Rigorous and fully computable a posteriori error bounds for eigenfunctions

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Joint work with Xuefeng Liu (Niigata University, Japan)

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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], [Gopalakrishnan, Grubišić, Ovall 2017], [Hu, Huang, Lin 2014], [Liu 2015], [Liu, Oishi 2013], [Plum 1990,1991], [Šebestová, V. 2014], [V. 2018], [Luo, Lin, Xie 2012], [Li, Lin, Xie 2013] and many others.

Introduction

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Two-sided bounds on eigenvalues:

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

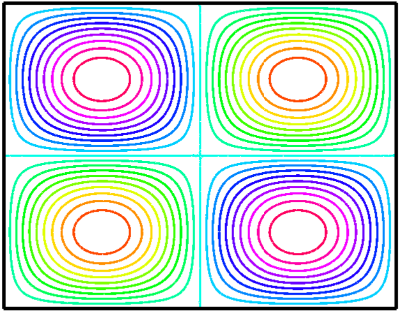
Approximate eigenfunctions: $\hat{u}_i$

Goal: fully computable error bound for eigenfuntions

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

Laplace eigenvalue problem in a rectangle

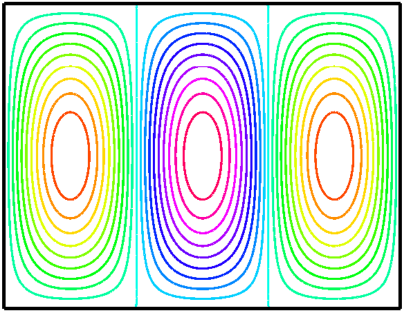
$\alpha = 1.29,\ \lambda_4 = 6.4037$



π

$\alpha\pi$

$\alpha = 1.30,\ \lambda_4 = 6.3254$

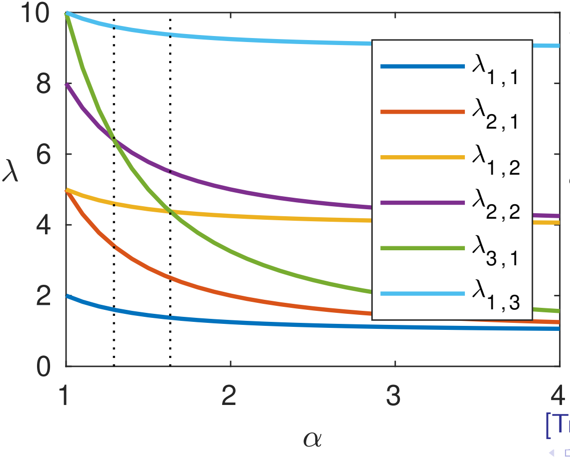


$\alpha\pi$

Laplace eigenvalue problem in a rectangle

$$-\Delta u_n = \lambda_n u_n \quad \text{in } \Omega = (0, \alpha\pi) \times (0, \pi)$$
$$u_n = 0 \quad \text{on } \partial\Omega$$

Dependence of eigenvalues on α



$$\lambda_{k,m} = \frac{k^2}{\alpha^2} + m^2$$

$$u_{k,m} = \sin\frac{kx}{\alpha}\sin(my)$$

$$\alpha^* = \sqrt{5/3} \approx 1.2910$$

[Trefethen, Betcke 2006]

Error bounds on eigenfunctions

Problem: Eigenfunctions may be ill-posed.

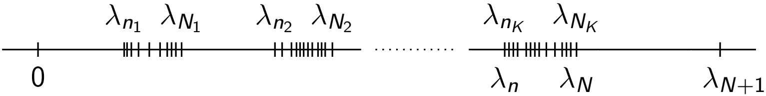
Solution:
(a) consider spaces of eigenfunctions

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

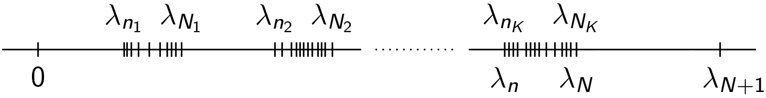
Error bounds on eigenfunctions in the energy norm



Theorem 1. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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

Error bounds on eigenfunctions in the energy norm



Theorem 1. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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Space of exact eigenfunctions

