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Xuefeng Liu

Guaranteed Computational Methods for Self-Adjoint Differential Eigenvalue Problems

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Preface

This monograph focuses on the study of eigenvalue problems of self-adjoint differential operators. It aims to explicate the recently developed methods that offer guaranteed computations for both eigenvalues and eigenfunctions. A central theme is the application of the Finite Element Method (FEM) as the primary numerical strategy for computations, accompanied by an in-depth discussion on theories of error estimation.

Eigenvalue problems of differential operators are of fundamental importance in both mathematics and engineering. Obtaining the upper eigenvalue bound, typically through the Rayleigh–Ritz method, is a relatively straightforward process. However, to obtain a rigorous lower eigenvalue bound is a challenging endeavor that requires complicated techniques and methodologies.

The recent progress in computer-assisted proofs for non-linear partial differential equations, such as the Navier–Stokes equation, necessitates explicit values or bounds of various quantities, most of which are governed by eigenvalues of the related differential operators. This situation highlights the critical need for the development and refinement of guaranteed computation methods for solving eigenvalue problems.

The following is a brief outline and highlights of the book:

Chapter 1 provides an overview of the literature regarding explicit eigenvalue bounds achieved through numerical methods. The chapter is enriched with examples of eigenvalue problems that demonstrate the need for guaranteed computation.

Chapter 2 presents recent advancements in quantitative error estimates, specifically error bounds with concrete values, for boundary value problems in partial differential equations. A primary focus is placed on a priori error estimation based on the hypercircle method, which provides a novel approach for the projection error estimation to be used in the analysis of eigenvalue problems.

Chapter 3 lays out a Galerkin projection-based method for obtaining explicit eigenvalue bounds. It deeply analyzes the eigenvalue problem formalized as $a(u, v) = \lambda b(u, v)$, including cases where either $a(\cdot, \cdot)$ or $b(\cdot, \cdot)$ is positive semi-definite.

Chapter 4 extends the theorem in Chap. 3 and applies it, in conjunction with the conforming and non-conforming finite element methods, to several traditional model eigenvalue problems involving the Laplace, the biharmonic, the Stokes, and the Steklov differential operators.

Chapter 5 provides a deep exploration of the Lehmann–Goerisch method, designed for the efficient computation of high-precision eigenvalue bounds. The implementation of the Lehmann–Goerisch method necessitates a rough lower bound for a specific eigenvalue, which can be obtained from the lower bound derived in Chaps. 3 and 4. This method takes the advantage of accurate approximate eigenfunctions computed by any means and subsequently delivers precise eigenvalue bounds. The effectiveness of this method is demonstrated via its application to the Laplacian and Steklov eigenvalue problems.

As a feature of this book, it discloses the affinity of the Lehmann–Goerisch method with finite element methods, which has not been well discussed in the existing literature. The relationship among the Lehmann–Goerisch method, Lehmann–Maehly method, and Kato's bound is thoroughly examined. Given that the original proof of this method was published in German, this book includes an English version of the proof with enhanced understanding and accessibility, while the original setting as posited by Goerisch is well preserved.

Chapter 6 is devoted to the guaranteed bounds for the approximation error encountered in eigenfunction calculations. The chapter explores three distinct algorithms depending on problem settings: the Rayleigh quotient-based algorithm, the residual-based algorithm, and the projection-based algorithm. Particular emphasis is placed on the residual-based error estimation, including an in-depth discussion on the Davis–Kahan theorem extended to weakly formulated eigenvalue problems. These algorithms have a common feature: they consider the angle between the exact eigenspace and the approximate one, thereby enabling them to handle cases where eigenvalues are tightly clustered.

Appendix introduces the Verified Finite Element Method (VFEM) library. Specifically designed for rigorous computations using finite element methods, the VFEM library is a valuable tool for practical computations that demand guaranteed results.

