate to replace the flow concept of annual income with a stock concept of wealth. Here the literature frequently suggests the objective of maximization of future net worth (or its present equivalent) subject to 'constraint goals' such as avoidance of financial collapse and adequate annual consumption expenditure.

If the system under study is only a part of the farm business then a different type of objective may be more suitable. For example, when modelling machinery renewal or pest control it may be reasonable to assume constant income and to seek management policies which minimize cost levels.

In studying an agricultural system the researcher should decide whether or not he is interested in identifying optimal management policies. Many systems research studies are positive in orientation. That is, they are exploratory in nature and designed to increase understanding of the operation of the system rather than to produce prescriptions or recommendations for management. In other cases the number of controllable or management variables is

so great that optimization may not be possible anyway, or may be unacceptably expensive in terms of computing time.

A fundamental question is whether farmers are optimizers or whether merely 'satisficers' aiming for satisfactory levels of profits provided other objectives are achieved [Simon, 1957]. And even if the farmer is a profit maximizer, it may be sufficient for the adviser to demonstrate how he can improve (rather than optimize) performance, and relatively simple experimental designs will be adequate for this purpose. Further, the farmer may already have management changes in mind and the adviser by demonstrating that these particular changes will be profitable, provides useful decision support to the farmer.

The decision to seek or not to seek optimal management policies, therefore, is not automatic, and must be considered in relation to the particular problem under study. In the past the absence of attempts to identify optimal management policies in systems studies has probably stemmed more from the lack of knowledge about suitable experimental designs rather than from a definite decision not to seek optimal policies. Certainly, the mathematics behind some of the optimum-seeking design procedures is not simple and many of the books on numerical search techniques make extensive use of matrix algebra and symbolic notation. This Report attempts to overcome the above problems by presenting the essential features of optimization procedures in simple language with a minimum of mathematics and using extensive examples and diagrams.

While the terminology introduced earlier is again applicable to management-oriented simulation, it is more convenient to introduce some new terminology. In particular, the experimental factors are now called decision or policy variables, and the factors beyond the control of the experimenter are called non-controllable exogenous variables or 'states of nature'. Each treatment is a management policy or strategy. The concept of a response is replaced by a

criterion of business performance or manager's utility. The aim of a simulation experiment is to determine the management policy which will optimize the performance criterion. Symbolic representation of the farm management problem to be solved by simular experimentation may be expanded to:

$$\text{optimize } Z = g(P)$$

where $P = f(X, Y, S, A)$

Z is the multidimensional objective or utility function of management;

X is a vector of policy variables ($X \geqslant 0$);

Y is a vector of non-controllable or environmental variables;

S is a vector of initial resource supplies constraining resource use; and

A is a vector of the system's parameters.[3]

The above discussion may be illustrated with reference to a farm enterprise planning example. Suppose an irrigation farmer with limited water supplies wishes to determine the most suitable combination of areas of irrigated wheat and lucerne to grow.[4] (The balance of his land may be sown to dryland pasture.) The relation to be investigated may be summarized as:

$$\text{Profit} = f(\text{area of wheat, area of lucerne, rainfall, prices})$$

The model represented by f may be simply a small number of accounting identities for determining the financial effects of varying

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[3] For further details of this kind of formulation see Anderson [1974], Emshoff and Sisson [1970] and Harrison and Longworth [1977].

[4] Of course, modelling and simulation is only one of a number of management research techniques which could be addressed to this problem. In fact, there is available a continuum of approaches varying from quick low-cost expedients (budgeting) through mathematical and dynamic programming to the relatively slow and expensive systems approach. These alternative methodologies are reviewed and compared by Harrison [1976, Ch. 3].

the areas of the two crops under irrigation. Alternatively, it may be a highly complex systems model which takes account of available soil moisture, light interception of plants, photosynthetic activity, starch accumulation, dry matter production, labour demands, cash flows and so on. In any case, from the farm planning point of view the model is simply a procedure for predicting the level of profit for any given management policy or crop area combination under any given bioeconomic environment. This procedure is repeated for each treatment during the simulation experiment. For example, irrigating 40 ha of wheat and 10 ha of lucerne would be one treatment; irrigating 20 ha of each would be another. If the model is deterministic then each treatment is evaluated once only but in the case of a stochastic model it is necessary to replicate each treatment a number of times.

Procedures for determining the sequence of management policies or treatments which must be evaluated in the simulation experiment so as to locate the most profitable levels of policy or decision variables at a reasonable computing cost are expounded in subsequent chapters. Initially, management problems will be considered in which there is only one policy variable (univariate optimization) then this will be extended to the case of two variables (as above) and finally to the general or n-variable case. Traditional or simultaneous designs will be discussed first, then the more efficient but more complex sequential designs.

While the above farm planning problem will be used to illustrate the design procedures, the methods are quite general and could equally well be applied to other biological or bioeconomic systems.

1.6 Summary

This chapter has viewed the systems approach to agricultural research in terms of a number of more or less clearly defined stages. It was shown that important among these is experimentation with the model to derive information about the real system it represents. Any experiment, real or simular, involves evaluation of response from two or more treatments in which experimental factors are set at different combinations of levels. As indicated, variability in response due to factors outside the control of the experimenter usually leads to replication of treatments. The special nature of simulation experiments with regard to cost, time and control over variability allows use of hill-climbing designs to locate optimal levels of a relatively large number of experimental factors. These designs are particularly useful in farm management research where the aim is to determine management policies which will best achieve the objectives of the farmer.

CHAPTER 2

TRADITIONAL EXPERIMENTAL DESIGNS

Traditional experimental designs, sometimes referred to as tabulation methods, require that all treatments be specified or listed prior to the commencement of the experiment. The treatments are chosen simultaneously, even though they may be evaluated one at a time (as in computer simulation experiments). While these designs fail to take advantage of the special features of experiments with computer models as outlined in Chapter 1, they are simpler to use than optimum-seeking sequential designs and are adequate for optimization purposes when the number of factors is not large. Also, they are sometimes used in conjunction with 'hill-climbing' designs, both for exploratory experimentation and for the closing stages of the search.

In this chapter the design and analysis of simulation experiments using traditional or tabulation methods will be reviewed for the single variable, bivariate and multivariate cases in turn. The discussion will be limited to three of the most widely used designs, viz. the full factorial, fractional factorial and central composite design.

To make the discussion more meaningful it will be assumed that a systems model of a Canterbury (N. Z.) irrigation farm has been developed and has satisfied tests of validity. This model is to be used to determine areas of the various crops and pastures which the farmer should grow if his objective is to maximize net income. The following discussion will consider the alternative situations in which the model is deterministic and in which it is stochastic. (In the latter case amount of rainfall each week, crop yields and product prices are allowed to vary randomly between years.)

2.1 Single Factor Experiments

The simplest case of an optimization experiment is to evaluate performance under just two alternative treatments or policies. The one with the highest net income would be chosen as optimal. Thus if irrigated wheat areas of 40 and 60 ha result in incomes of $22,000 and $25,000 (with areas of all other crops and pastures held fixed), then the latter level is to be recommended. If the model is stochastic then each treatment could be replicated say 10 times and mean net income compared using the student t test. We may then choose the policy with the greatest mean income or, alternatively, apply the more stringent criterion that mean income must differ significantly by at least some minimum amount of economic substance (say $1,000) before a choice is made. If identical starting numbers or seeds are used in the generation of environmental sequences for corresponding replicates of the two treatments then a test on differences in incomes between paired replicates is appropriate.[5] This blocking procedure for comparing treatments under the same environmental conditions allows significant response differences to be detected with fewer replicates than that required under independent seeding.

Often it is desirable to include several levels of the experimental factor, e.g. wheat areas of zero, 50, 100 and 150 ha. If the model is deterministic only one replicate of each of these treatments is evaluated and the level resulting in greatest income is chosen as optimal. For a stochastic model the t test is replaced by one way analysis of variance (ANOVA) and mean incomes for each treatment compared on the basis of least significant difference. One or more treatments may then be found superior to others. It should be noted, however, that the ANOVA technique assumes independence of replicates

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[5] These t tests are described in most introductory statistics tests, e.g. Mendenhall and Reinmuth [1978: 288, 296].

between treatments and is not valid when the random number generators are identically seeded. In fact, there is then no unexplained variation to be partitioned, any observed differences between mean incomes being due solely to treatments [Chudleigh, 1971: 239].

An alternative form of analysis is regression or curve fitting. This may be used regardless of whether the model is deterministic or stochastic (either independently or identically seeded) and provides more information than ANOVA by interpolation between factor levels. As a result, the wheat area corresponding to maximum income can be located with greater precision. Under this approach, an equation describing the response relationship is obtained by regressing predicted incomes (individual values or treatment means) on wheat area using an ordinary least squares regression package. The form of function most often adopted is the second-order polynomial

$$Z = m_0 + m_1 x + m_2 x^2$$

where Z is income, x is wheat area and the coefficients m_1 and m_2 define the position and shape of the curve. A stationary point on this curve occurs where the derivative $\frac{dZ}{dx}$ is zero (i.e. where $x = \frac{-m_1}{2m_2}$ and this is the income maximizing level provided the second derivative ($2m_2$) is negative. The above are known as the necessary and sufficient conditions for a maximum and will be extended later to multivariate cases.

2.2 The Factorial Design in Two Variables

Where there are two experimental factors or policy variables of interest, appropriate levels of each may be combined in a complete grid or full factorial design. The crosses in Table 2.1 represent the 16 factor combinations or treatments arising when areas of wheat and lucerne under irrigation can each take four levels. (The balance of the land may be sown to pastures.) Analysis options include two-way analysis of variance and least squares regression. A stochastic model

and independent seeding are again necessary for ANOVA to be applicable. A second-order polynomial function derived by regression analysis would include curvature terms for both factors plus a measure of interaction between them (an $x_1 x_2$ term) as follows:

$$Z = m_0 + m_1 x_1 + m_2 x_2 + m_3 x_1^2 + m_4 x_2^2 + m_5 x_1 x_2$$

TABLE 2.1

Full Factorial Design with Two Policy Variables Each at Four Levels

Area of lucerne (ha)	Area of wheat (ha) 0	50	100	150
0	x	x	x	x
20	x	x	x	x
40	x	x	x	x
60	x	x	x	x

A stationary point on this response surface is found by solving the simultaneous equations which result when the partial derivatives of Z with respect to x_1 and x_2 are set to zero, i.e.

$$\frac{\partial Z}{\partial x_1} = m_1 + 2m_3 x_1 + m_5 x_2 \quad \text{and}$$

$$\frac{\partial Z}{\partial x_2} = m_2 + 2m_4 x_2 + m_5 x_1$$

so $2m_3 x_1 + m_5 x_2 = -m_1$ and

$$m_5 x_1 + 2m_4 x_2 = -m_2$$

whence $$x_1 = \frac{2m_1 m_4 - m_2 m_5}{m_5^2 - 4m_3 m_4}$$

$$x_2 = \frac{2m_2 m_3 - m_1 m_5}{m_5^2 - 4m_3 m_4}$$

The sufficient condition for a maximum is defined in terms of the first and second partial derivatives, i.e.

$$\frac{\partial Z}{\partial x_1} < 0, \quad \frac{\partial Z}{\partial x_2} < 0 \quad \text{and}$$

$$\frac{\partial^2 Z}{\partial x_1^2} \frac{\partial^2 Z}{\partial x^2} > \left(\frac{\partial^2 Z}{\partial x_1 \partial x_2}\right)^2$$

which simplifies to $m_3 < 0$, $m_4 < 0$ and $m_3 m_4 > m_5^2$. If these conditions are not met then a minimum or saddle point has been located, indicating that income is highest at some other treatment, perhaps one on the boundary of the experimental region.

The fitting of response surfaces and location of stationary points has an important role in finishing off optimization experiments and will be reconsidered later in that context.

2.3 Designs for Three or More Factors

The full factorial design may be extended readily to cases of three or more experimental factors, but at the expense of rapidly increasing the size of the experiment. When there are k factors at n levels with each treatment replicated m times a total of mn^k encounters with the model is needed. Thus if there are seven controllable factors (a relatively small number for models of many bioeconomic systems) and each is assigned four levels then it is necessary to evaluate 4^7 or 16,384 treatments, each of which may be replicated say 10 times. While the cost of this experiment would vary with the size and complexity of the systems model and cost of computer time, let us make some reasonable assumptions in order to arrive at a cost estimate. Supposing each response evaluation requires one second of processor time, at a cost of $100 per hour, the cost of the whole experiment will be approximately $4,500 (without allowing for printing and paper charges, etc.). The full factorial design may, therefore, be unmanageably large and unacceptably expensive. This example

illustrates that simulation experiments implemented on a computer - like real experiments with plants, animals or other physical media - are not costless, and that their designs are constrained by the research budget.

One means of reducing cost is to use a fractional (incomplete, partial) factorial in which some combinations of factor levels are omitted. This enables us to fit a second-order polynomial function to the simulation output from evaluation of far fewer treatments than needed in the full factorial. The analysis of response is less complete than that possible with a full factorial design since interaction effects of higher than second order are confounded with main factor effects. A fractional factorial requiring only one sixteenth of the number of treatments of the full factorial where seven factors are to be investigated is presented by Hunter and Naylor [1969: 46]. The main use of fractional factorials (of which the Latin square is a special case) is for screening of factors or identification of those variables having greatest effect on response.

A further improvement over the fractional factorial, especially when there are three or more experimental factors of interest, is to be achieved through use of response surface methodology (RSM). In essence, RSM consists of a group of designs developed specifically for generating data with which to estimate an equation to the response surface [Box, 1954; Burdick and Naylor, 1968; Dillon, 1977]. The usual form of equation is again the second-order polynomial, including linear (x_i), quadratic (x_i^2) and interaction ($x_i x_j$) terms. Particularly efficient among the response surface designs is the central composite design which, because of its extensive use in bioeconomic simulation studies, will now be discussed in some detail.

2.4 Central Composite Designs

A typical central composite design for k experimental factors consists of the full factorial design with only two levels of each factor (2^k design points) augmented by 2k outside or 'star' points or treatments plus a treatment at the centre of the design. Returning to our farm planning example, suppose areas of irrigated wheat and lucerne are set at 40 and 60 ha, and 20 and 30 ha, respectively. For convenience we may code these factor levels using the transformations

$$x_1 = \frac{\text{area of wheat} - 50}{10} \quad \text{and}$$

$$x_2 = \frac{\text{area of lucerne} - 25}{5}$$

The levels of the two variables now take values of +1 and -1 on the new coded scale and the 2^2 full factorial design would consist of the first four treatments in Table 2.2. A central composite design is formed by adding treatments 5 to 8 outside each face of the 'square' inscribed by treatments 1 to 4, plus treatment 9 at the centre point. The complete design is illustrated in Figure 2.1.

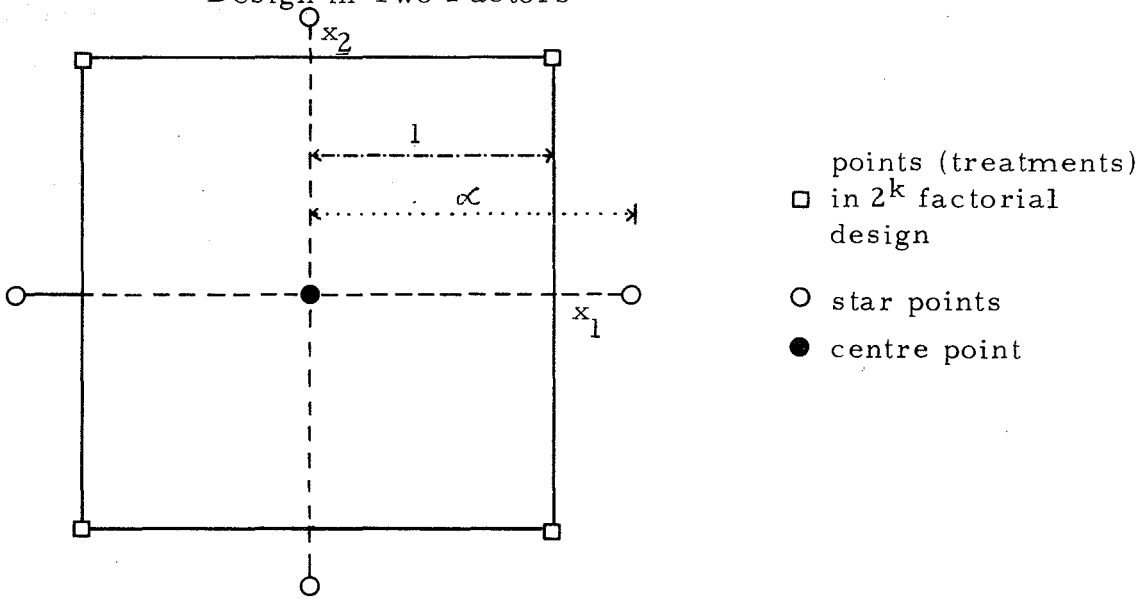
TABLE 2.2

Central Composite Design in Two Factors

Treatment No.	x_1	x_2	
1	1	1)	
2	1	-1)	2^2 factorial
3	-1	1)	
4	-1	-1)	
5	α	0)	
6	$-\alpha$	0)	star
7	0	α)	points
8	0	$-\alpha$)	
9	0	0	centre point

FIGURE 2.1

Illustration of Central Composite Design in Two Factors



Although there are only nine treatments in this design (as against 16 in the 4^2 factorial presented earlier), each of the factors is set at five different levels, viz. $-\alpha$, -1, 0, 1 and α. A typical central composite design in three factors would consist of the 15 treatments as in Table 2.3, and Figure 2.2.

TABLE 2.3

Central Composite Design in Three Factors

Treatment No.	x_1	x_2	x_3
1	1	1	1
2	1	1	-1
3	1	-1	1
4	1	-1	-1
5	-1	1	1
6	-1	1	-1
7	-1	-1	1
8	-1	-1	-1
9	α	0	0
10	$-\alpha$	0	0
11	0	α	0
12	0	$-\alpha$	0
13	0	0	α
14	0	0	$-\alpha$
15	0	0	0

The value of α or the distance of the star points from the design centre is chosen to give a compromise between precision and bias, both of which increase as α is increased. Usually a value is adopted which will make the design either orthogonal or rotatable. The orthogonal design has been found useful for fitting a performance function to simulation output which enables response to be predicted for different budgetary assumptions (factor levels) without having to rerun the model [McLintock, 1972] . Each parameter in the equation of the response surface is estimated independently of all other parameters, facilitating the fitting of the equation and subsequent partitioning of variance according to its possible causes. The total numbers of treatments and appropriate α values for the orthogonal designs with 2 to 8 factors are listed in Table 2.4 (from McLintock, p. 81).

Rotatable designs have been developed specifically for fitting second and higher order polynomials to response data [Hunter and Naylor, 1969: 48] and the rotatable central composite is perhaps the most useful of all simultaneous designs for agricultural simulation work. When fitting a response surface the precision is greatest (i.e. standard error of estimate smallest) at the centre of the design.

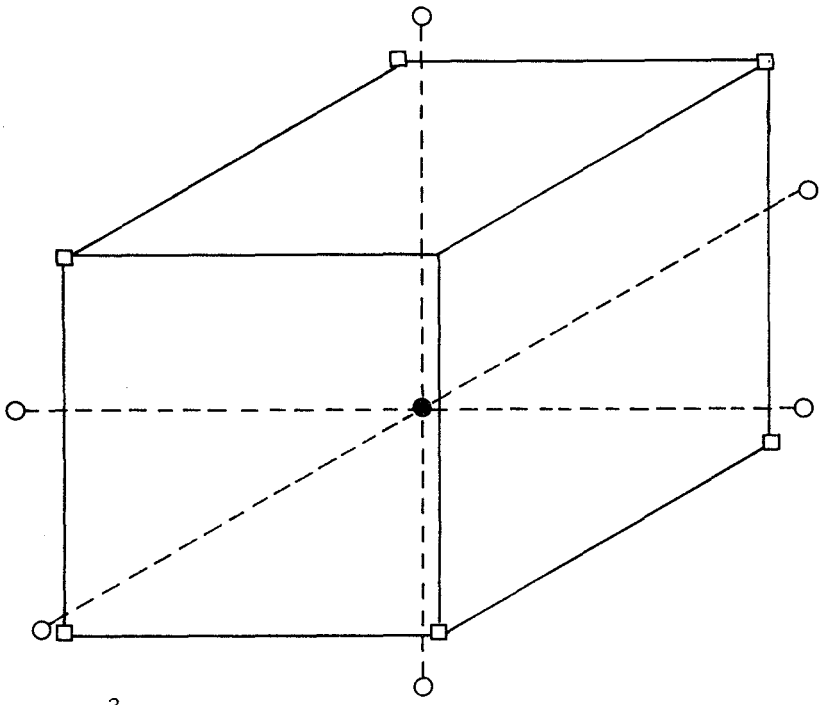
TABLE 2.4

Treatment Numbers and α Values for Orthogonal Central Composite Design

Number of factors	Number of treatments	Value of 'α' to make design orthogonal
2	9	1.00
3	15	1.215
4	25	1.414
5	43	1.547
6	77	1.761
7	143	1.910
8	273	2.045

FIGURE 2.2

Illustration of Central Composite Design in Three Factors



□ points in 2^3 factorial
○ star points
● centre point

In a rotatable design the standard error of estimate is the same for all points that are the same distance from the centre, regardless of their direction from the centre. This equal-precision property is desirable when little is known about the shape of the response surface on the borders of the design region. The centre treatment is sometimes replicated a number of times to provide a measure of variability of response. The number of design points (including replicates of the centre point) and values of α for rotatable designs in 2 to 6 factors are as follows (from Cochran and Cox, 1957: 347).

TABLE 2.5

Number of Design Points and α Values
for a Rotatable Central Composite Design

Number of factors	Number of points in			Total points	Value of α
	2^k Factorial	Star	Centre		
2	4	4	5	13	1.414
3	8	6	6	20	1.682
4	16	8	7	31	2.000
5	16	10	6	32	2.000
6	32	12	9	53	2.378

In this table the designs in five and six factors employ only one half of the full factorial design. Lists of treatments to be included in these cases are provided by Cochran and Cox [1957: 371, 372].

While the treatments of the above designs may be completely randomized (i.e. different environmental sequences used for each), the precision of the experiment is increased if treatments are divided into two or three groups or incomplete blocks [Cochran and Cox, 1957: 353]. These blocks may correspond to different simulated climatic sequences [Johnston, 1973: 170; Hughes, 1973: 89]. The same seeds are used to generate stochastic environments within blocks but different seeds are used between blocks. The block or climate effects are then incorporated in the response function by means of dummy or 0-1 variables.

2.5 Summary

Some of the more common traditional designs for experiments with systems models have been outlined in this chapter. The simplest of these is the full factorial. When more than about three factors are present use of a fractional factorial may be preferable. Still greater efficiency in locating optima is possible through response surface methodology, and especially by the use of a central composite design. Here a two-level full factorial (or fractional factorial if the number of factors is large) is augmented by star and centre treatments. The central composite design may be divided into incomplete blocks to test the effect of different simular environments on treatments (management policies). While the designs presented here indicate that a good deal of progress can be made with traditional or tabulation methods, the cost of the experiment becomes rather large for more than about six factors, and use of optimum-seeking sequential designs (introduced in the next chapter) is to be preferred.

CHAPTER 3

UNIVARIATE SEARCH

The determination of an optimal value for a single controllable factor within a systems model is generally a simple matter. However, a well designed univariate search routine may be most useful to the systems researcher for two reasons. Firstly, one may wish to locate optima with high precision yet prior knowledge of the optimal region may be inadequate to place treatments sufficiently close together when using a pre-specified design layout. Secondly, and more importantly, many multivariate search methods proceed by way of a series of unidirectional searches. Sometimes these directions are parallel to the factor level axes while in other cases two or more factors are adjusted in a fixed ratio to each other. Since the number of unidirectional searches in a single multivariate optimum-seeking experiment may run into the hundreds, it is essential to employ an efficient unidirectional optimization procedure.

The discussion of univariate search methods at this stage also provides a useful background to later chapters by illustrating a number of concepts common to all numerical optimization techniques.

While a large number of univariate search techniques have been devised (for example, see Wilde, 1965) only two will be discussed here, viz. a naive interval narrowing procedure and the highly efficient Powell method. In each case it will be assumed that the variable is quantitative and can take a continuous range of values.

3.1 Interval Narrowing

In this section a method to find the approximate optimal level of a single controllable factor by progressively narrowing the interval of search will be developed along intuitive lines. Although interval narrowing is not an efficient search procedure the example is convenient for illustrating some concepts and problems of adapting a numerical optimization procedure to the design of simulation experiments.

