## Matrix, Numerical, and Optimization Methods in Science and Engineering

Address vector and matrix methods necessary in numerical methods and optimization of systems in science and engineering with this unified text. The book treats the mathematical models that describe and predict the evolution of our processes and systems, and the numerical methods required to obtain approximate solutions. It explores the dynamical systems theory used to describe and characterize system behavior, alongside the techniques used to optimize their performance. The book integrates and unifies matrix and eigenfunction methods with their applications in numerical and optimization methods. Consolidating, generalizing, and unifying these topics into a single coherent subject, this practical resource is suitable for advanced undergraduate students and graduate students in engineering, physical sciences, and applied mathematics.

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**The heavens declare the glory of God;**
**the skies proclaim the work of his hands.**
**Day after day they pour forth speech;**
**night after night they display knowledge.**
**There is no speech or language**
**where their voice is not heard.**
**Their voice goes out into all the earth,**
**their words to the ends of the world.**
**(Psalm 19:1–4)**

# Contents

# Preface

So much of the mathematics that we know today was originally developed to treat particular problems and applications – the mathematics and applications were inseparable. As the years went by, the mathematical methods naturally were extended, unified, and formalized. This has provided a solid foundation on which to build mathematics as a standalone field and basis for extension to additional application areas, sometimes, in fact, providing the impetus for whole new fields of endeavor. Despite the fact that this evolution has served mathematics, science, and engineering immeasurably, this tendency naturally widens the gaps between pure theoretical mathematics, applied mathematics, and science and engineering applications as time progresses. As such, it becomes increasingly difficult to strike the right balance in textbooks and courses that encourages one to learn the mathematics in the context of the applications to which the scientist and engineer are ultimately interested.

Whatever the approach, the goal should be to increase the student's intellectual dexterity in research and/or practice. This requires a depth of knowledge in the fundamentals of the subject area along with the underlying mathematical techniques on which the field is based. Given the volume of theory, methods, and techniques required in the arsenal of the researcher and practitioner, I believe that this objective is best served by how the mathematical subjects are discretized into somewhat self-contained topics around which the associated methods and applications are hung.

The objective of the present text is to integrate matrix methods, dynamical systems, numerical methods, and optimization methods into a single coherent subject and extend our skill to the level that is required for graduate-level study and research in science and engineering through **consolidation**, **generalization**, and **unification** of topics. These objectives guide the choice and ordering of topics and lead to a framework that enables us to provide a unified treatment of the mathematical techniques so that the reader sees the entire picture from mathematics – without overdoing the rigor – to methods to applications in a logically arranged, and clearly articulated, manner. In this way, students retain their focus throughout on the most challenging aspects of the material to be learned – the mathematical methods. Once they have done so, it is then straightforward to see how these techniques can be extended to more complicated and disparate applications in their chosen field.

Because engineers and scientists are naturally curious about applications, we merely need to tap into this curiosity to provide motivation for mathematical developments. Consequently, the keys to learning mathematics for scientists and engineers are to (1) sufficiently motivate the need for it topic by topic, and (2) apply it right away and often. In order to leverage the reader's inherent interest in applications, therefore, the overall pattern of the text as a whole as well as within each topic is to *motivate* → *learn* → *interpret* → *apply* → *extend*. This approach more clearly uses the applications to help the student learn the fundamental mathematical techniques, and it also provides deeper insight into the applications by unifying the underlying mathematics. It encourages a deeper understanding of matrix methods and its intimate connection with numerical methods and optimization. The primary virtue of this approach is that the reader clearly sees the connections, both mathematical and physical, between a wide variety of topics.

For a subject as ubiquitous as matrix methods, great care must be exercised when selecting specific topics for inclusion in such a book lest it become an unwieldy encyclopedia. The most compelling answer to the question, "Why do scientists and engineers need a deep knowledge of matrix methods?" is that they provide the mathematical foundation for the numerical methods, optimization, and dynamical systems theory that are central to so much of modern research and practice in the physical sciences and engineering.

