Verified Eigenvalue Calculation for the Laplace Operator

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Abstract. This paper proposes a method for estimating eigenvalues and eigenvectors based on a computable residual. We provide guaranteed upper and lower bounds for eigenvalues and establish first-order and second-order error estimates. Additionally, error bounds for eigenvectors are provided, ensuring precise estimates for both eigenvalues and eigenvectors. Numerical experiments have validated the results. Furthermore, the interval algorithm is used for the calculation of residual function, and the resulting eigenvalue bounds are expected to be mathematically accurate.

Keywords: Error bounds · eigenvalue problem · self-adjoint operators.

1 Introduction

The solution of eigenvalue problems for operators arises in numerous applications in numerical analysis and scientific computing. These problems are central to diverse fields such as quantum mechanics, elasticity theory, and stability analysis. Given a linear self-adjoint operator A, its eigenvalues and eigenvectors are often of primary interest.

A standard approach for computing eigenvalues and eigenvectors of large matrices is the Rayleigh-Ritz method, which approximates the eigenvalue problem within a subspace. For the Laplace operator, we typically employ finite element discretization. Following this discretization, iterative methods—such as the power method, inverse power method, and Lanczos method—are commonly applied. The numerical solution process introduces several types of errors, including discretization errors and floating-point arithmetic errors. When using the conforming finite element method, the computed eigenvalue is usually larger than the exact eigenvalue due to the min-max principle. Consequently, determining a precise interval for the analytical eigenvalue, or its rigorous upper and lower bounds, remains a significant challenge.

In recent decades, guaranteed upper and lower bounds for eigenvalue problems have been a research focus. Methods for estimating these bounds generally fall into two categories: a priori estimates and a posteriori estimates [1]. Based on prior error estimates, Liu [5] provided a lower-order estimate for the Laplace eigenvalue problem by accurately estimating the constants in the projection operator. The theory in [4, 2] applies to arbitrarily coarse meshes and provides

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convincing numerical results in various test cases. Hu et al.[3], Luo et al. [6] and Yang et al. [8] also derived (guaranteed) eigenvalue estimates for the nonconforming finite element method.

In this paper, we propose a method for estimating eigenvalues and eigenvectors of linear operators. The approach is based on a computable residual function that quantifies the discrepancy between approximate and exact eigenvalues. Using this residual, we derive explicit upper and lower bounds for the eigenvalues, which are independent of unknown constants. The residual function is fully computable, and we further establish first- and second-order error estimates for the eigenvalues. In addition to the approximation error arising from the finite-dimensional discretization of the original infinite-dimensional problem, and the iterative solution error arising from numerical computation, we also account for rounding errors in floating-point arithmetic. The IEEE Standard enables the estimation of rounding errors through the use of interval arithmetic [7].

The structure of this paper is as follows: In the Section 2 we introduce the eigenvalue problem. The Section 3 provides the upper and lower bound estimates, while the Section 4 presents numerical validation of the theoretical results.

2 Eigenvalue problem

Consider the eigenvalue problem for the Laplace operator Δ on a domain $\Omega \subset \mathbb{R}^n$, defined as:

$$-\Delta u = \lambda u \quad \text{in} \quad \Omega,$$

where $\Delta = \nabla^2$ is the Laplace operator, λ is the eigenvalue, and u is the corresponding eigenvector (eigenfunction). We also have boundary conditions $u|_{\partial\Omega} = 0$ (Dirichlet boundary conditions), though other boundary conditions can be chosen depending on the specific problem.

Multiply both sides by a test function $v \in H_0^1(\Omega)$ and integrate, obtaining the weak form:

$$\text{Find} \quad (\lambda, u) \quad \text{such that} \quad (\nabla u, \nabla v) = \lambda(u, v) \quad \forall v \in H_0^1(\Omega),$$

where $(\cdot, \cdot)$ represents the standard inner product:

$$(u, v) = \int_\Omega uv \, dx, \quad (\nabla u, \nabla v) = \int_\Omega \nabla u \cdot \nabla v \, dx.$$

The key idea in finite element methods is to approximate the solution by choosing a suitable finite-dimensional space of test and trial functions. Let $V_h \subset H_0^1(\Omega)$ be a finite-dimensional subspace. We can obtain a discrete system of linear equations:

$$Su_h = \lambda_h M u_h,$$

where:

$$S_{ij} = (\nabla\varphi_i, \nabla\varphi_j), \quad M_{ij} = (\varphi_i, \varphi_j),$$

and $u_h = [u_1^h, u_2^h, \ldots, u_N^h]^T$ is the vector of coefficients in the finite element basis.