Recalling our farm planning model, suppose the experimenter wishes to determine the most profitable area of just one crop, viz. irrigated wheat. Assume that the response curve relating net farm income to wheat area is 'well behaved' or convex upwards in the range zero to 150 ha and the true but unknown optimum is 86.7 ha. The experiment is commenced with an initial guess of the optimal level; say this is 40 ha. Evaluation of this treatment with the systems model reveals a net income of $22,000. Further treatments are located at intervals of 20 ha. Since the response to each treatment is known before the next treatment is placed, the number of steps will be kept to a minimum. Suppose predicted income levels are $25,000 at 60 ha, $26,000 at 80 ha and $25,500 at 100 ha. The interval containing the optimum is now narrowed to 60 to 100 ha and areas outside this range are excluded from further consideration. This completes the first iteration of the search. In order to make further progress, let us now reduce the step size by a factor of 5 (i.e. to 4 ha) and commence a second iteration from our current best treatment of 80 ha. Treatments would now be placed at 84 ha, 88 ha and 92 ha (at which point income declines indicating that the optimum has again been overshot). The range of interest has now been narrowed to 84 to 92 ha. Step size is further reduced to 4/5 or 0.8 ha. A treatment at 88.8 ha reveals a decline in income relative to the previous best treatment, so backward stepping takes place, with treatments at 87.2 ha, 86.4 ha and 85.6 ha. The complete sequence of treatments for three search iterations is listed in Table 3.1.

TABLE 3.1

Experimental Design for Univariate Search by Inverval Narrowing

		Wheat area (ha)			
		Treatment number			
		1	2	3	4
Iteration	1	40	60	80	100
number	2	84	88	92	
	3	88.8	87.2	86.4	85.6

After 11 treatments the interval containing the optimum has been narrowed to 85.6 to 87.2 ha. At this stage the experimenter may decide upon the optimum by (i) accepting the best treatment evaluated (86.4 ha); (ii) interpolating between the closest factor levels; or (iii) carrying out a further search iteration.

The above account illustrates a number of typical features of optimum-seeking experimental designs. An initial guess of the optimal factor level is made, and improved values are obtained through a series of search iterations. Convergence to the optimum is at first rapid but then becomes increasingly slower. The total number of treatments needed depends on the closeness of the initial guess to the optimum and on the settings of the search parameters (here, initial step size and reduction to step size between iterations). The termination rule involves a compromise between the precision with which the optimum is estimated and the cost of evaluating additional treatments. All of the above characteristics are common to most optimum-seeking designs.

3.2 Powell's Method

A highly efficient univariate search method has been devised by Powell [1964] to find the level of a variable corresponding to a minimum function (or response) value. Essentially, the method involves placing treatments at three levels of the variable factor

(a, b and c), regressing a quadratic function through the predicted response values (Z_a, Z_b and Z_c) and locating the stationary point on the fitted equation. Special features are included to ensure that the stationary point is a minimum and for taking advantage of the fact that a quadratic equation will fit three points exactly. Also, a limit is placed on the extent of adjustment from the initial factor level towards the estimated minimum.

For convenience, a, b and c are defined as differences from the initial guess of the optimal x value. Treatments are first evaluated at x (where a = o) and at b = x + Δx where Δx is a forward step in the level of the factor. The position of the third treatment depends on whether the response is found to be increasing or decreasing, i.e.

if $Z_b < Z_a$ place c at x + 2 Δx, and

if $Z_b > Z_a$ place c at x - Δx,

as illustrated in cases (i) and (ii) of Figure 2.1. The quadratic passing through Z_a, Z_b and Z_c will have a stationary point at

$$x^* = x + d$$

where $$d = \tfrac{1}{2} \frac{(b^2 - c^2) Z_a + (c^2 - a^2) Z_b + (a^2 - b^2) Z_c}{(b - c) Z_a + (c - a) + Z_b + (a - b) Z_c}$$

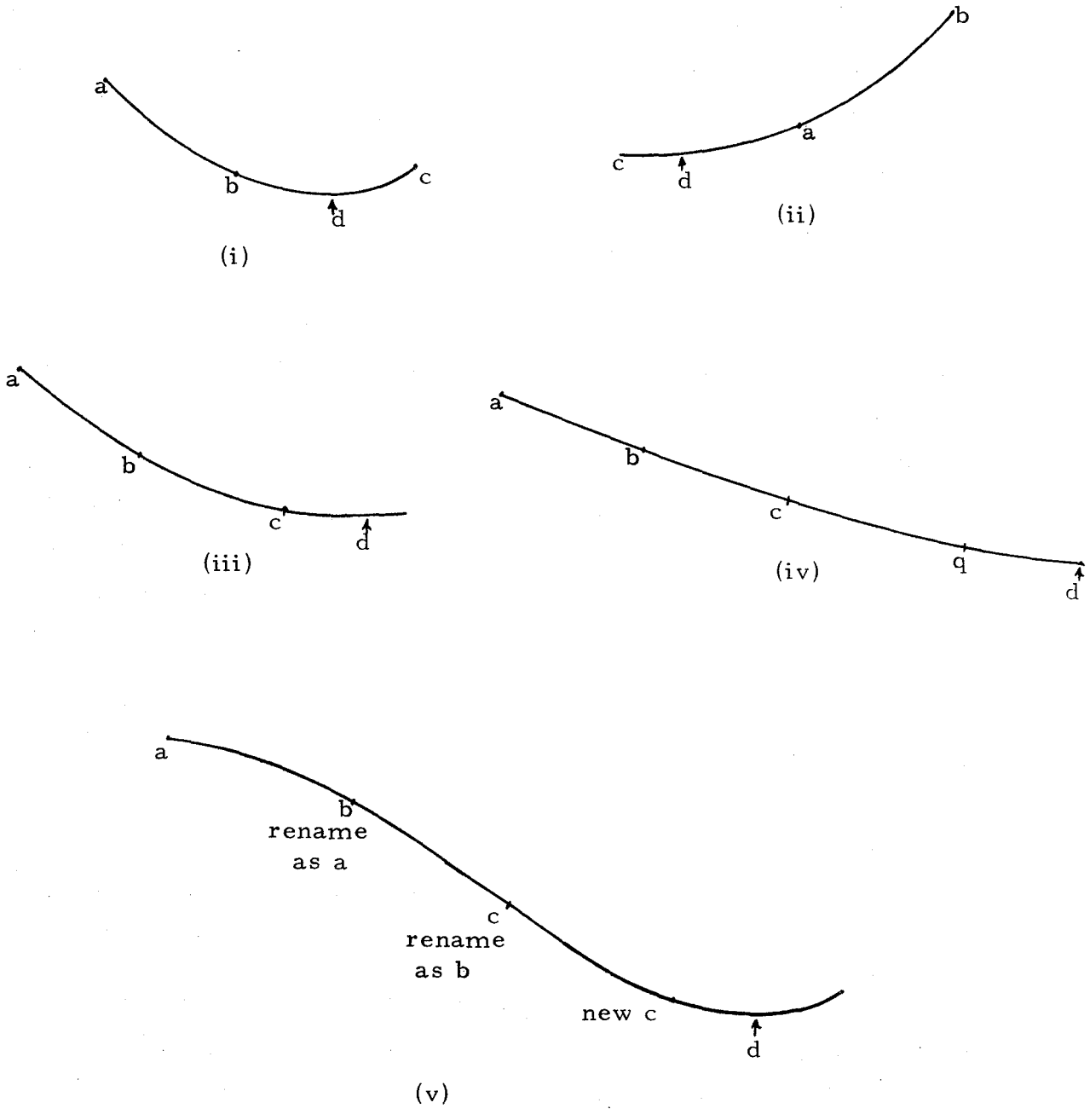
and this will be a minimum value if

$$\frac{(b-c) Z_a + (c-a) Z_b + (a-b) Z_c}{(a-b)(b-c)(c-a)} < 0$$

Note that the equation of the quadratic function need not be calculated explicitly.

FIGURE 3.1

Treatment Placements in Powell's Univariate Minimization Method



For the farm planning example, suppose wheat areas of 40, 60 and 80 ha are found to give incomes of \$22,000, \$25,000 and \$26,000 respectively. Here x = 40, and on negating the Z values to facilitate maximization,

$$d = \tfrac{1}{2} \frac{(20^2 - 40^2)\ (-22000) + (40^2)\ (-25000) + (-20^2)\ (-26000)}{(20 - 40)\quad (-22000) + (40)\quad (-25000) + (-20)\quad (-26000)} \text{ ha}$$

$$= 40 \text{ ha, and}$$

$$x^* = 40 \text{ ha} + 40 \text{ ha} = 80 \text{ ha.}$$

The optimal level will at times fall outside the range of treatments evaluated, as in case (iii) of Figure 3.1. Such extrapolation can be hazardous, particularly when the pattern of response is irregular as is likely with a stochastic model. This is illustrated in case (iv) where the three performance values are almost collinear (in a straight line) and d lies far to the right of c. To avoid running "off the edge" of the response curve or surface, the Powell method restricts the size of d to a maximum adjustment parameter q.

When the sufficiency condition is not satisfied the stationary point is a maximum and continued stepping is necessary. This is illustrated in case (v) where b and c are renamed as a and b, and a new treatment c is placed at $x + 3\Delta x$. In this case 'a' is no longer zero (which is the reason why the 'a' term is retained in the above formulae).

The estimate of the optimum obtained by this method may not be very precise, particularly if Δx is large and the response curve is not quadratic in shape. This could be overcome by repeating or iterating the procedure commencing with x at the new optimum and using a reduced step size. It is to be noted, however, that the Powell method is designed for multivariate optimization where pursuit of high accuracy during individual searches is not warranted.

On the other hand, Powell's method is highly efficient, locating the minimum with only two treatments in addition to the initial guess when the response curve is concave upwards. Further, by retaining curvature information (the second derivative) from the first iteration, minimization in subsequent iterations can be achieved with only one new treatment. This further refinement will not be elaborated since experience suggests it is not very successful for experiments with models of agricultural systems.

Appendix II presents a computer subroutine for univariate minimization using a quadratic interpolation procedure similar to that of Powell. This subroutine is linked to a main program, containing a simple test function. The FORTRAN listing of the main program and subroutine are provided, along with the computer output for the test function.

CHAPTER 4

STEEPEST ASCENT

The application of numerical optimization procedures to the design of simulation experiments aimed at locating levels of two or more factors which are simultaneously optimal is introduced in this chapter. It is illuminating to compare this application of search methods over a response surface with the physical analogy of mountain climbing. In many ways computer 'hill-climbing' is just as difficult and demanding as climbing real mountains. While not dangerous in a physical sense, it is fraught with frustrations and hazards with respect to failure to make progress and false summits, particularly when the response surface is multimodal (c.f. a mountain range).[6] Even when the surface is unimodal, convergence to the optimum may be difficult to achieve if the slopes are not regular and differ markedly with respect to factor axes, and if strong response interaction exists between the various factors.

One of the oldest hill-climbing procedures, and probably the easiest to understand, is the method of steepest ascent. Steepest ascent (or steepest descent) has probably been used more frequently than any other optimum-seeking design (and has even found application in agricultural systems research [Zusman and Amiad, 1965; Toft, 1970], but is not very efficient and fails to converge on optimal values in

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[6] Often the term "hypersurface" is used to represent a surface in more then two dimensions. An excellent introduction to the geometry of response surfaces and to simple hill-climbing methods, interspersed with appropriate excerpts from "Excelsior" by Nietzsche, is to be found in the books by Wilde [1964, 1967].

many situations. However, a discussion of steepest ascent is useful for illustrating many of the concepts involved in computer hill-climbing, and the basic procedure may be modified to make it reasonably effective. In this chapter the basic steepest ascent method will be explained and then refinements to the procedure will be outlined. Following Wilde, the search will be discussed in three stages, viz. opening gambit; mid-game tactics; and end-game tactics. The third of these stages is included in the refined version only. The discussion is limited initially to the two variable cases for simplicity of exposition and to allow diagrammatic representation. However, the algebra of the multivariate generalization is presented at the end of each section.

4.1 Basic Steepest Ascent

As with univariate search the opening gambit involves nominating an initial combination of factor levels (or management policy) which is feasible though perhaps not very desirable, then improving on this policy in an iterative fashion. It is, however, quite important to use prior knowledge to choose a good initial treatment. If the real system which has been modelled is in existence then the current management policy usually provides a suitable first treatment. If little is known about the nature of the response surface or the system is not yet in existence, then an exploratory experiment using a fixed design such as an incomplete factorial may be carried out to determine a suitable search base.

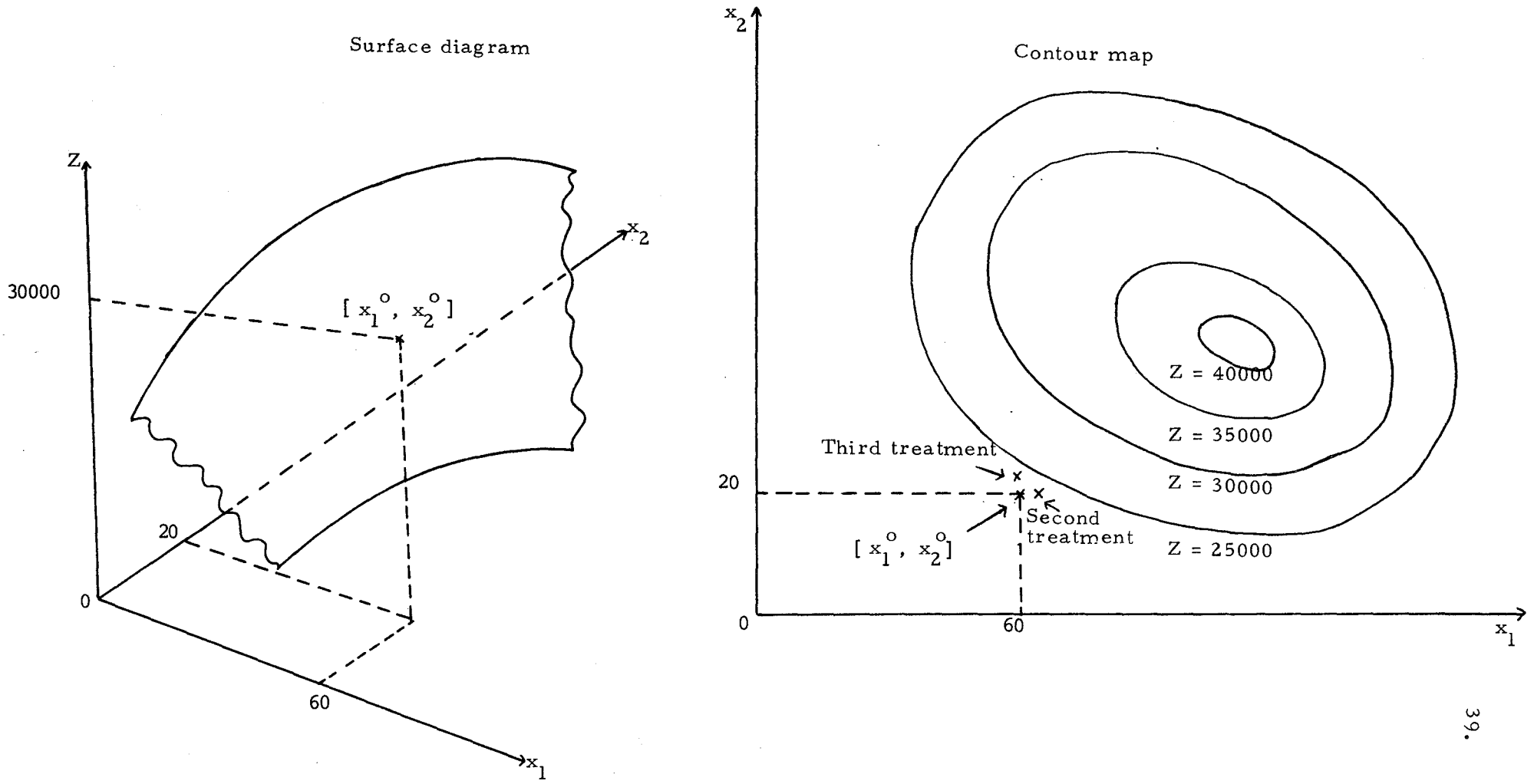
Let us designate the initial factor levels or decision vector as

$$X^o = (x_1^o , x_2^o)$$

The systems model is used to evaluate this treatment and predicts a response of Z_o. The decision space, unknown response surface and initial treatment are illustrated in Figure 4.1. Response is depicted by both a surface diagram in three dimensions and a contour map in two dimensions. The latter type of diagram, where the axes represent

FIGURE 4.1

Diagrammatic Representation of The Experimental Region and Response Surface for Two Variable Factors



factor levels and where factor combinations resulting in equal responses are linked by continuous curves, will be used in subsequent illustrations.

To take up the farm planning example, suppose the initial guess (or current plan) is to grow 60 ha of wheat and 20 ha of lucerne. Evaluation of this policy (treatment) with the systems model leads to a predicted net income of \$20,000, i.e.

$$X^o = (60 , 20) \quad \text{and} \quad Z_o = 20000.$$

Mid-game tactics consisting of <u>linear</u> searches over the response surface are now initiated. First, the equation to the plane touching the response surface (called the <u>tangent plane</u>) at X^o must be estimated. The direction of greatest steepness on this planar approximation to the (unknown) response surface indicates the most direct path to the optimal policy. By placing a sequence of treatments in this direction it should be possible to make rapid improvement in the response criterion, c.f. a mountain climber taking the shortest but most sheer route to the summit. When continued stepping in this ascent direction fails to make further improvement in the criterion, a new steepest ascent direction is established and another sequence of treatments evaluated. These iterations are continued until no further progress is possible.

The tangent plane is defined by the equation

$$\Delta Z = m_1 \Delta x_1 + m_2 \Delta x_2$$

where ΔZ is the change in response resulting from small changes Δx_1 and Δx_2 in factors x_1 and x_2 respectively. The parameters m_1 and m_2 are slopes of the plane with respect to each factor axis and are found by evaluating treatments in which x_1 and x_2 are <u>forward differenced</u> in turn, i.e.

$$X^1 = (x_1^o + \Delta x_1, x_2)$$

$$X^2 = (x_1^o, x_2^o + \Delta x_2),$$

and then calculating

$$m_1 = \frac{Z_1 - Z_o}{\Delta x_1} \quad \text{and} \quad m_2 = \frac{Z_2 - Z_o}{\Delta x_2}$$

where Z_1 and Z_2 are the respective response values.

The direction of steepest ascent is defined in terms of the slope coefficients m_1 and m_2. Specifically, it is that direction in the x_1 - x_2 plane such that changes are made to each factor in proportion to the slope with respect to that factor. If m_1 is greater than m_2 then each new treatment will involve a large increase in x_1 relative to that for x_2. On the other hand if m_2 is the larger then the greatest adjustment will be made to x_2. It is to be noted that both factors are adjusted simultaneously when placing treatments during the linear search.

Although the ascent direction is readily defined (as above), the selection of actual step sizes presents a problem. We could, for example, make changes in x_1 and x_2 of δx_1 and δx_2 where these simultaneous increments are defined by

$$\delta x_1 = \frac{m_1}{m_1 + m_2} L \quad \text{and} \quad \delta x_2 = \frac{m_2}{m_1 + m_2} L$$

and L is a parameter which has been introduced to govern the step length or distance between successive treatments. This would be satisfactory if m_1 and m_2 both had the same sign, but if one were positive and the other negative then step length would be unpredictable, and in the extreme case where $m_1 + m_2 = 0$ an infinitely large step would be taken. The problem is overcome by squaring the slope coefficients then taking the square root of the sum of their squares, i.e.

$$\delta x_1 = \frac{m_1}{\sqrt{m_1^2 + m_2^2}} L \quad \text{and} \quad \delta x_2 = \frac{m_2}{\sqrt{m_1^2 + m_2^2}} L .$$

Suppose that in the farm planning example x_1 and x_2 are each one hectare, Z_1 = \$21,500 and Z_2 = \$20,500 and L = 20 ha. Then

$$m_1 = \frac{21500 - 20000}{1} = 1.5, \quad m_2 = \frac{20500 - 20000}{1} = 0.5,$$

$$\sqrt{m_1^2 + m_2^2} = 1.58,$$

$$\delta x_1 = \frac{1.5}{1.58} 20 = 19.0 \quad \text{and} \quad \delta x_2 = \frac{0.5}{1.58} 20 = 6.3.$$

Successive treatments would be placed at

X_1 = (60 + 19, 20 + 6.3)

X_2 = (60 + 38, 20 + 12.7)

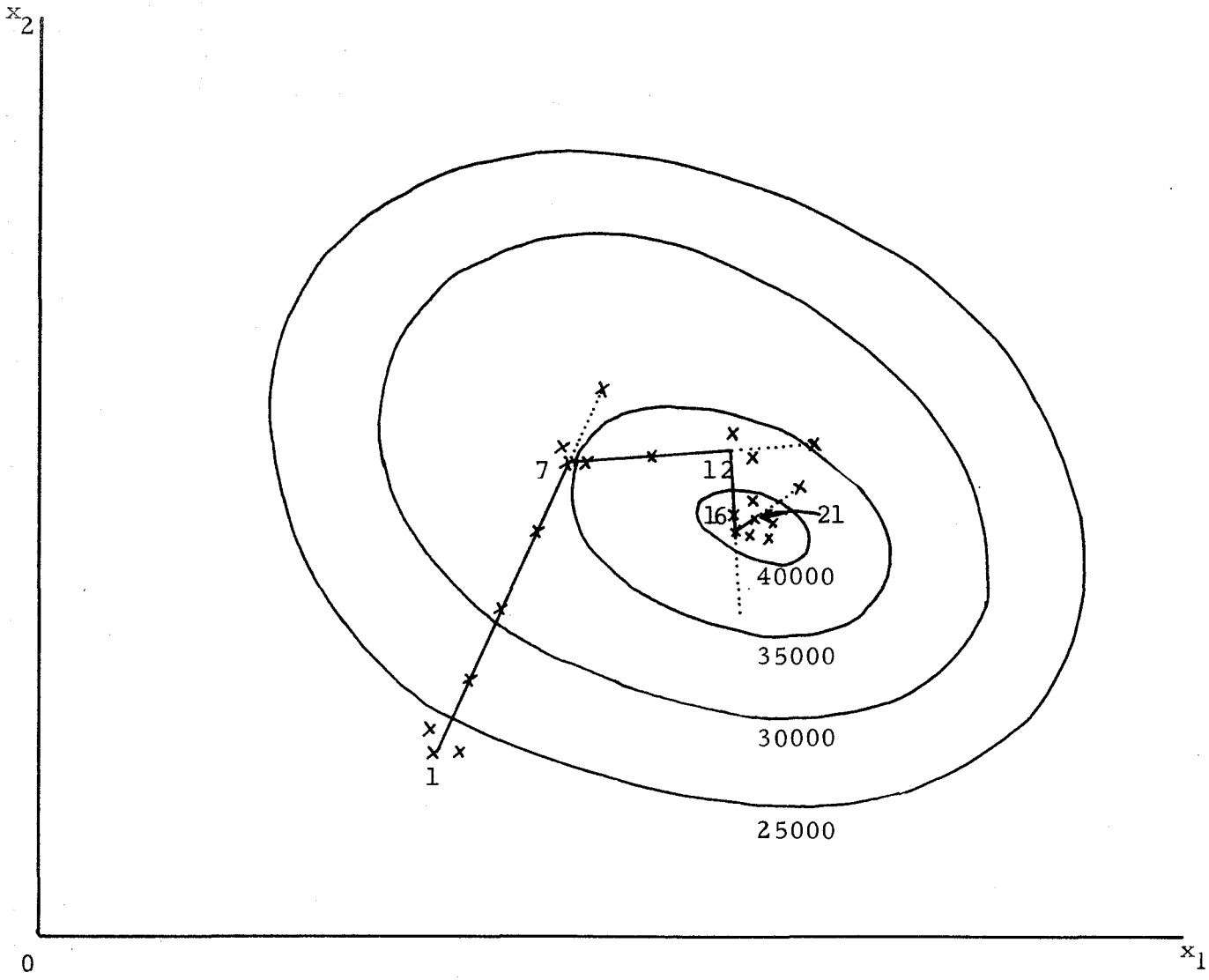
X_3 = (60 + 57, 20 + 19)

and so on.

Steps would be continued in this search direction while ever Z continued to improve. The first step for which Z declines is discarded and the previous treatment, which is the optimum for this iteration, is used as a new search base. The equation to the tangent plane is estimated at this improved position on the response surface and successive treatments in a new direction of steepest ascent are evaluated. Search iterations are carried out until no improvement in the performance criterion is achieved on the first step in a new ascent direction. The step size parameter is then reduced (e.g. L may be reduced from 20 to 4) and more closely spaced treatments in the currently defined search direction are evaluated. Note that no advantage would be gained by reducing Δx_1 and Δx_2 and re-establishing the equation to the tangent plane, since these forward differences are set initially at the smallest meaningful change in the level of each factor. The reduced step size may allow further iterations to be carried out, and further reductions may be made to step size when

FIGURE 4.2

Sequence of Treatments Under Steepest Ascent Design



the search again fails to progress. Eventually, no improvement in the performance criterion is possible with the smallest meaningful step size, and mid-game tactics (and basic steepest ascent) have been completed. A typical pattern of the experimental layout is provided in Figure 4.2.

