OPTIMIZATION

by F. Horn

1. Introduction

A prerequisite for optimization is the existence of a mathematical model for the system we wish to optimize. It is convenient to distinguish between physical models and empirical models, although strictly speaking any model is empirical. In the case of a "physical model" experience is used which has accumulated over a comparatively long time period and which has been condensed into physical laws and data. In deriving an "empirical model" the experience utilized is of more recent nature and has been obtained by empirically relating the input and output of an existing system which is either identical or directly related to the system to be optimized. Therefore, there is no sharp dividing line between the two types of models. The physical approach (i. e., the use of physical models) has the advantage of greater generality; that is, a larger class of possible designs and operations can be taken into account. It has the disadvantage that the accuracy of the results is limited by the lack of exact data and by insufficient knowledge of the mechanism of the processes going on in the system under consideration. The opposite is true for the empirical approach to optimization (i. e., the use of empirical models). Here the model may be applicable only to a small neighborhood of the present operating conditions of an existing system but within this neighborhood the accuracy of the model can be much higher than the accuracy of an even very sophisticated physical model. In any practical optimization problem one should try to combine the physical and the empirical approach.

The mathematical optimization problem obtained by using mathematical models is characterized by the properties of the functions and their domains occurring in the statement of the problem. There is a large number of such properties (e. g., continuity, differentiability, unimodality, compositeness, linearity, convexity, etc.) and an even larger number of possible combinations of such properties. It is impossible to cover in one paper the various cases for which effective optimization methods have been devised. In the general field of chemical engineering com-

Editor's Note: Mr. Horn is Professor of Chemical Engineering at Rice University.

positeness seems to be the most interesting property of a function and therefore, special attention will be given to this case (section 3). An optimization method may lead to the optimum with certainty or it may be merely a device to improve on an existing situation without necessarily yielding the absolute optimum. The latter case is of particular interest in practical applications and will be discussed in section 4. In the following section (2) some of the fundamental concepts of optimization will be explained.

2. Policy Space and Objective Variables

The objective in optimization is to make the best choice among various possible choices or policies. In order to apply mathematical methods one has to represent the "various possible choices" by mathematical objects and to define what "best choice" means. In many practically important problems the possible choices can be represented by points in a space spanned by coordinates $x_1, x_2, \ldots x_n$, which are real numbers. Suppose we have two variables x_1 (e. g., a flow rate) and x_2 (e.g., a temperature or another flow rate) which can be chosen between the limits a_1, b_1 and a_2, b_2 respectively. Then the set of admissable combinations or policies (x_1, x_2) from which we have to pick up the best combination can be represented by the rectangular region shown in Fig. 1. We

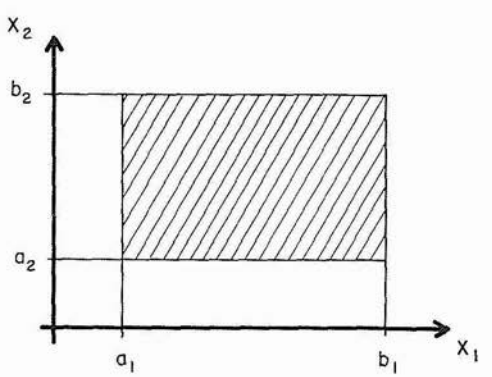

FIG. 1 - GEOMETRICAL REPRESENTATION OF A SIMPLE POLICY SPACE

refer to this region as the decision space or the policy space. The elements of the policy space are the points (x_1, x_2) of which it consists. The term

policy space will be used generally for the set of possible policies even if this set has too few or too many elements to be represented by what is called space in ordinary language. A finite policy space contains only a finite number of policies. For instance, in the problem of whether a batchwise or a continuous operation will give better results, the policy space contains only two elements. An infinite policy space contains infinitely many elements. The example represented by Fig. 1 is of this type. In the problem of finding a function, e. g., the flow rate of some substance, as function of the time, which will optimize the performance of a system, the policy space consists of all possible functions; i. e., it is a function space. The problem of finding the best element in a function space is called a variational problem. The function space is another example of an infinite policy space.

Often it is convenient to define the policy space as subspace of a larger space. The statements specifying the subspace are then called the restrictions. For the example given by Fig. 1 the restrictions are

$$\begin{aligned} a_1 \leq x_1 \leq b_1 \\ a_2 \leq x_2 \leq b_2 \end{aligned} \tag{1}$$

In a general function space we could impose the restrictions that the functions should be continuous or differentiable. In many cases the restrictions can be written as relations between real numbers. Then one can distinguish between equality and inequality restrictions. The restrictions (1) are inequality restrictions. The restriction

$$(x_1 - a_1)^2 + (x_2 - a_2)^2 = r^2 \tag{2}$$

is an equality restriction. This equation restricts the possible choices to the points on a circle of radius r about the point (a_1, a_2).

