OPTIMIZATION THEORY IN THE CHEMICAL ENGINEERING CURRICULUM

Douglass J. Wilde
Department of Chemical Engineering
University of Texas

Introduction

This article is intended to acquaint teachers of chemical engineering with the theory of optimization, which has developed so rapidly in eleven years that it is now finding its way into the practice, literature, and curricula of our profession. Optimization theory is composed of technical methods for computing the greatest (or least) value of some criterion of value or effectiveness measuring the performance of a system being studied. Since optimization involves, roughly speaking, finding the best way to do things, it has obvious applications in the chemical industry, where small changes in efficiency can spell the difference between success and failure. Today as always many important decisions can be made simply by choosing some measure of effectiveness and then optimizing it.

To justify the inclusion of this new material into the already crowded curriculum we cannot be content with describing the technical content of optimization theory. We must also show why the profession needs it and how it might be fit into existing graduate and undergraduate programs. Moreover, we must assess the pedagogical value of optimization theory in developing engineering judgment, scientific objectivity, and intellectual creativity in our students.

To begin we shall advance two arguments suggesting the chemical engineers' need for optimization theory. The first of these will be speculative, analyzing the role of optimization in engineering decision-making. The second will be historical, showing how our very lack of attention to optimization theory has created demands for operations analysts and management scientists to solve problems which could well be handled by engineers.

In the heart of the article we shall combine a review of optimization theory with description of a three-hour, one semester course already given to chemical engineering seniors having no special preparation. This resume will include references to recent developments of pedagogical interest. As each phase of the theory is discussed, its most important industrial applications will be mentioned so that the "why" may be unfolded at the same time as the "what" and "how". It is quite possible that a professor may not wish to offer an entire course in optimization theory, preferring instead to incorporate parts of the theory into various existing courses. Indeed, one would hope that eventually optimization theory would be absorbed into the curriculum in this way. To facilitate such gradual integration we shall indicate where each of the three main parts of optimization theory may be pertinent to such existing courses as plant design, kinetics, control, economics, and mathematics. Thus optimization theory may be introduced suddenly or gradually depending on local circumstances.

Finally we shall show how study of optimization theory gives a student a set of rules potentially valuable to him in making complex decisions. The rules and procedures are of course worthwhile in themselves, but equally important is the fact that their study reinforces the student's confidence in the rational scientific approach to problems. Optimization theory gives good training in the analysis of functions of many variables (via multidimensional geometry) and in the use of precise, logical reasoning. Moreover, the very novelty of the mathematics and the newness of the theory are great stimulants to the creativity and imagination of the students.

The Need For Optimization Theory

Let us examine two arguments tending to justify the need of the chemical engineering profession for optimization theory. First consider the typical engineering project. Theoretical principles are combined with experimental data to describe the system under study. It is rare that such a study is made for the sake of knowledge alone; ultimately the information is to be used for making some sort of decision -- build a new plant, replace a heater, or change a catalyst. Without optimization theory, such decisions must often be made impetuously, or at best, after laborious case studies, despite the good engineering that went into the study itself. Such a situation is intellectually (and often economically) unsatisfying.

Secondly, consider the rapid growth of the new profession of "operations research" or "management science", defined by most of their practitioners as "the scientific preparation of decisions". This sounds suspiciously like engineering, and on examination of their methods for making decisions, we find three steps: (1) rational (preferably mathematical) description of the system, (2) choice of a measure of effectiveness, and (3) optimization of that measure. Now in most industrial problems, rational description is precisely the job ofthe engineer, while the choice of a measure of effectiveness is either obvious or impossible. Thus the only difference between industrial operations research and engineering is usually that the former profession has better optimization techniques. We submit then that the rise of operations research has been due not only to the ability and imagination of its own pioneers, who contributed much to the theory of optimization, but also to the failure of the engineers to study optimization problems. Our loss has been their gain.

