Preface

Chemical engineering applications have been a source of challenging optimization problems for over 50 years. For many chemical process systems, detailed steady state and dynamic behavior can now be described by a rich set of detailed nonlinear models, and relatively small changes in process design and operation can lead to significant improvements in efficiency, product quality, environmental impact, and profitability. With these characteristics, it is not surprising that systematic optimization strategies have played an important role in chemical engineering practice. In particular, over the past 35 years, nonlinear programming (NLP) has become an indispensable tool for the optimization of chemical processes. These tools are now applied at research and process development stages, in the design stage, and in the online operation of these processes. More recently, the scope of these applications is being extended to cover more challenging, large-scale tasks including process control based on the optimization of nonlinear *dynamic* models, as well as the incorporation of nonlinear models into strategic planning functions.

Moreover, the ability to solve large-scale process optimization models cheaply, even online, is aided by recent breakthroughs in nonlinear programming, including the development of modern barrier methods, deeper understanding of line search and trust region strategies to aid global convergence, efficient exploitation of second derivatives in algorithmic development, and the availability of recently developed and widely used NLP codes, including those for barrier methods [81, 391, 404], sequential quadratic programming (SQP) [161, 159], and reduced gradient methods [119, 245, 285]. Finally, the availability of optimization modeling environments, such as AIMMS, AMPL, and GAMS, as well as the NEOS server, has made the formulation and solution of optimization accessible to a much wider user base. All of these advances have a huge impact in addressing and solving process engineering problems previously thought intractable. In addition to developments in mathematical programming, research in process systems engineering has led to optimization modeling formulations that leverage these algorithmic advances, with specific model structure and characteristics that lead to more efficient solutions.

This text attempts to make these recent optimization advances accessible to engineers and practitioners. Optimization texts for engineers usually fall into two categories. First, excellent mathematical programming texts (e.g., [134, 162, 294, 100, 227]) emphasize fundamental properties and numerical analysis, but have few specific examples with relevance to real-world applications, and are less accessible to practitioners. On the other hand, equally good engineering texts (e.g., [122, 305, 332, 53]) emphasize applications with well-known methods and codes, but often without their underlying fundamental properties. While their approach is accessible and quite useful for engineers, these texts do not aid in a deeper understanding of the methods or provide extensions to tackle large-scale problems efficiently.

To address the modeling and solution of large-scale process optimization problems, it is important for optimization practitioners to understand

- which NLP methods are best suited for specific applications,
- how large-scale problems should be formulated and what features should be emphasized, and
- how existing methods can be extended to exploit specific structures of large-scale optimization models.

This book attempts to fill the gap between the math programming and engineering texts. It provides a firm grounding in fundamental algorithmic properties but also with relevance to real-world problem classes through case studies. In addressing an engineering audience, it covers state-of-the-art gradient-based NLP methods, summarizes key characteristics and advantages of these methods, and emphasizes the link between problem structure and efficient methods. Finally, in addressing a broader audience of math programmers it also deals with steady state and dynamic models derived from chemical engineering.

The book is written for an audience consisting of

- engineers (specifically chemical engineers) interested in understanding and applying state-of-the-art NLP algorithms to specific applications,
- experts in mathematical optimization (in applied math and operations research) who are interested in understanding process engineering problems and developing better approaches to solving them, and
- researchers from both fields interested in developing better methods and problem formulations for challenging engineering problems.

The book is suitable for a class on continuous variable optimization, but with an emphasis on problem formulation and solution methods. It is intended as a text for graduate and advanced undergraduate classes in engineering and is also suitable as an elective class for students in applied mathematics and operations research. It is also intended as a reference for practitioners in process optimization in the area of design and operations, as well as researchers in process engineering and applied mathematics.

The text is organized into eleven chapters, and the structure follows that of a short course taught to graduate students and industrial practitioners which has evolved over the past 20 years. Included from the course are a number of problems and computer projects which form useful exercises at the end of each chapter.

The eleven chapters follow sequentially and build on each other. Chapter 1 provides an overview of nonlinear programming applications in process engineering and sets the motivation for the text. Chapter 2 defines basic concepts and properties for nonlinear programming and focuses on fundamentals of unconstrained optimization. Chapter 3 then develops Newton's method for unconstrained optimization and discusses basic concepts for globalization methods; this chapter also develops quasi-Newton methods and discusses their characteristics.

Chapter 4 then follows with fundamental aspects of constrained optimization, building on the concepts in Chapter 2. Algorithms for equality constrained optimization are derived in Chapter 5 from a Newton perspective that builds on Chapter 3. Chapter 6 extends this approach to inequality constraints and discusses algorithms and problem formulations that are essential for developing large-scale optimization models. Chapter 7 then discusses steady state process optimization and describes the application of NLP methods to modular and equation-oriented simulation environments.

Chapter 8 introduces the emerging field of dynamic modeling and optimization in process systems. A survey of optimization strategies is given and current applications are summarized. The next two chapters deal with two strategies for dynamic optimization. Chapter 9 develops optimization methods with embedded differential-algebraic equation (DAE) solvers, while Chapter 10 describes methods that embed discretized DAE models within the optimization formulation itself. Chapter 11 concludes this text by presenting complementarity models that can describe a class of discrete decisions. Embedded within nonlinear programs, these lead to mathematical programs with complementarity constraints (MPCC) that apply to both steady state and dynamic process optimization models.

Finally, it is important to mention what this book does not cover. As seen in the table of contents, the book is restricted to methods and applications centered around gradient-based nonlinear programming. Comprising the broad area of optimization, the following topics are not considered, although extensive citations are provided for additional reading:

- *Optimization in function spaces*. While the text provides a practical treatment of DAE optimization, this is developed from the perspective of finite-dimensional optimization problems. Similarly, PDE-constrained optimization problems [51, 50] are beyond the scope of this text.

- *Iterative linear solvers*. Unlike methods for PDE-based formulations, indirect linear solvers are almost never used with chemical process models. Hence, the NLP strategies in this book will rely on direct (and often sparse) linear solvers with little coverage of iterative linear solvers.

- *Optimization methods for nondifferentiable functions*. These methods are not covered, although some nondifferentiable features may be addressed through reformulation of the nonlinear program. Likewise, derivative-free optimization methods are not covered. A recent treatment of this area is given in [102].

- *Optimization problems with stochastic elements*. These problems are beyond the scope of this text and are covered in a number of texts including [57, 216].

- *Optimization methods that ensure global solutions*. The NLP methods covered in the text guarantee only local solutions unless the appropriate convexity conditions hold. Optimization methods that ensure global solutions for nonconvex problems are not covered here. Extensive treatment of these methods can be found in [144, 203, 379].

- *Optimization methods for problems with integer variables*. These methods are beyond the scope of this book. Resources for these mixed integer problems can be found in [53, 143, 295].

Nevertheless, the NLP concepts and algorithms developed in this text provide useful background and a set of tools to address many of these areas.

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