The above procedure may be extended readily to the general or n-factor case. Here n slope coefficients must be estimated as

$$m_i = \frac{Z_i - Z_o}{\Delta x_i}$$

and the adjustment to each variable factor when stepping in the direction of steepest ascent is given by

$$\delta x_i = \frac{m_i}{\sqrt{\sum_{j=1}^{n} m_j^2}} L \ .$$

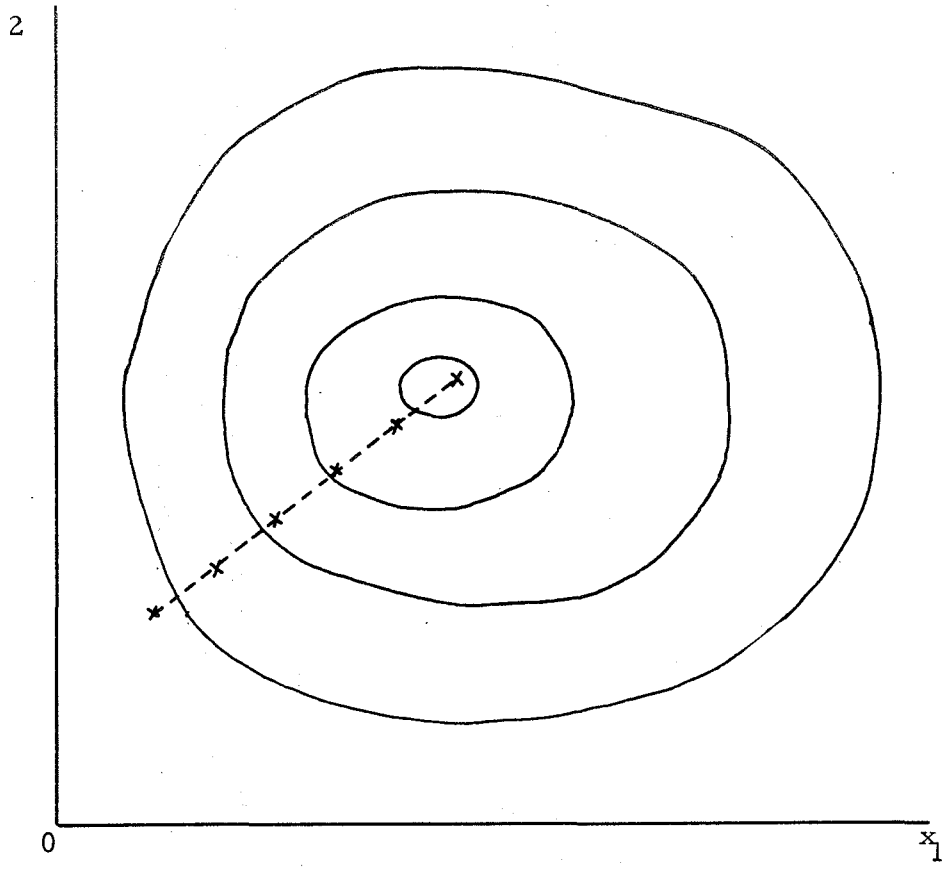
A FORTRAN program for the general case and computer printout of the ascent steps for a test function in three variables are presented as Appendix III.

4.2 A Refined Version of Steepest Ascent

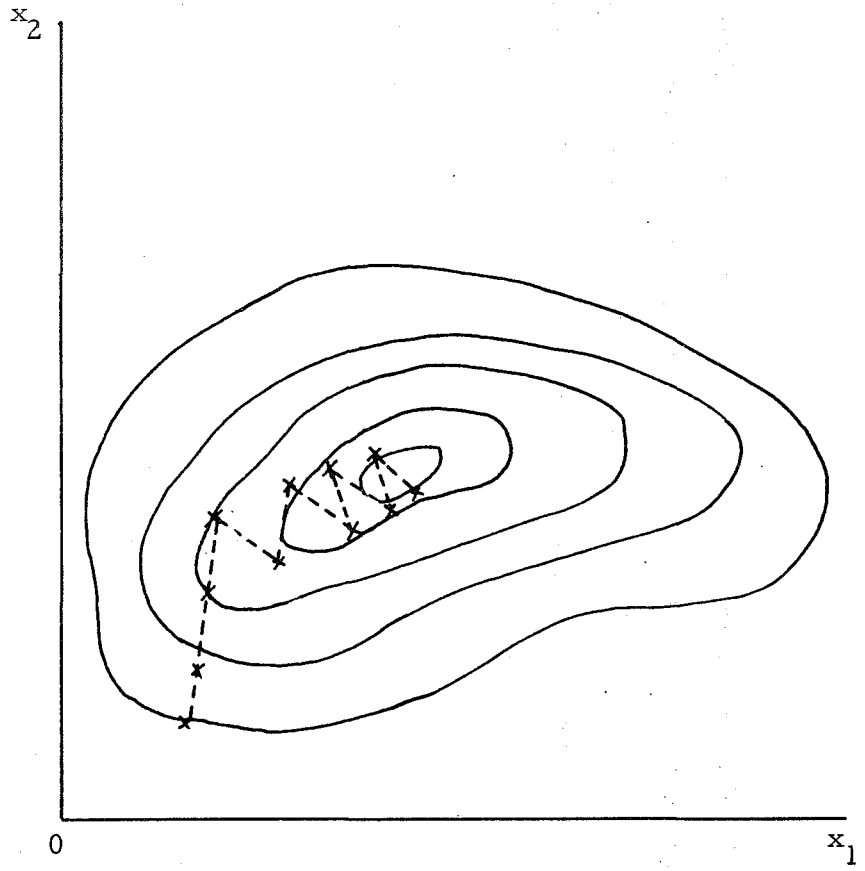
The basic steepest ascent procedure has a number of weaknesses from a theoretical and practical viewpoint. When the contours of the response surface are approximately circular, indicating little or no interaction between variables, very rapid progress will be made towards the optimum. But if these contours are in any way irregular, then the direction of steepest ascent quickly changes as treatments are placed further away from the search base, and the search may progress slowly along a zig-zag path. These two cases are illustrated in Figure 4.3.

FIGURE 4.3

Steepest Ascent Paths for High and Low Interaction Between Factors



Low interaction between factors



High interaction between factors

Another deficiency of the basic procedure is the fixed step size which means that the optimum in any ascent direction is always under-reached or overshot. (This may be likened to a golfer approaching a hole but repeatedly hitting his chip shots a fixed distance and passing backwards and forwards over the top of the green.) Reduction in step size (changing to a more angled or higher iron) in concluding iterations partially overcomes this problem, but a superior approach is to optimize on each ascent. That is, during each ascent in a fixed direction, the highest point on the ridge (as opposed to the higher of the steps before and after the crest) is located and used as the new search base. This may be achieved using a univariate search method such as that of Powell. Note that while two policy variables (x_1 and x_2) are being adjusted at each step, the optimization is carried out with respect to step length and this is a single variable.

At this stage it is necessary to introduce the concept of a search direction vector.[7] This is a vector containing elements which indicate the relative rates at which each variable is to be adjusted in the ascent direction. For example, the adjustments in the first iteration above were

$$U = [\,19 \quad 6.3\,]$$

and steps were placed at

$$X^o + U, \quad X^o + 2U, \quad X^o + 3U \qquad \text{and so on,}$$

or in general at $X^o + bU$. Here U is the search direction vector, and the fixed step size is a consequence of b being incremented by one-unit values. The search is linear because fixing U throughout the iteration fixes the direction of steps in the x_1 - x_2 plane.

---

[7] The remainder of this chapter draws increasingly on matrix-vector notation. An elementary introduction to the mathematical concepts used here is to be found in Yamane [1968].

The basic steepest ascent procedure may be refined by carrying out linear optimizations during each iteration, i.e. by finding the value of $\underline{b}$ for which Z is a maximum. Commencing each iteration on the crest of the ridge allows more rapid convergence towards the optimum, eliminating zig-zagging provided the ridge is approximately linear.

Another refinement to steepest ascent is to carry out a non-linear local exploration of the response surface in the vicinity of the best treatment located by the linear searches; this is what Wilde refers to as end-game tactics. A quadratic function can be fitted around the final search base at the cost of a small number of additional treatments. Greater precision in estimates of the optimal factor levels can then be obtained using differential calculus. More importantly, information about the shape of the response surface in the vicinity of the optimum is obtained. This may reveal that the stationary point is a saddle point rather than a maximum as required. Also, the variation in the response criterion when small changes are made to levels of each of the policy variables is readily ascertained, shedding light on the sensitivity of performance to policy changes. The procedure for non-linear local exploration will now be outlined.

Following Wilde (and using a slightly different notation to that of Chapter 2), the response surface is represented by the Taylor series for a function of two variables with terms of higher than second order neglected, i.e.

$$\Delta Z = m_1 \Delta x_1 + m_2 \Delta x_2 + \tfrac{1}{2}(m_{11} (\Delta x_1)^2 + 2m_{12} \Delta x_1 \Delta x_2 + m_{22} (\Delta x_2)^2)$$

Here the performance and policy variables are expressed in <u>difference</u> form, m_1 and m_2 are the slopes with respect to each co-ordinate axis, m_{11} and m_{22} are the curvature terms and m_{12} measures interaction between x_1 and x_2. To estimate these coefficients, the <u>triangular</u> experimental design used to determine the final tangent plane is augmented by three further treatments; two of these consist of <u>backward differencing</u> the variables in turn (to give a crucifix pattern)

while in the third they are forward differenced simultaneously. The resulting search pattern, with distances between treatments exaggerated, is illustrated in Figure 4.4.

Let Z_i^+ and Z_i^- represent the response criterion when variable i is forward and backward differenced respectively, and Z^{++} be response when both are forward differenced simultaneously. To find m_1, note that when $\Delta x_2 = 0$,

$$\Delta Z_1^+ = Z_1^+ - Z_o = m_1 \Delta x_1 + \tfrac{1}{2} m_{11} (\Delta x_1)^2 \qquad (1) \text{ and}$$

$$\Delta Z_1^- = Z_1^- - Z_o = m_1 (-\Delta x_1) + \tfrac{1}{2} m_{11} (-\Delta x_1)^2$$

$$= - m_1 \Delta x_1 + \tfrac{1}{2} m_{11} (\Delta x_1)^2 \qquad (2)$$

Subtracting (2) from (1):

$$Z_1^+ - Z_1^- = 2 m_1 \Delta x_1$$

hence $$m_1 = \frac{Z_1^+ - Z_1^-}{2 \Delta x_1}$$

and similarly

$$m_2 = \frac{Z_2^+ - Z_2^-}{2 \Delta x_2}$$

To find m_{11}, sum (1) and (2):

$$Z_1^+ + Z_1^- - 2 Z_o = m_{11} (\Delta x_1)^2$$

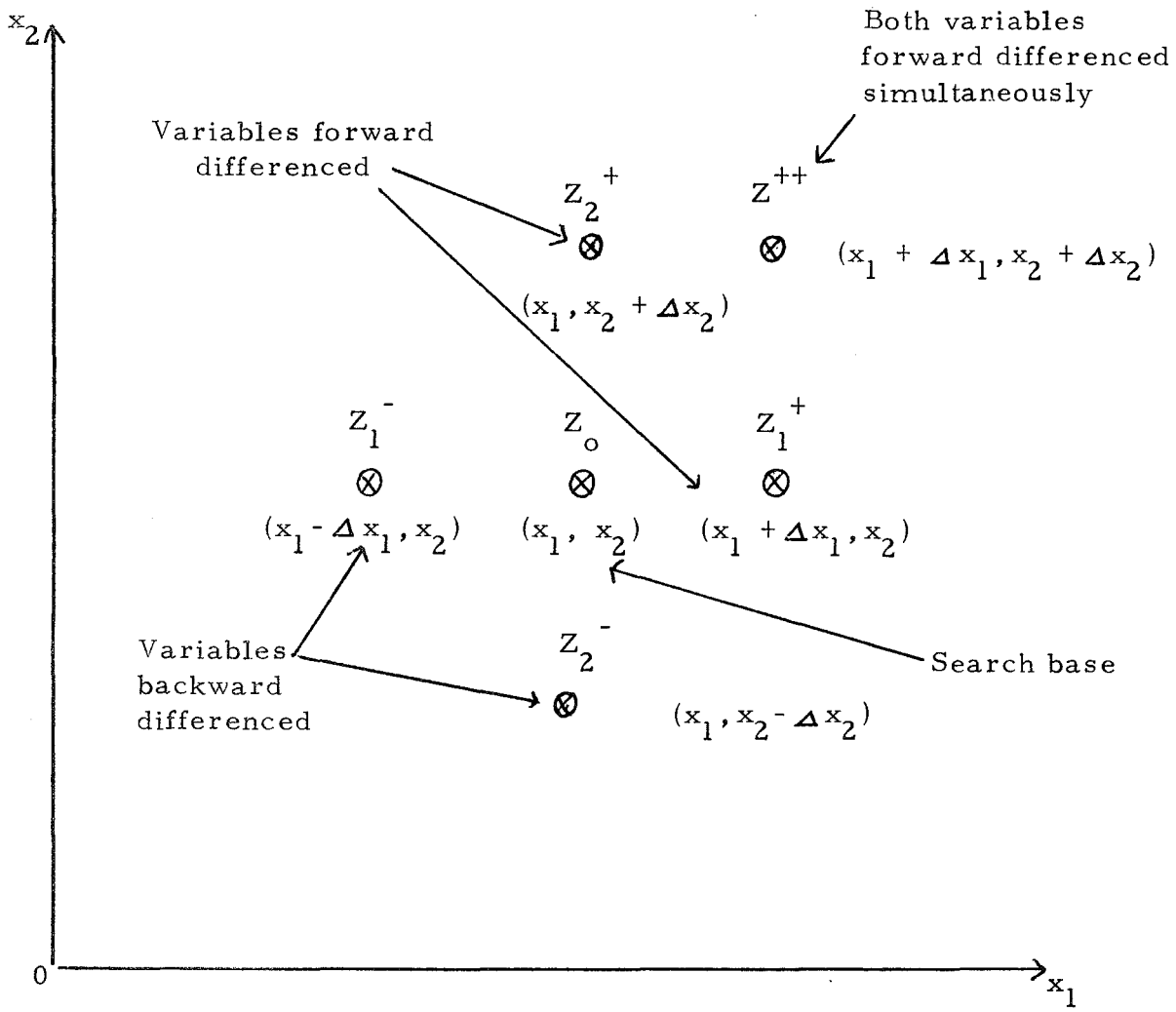
hence $$m_{11} = \frac{Z_1^+ + Z_1^- - 2 Z_o}{(\Delta x_1)^2}$$

and similarly

$$m_{22} = \frac{Z_2^+ - Z_2^- - 2 Z_o}{(\Delta x_2)^2}$$

FIGURE 4.4

Pattern of Treatments for Non-Linear Local Exploration



Having obtained m_1, m_2, m_{11} and m_{22}, the remaining coefficient m_{12} may be calculated from the Taylor series as

$$m_{12}\,\Delta x_1\,\Delta x_2 = \Delta Z - m_1\Delta x_1 - m_2\Delta x_2 - \tfrac{1}{2}m_{11}(\Delta x_1)^2 - \tfrac{1}{2}m_{22}(\Delta x_2)^2$$

i.e.,

$$m_{12} = \frac{Z^{++} - Z_o - m_1\Delta x_1 - m_2\Delta x_2 - \tfrac{1}{2}m_{11}(\Delta x_1)^2 - \tfrac{1}{2}m_{22}(\Delta x_2)^2}{\Delta x_1\Delta x_2}$$

The adjustments in x_1 and x_2 necessary to maximize ΔZ (and hence Z) are now obtained as follows:

$$\frac{\partial \Delta Z}{\partial \Delta x_1} = m_1 + m_{11}\Delta x_1 + m_{12}\Delta x_2 = 0 \qquad \text{and}$$

$$\frac{\partial \Delta Z}{\partial \Delta x_2} = m_2 + m_{22}\Delta x_2 + m_{12}\Delta x_1 = 0$$

$$\therefore \quad m_{11}\Delta x_1 + m_{12}\Delta x_2 = -m_1 \qquad \text{and}$$

$$m_{12}\Delta x_1 + m_{22}\Delta x_2 = -m_2$$

These two equations may be solved for x_1 and x_2 in the manner described in Chapter 2. Alternatively (and more conveniently when one wishes to generalize the procedure for $\underline{n}$ variables and program it on a computer) the solution may be expressed in matrix vector notation. Here each policy is represented by the column vector

$$X = \begin{bmatrix} x_1 \\ \\ x_2 \end{bmatrix}$$

rather than the co-ordinate pair (x_1, x_2). The forward differences form another column vector

$$U = \begin{bmatrix} \Delta x_1 \\ \\ \Delta x_2 \end{bmatrix}$$

as do the slopes of the response surface

$$g = \begin{bmatrix} m_1 \\ \\ m_2 \end{bmatrix}$$ (called the Jacobian gradient vector).

The curvature and interaction terms may be written as a matrix:

$$H = \begin{bmatrix} m_{11} & m_{12} \\ \\ m_{12} & m_{22} \end{bmatrix} ;$$

this is called the matrix of the quadratic form or the Hessian matrix. In matrix-vector notation the Taylor series becomes

$$\Delta Z = g'U + \tfrac{1}{2}U'HU$$

where g' and U' are the row vector transposes of g and U respectively. The simultaneous equations resulting from setting the partial derivatives to zero become

$$H\,U = -g$$

and the solution is

$$U^* = -H^{-1}g$$

where $U^* = \begin{bmatrix} \delta x_1 \\ \\ \delta x_2 \end{bmatrix}$ and H^{-1} is the inverse of the Hessian matrix.

The stationary point on the response surface X* is then found as

$$X^* = X + U^*.$$

This will be a maximum provided

$$m_{11} < 0 \qquad \text{and} \qquad |H| > 0$$

where $|H|$ is the Hessian determinant and is given by

$$|H| = m_{11}m_{22} - m_{12}^2$$

Once the coefficients of the Taylor series have been estimated it is a simple matter to predict the sensitivity of performance to policy changes. For example, if x_2 were fixed ($\Delta x_2 = 0$) and x_1 increased by Δx_1 units then

$$\Delta Z = m_1 \Delta x_1 + \tfrac{1}{2} m_{11} (\Delta x_1)^2$$

and the elasticity of response with respect to the factor x_1 could be obtained as

$$e_{x_1} = \frac{\Delta Z / \Delta x_1}{Z^* / x_1^*}$$

where Z^* and x_1^* are optimal levels.

The refinements of linear optimizations and non-linear local exploration are readily extended to the n-variable case. Here the Taylor series approximating the response hypersurface becomes

$$\Delta Z = \sum_{i=1}^{n} m_i \Delta x_i + \tfrac{1}{2} \sum_{i=1}^{n} m_{ii} (\Delta x_i)^2 + \sum_{i=1}^{n} \sum_{i \neq j \; j=1}^{n} m_{ij} \Delta x_i \Delta x_j$$

The coefficients of this relationship are obtained in the same manner as above (but replacing 1 and 2 by i and j for all combinations of i and j).

The stationary point on the response hypersurface is again at

$$X^* = X + U^*$$

where $U^* = -H^{-1}g$

and $g = \begin{bmatrix} m_1 \\ m_2 \\ . \\ . \\ . \\ m_n \end{bmatrix}$; $H = \begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ . & & & \\ . & & & \\ . & & & \\ m_{n1} & m_{n2} & \cdots & m_{nn} \end{bmatrix}$;

and $U^* = \begin{bmatrix} \delta x_1 \\ \delta x_2 \\ . \\ . \\ . \\ \delta x_n \end{bmatrix}$.

The test ensuring that X^* is a maximum (rather than a minimum or saddle point) is now more difficult and relies on advanced mathematics.[8]

A FORTRAN listing for the refined steepest ascent method together with computer output of the design points for a test function in three variables is provided as Appendix IV.

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[8] For the more mathematically inclined, X^* is a maximum if H is negative definite which is the case if the principal minors of H alternate in sign, commencing with a negative. In the computer program of Appendix IV the principal minors are obtained as the successive products of pivotal elements during Gaussian reduction of the Hessian matrix.

4.3 Summary

Multivariate search has been introduced by reference to the method of steepest ascent. While the basic steepest ascent procedure is relatively inefficient, modifications have been outlined which make the method adequate for a range of design problems. An understanding of these modifications requires advanced knowledge of matrix algebra. The discussion of steepest ascent, along with its mountain climbing analogy, has provided a background for the examination of more modern and more efficient optimum-seeking designs.

CHAPTER 5

DIRECT SEARCH METHODS

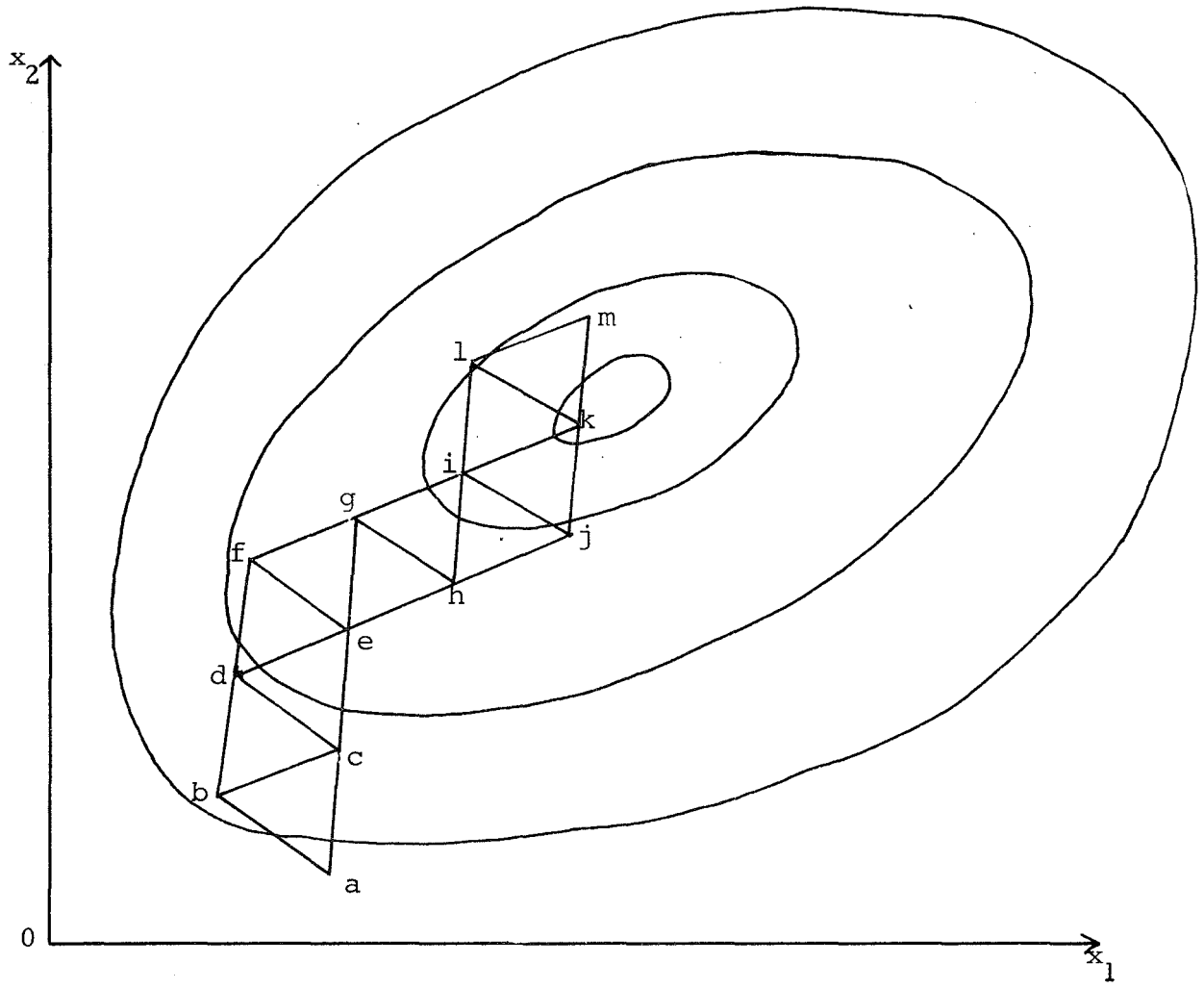
Direct search differs from gradient search methods such as steepest ascent in that the search directions are not based on estimated partial derivatives or slopes of the response surface. While a large number of direct search methods have been devised, only four will be considered in this chapter. First, brief descriptions of the simplex method and the alternating variable method will be provided. These are both conceptually simple, though not particularly effective, and the latter provides useful background to the method of conjugate directions. The major part of the chapter will be devoted to conjugate directions and random search, two procedures which appear to have great potential for designing experiments with models of agricultural systems.

5.1 The Simplex Method

This optimization procedure, not to be confused with the simplex method of linear programming, derives its name from the fact that a moving simplex is used during the search. A simplex in an n-dimensional space is a figure having plane sides and n + 1 vertices, e.g. a triangle in the x_1 - x_2 plane. The simplex method has been used for optimization of economic systems by Meier [1967, 1969].