Optimization Theory

Before 1951, optimization had hardly been studied at all since the development of the calculus of variations two centuries earlier and today most engineers know only one method for finding an optimum -- the differential calculus. By this method one expresses the criterion of effectiveness as a function of the independent variables, equates the first derivations to zero and then solves the resulting equations. But in industrial problems it is rarely possible to perform all these steps, and even when it is, the "solution" is often unattainable because of physical restrictions on the process. We shall distinguish three branches of optimization theory here, classifying them according to the very obstacles preventing their solution by the differential calculus. The three types of problems are: (1) experimental problems in which the measure of effectiveness is unknown and must be determined by direct experiment, (2) feasibility problems in which the apparent optimum lies outside the physical constraints on the system, and (3) interaction problems in which there are so many variables that the problem must be decomposed and solved in pieces.

Each type of problem can be covered in one semester-hour of undergraduate work, either all at once in a single three hour course or as parts of other existing courses. There are optimization problems which do not fit into these three categories, but we are limiting ourselves here to material that can be taught to a senior engineering student in one semester and be of use to him when he graduates.

After each type of problem is described, its historical development will be traced and references of either research or pedagogical interest cited. Then applications will be mentioned and finally, possible locations in the curriculum will be suggested.

Experimental problems

In an experimental problem one knows almost nothing about the dependence of the measure of effectiveness on the independent variables, and the only way to obtain information about this dependence is to take measurements. Kiefer (1.) has described a highly efficient way to carry out the search when there is but one independent variable and no experimental error, as for example in the calculation of the optimal number of stages in a distillation column or evaporator. A description of this Fibonacci search procedure in engineering terms is given in (2.) It is interesting perhaps that with this technique one could find the best case out of a possible twenty after only seven case studies.

Unfortuntely the elegant Fibonacci technique cannot be extended to situations with more than one independent variable, and in 1951, the year of revival of interest in optimization, Box and Wilson (3.) suggested their method of steepest ascent for multivariable problems. Recently newer approaches to this problem have been advanced -- the geometric techniques of Buehler, Shah, and Kempthorne (4.) and the author (5.), as well as the logical methods of Hooke and Jeeves (6.) and Mugele (7.).

The presence of experimental error requires different methods, known in general as stochastic approximation procedures. Dvoretzky (8.) has generalized the early methods of Robbins and Munro (9.) and Kiefer and Wolfowitz (10.), an acceleration technique has been proposed by Kesten (11.), and multivariable extensions have been developed by Blum (12.). Some of these procedures have been reviewed from the chemical engineers' point of view by Lapidus et. al. (13.).

These methods are applicable to design and operating problems involving either complicated computations or significant measurement error. The Fibonacci technique could conceivably fit into a plant design or economics course, or even into the exposition of staged unit operations. Mutivariable procedures are more appropriate in plant design courses, and the insight they give into multidimensional geometry could well suit them for inclusion in an advanced mathematics course. Stochastic approximation, since it depends on some probability theory, would be appropriate in an engineering statistics or probability course. In our experience the theory of experimental search for an optimum has been extremely stimulating to students, who seem to be inspired by it to surprisingly original contributions.

The author is presently completing a monograph on experimental optimization, reviewing and explaining all these developments, hopefully in language that an engineering senior can understand. Engineering professors can obtain a free preliminary draft of this material by writing the author, who would be grateful for suggestions and corrections.

Feasibility Problems

When, as is often the case in the industrial world, the ranges of variation of the independent variables are limited, it is sometimes physically impossible to attain the conditions where the first derivatives of the efficiency criterion all vanish. Such restrictions give rise to feasibility problems because only feasible conditions, those respecting all the constraints, can be considered. The technical term "mathematical programming" (not to be confused with the "programming" of computers) is often applied to such problems. The year 1951 also marks the beginning of the theory of mathematical programming. In that year Dantzig published his "simplex method" for solving the linear case. Since that time literally hundreds of articles have appeared on applications of the simplex method, and many petroleum companies have justified the installation of large electronic computers on the improvements in refinery scheduling and product blending made possible by mathematical programming.

