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OPTIMIZATION METHODS

FOR

COMPUTER-AIDED DESIGN

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Abstract This paper surveys recent automatic optimization methods which either have found or should find useful application in the optimal design of microwave networks by digital computer. Emphasis is given to formulations and methods which can be implemented in situations when the classical synthesis approach (analytic or numerical) is inappropriate. Objectives for network optimization are formulated including minimax and least pth. Detailed consideration is given to methods of dealing with parameter and response constraints by means of transformations or penalties. In particular, the formulation of problems in terms of inequality constraints and their solution by sequential unconstrained minimization is discussed. Several one-dimensional and multidimensional minimization strategies are summarized in a tutorial manner. Included are Fibonacci and Golden Section search, interpolation methods, pattern search, Rosenbrock's method, Powell's method, simplex methods, and the Newton-Raphson, Fletcher-Powell and least squares methods. Relevant examples of interest to microwave circuit designers illustrating the application of computer-aided optimization techniques are presented. The paper also includes a classified list of references.

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I INTRODUCTION

Fully automated design and optimization is surely one of the ultimate goals of computer-aided design. The amount of human intervention required to produce an acceptable design, even though this is often unavoidable, should, therefore, be regarded as a measure of our ignorance of the problem, our inability to specify our objectives in a meaningful way to the computer or our failure to anticipate and make provisions for dealing with the possible hazards which could be encountered in the solution of the problem.

An on-line facility which permits the user to propose a circuit configuration, analyze it and display the results may well be an invaluable educational and research tool providing the user with insight into certain aspects of his design problem. But even with the fastest analysis program it would be misleading to suggest that this method can be efficiently applied to the design and optimization of networks involving more than a few variables and anything other than the simplest of parameter and response constraints. For a fairly complex network optimization problem the number of effective response evaluations can easily run into the thousands even with the most efficient currently available automatic optimization methods before a local optimum is reached — and then only for that predetermined configuration.

Fully automated network design and optimization is still some way off. In the meantime, very effective use of the computer can be made by allowing the computer to optimize a network of predetermined allowable configuration automatically. If the results are unsatisfactory in some way, one could change the objective function, impose or relax constraints, try another strategy, alter the configuration, etc., whichever course of action is appropriate, and try again. Obviously, this can be executed either by batch processing or from an on-line terminal. There is no reason why the on-line designer should not avail himself of an efficient optimization program as well as an analysis program.

With the objective, therefore, of encouraging more effective use of computers, this paper surveys recent automatic optimization methods which either have found or should find useful application in computer-aided network design. Emphasis is given to formulations and methods which can be implemented in practical situations when the classical synthesis approach (analytic or numerical) is inappropriate. Objectives for network optimization including minimax and least pth are formulated and discussed.

Detailed consideration is given to methods of dealing with parameter constraints by means of transformations or penalties. This is rather important for microwave networks where the practical ranges of parameter values can be quite narrow, e.g., characteristic impedance values for transmission lines extend from about 15 to 150 ohms. The configuration, the overall size, the suppression of unwanted modes of propagation, considerations for parasitic discontinuity effects, the stabilization of an active device can all result in constraints on the parameters. Response constraints, which are less easy to deal with than parameter constraints, are also considered in some detail. In particular, the formulation of problems in terms of inequality constraints and their solution by sequential unconstrained minimization is discussed.

Several one-dimensional and multidimensional minimization strategies are summarized in a tutorial manner. Included are Fibonacci and Golden Section search, interpolation methods, pattern search and some variations including Rosenbrock's method, Powell's method, simplex methods, and the Newton-Raphson, Fletcher-Powell and least squares methods. Slightly more emphasis has been accorded to direct search methods than to gradient methods because they appear to date to have been more frequently employed in microwave network optimization. It is probably not widely appreciated that most direct search methods are superior, in general, to the classical steepest descent method and compare rather favourably with other gradient methods as far as efficiency and reliability are concerned. It is generally only near the minimum that differences in efficiency begin to manifest themselves between quadratically convergent and non-quadratically convergent methods — but quadratic convergence is not the prerogative of gradient methods as classified in this paper.

Section II introduces fundamental concepts and definitions. Section III formulates objectives for network optimization. Section IV deals with constraints. Section V describes one-dimensional optimization strategies, followed by Section VI which describes multidimensional direct search strategies and Section VII which describes multidimensional gradient strategies. Section VIII reviews some recent papers which report the application of various methods to network optimization. Finally, the references are divided into broad classifications: references of general interest [1-22], references recommended for direct search methods [23-55] and gradient methods [56-83], references dealing with applications to network design [84-119] and some miscellaneous references [120-126].

Inevitably, the material presented in this paper tends to reflect some of the author's current interests. Conspicuous omissions include Chebyshev polynomial and rational function approximation techniques using the Remez method or its generalizations [17,115,125]; and a discussion of optimization by hybrid computer in which the system is simulated on an analog computer while the optimization strategy is controlled by the digital computer [120,122]. The author apologizes in advance to all those researchers whose contributions he may not have done full justice to. He hopes, however, that the references adequately represent the state of the art of automatic optimization methods for computer-aided design. The use of such automatic computer-aided methods in microwave network design is not so well established as the use of computers in the numerical solution of electromagnetic field problems [126]. For this reason, there are not yet many microwave references to choose from to illustrate the optimization techniques.

II FUNDAMENTAL CONCEPTS AND DEFINITIONS

The problem is to minimize U where

$$U = U(\underline{\phi}) \tag{1}$$

and where

$$\underline{\phi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_k \end{bmatrix} . \tag{2}$$

U is called the objective function and the vector $\underline{\phi}$ represents a set of independent parameters. Minimizing a function is the same as maximizing the negative of the function, so there is no loss of generality.

In general, there will be constraints that must be satisfied either during optimization or by the optimum solution. Each parameter might be constrained explicitly by an upper and lower bound as follows:

$$\phi_{\ell i} \leq \phi_i \leq \phi_{ui} \qquad i = 1, 2, \ldots \; k \tag{3}$$

where ϕ_ℓ and ϕ_u are lower and upper bounds, respectively. Furthermore, the problem could be constrained by a set of h implicit functions

$$c_j(\underline{\phi}) \geq 0 \qquad j = 1, 2, \ldots \; h . \tag{4}$$

Any vector $\underline{\phi}$ which satisfies the constraints is termed feasible. It lies in a feasible region R (closed if equalities are admissible as in (3) or (4), open otherwise) as expressed by: $\underline{\phi} \in R$. It is assumed that $U(\underline{\phi})$ can be obtained for any $\underline{\phi} \in R$ either by calculation or by measurement.

Fig. 1 shows a 2-dimensional contour sketch which illustrates some features encountered in optimization problems. A hypercontour, described by the relation

$$U(\underline{\phi}) = U_{const.} \tag{5}$$

is the multidimensional generalization of a contour. The feasible region in Fig. 1 is determined by fixed upper and lower bounds on $\underline{\phi}$. The feasible region is seen to contain one <u>global minimum</u>, one <u>local minimum</u> and one <u>saddle point</u>. A minimum may be located by a point $\check{\underline{\phi}}$ on the <u>response hypersurface</u> generated by $U(\underline{\phi})$ such that

$$\check{U} = U(\check{\underline{\phi}}) < U(\underline{\phi}) \tag{6}$$

for any $\underline{\phi}$ in the immediate feasible neighbourhood of $\check{\underline{\phi}}$. (Since methods which guarantee convergence to a global minimum are not available, the discussion must restrict itself to consideration of local minima.) A saddle point is distinguished by the fact that it can appear to be a maximum or a minimum depending upon the direction being investigated. A more formal definition of a minimum follows.

The first three terms of the multidimensional Taylor series are given by

$$U(\underline{\phi} + \underline{\Delta\phi}) = U(\underline{\phi}) + \underline{\nabla U}^T \underline{\Delta\phi} + \frac{1}{2} \underline{\Delta\phi}^T \underline{H} \, \underline{\Delta\phi} + \ldots \tag{7}$$

where

$$\underline{\Delta\phi} = \begin{bmatrix} \Delta\phi_1 \\ \Delta\phi_2 \\ \vdots \\ \Delta\phi_k \end{bmatrix} \tag{8}$$

represents the parameter increments,

$$\underline{\nabla U} = \begin{bmatrix} \frac{\partial U}{\partial \phi_1} \\ \frac{\partial U}{\partial \phi_2} \\ \vdots \\ \frac{\partial U}{\partial \phi_k} \end{bmatrix} \tag{9}$$

is the gradient vector containing the first partial derivatives and

$$\underline{H} = \begin{bmatrix} \frac{\partial^2 U}{\partial \phi_1^2} & \frac{\partial^2 U}{\partial \phi_1 \partial \phi_2} & \cdots & \frac{\partial^2 U}{\partial \phi_1 \partial \phi_k} \\ \frac{\partial^2 U}{\partial \phi_2 \partial \phi_1} & \cdot & & \cdot \\ \vdots & & \cdot & \cdot \\ & & \cdot & \cdot \\ \frac{\partial^2 U}{\partial \phi_k \partial \phi_1} & \cdots & & \frac{\partial^2 U}{\partial \phi_k^2} \end{bmatrix} \tag{10}$$

is the matrix of second partial derivatives, the Hessian matrix. Assuming the first and second derivatives exist, a point is a minimum if the gradient vector is zero and the Hessian matrix is positive definite at that point.

A unimodal function may be defined in the present context as one which has a unique optimum in the feasible region. The presence of discontinuities in the function or its derivatives need not affect its unimodality. The example of Fig. 1 has two minima so it is called bimodal. A strictly convex function is one which can never be underestimated by a linear interpolation between any two points on its surface. Similarly, a strictly concave function is one whose negative is strictly convex. Examples of unimodal, convex and concave functions of one variable are illustrated in Fig. 2. (The word "strictly" is ommitted if equality of the function and a linear interpolation can occur.)

If the first and second derivatives of a function exist then strict convexity, for example, implies that the Hessian matrix is positive definite and vice versa. Consider the narrow curved valley shown in Fig. 3(a). It is possible to underestimate U by a linear interpolation along a contour, for example, which indicates that the function is nonconvex. Contours of this type do present some difficulties to optimization strategies. Ideally, one would like contours to be in the form of concentric hyperspheres, and one should attempt to scale the parameters to this end, where possible.

Fig. 3 shows contours of other two-dimensional optimization problems which present difficulties in practice. In Fig. 3(b), the minimum lies on a path of discontinuous derivatives; the constraint boundaries in Fig. 3(c) define a non-convex feasible region (a feasible region is convex if the straight line joining any two points lies entirely within the region); in Fig. 3(d) the minimum lies at a discontinuity in the function. Theorems which invoke the classical properties of optima or such concepts as convexity may not be so readily applicable to the problems illustrated in Figs. 3(b), (c) and (d), and yet the minima involved are quite unambiguously defined.

A number of the general references [1,17,19,20] give good introductions to the fundamental concepts and definitions used in the literature generally. Unfortunately, because of the diverse background of the authors concerned, there exists a profusion of different nomenclature. (The present author has probably added to this confusion.)

III OBJECTIVES FOR NETWORK OPTIMIZATION

In this section some objective function formulations for network optimization will be presented and discussed. The emphasis is on formulations which can allow explicit and implicit constraints, e.g. on the network parameters and responses, to be taken into account. This is felt to be particularly important in microwave network optimization where the range of permissible parameter values is often fairly narrow, the choice of physical configurations may be limited and parasitic effects can be acute. Thus, formulations which remain close to physical reality and aim towards physical and practical realizability are preferred, at least by this author.

Direct Minimax Formulation

An ideal objective for network optimization is

minimize U

where

$$U = U(\underline{\phi}, \psi) = \max_{[\psi_\ell, \psi_u]} [w_u(\psi)(F(\underline{\phi},\psi) - S_u(\psi)), - w_\ell(\psi)(F(\underline{\phi},\psi) - S_\ell(\psi))] \tag{11}$$

where $F(\underline{\phi}, \psi)$ is the response function

$\underline{\phi}$ represents the network parameters

ψ is an independent variable, e.g. frequency or time

$S_u(\psi)$ is a desired upper response specification

$S_\ell(\psi)$ is a desired lower response specification

$w_u(\psi)$ is a weighting factor for $S_u(\psi)$

$w_\ell(\psi)$ is a weighting factor for $S_\ell(\psi)$

ψ_u is the upper bound on ψ

ψ_ℓ is the lower bound on ψ.

This formulation is illustrated by Fig. 4. Fig. 4(a) shows a response function satisfying arbitrary specifications; Fig. 4(b) shows a response function failing to satisfy a bandpass filter specification; Fig.. 4(c) shows a response function just satisfying a possible amplifier specification. $F(\underline{\phi}, \psi)$ will often be expressible as a continuous function of $\underline{\phi}$ and ψ. But $S_\ell(\psi)$, $S_u(\psi)$, $w_\ell(\psi)$ and $w_u(\psi)$ are likely to be discontinuous.

The following restrictions are imposed:

$$S_u(\psi) \geq S_\ell(\psi) \tag{12}$$

$$w_u(\psi) > 0 \tag{13}$$

$$w_{\ell}(\psi) > 0. \tag{14}$$

Under these conditions $w_u(\psi)(F(\underline{\phi}, \psi) - S_u(\psi))$ and $-w_{\ell}(\psi)(F(\underline{\phi}, \psi) - S_{\ell}(\psi))$ are both positive when the specifications are not met; they are zero when the specifications are just met; and they are negative when the specifications are exceeded. The objective is, therefore, to minimize the maximum (weighted) amount by which the network response fails to meet the specifications; or to maximize the minimum amount by which the network response exceeds the specifications. Note the special case when

$$S_u(\psi) = S_{\ell}(\psi) = S(\psi) \tag{15}$$

and

$$w_u(\psi) = w_{\ell}(\psi) = w(\psi) \tag{16}$$

which reduces (11) to

$$U = \max_{[\psi_{\ell}, \psi_u]}[|w(\psi)(F(\underline{\phi},\psi) - S(\psi))|]. \tag{17}$$

This form may be recognized as the more conventional Chebyshev type of objective.

The direct minimax formulation, the optimum of which represents the best possible attempt at satisfying the design specifications within the constraints of the particular problem, appears to have received little attention in the literature on network optimization. This is chiefly due to the fact that discontinuous derivatives are generated in the response hypersurface when the maximum deviation jumps abruptly from one point on the ψ-axis to another, and that multidimensional optimization methods which deal effectively with such problems are rather scarce [89,100].

In spite of these difficulties, some success with objectives in the form of (17) has been reported [23,88]. But it is felt that considerable research into methods for dealing with objectives in the form of (11) remains to be done.

Formulation in Terms of Inequality Constraints

A less direct formulation than the previous one, but one which seems to have provided considerable success, is the formulation in terms of inequality constraints on the network response described by Waren, Lasdon and Suchman [18]. Their formulation will be slightly adjusted to fit in with the present notation.

The problem is

$$\text{minimize } U$$

subject to

$$U \geq w_{ui}(F_i(\phi) - S_{ui}) \qquad i \in I_u \tag{18}$$

$$U \geq - w_{\ell i}(F_i(\phi) - S_{\ell i}) \qquad i \in I_\ell \tag{19}$$

and other constraints, e.g. as in (3) where U is now an additional independent variable and where the subscript i refers to quantities (already defined) evaluated at discrete values of ψ which form the set $\{\psi_i\}$ in the interval $[\psi_\ell, \psi_u]$. The index sets I_u and I_ℓ, which are not necessarily disjoint, contain those values of i which refer to the upper and lower specifications, respectively. Thus, in the case of Fig. 4(a), the index set I_u and I_ℓ could be identical. For Fig. 4(b), the set I_u would refer to the passband and the set I_ℓ to the stop-bands. In Fig. 4(c), there might be an intersection between I_u and I_ℓ.