As an extended content of this book, the author prepared a web page located at http://www.xfliu.org/EVP2024/ to feature a comprehensive table of constants commonly used in numerical analysis. Examples include error constants for various interpolation operators and constants within the Sobolev embedding theorems. These constants are typically calculated by solving corresponding eigenvalue problems with the techniques introduced in this book.

The author wishes to express his great appreciation to Fumio Kikuchi for carefully reading the proof of this book and providing helpful revision advice. Thanks also go to Takuya Tsuchiya and Ryoki Endo for their feedback on partial chapters.

Tokyo, Japan Xuefeng Liu
March 2024

Contents

Chapter 1
Introduction to Eigenvalue Problems

Abstract This chapter provides an overview of the literature concerning explicit eigenvalue bounds achieved through numerical methods. It outlines the rapid progress in the field of guaranteed eigenvalue computation over the past decade, while also highlighting its relationship with early work such as Birkhoff's result. Examples of eigenvalue problems demonstrate the need for guaranteed computation. The chapter also discusses the settings of function spaces and basic usage of finite element methods.

Keywords Eigenvalue problem · Explicit eigenvalue bounds · Finite element method (FEM) · Birkhoff's result

This chapter provides a comprehensive overview of research focusing on rigorous eigenvalue bounds. To illustrate the motivation of studying eigenvalue problems, two specific problems associated with the Poincaré constant are introduced, complemented by numerical results.

1.1 Overview of Research on Rigorous Eigenvalue Bounds

Eigenvalue problems related to differential operators constitute a pivotal theme within numerical analysis. A vast amount of research papers have been dedicated to the error analysis of numerical schemes for these problems. When dealing with irregular domains, unlike special geometries such as rectangles or disks where a closed form of the eigensystem can be easily derived, the finite element method (FEM) becomes the preferred approach. For a thorough understanding of the fundamental approximation theories linked to eigenvalue problems, readers are referred to Babuška–Osborn [4] and Weinberger [88], while Boffi [7] and Sun–Zhou [83] provide surveys of methods based on the finite element method.

Over the past two decades, verified computation has found successful application in the investigation of nonlinear differential equations through computer-assisted

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proofs. This topic is comprehensively discussed in the recent monograph by Nakao–Watanabe–Plum [69]. Such investigations require the rigorous calculation of linear operator norms and the explicit values of various error constants, which invariably leads to solving eigenvalue problems of differential operators. This consequently urges the pursuit of guaranteed computational methods for eigenvalue problems.

For differential operators like the Laplacian, it is known that upper eigenvalue bounds can easily be obtained using the Rayleigh–Ritz method with trial functions, e.g., using polynomial or trigonometric functions or finite element methods. However, finding lower eigenvalue bounds remains a difficult problem and has drawn the interest of many researchers. In the literature, various techniques have been developed for providing lower eigenvalue bounds. Most of the classical methods, e.g., the Weinstein–Aronszajn intermediate method [35, 89] and the point-matching method [27], require a priori information about the eigenvalue range, which is not easy to validate in solving practical problems, and will not be dealt with in this book.