After some mathematical representation for the set of possible policies (i. e., the policy space) has been found, a criterion is needed for selecting the best policy. The most direct approach in any practical problem is to take as criterion the profit (expressed in dollars) one can expect as consequence of the choice of a policy. It may be more convenient, however, to base the criterion on some other variable which is known to be related to the profit, such as the amount of the desired substance produced, the purity of the product, or the cost of the process. In any case we have to know a functional relationship between the policy and the variable indicating the profit. This functional relationship is called the objective function and the variable indicating the profit is called the objective variable. The objective function can always be defined in such a way that a better policy is indicated by a larger objective function. If some cost is the decisive factor for the profit the negative cost can be taken as the objective variable.

For the decision space shown in Fig. 1 the objective function can be written in the form:

$$z = f(x_1, x_2) \tag{3}$$

The question arises whether or not there is a best point (x_1^*, x_2^*) in the sense that this point satisfies the restrictions (1) and that

$$f(x_1^*, x_2^*) \geq f(x_1, x_2) \tag{4}$$

for all points (x_1^*, x_2^*) satisfying the restrictions. In the case in question the existence of at least one such best point is guaranteed by a well-known mathematical theorem[1] if the function f is continuous. The value $f(x_1^*, x_2^*)$ is called the maximum of the function f on the objective space and the point (x_1^*, x_2^*) is called the optimum point or the optimum policy. There may be more than one optimum policy. It may be expected intuitively that the originating of an optimum problem from a practical situation guarantees the existence of an optimum policy. On account of the theorem mentioned above the ill-formulation of a problem is indeed unlikely if the policies can be represented by a finite set of real numbers (i. e., $x_1, x_2, \ldots x_n$). However, in the case of variational problems physical intuition often does not prevent ill-formulation.

It is convenient to generalize the concept of optimization developed thus far by considering cases with more than one objective variable. The usefulness of this will be discussed by means of an example. Suppose that a raw material A is to be transformed by chemical reaction into a substance Z_1 and that if the reaction is carried out inevitably some part of A is converted into an undesired isomer Z_2 which not only reduces the amount of Z_1 obtained but also makes the separation and purification of Z_1 more difficult. In Fig. 2 the box R represents the reaction process and the box S represents the separation and other processes carried out with the product (including selling). Only the flow of relevant information is indicated in this figure. Amount and quality of raw material are assumed to be given and constant and are therefore not indicated by arrows. The mixture obtained by the reaction process is characterized by the conversions z_1 to Z_1 and z_2 to Z_2. We shall assume that the reaction process is comparatively cheap so that the cost of this process can be neglected against the cost of the separation and the cost of raw material. In this case the profit z will be determined by z_1, z_2 and the decisions entering in separation, etc. That is, the decisions carried out in connection with the reaction process influence the profit only insofar as they influence the conversions z_1 and z_2.

Let us assume that for the problem in question the conversions to desired and undesired products are determined by the reaction time and by the way in which a given total amount of water is added during the

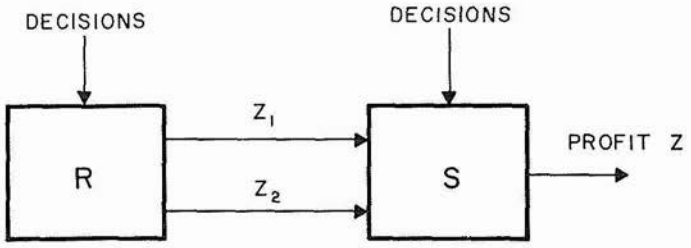

FIG. 2 - MODEL OF A SIMPLE CHEMICAL PROCESS CONSISTING OF REACTION UNIT R AND SEPARATION UNIT S.