At a minimum at least one of the constraints (18) or (19) must be an equality otherwise U could be further reduced without any violation of the constraints. If $\check{U} < 0$ then the minimum amount by which the network response exceeds the specifications has been maximized. If $\check{U} > 0$ then the maximum amount by which the network response fails to meet the specifications has been minimized. It is clear that both this and the previous formulations have ultimately similar objectives. Indeed, if the sets I_u and I_ℓ are infinite then the optimum solutions given by both formulations may be identical. Not surprisingly such a problem may be described as one which has an infinite number of constraints. However, with finite I_u and I_ℓ the present formulation can be used in an optimization process which avoids the generation of discontinuous derivatives within the feasible region, as will be seen later (Section IV).

A special case again arises when

$$S_{ui} = S_{\ell i} = S_i \tag{20}$$

$$w_{ui} = w_{\ell i} = w_i \tag{21}$$

$$I_u = I_\ell = I \tag{22}$$

which reduces (18) and (19) to

$$U \geq w_i(F_i(\underline{\phi}) - S_i) \qquad i \in I \tag{23}$$

$$U \geq - w_i(F_i(\underline{\phi}) - S_i) \tag{24}$$

This formulation, which is an approximation to (17), has been successfully used by Ishizaki and Watanabe [102,103] (see Section VIII).

Weighting Factors

A discussion of the weighting factors is appropriate at this stage. Essentially, their task is to emphasize or deemphasize various parts of the response to suit the designer's requirements. For example, if one of the factors is unity and the other very much greater than unity then if the specifications are not satisfied, a great deal of effort will be devoted to forcing the response associated with the large weighting factor to meeting the specifications at the expense of the rest of the response. Once the specifications are satisfied, then effort is quickly switched to the rest of the response while the response associated with the large weighting factor is virtually left alone. In this way, once certain parts of the network response reach acceptable levels they are effectively maintained at those levels while further effort is spent on improving other parts.

Least pth Approximation

A frequently employed class of objective functions may be written in the generalized form

$$U = U(\underline{\phi},\underline{\psi}) = \sum_{i=1}^{n} |w_i(F_i(\underline{\phi}) - S_i)|^p = \sum_{i=1}^{n} |e_i(\underline{\phi})|^p \quad (25)$$

where

$$\underline{\psi} = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{bmatrix} \quad (26)$$

and where the subscript i refers to quantities evaluated at the sample point ψ_i . Thus, the objective is essentially to minimize the sum of the magnitudes raised to some power p of the weighted deviations $e_i(\underline{\phi})$ of the network response from a desired response over a set of sample points $\{\psi_i\}$. p may be any positve integer.

The sample points are commonly spaced uniformly along the ψ-axis in the interval $[\psi_\ell,\psi_u]$. If the objective is effectively to minimize the area under a curve then sufficient sample points must be used to ensure that (25) is a good approximation to the area. However, it should be remembered that function evaluations are often by far the most time consuming parts of an optimization process. So the number of sample points should be carefully chosen for the particular problem under consideration. These arguments apply, of course, to any formulation which involves sampling.

With $p = 1$, (25) represents the area under the deviation magnitude curve if sufficient sample points are used. With $p = 2$ we have a least squares type of formulation. Obviously, the higher the value of p the more emphasis will be given to those deviations which are largest. So if the requirement is to concentrate more on minimizing the maximum deviation a sufficiently large value of p must be chosen [17,79,100]. The basis of such a formulation is the fact that

$$\max_{[\psi_\ell,\psi_u]} [|e(\underline{\phi},\psi)|] = \lim_{p\to\infty} \left[\frac{1}{\psi_u - \psi_\ell}\int_{\psi_\ell}^{\psi_u} |e(\underline{\phi},\psi)|^p \, d\psi\right]^{\frac{1}{p}} \tag{27}$$

when $|e(\underline{\phi},\psi)|$ is defined in the interval $[\psi_\ell,\psi_u]$. In terms of a sampled response deviation the corresponding statement is

$$\max_i[|e_i(\underline{\phi})|] = \lim_{p\to\infty} [\sum_i |e_i(\underline{\phi})|^p]^{\frac{1}{p}} . \tag{28}$$

In practice, values of p from 4 to 10 may provide an adequate approximation for engineering purposes to the ideal objective. A good choice of the weighting factors w_i will also assist in emphasizing or deemphasizing parts of the response deviation. It may also be found advantageous to switch objective functions, number of sample points or weighting factors after any complete optimization if the optimum is unsatisfactory. For example, one may optimize with the weighting factors set to unity and with $p = 2$. If the maximum deviation is larger than desired, one could select appropriate scale factors and/or a higher value of p and try again from the previous "optimum".

Combined Objectives

The objective function can consist of several objectives. Indeed, the form of (11) and (25) suggest such a possibility. For example, we could have a linear combination

$$U = \alpha_1 U_1 + \alpha_2 U_2 + \ldots \tag{29}$$

where U_1, U_2, ... could take the form of (25). For an amplifier a compromise might have to be reached between gain and noise figure [93]; another example is the problem of approximating the input resistance and reactance of a model to experimental data [100]. The factors α_1, α_2, ... would then be given values commensurate with the importance of U_1, U_2, ..., respectively. If, however, these objectives can be represented instead as inequality constraints, alternative approaches are possible (Section IV).

IV CONSTRAINTS

Discussions on how to handle constraints in optimization invariably follow discussions on unconstrained optimization methods in most publications. This is unfortunate because the nature of the constraints and the way they enter into the problem can be deciding factors in the selection of an optimization strategy. And it is rare to find a network design problem which is unconstrained.

This section deals in particular with methods of reducing a constrained problem into an essentially unconstrained one. This can be accomplished by transforming the parameters and leaving the objective function unaltered, or by modifying the objective function by introducing some kind of penalty.

Transformations for Parameter Constraints

Probably the most frequently occuring constraint on the parameter values are upper and lower bounds as indicated by (3). These can be handled by defining ϕ_i' such that [3]

$$\phi_i = \phi_{\ell i} + (\phi_{ui} - \phi_{\ell i})\sin^2 \phi_i' . \tag{30}$$

If the periodicity caused by this transformation is undesirable and the constraints are in the form

$$\phi_{\ell i} < \phi_i < \phi_{ui} \tag{31}$$

which defines an open feasible region, one could try [86]

$$\phi_i = \phi_{\ell i} + \frac{1}{\pi}(\phi_{ui} - \phi_{\ell i})\cot^{-1} \phi_i' \tag{32}$$

where $-\infty < \phi_i' < \infty$ but where only solutions within the range

$$0 < \cot^{-1} \phi_i' < \pi \tag{33}$$

are allowed. This transformation has a penalizing effect upon the parameters in the vicinity of the upper and lower bounds. So if the optimum values are expected to lie away from the bounds this transformation may also introduce a favorable parameter scaling [86].

When the constraints are in the form

$$\phi_i \geq \phi_{\ell i} \tag{34}$$

one can use

$$\phi_i = \phi_{\ell i} + \phi_i'^2 \quad . \tag{35}$$

For

$$\phi_i > 0 \tag{36}$$

one can use

$$\phi_i = e^{\phi_i'} \quad . \tag{37}$$

Other transformations of variables can be found [3]. Well chosen transformations may not only reduce an essentially constrained optimization problem to an unconstrained one but might also improve parameter scaling.

Consider the constraint

$$\ell_{ij} \leq \frac{\phi_i}{\phi_j} \leq u_{ij} \tag{38}$$

which restricts the ratio of two parameters to be within a permissible range $[\ell_{ij}, u_{ij}]$. This type of constraint can occur when parasitic effects need to be taken into account [17, 88]. Suppose we consider the example

$$\ell \leq \frac{\phi_2}{\phi_1} \leq u \tag{39}$$

$$\phi_1 > 0 \tag{40}$$

$$\phi_2 > 0 \tag{41}$$

where $\ell > 0$ and $u > 0$. It may be verified that the transformations

$$\phi_1 = e^{z_1} \cos(\theta_\ell + (\theta_u - \theta_\ell)\sin^2 z_2) \tag{42}$$

and

$$\phi_2 = e^{z_1} \sin(\theta_\ell + (\theta_u - \theta_\ell)\sin^2 z_2) \tag{43}$$

where

$$0 < \theta_\ell = \tan^{-1}\ell < \theta_u = \tan^{-1}u < \frac{\pi}{2} \qquad (44)$$

ensure that for any z_1 and z_2 the constraints (39) to (41) are always satisfied.

Inequality Constraints in General

Unfortunately, one cannot always conveniently transform the parameters to incorporate constraints. With implicit constraints of the form of (4) transformations may be out of the question. ψ-dependent constraints in network optimization may, without loss of generality, be written as

$$c_j(\underline{\phi}, \psi) \geq 0 \qquad j = 1, 2, \ldots h \qquad (45)$$

in the interval $[\psi_\ell, \psi_u]$ or, at particular points ψ_i

$$c_j(\underline{\phi}, \psi_i) \geq 0 \qquad \begin{cases} i = 1, 2, \ldots n \\ j = 1, 2, \ldots h \end{cases} \qquad (46)$$

A microwave problem having constraints of this form has been described by Bandler [87]. It concerns a stabilizing network of a tunnel-diode amplifier where the objective was to minimize the square of the input reactance of the network at selected frequencies while maintaining certain specifications on the input resistance and reactance at different frequencies.(See Fig. 15).

If one is lucky, of course, one might be able to rely on the constraints not being violated. If, for example, a certain parameter must be positive but it is clear from the network configuration that as the parameter tends to zero the response deteriorates anyway then it may not be necessary to constrain the parameter. However, one can not always rely on good fortune so various methods for dealing with inequality constraints in general need to be discussed.

Let all the inequality constraints in a particular problem including the ψ-dependent ones be contained in the vector of m functions

$$\underline{g}(\underline{\phi}) = \begin{bmatrix} g_1(\underline{\phi}) \\ g_2(\underline{\phi}) \\ \vdots \\ g_m(\underline{\phi}) \end{bmatrix} \tag{47}$$

where the feasible region is defined by[1]

$$\underline{g}(\underline{\phi}) \geq \underline{0} . \tag{48}$$

For example, constraints in the form of (3) may be written

$$\begin{aligned} \phi_i - \phi_{\ell i} &\geq 0 \\ \phi_{ui} - \phi_i &\geq 0 . \end{aligned} \tag{49}$$

Finding a Feasible Point

Finding a feasible point to serve as the initial point in the constrained optimization process may not be easy. It may be found by trial and error [87] or by unconstrained optimization as follows:

Minimize

$$-\sum_{i=1}^{m} w_i g_i(\underline{\phi}) \qquad w_i \begin{cases} = 0 & g_i(\underline{\phi}) \geq 0 \\ > 0 & g_i(\underline{\phi}) < 0 \end{cases} \tag{50}$$

A minimum of zero indicates that a feasible point has been found.

Penalties for Non-Feasible Points

Assuming that the initial solution is feasible, the simplest way of disallowing a constraint violation is by rejecting any set of parameter values which produces a non-feasible solution. This may be achieved in direct search methods during optimization either by freezing the violating parameter(s) temporarily or by imposing a sufficiently large penalty on the objective function when any violation occurs. Thus, we may add the term

[1] It is hoped that the reader will not be too upset by $\underline{g}(\underline{\phi}) \geq \underline{0}$ which is used for $g_i(\underline{\phi}) \geq 0$, i = 1, 2, ... m.

$$\sum_{i=1}^{m} w_i g_i^2(\underline{\phi}) \qquad w_i \begin{cases} = 0 & g_i(\underline{\phi}) \geq 0 \\ > 0 & g_i(\underline{\phi}) < 0 \end{cases} \tag{51}$$

to the objective function. As long as the constraints are satisfied the objective function is not penalized. However, non-feasible points can be obtained with this formulation. An alternative which can prevent this is simply to set the objective function to its most unattractive value when $g_i(\underline{\phi}) < 0$. In practice such a value may be easy to determine on physical grounds.

There are disadvantages inherent in this simple approach to dealing with constraints. Depending on the type of penalty used, the objective function may be discontinuous or have steepvalleys at the boundaries of the feasible region, and its first or second derivatives may be discontinuous.

Any method which does not modify the objective function in the feasible region and simply causes non-feasible points to be rejected can run into the following difficulty: Consider the point A on the constraint boundary in Fig. 5. Clearly any exploration along a co-ordinate direction from A will result either in a non-feasible point or in an increase in the objective function. Similarly, any excursion along the path of steepest descent (see Section VII) results in a non-feasible point. This problem does not occur at B, however. Note that direct search methods (Section VI) in particular those good at following narrow curved valleys, might be able to make reasonable progress once a feasible direction is found. A rotation of co-ordinates might also alleviate the problem to some extent.

The Created Response Surface Technique[2]

This approach originally suggested by Carroll [60] and developed further by Fiacco and McCormick [63,64] involves the transformation of the constrained objective into a penalized unconstrained objective of the form

[2]References pertinent to this subsection have been included under gradient methods because of their association with gradient methods of minimization.

$$P(\underline{\phi}, r) = U(\underline{\phi}) + r \sum_{i=1}^{m} \frac{1}{g_i(\underline{\phi})} \tag{52}$$

where $r > 0$.

Define the interior of the region R of feasible points as[1]

$$R^o = \{\underline{\phi} | \underline{g}(\underline{\phi}) > \underline{0}\} \tag{53}$$

where

$$R = \{\underline{\phi} | \underline{g}(\underline{\phi}) \geq \underline{0}\} . \tag{54}$$

Starting with a point $\underline{\phi}$ and a value of r, initially r_1, such that $\underline{\phi} \in R^o$ and $r_1 > 0$ minimize the unconstrained function $P(\underline{\phi}, r_1)$. The form of (52) leads one to expect that a minimum will lie in R^o, since as any $g_i(\underline{\phi}) \to 0$, $P \to \infty$. The location of the minimum will depend on the value of r_1 and is denoted $\check{\underline{\phi}}(r_1)$.

This procedure is repeated for a strictly monotonic decreasing sequence of r values, i.e.,

$$r_1 > r_2 > \ldots r_j > 0 \tag{55}$$

each minimization being started at the previous minimum. For example, the minimization of $P(\underline{\phi}, r_2)$ would be started at $\check{\underline{\phi}}(r_1)$. Every time r is reduced, the effect of the penalty is reduced, so one would expect in the limit as $j \to \infty$ and $r_j \to 0$ that $\check{\underline{\phi}}(r_j) \to \check{\underline{\phi}}$ and, consequently, that $U \to \check{U}$, the constrained minimum.

During minimization, should a non-feasible point be encountered in some current search direction it can simply be rejected since a minimum can always be found in R^o by interpolation. If an interior feasible point is not initially available, an attempt to find one can be made either as indicated previously, or by repeated application of the present method [63]. In the latter case, the objective function in (52) is replaced by the negative of any violating constraint function and the satisfied constraints are included as the penalty term. When

[1] It is hoped that the reader will not be too upset by $\underline{g}(\underline{\phi}) \geq \underline{0}$ which is used for $g_i(\underline{\phi}) \geq 0$, $i = 1, 2, \ldots m$.

the constraint is satisfied, the minimization process is stopped and the procedure is repeated for another violating constraint.

Conditions which guarantee convergence have been proved by Fiacco and McCormick. They invoke the requirements that $U(\underline{\phi})$ be convex and the $g_i(\underline{\phi})$ be concave (see Section II) so that $P(\underline{\phi}, r)$ is convex. However, it is not unlikely that this method will work successfully on problems for which convergence cannot be readily proved.