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In this paper, we employ a global spectral method to solve the problem. Compared with traditional finite element methods, spectral methods offer superior accuracy and computational efficiency through the use of globally orthogonal basis functions for solution representation.

After discretizing the problem using global basis functions, we obtain a matrix eigenvalue problem that could conventionally be solved using methods like the power method or inverse power method. However, in this work, we employ a gradient flow approach instead. This method offers unconditional energy stability, making it particularly advantageous for our purposes.

$$\frac{\tilde{u}_h^{n+1} - u_h^n}{\Delta t} = M^{-1} S u_h^{n+1},$$
$$u_h^{n+1} = \tilde{u}_h^{n+1} / (\tilde{u}_h^{n+1}, \tilde{u}_h^{n+1}).$$

One key advantage of using the gradient flow method is that it is well-suited for solving eigenvalue problems in the context of non-linear and large-scale systems, where other methods might fail to converge or require extensive computational resources.

3 Guaranteed Bounds

In this section, we provide upper and lower bound estimates for the eigenvalues. Define $\{(\lambda_i, u_i), i \in \mathbb{N}\}$ are the exact eigen-pairs of the operator $A = -\Delta$, where $\lambda_1 \leq \lambda_2 \leq \lambda_2 \leq \cdots \lambda_{k-1} \leq \lambda_k \leq \cdots$. We assume the numerical scheme provides an approximate u_h intended to approximate the k-th exact eigenvector u_k. The corresponding eigenvalue λ_k is then computed using the following equation. We note that even the numerical scheme gives us also λ_k, we do not use it, and we update λ_k by

$$\lambda_h = \frac{(Au_h, u_h)}{(u_h, u_h)}.$$

And we define the residual vector as

$$r_h = \frac{Au_h - \lambda_h u_h}{\|u_h\|_{L^2(\Omega)}}.$$

First, we present a guaranteed numerical bound for eigenvalues known as D. Weinstein's bound in the literature.

Lemma 1. *We assume among all the exact eigenvalues of A, the eigenvalue λ_k is the one closest to λ_h, that is $|\lambda_k - \lambda_h| \leq |\lambda_i - \lambda_h|, \forall i \in \mathbb{N}$. Then we have*

$$\lambda_h - \delta \leq \lambda_k \leq \lambda_h + \delta,$$

where $\delta = \|r_h\|_{L^2(\Omega)}$.

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Proof. We first expand u_h in terms of $\{u_i, i \in \mathbb{N}\}$,

$$u_h = \sum_{i=1}^{\infty} \alpha_i u_i, \quad \alpha_i = (u_h, u_i),$$

We then note that

$$r_h = Au_h - \lambda_h u_h = \sum_{i=1}^{\infty} \alpha_i (Au_i - \lambda_h u_i) = \sum_{i=1}^{\infty} \alpha_i (\lambda_i - \lambda_h) u_i.$$

We can obtain,

$$\|r_h\|^2_{L^2(\Omega)} = \sum_{i=1}^{\infty} \alpha_i^2 (\lambda_i - \lambda_h)^2 \geq \sum_{i=1}^{\infty} \alpha_i^2 (\lambda_k - \lambda_h)^2 = (\lambda_i - \lambda_h)^2.$$

□

Remark 1. In our calculation, the first step is to calculate the first eigenpair (λ_1, u_1) using the regular floating numbers, the second step is to obtain a guaranteed interval estimate for $\delta = \|r_h\|_{L^2(\Omega)}$ and then for λ_k by using the Interval Arithmetic (IA) technique: $\delta \in [\delta_m, \delta_M]$ and $\lambda_k \in [\lambda_{k,m}, \lambda_{k,M}]$, where $[\delta_m, \delta_M] = \mathrm{IA}\left(\|r_h\|_2\right)$, $\lambda_{k,m} = \mathrm{IA}_m\left(\lambda_h - \delta_M\right)$, and $\lambda_{k,m} = \mathrm{IA}_M\left(\lambda_h + \delta_M\right)$.