reaction. A policy is then represented by a time t_e and an increasing function f(t) which assumes a given value at the time t_e (see Fig. 3). Since a functional relationship has to be optimized the problem is a variational problem. For given policy and given reaction kinetics z_1 and z_2 can be obtained by integrating the kinetic differential equations for the reactor. To each policy there belongs one point in a $z_1 - z_2$ diagram. One may ask for the set of points in this diagram obtained by considering all possible policies. This problem has been solved for a particular reaction system (introduction of a sulfo-group which can enter at two different positions) and the result is shown in Fig. 3. Not only the shape of this region is of interest but also the fact that any point at the boundary of the region can be obtained with only one particular water-policy while each point inside this region can be obtained by infinitely many policies. Without knowing the separation process in detail one can say that the profit will increase if z_1 increases and z_2 is kept constant, or if z_2 decreases and z_1 is kept constant. Because of this the optimum reaction process cannot correspond to an interior point of the region but only to a boundary point. More specifically the optimum operation must correspond to a point on the boundary between the points A and B. In this way we have, even without detailed knowledge of the separation processes, the huge entity of policies reduced to a comparatively small subset of policies, that is, to the set of policies corresponding to boundary points between A and B. Once these boundary points are known the optimization of the separation processes can be carried out without any other knowledge about the reaction process.

The variables z_1 and z_2 in the problem considered above are examples for objective variables. In general, the objective variables represent the

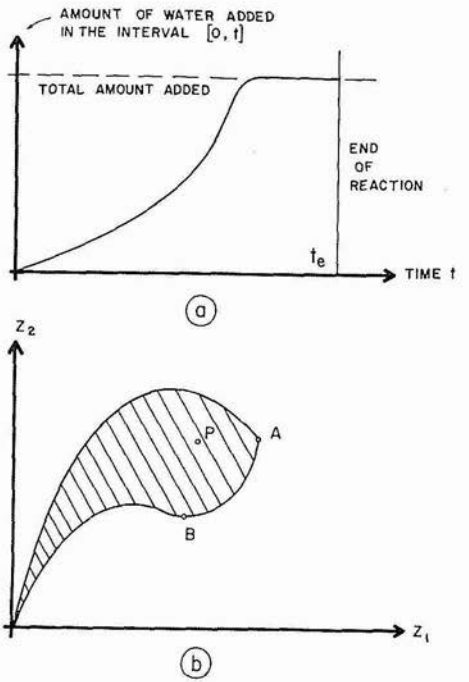

FIG. 3 - WATERPOLICY (UPPER DIAGRAM) AND ATTAINABLE REGION (LOWER DIAGRAM).
EACH POLICY TRANSFORMS INTO ONE POINT OF THE ATTAINABLE REGION.
E.G. THE POLICY SHOWN IN (a) MAY TRANSFORM INTO POINT P IN (b).
THERE ARE INFINITELY MANY POLICIES WHICH GENERATE P , BUT THERE IS ONLY ONE POLICY FOR EACH BOUNDARY POINT OF THE REGION.

links connecting the system under consideration with its environment. To each policy affecting the system there belongs a point or a set of points in the space spanned by the z_i The set of points obtained by considering all possible decisions is called the attainable region. If the attainable region is known, the optimum problem for the environment (the separation in the example given above) can be solved without any further knowledge about the system (the reaction process in the example). The boundary points of the attainable region are of special interest. The problem of finding boundary points is similar to the ordinary optimization problem with only one objective variable. In the latter case the problem can always be formulated in such a way that the attainable points on the profit line form a region as shown in Fig. 4. The maximum profit corresponds to the boundary point of this attainable region.

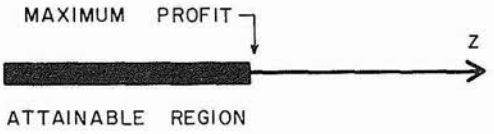

FIG. 4 - ONE DIMENSIONAL ATTAINABLE REGION

3. Optimization and the Structure of the Functional Relationship

Any optimization method has to rely on certain properties of the objective function such as continuity, differentiability, or linearity. In this section the property of a function to be composed of several functions will be considered. As an example take the function

$$z = f(x_1, x_2, x_3, x_4, x_5, x_6) \tag{5}$$

It is easy to show that it always will be possible to define two functions $y_1(x_1, x_2)$ and $y_2(x_2, x_3, x_4, x_5, x_6)$ and one function $F(y_1, y_2)$ in such a way that

$$f = F[y_1(x_1, x_2), y_2(x_2, x_3, x_4, x_5, x_6)]$$

On the other hand, it may or may not be that a particular f can be expressed in the form

$$f = F[y_1(x_1, x_2, x_3), y_2(x_4, x_5, x_6)] \tag{6}$$

If the function can be expressed in this form then one may ask whether this nontrivial fact can be utilized in the problem of maximizing the objective variable z. Cases in which the objective function can be shown to be nontrivially composite are quite frequent. Consider a process which consists of two subprocesses as shown in Fig. 5. The output y_1, y_2 of