To apply the created response surface technique to the formulation in terms of inequality constraints used by Waren et al. [18] and introduced in Section III, (52) may be rewritten as

$$P(\underline{\phi}, U, r) = U + r \sum_{i=1}^{m} \frac{1}{g_i(\underline{\phi}, U)} . \tag{56}$$

This brings out explicitly the fact that U is both the objective to be minimized and an independent parameter. The constraints $\underline{g}(\underline{\phi})$ are from (18) and (19)

$$U - w_{ui} (F_i(\underline{\phi}) - S_{ui}) \geq 0 \qquad i \in I_u \tag{57}$$

$$U + w_{\ell i} (F_i(\underline{\phi}) - S_{\ell i}) \geq 0 \qquad i \in I_\ell \tag{58}$$

and, for example, (49). Waren et al. [18] describe a method for allowing for parameter constraints to be initially violated so that a "reasonably good" initial design can be found. However, the method does not seem to guarantee that these constraints will be ultimately satisfied.

As might be expected, a bad initial value of r will slow down convergence onto each response surface minimum (as indeed a bad initial $\underline{\phi}$ will). Too large a value of r_1 will cause the first few minima of P to be relatively independent of U, whereas too small a value will render the penalty term ineffective, except near the constraint boundaries where the surface rises very steeply. Once the process is started, however, a constant reduction factor of 10 can be used for successive r values. Another disadvantage of this sequential unconstrained minimization technique (SUMT) is that second-order minimization methods are generally required for reasonably fast convergence to the constrained minimum.

Discussions and extensions of these techniques abound in the literature [63,64,69,72,77,83]. A book on applications of SUMT is also available [4].

Sufficient Conditions for a Constrained Minimum

Assuming $\underline{g}(\underline{\phi})$ to be concave and differentiable and $U(\underline{\phi})$ to be convex and differentiable, a constrained minimum at $\underline{\phi} = \check{\underline{\phi}}$ will satisfy

$$\underline{\nabla} U(\check{\underline{\phi}}) = \sum_{i=1}^{m} u_i \, \underline{\nabla} g_i(\check{\underline{\phi}}) \tag{59}$$

$$\underline{u}^T \underline{g}(\check{\underline{\phi}}) = 0 \tag{60}$$

where $\underline{u}$ is a column vector of non-negative constants and $\underline{\nabla} g_i$ is the gradient vector of the ith constraint function. These are the Kuhn-Tucker relations [123]. They state that $\underline{\nabla} U(\check{\underline{\phi}})$ is a non-negative linear combination of the gradients $\underline{\nabla} g_i(\check{\underline{\phi}})$ of those constraints which are active at $\check{\underline{\phi}}$. An interpretation of these ideas is sketched in Fig. 6. Note that these relations are not, for example, applicable to the case of Fig. 3(c), which is a serious drawback.

Other Methods for Handling Constraints

Other methods for handling constraints include, for example, Rosen's gradient projection method [73,74], Zoutendijk's method of feasible directions [22] and the method of Glass and Cooper [33]. These methods employ changes in strategy when constraint violations occur. They do not require a transformation of parameters or a penalty function. Thus, they can deal with difficulties such as the one illustrated by Fig. 5 and find a feasible direction yielding an improvement in the objective function. Further details may be found in some of the general references [16,19,20]. Alternative methods for dealing with constraints are also indicated, where appropriate, in the following sections.

V ONE-DIMENSIONAL OPTIMIZATION STRATEGIES

Many multidimensional optimization strategies employ one-dimensional techniques for searching along some feasible direction to find the minimum in that direction. A brief discussion of efficient one-dimensional strategies is, therefore, appropriate at this stage.

The methods can be divided into two classes, (1) the minimax direct elimination methods — minimax, because they minimize the maximum interval which could contain the minimum — and (2) the approximation methods. The latter are generally effective on smooth functions, but the former can be applied to arbitrary unimodal functions.

Fibonacci Search

The most effective direct elimination method is the Fibonacci search method [25,28,40,47,49,52]. It is so-called because of its association with the Fibonacci sequence of numbers defined by

$$\begin{aligned} &F_0 = F_1 = 1 \\ &F_i = F_{i-1} + F_{i-2} \qquad i = 2, 3, \ldots \end{aligned} \tag{61}$$

the first six terms, for example, being 1,1,2,3,5,8. Assume that we have obtained an initial interval $[\phi_\ell^1, \phi_u^1]$ over which the objective function is unimodal. At the jth iteration of the Fibonacci search using n function evaluations $(n \geq 2)$ we have

$$\phi_a^j = \frac{F_{n-1-j}}{F_{n+1-j}} I^j + \phi_\ell^j \tag{62}$$

$$\phi_b^j = \frac{F_{n-j}}{F_{n+1-j}} I^j + \phi_\ell^j \tag{63}$$

$j = 1, 2, \ldots n-1$ (for (62) and (63))

where

$$I^j = \phi_u^j - \phi_\ell^j \tag{64}$$

is the interval of uncertainty at the start of the jth iteration. An example for $n = 4$ is illustrated in Fig. 7. Observe that each iteration except the first actually requires only one function evaluation due to symmetry. This fact is summarized by the relationship

$$\text{If} \quad \begin{array}{l} U_a^j > U_b^j \\ U_a^j < U_b^j \end{array} \quad \text{then} \quad \begin{array}{l} \phi_\ell^{j+1}=\phi_a^j \ , \ \phi_a^{j+1}=\phi_b^j \ , \ \phi_u^{j+1}=\phi_u^j \\ \phi_\ell^{j+1}=\phi_\ell^j \ , \ \phi_b^{j+1}=\phi_a^j \ , \ \phi_u^{j+1}=\phi_b^j \end{array} \quad \text{and} \quad \begin{array}{l} U_a^{j+1} = U_b^j \\ U_b^{j+1} = U_a^j \end{array} \tag{65}$$

Note that the very last function evaluation should, according to this algorithm, be made where the previous one was made. It can, therefore, be ommitted if only the minimum value is desired. But to reduce the interval of uncertainty the last function evaluation should be made as close as possible to the previous one, either to the right or to the left.

The interval of uncertainty after j iterations is

$$I^{j+1} = \phi_u^j - \phi_a^j = \phi_b^j - \phi_\ell^j \tag{66}$$

reducing the interval I^j by a factor

$$\frac{I^j}{I^{j+1}} = \frac{F_{n+1-j}}{F_{n-j}} \ . \tag{67}$$

After $n - 1$ iterations, assuming infinite resolution, the total reduction ratio is

$$\frac{I^1}{I^n} = \frac{F_n}{F_{n-1}} \cdot \frac{F_{n-1}}{F_{n-2}} \cdots \frac{F_2}{F_1} = F_n \ . \tag{68}$$

For an accuracy of σ the values of n must be such that

$$F_{n-1} < \frac{\phi_u^1 - \phi_\ell^1}{\sigma} \leq F_n \ . \tag{69}$$

In the example of Fig. 7 the initial interval has been reduced by a factor of 5 after 4 function evaluations. Eleven evaluations would have reduced the interval by a factor of 144.

Search by Golden Section

Almost as effective as Fibonacci search, but with the advantage that n need not be fixed in advance, is the one-dimensional search method using the Golden Section [47,49,52].

It is readily shown for Fibonacci search that

$$I^j = I^{j+1} + I^{j+2} \qquad (70)$$

as may be verified by the example of Fig. 7. The same relationship between the intervals of uncertainty is true for the present method, with an added restriction that

$$\frac{I^j}{I^{j+1}} = \frac{I^{j+1}}{I^{j+2}} = \tau \qquad (71)$$

which leads to

$$\tau^2 = \tau + 1 \qquad (72)$$

the solution of interest being $\tau = \frac{1}{2}(1 + \sqrt{5}) = 1.6180 \ldots$ The division of a line according to (70) and (71) is called the Golden Section of a line.

The reduction ratio after n function evaluations is

$$\frac{I^1}{I^n} = \tau^{n-1} \quad . \qquad (73)$$

It can be shown that for Fibonacci search as $n \to \infty$

$$\frac{I^1}{I^n} = F_n \approx \frac{\tau^{n+1}}{\sqrt{5}} \quad . \qquad (74)$$

The ratio of effectiveness of the Fibonacci search as compared with the Golden Section is, therefore,

$$\frac{F_n}{\tau^{n-1}} \approx \frac{\tau^2}{\sqrt{5}} = 1.1708 \quad . \qquad (75)$$

Furthermore as $n \to \infty$

$$\frac{F_n}{F_{n-1}} \approx \tau \ . \tag{76}$$

Comparing (67) and (71) for $j = 1$ we see that the Fibonacci search and the Golden Section search start at practically the same point, the latter method ultimately providing an interval of uncertainty only some 17% greater than the former.

Golden Section search is frequently preferred because the number of function evaluations need not be fixed in advance.

Interpolation Methods

Several methods for finding a minimum have been proposed which repetitively fit a low order polynomial through a number of points until the minimum is obtained to the desired accuracy [28,41,47]. The essence of a typical method involving quadratic interpolation may be explained as follows:

At the jth iteration we have a unimodal function over $[\phi_\ell^j, \phi_u^j]$ with an interior point ϕ_m^j. Let $a = \phi_\ell^j$, $b = \phi_m^j$ and $c = \phi_u^j$. Then the minimum of the quadratic through a, b and c is at

$$d = \frac{1}{2}\,\frac{(b^2-c^2)U_a + (c^2-a^2)U_b + (a^2-b^2)U_c}{(b-c)U_a + (c-a)U_b + (a-b)U_c} \ . \tag{77}$$

Then ϕ_ℓ^{j+1}, ϕ_m^{j+1} and ϕ_u^{j+1} are obtained as follows:

$$\text{If} \begin{cases} b > d \text{ and } \begin{cases} U_b > U_d & \phi_\ell^{j+1} = a\ ,\ \phi_m^{j+1} = d\ ,\ \phi_u^{j+1} = b \\ U_b < U_d & \phi_\ell^{j+1} = d\ ,\ \phi_m^{j+1} = b\ ,\ \phi_u^{j+1} = c \end{cases} \\ b < d \text{ and } \begin{cases} U_b > U_d & \phi_\ell^{j+1} = b\ ,\ \phi_m^{j+1} = d\ ,\ \phi_u^{j+1} = c \\ U_b < U_d & \phi_\ell^{j+1} = a\ ,\ \phi_m^{j+1} = b\ ,\ \phi_u^{j+1} = d \end{cases} \end{cases} \tag{78}$$

The procedure may be repeated for greater accuracy, convergence being guaranteed.

This method and certain others like it, are said to have second order convergence. For this reason they can be more efficient on smooth, well-behaved functions than the Fibonacci search.

Finding Unimodal Intervals

The methods described so far rely on knowing in advance the unimodal interval which contains the desired minimum otherwise convergence onto it can not be guaranteed. Two situations can arise in practice which require a more cautious strategy.

One is that a given function is expected to be unimodal but the bounds on the unimodal interval are not known in advance. In this case, a quadratic extrapolation method similar to the interpolation method already discussed can be employed repetitively until the minimum is bounded [41,47]. Alternatively, a sequence of explorations may be performed until such bounds can be established. The second situation is when a given function is expected to be multimodal. In this case, it is advisable to proceed even more cautiously. The function should be evaluated at a sufficient number of uniformly spaced points to determine the unimodal intervals. Once unimodal intervals are established they can be shrunk further by a more efficient method. An example of a multimodal search strategy is the ripple search method [23].

VI MULTIDIMENSIONAL DIRECT SEARCH STRATEGIES

Methods which do not rely explicitly on evaluation or estimation of partial derivatives of the objective function at any point are usually called direct search methods. Broadly speaking, they rely on the sequential examination of trial solutions in which each solution is compared with the best obtained up to that time, with a strategy generally based on past experience for deciding where the next trial solution should be located.

Falling into the category of direct search are: random search; one-at-a-time search [25,50,53]; simplex methods [26,27,38,45,47]; pattern search and its variations [23,24,29,30,33-35,44,46,48,50,51,53,54] and some quadratically convergent methods [27,31,41,55]. Multidimensional extensions of Fibonacci search have also been reported [36,37]. Elimination methods are not as successful, however, as some of the climbing methods to be discussed.

One-at-a-time Search

In this method first one parameter is allowed to vary, generally until no further improvement is obtained, and then the next one, and so on. Fig. 8 illustrates the behaviour of this method. It is clear that progress will be slow on narrow valleys which are not oriented in the direction of any coordinate axis.

Pattern Search

The pattern search strategy of Hooke and Jeeves [34,50,53], however, is able to follow along fairly narrow valleys because it attempts to align a search direction along the valley. Fig. 9 shows an example of the pattern search strategy.

The starting point $\underline{\phi}^1$ is the first base point $\underline{b}^1$. In the example the first exploratory move from $\underline{\phi}^1$ begins by incrementing ϕ_1 and resulting in $\underline{\phi}^2$. Since $U^2 < U^1$, $\underline{\phi}^2$ is retained and exploration is continued by incrementing

ϕ_2. $U^3 < U^2$ so $\underset{\sim}{\phi}^3$ is retained in place of $\underset{\sim}{\phi}^2$. The first set of exploratory moves being complete, $\underset{\sim}{\phi}^3$ becomes the second base point $\underset{\sim}{b}^2$. A pattern move is now made to $\underset{\sim}{\phi}^4 = 2\underset{\sim}{b}^2 - \underset{\sim}{b}^1$, i.e., in the direction $\underset{\sim}{b}^2 - \underset{\sim}{b}^1$, in the hope that the previous success will be repeated. U^4 is not immediately compared with U^3. Instead, a set of exploratory moves is first made to try to improve on the pattern direction. The best point found in the present example is $\underset{\sim}{\phi}^5$ and, since $U^5 < U^3$, it becomes $\underset{\sim}{b}^3$, the third base point. The search continues with a pattern move to $\underset{\sim}{\phi}^8 = 2\underset{\sim}{b}^3 - \underset{\sim}{b}^2$.

When a pattern move and subsequent exploratory moves fail (as around $\underset{\sim}{\phi}^{13}$), the strategy is to return to the previous base point. If the exploratory moves about the base point fail (as at $\underset{\sim}{\phi}^8$) the pattern is destroyed, the parameter increments are reduced and the whole procedure restarted at that point. The search is terminated when the parameter increments fall below prescribed levels.

Constraints can be taken into account by addition of penalties as described by Weisman and Wood [48], or by the method of Glass and Cooper [33] who describe an alternate strategy for dealing with constraints. Algorithms of pattern search are available in the literature [24,35].

A variation of pattern search called spider, which seems to have enjoyed some success in microwave network optimization [53], has been described by Emery and O'Hagan [30]. The essential difference is that the exploratory moves are made in randomly chosen orthogonal directions. For this reason, there is less likelihood of the search terminating at a false minimum either in a sharp valley or at a constraint boundary as in Fig. 5. Spider can, therefore, be recommended as a useful general purpose direct search method.

Another variation of pattern search called razor search [23] has recently been proposed by Bandler and Macdonald to deal with "razor sharp" valleys, i.e., valleys along which a path of discontinuous derivatives lies. Such situations arise in direct minimax response formulations (Section III). An example [23,89] is shown in Fig. 10. When the basic pattern search strategy fails it is assumed that a sharp valley whose contours lie entirely within a quadrant of the coordinate axes has been encountered (or for that matter a constraint boundary as in Fig. 5) so a random move is made. When pattern search fails again it is assumed that the same valley (or boundary) is responsible and an attempt to establish a new pattern in the direction of the minimum is tried. The method has been successfully applied to microwave network optimization [23,88].