As an example, consider the initial triangle with equally spaced treatments, a, b and c at the three vertices in Figure 5.1. This triangle can be moved uphill by reflection or flipping over in a direction opposite the lowest vertex. Thus if evaluation of these treatments with the systems model reveals that Z_a is lower than both Z_b and Z_c then treatment a will be discarded and a new simplex formed by placing treatment d equidistant from b and c on the opposite

FIGURE 5.1



Sequence of Treatments for Simplex Design
Method in Two Factors

side of the b - c face. This new treatment is now evaluated. Supposing it is found that Z_b is less than both Z_c and Z_d, the next treatment will be placed at e. The simplex is moved up the response surface in this manner until treatment k in the vicinity of the summit has been evaluated. At this stage further search involves revolution of the triangle about the region of optimality, and the search is concluded after one such revolution.

Modifications to the basic procedure such as changing the size or shape of the simplex during the experiment have been found to increase efficiency and precision. A study by Box [1966] has indicated that the simplex method is not very satisfactory when there are more than three experimental factors, although more recently Galbraith [1978] has suggested use of this design procedure for up to eight factors.

5.2 Alternating Variable Search

The alternating variable method consists of carrying out linear optimizations with respect to each variable in turn, the sequence of linear optimization being repeated on each iteration of the search. The sequence of treatments for an experiment with two controllable factors takes the form of a contracting staircase as in Figure 5.2.

To define alternating variable search more precisely, let

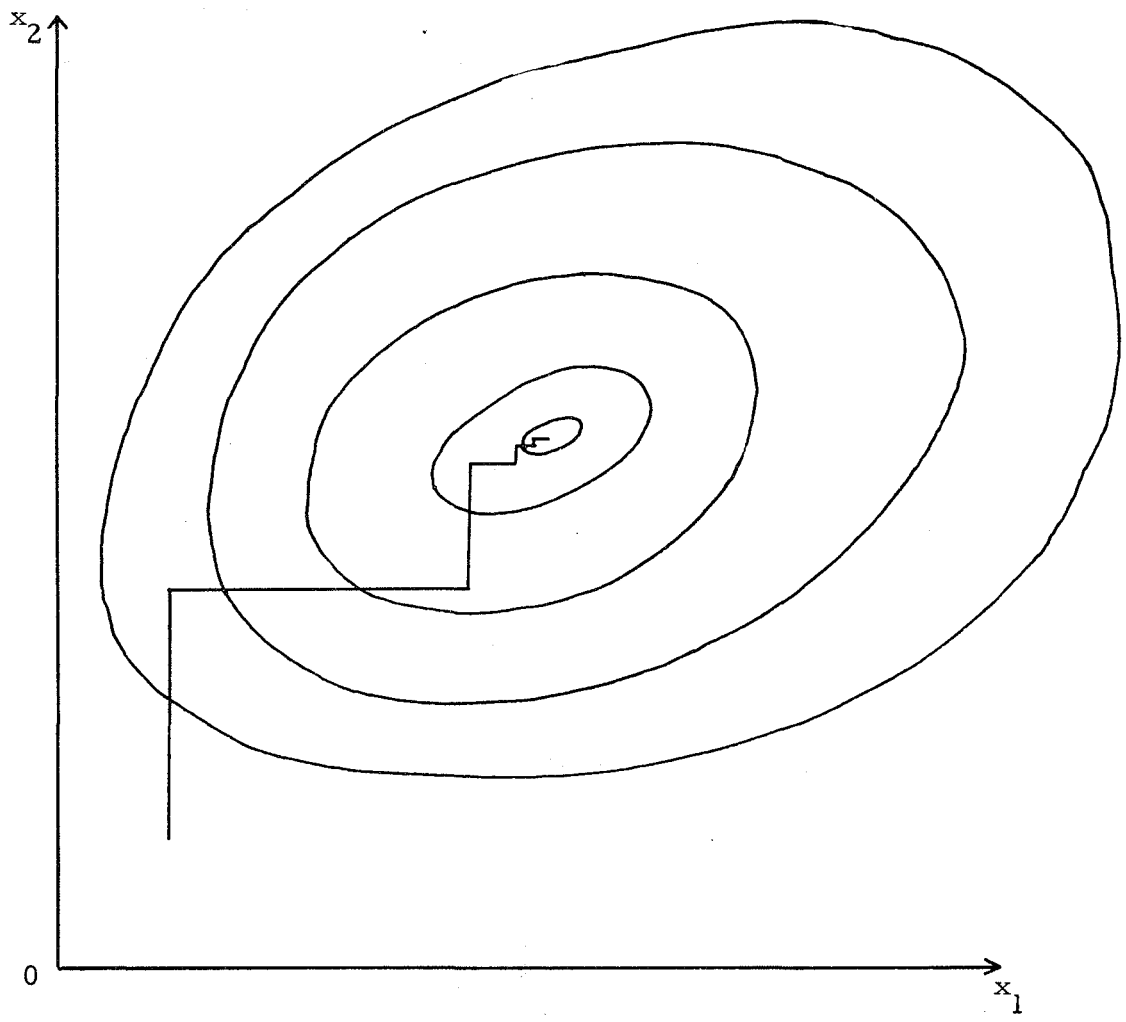
$$X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$ the policy vector; and

$$U = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad U_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$ the direction

vectors for searches parallel to the co-ordinate axes. Each search iteration involves treatments placed so as to

FIGURE 5.2

Ascent Path in Alternating Variable Search



(i) find β_1 to maximize $f(X_0 + \beta_1 U_1)$ and move to $X_1 = X_0 + \beta_1 U_1$; and

(ii) find β_2 to maximize $f(X_1 + \beta_2 U_2)$ and move to $X_2 = X_1 + \beta_2 U_2$ as the new search base X_0.

The linear optimizations may be carried out using any univariate search technique, the Powell method outlined in Chapter 3 being particularly attractive because of the low number of treatments required.

Although intuitively appealing in its simplicity, alternating variable search is not to be recommended because of slow progress or outright failure when a moderate or high degree of interaction exists between variables. Here the search is liable to become 'hung-up' on a sharp ridge which may be well below the response summit, as illustrated in Figure 5.3.

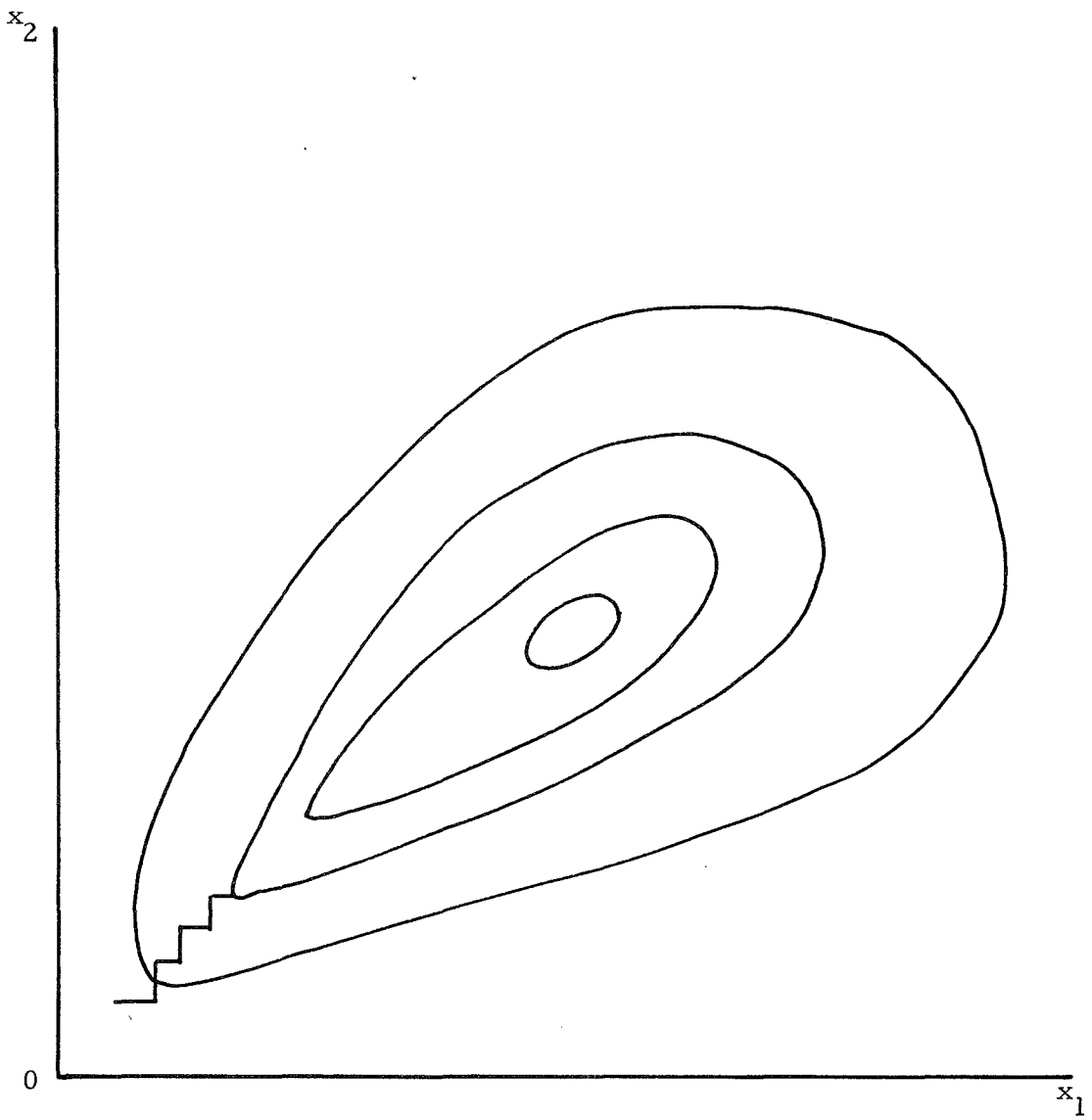
5.3 The Method of Conjugate Directions

This is a numerical procedure for finding the minimum of a function of n variables. In its current form, attributed to Powell [1964], it is highly efficient (requires few treatments) and is quite robust, working well on a variety of problems where other methods would fail. Use of conjugate directions search in connection with models of economic systems has been advocated by Emshoff and Sisson [1970] and the method has been applied to design of simulation experiments with a farm planning model by Harrison and Longworth [1977]. The Powell procedure is not intended for problems with fewer than three variables, and the following discussion will relate to the general or n-variable case, precluding diagrammatic representation.

The definition of conjugate search direction vectors rests on matrix-vector algebra similar to that introduced in Chapter 4. A quadratic form or quadratic function in n variables may be written as

FIGURE 5.3

Failure of Alternating Variable Method Due to High Interaction Between Factors



$$Z = m_0 + m_1 x_1 + m_2 x_2 + \ldots + m_n x_m$$
$$+ \tfrac{1}{2}(m_{11} x_1^2 + m_{22} x_2^2 + \ldots + m_{nn} x_n^2$$
$$+ 2m_{12} x_1 x_2 + 2m_{13} x_1 x_3 + \ldots + 2m_{n-1} m_n x_{n-1} x_n)$$
$$= m_0 + g'X + \tfrac{1}{2} X'HX$$

where $X = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$; $g = \begin{bmatrix} m_1 \\ m_2 \\ \cdot \\ \cdot \\ \cdot \\ m_n \end{bmatrix}$ the Jacobian gradient vector;

X' and g' are the transposes of X and g respectively; and

$$H = \begin{bmatrix} m_{11} & m_{12} & \cdot & \cdot & \cdot & m_{1n} \\ m_{21} & m_{22} & \cdot & \cdot & \cdot & m_{2n} \\ \cdot & & & & & \\ \cdot & & & & & \\ \cdot & & & & & \\ m_{n1} & m_{n2} & \cdot & \cdot & \cdot & m_{nn} \end{bmatrix}$$, the Hessian

matrix. Now if U_1 to U_n are the search direction vectors (initially

$$U_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \quad U_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \ldots U_n = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 1 \end{bmatrix}),$$

then any pair U_i and U_j are said to be conjugate with respect to the matrix H if

$$U_i' H U_j = 0 \quad \text{for } i \neq j.$$

The minimum of a quadratic form can be obtained by optimizing just once in each of the mutually conjugate directions. This property, known as quadratic convergence, means that the method of conjugate

directions will locate the exact minimum of a quadratic form, and with a relatively small number of treatments. Since many response surfaces can be approximated closely by a quadratic form in the region of the optimum, the method is well suited to a variety of problems.

The search begins by choosing an initial vector X then locating improved vectors in an iterative fashion where each iteration consists of a series of linear optimizations. The directions of these linear searches are U_1, U_2, . . . U_n (as indicated above) so that the first iteration of the search is identical to that of the alternating variable method. At the end of each iteration, and subject to a test criterion being fulfilled, one of the original search directions is deleted and a new direction inserted in its place. This new search direction involves simultaneous adjustments in the levels of all variables. If the response hypersurface is quadratic in form, the new search directions will be pairwise mutually conjugate.

Earlier versions of the method of conjugate directions introduced new direction vectors at every iteration. Powell noted that the search directions may become linearly dependent, leading to failure of the search, and only allowed direction vectors to be replaced when not likely to reduce search efficiency.

One iteration of the Powell method consists of the following steps:

1. For i = 1, 2, ... n find β_i to minimize $f(X_{i-1} + \beta_i U_i)$ and define $X_i = X_{i-1} + \beta_i U_i$.
2. Find the integer m, $1 \leqslant m \leqslant n$, such that $f(X_{m-1}) - f(X_m)$ is a maximum and define $\Delta = f(X_m)$.
3. Define $f_1 = f(X_0)$ and $f_2 = f(X_n)$, and obtain $f_3 = f(2X_n - X_0)$.
4. If $f_3 > f_1$ and/or
$$(f_1 - 2f_2 + f_3)(f_1 - f_2 - \Delta)^2 \geqslant \tfrac{1}{2}\Delta (f_1 - f_3)^2 ,$$

retain the search directions of this iteration and use X_n (or $2X_n - X_0$ if this results in a smaller function value)[9] as the next X_0. Otherwise,

5. Set $U = X_n - X_0$ and find β such that $f(X_n + \beta U)$ is a minimum and use $X_n + \beta U$ as the new X_o. Also, replace U_m by U in the matrix of search directions, i.e. set $(U_1, \ldots U_{m-1}, U_{m+1}, \ldots U_n, U)$ to $(U_1, U_2, \ldots U_n)$ for the next iteration.

Estimation of the β coefficient in each linear optimization uses the Powell method of univariate search as outlined in Chapter 3.[10] Step sizes for placement of treatments to fit the quadratic and for restricting the size of β to avert overstepping are based on the largest element (positive or negative) in the current direction vector.

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[9] This modification to the Powell procedure is suggested by Box et al. [1969].

[10] Powell [1964] suggests calculation of the second partial derivative for each search direction the first time that direction is used. These second derivatives are employed in subsequent linear optimizations so that only one additional treatment is required to predict the minimum. In an application to farm planning [Harrison, 1976], changes in slopes of the response hypersurface due to non-quadratic curvature and stochastic fluctuations led to large differences in curvature in the same search directions on different iterations and repeated use of initial estimates of second derivatives was found to impair search efficiency.

Various rules may be applied for terminating the search. Powell uses a very safe criterion, based on the level of precision of each variable, but this is rather expensive in terms of number of treatment evaluations.

A FORTRAN program for minimization by the method of conjugate directions is provided in Appendix V, together with computer output for a test function in three variables and brief notes on the program. The stopping rule built into this procedure is that the response does not improve (i.e. decrease) during the last iteration, or the limit imposed on number of treatments has been reached, whichever occurs first. It is to be recalled that minimization procedures may be adapted for maximization merely by negating the response criterion, i.e., giving it a minus sign.

5.4 Random Search

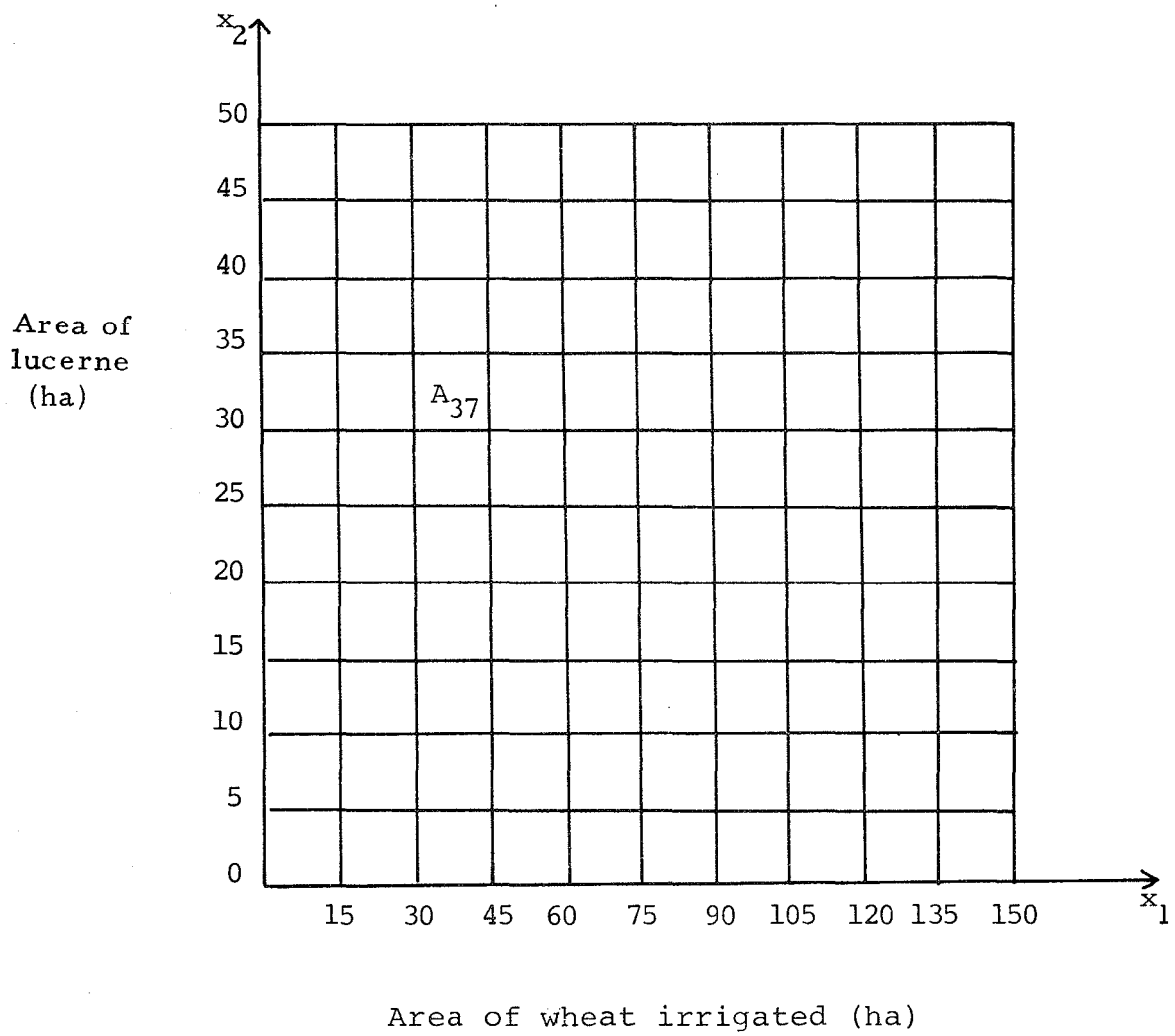
The method of random search consists basically of specifying a range of values which each variable may take, and sampling a value of each variable at random from the respective ranges to form each treatment. A pre-specified number of treatments are evaluated and the results are sorted to pick out the treatment with the optimal (highest) response value. The procedure is similar to that used for selecting farm plans in Monte Carlo programming.

A review of the many books on numerical optimization reveals little information on random search. Fletcher [1965] and Box et al. [1969] summarily dismiss the method as inefficient, and mathematicians in general appear to have a distinct leaning towards non-probabilistic methods.

The reason for this lack of interest may be illustrated by an example. Suppose there are two policy variables - the areas of wheat and lucerne - and optimal levels can be assumed to be in the ranges of zero to 150 ha and zero to 50 ha respectively. Let us split up each range into 10 sub-intervals of equal width, dividing the experimental region into a grid as in Figure 5.4. Each of the rectangles

FIGURE 5.4

Experimental Region for Two Factors Divided into a 10 x 10 Grid



in this figure may be designated as A_{ij} where the subscripts i and j refer to area sub-intervals for wheat and lucerne respectively. For example, A_{37} represents 30 to 45 ha of wheat and 30 to 35 ha of lucerne. The optimal levels of x_1 and x_2 will lie in one of the 100 rectangles, and it will be assumed that optimization consists of selecting the correct rectangle.

Let us now compare the efficiency of (i) tabulation with the full 10x10 factorial design placing one treatment in each rectangle and (ii) random search also with 100 treatments. Since the factorial design fully explores the experimental region the optimal policy will be located with certainty. On the other hand, in random search each individual rectangle (such as A_{37}) has a probability of .01 or being chosen, and a probability of .99 of not being chosen, in each selection of a treatment. In 100 treatments the probability that an individual rectangle will not be selected is $(.99)^{100}$. Thus the probability that the optimal factor combination will be selected is $1 - (.99)^{100}$ or .63. If the number of treatments were reduced to 50 then there would only be about four chances in 10 of the optimal policy being located.

Another way of measuring search efficiency is to calculate the number of treatments needed to place at least one treatment in a sub-region of given size within the experimental region, at a specified probability level. These numbers have been tabulated by Boehlje [1973] and are surprisingly large for even a substantial fraction of the overall x_1 - x_2 region. For example, 44 treatments are required to place at least one treatment in a sub-region of one tenth of the experimental region (equivalent to about one third of the range for each factor) with a probability of .99.

The above discussion reveals that random search is most inefficient, even by comparison with full factorial designs. However, by modifying the procedure to include learning and extension (explained presently) a surprising increase in efficiency can be achieved. Also, random search has a number of advantages over non-random

optimum seeking designs for management oriented systems studies:

(i) it is conceptually simple, not relying on difficult mathematics and is an easy program for a computer;

(ii) integer factor levels or policy variables such as purchase of items of farm equipment can be handled without difficulty;

(iii) policy variables may be made mutually exclusive,[11] complementary or conditionally complementary;

(iv) no matter how many policy variables are included, a solution is obtained (whereas other methods may make no progress) and this solution is usually at least reasonable; and

(v) random search copes with non-convex (including multi-modal) response hypersurfaces more successfully than alternative search procedures.

These considerations suggest that random search is greatly underrated as an experimental design procedure. The most important single development for enhancing its usefulness is the inclusion of learning mechanisms.

Random search with learning. The efficiency of random search is increased substantially by heuristic learning,[12] whereby the probabilities of selecting particular factor levels are adjusted during the experiment. Those levels which are found to produce high response early in the search have their probabilities adjusted upwards, concentrating the later part of the search on promising areas of the experimental region.

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[11] If two or more of the policy variables form a mutually exclusive subset then only one variable from this subset can take a non-zero value.

[12] Defined as learning by experience.

Various forms of probability adjustment may be used. It is necessary to define discrete values of each variable, and these may take the form of either integer values or midpoints of a number of classes or ranges. Initially equal probability weights are attached to each discrete value, i.e. sampling is carried out from uniform probability distributions. The adjustment of probabilities is facilitated by selecting weight coefficients for each discrete value which can never become negative and which are asymptotic to zero; for example, an expression of the form a^v where a is a positive constant and where v may be adjusted upwards or downwards.[13]

Random search with learning has been used in conjunction with systems models to determine optimal long-run plans for hog/corn farms in Indiana. The method originates from a dissertation by Lee [1971] and is described briefly in published reports [Eisgruber and Lee, 1971; Boehlje, 1973; Furtan and Lee 1975]. The procedure outlined here is based on Boehlje [1973] but with simplifying changes to the notation.

Suppose there are two decision variables x_i, $i = 1,2$, and each can take a number of mutually exclusive discrete values x_{ij}, $j = 1$ to n_i. Initially, for each policy variable, a choice distribution w_{ij} is defined as

$$w_{ij} = 2^{e_{ij}}$$

where e_{ij} is the learning parameter, and is initialized at a specified integer number (e.g. 3) for each value of the variable, i.e. for $i = 1$ to 2 and $j = 1$ to n_i. This defines a uniform distribution for each variable, the probabilities being

---

[13] Here $a^v > 0$ for all v and $a^v \to 0$ as $v \to -\infty$.

$$P\left(x_{1j_1}\right) = \frac{w_{1j_1}}{\sum_{j_1=1}^{n_1} w_{1j_1}}, \quad j_1 = 1 \text{ to } n_1, \text{ and}$$

$$P\left(x_{2j_2}\right) = \frac{w_{2j_2}}{\sum_{j_2=1}^{n_2} w_{2j_2}}, \quad j_2 = 1 \text{ to } n_2.$$

A uniform pseudorandom number m in the range 0 to 1 is then generated and is used to locate the s alternative value of x_1 where

$$\sum_{j_1=1}^{s-1} P(x_{1j_1}) < m \leqslant \sum_{j_1=1}^{s} P(x_{1j_1})$$

a random value of x_2 being obtained in the same manner.