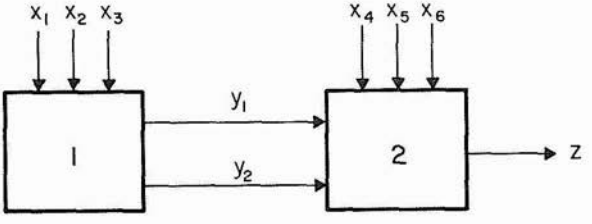

FIG. 5 - PROCESS CONSISTING OF TWO STAGES

subprocess 1 depends on the variables x_1, x_2, and x_3 and the output of subprocess 2 depends on its input which is equal to the output of subprocess 1 and on the variables x_4, x_5, and x_6. In this case the objective function can be written as in equation (6).

A somewhat more general situation is shown in Fig. 6. Here a set of N

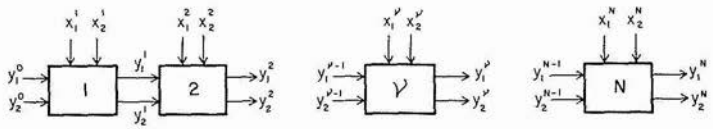

FIG. 6 - SEQUENCE OF N STAGES WITH TWO STATE - AND TWO DECISION VARIABLES PER STAGE

subprocesses or stages is operated such that the output of each stage except the first depends on the output of the previous stage and on some variable x. In such a case the output variables are also called the state variables and the variable x the decision variable. Fig. 6 shows a process in which there are two state and two decision variables for each stage. The following discussion can be extended easily to processes with an arbitrary number of state and decision variables for each stage. It will be assumed that the objective variable z depends on the output of the last stage only

$$z = F(y_1^N, y_2^N) \tag{7}$$

The relations between input and output of a stage are given by

$$\begin{aligned} y_1^\nu &= g_1^\nu (y_1^{\nu-1}, y_2^{\nu-1} ; x_1^\nu, x_2^\nu) \\ y_2^\nu &= g_2^\nu (y_1^{\nu-1}, y_2^{\nu-1} ; x_1^\nu, x_2^\nu) \end{aligned} \tag{8}$$

The objective of optimization is to choose the decision variables x_1^1, x_2^1; x_1^2, x_2^2, . . . in such a way that z becomes a maximum for given values y_1^0 and y_2^0 at the input of the first stage. This type of problem is encountered frequently in chemical engineering. The stages may represent reaction or separation processes, the state variables may refer to the composition of the material leaving a stage, and the decision variables may refer to temperatures or residence times. The objective variable z may be the value of the product leaving the last stage. It is therefore a function of the state variables of the stage N. If the cost of the operations represented by the stages has to be taken into account this can be taken care of by introducing a new state variable for each stage which represents the accumulated cost from the first stage to the stage under consideration.

The formidable problem of optimizing the whole process can be broken down into a set of more amenable problems by considering one stage after the other. Depending on whether the procedure starts at the first or the last stage this method will be called forward or backward optimization.

Forward Optimization Technique

Let us consider the space spanned by the variables y_1^1, and y_2^1. An attainable point in this space is defined as a point with coordinates corresponding to an output which can be obtained for the given input y_1^0, y_2^0 and for some admissable decision variables x_1^1, x_2^1. The term admissable refers to the possibility of having restrictions for the variables x_1^1, x_2^1. For the sake of the argument it will be assumed that the attainable region thus defined has a shape as indicated in Fig. 7b. If this region has been

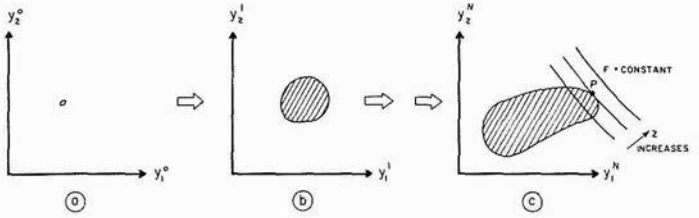

FIG. 7 - TRANSFORMATION OF ATTAINABLE REGIONS BY THE FORWARD METHOD. P CORRESPONDS TO THE OPTIMUM.

found, the attainable region in the y_1^2, y_2^2 space can then be constructed by determining all points in this space which can be obtained by some admissable decisions x_1^2, x_2^2 from some point belonging to the attainable region in the y_1^1, y_2^1 space. By repeated transformation of attainable regions, eventually the attainable region in the y_1^N, y_2^N space can be obtained. The optimization problem now is reduced to the problem of finding the maximum of the function $F(y_1^N, y_2^N)$ on the attainable region of the space spanned by the state variables of stage N. If the function F has the property that it cannot have a maximum for unrestricted arguments y_1^N and y_2^N the maximum must occur at the boundary of the attainable region. This case is shown in Fig. 7c. The best operating point corresponds to a point of tangency between the border of the attainable region and one of the contour lines

$$F(y_1^N, y_2^N) = \text{Constant}$$

of the function F.