Rotating Coordinates

Rosenbrock's strategy [44] is to carry on exploring in directions parallel to the current coordinate axes until one success followed by one failure has occurred in each direction. Whenever a move is successful (objective function does not become greater than the current best value) the associated increment is multiplied by a factor α; whenever a move fails the increment is multiplied by $-\beta$. When the jth exploratory stage is complete, the coordinates are rotated as described below. First,

$$\begin{aligned} \underline{v}_k &= d_k \, \underline{u}_k^j \\ \underline{v}_i &= d_i \, \underline{u}_i^j + \underline{v}_{i+1} \qquad i = k-1, \ldots 1 \end{aligned} \tag{79}$$

where $\underline{u}_1^j, \underline{u}_2^j, \ldots \underline{u}_k^j$ are the orthogonal directions during the jth stage (initially the coordinate directions) and $d_1, d_2, \ldots d_k$ are the distances moved in the respective directions since the previous rotation of the axes. The new set of orthogonal unit vectors $\underline{u}_1^{j+1}, \underline{u}_2^{j+1}, \ldots \underline{u}_k^{j+1}$, the first of which always lies in the direction of total progress made during the jth stage, are obtained from (79) using the Gram-Schmidt procedure:

$$\left.\begin{aligned} \underline{w}_1 &= \underline{v}_1 \\ \underline{u}_1^{j+1} &= \frac{\underline{w}_1}{||\underline{w}_1||} \\ \underline{w}_i &= \underline{v}_i - \sum_{p=1}^{i-1} (\underline{v}_i^T \underline{u}_p^{j+1}) \underline{u}_p^{j+1} \\ \underline{u}_i^{j+1} &= \frac{\underline{w}_i}{||\underline{w}_i||} \end{aligned}\right\} \quad i = 2, 3, \ldots k \tag{80}$$

The process is then repeated. The search may be terminated after a predetermined number of function evaluations or when the total progress made during each of several successive exploratory stages becomes smaller than a predetermined value.

Fig. 11 shows a contour plot of Rosenbrock's test function which is frequently used for testing new strategies. Experimentally, Rosenbrock found that $\alpha = 3$, $\beta = -\frac{1}{2}$ gives a good efficiency. Constraints can be taken into account by Rosenbrock's boundary zone approach [44,47].

Swann [46] has described an improvement of Rosenbrock's method which employs linear minimizations once along each direction in turn, after which the coordinates are rotated [27,31,47].

More efficient methods of rotating the coordinate directions for Rosenbrock's and Swann's methods have been recently proposed [39,43].

Powell's Method

An efficient method devised by Powell [41] is based on the properties of conjugate directions defined by a quadratic function, namely

$$U(\underline{\phi}) = \underline{\phi}^T \underline{A} \underline{\phi} + \underline{b}^T \underline{\phi} + c \tag{81}$$

where $\underline{A}$ is a kxk constant matrix, $\underline{b}$ is a constant vector and c is a constant. The directions $\underline{u}_i$ and $\underline{u}_j$ are conjugate with respect to $\underline{A}$ if

$$\underline{u}_i^T \underline{A} \underline{u}_j = 0 \qquad i \neq j . \tag{82}$$

A two-dimensional example is shown in Fig. 12(a). The consequences of having mutually conjugate directions is that the minimum of a quadratic function can be located by searching for a minimum along each of the directions once.

The jth iteration involves a search for a minimum along k linearly independent directions $\underline{u}_1^j, \underline{u}_2^j, \ldots \underline{u}_k^j$. At the first iteration these are the coordinate directions. Denoting the starting point of the iteration $\underline{\phi}^0$, and the point arrived at after k minimizations $\underline{\phi}^k$, a new direction

$$\underline{u} = \underline{\phi}^k - \underline{\phi}^0 \tag{83}$$

is defined along which another search for a minimum is carried out. $\underline{u}_1^j$ is then discarded and the linearly independent directions for the (j+1)th iteration are defined as

$$[\underline{u}_1^{j+1}, \underline{u}_2^{j+1}, \ldots \underline{u}_k^{j+1}] = [\underline{u}_2^j, \underline{u}_3^j, \ldots \underline{u}_k^j, \underline{u}] \tag{84}$$

and the process is repeated.

If a quadratic is being minimized then after k iterations all the directions are mutually conjugate insuring quadratic convergence. One iteration of Powell's method is represented in Fig. 12(b). In its final form, the method is somewhat more involved than indicated here (see Powell [41] for details, and for the quadratically convergent linear minimization technique). In order to prevent the directions from becoming linearly dependent allowance is made for discarding directions other than $\underline{u}_1^j$. Comparisons with other methods are available [27,31]. Zangwill [55] has simplified Powell's modified method and presented a new one based on Powell's.

Simplex Methods

Simplex methods of nonlinear optimization [26,27,38,45,47] involve the following operations. A set of k+1 points are set up in the k-dimensional $\underline{\phi}$-space to form a simplex. The objective function is evaluated at each vertex and an attempt to form a new simplex by replacing the vector with the greatest value of the objective function by another point is made.

An efficient simplex method has been presented by Nelder and Mead [38]. The basic move is to reflect the vertex with the greatest value with respect to the centroid of the simplex formed by the remaining vertices. Depending on the outcome, the procedure is repeated or expansion, contraction or shrinking tactics are employed. Although remarkably efficient for up to four parameters, progress may be slow on problems having more than four parameters [27].

A two-dimensional example of a simplex strategy is given in Fig. 13. Examples of expansion ($\underline{\phi}^4$ to $\underline{\phi}^5$) and contraction ($\underline{\phi}^6$ to $\underline{\phi}^7$ and $\underline{\phi}^{10}$ to $\underline{\phi}^{11}$) are shown. Shrinking of the simplex about the vertex having the lowest value follows an unsuccessful attempt at contraction.

A simplex method developed for constrained optimization has been presented by Box [26,27,47].

VII MULTIDIMENSIONAL GRADIENT STRATEGIES

In this section methods are described which utilize partial derivative information to determine the direction of search. The appropriate partial derivatives (which are assumed to exist) may be obtained either by evaluating analytic expressions or by estimation.

The first derivatives can, for example, be estimated from the differences in the objective function produced by small perturbations in the parameter values, say .01 - 1% [78]. If the perturbations are too large the estimation will be inaccurate; if they are too small they can still be inaccurate through numerical difficulties. The presence of a narrow curved valley can further confound the issue. Thus, numerical estimation of derivatives must be made somewhat apprehensively

Steepest Descent

Referring to the multidimensional Taylor series expansion of (7) and neglecting the third term it is clear that a first order change ΔU in the objective function is given by

$$\Delta U = \underline{\nabla} U^T \underline{\Delta\phi} . \tag{85}$$

It is readily shown that maximum change occurs in the direction of the gradient vector $\underline{\nabla} U$. The steepest descent direction is, therefore, given by

$$\underline{s} = - \frac{\underline{\nabla} U}{||\underline{\nabla} U||} \tag{86}$$

where the unit vector $\underline{s}$ is the negative of the normalized gradient vector.

At the jth iteration of a simple steepest descent strategy we would have

$$\underline{\phi}^{j+1} = \underline{\phi}^j + \alpha^j \underline{s}^j \tag{87}$$

where α^j is a positive scale factor. It is usual to proceed in the $\underline{s}^j$ direction until no further improvement is obtained, evaluate $\underline{s}^{j+1}$, and continue called the generalized Newton-Raphson method [72,77].

Although quadratically convergent, the method has several disadvantages. $\underline{H}$ must be positive definite, implying that the function must be convex (see Section II), or divergence could occur. To counteract this tendency (91) can be modified to

$$\underline{\phi}^{j+1} = \underline{\phi}^{j} - \alpha^{j}\underline{H}^{-1}\underline{\nabla}U^{j} \tag{92}$$

where α^j is chosen to minimize U^{j+1} in the direction indicated by $-\underline{H}^{-1}\underline{\nabla}U^j$. But even this may be ineffective [72]. Thus, unlike steepest descent, the Newton-Raphson method may fail to converge from a poor starting point. Furthermore, the computation of $\underline{H}$ and its inverse are time consuming operations.

Fletcher-Powell

Generally acknowledged to be one of the most powerful minimization methods currently available when first derivatives are analytically defined, the Fletcher-Powell method [66] combines some of the more desirable features of steepest descent and the Newton-Raphson method. It is a development of Davidon's variable metric method [61]. A brief discussion of the method follows.

Redefine $\underline{H}$ as any positive definite matrix. Then at the jth iteration

$$\underline{\phi}^{j+1} = \underline{\phi}^{j} + \alpha^{j}\underline{s}^{j} \tag{93}$$

where

$$\underline{s}^{j} = -\underline{H}^{j}\underline{\nabla}U^{j} . \tag{94}$$

Here, $\underline{H}^j$ is the jth approximation to the inverse of the Hessian matrix. The initial approximation to $\underline{H}$ is usually the unit matrix. Notice that, in this case, the first iteration is in the direction of steepest descent (cf. (87)). The α^j are chosen to minimize U^{j+1}. $\underline{H}$ is continually updated during minimization (hence the name variable metric) such that [72]

$$\underline{\phi}^{j+1} - \underline{\phi}^{j} = \underline{H}^{j+1}[\underline{\nabla}U^{j+1} - \underline{\nabla}U^{j}]. \tag{95}$$

Thus, only first derivatives are required to update $\underline{H}$.

In practice the following procedure is adopted. Let

$$\underline{\Delta\phi}^j = \alpha^j \underline{s}^j \tag{96}$$

$$\underline{g}^j = \underline{\nabla}U^{j+1} - \underline{\nabla}U^j . \tag{97}$$

Set

$$\underline{H}^{j+1} = \underline{H}^j + \underline{A}^j + \underline{B}^j \tag{98}$$

where

$$\underline{A}^j = \frac{\underline{\Delta\phi}^j \; \underline{\Delta\phi}^{jT}}{\underline{\Delta\phi}^{jT} \; \underline{g}^j} \tag{99}$$

and

$$\underline{B}^j = \frac{-\underline{H}^j \underline{g}^j \underline{g}^{jT} \underline{H}^j}{\underline{g}^{jT} \underline{H}^j \underline{g}^j} . \tag{100}$$

The process is repeated from $\underline{\phi}^{j+1}$, replacing j by $j+1$.

Fletcher and Powell prove by induction that if $\underline{H}^j$ is positive definite then $\underline{H}^{j+1}$ is also positive definite, since $\underline{H}^0$ is taken as positive definite. Fletcher and Powell further prove that on a quadratic function, $\underline{H}^k$ is the inverse of the Hessian matrix and $\underline{\nabla}U^k = \underline{0}$. However, because of, say, accumulated round-off errors, one extra iteration corresponding to a Newton-Raphson iteration may be required. It is possible for divergence to occur if the α^j are not accurately chosen to minimize the function along $\underline{s}^j$. A check for this can be made and $\underline{H}$ reset to the unit matrix, if necessary.

Algorithms of the Fletcher-Powell method are available [59,65,80]. Several comparisons of its performance with other gradient methods have also been published [58,59,71,78]. The reader might also be interested in related methods and extensions which have been proposed [62,67,68,76], in particular, Stewart's modification [76] to accept difference approximations of the derivatives, and Davidon's recent <u>variance</u> algorithm [62].

Least Squares

When the objective function can be represented as a sum of squares of a set of functions, special techniques are available [56,59,78,82]. In this case

(25) becomes

$$U = \sum_{i=1}^{n} [e_i(\underline{\phi})]^2 \tag{101}$$

with $n \geq k$. Define the vector

$$\underline{e}(\underline{\phi}) = \begin{bmatrix} e_1(\underline{\phi}) \\ e_2(\underline{\phi}) \\ \vdots \\ e_n(\underline{\phi}) \end{bmatrix} \tag{102}$$

Then (101) can be written as

$$U = \underline{e}^T \underline{e} \tag{103}$$

and

$$\underline{\nabla} U = 2\underline{J}^T \underline{e} \tag{104}$$

where

$$\underline{J} = \begin{bmatrix} \frac{\partial e_1}{\partial \phi_1} & \frac{\partial e_1}{\partial \phi_2} & \cdots & \frac{\partial e_1}{\partial \phi_k} \\ \frac{\partial e_2}{\partial \phi_1} & \ddots & & \frac{\partial e_2}{\partial \phi_k} \\ \vdots & & \ddots & \vdots \\ \frac{\partial e_n}{\partial \phi_1} & \cdots & & \frac{\partial e_n}{\partial \phi_k} \end{bmatrix} \tag{105}$$

is an nxk Jacobian matrix. Using the first two terms of a Taylor series expansion

$$\underline{e}(\underline{\phi} + \underline{\Delta\phi}) \approx \underline{e}(\underline{\phi}) + \underline{J}\underline{\Delta\phi} \; . \tag{106}$$

Assuming $\underline{J}$ does not change from $\underline{\phi}$ to $\underline{\phi} + \underline{\Delta\phi}$ we may write (from (104))

$$\underline{\nabla} U(\underline{\phi} + \underline{\Delta\phi}) \approx 2\underline{J}^T[\underline{e} + \underline{J}\underline{\Delta\phi}] \; . \tag{107}$$

The least squares method then is to solve

$$\underline{J}^T \underline{e} + \underline{J}^T \underline{J} \, \underline{\Delta\phi} = \underline{0} \tag{108}$$

for the k components of $\underline{\Delta\phi}$ causing the gradient at $\underline{\phi} + \underline{\Delta\phi}$ to vanish. Note that $\underline{J}^T\underline{J}$ is a square matrix of rank k so that

$$\underline{\Delta\phi} = - [\underline{J}^T\underline{J}]^{-1}\underline{J}^T\underline{e} \ . \tag{109}$$

But from (104) $2\underline{J}^T\underline{e} = \underline{\nabla}U$. Now compare (109) with (90). Hence, the term $2\underline{J}^T\underline{J}$ corresponds to the Hessian matrix. The least squares method (sometimes called the Gauss method) is, therefore, analogous to the Newton-Raphson method. U is minimized when $[\underline{J}^T\underline{J}]^{-1}$ is positive definite which is generally true under the assumptions of the problem.

To avoid divergence, however, the jth iteration is often taken as

$$\underline{\phi}^{j+1} = \underline{\phi}^j + \alpha^j \underline{\Delta\phi}^j \tag{110}$$

where α^j, as for the previous methods, may be chosen so as minimize U^{j+1}. With $\alpha^j < 1$ we have one possible form of <u>damped least squares</u>.

Other variations to the least squares method to improve convergence are available [78, 82]. Powell [42] has presented a procedure for least squares which does not require derivatives, these being approximated by differences.

<u>Least pth</u>

Temes and Zai [79] have recently generalized the least squares method to a <u>least pth method</u>, where p is any positive even integer. They report improved convergence but also discuss damping techniques similar to those used in least squares. The advantages of using a large value of p as far as reducing the maximum response deviation is concerned are discussed in Section III, so the method should be of considerable interest to network designers. The derivation is analogous to the least squares method which falls out as a special case.

VIII APPLICATION TO NETWORK OPTIMIZATION

A list is appended of selected references [84-119] on the application of various methods to the optimal design of networks which should be of interest to microwave engineers. Most of these are briefly discussed and commented upon in this section.

Least pth Objectives

Weighted least squares objectives with the sample points nonuniformly distributed along the frequency axes have been used to design LC ladder filters in the presence of loss [95,110]. Desoer and Mitra [95] used a steepest descent method, while Murata [110] used s simple direct search method. A comparison of the rather unfavourable results obtained by these formulations with alternative formulations is presented by Temes and Calahan [116].

Sheibe and Huber [112] used a least squares objective function with the created response surface technique (Section IV) to optimize a transistor amplifier subject to various parameter constraints including realistic Q values. Their aim was to fit the gain curve to a desired trapezoidal shape. It turned out that the Q value of one of the tuned circuits was forced to its maximum value, and the response at higher frequencies was rather poor.

An investigation into the design and optimization of LC ladder networks to match arbitrary load immittances to a constant source resitance has been reported by Hatley [100]. After experimentation with several objective functions of the form of (25) on a 6-element resistively terminated LC transformer, $\sum_i |\rho_i(\underline{\phi})|^4$ was chosen, where ρ is the reflection coefficient, even though $\max |\rho|$ was .08870 after optimization as compared with the known optimum value of .07582. A new minimization technique called the method of quadratic eigenspaces is presented and compared with the Fletcher-Powell method. Examples are presented involving antenna matching, the antennas being characterized by measured data rather than models.