Perhaps the most prevalent and ubiquitous applications of matrix methods are in the numerical techniques for obtaining approximate solutions to algebraic and differential equations that govern the behavior of mechanical, electrical, chemical, and biological systems. These numerical methods pervade all areas of science and engineering and pick up where analytical methods fail us. It is becoming increasingly clear that serious researchers and practitioners must have a solid foundation in both matrix methods and numerical techniques. The most effective way to articulate such foundational material is in a unified and comprehensive manner – a token chapter on elementary numerical methods is insufficient. On the other hand, undergraduate texts in numerical methods for engineers and scientists generally only require a minimal background in linear algebra. However, a bit more formal understanding of vectors, matrices, linear systems of algebraic equations, and eigenproblems can significantly enhance the learning of such subjects. The strategy of this text clearly highlights and leverages the integral and essential nature of linear algebra in numerical methods.

The present text has been written in the same style as *Variational Methods with Applications in Science and Engineering* (Cassel, 2013) with the same emphasis on broad applications in science and engineering. Observe in Figure 0.1 how the topics from the two books complement and overlap one another. The present book consists of three parts: Part I – Matrix Methods, Part II – Numerical Methods, and Part III – Least Squares and Optimization. Of course, all of these subjects are treated within a unified framework with matrix methods providing the catalyst. After completing Part I, the reader can choose to proceed directly to Part II on numerical methods or Part III on least-squares and optimization. Part I provides all of the prerequisite material for both parts. Although there will be some numerical methods introduced in Part III, none of them depend on material in Part II.

In Part I on matrix methods, the focus is on topics that are common to numerous areas of science and engineering, not subject-specific topics. Because of our interest

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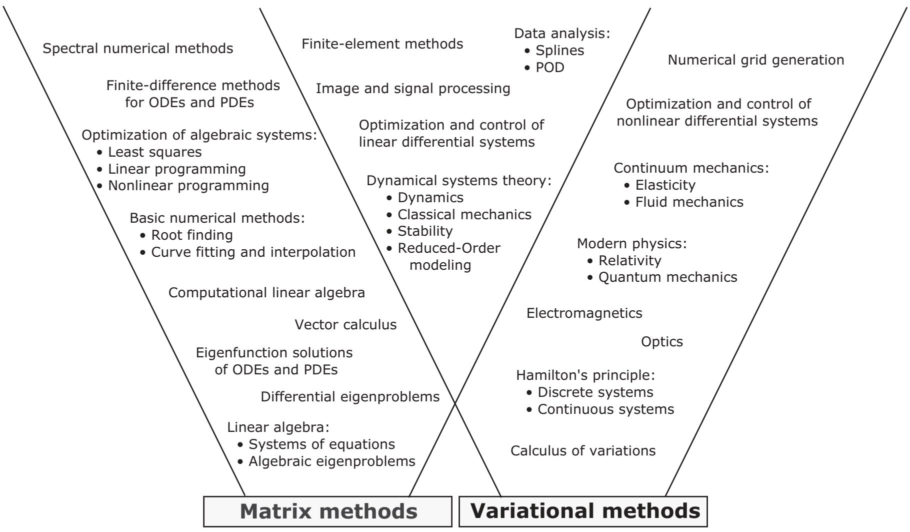


**Figure 0.1** Correspondence of topics in matrix methods and variational methods with applications in science and engineering.

in continuous, as well as discrete, systems, "matrix methods" is interpreted loosely to include function spaces and eigenfunction methods. Far from being a recounting of standard methods, the material is infused with a strong dose of the applications that motivate them – including to dynamical systems theory. We progress from the basic operations on vectors and matrices in Chapter 1 in a logical fashion all the way to the singular-value decomposition at the end of Chapter 2 that is at the heart of so many modern applications to discrete and continuous systems. Integrating and juxtaposing the differential eigenproblem in Chapter 3 with its algebraic counterpart in Chapter 2 also serves to unify topics that are often separated and presented in different settings and courses. The methods articulated in Part I are appropriate for relatively small systems that can be solved exactly by hand or using symbolic mathematical software. Despite this obvious limitation, they are essential knowledge and provide a starting point for all subsequent discussion of numerical methods and optimization techniques.