This book mainly focuses on the finite element method and introduces the Galerkin projection-based algorithm developed for the purpose of rigorous bounds for the eigenvalues in Chaps. 2–4. The idea of using the projection error estimation to obtain eigenvalue bounds can be found in an early paper by Birkhoff et al. [6] in 1966, where the eigenvalue bounds for smooth Sturm–Liouville systems are provided by using projection to piecewise-cubic polynomials. In a preprint [54] in 2011 and later a paper [56] in 2013, the author extends the idea of Birkhoff and proposes guaranteed two-sided bounds for the Laplacian eigenvalue problem by using the Galerkin projection associated with conforming finite element methods. The proposed eigenvalue bounds can naturally handle problems defined over bounded polygonal domains of arbitrary shapes. The projection-based method is further extended to handle general compact self-adjoint differential operators [50] and the eigenvalue problem formulated by positive semi-definite bilinear forms [51], where zero eigenvalue may appear (e.g., the case of the Steklov eigenvalue problem). Meanwhile, the non-conforming finite element method is utilized to provide easy-to-obtain estimation for the projection error. In 2011, Kobayashi [45, 46] applied the Crouzeix–Raviart FEM and the Fujino–Morley FEM to bound the interpolation error constants, which are related to the first eigenvalue of differential operators. In 2014, Carstensen et al. [16, 18] utilized the Crouzeix–Raviart FEM and the Fujino–Morley FEM to give lower eigenvalue bounds for the leading eigenvalues of the Laplace and the biharmonic differential operators, which hinge on a "separation condition." In [50], the author proposed a general framework to take advantage of both the conforming and non-conforming FEM to obtain lower eigenvalue bounds, where the requirement of a "separation condition" is confirmed to be unnecessary.

The projection-based method has been successfully applied to various eigenvalue problems, including the biharmonic operator [49, 60], the Stokes operator [53, 91], the Steklov operator [94], the Maxwell operator [30], fluid–solid vibrations [98], high-order elliptic operators [39], and elastic problems [97].

The Lehmann–Goerisch method, to be introduced in Chap. 5, is a very useful approach to obtain sharp eigenvalue bounds when rough eigenvalue bounds and good eigenfunction approximations are available. Such a method is regarded as a generalization of Kato's eigenvalue bound [42]; see the discussion in Remark 5.4. The relation with its preceding theorems, e.g., Lehmann–Maehly's method, Temple's bound, and Collatz's bound, are discussed in Chap. 5.

Next, we introduce other useful approaches to bound eigenvalues, the details of which are skipped in this book.

Based on the Lehmann–Goerisch method, Plum [72] develops the homotopy method to solve the eigenvalue problem by considering the homotopy process with a family of eigenvalue problems that connect to a base problem with explicit spectral bounds. A distinct advantage of this method is that it accommodates a wide range of eigenvalue problems by strategically linking the target problem with the base problem via the homotopy process. However, this technique necessitates the closed form of the base problem and the monotonicity of eigenvalues within the homotopy process, which usually requires case-by-case theoretical techniques.

Nakao et al. [69, 70, 87] developed methods that provide eigenvalue bounds by identifying ranges where eigenvalues exist and cannot exist. The eigenvalue problem is transformed into an investigation of solution existence and uniqueness for certain nonlinear partial differential equations, for which existing techniques such as [68, 73] can be used.

Recently, Carstensen et al. have developed FEM schemes designed to generate direct lower eigenvalue bounds [14, 19, 20]. A notable merit of these methods lies in their applicability to graded meshes generated through adaptive computation, albeit at the cost of parameter tuning or an expanded degree of freedoms within the newly developed FEM schemes.

To conclude this section, we shall also present the existing literature on eigenvalue bounds, which exhibit limitations or pose unresolved issues when applied to derive explicit eigenvalue bounds. For special domains with well-constructed meshes, it is proved that the approximate eigenvalues from the mass lumping method provide lower eigenvalue bounds directly [40, 41]. Many non-conforming FEMs also provide lower eigenvalue bounds asymptotically, i.e., when the mesh is fine enough, the computed eigenvalues converge to the exact values from below; see early results of Armentano–Durán [2] and the work surveyed in [38, 61, 93]. However, it is still not clear how to verify the required precondition, i.e., the mesh size being small enough, to ensure the asymptotic lower bounds.

1.2 Model Eigenvalue Problems

Let us first consider the model eigenvalue problem of the Laplace operator. Later in Chap. 4, we will investigate eigenvalue problems more deeply.

Let $\Omega \subset \mathbb{R}^2$ be a bounded connected domain with a Lipschitz boundary. The case of non-convex Ω is allowed. The Dirichlet Laplacian eigenvalue problem is to