The application of the least pth method developed by Temes and Zai [117] (Section VII) was applied to the optimization of a four-variable RC active equalizer with $p = 10$. The maximum deviation from the desired specification for $p = 2$ was found to be 33% higher. Temes and Zai demonstrated the non-uniqueness of the optimum — they obtained different solutions with different starting points. Indeed, two of the four elements were found to be essentially redundant. The necessity of some experimentation, in general, before accepting an apparently optimal solution (by any numerical optimization procedure) is shown by this example. It is interesting to speculate that since the least pth solution will generally not be the minimax solution, although they could be fairly close, it may be possible to obtain a smaller maximum deviation than given by the least pth solution while still searching for it. The optimization program could check for this possibility.

Inequality Constraints

Two distinct methods of optimizing networks when the objectives are formulated in terms of inequality constraints (Section III) and when minimax solutions are required have been reported.

One of these [102,103] reduces the nonlinear programming problem to a series of linear programming problems. The constraints are in the form of (23) and (24). The response function $F_i(\underline{\phi})$ or the deviation $e_i(\underline{\phi})$ is linearized at a particular stage in the optimization process and the linear programming problem thus created can be solved by the simplex method of linear programming [9,20] to reduce U for that stage. Unfortunately, however, because of the linear approximations made, it is possible that the original constraints are violated and that U is not actually minimized. Sufficient under-relaxing (or damping) may be required to guarantee that $U^{j+1} < U^j$ and that in the limit the process converges to the desired minimax response. A detailed discussion of this method is presented by Temes and Calahan [116]. The paper by Ishizaki and Watanabe [103] presents examples including the design of attenuation equalizers and group delay equalizers. It is felt that their method should have wide application. The reader may also be interested in another recent contribution for nonlinear minimax approximation [124].

The other method which is reviewed by Waren et al [119], uses the sequentail unconstrained minimization technique, the advantages and disadvantages of which are discussed in Section IV. They recommend quadratically convergent minimization methods such as the Fletcher-Powell method (Section VII) or Powell's method (Section VI) for rapid convergence to each response surface minimum. Several successful applications have been reported [85,106,107,118,119]. For example, cascade crystal-realizable lattice filters have been optimized from approximate initial designs, including realistic losses and bounds on the element values [107,118,119]. Also of interest to microwave engineers might be the optimization of linear arrays, where allowing additional degrees of freedom can result in improved designs [106], and the more recent extension to planar arrays [119].

Microwave Networks

Several reports of the application of computer-aided optimization methods of varying sophistication to microwave network problems can be found in the literature [84,86-90,93,97,99,101,104,108,114]. A number of these [88,90,104,108] are found elsewhere in this issue.

One example which demonstrates the effectiveness of computer-aided optimization techniques [87] involved the optimization of the transmission-line network shown in Fig. 15 which was to be used for stabilizing and biasing a tunnel-diode amplifier. The requirements of stability and low noise broadband amplification in conjunction with the rest of the circuitry (rectangular waveguide components including circulator, matching network and tuning element) imposed nonsymmetrical response restrictions on the input resistance and reactance of the network as shown in Fig. 15. Upper and lower bounds on the final parameter values were also imposed. The objective was to minimize the sum of squares of the input reactance at selected frequencies. A simple direct search method was used, which rejected non-feasible solutions, an initial feasible solution being found by trial and error. An alternative, and perhaps more elegant, approach would have been the implementation of the sequential unconstrained minimization technique.

Another area in which the computer can be effectively used is the design and optimization of broadband integrated microwave transistor amplifiers [93,97, 99]. A block diagram of a two-stage amplifier is shown in Fig. 16. The transistors are usually characterised experimentally at selected frequencies in the band of interest and under the conditions (e.g., operating power level) in which they are to be used. The representation can, for example, be in the form of input and output admittance [97], ABCD matrix [93] or scattering matrix [99]. It may also be an advantage to fit the measured data versus frequency to a suitable function in a least-squares sense [93,97].

The input,output and interstage matching networks usually consist of noncommensurate transmission lines and stubs. The line lengths and characteristic impedances are allowed to vary within upper and lower bounds during the optimization of the amplifier. The spider search method (Section VI) has been applied to the design of such matching networks [97]. The objective functions commonly take the form of (25) with $p = 1$ or 2. It is felt, however, that better designs might be achieved by using larger values of p or a minimax objective like (17) to reduce, for example, the maximum deviation of the gain versus frequency from the desired gain. The method of Temes and Zai [117] would be quite appropriate in the former case, while the razor search method [90] could be used in the latter. Since it is difficult to realize component values in integrated circuitry very accurately, the optimal solution should also satisfy appropriate sensitivity constraints.

Multisection inhomogeneous rectangular waveguide impedance transformers (Fig. 17) have been optimized in a minimax equal-ripple sense [88] by the razor search strategy [90] (see Section VI). Suitable parameter constraints — the parameters were the physical dimensions — were imposed to ensure dominant mode propagation and reasonably small junction discontinuity effects which could be taken into account during optimization. Improvements in performance coupled with reduction in size over previous design methods are reported [88].

Automated Design

Approaches to automated network design and optimization which can permit new elements to be "grown" have been suggested by Rohrer [111] and Director and Rohrer [96]. The latter paper, a significant contribution, discusses design in the frequency domain of circuits comprising certain types of lumped, linear, time-invariant elements. A technique is presented whereby the gradient vector of a least squares type of objective function is shown to require only two analyses over the frequency range of interest regardless of the number of variable parameters! And because this gradient depends only on currents and voltages, gradients with respect to nonexistent elements can be calculated. If such a gradient indicates an increase in an element value an appropriate element is grown in the appropriate location. The authors consider an example of broadbanding a transistor amplifier in which they allow for the possibility of growing a number of capacitors. Apparently one has to specify in advance the locations where elements can grow.

IX CONCLUSIONS

It is hoped that this paper will not only encourage the use of efficient optimization methods, but will also stimulate the engineer into developing new ones more suited to his design problems. After all, as exemplified by this paper, few optimization strategies have been reported so far which were originally developed with electrical networks in mind. It is also hoped that the present almost instinctive preoccupation with least squares formulations may give way to more attention being paid to minimax objectives and efficient methods of realizing them. Least squares objectives may be flexible and easy to optimize. It is probably their flexibility, however, which is their undoing since any designer who is essentially trying to fit a network response between certain upper and lower levels and is using a least squares objective function may have to employ more human intervention than necessary to achieve an acceptable design. On the other hand, the designer who is employing a minimax objective directly and does not recognize the possible dangers, e.g. of discontinuous derivatives, can easily obtain an equal-ripple response which is still far from the optimum. On-line designers optimizing a network manually with the objective of minimizing the maximum deviation of the network response from a desired response are equally prone to these dangers. An equal ripple solution need not necessarily be the minimax solution.

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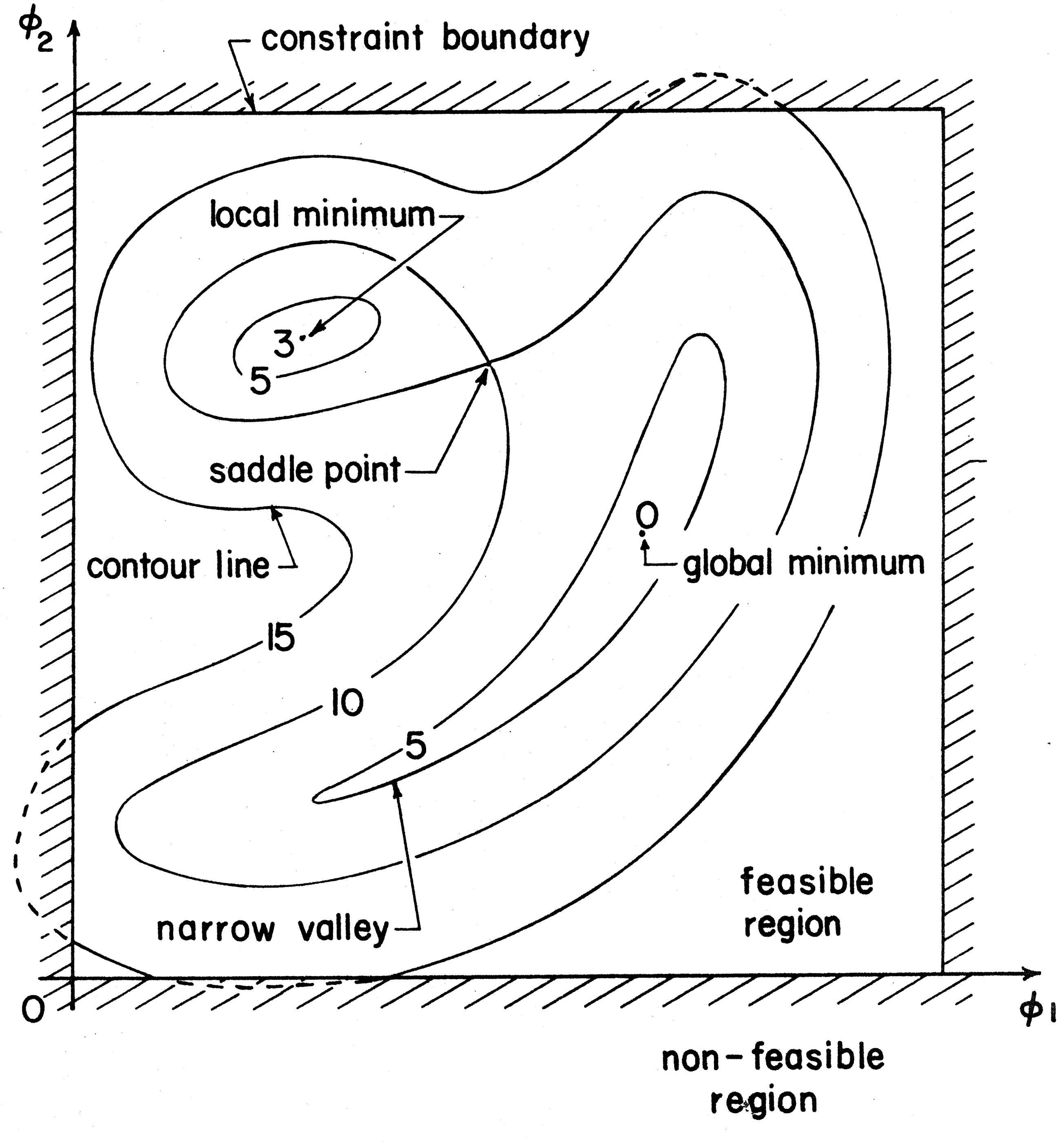

Fig. 1 Two-dimensional contour sketch illustrating some features encountered in optimization problems.

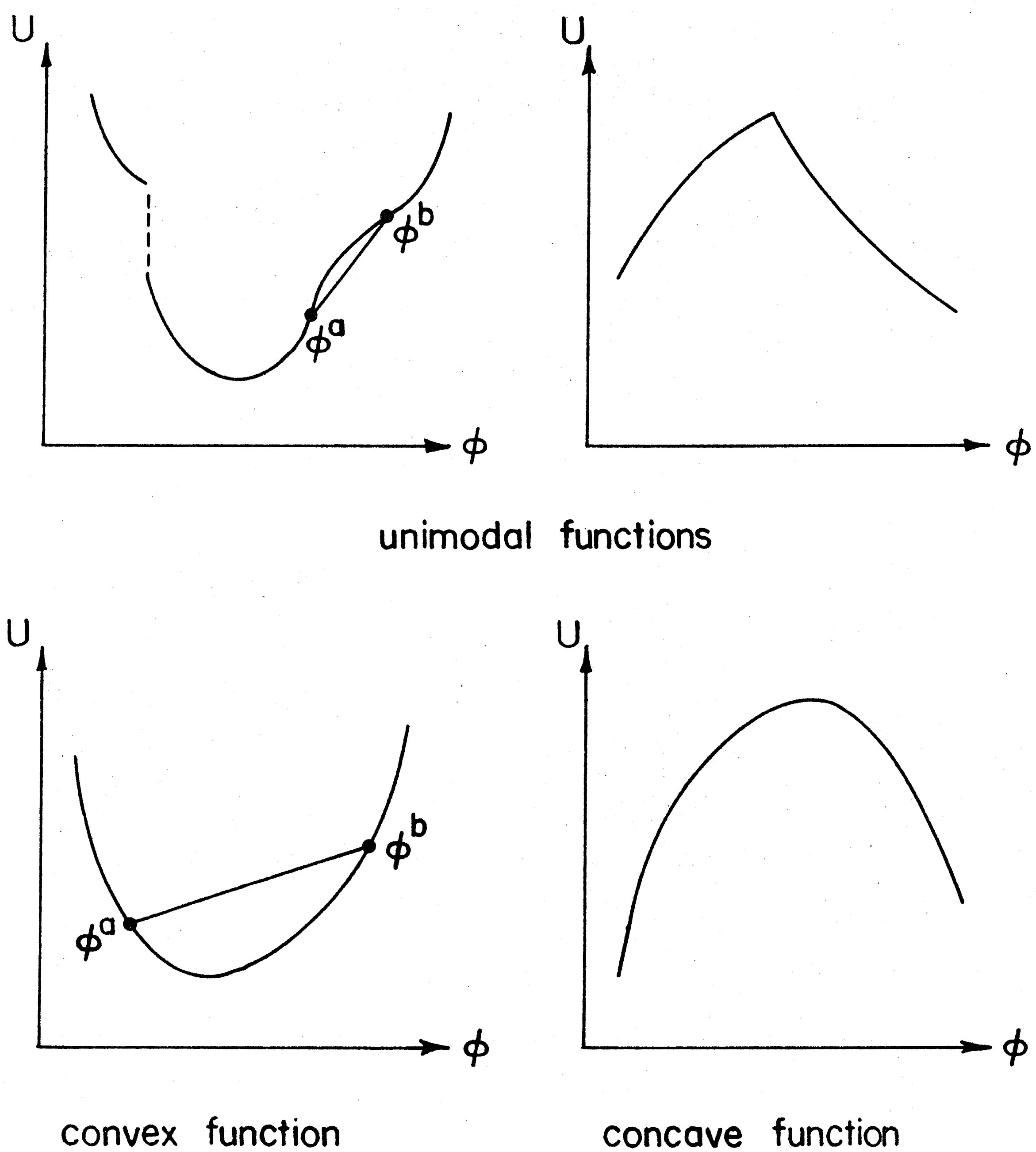

Fig. 2 Examples of unimodal, convex and concave functions of one variable.