The search proceeds in three stages. The first or initialization phase involves repeated sampling from these uniform distributions, the level of response being evaluated for each X set. The highest criterion value in the initialization phase is taken as a base performance or norm Z_0 against which to compare alternative policies in the learning phase. Throughout the learning phase the weights and hence probabilities of different factor levels are adjusted according to the formula

$$w_{ij_i} = 2^{e_{ij_i} + \Delta e_{ij_i}}$$

where $\Delta e_{ij_i} = \dfrac{f(x_{1j_1}, x_{2j_2}) - Z_0}{k}$

and where $f(x_{1j_1}, x_{2j_2})$ is performance under a particular treatment and k is a parameter governing rate of learning. For example, suppose Z_0 = \$20,000, k is set at 5000, and the first random selection of factor levels during the learning phase yields $j_1=3$ and $j_2=7$. Evaluation of this treatment (x_{13}, x_{27} or grid square A_{37}) reveals a farm net income of \$22,000. By the above formula

$$\Delta e_{13} \text{ and } \Delta e_{27} = \frac{22000 - 20000}{5000} = .4$$

and hence

$$w_{1,3} = 2^{3+.4} \quad \text{and} \quad w_{2,7} = 2^{3+.4}$$

New probability distributions are obtained for each factor in which one weight is adjusted as above and all other weights remain unaltered. The effect of these calculations would be to increase slightly the probability associated with the third wheat area and seventh lucerne area with corresponding reductions to remaining probabilities. The weights and probabilities for each value of each factor are recomputed before the next treatment is selected.

The learning phase is continued for a fixed number of treatments, producing distributions for each variable which may be quite non-uniform and skewed. The rate of learning or value of k is a critical consideration, and must be chosen to suit the particular problem. If the adjustment of probabilities is too slow, then the search will be inefficient and unduly costly. On the other hand, rapid adjustment may lock the search into a local optimum rather than seeking out a global optimum; i.e. too fast learning means jumping to conclusions.

In the final sampling stage the probability distributions are locked in and a set number of treatments are evaluated. The treatment resulting in the highest criterion value is selected as the optimal policy.

The number of treatments in each of the three stages also has an important bearing on efficiency of the search. These numbers,

and the learning rate parameter, can only be decided after carrying out trial searches with the systems model.

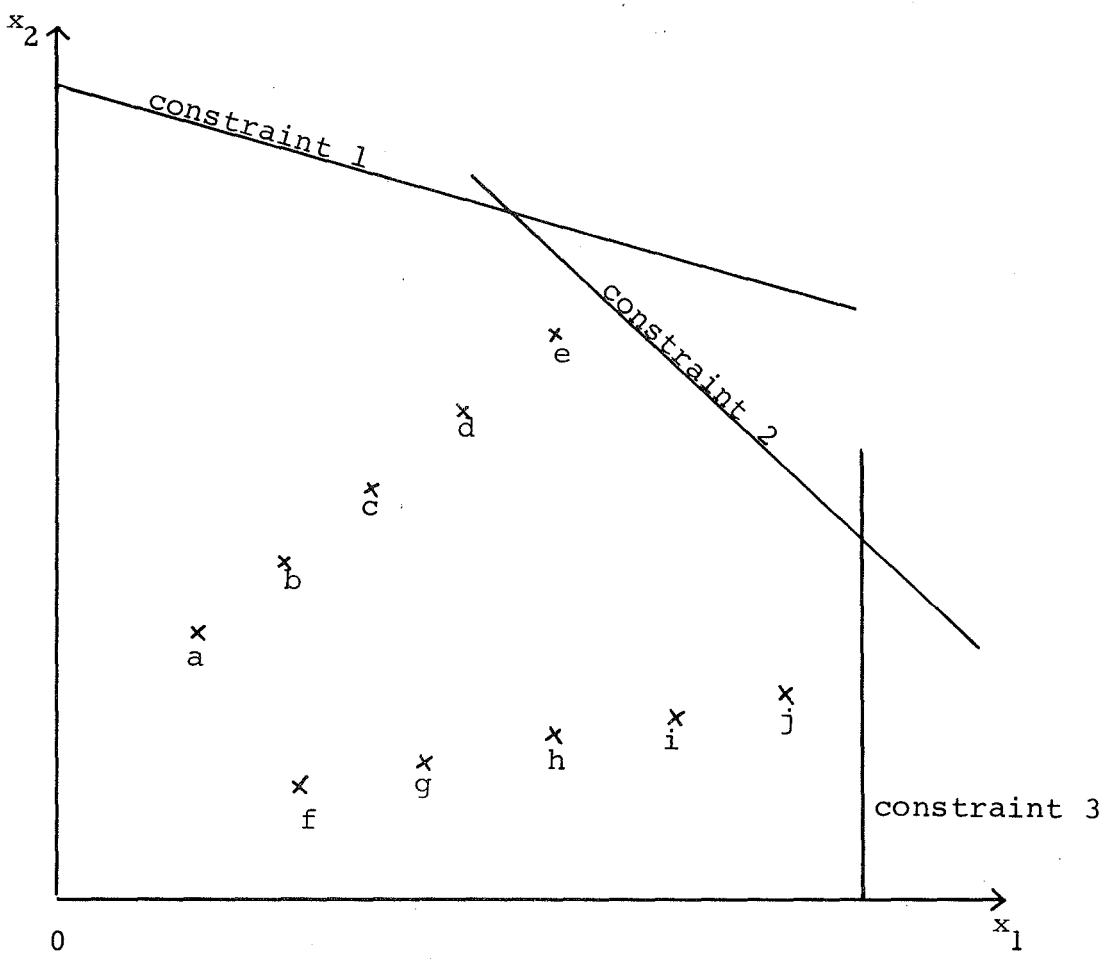
A FORTRAN program for random search with learning together with output from a test problem are provided as Appendix VI.

Extension or hill-climbing. This is a further modification to random search which concentrates treatments in promising areas of the experimental region. The extension procedure was developed originally for use in Monte Carlo programming, e.g. see Carlsson et al. [1969]. Basically, it involves systematically forming new treatments from those selected at random by increasing the level of each factor or policy variable in the direction of the constraint boundaries. The variables are adjusted by fixed increments at each step, and the sequence of new treatments is terminated when either the supply of a resource is exhausted or the response criterion decreases. This modification is useful for resource allocation problems where a solution in the interior of the experimental region or decision space is clearly inferior to a solution on the boundary of the constraint set.

The concept of extension or hill-climbing is illustrated with respect to a two factor experiment in Figure 5.5. Treatment a represents a randomly selected pair of values for x_1 and x_2. Another random number is obtained to indicate the ratios by which the variables will be adjusted; for example, if the number is .33 then x_1 and x_2 will be incremented in the ratio 1:2, successive treatments being placed at b, c, d and e. Treatment f is then selected at random, and another random adjustment factor is obtained leading to treatments g to j. The extension procedure has not been included in the computer program of Appendix VI.

FIGURE 5.5

Hill-Climbing or Extension with Random Search



5.5 Summary

Some of the more useful design procedures for optimization experiments with agricultural systems models have been introduced in this chapter. Included are the highly efficient and robust method of conjugate directions and the method of random-search-with-learning which has important advantages for some farm management applications. The problem of constraining treatments according to resource supplies has been briefly alluded to, and this and other aspects of the practical application of optimum-seeking designs will be discussed in the next and final chapter.

CHAPTER 6

RELATED ISSUES AND CONCLUDING COMMENTS

The problems of applying optimum-seeking designs to situations of multi-modal response surfaces, stochastic variation in response and resource constraints on factor levels are examined in this chapter. Also, the use of numerical optimization routines for tuning or parameter estimation during model construction is discussed briefly. The chapter concludes with comments on the choice of design procedure and suggestions for further reading.

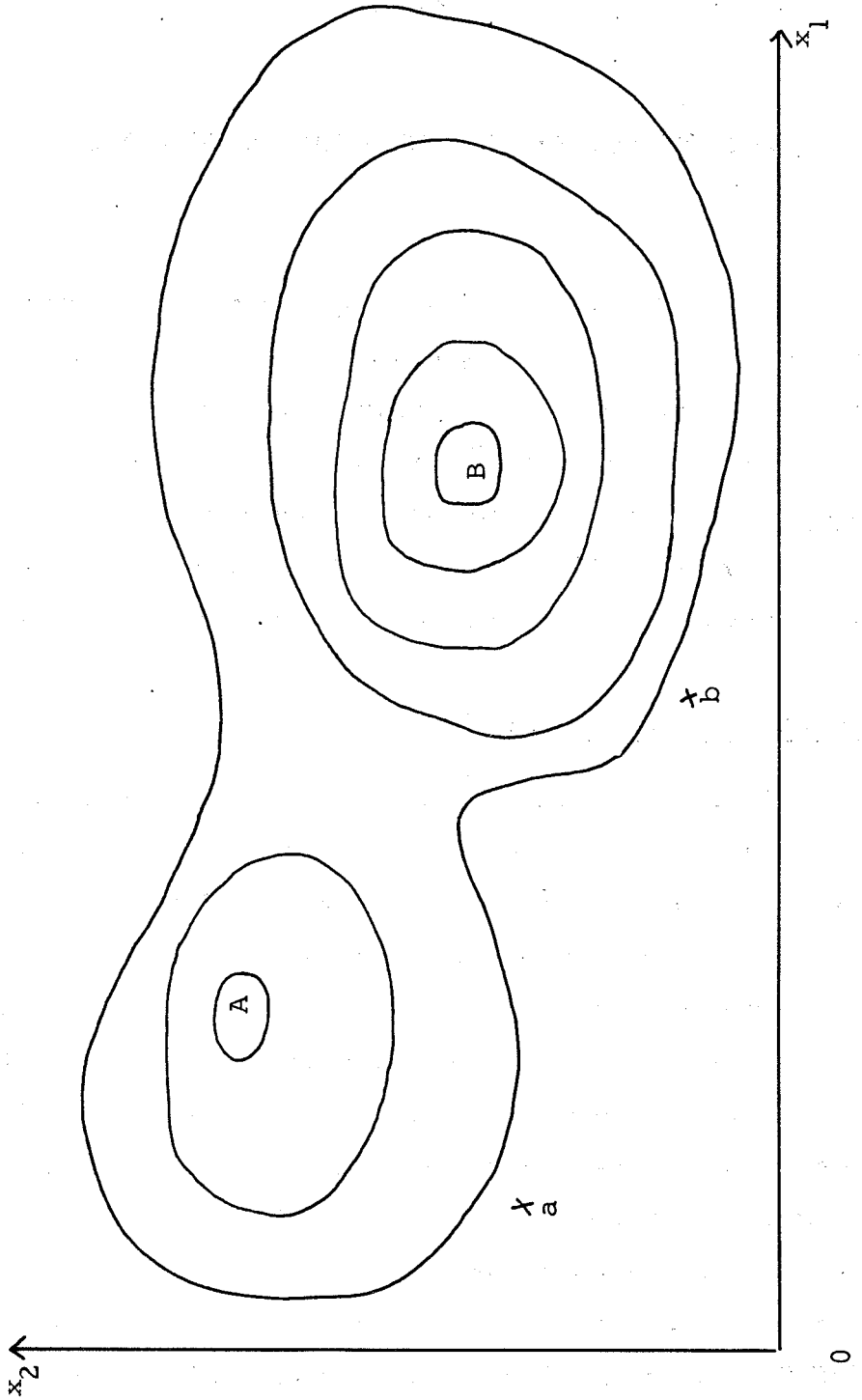
6.1 Multi-modal Response Surfaces

The discussion of search procedures has been confined mainly to response surfaces (or hypersurfaces) with unique optima. However, in practice several optima often will exist. Figure 6.1 depicts a response surface with two optimal regions, A and B. B has the higher response value and is therefore the global optimum, while A is a local optimum. A hill-climbing search, if effective, would converge to one of these regions, the peak located depending on the slope of the surface in the vicinity of the initial treatment. If the initial guess was point a then local optimum A would be located; whereas, a search originating from b would terminate on the true optimum B. As previously noted, random search is to some extent capable of discerning between local and global optima provided the rate of learning is not too great.

An experimental region in two or more factors may contain a large number of local optima, but of course only one global optimum. In general it cannot be guaranteed that the initial guess will be sufficiently good that the search will converge towards this global optimum;

FIGURE 6.1

Bimodal Response Surface



hence it is advisable to carry out a number of optimum-seeking experiments using different initial treatments, at least during familiarization with a systems model. If these searches terminate on dissimilar policies then either the response surface is not 'well-behaved' or the optimization procedure has not functioned satisfactorily, and either case warrants further investigation.

6.2 Stochastic Variation and Extent of Replication

If the systems model is stochastic then evaluation of only one replicate for each treatment would lead to an erratic search, the contours of the response surface being blurred by random variation in performance. This problem may be overcome by evaluating a number of replicates for each treatment. If a criterion based on the outcome over all replicates - such as mean net income - is adopted, then response values will be less affected by random influences.[14]

The appropriate sample size in terms of number of replicates is rather difficult to determine. Some guidance may be obtained from classical statistical theory which holds that the sample size required to estimate a population mean with an error of not more than E at the 100 $(1 - \alpha)$ per cent confidence level is given by the smallest n satisfying

$$n \geqslant \frac{z_{\alpha/2}^{2} s^{2}}{E}$$

where $z_{\alpha/2}$ is the standard normal variate (tabulated in most statistics textbooks). Here s is the estimated standard deviation of the performance criterion, which may be obtained by evaluating a small number of replicates (say 20) of a representative treatment.

---

[14] Variance of mean response is smaller than that of individual replicates by the factor of square root of number of replicates i.e. $\text{Var}(\bar{Z}) = \text{Var}(Z)/\sqrt{n}$.

In practice this approach is usually of limited value because the number of replicates is restricted by availability of computing funds. In any case the objective of the experiments is normally the ranking of alternative treatments or management policies rather than precise estimation of response, and this may reduce the extent of replication required. Also the classical approach does not take account of variance reduction through blocking of replicates for each treatment. As a general rule it is suggested that the number of replicates for optimum-seeking experiments need not be more than 30, and that as few as 5 or 10 will sometimes be adequate. Even these numbers exceed the extent of replication normally regarded as acceptable in real agricultural experiments.

6.3 Dealing with Constraints

The values taken by policy variables frequently will be restricted by non-negativity and resource constraints. Non-negativity constraints take the form

$$x_j \geqslant 0 \qquad \text{for} \qquad j = 1 \text{ to } n.$$

For example, it is not possible to grow a negative area of irrigated wheat or lucerne. With the exception of random search (where ranges are placed on factor levels) the procedures outlined earlier may converge on policies for which some of the x_j are negative, even though such policies are absurd and can cause the systems model to behave unpredictably. In models of systems at a high level of aggregation, such as the farm-firm, levels of policy variables may also be constrained by limited supplies of land, labour and capital, and through crop rotation and other husbandry considerations. Such constraints are less direct, and tend to act on the variable factors collectively rather than individually. For example, if the combined area of wheat and lucerne under irrigation is limited by water availability then an increase in the area of lucerne necessitates a reduction in the area of wheat. This introduces negative interaction between factors (the response contours being ellipsodial with principal axes running downwards and to the right) and may render 'hill-climbing' more difficult.

Non-negativity and resource constraints may be taken into account through use of constrained optimization techniques (such as linear programming) but these may place unacceptable rigidity on the structure of the model. Quite often optimum-seeking designs may be used in conjunction with the systems approach if relatively minor modifications are made to the model. One such modification is the barrier penalty function or penalty charge on infeasible factor levels. For example, if the x_j are to take only non-negative values than the response criterion may be altered from Z to Z-P where

$$P = \sum_{j=1}^{h} k_j (\min(0, x_j))^2$$

and the k_j are positive penalty function coefficients. Here, if any x_j is negative then an artificial cost of $k_j x_j^2$ is incurred, the magnitude of which depends on the setting of k_j. Small values (of the order of 0.1) are desirable as this prevents creation of steep valleys at the edge of the response hypersurface and distortion of the search away from near-zero factor levels.

A similar device may be used for constraining upper levels of factors of policy variables to take account of limited resource supplies, e.g. see Harrison [1976: 205]. A complication which arises with stochastic multi-period models is that constraint boundaries may vary over time, e.g. when cash receipts and hence finance for expenditure in later years depends on wheat prices in early years. In this case feasible (and optimal) policies may differ between replicates, and the magnitudes of penalty function coefficients will determine whether a consistently feasible policy or an opportunistic and more profitable (though sometimes infeasible) policy is selected.

6.4 Parameter Identification or Model Tuning

Numerical search methods have an important application, quite apart from design of simulation experiments, for estimating parameters of functional relationships during construction of systems models.

While statistical inference techniques such as regression analysis are to be preferred for establishing relationships because they provide measures of precision as well as estimates of parameter values, the complexity of the hypothesized relationship may preclude use of statistical analysis. Numerical search then provides a systematic alternative to trial and error for fine-tuning of the model.

Suppose the researcher has historical records of output V and of a number of causal variables Y for some particular relationship or submodel, and hypothesizes a complex relationship between them. Output is then a function of the set of parameters in the relationship, represented by the vector A, i.e. $V = f(A)$. A search over the region of possible parameter values is carried out with an optimum-seeking method to minimize the sum of squares of prediction errors, $\sum(V - f(A))^2$. Each treatment of the search is a different parameter set A, and the submodel is used to evaluate the response criterion V. For example, when constructing the farm planning model we may have measurements of available soil moisture and of rainfall, irrigation, temperature and windspeed. A submodel relating soil moisture to rainfall and other environmental variables is hypothesized, and parameter values for this relationship which best explain observed soil moisture are estimated by numerical optimization. Further discussion of parameter estimation by numerical search procedures is provided by Emshoff and Sisson [1970], while applications in agricultural modelling are discussed by Stol [1975], Harrison [1976], Highland et al. [1976] and Galbraith [1978].

6.5 Choice of Search Method

The choice of a suitable experimental design for determining optimal factor levels (or optimal parameter values) is not clear-cut, and will depend on the nature of the systems model, number and type of controllable factors and availability of computer packages for optimization. For experiments involving three or less factors it is

probable that a simultaneous design or tabulation method such as the full factorial or central composite design will be adequate. Where optimal policies are sought with respect to a larger number of factors, cost considerations may dictate use of an optimum-seeking design. Comparisons between numerical optimization methods may be made in terms of the number of function evaluations or treatments needed to find the optimum of a given test problem. It must be recognized that results of such comparisons are not independent of the test problem selected or of settings on the search parameters. A comparative study by Fletcher [1965] indicated that tabulation methods, random search (without learning) and the alternating variable method are very inefficient, and that conjugate directions is one of the most efficient procedures.

Selection of an appropriate design procedure can also be guided by an examination of the characteristics of the optimization problem, and on this basis the British Atomic Energy Research Establishment (A.E.R.E.) had devised a sequential elimination procedure or key to choice of method [Hooper, 1973].

A number of comments may be made concerning choice between the five methods for which computer programs are provided in this Report.[15]

Method 1 : Univariate Optimization:

This is a relatively precise and efficient method of univariate search. It has been found useful at Lincoln College for estimating depreciation rates to explain current market values on different classes of farm machinery [Davey, 1977] and for determining the internal rate of return in project evaluation [Gale and Harrison, 1977]. Typically, seven to ten treatments are required to locate the optimum.

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[15] Other sources of computer programs for numerical optimization include the A.E.R.E. subroutine library (available to outside users for a modest charge [Hooper, 1973]) and the FORTRAN listings published by Keuster and Mize [1973].

Method 2 : Basic Steepest Ascent:

The steepest ascent procedure for multivariate optimization is very simple and may locate acceptable near-optimal combinations of factor levels for a small number of non-interacting factors. The number of treatments required is relatively low.

Method 3 : Refined Steepest Ascent:

Steepest ascent with linear optimization and non-linear local exploration is more precise than method 2, and generates additional information on the shape of the response surface in the region of the optimum. A problem which sometimes arises is that the stationary point located by non-linear exploration is not a maximum; this is most likely to occur if mid-game tactics do not converge sufficiently close to the optimal policy.[16] A moderately large number of treatments may be required with this method.[17]

Method 4 : Conjugate Directions:

The method of conjugate directions is efficient, robust and (like 3) quadratically convergent. It will not terminate on a saddle point but occasionally fails to introduce new search directions, thus deteriorating to an alternating variable search. The number of treatments is approximately the same as for method 3.

---

[16] The stationary point is a saddle point (or minimum) if the Hessian matrix is not negative definite, and this is indicated in the printout from the program.

[17] The number of treatments will be approximately $(n+3)i$ for linear optimizations plus $n(1+\frac{n-1}{2})$ for non-linear local exploration, where n is the number of variables and i is the number of iterations of mid-game tactics.

Method 5 : Random Search with Learning:

Work at Purdue University suggests that random search with learning is a much under-rated procedure. The reduction in number of treatments because optimization experiments do not have to be carried out from different starting points may make this the most suitable method for problems involving irregularly shaped response surfaces. Random search also has the capacity to handle a large number of experimental variables though the reliability of estimated optima in such cases is difficult to ascertain. The number of treatments in each of the three phases of the search is set by the user, and requires trade-off between precision and cost.

Of the search procedures not considered in this Report, the most important are the Quasi-Newton Methods [Broyden, 1972]. These are non-linear gradient methods of minimization, utilizing continually updated positive definite approximations to the Hessian matrix, and can only be explained with rather advanced mathematics. Quasi-Newton methods are highly efficient when they work (more so than any of the methods outlined in this Report), but they are subject to failure in certain applications.

The possibility also exists of using a combination of procedures within a single optimization experiment, switching from one to the other during the search. In this way, procedures with rapid convergence near the optimum, such as the Quasi-Newton methods, may be used for finishing off the search. Also, the combination of factor levels indicated as optimal from one simulation experiment may be used as the initial treatment for a further search, perhaps using a different method.

Some authors suggest that numerical optimization can be successful with respect to as many as 100 variables. However, one should be cautious about the reliability and cost of optimum-seeking designs for simulation experiments with large complex agricultural systems models containing more than about 10 to 15 policy variables.

6.6 Suggested Reading

A large number of books and articles dealing with numerical optimization are listed in the bibliography following this chapter. Highly recommended reading at an introductory level are the monograph of Box et al. [1969] and books by Adby and Demster [1974], Brent [1973] and Wilde [1964]. The more mathematically inclined may find Otega and Rheinboldt [1970] and Daniel [1971] and Polak [1971] of interest. Between these two extremes and giving a comprehensive coverage of the procedures are the works of Beveridge and Schecter [1970], Cooper and Steinberg [1970], Jacoby, Kowalik and Pizzo [1972], Walsh [1975] and many others. The above literature is orientated towards solving problems in mathematics and engineering. Although the procedures are readily transferable to design of simulation experiments, relatively little has been written in this context. The books of Naylor et al. [1966, 1968, 1971] discuss experiments with economic systems models but in the main limit attention to traditional designs. The survey article by Boehlje [1973] discusses agricultural applications with particular emphasis on random search.

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APPENDIX I

INTRODUCTION TO THE COMPUTER PROGRAMS

The five computer programs for optimum-seeking experimental designs are presented in Appendix II through to VI. These programs are written in FORTRAN for a Burroughs B6700 computer but are designed for ease of adaption to other makes of machine. The operating system under which the programs were developed has unusual features with respect to line spacing control and loss of constants (but not arrays) in subroutines on return to the main program, and these are overcome by adding dummy WRITE statements and COMMON statements respectively. Each optimization procedure has been programmed as

(i) a main program containing a test function which is to be optimized and a subroutine call statement. In agricultural systems applications the systems model would replace the test function.

(ii) a subroutine which generates a new set of factor levels (i.e. a new treatment) every time it is called.

The programs are currently designed to allow a maximum of 10 experimental factors, although this limit can be relaxed by revising the DIMENSION statements. The initial guess or first treatment is specified in a DATA statement in the main program, as is an upper limit on the number of treatments to avoid excessive use of computer time.

The FORTRAN subroutines for each of the five optimization procedures follow the same general layout, and this is illustrated in Figure I-1 for the method of steepest ascent. The subroutine initially reserves space for arrays (in a DIMENSION statement), specifies search parameters (as DATA), makes type declarations (INTEGER and REAL)

and indicates which constants and arrays are common to the main program and subroutine (or are to be retained in the subroutine between successive calls). The first time the subroutine is entered a number of initial conditions are established. At the heart of the layout in Figure I-1 is a branching (GO TO) statement conferring control to different segments of the subroutine depending on the value of a test criterion, ITEST. Each segment carries out a specific part of the search and ends with a RETURN to the main program where the treatments are evaluated. Branching to a given segment is repeated for a number of treatments, until that particular phase of the search iteration is completed, e.g. control returns to the segment placing treatments in the direction of steepest ascent until response falls relative to the previous treatment.

FIGURE I-1

Layout of the Steepest Ascent Subroutine

```
      Type statements (REAL and INTEGER), DIMENSION, COMMON, DATA.
      IF (ITREAT.GT.1) GO TO 2
      .
      .
      . Initial conditions
      .
      .
 2    GO TO (30, 40, 50), ITEST
      .
      .
      . Es tablish slopes of the tangent hyperplane
      .
      .
      ITEST = 1
      RETURN
30    . . . . .
      .
      .
      . Step in the direction of steepest ascent
      .
      .
      .
      ITEST = 2
      RETURN
40    . . . . .
      . Take a step backwards, or reduce step size
      .
      .
      .
      ITEST = 3
      RETURN
50    . . . . .
      .
      . Terminate search
      .
      .
      .
      RETURN
      END
```

None of the programs contain READ statements, all information for the search being defined in the DATA statements. The interpretation of these data is explained in the following appendices. Output of results is formated with row rather than column headings to avoid confusion with any other information from the experiment which the user may wish to have printed.