By means of repeated transformation of attainable regions the overall effort for solving the optimization problem can be reduced considerably. Let us consider a possible numerical or experimental procedure. In any

such procedure infinite sets have to be approximately represented by finite sets. For instance, for each of the decision variables x, not infinitely many but only a finite number, a, of values may be taken into account. The total number of policies to be compared then is a^{2N}. If the serial structure of the system under consideration is not utilized all those policies have to be tried and the results compared. In the method of forward optimization the number of calculations or experiments per stage is approximately a^2b^2 if b is the number of values to be taken into account for each state variable. The numbers a and b which ensure reasonable accuracy will strongly depend on the particular problem. It may be that

$$a^{2N} \gg a^2b^2 \tag{9}$$

and then the method of forward optimization will be superior to a method which does not take advantage of the chainlike structure of the system. It can be seen that the condition (9) is likely to be satisfied if N is not a small number.

Backward Optimization Technique or Dynamic Programming

Let us consider now the spaces spanned by the variables y_1^ν, y_2^ν, and z. For a particular ν such a space represents the subsystem consisting of the stages $\nu+1, \nu+2, \ldots N$. A point with the coordinates y_1, y_2, z is attainable if for the state variables at stage ν corresponding to the first two coordinates there exist admissable $x_1^{\nu+1}$, $x_2^{\nu+1}$, $x_1^{\nu+2} \ldots . x_1^N$, x_2^N such that the value of the objective variable corresponding to the third coordinate is obtained. If the attainable points in the y_1^0, y_2^0, z space are known as well as the method by which they are generated, the optimum problem is solved, that is, not only for one particular input but for all possible inputs y_1^0, y_2^0. The attainable region in the y_1^N, y_2^N, z space is known a priori because this point set is the surface represented by the function $z=F(y_1^N, y_2^N)$. Thus all that is needed to solve the optimization problem is a procedure to transform the attainable region in the $y_1^{\nu+1}$, $y_2^{\nu+1}$, z space into the attainable region in the y_1^ν, y_2^ν, z space. By consecutively applying this procedure to the known attainable region at stage N eventually the attainable region in the y_1^0, y_2^0, z space can be found. The transformation of attainable regions can be carried out in the following way (see Fig. 8): to each state y_1, y_2 all possible operations in stage $\nu+1$ represented by all the admissable combinations of $x_1^{\nu+1}$, $x_2^{\nu+1}$ are applied. Each operation leads to a state $y_1^{\nu+1}$, $y_2^{\nu+1}$. The whole range of z values, which together with this state represent attainable points in the $y_1^{\nu+1}$, $y_2^{\nu+1}$, z space, is then combined with the original state y_1, y_2 to form attainable points in the y_1^ν, y_2^ν, z space. Each point is considered attainable in this latter space if it is generated by at least one operation. As in the forward optimization technique, a^2b^2 experiments or calculations are

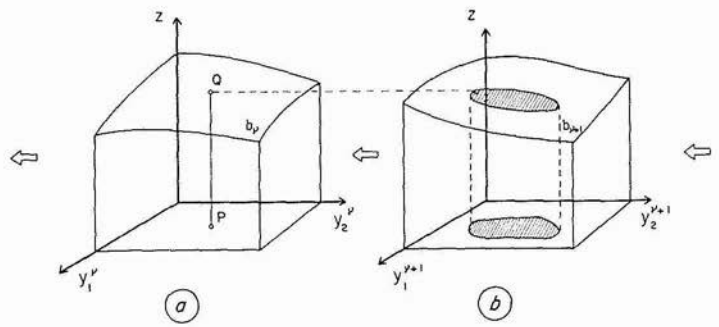

FIG. 8 - TRANSFORMATION OF ATTAINABLE REGIONS BY THE BACKWARD METHOD.
THE SURFACES b_ν AND $b_{\nu+1}$ ARE THE UPPER BOUNDARIES OF THE ATTAINABLE REGIONS.
THE LOWER SHADED REGION IN (b) REPRESENTS THE SET OF STATES $y_1^{\nu+1}, y_2^{\nu+1}$ WHICH CAN BE OBTAINED FROM THE STATE y_1^ν, y_2^ν REPRESENTED BY P, BY ADMISSIBLE DECISIONS $x_1^{\nu+1}$, $x_2^{\nu+1}$
THE DISTANCE $\overline{PQ}$ IS EQUAL TO THE MAXIMUM ELEVATION OF THE SURFACE $b_{\nu+1}$ OVER THE LOWER SHADED REGION.

