Variable Elimination for Optimization with Difficult Explicit Inequality Constraints

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One of the foremost difficulties in optimization is the handling of nonlinear inequality constraints. Most optimization algorithms have difficulty in following constraints, and slow convergence or failure often results if the optimum lies near one or more constraints or if the search must follow a constraint in reaching the optimum (Gaines and Gaddy, 1976; Gould, 1971). Penalty functions are sometimes helpful, but for heavily constrainted problems, failures are common (Beveridge and Schechter, 1970). Random search procedures have been found to be successful in following constraints, although their convergence efficiency, in some cases, is not rapid (Heuckroth et al., 1976).

The purpose of this note is to present a method for handling difficult explicit inequality constraints which may result in considerably improved efficiencies. This method is applied to six heavily constrainted example problems, and a comparison with previous solutions is presented. These problems are solved using the adaptive random search procedure, but the method is applicable to any algorithm.

Table 2. Comparative Results for Example 6

Variable	Gisvold and Moe solution	ARS solution
x_1	0.788	0.28543
x_2	0.732	0.61082
x_3	42	60
x_4	12.5	12.5
x_5	8.9	8.9
x_6	15.5	15.5
x_7	15.13	15.13
x_8	17.5	19.0
x_9	21.36	21.36
x_{10}	19.0	19.0
Y	220.203	215.043
Function evaluations:	3 263	1 663*

* Average for ten runs.

Table 1. Computational Requirements for Example Problems

Example No.	Function evaluations other studies	Avg.* No. function evaluations to 0.1% Heuckroth et al. (1976)	Elimination method
1	1 952†	3 874	245
2	1 759†	1 754	277
3	394†	387	329
4	3 487**	462	30
5	336†	484	13.4

* Average for fifty runs.
† Luus and Jaakola (1973).
** Keefer (1973).

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VARIABLE ELIMINATION

The variable elimination method is based upon the assumption that the optimum lies near one or more inequality constraints. During the search, when a constraint is encountered, the constraint equation is solved, as an equality, for one of the independent variables, thus eliminating a variable and constraint from the search. The search is then continued in one less dimension. When convergence slows, the problem is returned to its original form, and the search is continued to determine whether the optimum lies away from the constraint.

Elimination of a variable requires that an algebraic solution of the constraining equation be possible for at least one variable. Theoretically, any variable can be eliminated, with the improvement in efficiency depending upon the shape of the resulting function. If more than one constraint is encountered, elimination of additional variables is possible.

The decision as to which constraint to eliminate should be determined by the progress of the search. With no prior knowledge of the shape of the function, the best procedure is to allow variable elimination when the search approaches a predetermined value (say 2%) of any constraint. This necessitates solving, in advance, each constraint equation for a variable and programming these solutions for use should that constraint be encountered.

EXAMPLE PROBLEMS

Six example problems were solved to test the usefulness of the variable elimination method. Five of these problems were taken from Heuckroth et al. (1976) and are adequately described elsewhere in the literature. These will be referred to as examples 1 to 5. In each of the examples, the optimum lies near an explicit inequality constraint, and examples 1 and 2 are particularly heavily constrained. In the other problem presented by Heuckroth et al. (1976), the solution does not lie near a constraint; therefore, this example was not included in this study.

An additional example problem was chosen from Gisvold and Moe (1972). This example involves design of a corrugated bulkhead, with eight discrete and two continuous independent variables. There are twenty-eight nonlinear inequality constraints surrounding the optimum, and this problem presents a severe test for the variable elimination procedure.

Each of the above examples was solved using the adaptive random search procedure (Heuckroth et al., 1976). Range reduction was used, but skewing was not tried. The efficiencies are reported as the average number of function evaluations (fifty runs) required to reach 0.1% of the optimum. Starting points were the same as reported for other solutions.

RESULTS AND DISCUSSION

A comparison of the efficiency of the elimination procedure with other solutions for examples 1 to 5 is shown in Table 1. Significant improvements are noted for each problem, except example 3, which was not heavily constrained. The computational effort was reduced by factors of 5 to 20 over the best results reported previously. Greatest improvement was achieved, as expected, for those solutions which lie near an inequality constraint.

Perfect reliability was achieved in each of the solutions, that is, all fifty runs converged to the optimum. In each case, the variable eliminated from a constraint equation was simply that variable which resulted in the simplest equations for solution. Even better efficiency might result with different variable selection. Elimination was accomplished when the search reached 1 to 5% of the constraint value. For constraint values of 0, variable elimination was made when the constraint value was 0.05.

In cases where the optimum lies near more than one constraint, it may not be possible to solve the resulting equations to eliminate all variables. This was found to be the case for example 2, which bordered on two constraints. However, elimination of just one variable, in this case, resulted in a significant improvement in efficiency.

A comparison of the solution of example 6 with that of Gisvold and Moe (1972) is given in Table 2. To reach the optimum of this problem, the search must proceed down a tunnel formed by four constraining equations. Thus, elimination of several variables simultaneously was necessary. Elimination was achieved when the search reached 5% of any of the constraints.

As noted, the elimination method, with the adaptive random search, resulted in a substantial reduction in the computational effort in solving this problem. A better optimum was also located. It should be noted that this problem is mixed integer. No special programming is necessary to apply the adaptive random search to this type of problem.

SUMMARY AND CONCLUSIONS

The variable elimination method can be readily applied to several different types of optimization problems. The procedure significantly improves the efficiency of problems with difficult explicit constraints. Perfect reliability was achieved in reaching the optimum of each example. This method should be quite useful in solving problems in which the inequality constraints are explicit and solvable for at least one variable.

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Determination of Birth and Growth Rate of Secondary Nuclei: SSBCR Crystallizer

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Although the secondary nucleation is well known and has been extensively studied (Clontz and McCabe, 1971; Cise and Randolph, 1972; Strickland-Constable, 1972; Ottens and de Jong, 1973; Sung et al., 1973; Bauer et al., 1974; Garside and Jancic, 1976), many aspects of the phenomenon are still quite uncertain, especially in the area of growth of secondary nuclei. Perhaps the uncertainties stem in part from lack of experimental and analytical methods for the determination of birth and growth rate of secondary nuclei which would be equivalent in their effectiveness to the MSMPR methods pioneered by Randolph and Larson (1962, 1971) and proven powerful for the studies of primary crystallization.

It is known that McCabe's ΔL law does not necessarily hold for the growth of secondary nuclei. Therefore, the population balance of MSMPR can not be used for the determination of birth and growth rate of secondary nuclei unless certain assumptions (Randolph and Cise, 1972) are made. To overcome this difficulty, Garside and Jancic (1976) formed secondary nuclei in an MSMPR crystallizer and then grew the nuclei in a stirred batch crystallizer, effectively eliminating birth rate in the population balance. A differential method was used to obtain growth rate from experimental data.

An experimental method of a single-seeded batch crystallizer with an in situ Coulter counter can be combined with the analytical method of population balance (Randolph and Larson, 1971) to obtain the birth and growth rate of secondary nuclei. Consider a single-seeded, stirred batch crystallizer. If the seed crystal is removed from the crystallizer at time $t = t_r$ and the secondary nuclei formed are allowed to grow, the population balance yields

$$\frac{\partial}{\partial t} n(t, L) + \frac{\partial}{\partial L} G(L)\, n(t, L) = b_n(L;\ t \leq t_r,\ L \geq L_c) \tag{1}$$

Integrating Equation (1) with respect to time, we have

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