The first step (numerical computation) introduces multiple potential error sources: discretization error from approximating the infinite-dimensional space with a finite-dimensional subspace; domain truncation error, particularly significant for quantum systems like the hydrogen atom requiring unbounded-domain approximation; iterative convergence error inherent in numerical approximation schemes; and floating-point round-off error due to finite-precision arithmetic limitations. The second step yields a guaranteed interval estimate for the eigenvalue λ_k. This overestimation arises from two primary sources: (i) the inherent non-sharpness of our *a posteriori* error estimator (as seen in the bounding estimate $\lambda_h - \delta \leq \lambda_k \leq \lambda_h + \delta$), and (ii) the application of interval arithmetic during the post-processing step. Both factors contribute conservatively to the final error bounds.

Theorem 1. *We assume among all the exact eigenvalues of A, the eigenvalue λ_1 is the one closest to λ_h; that is, $|\lambda_1 - \lambda_h| \leq |\lambda_i - \lambda_h|, \forall i \in \mathbb{N}$. Let $\lambda_{2,L}$ is a lower approximate of λ_2. Then we have*

$$\sin \alpha(u_h, u_1) \leq \frac{\delta}{\lambda_{2,L} - \lambda_h}, \|u_h - u_1\|_{L^2(\Omega)} \leq \left(\frac{\delta}{\lambda_{2,L} - \lambda_h}\right) \sqrt{1 + \left(\frac{\delta}{\lambda_{2,L} - \lambda_h}\right)^2},$$

where $\delta := \|r_h\|_{L^2(\Omega)}$.

Proof. We expand u_h in terms of $\{u_i, i \in \mathbb{N}\}$, $u_h = \sum_{i=1}^{\infty} \alpha_i u_i, \alpha_i := (u_h, u_i)$, we have

$$\sin^2 \alpha(u_h, u_1) = 1 - \cos^2 \alpha(u_h, u_1) = 1 - \alpha_1^2$$

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As

$$r_h = Au_h - \lambda_h u_h = \sum_{i=0}^{\infty} \alpha_i (Au_i - \lambda_h u_i) = \sum_{i=0}^{\infty} \alpha_i (\lambda_i - \lambda_h) u_i,$$

we have

$$\|r_h\|^2_{L^2(\Omega)} = \sum_{i=1}^{\infty} \alpha_i^2 (\lambda_i - \lambda_h)^2 \geq \sum_{i=2}^{\infty} \alpha_i^2 (\lambda_2 - \lambda_h)^2 = (1 - \alpha_1^2)(\lambda_2 - \lambda_h)^2.$$

For $(1-\alpha_1)^2 \leq (1-\alpha_1^2)^2 = \sin^4 \alpha(u_h, u_1)$, we obtain,

$$\|u_h - u_1\|_2^2 = (1-\alpha_1)^2 + \sum_{i \geq 2} \alpha_i^2 = (1-\alpha_1)^2 + 1 - \alpha_1^2 \leq \sin^4 \alpha(u_h, u_1) + \sin^2 \alpha(u_h, u_1),$$

implying

$$\begin{aligned} \|u_h - u_1\|_{L^2(\Omega)} &\leq \sin \alpha(u_h, u_1) \sqrt{1 + \sin^2 \alpha(u_h, u_1)} \\ &\leq \left(\frac{\delta}{\lambda_{2,L} - \lambda_h} \right) \sqrt{1 + \left(\frac{\delta}{\lambda_{2,L} - \lambda_h} \right)^2}. \end{aligned}$$

□

Next, we give a second-order result.

Theorem 2. *We assume among all the exact eigenvalues of A, the eigenvalue λ_1 is the one closest to λ_h; that is, $|\lambda_1 - \lambda_h| \leq |\lambda_i - \lambda_h|, \forall i \in \mathbb{N}$. We assume $\lambda_h = \frac{(Au_h, u_h)}{(u_h, u_h)}$ precisely (without any errors including round-off errors). Then we have*

$$\lambda_h - \frac{\delta^2}{(1 - \sin^2 \alpha(u_h, u_1))(\lambda_2 - \lambda_1)} \leq \lambda_1 \leq \lambda_h,$$

where $\delta := \|r_h\|_{L^2(\Omega)}$. As a result,

$$\lambda_h - \frac{\delta^2}{\lambda_2 - \lambda_1} \leq \lambda_1 \leq \lambda_h.$$