The test functions (surrogates for the systems model) are simple polynomials with known optima. The function for univariate minimization (Appendix II) is

$$Z = x^4 + 3$$

which has a <u>minimum</u> value of $Z = 3$ at $x = 0$. The function for multivariate search is

$$Z = (x_1 - 2x_2)^2 + (x_2 - 2x_3)^2 + (3x_1 - 2x_3)^2 - 2x_1 + x_2 - 3x_3 + 10$$

which has a <u>minimum</u> of $Z = 9.2813$ at $x = \begin{bmatrix} .3439 \\ .2344 \\ .3281 \end{bmatrix}$.

To facilitate maximization the sign of Z is changed from positive to negative when using the methods of steepest ascent (Appendix III and IV) and random search with learning (Appendix VI).

The five subroutines are designed for coupling to the program of systems model with little or no reprogramming. However, the initial factor levels and search parameters as defined in DATA statements would need to be adjusted on a trial-and-error basis to determine settings most appropriate to the particular application.

APPENDIX II

UNIVARIATE SEARCH

This program minimizes a 'function' in one variable by repeated quadratic interpolation. Each interpolation follows the Powell method outlined in Chapter 3. However, stepping is continued until three treatments a, b and c bracket the value of X for which Z is a minimum, removing the need for the sufficiency test on the stationary point and for limiting the extent of adjustment in the direction of the minimum.

The parameters in the listing of this program have the following meanings:

Main program

TMAX = maximum number of treatments before the search must terminate (here 15).

X = initial factor level (here 10.0).

Subroutine

D = initial step size (here 3.0)

NRED = number of reductions on step size (here 1),

SRED = extent of reduction in step size. (Here SRED = 6 so L is reduced to 3/6 or 0.5 for the second quadratic interpolation).

The listings of the main program and subroutine and the search output follow. In this case six treatments are needed before the minimum is bracketed, and the first iteration is completed with a quadratic interpolation leading to treatment no. 7. The search terminates after 10 treatments with X = -.0556 and Z equal to the target value of 3.0 correct to at least four decimal places.

B6700 F O R T R A N C O M P I L A T I O N M A R K 2.9.190

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U N I V
= = = =

```
FILE  5=FILE5,UNIT=READER

FILE  6=FILE6,UNIT=PRINTER


      INTEGER TMAX
      COMMON XO,A,B,C,ZA,ZB,ZC,ITEST,ITN,STEP
      DATA IN/5/,IO/6/,X/10./,TMAX/15/
      ITREAT = 0
1     ITREAT = ITREAT + 1
      Z = X**4 + 3.
      CALL OPT1(ITREAT,TMAX,X,Z)
      IF (ITREAT.LT.TMAX) GO TO 1
      STOP
      END
```

```
      SUBROUTINE OPT1(ITREAT,TMAX,X,Z)
      REAL NUM
      INTEGER TMAX
      COMMON XO,A,B,C,ZA,ZB,ZC,ITEST,ITN,STEP
      DATA IO/6/, D/3./, NRED/1/, SRED/6./
      IF (ITREAT.EQ.1) WRITE (IO,8)
8     FORMAT (1X,'INITIAL ESTIMATE'/)
      WRITE (IO,10) ITREAT,X,Z
10    FORMAT (3X, 'TREATMENT NO',I3,7X,'X =',F12.4,7X,'Z =',F12.4/)
      IF (ITREAT.GT.1) GO TO 18
      ITEST = 0
      ITN = 0
18    GO TO (20,30,40), ITEST
      ITN = ITN + 1
      WRITE (IO,12) ITN
12    FORMAT (1X,'ITERATION NUMBER',I2/)
      XO = X
      A = 0.
      ZA = Z
      B = D
      X = X + B
      ITEST = 1
      RETURN
C
20    IF (Z.GT.ZA) GO TO 22
      STEP = D
      ZB = Z
      GO TO 24
22    STEP = 0. - D
      TEMP = B
      B = A
      A = TEMP
      ZB = ZA
      ZA = Z
24    ITEST = 2
      C = B + STEP
      X = XO + C
      RETURN
C
30    ZC = Z
      IF (ZC.LT.ZB) GO TO 32
C  MINIMUM BRACKETED BY A AND C. CALCULATE OPTIMAL STEP SIZE
      NUM = (B*B-C*C)*ZA + (C*C-A*A)*ZB + (A*A-B*B)*ZC
      DEN = 2. * ((B-C)*ZA + (C-A)*ZB + (A-B)*ZC)
      BETA = NUM / DEN
      X = XO + BETA
      D = D / SRED
      NRED = NRED - 1
      ITEST = 0
      IF (NRED.LT.0) ITEST = 3
      RETURN
C
C  MINIMUM NOT BRACKETED. TAKE A FURTHER STEP
32    A = B
      ZA = ZB
      B = C
      ZB = ZC
      C = B + STEP
      X = XO + C
      RETURN
C
40    ITREAT = TMAX
      RETURN
      END
```

INITIAL ESTIMATE

TREATMENT NO 1	X =	10.0000	Z =	10003.0000

ITERATION NUMBER 1

TREATMENT NO 2	X =	13.0000	Z =	28564.0000
TREATMENT NO 3	X =	7.0000	Z =	2404.0000
TREATMENT NO 4	X =	4.0000	Z =	259.0000
TREATMENT NO 5	X =	1.0000	Z =	4.0000
TREATMENT NO 6	X =	-2.0000	Z =	19.0000
TREATMENT NO 7	X =	-0.3333	Z =	3.0123

ITERATION NUMBER 2

TREATMENT NO 8	X =	0.1667	Z =	3.0008
TREATMENT NO 9	X =	0.6667	Z =	3.1975
TREATMENT NO 10	X =	-0.0556	Z =	3.0000

APPENDIX III

BASIC STEEPEST ASCENT

This program follows the procedure outlined in Chapter 4. The parameters as listed in the DATA statements have the following interpretations:

Main program

X = initial treatment, i.e. initial levels of the three experimental factors, here $\begin{bmatrix} 5.0 \\ -8.0 \\ 10.0 \end{bmatrix}$

TMAX = maximum number of treatments before the search must terminate (here 40).

Subroutine

NVAR = number of factors (here 3),

S(1), S(2), S(3) = size of forward differences for variables 1 to 3, here all 0.1.

L = step size parameter (here 2.0).

NRED = number of reductions in step size during the search (here 1).

SRED = extent of reduction in step size. (Here L is divided by 5.)

The experiment with the test function proceeds through three iterations, terminating because no further progress is possible, even with a reduced step size, on the 24th treatment. (The jump in treatment numbering from 23 to 40 is associated with the stopping procedure.) Final factor levels are all within 0.7 of the optimal values as indicated in Appendix I, although the response level of -18.49 is some distance from the maximum of -10.

100.

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S T A S
= = = =

```
FILE  5=FILE5,UNIT=READER

FILE  6=FILE6,UNIT=PRINTER


      INTEGER TMAX
      DIMENSION X(10)
      COMMON X
     1 ,IVAR,ITEST,ISTEP,ZL,DEN,ITN
      DATA IN/5/,IO/6/
      DATA X(1)/5./,X(2)/-8./,X(3)/10./,TMAX/40/
      ITREAT = 0
1     ITREAT = ITREAT + 1
      Z = (X(1)-2.*X(2))**2 + (X(2)-3.*X(3))**2 + (3.*X(1)-2.*X(3))**2
     1 - 2.*X(1) + X(2) - 3.*X(3) + 10.
      Z = -Z
      CALL OPT2(ITREAT,TMAX,Z)
      IF (ITREAT.LT.TMAX) GO TO 1
      STOP
      END
```

```
C  SUBROUTINE TO MAXIMIZE A FUNCTION OF SEVERAL VARIABLES USING THE
C  METHOD OF STEEPEST ASCENT

      SUBROUTINE OPT2(ITREAT,TMAX,Z)
      INTEGER TMAX
      REAL M,L
      DIMENSION X(10),S(10),M(10),D(10)
      COMMON X
     1 ,IVAR,ITEST,ISTEP,ZL,DEN,ITN
      DATA NVAR/3/,S(1)/.1/,S(2)/.1/,S(3)/.1/,L/2./,NRED/1/,SRED/5./,
     1 IO/6/
      IF (ITREAT.EQ.1) WRITE (IO,4)
4     FORMAT (1X,'INITIAL ESTIMATE'/)
      WRITE (IO,6) ITREAT,Z,(X(J),J=1,NVAR)
6     FORMAT (3X,'TREATMENT NO',I3,4X,'Z =',F10.4,4X,'X VALUES:',6F10.4/
     1 3X,4F10.4/)
      IF (ITREAT.GT.1) GO TO 2
      ITEST = 0
      IVAR = 0
      ITN = 1
      WRITE (IO,9) ITN
9     FORMAT (/1X,'ITERATION NO',I2/)
      ZL = Z
2     GO TO (30,40,50), ITEST
      IF (IVAR.EQ.0) GO TO 22
C  DERIVE EQUATION TO TANGENT HYPERPLANE
      M(IVAR) = (Z-ZL) / S(IVAR)
      X(IVAR) = X(IVAR) - S(IVAR)
      WRITE (IO,13) Z,ZL,M(IVAR)
13    FORMAT (3X,'CURRENT Z VALUE =',F15.4, 8X,'BASE Z VALUE =',F15.4,
     1 8X,'SLOPE =',F15.4)
22    IVAR = IVAR + 1
      X(IVAR) = X(IVAR) + S(IVAR)
      IF (IVAR.EQ.NVAR) ITEST = 1
      WRITE (IO,12) IVAR,S(IVAR),X(IVAR)
12    FORMAT (3X,'VARIABLE',I3,' FORWARD DIFFERENCED BY ', F9.4,' TO',
     1 F10.4)
      RETURN
C
C  DETERMINE DIRECTION OF STEEPEST ASCENT
30    M(NVAR) = (Z-ZL) / S(NVAR)
      WRITE (IO,13) Z,ZL,M(IVAR)
      X(NVAR) = X(NVAR) - S(NVAR)
      SSQ = M(1)*M(1)
      DO 32 IVAR=2,NVAR
32    SSQ = SSQ + M(IVAR)*M(IVAR)
      DEN = SQRT(SSQ)
38    ISTEP = 0
C  STEP IN STEEPEST ASCENT DIRECTION
      DO 34 IVAR=1,NVAR
34    D(IVAR) = M(IVAR) / DEN * L
      WRITE (IO,14) (D(J),J=1,NVAR)
14    FORMAT (3X,'ADJUSTMENTS TO X VALUES:',8F9.4)
36    ISTEP = ISTEP + 1
      WRITE (IO,15) ISTEP
15    FORMAT (3X,'STEP NO',I3)
      DO 35 IVAR=1,NVAR
35    X(IVAR) = X(IVAR) + D(IVAR)
      ZL = Z
      ITEST = 2
      RETURN
```

```
   CONTINUE
   IF (Z.GT.ZL) GO TO 36
   ISTEP = ISTEP - 1
   WRITE (IO,16) ISTEP
   FORMAT (3X,'X VALUES AT STEP',I2,1X,'TAKEN AS NEW SEARCH BASE')
FUNCTION VALUE DECREASING. STEP BACKWARDS
   Z = ZL
   DO 42 IVAR=1,NVAR
   X(IVAR) = X(IVAR) - D(IVAR)
   IF (ISTEP.GT.1) GO TO 44
FUNCTION HAS DECREASED ON FIRST STEP
   IF (NRED.GT.0) GO TO 46
   ITREAT = TMAX - 1
   ITEST = 3
   RETURN

REDUCE STEP SIZE
   L = L / SRED
   NRED = NRED - 1
   WRITE (IO,19) L
   FORMAT (3X,'STEP SIZE PARAMETER REDUCED TO',F10.4)
   GO TO 38
   IVAR = 1
   ITN = ITN + 1
   WRITE (IO,9) ITN
   X(IVAR) = X(IVAR) + S(IVAR)
   WRITE (IO,12) IVAR,S(IVAR),X(IVAR)
   ITEST = 0
   RETURN

   ITREAT = TMAX
   RETURN
   END
```

```
INITIAL ESTIMATE

  TREATMENT NO  1     Z =-1872.0000     X VALUES:     5.0000    -8.0000    10.0000

ITERATION NO 1

  VARIABLE  1 FORWARD DIFFERENCED BY     0.1000 TO     5.1000
  TREATMENT NO  2     Z =-1873.1000     X VALUES:     5.1000    -8.0000    10.0000
  CURRENT Z VALUE =      -1873.1000        BASE Z VALUE =      -1872.0000          SLOPE =      -11.0000
  VARIABLE  2 FORWARD DIFFERENCED BY     0.1000 TO    -7.9000
  TREATMENT NO  3     Z =-1856.1500     X VALUES:     5.0000    -7.9000    10.0000
  CURRENT Z VALUE =      -1856.1500        BASE Z VALUE =      -1872.0000          SLOPE =      158.5000
  VARIABLE  3 FORWARD DIFFERENCED BY     0.1000 TO    10.1000
  TREATMENT NO  4     Z =-1896.6300     X VALUES:     5.0000    -8.0000    10.1000
  CURRENT Z VALUE =      -1896.6300        BASE Z VALUE =      -1872.0000          SLOPE =      -246.3000
  ADJUSTMENTS TO X VALUES:  -0.0751   1.0815  -1.6807
  STEP NO  1
  TREATMENT NO  5     Z =-1339.8638     X VALUES:     4.9249    -6.9185     8.3193
  STEP NO  2
  TREATMENT NO  6     Z = -912.4123     X VALUES:     4.8499    -5.8369     6.6387
  STEP NO  3
  TREATMENT NO  7     Z = -589.6455     X VALUES:     4.7748    -4.7554     4.9580
  STEP NO  4
  TREATMENT NO  8     Z = -371.5634     X VALUES:     4.6998    -3.6738     3.2774
  STEP NO  5
  TREATMENT NO  9     Z = -258.1661     X VALUES:     4.6247    -2.5923     1.5967
  STEP NO  6
  TREATMENT NO 10     Z = -249.4534     X VALUES:     4.5496    -1.5107    -0.0840
  STEP NO  7
  TREATMENT NO 11     Z = -345.4255     X VALUES:     4.4746    -0.4292    -1.7646
  X VALUES AT STEP 6 TAKEN AS NEW SEARCH BASE

ITERATION NO 2

  VARIABLE  1 FORWARD DIFFERENCED BY     0.1000 TO     4.6496
  TREATMENT NO 12     Z = -259.1578     X VALUES:     4.6496    -1.5107    -0.0840
  CURRENT Z VALUE =      -259.1578        BASE Z VALUE =      -249.4534          SLOPE =      -97.0433
  VARIABLE  2 FORWARD DIFFERENCED BY     0.1000 TO    -1.4107
  TREATMENT NO 13     Z = -246.3232     X VALUES:     4.5496    -1.4107    -0.0840
  CURRENT Z VALUE =      -246.3232        BASE Z VALUE =      -249.4534          SLOPE =      31.3020
  VARIABLE  3 FORWARD DIFFERENCED BY     0.1000 TO     0.0160
  TREATMENT NO 14     Z = -244.5120     X VALUES:     4.5496    -1.5107     0.0160
  CURRENT Z VALUE =      -244.5120        BASE Z VALUE =      -249.4534          SLOPE =      49.4146
  ADJUSTMENTS TO X VALUES:  -1.7129   0.5525   0.8722
  STEP NO  1
  TREATMENT NO 15     Z =  -82.7154     X VALUES:     2.8367    -0.9582     0.7882
  STEP NO  2
  TREATMENT NO 16     Z =  -35.1333     X VALUES:     1.1239    -0.4057     1.6604
  STEP NO  3
  TREATMENT NO 17     Z = -106.7072     X VALUES:    -0.5890     0.1468     2.5326
  X VALUES AT STEP 2 TAKEN AS NEW SEARCH BASE

ITERATION NO 3

  VARIABLE  1 FORWARD DIFFERENCED BY     0.1000 TO     1.2239
  TREATMENT NO 18     Z =  -35.4508     X VALUES:     1.2239    -0.4057     1.6604
  CURRENT Z VALUE =      -35.4508        BASE Z VALUE =      -35.1333          SLOPE =      -3.1747
  VARIABLE  2 FORWARD DIFFERENCED BY     0.1000 TO    -0.3057
  TREATMENT NO 19     Z =  -33.4318     X VALUES:     1.1239    -0.3057     1.6604
  CURRENT Z VALUE =      -33.4318        BASE Z VALUE =      -35.1333          SLOPE =      17.0152
  VARIABLE  3 FORWARD DIFFERENCED BY     0.1000 TO     1.7604
  TREATMENT NO 20     Z =  -38.1753     X VALUES:     1.1239    -0.4057     1.7604
  CURRENT Z VALUE =      -38.1753        BASE Z VALUE =      -35.1333          SLOPE =      -30.4195
  ADJUSTMENTS TO X VALUES:  -0.1814   0.9723  -1.7383
  STEP NO  1
  TREATMENT NO 21     Z =  -18.4905     X VALUES:     0.9424     0.5666    -0.0779
  STEP NO  2
  TREATMENT NO 22     Z = -104.6484     X VALUES:     0.7610     1.5389    -1.8162
  X VALUES AT STEP 1 TAKEN AS NEW SEARCH BASE
  STEP SIZE PARAMETER REDUCED TO     0.4000
  ADJUSTMENTS TO X VALUES:  -0.0363   0.1945  -0.3477
  STEP NO  1
  TREATMENT NO 23     Z =  -27.4980     X VALUES:     0.9062     0.7611    -0.4255
  X VALUES AT STEP 0 TAKEN AS NEW SEARCH BASE
  TREATMENT NO 40     Z =  -18.4905     X VALUES:     0.9424     0.5666    -0.0779
```

APPENDIX IV

STEEPEST ASCENT (REFINED)

This subroutine follows the procedure outlined in the final section of Chapter 4. A series of linear optimizations are first carried out each following the Powell procedure but ensuring that the maximum is bracketed before taking a quadratic interpolation. The number of these linear optimizations is determined within the subroutine with reference to the maximum number of treatments allowed. No reductions are made to step size. When this phase of the search has been completed a non-linear local exploration is carried out. (Since the test function is a quadratic and the procedure is quadratically convergent, the exact optimum has been located.)

The parameters of the main program are as in Appendix III, as are NVAR, S and L of the subroutine.

In the experiment with the test function three iterations of linear search bring each of the factor levels to within one unit of the optimal value and the response criterion to -12.88. A small number of additional treatments are then evaluated, and a stationary point on the response hypersurface is located. A test applied to the Hessian matrix reveals that this stationary point is a maximum as required.

