OPTIMIZATION BY VARIATIONAL METHODS

BY MORTON M. DENN

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Preface

The development of a systematic theory of optimization since the mid-1950s has not been followed by widespread application to the design and control problems of the process industries. This surprising and disappointing fact is largely a consequence of the absence of effective communication between theorists and process engineers, for the latter typically do not have sufficient mathematical training to look past the sophistication with which optimization theory is usually presented and recognize the practical significance of the results. This book is an attempt to present a logical development of optimization theory at an elementary mathematical level, with applications to simple but typical process design and control situations.

The book follows rather closely a course in optimization which I have taught at the University of Delaware since 1965 to classes made up of graduate students and extension students from local industry, together with some seniors. Approximately half of the students each year have been chemical engineers, with the remainder made up of other types of engineers, statisticians, and computer scientists. The only formal mathematical prerequisites are a familiarity with calculus through Taylor series and a first course in ordinary differential equations, together with the maturity and problem awareness expected of students at this level. In two sections of Chapter 3 and in Chapter 11 a familiarity with partial differential equations is helpful but not essential. With this background it is possible to proceed in one semester from the basic elements of optimization to an introduction to that current research which is of direct process significance. The book deviates from the course in containing more material of an advanced nature than can be reasonably covered in one semester, and in that sense it may be looked upon as comprising in part a research monograph.

Chapter 1 presents the essential features of the variational approach within the limited context of problems in which only one or a finite number of discrete variables is required for optimization. Some of this material is familiar, and a number of interesting control and design problems can be so formulated. Chapter 2 is concerned with the parallel variational development of methods of numerical computation for such problems. The approach of Chapter 1 is then resumed in Chapters 3 to 5, where the scope of physical systems analyzed is gradually expanded to include processes described by several differential equations with magnitude limits on the decisions which can be made for optimization. The optimal control of a flow reactor is a typical situation.

In Chapters 6 and 7 much of the preceding work is reexamined and unified in the context of the construction of Green's functions for linear systems. It is only here that the Pontryagin minimum principle, which dominates modern optimization literature, is first introduced in its complete form and carefully related to the more elementary and classical material which is sufficient for most applications.

Chapter 8 relates the results of optimization theory to problems of design of practical feedback control systems for lumped multivariable processes.

Chapter 9 is an extension of the variational development of principles of numerical computation first considered in Chapter 2 to the more complex situations now being studied.

Chapters 10 and 11 are concerned with both the theoretical development and numerical computation for two extensions of process significance. The former deals with complex structures involving recycle and bypass streams and with periodic operation, while the latter treats distributed-parameter systems. Optimization in periodically operated and distributed-parameter systems represents major pertinent efforts of current research.

Chapter 12 is an introduction to dynamic programming and Hamilton-Jacobi theory, with particular attention to the essential equivalence in most situations between this alternate approach and the variational approach to optimization taken throughout the remainder of the book. Chapter 12 can be studied at any time after the first half of Chapters 6 and 7, as can any of the last five chapters, except that Chapter 9 must precede Chapters 10 and 11.

Problems appear at the end of each chapter. Some supplement the theoretical developments, while others present further applications.

In part for reasons of space and in part to maintain a consistent mathematical level I have omitted any discussion of such advanced topics as the existence of optimal solutions, the Kuhn-Tucker theorem, the control-theory topics of observability and controllability, and optimization under uncertainty. I have deliberately refrained from using matrix notation in the developments as a result of my experience in teaching this material; for I have found that the very conciseness afforded by matrix notation masks the significance of the manipulations being performed for many students, even those with an adequate background in linear algebra. For this reason the analysis in several chapters is limited to two-variable processes, where every term can be conveniently written out.

In preparing this book I have incurred many debts to colleagues and students. None will be discharged by simple acknowledgement, but some must be explicitly mentioned. My teacher, Rutherford Aris, first introduced me to problems in optimization and collaborated in the development of Green's functions as the unifying approach to variational problems. J. R. Ferron, R. D. Gray, Jr., G. E. O'Connor, A. K. Wagle, and particularly J. M. Douglas have been most helpful in furthering my understanding and have permitted me to use the results of our joint efforts. The calculations in Chapter 2 and many of those in Chapter 9 were carried out by D. H. McCoy, those in Section 10.8 by G. E. O'Connor, and Figures 6.1 to 6.4 were kindly supplied by A. W. Pollock. My handwritten manuscript was expertly typed by Mrs. Frances Phillips. For permission to use copyrighted material I am grateful to my several coauthors and to the following authors and publishers:

The American Chemical Society for Figures 4.2, 5.7, 5.8, 9.1, 9.2, 9.7 to 9.13, 10.5 to 10.15, 11.8 to 11.12, which appeared in *Industrial and Engineering Chemistry Monthly* and *Fundamentals Quarterly*.

