Rigorous and fully computable a posteriori error bounds for eigenfunctions

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Supported by the Neuron Impuls project no. 24/2016

Joint work with Xuefeng Liu (Niigata University, Japan)

Mafelap 2019, Brunel University, June 18–21

Introduction

Laplace eigenvalue problem

$$
\begin{aligned}
-\Delta u_i &= \lambda_i u_i \quad \text{in } \Omega \\
u_i &= 0 \qquad \text{on } \partial\Omega
\end{aligned}
$$

Two-sided bounds on eigenvalues:

$$\underline{\lambda}_i \leq \lambda_i \leq \overline{\lambda}_i$$

[Goerisch, Haunhorst 1985], [Kato 1949], [Lehmann 1949, 1950], [Barrenechea, Boulton, Boussaïd 2014], [Cancès, Dusson, Maday, Stamm, Vohralík 2017, 2018, 2019], [Carstensen, Gedicke 2014], [Carstensen, Gallistl 2014], [Hu, Huang, Lin 2014], [Liu 2015], [Liu, Oishi 2013], [Šebestová, V. 2014], [V. 2018], and many others.

Introduction

Laplace eigenvalue problem

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega$$
$$u_i = 0 \qquad \text{on } \partial\Omega$$

Two-sided bounds on eigenvalues:

$$\underline{\lambda}_i \leq \lambda_i \leq \overline{\lambda}_i$$

Approximate eigenfunctions: $\hat{u}_i$

Goal: fully computable error bound for eigenfuntions

$$\|\nabla u_i - \nabla \hat{u}_i\| \leq \eta(\underline{\lambda}_i, \overline{\lambda}_i, \hat{u}_i)$$

Error bounds on eigenfunctions

Problem: Eigenfunctions may be ill-posed.

Solution:
(a) consider spaces of eigenfunctions

- $\lambda_n, \lambda_{n+1}, \ldots, \lambda_N$ (cluster)
- $E = \text{span}\{u_n, u_{n+1}, \ldots, u_N\}$ (space of eigenfunctions)
- $\widehat{E} = \text{span}\{\hat{u}_n, \hat{u}_{n+1}, \ldots, \hat{u}_N\}$ (its approximation)

(b) bound the directed distance of spaces

- $\delta(E, \widehat{E}) \leq \eta(\underline{\lambda}_i, \overline{\lambda}_i, \hat{u}_i)$ [Meyer 2000]

Directed distance of spaces

Definition

Let E and $\widehat{E}$ be two subspaces of a Hilbert space V then

$$\delta(E, \widehat{E}) = \max_{\substack{v \in E \\ \|v\|=1}} \min_{\hat{v} \in \widehat{E}} \|v - \hat{v}\|$$

Properties

- if $\dim E = \dim \widehat{E}$ then $\delta(E, \widehat{E}) = \delta(\widehat{E}, E)$
- $\delta^2(E, \widehat{E}) = 1 - \min_{\substack{v \in E \\ \|v\|=1}} \max_{\substack{\hat{v} \in \hat{E} \\ \|\hat{v}\|=1}} |(v, \hat{v})|^2$

Example

Let $E = \text{span}\{u\}$ and $\widehat{E} = \text{span}\{\hat{u}\}$ then

$$\delta^2(E, \widehat{E}) = 1 - \frac{|(u, \hat{u})|^2}{\|u\|^2 \|\hat{u}\|^2} = 1 - \cos^2 \alpha = \sin^2 \alpha$$

$$\|u - \hat{u}\|^2 = \|u\|^2 + \|\hat{u}\|^2 - 2\|u\|\|\hat{u}\|\sqrt{1 - \delta^2(E, \widehat{E})}$$

Nonorthogonality

Definition: $$\hat{\epsilon}^2(E,E') = \max_{\substack{v\in E\\ \|v\|=1}} \max_{\substack{v'\in E'\\ \|v'\|=1}} (v,v')$$

Lemma

Let $v_1, v_2, \ldots, v_m$ and $v'_1, v'_2, \ldots, v'_{m'}$ be bases of $E, E' \subset V$.

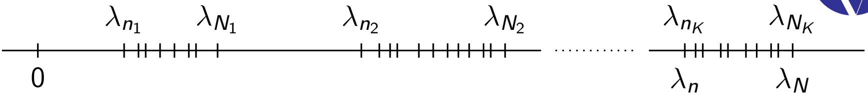
$$F = \left[(v_i, v'_j)\right]_{m\times m'}, \quad G = \left[(v_i, v_j)\right]_{m\times m}, \quad H = \left[(v'_i, v'_j)\right]_{m'\times m'}$$

Then

$$\hat{\epsilon}^2(E,E') = \lambda_{max}(FG^{-1}F^T, H) = \lambda_{max}(F^T H^{-1} F, G),$$

where $\lambda_{max}(A,B)$ denotes the maximum eigenvalue of $Ax = \lambda Bx$.