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S A S R
= = = =

```
ILE  5=FILE5,UNIT=READER

ILE  6=FILE6,UNIT=PRINTER


      INTEGER TMAX
      DIMENSION X(10)
      COMMON X
     1 ,IVAR,JVAR,ITEST,A,B,C,STEP,FA,FB,FC,DET,MAX,MIN,ISIGN,JSIGN,ITN
     2 ,NLIN,ZL
      DATA IN/5/,IO/6/
      DATA X(1)/5./,X(2)/-8./,X(3)/10./,TMAX/60/
      ITREAT = 0
      ITREAT = ITREAT + 1
      Z = (X(1)-2.*X(2))**2 + (X(2)-3.*X(3))**2 + (3.*X(1)-2.*X(3))**2
     1 - 2.*X(1) + X(2) - 3.*X(3) + 10.
      Z = -Z
      CALL OPT3(ITREAT,TMAX,Z)
      IF (ITREAT.LT.TMAX) GO TO 1
      STOP
      END
```

```
C  SUBROUTINE TO MAXIMIZE A FUNCTION OF SEVERAL VARIABLES BY THE METHOD
C  OF STEEPEST ASCENT WITH OPTIMIZATIONS IN ASCENT DIRECTIONS AND
C  NON-LINEAR LOCAL EXPLORATIONS IN THE VICINITY OF THE MAXIMUM

      SUBROUTINE OPT3(ITREAT,TMAX,Z)
      INTEGER TMAX
      REAL M,L,NUM
      DIMENSION X(10),XB(10),ZPLUS(10),M(10),U(10),H(10,10),
     1 E(10,10), S(10)
      DOUBLE PRECISION D(3)
      DATA D/'MAXIMUM','MINIMUM','SADDLE POINT'/
      COMMON X
     1 ,IVAR,JVAR,ITEST,A,B,C,STEP,FA,FB,FC,DET,MAX,MIN,ISIGN,JSIGN,ITN
     2 ,NLIN,ZL
      DATA NVAR/ 3/,S(1)/.1/,S(2)/.1/,S(3)/.1/,L/2./,IO/6/
      IF (ITREAT.EQ.1) WRITE (IO,4)
4     FORMAT (1X,'INITIAL ESTIMATE'/)
      WRITE (IO,5) ITREAT,Z,(X(J),J=1,NVAR)
5     FORMAT (3X,'TREATMENT NO',I3,4X,'Z =',F12.4,4X,'X VALUES:',6F10.4
     1 3X,4F10.4/)
      IF (ITREAT.GT.1) GO TO 2
      ITEST = 0
      IVAR = 0
      ITN = 0
      NLIN = TMAX - NVAR*(2+(NVAR-1)/2) - 6
C
2     GO TO (30,40,50,22,30,70,80,90,100,140), ITEST
22    IF (IVAR.GT.0) GO TO 26
      ITN = ITN + 1
      IF (ITEST.EQ.0) WRITE (IO,3) ITN
3     FORMAT (/1X,'ITERATION NO',I2/)
      IF (ITEST.EQ.4) WRITE (IO,164)
164   FORMAT (1H1,1X,'NON-LINEAR LOCAL EXPLORATION'/)
C  STORE CURRENT SEARCH BASE XB
      DO 24 J=1,NVAR
24    XB(J) = X(J)
      A = 0.
      FA = Z
      ZL = Z
      GO TO 28
26    M(IVAR) = (Z-FA) / S(IVAR)
      IF (ITEST.EQ.0) WRITE (IO,7) Z,FA,M(IVAR)
7     FORMAT (3X,'CURRENT Z =',F15.4,8X,'BASE Z =',F15.4,8X,'SLOPE =',
     1 F12.4)
      X(IVAR) = X(IVAR) - S(IVAR)
      ZPLUS(IVAR) = Z
28    IVAR = IVAR + 1
      X(IVAR) = X(IVAR) + S(IVAR)
      IF (IVAR.EQ.NVAR) ITEST = ITEST + 1
      WRITE (IO,8) IVAR,S(IVAR),X(IVAR)
8     FORMAT (3X,'VARIABLE',I3,' FORWARD DIFFERENCED BY ',F10.4,' TO',
     1 F10.4)
      RETURN
C
C  DETERMINE DIRECTION OF STEEPEST ASCENT
30    M(NVAR) = (Z-FA) / S(NVAR)
      ZPLUS(NVAR) = Z
      IF (ITEST.EQ.1) WRITE (IO,7) Z,FA,M(IVAR)
      X(NVAR) = X(NVAR) - S(NVAR)
      IF (ITEST.NE.5) GO TO 32
      ITEST = 6
```

```
C
C  MAXIMUM NOT BRACKETED. TAKE A FURTHER STEP
52     A = B
       FA = FB
       B = C
       FB = FC
       C = B + STEP
       DO 57 J=1,NVAR
57     X(J) = XB(J) + C * U(J)
       WRITE (IO,13)
13     FORMAT (3X,'THIRD OR LATER STEP')
       RETURN
C  NON-LINEAR LOCAL EXPLORATION
70     IVAR = 1
       X(1) = X(1) - S(1)
       ITEST = 7
       WRITE (IO,14) IVAR,S(IVAR),X(IVAR)
14     FORMAT (3X,'VARIABLE',I3,' BACKWARD DIFFERENCED BY',F10.4,' TO',
      1 F10.4)
       RETURN
C
C  CALCULATE LINEAR AND QUADRATIC TERMS OF TAYLOR SERIES FOR VBLE IVAR
80     M(IVAR) = (ZPLUS(IVAR)-Z) / (2.*S(IVAR))
       H(IVAR,IVAR) = (ZPLUS(IVAR)+Z-2.* FA  ) / (S(IVAR)*S(IVAR))
       X(IVAR) = X(IVAR) + S(IVAR)
       IVAR = IVAR + 1
       X(IVAR) = X(IVAR) - S(IVAR)
       IF (IVAR.EQ.NVAR) ITEST = 8
       WRITE (IO,14) IVAR,S(IVAR),X(IVAR)
       RETURN
C
90     X(NVAR) = X(NVAR) + S(NVAR)
       M(NVAR) = (ZPLUS(NVAR)-Z) / (2.*S(NVAR))
       H(NVAR,NVAR) = (ZPLUS(NVAR)+Z-2.* FA  ) / (S(NVAR)*S(NVAR))
C  CALCULATE INTERACTION TERMS OF TAYLOR SERIES
       IVAR = 1
       JVAR = 2
       X(1) = X(1) + S(1)
       X(2) = X(2) + S(2)
       ITEST = 9
       WRITE (IO,15) IVAR,JVAR
15     FORMAT (3X,'VARIABLE',I3,' AND',I3,' FORWARD DIFFERENCED')
       RETURN
C
100    H(IVAR,JVAR) = (Z- FA  -M(IVAR)*S(IVAR)-M(JVAR)*S(JVAR) - H(IVAR,
      1IVAR)*S(IVAR)*S(IVAR)/2. - H(JVAR,JVAR)*S(JVAR)*S(JVAR)/2.) /
      2 (S(IVAR)*S(JVAR))
       X(JVAR) = X(JVAR) - S(JVAR)
       IF (JVAR.EQ.NVAR) GO TO 102
       JVAR = JVAR + 1
       X(JVAR) = X(JVAR) + S(JVAR)
       WRITE (IO,15) IVAR,JVAR
       RETURN
```

```
C
32      SSQ = M(1)*M(1)
        DO 36 J=2,NVAR
36      SSQ = SSQ + M(J)*M(J)
        DIV = SQRT(SSQ)
        DO 38 J=1,NVAR
        U(J) = M(J) / DIV * L
38      X(J) = XB(J) + U(J)
        WRITE (IO,10) (U(J),J=1,NVAR)
10      FORMAT (3X,'ADJUSTMENTS TO X VALUES:',10F9.4)
        B = 1.
        ITEST = 2
        WRITE (IO,9)
9       FORMAT (3X,'FIRST STEP IN DIRECTION OF STEEPEST ASCENT')
        RETURN
C
C   DEFINE SECOND STEP IN ASCENT DIRECTION
40      IF (Z.LT.FA) GO TO 42
C   FUNCTION INCREASING SO STEP FORWARD
        FB = Z
        STEP = 1.
        ITEST = 3
        GO TO 44
C   FUNCTION DECREASING SO STEP BACKWARDS
42      STEP = -1
        TEMP = B
        B = A
        A = TEMP
        FB = FA
        FA = Z
44      C = B + STEP
        DO 46 J=1,NVAR
46      X(J) = XB(J) + C * U(J)
        WRITE (IO,11)
11      FORMAT (3X,'SECOND STEP')
        RETURN
C
C   LOCATE MAXIMUM OR CONTINUE STEPPING
50      FC = Z
        IF (FC.GT.FB) GO TO 52
C   MAXIMUM BRACKETED BY A,B AND C. CALCULATE OPTIMAL STEP SIZE
        NUM = (B*B-C*C)*FA + (C*C-A*A)*FB + (A*A-B*B)*FC
        DEN = 2. * ((B-C)*FA + (C-A)*FB + (A-B)*FC)
        BETA = NUM / DEN
        DO 60 J=1,NVAR
60      X(J) = XB(J) + BETA * U(J)
        IVAR = 0
        ITEST = 0
        IF (Z.LT.ZL.OR.ITREAT.GE.NLIN) ITEST = 4
        WRITE (IO,12) BETA
12      FORMAT (3X,'LINEAR OPTIMIZATION; BETA =',F12.4)
        RETURN
```

```
C
102   IVAR = IVAR + 1
      IF (IVAR.EQ.NVAR) GO TO 110
      X(IVAR-1) = X(IVAR-1) - S(IVAR-1)
      JVAR = IVAR + 1
      X(IVAR) = X(IVAR) + S(IVAR)
      X(JVAR) = X(JVAR) + S(JVAR)
      WRITE (IO,15) IVAR,JVAR
      RETURN
C  CALCULATE ELEMENTS OF HESSIAN MATRIX H BELOW THE DIAGONAL
110   DO 112 I=1,NVAR
      DO 112 J=1,NVAR
112   H(J,I) = H(I,J)
      WRITE (IO,16)
16    FORMAT (3X,'JACOBIAN GRADIENT VECTOR')
      WRITE (IO,18) (M(J),J=1,NVAR)
      WRITE (IO,17)
17    FORMAT (3X,'HESSIAN MATRIX')
      DO 114 I=1,NVAR
114   WRITE (IO,18) (H(I,J),J=1,NVAR)
18    FORMAT (3X,10F12.4)
C  OBTAIN THE INVERSE OF H (=E), AT THE SAME TIME TESTING FOR NEGATIVE
C  DEFINATENESS
      MAX = 0
      MIN = 0
      ISIGN = 1
      DET = 1.
      DO 120 I=1,NVAR
      DO 120 J=1,NVAR
      E(I,J) = 0.
      IF (I.EQ.J) E(I,J) = 1.
120   CONTINUE
C  FOR EACH ROW
      DO 122 I=1,NVAR
C   DIVIDE THROUGH BY PIVOT ELEMENT
      PIV = H(I,I)
      DET = DET * PIV
      IF (DET.LT.0.) MIN = MIN + 1
      ISIGN = ISIGN * (-1)
      JSIGN = 1
      IF (DET.LT.0.) JSIGN = -1
      IF (JSIGN.NE.ISIGN) MAX = MAX + 1
      MIN = MIN + JSIGN
      DO 124 J=1,NVAR
      H(I,J) = H(I,J) / PIV
124   E(I,J) = E(I,J) / PIV
C   FOR EACH OTHER ROW
      DO 126 K=1,NVAR
      IF (K.EQ.I) GO TO 126
      TEMP = H(K,I)
C    FOR EACH ELEMENT
      DO 128 J=1,NVAR
      H(K,J) = H(K,J) - TEMP * H(I,J)
128   E(K,J) = E(K,J) - TEMP * E(I,J)
126   CONTINUE
122   CONTINUE
C  CALCULATE REQUIRED ADJUSTMENTS IN X
      DO 130 I=1,NVAR
      U(I) = 0.
      DO 132 J=1,NVAR
132   U(I) = U(I) - E(I,J)*M(J)
130   CONTINUE
C  CALCULATE OPTIMAL X VALUES
      DO 134 J=1,NVAR
134   X(J) = XB(J) + U(J)
      IF (MAX.EQ.0) J = 1
      IF (MIN.EQ.NVAR) J = 2
      IF (MAX.NE.0.AND.MIN.NE.NVAR) J = 3
      WRITE (IO,162) D(J)
162   FORMAT (/3X,'THE STATIONARY POINT IS A ',A12/)
      ITREAT = TMAX - 1
      ITEST = 10
140   RETURN
      END
```

```
INITIAL ESTIMATE

  TREATMENT NO  1     Z =  -1872.0000     X VALUES:     5.0000    -8.0000    10.0000

ITERATION NO 1

  VARIABLE  1 FORWARD DIFFERENCED BY      0.1000 TO     5.1000
  TREATMENT NO  2     Z =  -1873.1000     X VALUES:     5.1000    -8.0000    10.0000
  CURRENT Z =      -1873.1000          BASE Z =      -1872.0000          SLOPE =     -11.0000
  VARIABLE  2 FORWARD DIFFERENCED BY      0.1000 TO    -7.9000
  TREATMENT NO  3     Z =  -1856.1500     X VALUES:     5.0000    -7.9000    10.0000
  CURRENT Z =      -1856.1500          BASE Z =      -1872.0000          SLOPE =     158.5000
  VARIABLE  3 FORWARD DIFFERENCED BY      0.1000 TO    10.1000
  TREATMENT NO  4     Z =  -1896.6300     X VALUES:     5.0000    -8.0000    10.1000
  CURRENT Z =      -1896.6300          BASE Z =      -1872.0000          SLOPE =    -246.3000
  ADJUSTMENTS TO X VALUES:  -0.0751   1.0815  -1.6807
  FIRST STEP IN DIRECTION OF STEEPEST ASCENT
  TREATMENT NO  5     Z =  -1339.8638     X VALUES:     4.9249    -6.9185     8.3193
  SECOND STEP
  TREATMENT NO  6     Z =   -912.4123     X VALUES:     4.8499    -5.8369     6.6387
  THIRD OR LATER STEP
  TREATMENT NO  7     Z =   -589.6455     X VALUES:     4.7748    -4.7554     4.9580
  THIRD OR LATER STEP
  TREATMENT NO  8     Z =   -371.5634     X VALUES:     4.6998    -3.6738     3.2774
  THIRD OR LATER STEP
  TREATMENT NO  9     Z =   -258.1661     X VALUES:     4.6247    -2.5923     1.5967
  THIRD OR LATER STEP
  TREATMENT NO 10     Z =   -249.4534     X VALUES:     4.5496    -1.5107    -0.0840
  THIRD OR LATER STEP
  TREATMENT NO 11     Z =   -345.4255     X VALUES:     4.4746    -0.4292    -1.7646
  LINEAR OPTIMIZATION; BETA =      5.5832
  TREATMENT NO 12     Z =   -240.3616     X VALUES:     4.5809    -1.9615     0.6165

ITERATION NO 2

  VARIABLE  1 FORWARD DIFFERENCED BY      0.1000 TO     4.6809
  TREATMENT NO 13     Z =   -249.4683     X VALUES:     4.6809    -1.9615     0.6165
  CURRENT Z =      -249.4683          BASE Z =      -240.3616          SLOPE =     -91.0666
  VARIABLE  2 FORWARD DIFFERENCED BY      0.1000 TO    -1.8615
  TREATMENT NO 14     Z =   -236.3479     X VALUES:     4.5809    -1.8615     0.6165
  CURRENT Z =      -236.3479          BASE Z =      -240.3616          SLOPE =      40.1374
  VARIABLE  3 FORWARD DIFFERENCED BY      0.1000 TO     0.7165
  TREATMENT NO 15     Z =   -237.4742     X VALUES:     4.5809    -1.9615     0.7165
  CURRENT Z =      -237.4742          BASE Z =      -240.3616          SLOPE =      28.8736
  ADJUSTMENTS TO X VALUES:  -1.7576   0.7747   0.5573
  FIRST STEP IN DIRECTION OF STEEPEST ASCENT
  TREATMENT NO 16     Z =    -86.3018     X VALUES:     2.8233    -1.1868     1.1738
  SECOND STEP
  TREATMENT NO 17     Z =    -37.3243     X VALUES:     1.0656    -0.4121     1.7310
  THIRD OR LATER STEP
  TREATMENT NO 18     Z =    -93.4293     X VALUES:    -0.6920     0.3626     2.2883
  LINEAR OPTIMIZATION; BETA =      1.9661
  TREATMENT NO 19     Z =    -37.2639     X VALUES:     1.1252    -0.4384     1.7121

ITERATION NO 3

  VARIABLE  1 FORWARD DIFFERENCED BY      0.1000 TO     1.2252
  TREATMENT NO 20     Z =    -37.5352     X VALUES:     1.2252    -0.4384     1.7121
  CURRENT Z =      -37.5352          BASE Z =      -37.2639          SLOPE =      -2.712
  VARIABLE  2 FORWARD DIFFERENCED BY      0.1000 TO    -0.3384
  TREATMENT NO 21     Z =    -35.4981     X VALUES:     1.1252    -0.3384     1.7121
  CURRENT Z =      -35.4981          BASE Z =      -37.2639          SLOPE =      17.657
  VARIABLE  3 FORWARD DIFFERENCED BY      0.1000 TO     1.8121
  TREATMENT NO 22     Z =    -40.4582     X VALUES:     1.1252    -0.4384     1.8121
  CURRENT Z =      -40.4582          BASE Z =      -37.2639          SLOPE =     -31.943
  ADJUSTMENTS TO X VALUES:  -0.1482   0.9649  -1.7456
  FIRST STEP IN DIRECTION OF STEEPEST ASCENT
  TREATMENT NO 23     Z =    -18.0583     X VALUES:     0.9770     0.5265    -0.0334
  SECOND STEP
  TREATMENT NO 24     Z =   -102.9697     X VALUES:     0.8288     1.4914    -1.7790
  LINEAR OPTIMIZATION; BETA =      0.6845
  TREATMENT NO 25     Z =    -12.8752     X VALUES:     1.0238     0.2221     0.5174
```

NON-LINEAR LOCAL EXPLORATION

VARIABLE 1 FORWARD DIFFERENCED BY	0.1000 TO	1.1238			
TREATMENT NO 26 Z = -14.1130	X VALUES:	1.1238	0.2221	0.5174	
VARIABLE 2 FORWARD DIFFERENCED BY	0.1000 TO	0.3221			
TREATMENT NO 27 Z = -12.5273	X VALUES:	1.0238	0.3221	0.5174	
VARIABLE 3 FORWARD DIFFERENCED BY	0.1000 TO	0.6174			
TREATMENT NO 28 Z = -12.6886	X VALUES:	1.0238	0.2221	0.6174	
TREATMENT NO 29 Z = -12.8752	X VALUES:	1.0238	0.2221	0.5174	
VARIABLE 1 BACKWARD DIFFERENCED BY	0.1000 TO	0.9238			
TREATMENT NO 30 Z = -11.8373	X VALUES:	0.9238	0.2221	0.5174	
VARIABLE 2 BACKWARD DIFFERENCED BY	0.1000 TO	0.1221			
TREATMENT NO 31 Z = -13.3230	X VALUES:	1.0238	0.1221	0.5174	
VARIABLE 3 BACKWARD DIFFERENCED BY	0.1000 TO	0.4174			
TREATMENT NO 32 Z = -13.3217	X VALUES:	1.0238	0.2221	0.4174	
VARIABLE 1 AND 2 FORWARD DIFFERENCED					
TREATMENT NO 33 Z = -13.7252	X VALUES:	1.1238	0.3221	0.5174	
VARIABLE 1 AND 3 FORWARD DIFFERENCED					
TREATMENT NO 34 Z = -13.8065	X VALUES:	1.1238	0.2221	0.6174	
VARIABLE 2 AND 3 FORWARD DIFFERENCED					
TREATMENT NO 35 Z = -12.2807	X VALUES:	1.0238	0.3221	0.6174	

JACOBIAN GRADIENT VECTOR

-11.3788	3.9789	3.1658

HESSIAN MATRIX

-20.0000	4.0000	12.0000
4.0000	-10.0000	6.0000
12.0000	6.0000	-26.0000

THE STATIONARY POINT IS A MAXIMUM

TREATMENT NO 60	Z = -9.2813	X VALUES:	0.3438	0.2344	0.3281

APPENDIX V

CONJUGATE DIRECTIONS

This program follows the conjugate directions method as outlined in Chapter 5. The parameters defined in DATA statements have the following interpretations.

Main program

As in Appendix III.

Subroutine

NVAR = number of experimental factors (here 3),

L(1), L(2), L(3) = step size parameters for variables 1 to 3 (here each 2.0).

Q = maximum step size (here 12.0).

DMIN = minimum improvement in response from a full search iteration for which the experiment is to be continued (here 1.0).

MIT = maximum number of iterations before the search must terminate (here 4).

This method, which is also quadratically convergent, locates the exact minimum of the test function (Z = 9.2813) and corresponding factor levels in three iterations or 47 treatments.

114.

B6700 F O R T R A N C O M P I L A T I O N M A R K 2.9.190

TUESDAY, 05/16/78 04:57 PM

C D I R
= = = = =

```
FILE  5=FILE5,UNIT=READER

FILE  6=FILE6,UNIT=PRINTER


      INTEGER TMAX
      DIMENSION X(10)
      COMMON X
     1 ,I,ITEST,M,DELTA,A,B,C,FA,FB,FC,F1,F2,F3,ZL,ZBASE,S,UMAX,ITN
      DATA IN/5/,IO/6/
     ,  DATA X(1)/5./,X(2)/-8./,X(3)/10./,TMAX/60/
      ITREAT = 0
1     ITREAT = ITREAT + 1
      Z = (X(1)-2.*X(2))**2 + (X(2)-3.*X(3))**2 + (3.*X(1)-2.*X(3))**2
     1 - 2.*X(1) + X(2) - 3.*X(3) + 10.
      CALL OPT4(ITREAT,TMAX,Z)
      IF (ITREAT.LT.TMAX) GO TO 1
      STOP
      END
```

```
C  SUBROUTINE TO MAXIMIZE A FUNCTION OF SEVERAL VARIABLES USING THE
C  METHOD OF CONJUGATE DIRECTIONS

      SUBROUTINE OPT4(ITREAT,TMAX,Z)
      INTEGER TMAX
      REAL L,NUM
      DIMENSION X(10),L(10),W(10),U(10,10),XO(10),XN(10),XB(10)
      COMMON X
     1 ,I,ITEST,M,DELTA,A,B,C,FA,FB,FC,F1,F2,F3,ZL,ZBASE,S,UMAX,ITN
      DATA NVAR/3/,L(1)/2./,L(2)/2./,L(3)/2./,Q/12./,IO/6/
     1 ,DMIN/1./,MIT/4/
      IF (ITREAT.EQ.1) WRITE (IO,3)
3     FORMAT (1X,'INITIAL ESTIMATE'/)
      WRITE (IO,4) ITREAT,Z,(X(J),J=1,NVAR)
4     FORMAT (3X,'TREATMENT NO',I3,4X,'Z =',F12.4,4X,'X VALUES:',6F12.4/
     1 3X,4F12.4/)
      IF (ITREAT.GT.1) GO TO 10
C  STORE ITERATION SEARCH BASE
      DO 32 J=1,NVAR
32    XO(J) = X(J)
C  SET UP INITIAL SEARCH DIRECTION VECTORS
      DO 12 I=1,NVAR
      DO 12 J=1,NVAR
      U(I,J) = 0.
      IF (I.EQ.J) U(I,J) = 1.
12    CONTINUE
      I = 0
      ITEST = 0
      ITN = 0
      ZBASE = 999999
10    CONTINUE
C
      GO TO (70,80,50,60,70,80,50), ITEST
C  BEGIN NEW LINEAR MINIMIZATION
20    I = I+1
      IF (I.EQ.1) ITN = ITN + 1
      IF (I.EQ.1) WRITE (IO,5) ITN
5     FORMAT (/1X,'ITERATION NO',I2/)
21    ITEST = ITEST + 1
      WRITE (IO,114) I
114   FORMAT (3X,'SEARCH IN DIRECTION NO',I3)
      A = 0.
      FA = Z
      UMAX = U(I,1)
      UMIN = U(I,1)
      DO 16 J=2,NVAR
      IF (U(I,J).GT.UMAX) UMAX = U(I,J)
      IF (U(I,J).LT.UMIN) UMIN = U(I,J)
16    CONTINUE
      UMAX = AMAX1(UMAX,ABS(UMIN))
      S = L(I) / UMAX
      B = S
      WRITE (IO,116) S
116   FORMAT (3X,'STEP SIZE PARAMETER SET AT',F10.4)
C  STORE BASE TREATMENT FOR CURRENT LINEAR MINIMIZATION
      DO 18 J=1,NVAR
18    XB(J) = X(J)
C  SPECIFY FIRST TREATMENT OF LINEAR OPTIMIZATION
19    DO 14 J=1,NVAR
14    X(J) = XB(J) + B * U(I,J)
      IF (ITEST.EQ.5) RETURN
      IF (I.GT.1) GO TO 30
      DELTA = 0.
      M = 1
```

```
C  RECORD WHETHER IMPROVEMENT IS GREATER THAN IN PREVIOUS LINEAR OPTIMNS
30     DIFF = ZL - Z
       IF (DIFF.L.T.DELTA) GO TO 34
       DELTA = DIFF
       M = I-1
34     ZL = Z
       ITEST = 1
       RETURN
C
50     F2 = Z
       ITEST = ITEST + 1
       DO 36 J=1,NVAR
36     X(J) = 2. * XN(J) - XO(J)
       DIFF = ZL - Z
       IF (DIFF.GT.DELTA) M = NVAR
       IF (DIFF.GT.DELTA) DELTA = DIFF
       WRITE (IO,120)
120    FORMAT (3X,'DOUBLE ITERATION STEP')
       RETURN
C
C  RETURN FROM EVALUATION OF DOUBLE ITERATION STEP (X=2XN-XO)
60     F3 = Z
       WRITE (IO,118) F1,F2,F3,M,DELTA
118    FORMAT (3X,'F1 =',F12.4,5X,'F2 =',F10.4,5X,'F3 =',F10.4,5X,
      1 'M =',I2,5X,'DELTA =',F10.4)
       IF (F3.GE.F1) GO TO 38
       T1 = (F1-2.*F2+F3) * (F1-F2-DELTA)**2
       T2 = DELTA * (F1-F3)**2 / 2.
       IF (T1.GE.T2) GO TO 38
C  INTRODUCE NEW SEARCH DIRECTION VECTOR
       DO 42 K=M,NVAR-1
       DO 44 J=1,NVAR
44     U(K,J) = U(K+1,J)
42     CONTINUE
       DO 46 J=1,NVAR
46     U(NVAR,J) = XN(J) - XO(J)
       WRITE (IO,124) (U(NVAR,J),J=1,NVAR)
124    FORMAT (3X,'NEW SEARCH DIRECTION VECTOR:',10F10.4)
       DO 47 J=1,NVAR
47     X(J) = XN(J)
       Z = F2
       GO TO 21
38     IF (F3.LT.F2) GO TO 48
C  SET NEW ITERATION BASE AS XN
       DO 56 J=1,NVAR
56     XO(J) = XN(J)
       GO TO 54
C  SET NEW ITERATION BASE AS 2XN-XO
48     DO 52 J=1,NVAR
52     XO(J) = 2. * XN(J) - XO(J)
C  END OF ITERATION
54     ZIT = AMIN1(F2,F3)
       ZDIFF = ZBASE - ZIT
       IF (ZDIFF.LT.DMIN.OR.ITN.EQ.MIT) GO TO 58
       IF (ZIT.GT.ZBASE) GO TO 58
       ITEST = 0
       I = 0
       DO 55 J=1,NVAR
55     X(J) = XO(J)
       Z = ZIT
       GO TO 20
C  END OF OPTIMIZATION
58     ITREAT = TMAX
       RETURN
```

```
C
C  TAKE A SECOND STEP
70     FB = Z
       ITEST = ITEST + 1
       C = 2. * S
       IF (FB.GT.FA) C = 0. - S
76     DO 78 J=1,NVAR
78     X(J) = XB(J) + C * U(I,J)
       RETURN
C
C  THIRD OR LATER STEP IN LINEAR MINIMIZATION
80     FC = Z
       DEN = 2. * ((B-C)*FA + (C-A)*FB + (A-B)*FC)
       TEST = DEN / ((A-B)*(B-C)*(C-A))
       IF (TEST.LT.0.) GO TO 90
       IF (FB.GT.FA) GO TO 88
C  FUNCTION DECREASING. TAKE A FURTHER STEP FORWARDS
       A = B
       FA = FB
       B = C
       FB = FC
       C = C + S
       GO TO 76
C  FUNCTION INCREASING. TAKE A STEP BACKWARDS
88     B = A
       FB = FA
       A = C
       FA = FC
       C = C - S
       GO TO 76
C
C  CALCULATE OPTIMAL STEP SIZE
90     NUM = (B*B-C*C)*FA + (C*C-A*A)*FB + (A*A-B*B)*FC
       BETA = NUM / DEN
       PROD = BETA * UMAX
       IF (ABS(PROD).GT.Q) BETA = BETA * ABS(Q/PROD)
C  PLACE NEW TREATMENT AT OPTIMAL POSITION
       DO 94 J=1,NVAR
       X(J) = XB(J) + BETA * U(I,J)
       IF (I.EQ.NVAR.AND.ITEST.EQ.2) XN(J) = X(J)
94     CONTINUE
       WRITE (IO,128) BETA
128    FORMAT (3X,'LINEAR OPTIMIZATION; BETA =',F12.4)
       IF (I.EQ.NVAR.AND.ITEST.EQ.6) GO TO 96
       IF (I.LT.NVAR) ITEST = 0
       IF (I.EQ.NVAR) ITEST = 3
       RETURN
C
C  END OF ITERATION (INTRODUCED DIRECTION). SET NEW ITERATION BASE
C  AT XN + BETA*UN
96     DO 98 J=1,NVAR
98     XO(J) = X(J)
       ITEST = 0
       I = 0
       RETURN
       END
```

```
INITIAL ESTIMATE

  TREATMENT NO  1     Z =    1872.0000     X VALUES:       5.0000      -8.0000      10.0000

ITERATION NO 1

  SEARCH IN DIRECTION NO  1
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO  2     Z =    1932.0000     X VALUES:       7.0000      -8.0000      10.0000
  TREATMENT NO  3     Z =    1892.0000     X VALUES:       3.0000      -8.0000      10.0000
  LINEAR OPTIMIZATION; BETA =      -0.5000
  TREATMENT NO  4     Z =    1869.5000     X VALUES:       4.5000      -8.0000      10.0000
  SEARCH IN DIRECTION NO  2
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO  5     Z =    1575.5000     X VALUES:       4.5000      -6.0000      10.0000
  TREATMENT NO  6     Z =    1321.5000     X VALUES:       4.5000      -4.0000      10.0000
  LINEAR OPTIMIZATION; BETA =     12.0000
  TREATMENT NO  7     Z =     705.5000     X VALUES:       4.5000       4.0000      10.0000
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO  8     Z =    1115.5000     X VALUES:       4.5000       4.0000      12.0000
  TREATMENT NO  9     Z =     399.5000     X VALUES:       4.5000       4.0000       8.0000
  LINEAR OPTIMIZATION; BETA =     -6.8846
  TREATMENT NO 10     Z =      89.3269     X VALUES:       4.5000       4.0000       3.1154
  DOUBLE ITERATION STEP
  TREATMENT NO 11     Z =    1940.7692     X VALUES:       4.0000      16.0000      -3.7692
  F1 =    1872.0000     F2 =     89.3269     F3 = 1940.7692     M = 2     DELTA = 1164.0000

ITERATION NO 2

  SEARCH IN DIRECTION NO  1
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 12     Z =     198.5577     X VALUES:       6.5000       4.0000       3.1154
  TREATMENT NO 13     Z =      60.0962     X VALUES:       2.5000       4.0000       3.1154
  LINEAR OPTIMIZATION; BETA =     -1.7308
  TREATMENT NO 14     Z =      59.3713     X VALUES:       2.7692       4.0000       3.1154
  SEARCH IN DIRECTION NO  2
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 15     Z =     101.8328     X VALUES:       2.7692       6.0000       3.1154
  TREATMENT NO 16     Z =      56.9098     X VALUES:       2.7692       2.0000       3.1154
  LINEAR OPTIMIZATION; BETA =     -1.1231
  TREATMENT NO 17     Z =      53.0648     X VALUES:       2.7692       2.8769       3.1154
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 18     Z =     160.0802     X VALUES:       2.7692       2.8769       5.1154
  TREATMENT NO 19     Z =      50.0494     X VALUES:       2.7692       2.8769       1.1154
  LINEAR OPTIMIZATION; BETA =     -1.0580
  TREATMENT NO 20     Z =      38.5134     X VALUES:       2.7692       2.8769       2.0574
  DOUBLE ITERATION STEP
  TREATMENT NO 21     Z =      15.5710     X VALUES:       1.0385       1.7538       0.9994
  F1 =      89.3269     F2 =     38.5134     F3 =    15.5710     M = 1     DELTA =    29.9556
  NEW SEARCH DIRECTION VECTOR:    -1.7308    -1.1231    -1.0580
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     1.1556
  TREATMENT NO 22     Z =      14.5071     X VALUES:       0.7692       1.5791       0.8348
  TREATMENT NO 23     Z =      27.7175     X VALUES:      -1.2308       0.2814      -0.3877
  LINEAR OPTIMIZATION; BETA =      1.3232
  TREATMENT NO 24     Z =      14.1157     X VALUES:       0.4791       1.3909       0.6575
```

```
ITERATION NO 3

  SEARCH IN DIRECTION NO  1
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 25     Z =      52.2107     X VALUES:       0.4791        3.3909        0.6575
  TREATMENT NO 26     Z =      16.0207     X VALUES:       0.4791       -0.6091        0.6575
  LINEAR OPTIMIZATION; BETA =      -0.9047
  TREATMENT NO 27     Z =      10.0228     X VALUES:       0.4791        0.4862        0.6575
  SEARCH IN DIRECTION NO  2
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 28     Z =      72.8798     X VALUES:       0.4791        0.4862        2.6575
  TREATMENT NO 29     Z =      51.1659     X VALUES:       0.4791        0.4862       -1.3425
  LINEAR OPTIMIZATION; BETA =      -0.2088
  TREATMENT NO 30     Z =       9.4561     X VALUES:       0.4791        0.4862        0.4487
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     1.1556
  TREATMENT NO 31     Z =      25.9314     X VALUES:      -1.5209       -0.8116       -0.7738
  TREATMENT NO 32     Z =      30.1975     X VALUES:       2.4791        1.7839        1.6713
  LINEAR OPTIMIZATION; BETA =       0.0662
  TREATMENT NO 33     Z =       9.3950     X VALUES:       0.3645        0.4118        0.3787
  DOUBLE ITERATION STEP
  TREATMENT NO 34     Z =      11.6044     X VALUES:       0.2499       -0.5673        0.0998
  F1 =      14.1157     F2 =      9.3950     F3 =     11.6044     M = 1     DELTA =      4.0929
  NEW SEARCH DIRECTION VECTOR:    -0.1146    -0.9791    -0.2789
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     2.0426
  TREATMENT NO 35     Z =      21.2874     X VALUES:       0.1304       -1.5882       -0.1910
  TREATMENT NO 36     Z =      26.4171     X VALUES:       0.5987        2.4118        0.9483
  LINEAR OPTIMIZATION; BETA =       0.1812
  TREATMENT NO 37     Z =       9.2813     X VALUES:       0.3438        0.2344        0.3281

ITERATION NO 4

  SEARCH IN DIRECTION NO  1
  STEP SIZE PARAMETER SET AT     2.0000
  TREATMENT NO 38     Z =      61.2813     X VALUES:       0.3438        0.2344        2.3281
  TREATMENT NO 39     Z =      61.2813     X VALUES:       0.3438        0.2344       -1.6719
  LINEAR OPTIMIZATION; BETA =       0.0000
  TREATMENT NO 40     Z =       9.2813     X VALUES:       0.3438        0.2344        0.3281
  SEARCH IN DIRECTION NO  2
  STEP SIZE PARAMETER SET AT     1.1556
  TREATMENT NO 41     Z =      27.8895     X VALUES:      -1.6563       -1.0634       -0.8944
  TREATMENT NO 42     Z =      27.8895     X VALUES:       2.3438        1.5322        1.5507
  LINEAR OPTIMIZATION; BETA =       0.0000
  TREATMENT NO 43     Z =       9.2813     X VALUES:       0.3438        0.2344        0.3281
  SEARCH IN DIRECTION NO  3
  STEP SIZE PARAMETER SET AT     2.0426
  TREATMENT NO 44     Z =      23.7385     X VALUES:       0.1096       -1.7656       -0.2415
  TREATMENT NO 45     Z =      23.7385     X VALUES:       0.5779        2.2344        0.8977
  LINEAR OPTIMIZATION; BETA =       0.0000
  TREATMENT NO 46     Z =       9.2813     X VALUES:       0.3438        0.2344        0.3281
  DOUBLE ITERATION STEP
  TREATMENT NO 47     Z =       9.2813     X VALUES:       0.3438        0.2344        0.3281
  F1 =       9.2813     F2 =      9.2813     F3 =      9.2813     M = 2     DELTA =      0.0000
```