Taylor and Francis, Ltd., for Figures 11.1 to 11.7 and Sections 11.2 to 11.7, a paraphrase of material which appeared in *International Journal of Control*.

R. Aris, J. M. Douglas, E. S. Lee, and Pergamon Press for Figures 5.9, 5.15, 9.3, and Table 9.8, which appeared in *Chemical Engineering Science*.

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D. D. Perlmutter and the American Institute of Chemical Engineers for Figures 8.1 and 8.2, which appeared in *AIChE Journal*.

Several of my colleagues at the University of Delaware have shaped my thinking over the years about both optimization and pedagogy, and it is my hope that their contributions to this book will be obvious at least to them. J. M. Douglas and D. D. Perlmutter have kindly read the entire manuscript and made numerous helpful suggestions for improvement. For the decision not to follow many other suggestions from students and colleagues and for the overall style, accuracy, and selection of material, I must, of course, bear the final responsibility.

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Introduction

OPTIMIZATION AND ENGINEERING PRACTICE

The optimal design and control of systems and industrial processes has long been of concern to the applied scientist and engineer, and, indeed, might be taken as a definition of the function and goal of engineering. The practical attainment of an optimum design is generally a consequence of a combination of mathematical analysis, empirical information, and the subjective experience of the scientist and engineer. In the chapters to follow we shall examine in detail the principles which underlie the formulation and resolution of the practical problems of the analysis and specification of optimal process units and control systems. Some of these results lend themselves to immediate application, while others provide helpful insight into the considerations which must enter into the specification and operation of a working system.

The formulation of a process or control system design is a trial-and-error procedure, in which estimates are made first and then information is sought from the system to determine improvements. When a sufficient mathematical characterization of the system is available, the effect of changes about a preliminary design may be obtained analytically, for the perturbation techniques so common in modern applied mathematics and engineering analysis have their foundation in linear analysis, despite the nonlinearity of the system being analyzed. Whether mathematical or experimental or a judicious combination of both, perturbation analysis lies at the heart of modern engineering practice.

Mathematical optimization techniques have as their goal the development of rigorous procedures for the attainment of an optimum in a system which can be characterized mathematically. The mathematical characterization may be partial or complete, approximate or exact, empirical or theoretical. Similarly, the resulting optimum may be a final implementable design or a guide to practical design and a criterion by which practical designs are to be judged. In either case, the optimization techniques should serve as an important part of the total effort in the design of the units, structure, and control of a practical system.

Several approaches can be taken to the development of mathematical methods of optimization, all of which lead to essentially equivalent results. We shall adopt here the variational method, for since it is grounded in the analysis of small perturbations, it is the procedure which lies closest to the usual engineering experience. The general approach is one of assuming that a preliminary specification has been made and then enquiring about the effect of small changes. If the specification is in fact the optimum, any change must result in poorer performance and the precise mathematical statement of this fact leads to *necessary conditions*, or equations which define the optimum. Similarly, the analysis of the effect of small perturbations about a nonoptimal specification leads to computational procedures which produce a better specification. Thus, unlike most approaches to optimization, the variational method leads rather simply to both necessary conditions and computational algorithms by an identical approach and, furthermore, provides a logical framework for studying optimization in new classes of systems.

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A. E. Rogers and T. W. Connolly: "Analog Computation in Engineering Design," McGraw-Hill Book Company, New York, 1960

R. G. E. Franks: "Mathematical Modeling in Chemical Engineering," John Wiley & Sons, Inc., New York, 1967

Perturbation methods for nonlinear systems are treated in such books as

W. F. Ames: "Nonlinear Ordinary Differential Equations in Transport Processes," Academic Press, Inc., New York, 1968

———: "Nonlinear Partial Differential Equations in Engineering," Academic Press, Inc., New York, 1965

R. E. Bellman: "Perturbation Techniques in Mathematics, Physics, and Engineering," Holt, Rinehart and Winston, Inc., New York, 1964

W. J. Cunningham: "Introduction to Nonlinear Analysis," McGraw-Hill Book Company, New York, 1958

N. Minorsky: "Nonlinear Oscillations," D. Van Nostrand Company, Inc., Princeton, N.J., 1962

Perhaps the most pertinent perturbation method from a system analysis viewpoint, the Newton-Raphson method, which we shall consider in detail in Chaps. 2 and 9, is discussed in