It is traditional in operations research curricula to spend a great deal of time on mathematical programming, especially the linear case, which is the simplest. Much of this time is consumed in introducing the student to matrix algebra. While matrix algebra is interesting in its own right, we have found that one can profitably develop mathematical programming without it and save considerable time. This is achieved by treating feasibility problems as simple extensions of the classical optimization problem solvable by the differential calculus. Since engineering students are more adept at manipulating derivatives than matrices, this approach has proven quite successful, and it has been possible to take a class through linear and quadratic programming, as well as the decomposition principle to be discussed later, in only six weeks. This differential approach, which we think has great pedagogical value, is illustrated in (2.) and justified theoretically in (14.)

Discussion of feasibility problems is appropriate in any economics or design course. The subject may also be used in applied mathematics courses as an application of matrix theory; Lapidus has used this approach in his new book (15.) With the differential approach, mathematical programming can be covered in any engineering calculus course, almost as an exercise in partial differentiation.

Interaction Problems

Sometimes the criterion of effectiveness depends on so many factors that it is impractical or impossible to find the optimum by classical methods. Often such problems are generated by the interaction of smaller systems with each other. In such cases it is occasionally possible to decompose the large problem into smaller ones, solve the sub-problems, and recombine these sub-optimal systems in such a way that the interactions are properly taken into account. This exploitation of the structure of a system is advantageous because the number of calculations tends to increase as the cube of the number of variables. Thus doubling the number of variables will ordinarily increase the computation load by a factor of eight. It the problem can be split in two, however, the number of calculations will only double or triple.

Bellman (16.) has shown how to decompose a series of decisions, each depending on the one preceding, by the method he calls "dynamic programming.' This technique, which might also be called "serial optimization", has many applications to such long range planning problems as capital investment, production scheduling, and maintenance planning. Application of dynamic programming to the design of chemical reactors has been described in Aris' recent monograph (17.) Nemmhauser has given a very clear example of design of a straight-line chemical plant by dynamic programming (18.) The conventional exposition of this subject using functional equations is often confusing to students, and we have found the block diagram approach of reference (2.) to be helpful in the classroom.

The solar system-satellite structure of many multiplant scheduling problems lends itself to analysis by Dantzig and Wolfe's decomposition principle when all the equations are linear (19.) A numerical example of the application of this principle to centralized planning is available (20.) This example illustrates the power and clarity of the differential approach mentioned earlier, and senior students have had little difficulty absorbing this material, considered quite abstruse by many operations analysts.

References (2), (16), and (17) give many applications of dynamic programming, whose ability to handle time-dependent problems makes the process dynamics and control course an attractive place for its introduction. Aris' work suggests that the kinetics and reactor design course would also be suitable. Again, plant design and economics offerings can be used to introduce serial optimization techniques. Related to dynamic programming is Pontryagin's maximum principle (21). The decomposition principle should be discussed as an extension of linear programming rather than as a separate topic for the differential formulation makes this extension relatively painless.

Pedagogical Values

In describing the outline of a course in optimization theory we have indicated how it is a good vehicle for developing mathematical maturity and respect for the scientific method on engineering students. But aside from the technical material, the decision rules themselves can build sound engineering judgment in the student that will help him make up his mind inteligently even when there is no time for detailed and rigorous analysis. Study of the one-variable experimental optimization problem gives insight into the important minimax concept and the somewhat startling concept of randomization. Analysis of multivariable problems unearths some rather disturbing facts about graphical reasoning and the paradoxes that can arise from failing to realize that engineers often work in non-Euclidean space (2.) Linear programming shows that it is sometimes economical to give a customer higher quality than he asks for at no increase in price. The classic "law of diminishing returns" is illustrated quite clearly in the study of quadratic programming. Anyone's point of view is affected by insight into the far-sighted philosophy of dynamic programming, which begins by analyzing the last rather than the first decision in a sequence. Perhpas the most surprising decision rule of all comes from study of the decomposition principle, which shows that a central planning board should ask branch managers for nonoptimal production plans. This is particularly significant because few organizations presently operate this way, at least intentionally.