APPENDIX VI

RANDOM SEARCH WITH LEARNING

This subroutine follows the procedure outlined in Chapter 5. The layout is slightly different from that of the previous four subroutines due to the nature of random search. In particular, experimental ranges are defined for the three factors and the number of equally spaced levels to be considered within these ranges is specified. If the program were to be used for discrete rather than continuous factors then actual levels (rather than ranges) could be defined as DATA in the main program. The parameters set out in DATA statements in the main program have the following interpretations:

NVAR = number of experimental factors (here 3).

N = vector of number of levels to be included for each factor;

here $N = \begin{bmatrix} 5 \\ 4 \\ 7 \end{bmatrix}$

LO and HI = vectors defining the experimental regions for each factor;

here $LO = \begin{bmatrix} -10 \\ -5 \\ -10 \end{bmatrix}$ and $HI = \begin{bmatrix} 10 \\ 10 \\ 20 \end{bmatrix}$, meaning

for example that X(1) is allocated five equally spaced levels over the range -10 to 10 (i.e. -10, -5, 0, 5 and 10).

NS = initial number or seed for the random number generator, here 524,287.

K = learning rate parameter (here 4000).

NT1 = number of treatments in the initial sampling phase (here 5).

NT2 = number of treatments in the learning phase (here 20).

NT3 = number of treatments in the final sampling phase (here 15).

No parameters are defined in the subroutine.

The greatest response level achieved during the initial sampling phase is Z = -920, and this is used as the standard of comparison when revising probabilities in the learning phase. The adjusted probability distributions for the three factors are listed after each treatment. At the end of the learning phase (after the 25th treatment) these distributions are decidedly peaked around factor levels nearest zero. Response values in the final sampling phase are generally high (near zero), a number of near-optimal treatments being generated.

TUESDAY, 05/16/78 07:50 PM

R S W L
= = = =

```
FILE  5=FILE5,UNIT=READER

FILE  6=FILE6,UNIT=PRINTER
C  MAIN PROGRAMME TO TEST RANDOM SEARCH ROUTINE


      REAL LO,K
      DIMENSION X(10,10),J(10),N(10),LO(10),HI(10)
      COMMON X,J,NT1,NT2,NT3,NS,ZNORM,NVAR,N,ITEST,K
      DATA IN/5/,IO/6/,NS/ 524287/,NT1/ 5/,NT2/20/,NT3/15/,K/4000./
      DATA NVAR/3/,N(1)/5/,N(2)/4/,N(3)/7/,LO(1)/-10./,LO(2)/ -5./,LO(3)
     1 /-10./,HI(1)/10./,HI(2)/10./,HI(3)/
      DO 10 I=1,NVAR
      S = (HI(I)-LO(I)) / (N(I)-1.)
      DO 12 L=1,N(I)
12    X(I,L) = LO(I) + (L-1)*S
10    CONTINUE
      NTOT = NT1 + NT2 + NT3
      ITREAT = 0
1     ITREAT = ITREAT + 1
      CALL OPT5(ITREAT,Z)
      Z = (X(1,J(1))-2.*X(2,J(2)))**2 + (X(2,J(2))-3.*X(3,J(3)))**2 +
     1 (3.*X(1,J(1))-2.*X(3,J(3)))**2 - 2.*X(1,J(1)) + X(2,J(2)) -
     2 3.*X(3,J(3)) + 10.
      Z = -Z
      IF (ITREAT.LE.NTOT) GO TO 1
      STOP
      END
```

```
C  SUBROUTINE TO FIND THE MAXIMUM FOR A FUNCTION OF SEVERAL VARIABLES
C  USING RANDOM SEARCH PLUS LEARNING

      SUBROUTINE OPT5(ITREAT,Z)
      REAL K
      DIMENSION X(10,10),N(10),SW(10),E(10,10),P(10,10),CP(10,11),
     1 D(10,10),J(10),W(10,10)
      DOUBLE PRECISION F(2)
      COMMON X,J,NT1,NT2,NT3,NS,ZNORM,NVAR,N,ITEST,K
      DATA IO/6/,F/'UPWARDS','DOWNWARDS'/
      IF (ITREAT.GT.1) GO TO 1
      WRITE (IO,3)
3     FORMAT (1X,'DISCRETE X VALUES'/)
      DO 18 I=1,NVAR
18    WRITE (IO,4) I,(X(I,L),L=1,N(I))
4     FORMAT (3X,'VARIABLE NO',I3,6X,10F10.2)
      WRITE (IO,5)
5     FORMAT (/1X,'INITIAL SAMPLING PHASE'/)
      NT2 = NT2 + NT1
      NT3 = NT3 + NT2
      ZNORM = -10000.
C  SET UP INITIAL CHOICE DISTRIBUTIONS
      DO 20 I=1,NVAR
      SW(I) = 0.
      DO 22 L=1,N(I)
      E(I,L) = 3.
      W(I,L) = 2.**E(I,L)
22    SW(I) = SW(I) + W(I,L)
20    CONTINUE
C  CALCULATE AND CUMULATE PROBABILITIES
      DO 24 I=1,NVAR
      CP(I,1) = 0.
      DO 26 L=1,N(I)
      P(I,L) = W(I,L) / SW(I)
26    CP(I,L+1) = CP(I,L) + P(I,L)
24    CONTINUE
      WRITE (IO,6)
6     FORMAT (/3X,'INITIAL PROBABILITIES'/)
      DO 28 I=1,NVAR
28    WRITE (IO,7) (P(I,L),L=1,N(I))
7     FORMAT (1X,10F8.4)
      WRITE (IO,8)
8     FORMAT (1X,' ')
      ITEST = 0
      GO TO 50
1     CONTINUE
      JTREAT = ITREAT - 1
      WRITE (IO,10) JTREAT,Z,(X(I,J(I)),I=1,NVAR)
10    FORMAT (3X,'TREATMENT NO',I3,5X,'Z =',F12.4,5X,'X VALUES:',6F12.4/
     1 1X,4F12.4/)
C
      GO TO (30,40,50), ITEST
C  UPDATE PERFORMANCE NORM
      IF (ZNORM.LT.Z) ZNORM = Z
      IF (ITREAT.EQ.NT1) ITEST = 1
      GO TO 50
```

```
C
30    IF (ZNORM.LT.Z) ZNORM = Z
      WRITE (IO,11)
11    FORMAT (/1X,'LEARNING PHASE'/)
      WRITE (IO,12) ZNORM
12    FORMAT (/3X,'PERFORMANCE STANDARD OR NORM =',F12.4/)
      WRITE (IO,8)
      ITEST = 2
      GO TO 50
C
C  REVISE PROBABILITY OF VALUE J(I) OF EACH VARIABLE I
40    ID = 1
      IF (Z.LT.ZNORM) ID = 2
      ADJT = (Z-ZNORM) / K
      DO 42 I=1,NVAR
      D(I,J(I)) = ADJT
      E(I,J(I)) = E(I,J(I)) + D(I,J(I))
      SW(I) = SW(I) - W(I,J(I))
      W(I,J(I)) = 2.**E(I,J(I))
42    SW(I) = SW(I) + W(I,J(I))
      DO 44 I=1,NVAR
      CP(I,1) = 0.
      DO 44 L=1,N(I)
      P(I,L) = W(I,L) / SW(I)
44    CP(I,L+1) = CP(I,L) + P(I,L)
      WRITE (IO,14) F(ID),(J(I),I=1,NVAR)
14    FORMAT (3X,'PROBABILITIES REVISED ',A12,'FOR X(I,J(I)), ALL I, J(I
     1) =',10I2)
      DO 46 I=1,NVAR
46    WRITE (IO,7)  (P(I,L),L=1,N(I))
      IF (ITREAT.LE.NT2) GO TO 50
      ITEST = 3
      WRITE (IO,17)
17    FORMAT (/1X,'FINAL SAMPLING PHASE'/)
C
C  SAMPLE A VALUE FROM EACH UNIVARIATE DISTRIBUTION
50    DO 64 I=1,NVAR
      R = RANDOM(NS)
      DO 66 L=1,N(I)
      IF (R.GT.CP(I,L+1)) GO TO 66
      J(I) = L
      GO TO 64
66    CONTINUE
64    CONTINUE
      RETURN
      END
```

DISCRETE X VALUES

VARIABLE NO 1 -10.00 -5.00 0.00 5.00 10.00
VARIABLE NO 2 -5.00 0.00 5.00 10.00
VARIABLE NO 3 -10.00 -5.00 0.00 5.00 10.00 15.00 20.00

INITIAL SAMPLING PHASE

INITIAL PROBABILITIES

0.2000 0.2000 0.2000 0.2000 0.2000
0.2500 0.2500 0.2500 0.2500
0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429

TREATMENT NO 1 Z = -6080.0000 X VALUES: -10.0000 -5.0000 15.0000
TREATMENT NO 2 Z = -2510.0000 X VALUES: 5.0000 5.0000 -10.0000
TREATMENT NO 3 Z = -4050.0000 X VALUES: -5.0000 0.0000 15.0000
TREATMENT NO 4 Z = -1940.0000 X VALUES: -10.0000 10.0000 0.0000
TREATMENT NO 5 Z = -920.0000 X VALUES: 10.0000 5.0000 0.0000

LEARNING PHASE

PERFORMANCE STANDARD OR NORM = -920.0000

TREATMENT NO 6 Z = -2010.0000 X VALUES: -10.0000 -5.0000 5.0000
PROBABILITIES REVISED DOWNWARDS FOR X(I,J(I)), ALL I, J(I) = 1 1 4
0.1715 0.2071 0.2071 0.2071 0.2071
0.2163 0.2612 0.2612 0.2612
0.1465 0.1465 0.1465 0.1213 0.1465 0.1465 0.1465
TREATMENT NO 7 Z = -1530.0000 X VALUES: -5.0000 5.0000 -10.0000
PROBABILITIES REVISED DOWNWARDS FOR X(I,J(I)), ALL I, J(I) = 2 3 1
0.1751 0.1903 0.2115 0.2115 0.2115
0.2221 0.2683 0.2414 0.2683
0.1337 0.1486 0.1486 0.1231 0.1486 0.1486 0.1486
TREATMENT NO 8 Z = -720.0000 X VALUES: -5.0000 -5.0000 -10.0000
PROBABILITIES REVISED UPWARDS FOR X(I,J(I)), ALL I, J(I) = 2 1 1
0.1740 0.1957 0.2101 0.2101 0.2101
0.2281 0.2662 0.2395 0.2662
0.1378 0.1479 0.1479 0.1225 0.1479 0.1479 0.1479
TREATMENT NO 9 Z = -980.0000 X VALUES: -5.0000 10.0000 0.0000
PROBABILITIES REVISED DOWNWARDS FOR X(I,J(I)), ALL I, J(I) = 2 4 3
0.1743 0.1941 0.2105 0.2105 0.2105
0.2288 0.2669 0.2401 0.2642
0.1380 0.1482 0.1466 0.1227 0.1482 0.1482 0.1482
TREATMENT NO 10 Z = -6240.0000 X VALUES: -5.0000 5.0000 20.0000
PROBABILITIES REVISED DOWNWARDS FOR X(I,J(I)), ALL I, J(I) = 2 3 7
0.1974 0.0874 0.2384 0.2384 0.2384
0.2675 0.3121 0.1117 0.3088
0.1515 0.1627 0.1610 0.1347 0.1627 0.1627 0.0647
TREATMENT NO 11 Z = -1980.0000 X VALUES: -10.0000 10.0000 -5.0000
PROBABILITIES REVISED DOWNWARDS FOR X(I,J(I)), ALL I, J(I) = 1 4 2
0.1699 0.0904 0.2466 0.2466 0.2466
0.2821 0.3291 0.1178 0.2710
0.1558 0.1392 0.1655 0.1385 0.1673 0.1673 0.0665
TREATMENT NO 12 Z = -530.0000 X VALUES: 0.0000 10.0000 5.0000
PROBABILITIES REVISED UPWARDS FOR X(I,J(I)), ALL I, J(I) = 3 4 4
0.1670 0.0889 0.2593 0.2424 0.2424
0.2768 0.3230 0.1156 0.2846
0.1543 0.1379 0.1639 0.1467 0.1657 0.1657 0.0659
TREATMENT NO 13 Z = -270.0000 X VALUES: -5.0000 0.0000 0.0000
PROBABILITIES REVISED UPWARDS FOR X(I,J(I)), ALL I, J(I) = 2 2 3
0.1652 0.0984 0.2566 0.2399 0.2399
0.2666 0.3481 0.1113 0.2741
0.1513 0.1352 0.1800 0.1439 0.1625 0.1625 0.0646
TREATMENT NO 14 Z = -250.0000 X VALUES: 5.0000 0.0000 0.0000
PROBABILITIES REVISED UPWARDS FOR X(I,J(I)), ALL I, J(I) = 4 2 3
0.1605 0.0956 0.2493 0.2617 0.2330
0.2556 0.3749 0.1067 0.2628
0.1481 0.1323 0.1977 0.1408 0.1590 0.1590 0.0632
TREATMENT NO 15 Z = -250.0000 X VALUES: 5.0000 0.0000 0.0000
PROBABILITIES REVISED UPWARDS FOR X(I,J(I)), ALL I, J(I) = 4 2 3

```
0.1555  0.0926  0.2415  0.2847  0.2257
0.2443  0.4025  0.1020  0.2512
0.1445  0.1291  0.2168  0.1374  0.1552  0.1552  0.0617
TREATMENT NO 16      Z =    -350.0000      X VALUES:        0.0000        0.0000       -5.0000
PROBABILITIES REVISED UPWARDS      FOR X(I,J(I)), ALL I, J(I) = 3 2 2
0.1517  0.0904  0.2600  0.2777  0.2202
0.2345  0.4264  0.0979  0.2411
0.1426  0.1407  0.2139  0.1356  0.1531  0.1531  0.0609
TREATMENT NO 17      Z =   -3720.0000      X VALUES:      -10.0000       -5.0000       10.0000
PROBABILITIES REVISED DOWNWARDS    FOR X(I,J(I)), ALL I, J(I) = 1 1 5
0.0992  0.0960  0.2761  0.2949  0.2338
0.1587  0.4687  0.1076  0.2650
0.1515  0.1495  0.2273  0.1441  0.1002  0.1627  0.0647
TREATMENT NO 18      Z =    -320.0000      X VALUES:        0.0000       -5.0000       -5.0000
PROBABILITIES REVISED UPWARDS      FOR X(I,J(I)), ALL I, J(I) = 3 1 2
0.0963  0.0931  0.2974  0.2863  0.2270
0.1731  0.4607  0.1058  0.2605
0.1491  0.1632  0.2237  0.1418  0.0985  0.1601  0.0637
TREATMENT NO 19      Z =   -2140.0000      X VALUES:       -5.0000        0.0000       10.0000
PROBABILITIES REVISED DOWNWARDS    FOR X(I,J(I)), ALL I, J(I) = 2 2 5
0.0980  0.0767  0.3028  0.2914  0.2311
0.1897  0.4088  0.1160  0.2856
0.1520  0.1663  0.2279  0.1445  0.0813  0.1631  0.0649
TREATMENT NO 20      Z =    -250.0000      X VALUES:        5.0000        0.0000        0.0000
PROBABILITIES REVISED UPWARDS      FOR X(I,J(I)), ALL I, J(I) = 4 2 3
0.0946  0.0741  0.2923  0.3160  0.2230
0.1806  0.4371  0.1104  0.2719
0.1478  0.1617  0.2490  0.1406  0.0791  0.1587  0.0631
TREATMENT NO 21      Z =   -3520.0000      X VALUES:       10.0000        0.0000      -10.0000
PROBABILITIES REVISED DOWNWARDS    FOR X(I,J(I)), ALL I, J(I) = 5 2 1
0.1029  0.0806  0.3180  0.3438  0.1547
0.2146  0.3310  0.1312  0.3231
0.0995  0.1709  0.2631  0.1485  0.0835  0.1677  0.0667
TREATMENT NO 22      Z =    -650.0000      X VALUES:        5.0000        5.0000       10.0000
PROBABILITIES REVISED UPWARDS      FOR X(I,J(I)), ALL I, J(I) = 4 3 5
0.1013  0.0793  0.3129  0.3544  0.1522
0.2133  0.3290  0.1366  0.3211
0.0991  0.1702  0.2621  0.1479  0.0872  0.1670  0.0664
TREATMENT NO 23      Z =   -1980.0000      X VALUES:       -10.0000       10.0000       -5.0000
PROBABILITIES REVISED DOWNWARDS    FOR X(I,J(I)), ALL I, J(I) = 1 4 2
0.0857  0.0807  0.3183  0.3606  0.1548
0.2255  0.3477  0.1444  0.2824
0.1020  0.1458  0.2698  0.1523  0.0898  0.1719  0.0684
TREATMENT NO 24      Z =   -1310.0000      X VALUES:       10.0000       -5.0000        0.0000
PROBABILITIES REVISED DOWNWARDS    FOR X(I,J(I)), ALL I, J(I) = 5 1 3
0.0866  0.0815  0.3215  0.3642  0.1461
0.2139  0.3529  0.1466  0.2866
0.1039  0.1484  0.2567  0.1550  0.0914  0.1750  0.0696
TREATMENT NO 25      Z =     -10.0000      X VALUES:        0.0000        0.0000        0.0000
PROBABILITIES REVISED UPWARDS      FOR X(I,J(I)), ALL I, J(I) = 3 2 3
0.0821  0.0773  0.3568  0.3453  0.1385
0.2017  0.3897  0.1383  0.2703
0.0995  0.1422  0.2879  0.1485  0.0875  0.1677  0.0667
```

FINAL SAMPLING PHASE

```
TREATMENT NO 26      Z =   -2230.0000      X VALUES:        5.0000        0.0000       15.0000
TREATMENT NO 27      Z =    -630.0000      X VALUES:        5.0000       10.0000       10.0000
TREATMENT NO 28      Z =    -530.0000      X VALUES:        0.0000       10.0000        5.0000
TREATMENT NO 29      Z =   -2340.0000      X VALUES:       10.0000       10.0000       -5.0000
TREATMENT NO 30      Z =   -3090.0000      X VALUES:        5.0000       10.0000      -10.0000
TREATMENT NO 31      Z =    -270.0000      X VALUES:        5.0000       10.0000        5.0000
TREATMENT NO 32      Z =    -520.0000      X VALUES:        0.0000       10.0000        0.0000
TREATMENT NO 33      Z =   -1930.0000      X VALUES:       10.0000        0.0000       -5.0000
TREATMENT NO 34      Z =    -590.0000      X VALUES:        0.0000       -5.0000        5.0000
TREATMENT NO 35      Z =   -2890.0000      X VALUES:        0.0000        0.0000       15.0000
TREATMENT NO 36      Z =     -10.0000      X VALUES:        0.0000        0.0000        0.0000
TREATMENT NO 37      Z =    -570.0000      X VALUES:       10.0000       10.0000       10.0000
TREATMENT NO 38      Z =    -560.0000      X VALUES:        5.0000       10.0000        0.0000
TREATMENT NO 39      Z =    -320.0000      X VALUES:        0.0000        0.0000        5.0000
TREATMENT NO 40      Z =    -250.0000      X VALUES:        5.0000        0.0000        0.0000
```

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