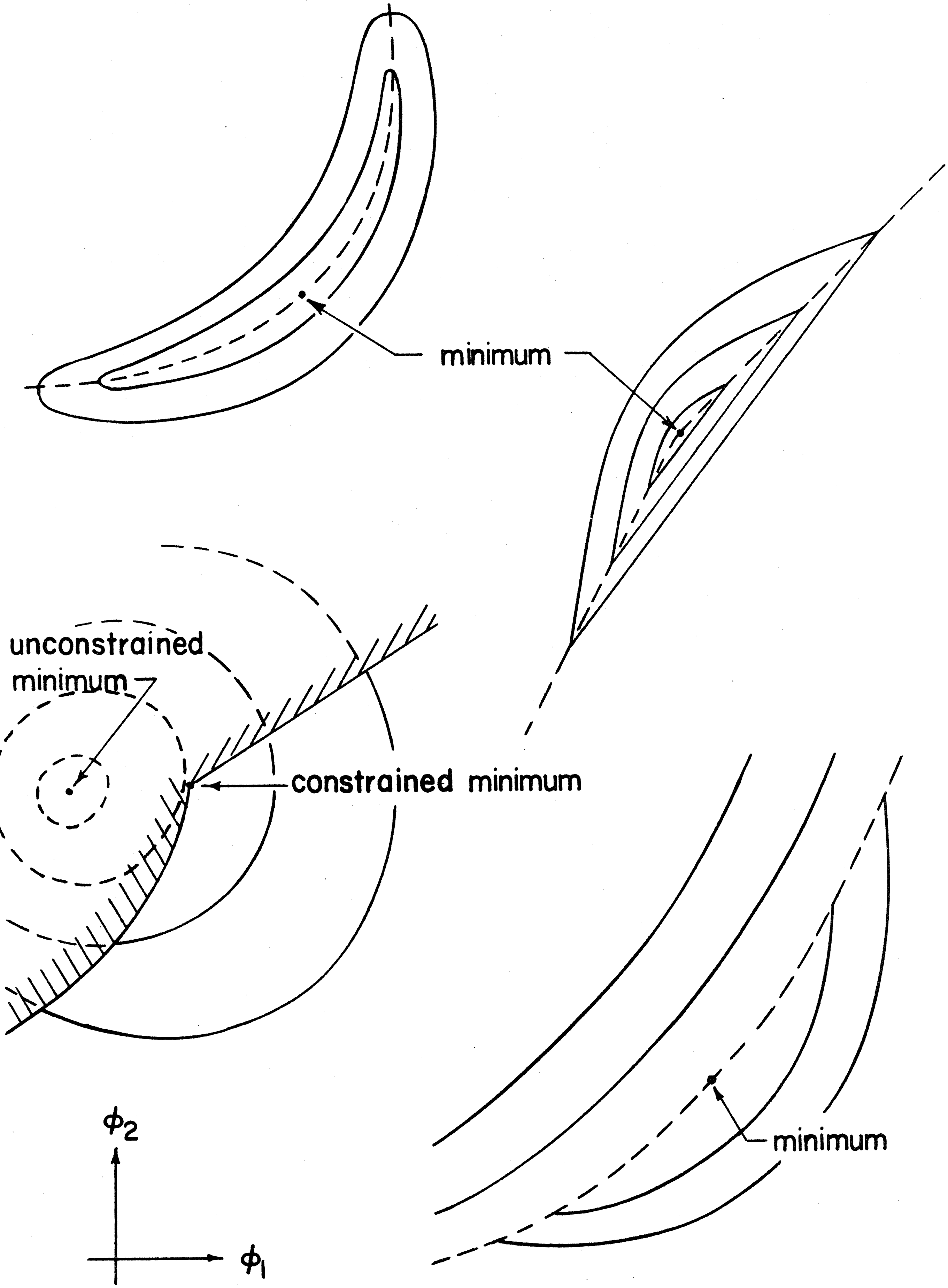

Fig. 3 Contours which present difficulties to optimization strategies, (a) a narrow curved valley, (b) a narrow valley along which a path of discontinuous derivatives lies, (c) a non-convex feasible region, and (d) a discontinuous function.

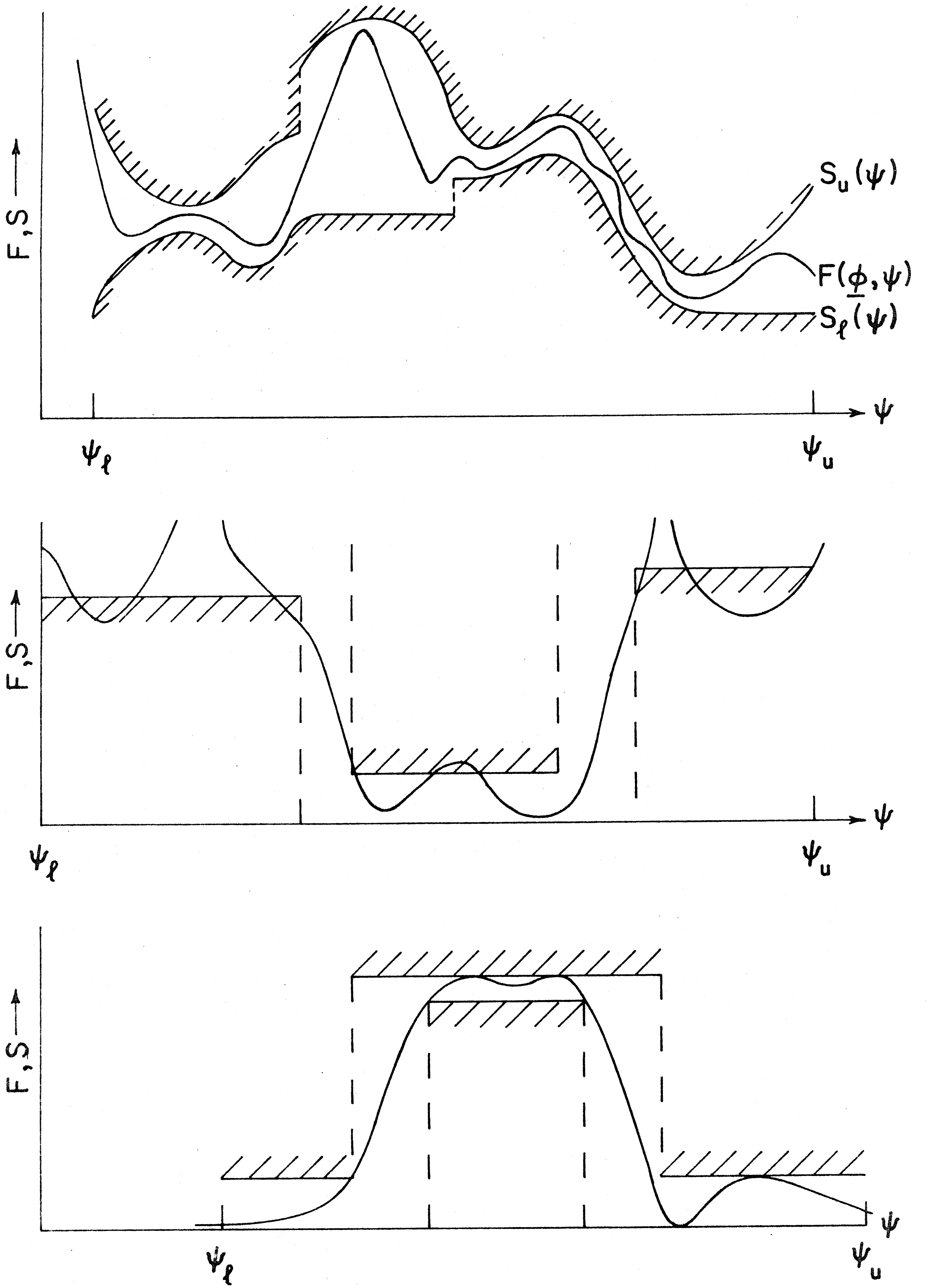

Fig. 4 (a) A response function satisfying arbitrary specifications,
(b) a response function failing to satisfy a bandpass filter specification,
(c) a response function just satisfying an amplifier specification.

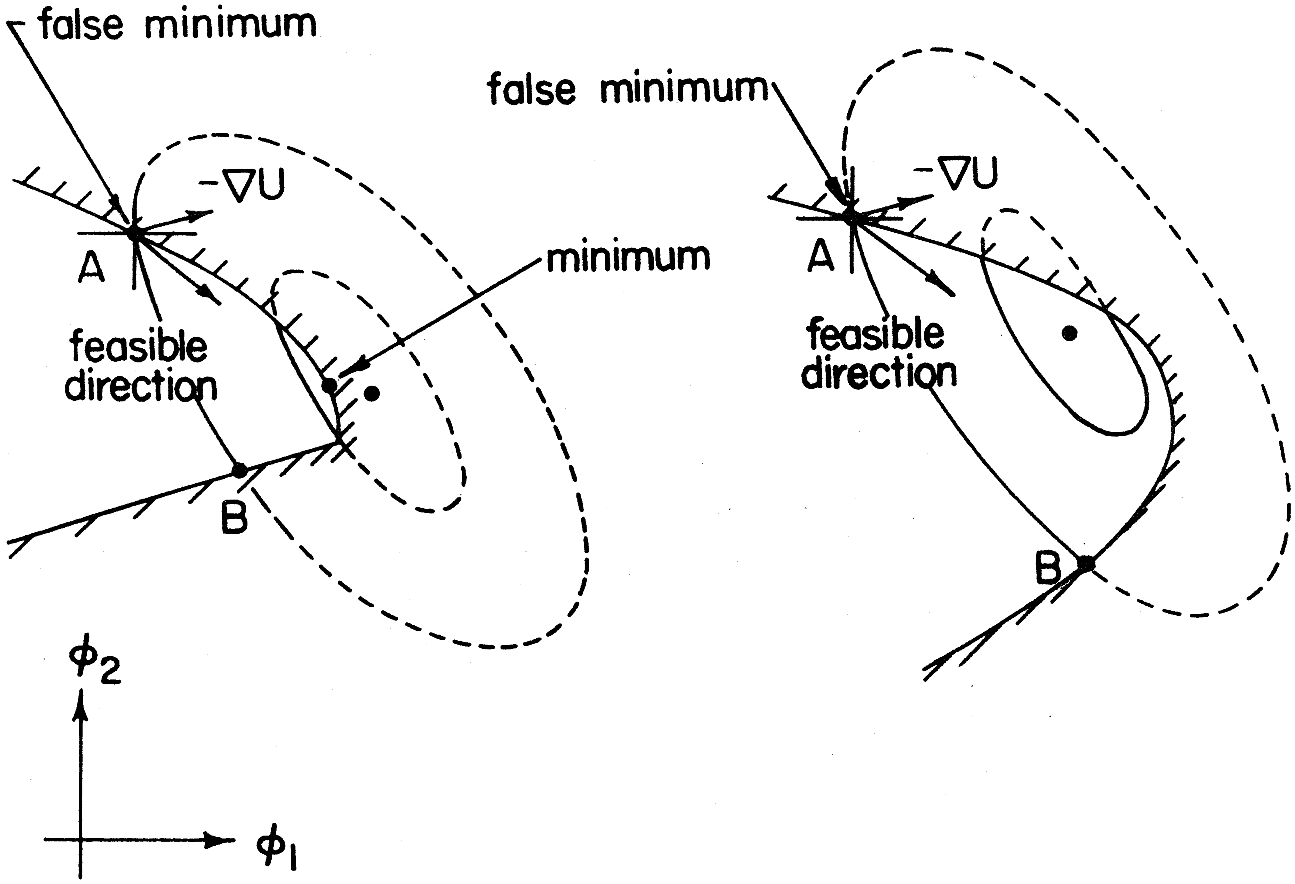

Fig. 5 Pitfalls in constrained minimization when non-feasible points are simply rejected.

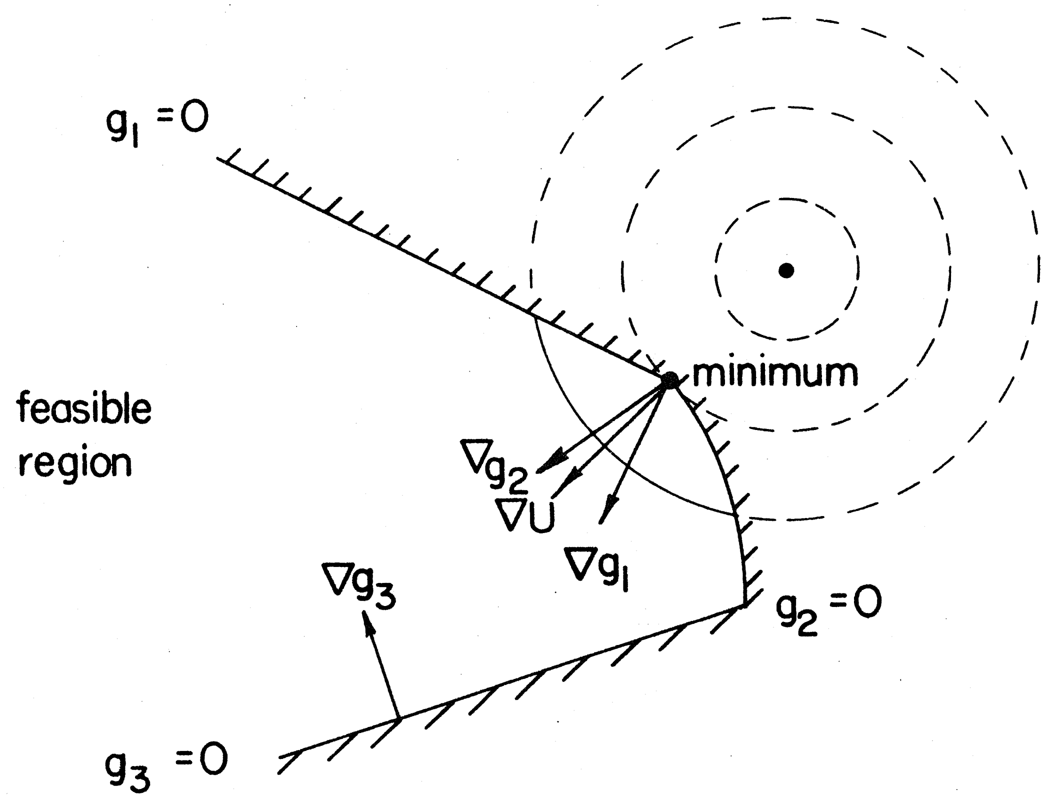

Fig. 6 An interpretation of the Kuhn-Tucker relations; $u_1 > 0$, $u_2 > 0$, $u_3 = 0$.

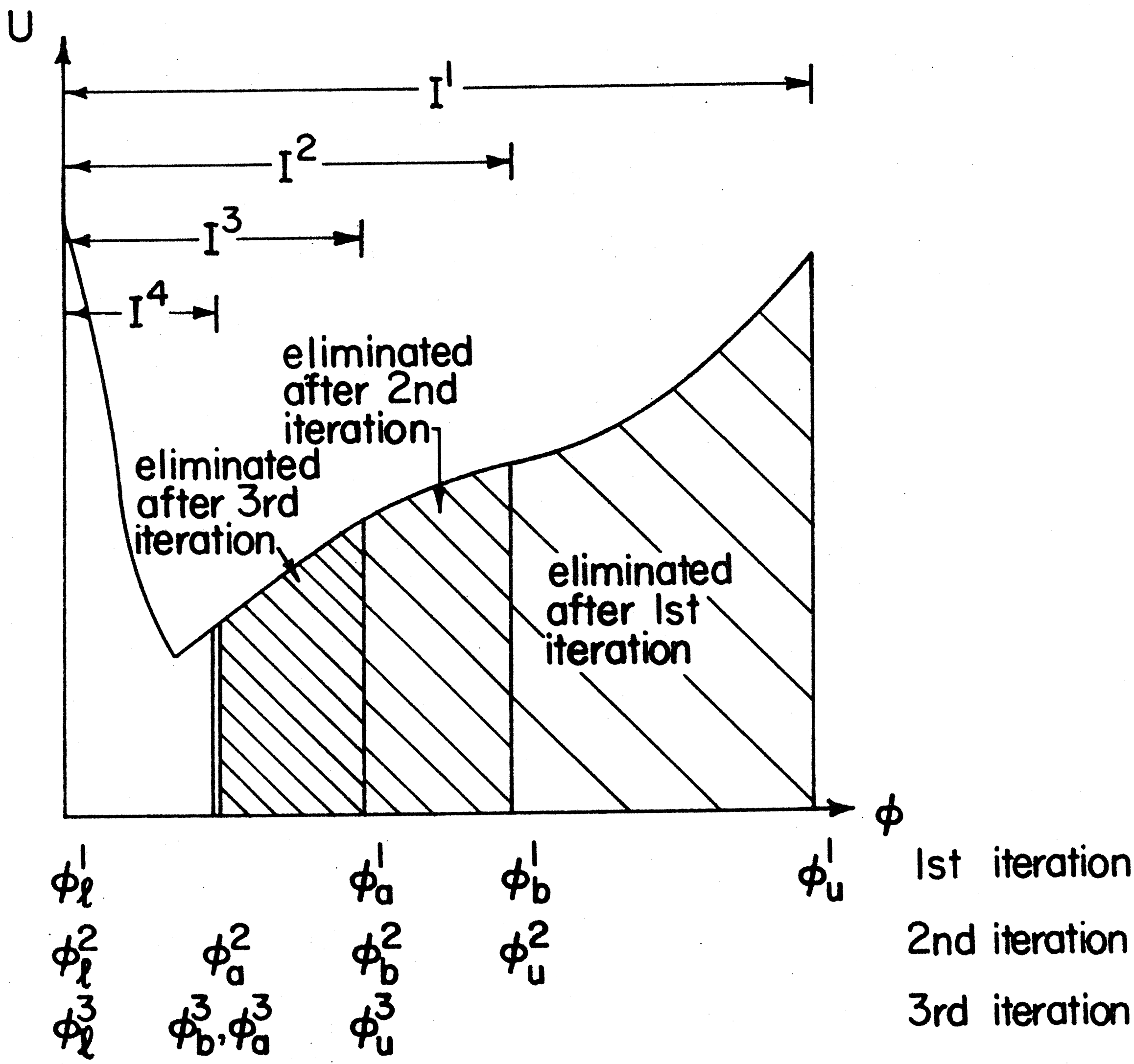

Fig. 7 A Fibonacci search scheme involving three iterations on a unimodal function of one variable.