needed in order to transform one attainable region into the other. Therefore, if the relation (9) is satisfied the backward optimization will be superior to a nonsequential technique.

It is interesting to compare both optimization techniques. In the forward method information is obtained (that is, the attainable region in the y_1^N, y_2^N, space) by means of which the solution for any objective function $F(y_1^N, y_2^N)$ can readily be achieved. On the other hand, this information is valid only for a particular input y_1^0, y_2^0 into the first stage. The opposite is true for the backward optimization method where for a particular objective function $F(y_1^N, y_2^N)$ optimum systems for various inputs y_1^0, y_2^0 are constructed. Which of the two methods, if any, should be applied to a particular problem depends largely on whether the one or the other type of information is of greater value. If the objective function is not yet exactly known, or even unknown, the forward method is the natural one, and if the problem has to be solved for various input conditions dynamic programming will be better suited than the forward method. In both methods, the system is separated at each step into two subsystems. In the forward method special attention is paid to the subsystem consisting of the stages $1, 2, \ldots \nu$. Its links with the environment are y_1^ν and y_2^ν (the input y_1^0, y_2^0 is considered fixed in this method). These variables are considered objective variables and accordingly the attainable region in the respective space is constructed. In dynamic programming special attention is paid to the subsystem $\nu + 1, \nu + 2, \ldots N$. Its

links with the environment are y_1, y_2, and z, and consequently attainable points in the space spanned by these variables are considered. The underlying principles of both methods can be seen to be essentially the same.

Thus far only the compositeness of the objective function has been utilized. If the objective function has no other useful property the methods described above can be of practical value. This would be the case, for instance, if there were indeed only a finite number of states and decisions or if a purely experimental procedure were to be followed. However, often the relevant relationships, e. g., the functions g_i in equation (8), are known and are differentiable with respect to their arguments. In this case advantage should be taken of the differentiability of the objective function as well as of its structural properties.

In the problem of optimizing the system shown in Fig. 6 the derivatives of the objective variable with respect to the decision variables at stage ν are given by:

$$\frac{\partial z}{\partial x_1^{\nu}} = \lambda_1^{\nu} \frac{\partial g_1^{\nu}}{\partial x_1^{\nu}} + \lambda_2^{\nu} \frac{\partial g_2^{\nu}}{\partial x_1^{\nu}}$$

$$\frac{\partial z}{\partial x_2^{\nu}} = \lambda_1^{\nu} \frac{\partial g_1^{\nu}}{\partial x_2^{\nu}} + \lambda_2^{\nu} \frac{\partial g_2^{\nu}}{\partial x_2^{\nu}} \tag{10}$$

Here for convenience new variables λ, the so-called adjoint variables, have been introduced. The λ's are determined by the relationships:

$$\lambda_1^N = \frac{\partial F}{\partial y_1^N} \qquad \lambda_2^N = \frac{\partial F}{\partial y_2^N} \tag{11}$$

$$\lambda_1^{\nu} = \frac{\partial g_1^{\nu+1}}{\partial y_1} \lambda_1^{\nu+1} + \frac{\partial g_2^{\nu+1}}{\partial y_1} \lambda_2^{\nu+1}$$

$$\lambda_2^{\nu} = \frac{\partial g_1^{\nu+1}}{\partial y_2} \lambda_1^{\nu+1} + \frac{\partial g_2^{\nu+1}}{\partial y_2} \lambda_2^{\nu+1} \tag{12}$$

$$= 0, 1, \ldots . N.$$

The adjoint variables have the following physical meaning: if the system is cut between the stages ν and $\nu + 1$ and all the decision variables in the part consisting of the stages $\nu + 1, \nu + 2, \ldots N$ are kept constant the objective variable z will be determined by the input into this part. That is, z can be considered as function of y_1 and y_2. The relations

$$\frac{\partial z}{\partial y_1^{\nu}} = \lambda_1^{\nu} \qquad \frac{\partial z}{\partial y_2^{\nu}} = \lambda_2^{\nu} \tag{13}$$

are then valid for the adjoint variables. By taking these relations as definitions one can easily derive equations (10) and (12) by means of the chain rule of differential calculus.