R. E. Bellman and R. E. Kalaba: "Quasilinearization and Nonlinear Boundary Value Problems," American Elsevier Publishing Company, New York, 1965

1

Optimization with Differential Calculus

1.1 INTRODUCTION

A large number of interesting optimization problems can be formulated in such a way that they can be solved by application of differential calculus, and for this reason alone it is well to begin a book on optimization with an examination of the usefulness of this familiar tool. We have a further motivation, however, in that all variational methods may be considered to be straightforward extensions of the methods of differential calculus. Thus, this first chapter provides the groundwork and basic principles for the entire book.

1.2 THE SIMPLEST PROBLEM

The simplest optimization problem which can be treated by calculus is the following: $\mathcal{E}(x_1,x_2, \ldots ,x_n)$ is a function of the n variables $x_1, x_2, \ldots, x_n$. Find the particular values $\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n$ which cause the function $\mathcal{E}$ to take on its minimum value.

We shall solve this problem in several ways. Let us note first that the minimum has the property that

$$\mathcal{E}(x_1,x_2, \ldots ,x_n) - \mathcal{E}(\bar{x}_1,\bar{x}_2, \ldots ,\bar{x}_n) \geq 0 \tag{1}$$

Suppose that we let $x_1 = \bar{x}_1 + \delta x_1$, where δx_1 is a small number in absolute value, while $x_2 = \bar{x}_2$, $x_3 = \bar{x}_3$, . . . , $x_n = \bar{x}_n$. If we divide Eq. (1) by δx_1, we obtain, depending upon the algebraic sign of δx_1,

$$\frac{\mathcal{E}(\bar{x}_1 + \delta x_1, \bar{x}_2, \ldots , \bar{x}_n) - \mathcal{E}(\bar{x}_1,\bar{x}_2, \ldots ,\bar{x}_n)}{\delta x_1} \geq 0 \qquad \delta x_1 > 0 \tag{2a}$$

or

$$\frac{\mathcal{E}(\bar{x}_1 + \delta x_1, \bar{x}_2, \ldots , \bar{x}_n) - \mathcal{E}(\bar{x}_1,\bar{x}_2, \ldots ,\bar{x}_n)}{\delta x_1} \leq 0 \qquad \delta x_1 < 0 \tag{2b}$$

The limit of the left-hand side as $\delta x_1 \to 0$ is simply $\partial \mathcal{E}/\partial x_1$, evaluated at $\bar{x}_1$, $\bar{x}_2$, . . . , $\bar{x}_n$. From the inequality (2*a*) this partial derivative is nonnegative, while from (2*b*) it is nonpositive, and both inequalities are satisfied only if $\partial \mathcal{E}/\partial x_1$ vanishes. In an identical way we find for all x_k, $k = 1, 2, \ldots, n$,

$$\frac{\partial \mathcal{E}}{\partial x_k} = 0 \tag{3}$$

at the minimizing values $\bar{x}_1$, $\bar{x}_2$, . . . , $\bar{x}_n$. We thus have n algebraic equations to solve for the n unknowns, $\bar{x}_1$, $\bar{x}_2$, . . . , $\bar{x}_n$.

It is instructive to examine the problem somewhat more carefully to search for potential difficulties. We have, for example, made a rather strong assumption in passing from inequalities (2*a*) and (2*b*) to Eq. (3), namely, that the partial derivative in Eq. (3) exists at the values x_1, x_2, . . . , x_n. Consider, for example, the function

$$\mathcal{E}(x_1,x_2, \ldots ,x_n) = |x_1| + |x_2| + \cdots + |x_n| \tag{4}$$

which has a minimum at $x_1 = x_2 = \cdots = x_n = 0$. Inequalities (1) and (2) are satisfied, but the partial derivatives in Eq. (3) are not defined at $x_k = 0$. If we assume that one-sided derivatives of the function $\mathcal{E}$ exist everywhere, we must modify condition (3) to

$$\lim_{x_k \to \bar{x}_k^-} \frac{\partial \mathcal{E}}{\partial x_k} \leq 0 \tag{5a}$$

$$\lim_{x_k \to \bar{x}_k^+} \frac{\partial \mathcal{E}}{\partial x_k} \geq 0 \tag{5b}$$

with Eq. (3) implied if the derivative is continuous.

In problems which describe real situations, we shall often find that physical or economic interpretations restrict the range of variables we

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