Proof. We expand u_h in terms of $\{u_i, i \in \mathbb{N}\}$, $u_h = \sum_{i=1}^{\infty} \alpha_i u_i, \alpha_i = (u_h, u_i)$. First $|\lambda_1 - \lambda_h| \leq |\lambda_i - \lambda_h|, \forall i \in \mathbb{N}$ implies $\lambda_h \leq \lambda_i, \forall i \geq 2$. We then note that

$$r_h = Au_h - \lambda_h u_h = \sum_{i=1}^{\infty} \alpha_i (Au_i - \lambda_h u_i) = \sum_{i=1}^{\infty} \alpha_i (\lambda_i - \lambda_h) u_i.$$

Due to the definition of $\lambda_h = \frac{(Au_h, u_h)}{(u_h, u_h)}$, we see that r_h is orthogonal to u_h. Thus,

$$0 = \left(\sum_{i=1}^{\infty} \alpha_i (\lambda_i - \lambda_h) u_i, \sum_{i=1}^{\infty} \alpha_i u_i \right) = \alpha_1^2 (\lambda_1 - \lambda_h) + \sum_{i=2}^{\infty} \alpha_i^2 (\lambda_i - \lambda_h),$$

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which implies $\lambda_h \geq \lambda_1$ and

$$\alpha_1^2(\lambda_h - \lambda_1) = \sum_{i=2}^{\infty} \alpha_i^2(\lambda_i - \lambda_h) \geq 0.$$

On the other hand,

$$\begin{aligned} \|r_h\|_{L^2(\Omega)}^2 &= \sum_{i=1}^{\infty} \alpha_i^2(\lambda_i - \lambda_h)^2 \geq \alpha_1^2(\lambda_h - \lambda_1)^2 + \sum_{i=2}^{\infty} \alpha_i^2(\lambda_i - \lambda_h)(\lambda_2 - \lambda_h) \\ &= \alpha_1^2(\lambda_h - \lambda_1)^2 + \alpha_1^2(\lambda_h - \lambda_1)(\lambda_2 - \lambda_h) \\ &= \alpha_1^2(\lambda_h - \lambda_1)(\lambda_2 - \lambda_1). \end{aligned} \tag{1}$$

Noting that

$$\sin^2 \alpha(u_h, u_1) = 1 - \cos^2 \alpha(u_h, u_1) = 1 - \alpha_1^2,$$

we have the desired result. □

We assume among all the exact eigenvalues of A, the eigenvalue λ_1 is the one closest to λ_h; that is $|\lambda_1 - \lambda_h| \leq |\lambda_i - \lambda_h|, \forall i \in \mathbb{N}$. Given u_h to approximate u_1, we obtain $\lambda_h = \frac{(Au_h, u_h)}{(u_h, u_h)}$ using Interval Arithmetic to get $\mathrm{IA}(\lambda_h) = [\lambda_{h,L}, \lambda_{h,U}]$. Let $\mathrm{IA}(\|r_h\|_{L^2(\Omega)}) = [\delta_L, \delta_U]$. Then we have

$$\mathrm{IA}_L\left(\lambda_{h,L} - \frac{\delta_L^2}{\lambda_{2,L} - \lambda_{1,U}}\right) \leq \lambda_1 \leq \lambda_{h,U},$$

where $\lambda_{2,L}$ is a guaranteed lower bound for λ_2, and $\lambda_{1,U}$ is a guaranteed upper bound for λ_1. Both $\lambda_{2,L}$ and $\lambda_{1,U}$ can be obtained from Lemma 1.