Concluding Summary

In this review we hope we have given information upon which chemical engineering professors can decide why and how they might introduce optimization theory, or parts of it, to their students. The demands of industry have made this necessary; research has made it possible; and pedagogical advances have made it practical. The rest is up to the profession itself.

REFERENCES

1. Kiefer, J., "Sequential Minimax Search for a Maximum", Proc. Amer. Math. Soc., 4 (1953), pp. 502-506.
2. Wilde, D.J., "Optimization Methods", a chapter in Advances in Chemical Engineering, Vol. III (T.B. Drew, J.W. Hoopers, Jr., and T. Vermeulen, eds.) Academic Press, New York 1962.
3. Box, G.E.P., and Wilson, K.B., "The Experimental Attainment of Optimum Conditions", J. Roy, Stat. Soc., BB (1951) pp. 1-20
4. Shah, B.V., Buehler, R.J., and Kempthorne, O., "The Method of Parallel Tangents (PARTAN) for Finding an Optimum", Iowa State Univ. Statistics Lab. Technical Report No. 2, Ames Iowa (April 1961).
5. Wilde, D.J., "The Contour Tangent Optimization Method", to appear in AIChE Journal.
6. Hooke, R., and Jeeves, T.A., "Direct Search Solution of Numerical and Statistical Problems", J. Assoc. Computing Mach. 8, 2 (April 1961), pp. 212-229.
7. Mugele, R.A. "A Monlinear Digital Optimizing Program for Process Control Systems", Proc-Western Joint Computer Conference (Spring 1962).
8. Dvoretzky, A., "On Stochastic Approximation", Proc. 3rd Berkeley Symp. Math. Stat. Prob. (J.Neyman, ed.), Berkeley, U. of California Press (1956), pp. 39-55.
9. Robbins, H., and Munro, S., "A Stochastic Approximation Method", Ann. Math. Stat., 23 (1951), --. 400-407.
10. Kiefer, J., and Wolfowitz, J., "Stochastic Estimation of the Maximum of a Regression Function", Ann. Math. Stat., 23 (1952) pp. 462-6.
11. Kesten, H., "Accelerated Stochastic Approximation", Ann. Math. Stat. 29, (1958), pp. 41-59.
12. Blum, J.R., "Multidimensional Stochastic Approximation Methods", Ann. Math. Stat., 25 (1954), pp. 737-44.
13. Lapidus, L, Stillman, R., Shapiro, S., and Shapiro, E., "Strategy for Optimizing Chemical Engineering Systems", AIChE Journal (Summer 1961).
14. Wilde, D.J., "Differential Calculus in Nonlinear Programming", to appear in Operations Research.
15. Lapidus, L. Digital Computation for Chemical Engineers, McGraw-Hill, New York (1962).
16. Bellman, R., Dynamic Programming, Princeton U. Press, Princeton (1957)
17. Aris, R., Optimal Design of Chemical Reactors -- Studies in Dynamic Programming. Academic Press, New York (1961).
18. Nemmhauser, G., Ph.D. dissertation Northwestern University
19. Dantzig, G.B., and Wolfe, P., "A Decomposition Principle for Linear Programs", Operations Research, 8 (Jan. 1960.)
20. Wilde, D.J., "Production Planning of Large Systems by the Decomposition Principle", to be presented at the AIChE annual meeting, Chicago, Dec. 1962.
21. Chang, S.S.L., Synthesis of Optimal Control Systems, McGraw-Hill, New York (1961).