Clusters of eigenvalues



Spaces of exact eigenfunctions

$E_k = \text{span}\{u_{n_k}, u_{n_k+1}, \dots, u_{N_k}\}, \quad k = 1, 2, \dots, K$

Spaces of approximate eigenfunctions

$\widehat{E}_k = \text{span}\{\hat{u}_{n_k}, \hat{u}_{n_k+1}, \dots, \hat{u}_{N_k}\}, \quad k = 1, 2, \dots, K$

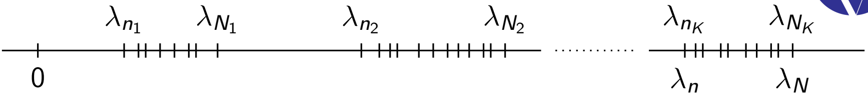
Assumption

$\dim \widehat{E}_k = N_k - n_k + 1$ for all $k = 1, 2, \dots, K$

Notation:

$n = n_K$ and $N = N_K$

The bound on eigenfunctions in energy norm



Directed distance: $\Delta(E_K, \widehat{E}_K) = \max\limits_{\substack{v \in E_K \\ \|\nabla v\| = 1}} \min\limits_{\hat{v} \in \widehat{E}_K} \|\nabla v - \nabla \hat{v}\|$

Nonorthogonality: $\hat{\zeta}(\widehat{E}_k, \widehat{E}_K) = \max\limits_{\substack{v \in \widehat{E}_k \\ \|\nabla v\| = 1}} \max\limits_{\substack{w \in \widehat{E}_K \\ \|\nabla w\| = 1}} (\nabla v, \nabla w)$

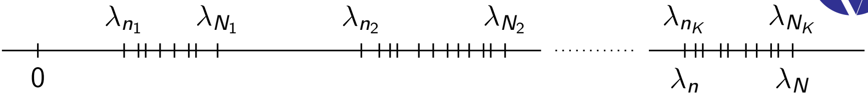
Theorem 1

$$\Delta^2(E_K, \widehat{E}_K) \le \frac{\rho\left(\hat{\lambda}_N^{(K)} - \lambda_n\right) + \lambda_n \hat{\lambda}_N^{(K)} \vartheta^{(K)}}{\hat{\lambda}_N^{(K)}(\rho - \lambda_n)},$$

where $\lambda_n < \rho \le \lambda_{N+1}$,

$$\hat{\lambda}_N^{(K)} = \max_{\hat{v} \in \widehat{E}_K} \frac{\|\nabla \hat{v}\|^2}{\|\hat{v}\|^2}, \quad \vartheta^{(K)} = \sum_{k=1}^{K-1} \frac{\rho - \lambda_{n_k}}{\lambda_{n_k}} \left[\hat{\zeta}(\widehat{E}_k, \widehat{E}_K) + \Delta(E_k, \widehat{E}_k)\right]^2.$$

Analogous bound on eigenfunctions in $L^2(\Omega)$ norm



Directed distance: $\delta(E,\widehat{E}) = \max\limits_{\substack{v\in E\\ \|v\|=1}} \min\limits_{\hat{v}\in\widehat{E}} \|v-\hat{v}\|$

Nonorthogonality: $\hat{\varepsilon}(\widehat{E}_k,\widehat{E}_K) = \max\limits_{\substack{v\in\widehat{E}_k\\ \|v\|=1}} \max\limits_{\substack{w\in\widehat{E}_K\\ \|w\|=1}} (v,w)$

Theorem 2

$$\delta^2(E_K,\widehat{E}_K) \le \frac{\hat{\lambda}_N^{(K)} - \lambda_n + \theta^{(K)}}{\rho-\lambda_n},$$

where $\lambda_n < \rho \le \lambda_{N+1}$,

$$\hat{\lambda}_N^{(K)} = \max_{\hat{v}\in\widehat{E}_K} \frac{\|\nabla\hat{v}\|^2}{\|\hat{v}\|^2}, \quad \theta^{(K)} = \sum_{k=1}^{K-1} (\rho-\lambda_{n_k}) \left[\hat{\epsilon}(\widehat{E}_k,\widehat{E}_K) + \delta(E_k,\widehat{E}_k)\right]^2.$$