Remark 2. When we get $(\lambda_h, u_h) \approx (\lambda_1, u_1)$ eigen-pair, u_h is not exactly u_1 due to round-off error (and other numerical errors like iteration error, truncation error etc). When employing the gradient flow method to compute the approximate eigenfunction u_h, the resulting solution predominantly captures the first eigenvector u_1 rather than $u_i, i \geq 2$. By subtracting the projection of u_h onto the first eigenmode u_1 from u_h itself, we obtain the residual component orthogonal to u_1: $u_{h,\neq 1} := u_h - (u_h, u_1)u_1$. Intuitively, we see $u_{h,\neq 1}$ contains mainly u_2 rather than $u_i,\ i \geq 3$. Similarly, because the residual vector $r_h = Au_h - \lambda_h u_h$ is orthogonal to u_h, which is close to u_1, it is also expected that r_h mainly contains u_2 rather than $u_i,\ i \neq 2$. Consequently, we can use r_h to get $(\lambda_{2,h}, u_{2,h})$, an approximation of (λ_2, u_2), by $u_{2,h} = \frac{r_h}{\|r_h\|_{L^2(\Omega)}}, \lambda_{2,h} = \frac{(Au_{2,h}, u_{2,h})}{(u_{2,h}, u_{2,h})}$. Then we use Lemma 1 to get a guaranteed interval for λ_2, then get $\lambda_{2,L}$.

4 Numerical examples

In this section, we validate the results using two examples with rectangular domains. We consider the spectral method for rectangular domains. The basis

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functions are Legendre polynomials, which are orthogonal polynomials defined globally.

$$L_0(x) = 1, L_1(x) = x, L_2(x) = \frac{3}{2}x^2 - \frac{1}{2}, ...$$
$$(n+1)L_{n+1}(x) = (2n+1)xL_n(x) - nL_{n-1}(x).$$

The k-th basis function and the j-th basis function are orthogonal on the interval $[-1, 1]$,

$$\int_{-1}^{1} L_k(x)L_j(x)dx = \frac{1}{k+\frac{1}{2}}\delta_{kj}.$$

We will use this basis function to solve the Laplace eigenvalue problem on two different rectangular domains $[0, \pi]^2$ and $[0, 1]^2$. The smallest exact eigenvalue for the $[0, \pi]^2$ domain is 2, and the smallest exact eigenvalue for the $[0, 1]^2$ domain is $2\pi^2$. We present the upper and lower bounds of the smallest eigenvalue, as shown in Tables 1 and 2.

Table 1. Results of $[0, 1]^2$.

Poly Degree	λ_h	$\lvert\lambda - \lambda_h\rvert$	Upper Bound	Lower Bound	Upper - Lower
4	2.02642367284675	2.64e-02	2.66724	1.38561	1.28e-00
6	2.00002942777066	2.94e-05	2.04342	1.95664	8.68e-02
8	2.00000000686899	6.87e-09	2.00107	1.99893	2.14e-03
9	2.00000000000054	5.40e-13	2.000013417	1.999986583	2.68e-05
11	2.00000000000001	1.02e-13	2.000000138	1.999999862	2.76e-06
12	1.99999999999992	7.99e-14	2.000000138	1.999999862	2.71e-06
13	1.99999999999998	2.00e-14	2.000000091	1.999999909	1.82e-07

Table 2. Results of $[0, \pi]^2$.

Poly Degree	λ_h	$\lvert\lambda - \lambda_h\rvert$	Upper Bound	Lower Bound	Upper - Lower
4	20	2.61e-01	26.3246	13.6754	1.26e01
6	19.7394992426336	2.90e-04	20.1678	19.3112	8.56e-01
8	19.7392088699728	6.78e-08	19.74975953	19.72865821	2.11e-02
10	19.7392088021836	4.90e-12	19.73934122	19.73907639	2.65e-04
11	19.7392088021788	9.90e-14	19.73921007	19.73920753	2.54E-06
12	19.7392088021789	1.99e-14	19.73920952	19.73920808	1.44E-06
13	19.7392088021791	3.40e-14	19.73920960	19.73920800	1.40E-06

From our numerical experiments, we can see that the residual can effectively provide upper and lower bounds for the true eigenvalues using interval arithmetic. Specifically, interval arithmetic maintains error bounds at computational step, avoiding the numerical uncertainties that may arise in traditional

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floating-point calculations, thus providing stronger mathematical guarantees for the computation of eigenvalues.

By accurately computing the residuals, we are able not only to obtain approximate eigenvalues but also to provide their exact upper and lower bounds, offering an effective guarantee for the reliability of the eigenvalues.

5 Conclusions

This paper presents an approach for estimating eigenvalues using a computable residual function. The method provides guaranteed upper and lower bounds for eigenvalues, along with first-order and second-order error estimates that enhance the precision of eigenvalue and eigenvector approximations.

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