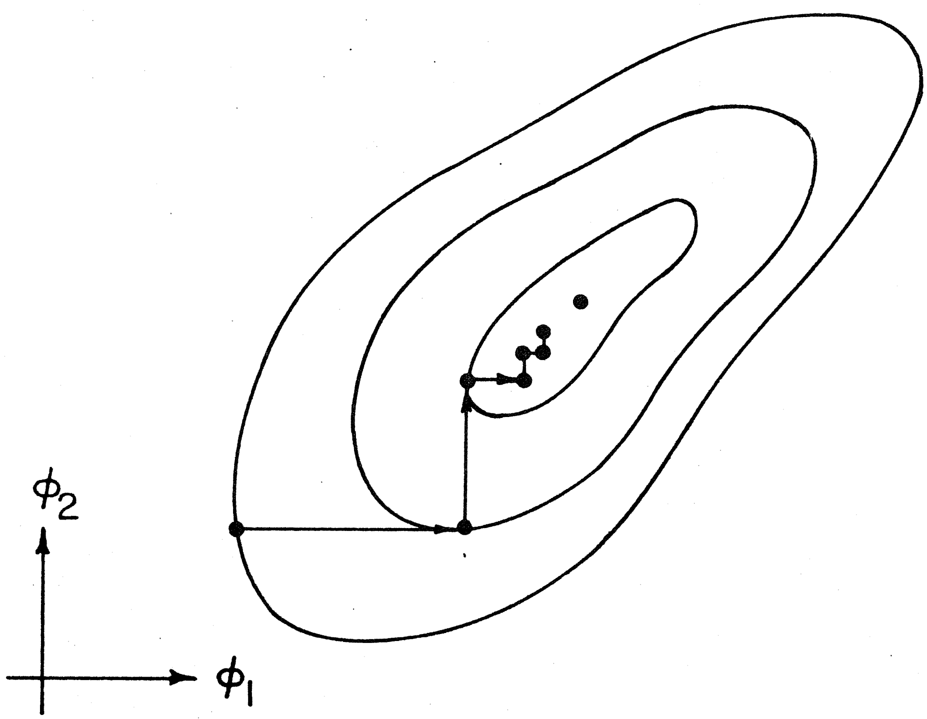

Fig. 8 Minimization by a one-at-a-time method.

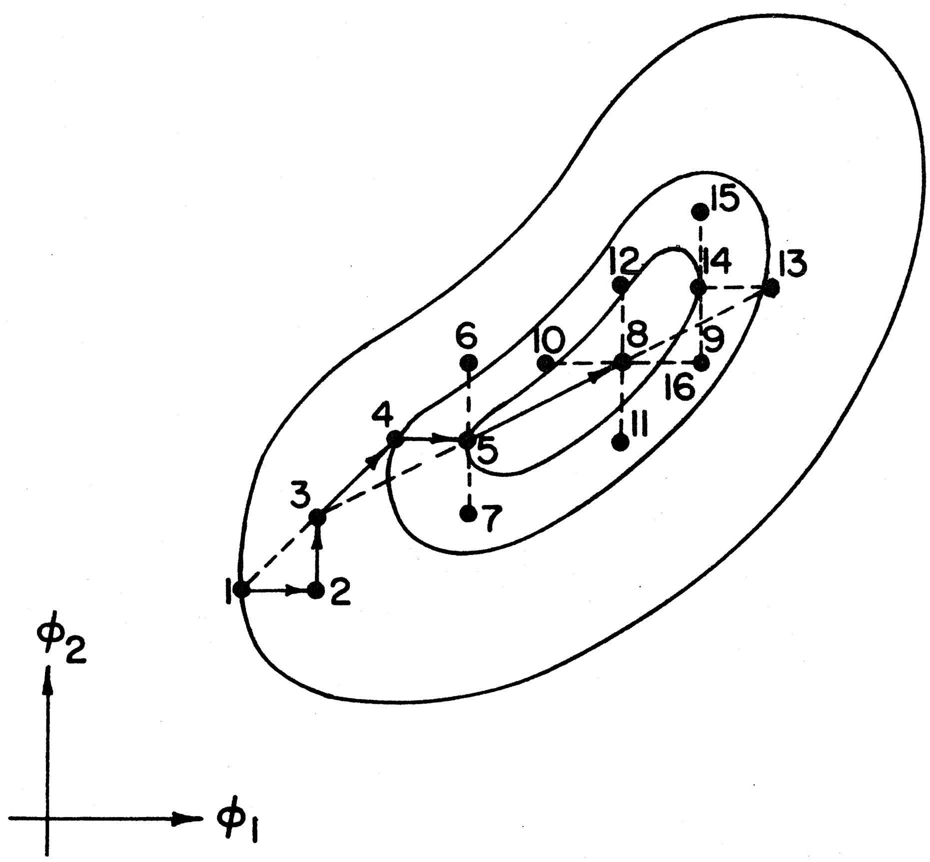

Fig. 9 Following a valley by pattern search.

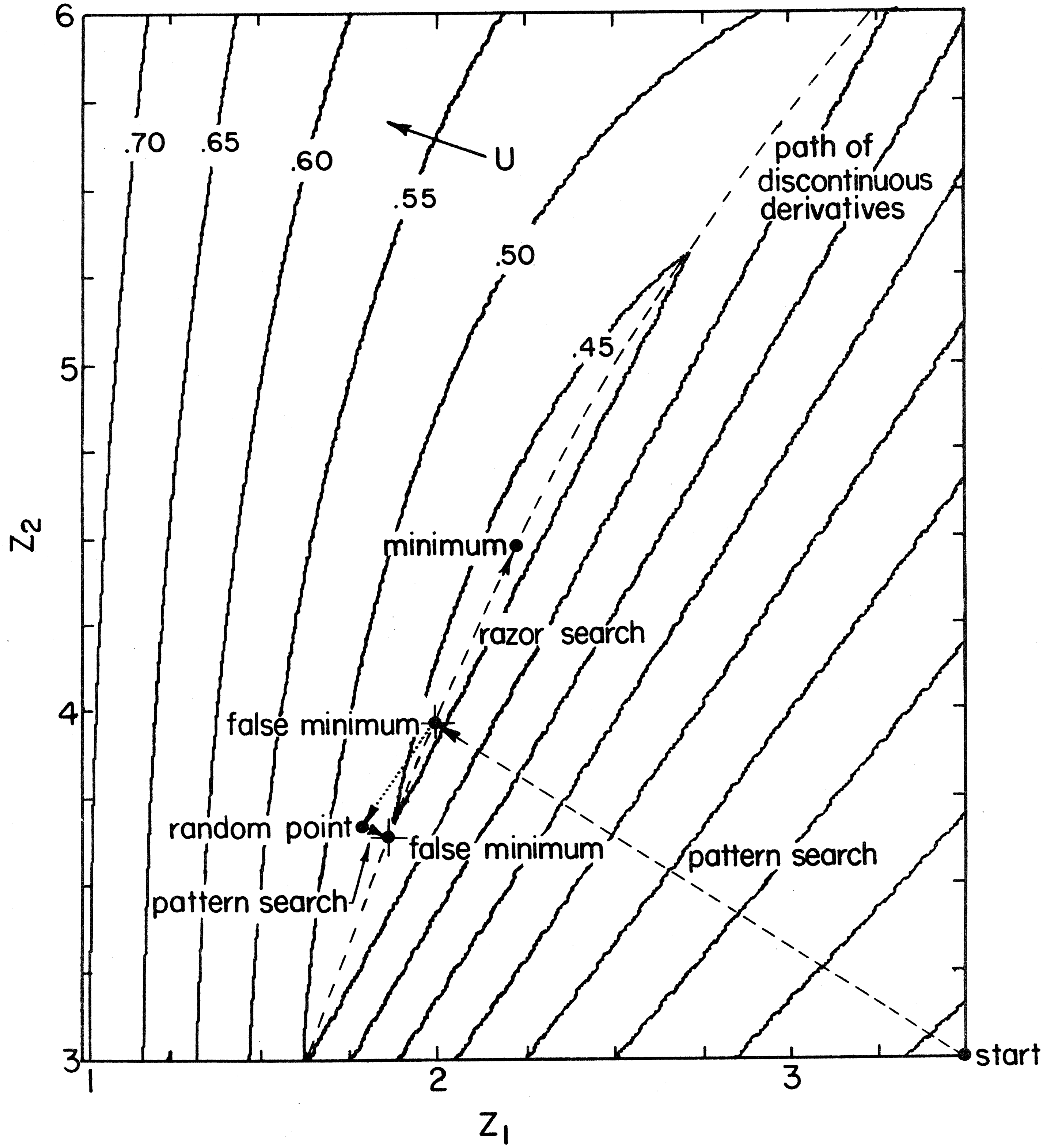

Fig. 10 Following a path of discontinuous derivatives along a narrow valley by razor search. The function is the maximum reflection coefficient over a 100% bandwidth of a 2-section 10:1 quarter-wave transmission-line transformer versus characteristic impedances Z_1 and Z_2.

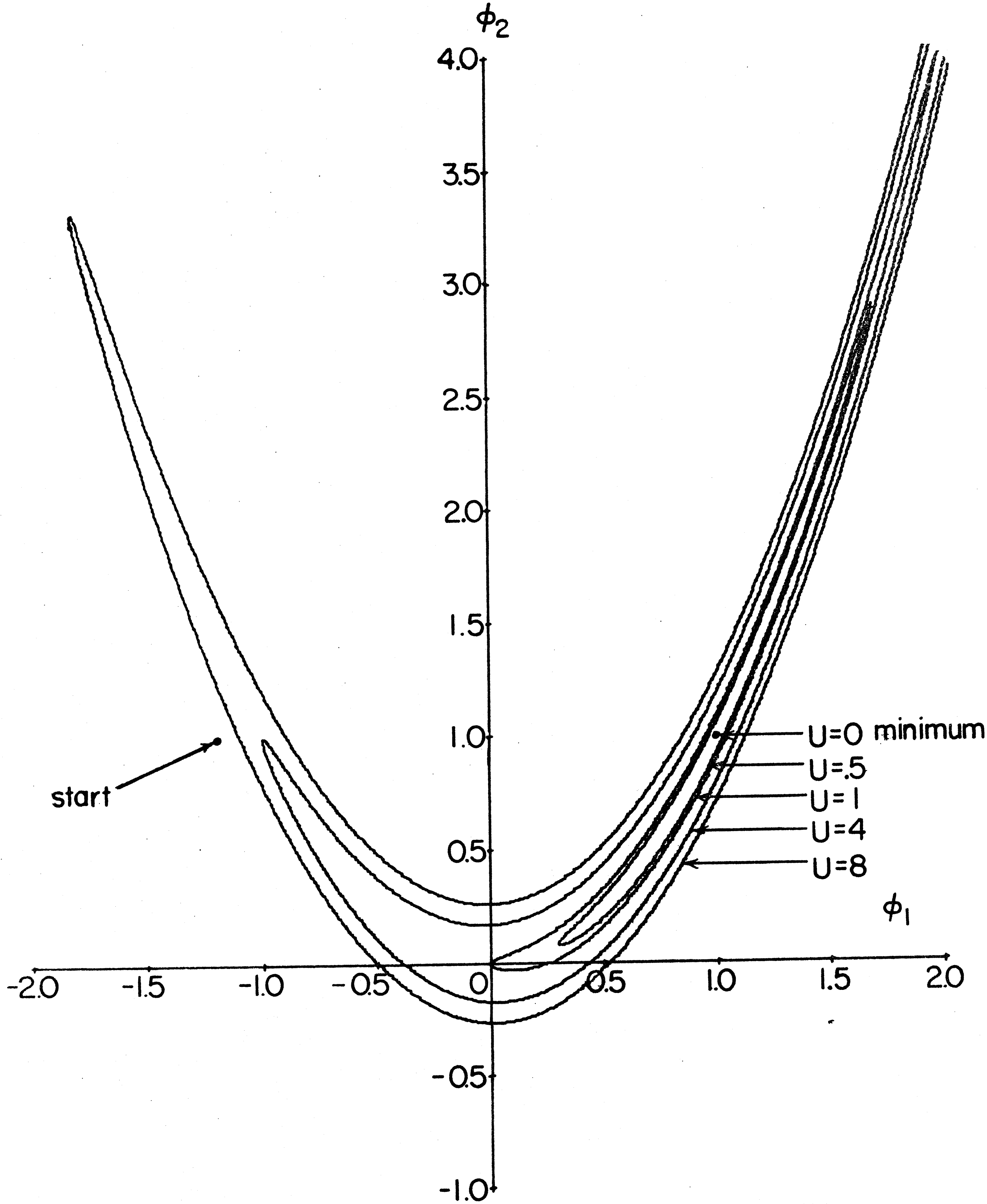

Fig. 11 Contours of a standard test problem: Rosenbrock's function $U = 100(\phi_2 - \phi_1^2)^2 + (1 - \phi_1)^2$.

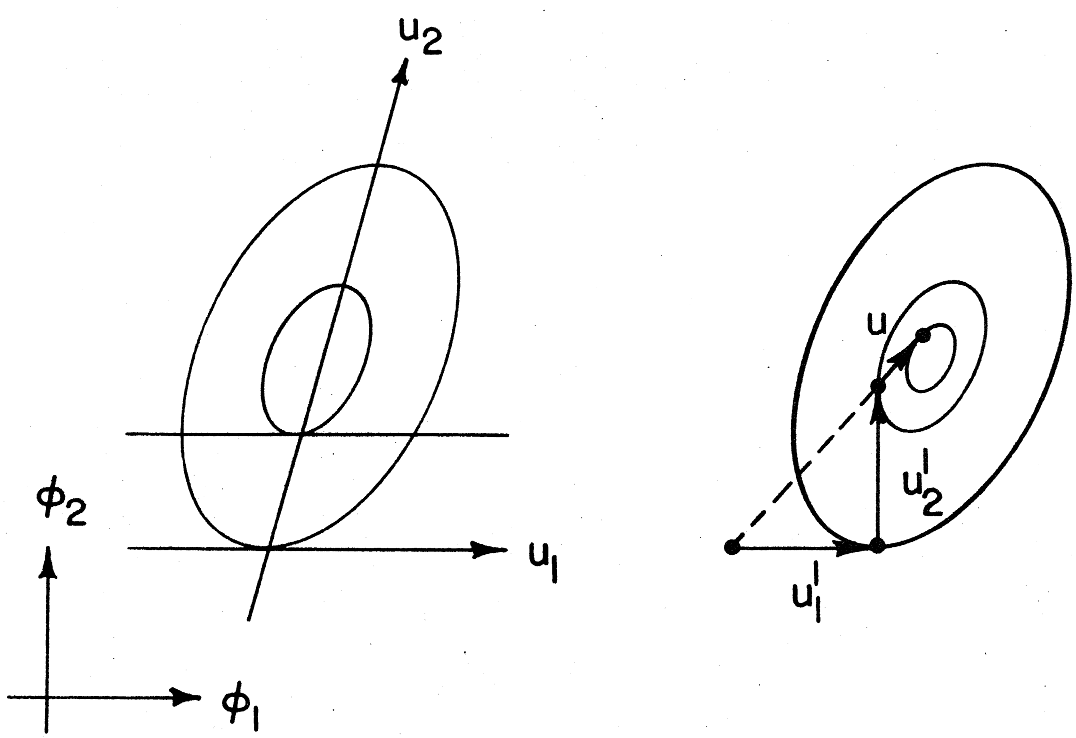

Fig. 12 Illustration of (a) conjugate directions $\underline{u}_1$ and $\underline{u}_2$, and (b) one iteration of Powell's method (the minimum is found in this problem after two iterations).