Optimal order bound in $L^2(\Omega)$ norm

Conforming finite element method:

$$E_{h,k} = \mathrm{span}\{u_{h,n_k}, u_{h,n_k+1}, \dots, u_{h,N_k}\}$$

Error constant for elliptic projection P_h:

$$\|u - P_h u\| \le C_h \|\nabla(u - P_h u)\| \le C_h^2 \|f\|$$

Note: $C_h = 0.493h$ for convex domains and linear conforming FEM

Theorem 3

$$\delta(E_k, E_{h,k}) \le \sqrt{\lambda_{N_k}}\, C_h \left(1 + \tau_k \sqrt{|\mathcal{C}(k)|}\right) \Delta(E_k, E_{h,k}),$$

where $\mathcal{C}(k) = \{n_k, n_k+1, \dots, N_k\}$, $|\mathcal{C}(k)| = N_k - n_k + 1$, and

$$\tau_k = \max_{j \in \mathcal{C}(k)} \max_{i \in \mathcal{C} \setminus \mathcal{C}(k)} \frac{\lambda_j}{|\lambda_{h,i} - \lambda_j|}.$$

Using Aubin–Nitsche, [Boffi 2010], [Liu, Oishi 2013]

Asymptotically sharp bound in the energy norm

Theorem 4

- Let $E = \text{span}\{u_n, \dots, u_N\}$ be a space of exact eigenfunctions.
- Let $\widehat{E} = \text{span}\{\hat{u}_n, \dots, \hat{u}_N\} \subset H_0^1(\Omega)$ have dimension $N - n + 1$.

Then

$$\Delta^2(E, \widehat{E}) \leq 2 - 2\lambda_n \left(\frac{1 - \delta^2(E, \widehat{E})}{\lambda_N \hat{\lambda}_N} \right)^{1/2},$$

where $\hat{\lambda}_N = \max_{\hat{v} \in \widehat{E}} \frac{\|\nabla \hat{v}\|^2}{\|\hat{v}\|^2}$.

Iterately improved bounds

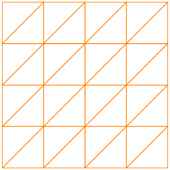
For $K = 1, 2, \ldots$ do

1. Compute the original bound on $\Delta(E_K, \widehat{E}_K)$
2. Compute the analogous bound on $\delta(E_K, \widehat{E}_K)$
3. Compute the optimal order bound on $\delta(E_K, \widehat{E}_K)$ using $\Delta(E_K, \widehat{E}_K)$
4. Compute asymptotically sharp bound on $\Delta(E_K, \widehat{E}_K)$ using $\delta(E_K, \widehat{E}_K)$
   (Use the minimum of 2. and 3.)
5. Compute improved bounds by repeating steps 3. and 4.
   (Use the best bounds on $\Delta(E_K, \widehat{E}_K)$ and $\delta(E_K, \widehat{E}_K)$ available.)

Example 1: Square

Laplace eigenvalue problem

$$\begin{aligned} -\Delta u_i &= \lambda_i u_i \quad && \text{in } \Omega = (0,1)^2 \\ u_i &= 0 && \text{on } \partial\Omega \end{aligned}$$

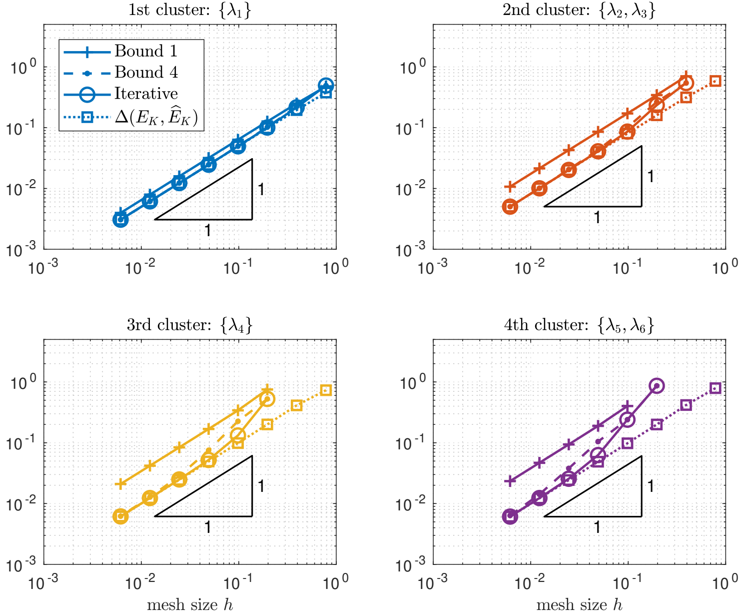


Exact eigenvalues:

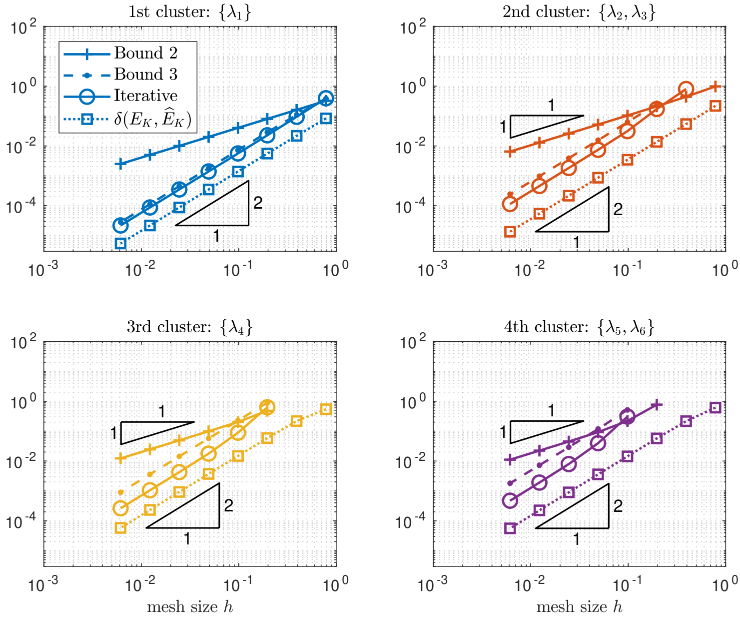
$$\underbrace{2\pi^2}_{\text{cluster 1}}, \quad \underbrace{5\pi^2,\ 5\pi^2}_{\text{cluster 2}}, \quad \underbrace{8\pi^2}_{\text{cluster 3}}, \quad \underbrace{9\pi^2,\ 9\pi^2}_{\text{cluster 4}}, \ldots.$$

Conforming linear finite elements: $u_{h,1},\ u_{h,2},\ u_{h,3},\ \ldots$

Example 1: Square – bounds in the energy norm



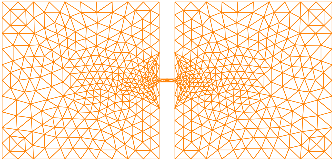
Example 1: Square – bounds in the $L^2(\Omega)$ norm



Example 2: Dumbbell

Laplace eigenvalue problem

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega$$
$$u_i = 0 \quad \text{on } \partial\Omega$$