Let us assume now that the decision variables are unrestricted. Then for an optimum system the conditions

$$\frac{\partial z}{\partial x_1^{\nu}} = 0 \qquad \frac{\partial z}{\partial x_2^{\nu}} = 0 \tag{14}$$

must be satisfied for all ν. All together there are $6N + 2$ equations which must be satisfied for the optimum system: $2N$ equations (8), $2N + 2$ equations (11) and (12), and the $2N$ conditions obtained by setting the left hand sides in equations (10) equal to zero. There are also $6N + 2$ variables determining an optimum system: $2N$ state variables, $2N$ decision variables, and the $2N + 2$ adjoint variables. In general the $6N + 2$ equations admit only a finite number of solutions for the $6N + 2$ unknown variables. In exceptional cases infinitely many solutions exist. In any case the optimum conditions (14) reduce the set of all policies to a small subset in which the optimum policy must lie. For practical calculations it is important that the solutions of the $6N + 2$ equations mentioned above can be determined conveniently by either starting the solution procedure with the equations belonging to stage N or with the equations belonging to stage 1. The two methods correspond to forward and backward optimization discussed earlier. It is also possible to interpret these methods geometrically.

Only systems with a simple chainlike structure have been considered here. In chemical engineering the structure of systems is usually more complicated due to the presence of recycles. The methods discussed in this section can be adapted to cope with recycles. However, the effectiveness of these methods decreases as the structure of the system becomes more complex. For complex systems in general, search methods have to be employed. These are discussed in the next section.

4. Search Methods

In the previous section methods have been discussed which in principle lead to the optimum with certainty. In some cases (forward and backward optimization) all possible policies were, in effect, compared with each other and, in the method discussed last, necessary conditions (the equations [14]) were used to reduce the number of policies with the intent of picking the optimum policy from the small subset of policies which satisfy the necessary conditions. Due to the complexity of chemical systems these methods are sometimes impractical. If this situation arises a search method can be employed. The principle of the search methods is to assume arbitrarily a policy and to improve this policy repeatedly until no further significant improvement (that is, increase of the objective variable) can be obtained.

As an example let us consider a differentiable objective function which depends on two variables x_1 and x_2

$$z = f(x_1, x_2) \tag{15}$$

and which is represented by the contour diagram in Fig. 9. Consider the policy x_1', x_2' and suppose that the person faced with the optimum prob-

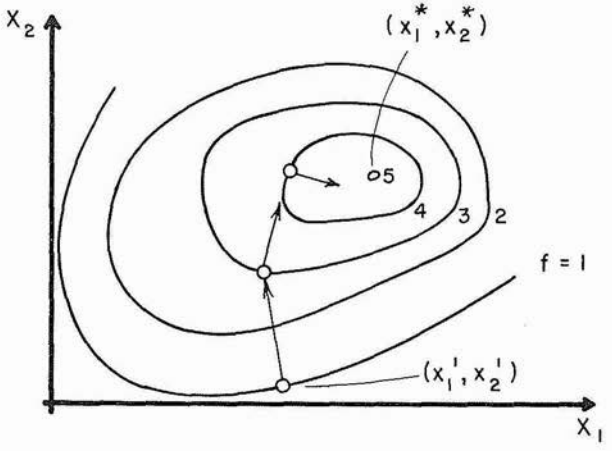

FIG. 9 - SUCCESSIVE IMPROVEMENTS OF A POLICY BY THE STEEPEST ASCENT METHOD.

lem knows only the values of the objective function and of its first derivatives at x_1', x_2' and has no other knowledge about the function. With this knowledge the original policy can be improved by changing the variables x_1' and x_2' in such a way that the point x_1', x_2' moves in the direction of the "steepest ascent," that is, the direction of the straight line perpendicular to the contour line through the original point. Mathematically, all points on this line are represented by:

$$x_1 = x_1' + s\,\frac{\partial f}{\partial x_1} \qquad x_2 = x_2' + s\,\frac{\partial f}{\partial x_2} \tag{16}$$

Where s=o and corresponds to the original point, the points with $s > o$ lie in the direction of steepest ascent from the original point. By choosing s positive but not too large (in order to avoid coming down on the other side of the hill) the original policy can be improved. This improvement can be carried out repeatedly as indicated in Fig. 9. At each step the step length must be chosen small enough to insure an increase of the objective function but it should not be selected too small to have sufficient progress at each step. In the example represented by Fig. 9 it is obvious that step length policies can be adopted which will make the procedure converge so that finally a good approximation for the optimum x_1^*, x_2^* is found. Fig. 10 shows a situation in which this search method would either lead to the optimal policy x_1^*, x_2^* or to the nonoptimal policy x_1^{**}, x_2^{**} depending

on the starting point. In practice the results can be checked by carrying out calculations for several starting points. The possibility of having missed the optimum becomes more and more unlikely as more starting points are explored.