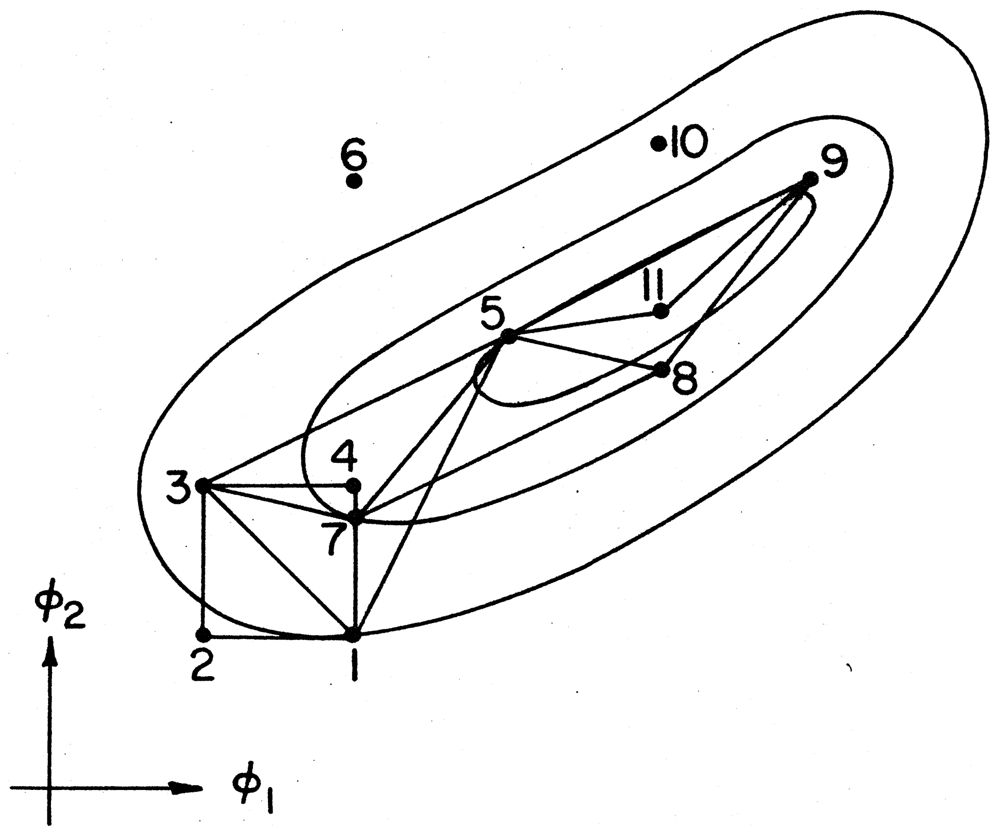

Fig. 13 Following a valley by the simplex method of Nelder and Mead.

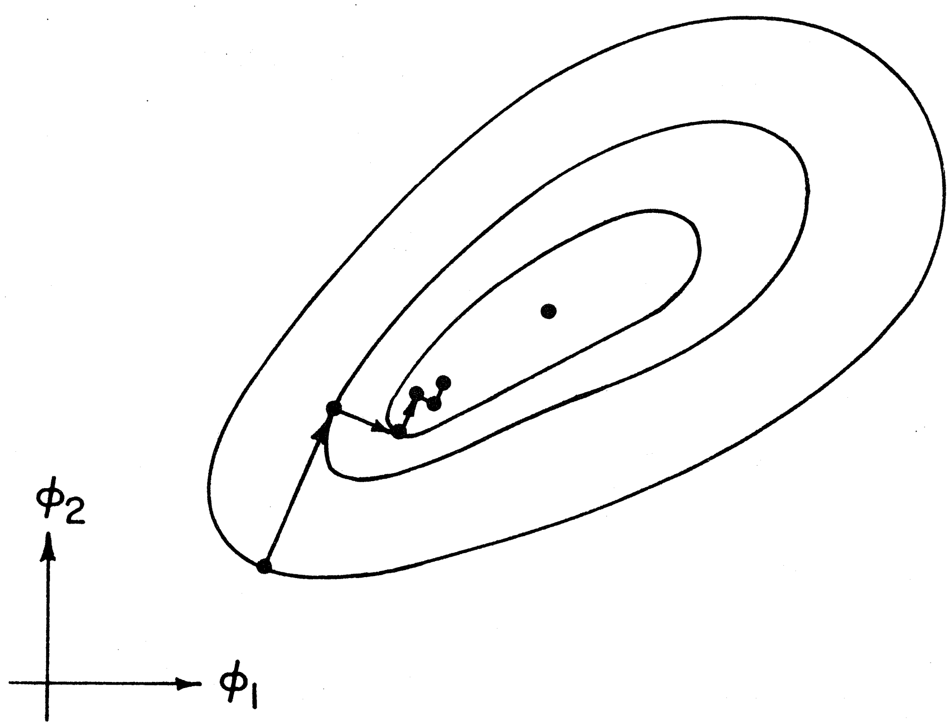

Fig. 14 Minimization by a steepest descent method (cf. Fig. 8).

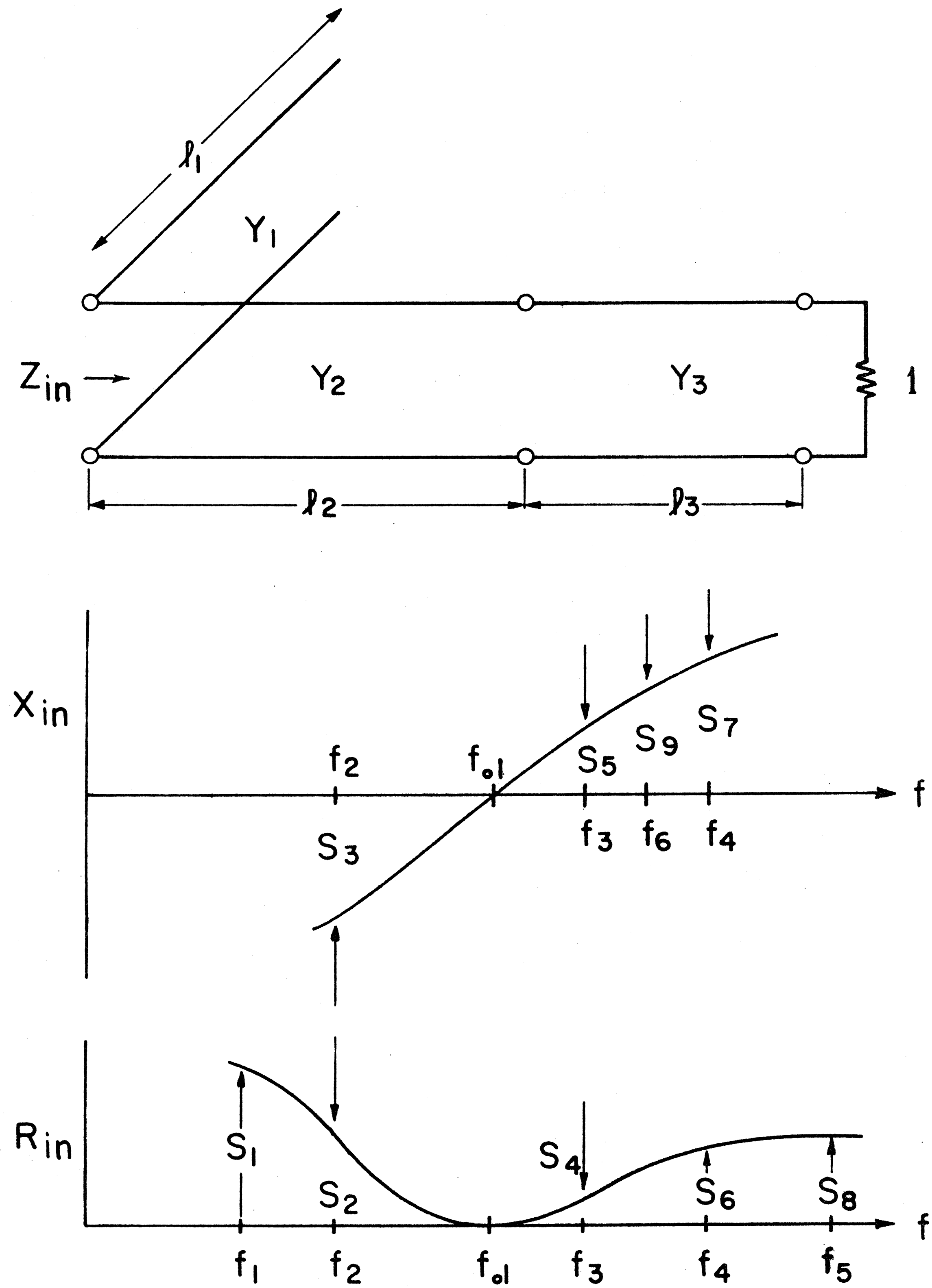

Fig. 15 Noncommensurate stabilizing network for a tunnel-diode amplifier with constraints on input resistance and reactance at certain frequencies.

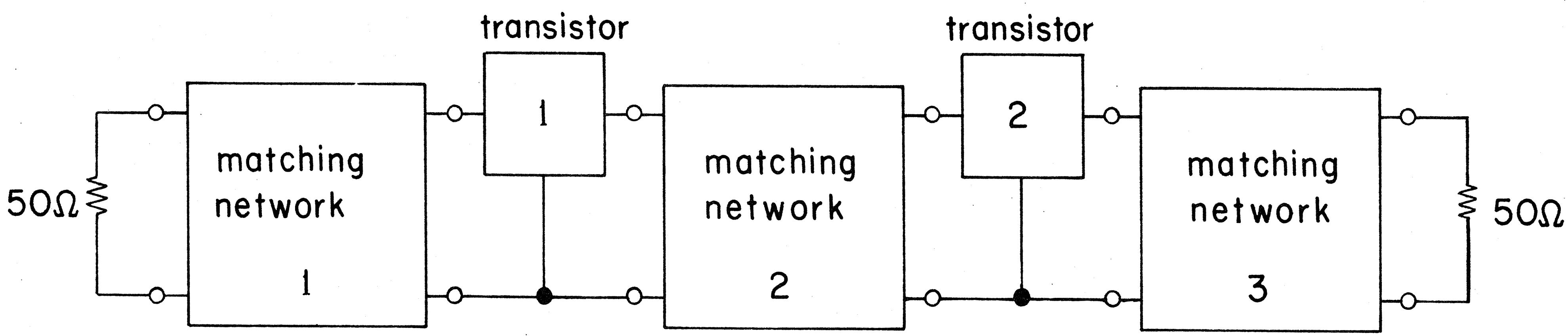

Fig. 16 Block diagram of a two-stage microwave transistor amplifier. The transistors are characterized experimentally. The matching networks usually consist of noncommensurate transmission lines and stubs.

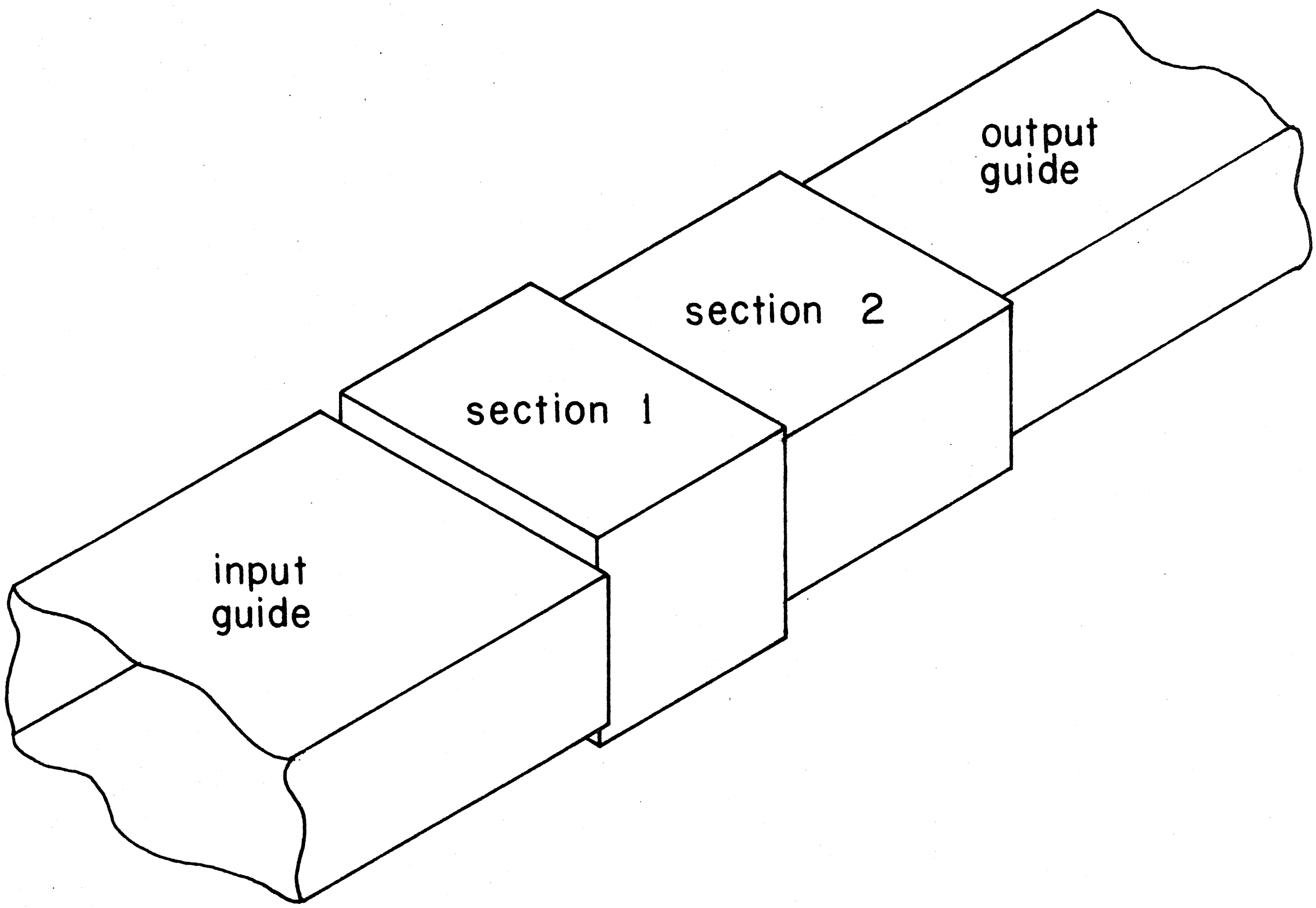

Fig. 17 An inhomogeneous rectangular waveguide impedance transformer. All guides are, in general, noncommensurate.