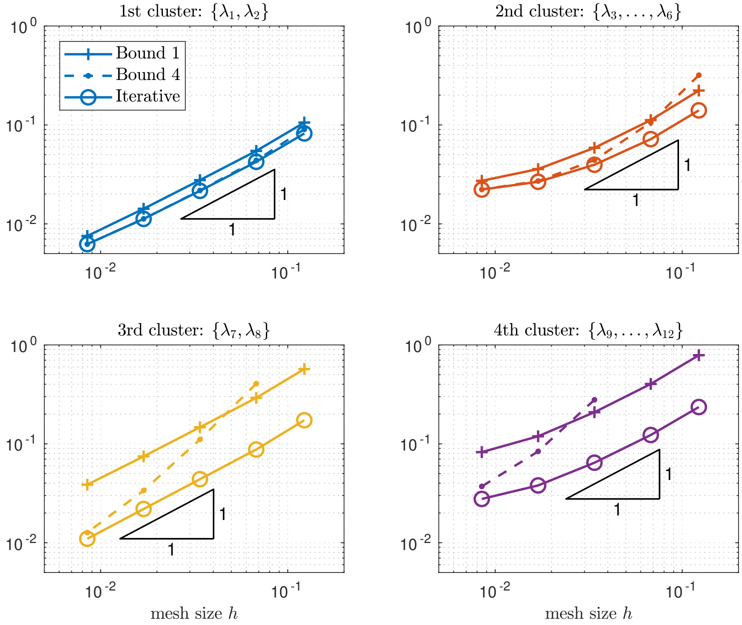


Exact eigenvalues – unknown, but close to

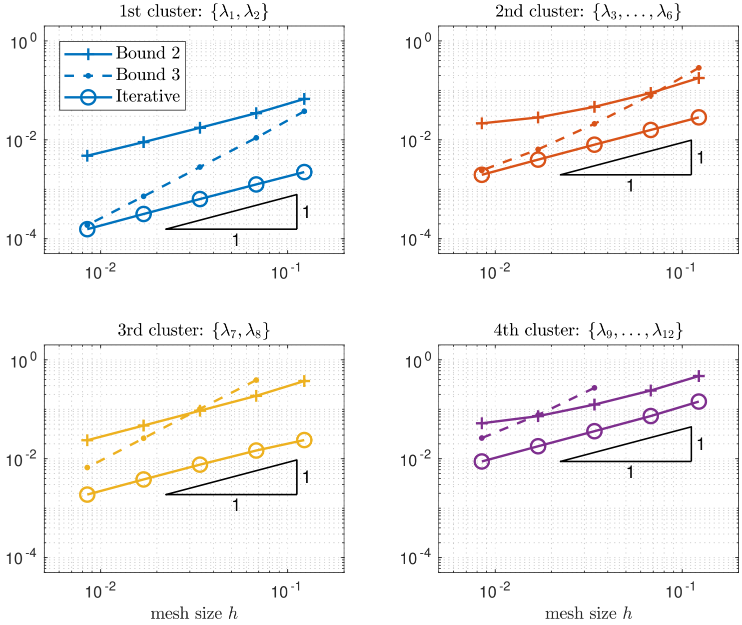
$$\underbrace{2\pi^2,\ 2\pi^2}_{\text{cluster 1}},\ \underbrace{5\pi^2,\ 5\pi^2,\ 5\pi^2,\ 5\pi^2}_{\text{cluster 2}},\ \underbrace{8\pi^2,\ 8\pi^2}_{\text{cluster 3}},\ \underbrace{9\pi^2,\ 9\pi^2, 9\pi^2,\ 9\pi^2}_{\text{cluster 4}},\ \ldots$$

Cluster	lower and upper bound
1	$\lambda_1 = 19.736^{729}_{634},\ \lambda_2 = 19.736^{729}_{635}$
2	$\lambda_3 = 49.33^{809}_{761},\ \lambda_4 = 49.33^{809}_{761},\ \lambda_5 = 49.348020^{8}_{5},\ \lambda_6 = 49.348020^{8}_{5}$
3	$\lambda_7 = 78.9568^{301}_{290},\ \lambda_8 = 78.9568^{301}_{290}$
4	$\lambda_9 = 98.6^{71154}_{69041},\ \lambda_{10} = 98.6^{71154}_{69041},\ \lambda_{11} = 98.6960^{41}_{39},\ \lambda_{12} = 98.6960^{41}_{39}$

Example 2: Dumbbell – bounds in the energy norm

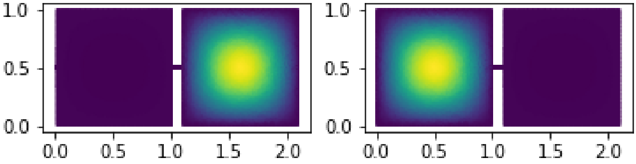


Example 2: Dumbbell – bounds in the $L^2(\Omega)$ norm

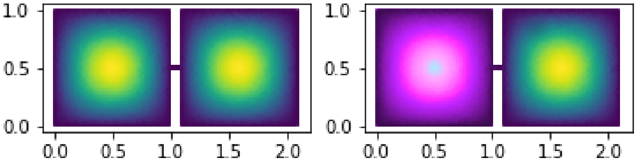


Are the computed eigenfunctions wrong?

Computed eigenfunctions



Exact eigenfunctions



- Both $\|\nabla u_1 - \nabla u_{h,1}\|$ and $\|\nabla u_2 - \nabla u_{h,2}\|$ are large,
- but $\Delta(E_1, E_{h,1})$ is small for $E_1 = \text{span}\{u_1,\ u_2\}$ and $E_{h,1} = \text{span}\{u_{h,1},\ u_{h,2}\}$.

Conclusions

- Fully computable upper bounds on the directed distance of spaces of eigenfunctions
- Only eigenvalues and approximate eigenfunctions needed
- Optimal rates of convergence (for clusters of zero width)
- Possibility of iterative improvement

Literature

Preprint

X. Liu, T. V.: Rigorous and fully computable a posteriori error bounds for eigenfunctions, arXiv:1904.07903

Generalization of:

[Birkhoff, de Boor, Swartz, Wendroff, 1966]

Alternative approach:

[Cancès, Dusson, Maday, Stamm, Vohralík, 2017]
[Cancès, Dusson, Maday, Stamm, Vohralík, 2018]
[Cancès, Dusson, Maday, Stamm, Vohralík, 2019]

Thank you for your attention

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