Whereas Part I primarily deals with the traditional methods used for hand calculations of small systems, Part II focuses on numerical methods used to approximate solutions of very large systems on computers. In order to solve moderate to large systems of algebraic equations, for example, we must revisit linear systems of algebraic equations and the eigenproblem to see how the methods in Part I can be adapted for large systems. This is known as *computational*, or *numerical, linear algebra* and is covered in Chapter 6. The remaining chapters in Part II encompass a broad range of numerical techniques in widespread use for obtaining approximate solutions to ordinary and partial differential equations. The focus is on finite-difference methods with limited coverage of finite-element and spectral methods primarily for comparison. Unifying all of these topics under the umbrella of matrix methods provides both a broader and deeper understanding of the numerical methods themselves and the issues that arise in their deployment. In particular, it encourages a unification of topics that is not possible otherwise.

Similar to Part II, those least-squares and optimization topics included in Part III are of general interest in a wide variety of fields involving discrete and continuous systems and follow directly from material discussed in Part I. We begin with a general treatment of the least-squares problem, which is used in least-squares regression curve fitting and interpolation for data analysis and is the basis for numerous optimization and control techniques used in research and practice. Root-finding techniques for algebraic systems are integrated with optimization methods used to solve linear and nonlinear programming problems. Finally, Chapter 13 builds on the optimization foundation to address data-driven methods in reduced-order modeling featuring a clear treatment of proper-orthogonal decomposition, also called principal component analysis, and its extensions. This treatment clearly highlights the centrality of Galerkin projection in such methods.

It goes without saying that each individual reader will wish that there was more material specifically related to applications in their chosen field of study, and certain application areas have received little or no attention. Because of the broad range of applications that draw on matrix methods, we are limited in how far we may proceed along the *mathematics* → *methods* → *applications* continuum to primarily focus on methods that have broad applicability in science and engineering. For example, there is no mention of machine learning and artificial intelligence as these also depend on probability and statistics, which are beyond the scope of this text. Similarly, other than a brief mention in the context of singular-value decomposition, there is no material directly addressing image and signal processing – except that the underlying Fourier analysis methods are covered. The reader is referred to chapter 11 of Cassel (2013) for an introduction to the variational approach to such data analysis.

This text is targeted at the advanced undergraduate or graduate engineering, physical sciences, or applied mathematics student. It may also serve as a reference for researchers and practitioners in the many fields that make use of matrix, numerical, or optimization methods. The prerequisite material required is an undergraduate-level understanding of calculus, elementary complex variables, and ordinary and partial differential equations typical of engineering and physical science programs. Because of the intended audience of the book, there is little emphasis on mathematical proofs except where necessary to highlight certain essential features. Instead, the material is presented in a manner that promotes development of an intuition about the concepts and methods with an emphasis on applications to numerical and optimization methods as well as dynamical systems theory.

This book could serve as the primary text or a reference for courses in linear algebra or matrix methods, linear systems, basic numerical methods, optimization and control, and advanced numerical methods for partial differential equations. At the Illinois Institute of Technology, the material covers a portion of an engineering analysis course for first-year graduate students in various engineering disciplines (which also includes complex variables and variational methods), an undergraduate numerical methods course for mechanical and aerospace engineers (we call it computational mechanics), and a graduate course in computational methods for partial differential equations, such as computational fluid dynamics (CFD) and heat transfer. In addition, it could serve as a supplement or reference for courses in dynamical systems theory, classical mechanics, mechanical vibrations, structural mechanics, or optimization.

I would like to thank the many students who have helped shape my thinking on how best to arrange and articulate this material, and I particularly appreciate the comments and suggestions of the reviewers who greatly assisted in improving this somewhat unconventional amalgamation of topics. I can be reached at cassel@iit.edu if you have any comments on the text.