The practical difficulties with search methods do not come so much from the occurrence of multiple hills (Fig. 10) as from the shapes of the

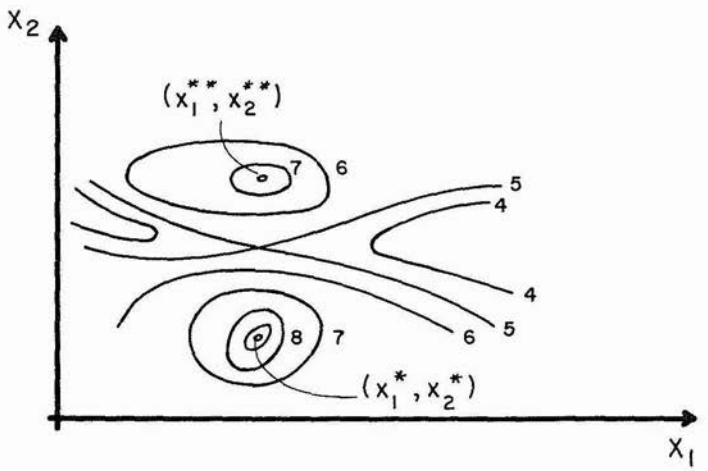

FIG. 10- CONTOUR DIAGRAM OF A FUNCTION WITH TWO LOCAL MAXIMA.

hills. Occasionally only a very narrow ridge leads to the optimum, and primitive search methods are not able to follow such ridges effectively, especially if the number of independent variables increases. The equations (16) and the following relevant equations are readily modified to cope with an arbitrary number of x variables, but for simplicity these equations are written for two dimensions only. Experience has shown that the method based on equations (16) is in many cases impractical because of slow convergence. The difficulties were removed when it was realized that, in the absence of any further information except the values of the objective function and of its first derivatives at the point to be improved, the direction of "steepest ascent" is, contrary to intuition, not a better choice than other directions corresponding to an increasing objective function. For instance, if equation (16) is replaced by

$$x_1 = x_1' + s\left(a_{11}\frac{\partial f}{\partial x_1} + a_{12}\frac{\partial f}{\partial x_2}\right)$$
$$x_2 = x_2' + s\left(a_{21}\frac{\partial f}{\partial x_1} + a_{22}\frac{\partial f}{\partial x_2}\right) \qquad (17)$$

where the coefficients a_{ik} satisfy

$$a_{11} > 0 \qquad a_{11}\,a_{22} - a_{12}\,a_{21} > 0 \qquad (18)$$

but are otherwise arbitrary, a method is obtained which on the average is as good as the method based on equations (16). Much better results can be obtained, however, if for a particular objective function special coefficients a_{ik} are selected or even better if the coefficients a_{ik} are changed at each improvement step according to information obtained in previous steps. The details of the method cannot be explained here. In principle the fact is utilized that in any search method the longer the search goes on the more potential information about the general shape of the objective function is available. While in the primitive search method (16) this information is wasted, in the more sophisticated method it is used for improving the improvement policy (characterized by the coefficients a_{ik}).

If the system represented by Fig. 6 were to be optimized by a search method the calculation would be as follows:

a) A policy $x_1^1, x_2^1; x_1^2, x_2^2, \ldots \quad x_1^N, x_2^N$ is selected.
b) The equations (8) are used to calculate all y's beginning at stage 1. Then z is calculated from equation (7).
c) λ_1^N and λ_2^N are calculated by means of equations (11). Then equations (12) are used to calculate all λ's starting at the last stage.
d) Now the derivatives of the objective function with respect to the decision variables are calculated by means of equations (10).
e) The improvement is carried out according to the search method adopted.

After step e) the improved policy is used again for the calculations in b). Then the sequence b) – e) is repeated. The whole procedure is repeated until no further significant increase of z can be obtained.

NOTE

1. A real valued continuous function defined on a closed and bounded subset of a n-dimensional Euclidian space possesses a maximum.