$E_K = \text{span}\{u_n, u_{n+1}, \ldots, u_N\}$

Notation

$n = n_K$ and $N = N_K$

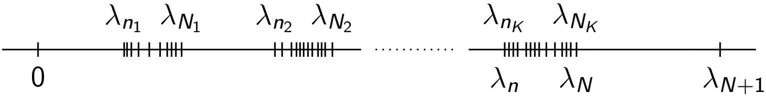
Space of approximate eigenfunctions

$\widehat{E}_K = \text{span}\{\hat{u}_n, \hat{u}_{n+1}, \ldots, \hat{u}_N\}$

Assumption: $\widehat{E}_K \subset H_0^1(\Omega)$

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

Error bounds on eigenfunctions in the energy norm



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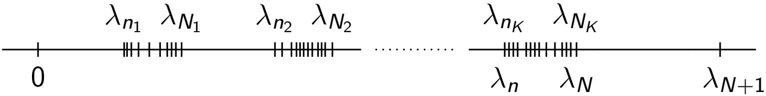
Directed distance

$$\Delta(E_K, \widehat{E}_K) = \max_{\substack{v \in E_K \\ \|\nabla v\| = 1}} \min_{\hat{v} \in \widehat{E}_K} \|\nabla v - \nabla \hat{v}\|$$

Note

If $\dim E_K = \dim \widehat{E}_K$ then $\Delta(E_K, \widehat{E}_K) = \Delta(\widehat{E}_K, E_K) = \operatorname{gap}(E_K, \widehat{E}_K)$.

Error bounds on eigenfunctions in the energy norm



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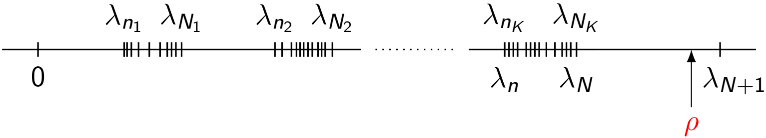
Example

If $E_K = \operatorname{span}\{u_n\}$ and $\widehat{E}_K = \operatorname{span}\{\hat{u}_n\}$ then

$$\Delta^2(E_K, \widehat{E}_K) = 1 - \frac{|(\nabla u_n, \nabla \hat{u}_n)|^2}{\|\nabla u_n\|^2 \|\nabla \hat{u}_n\|^2} = 1 - \cos^2 \alpha = \sin^2 \alpha$$

Error bounds on eigenfunctions in the energy norm



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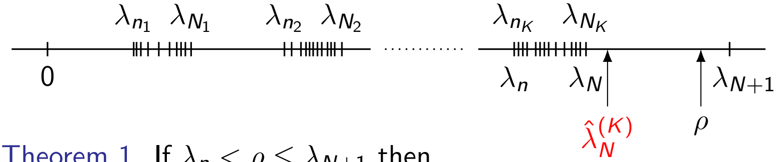
Set

$\rho = \underline{\lambda}_{N+1}$

Error bounds on eigenfunctions in the energy norm



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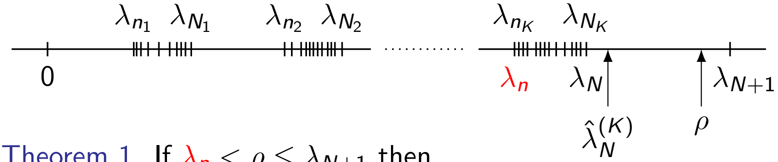
Approximation of λ_N

$$\hat{\lambda}_N^{(K)} = \max_{\hat{v} \in \widehat{E}_K} \frac{\|\nabla \hat{v}\|^2}{\|\hat{v}\|^2}$$

Error bounds on eigenfunctions in the energy norm



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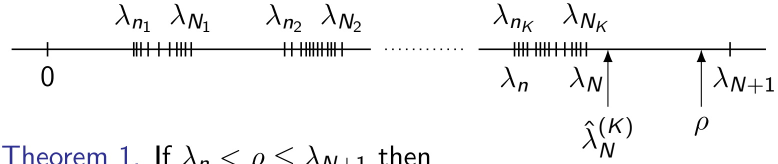
Use

$\underline{\lambda}_n \leq \lambda_n \leq \overline{\lambda}_n$

Error bounds on eigenfunctions in the energy norm



Theorem 1. If $\lambda_n < \rho \le \lambda_{N+1}$ then

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

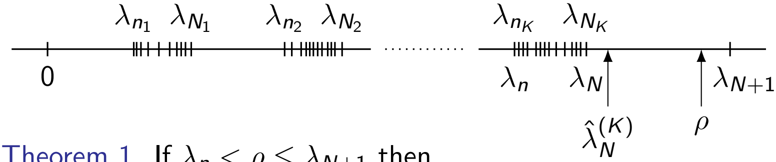
Errors in previous clusters

$$\vartheta^{(K)} = \sum_{k=1}^{K-1} \frac{\rho - \lambda_{n_k}}{\lambda_{n_k}} \left[\hat\zeta(\widehat{E}_k, \widehat{E}_K) + \Delta(E_k, \widehat{E}_k)\right]^2$$

Nonorthogonality

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

Error bounds on eigenfunctions in the energy norm



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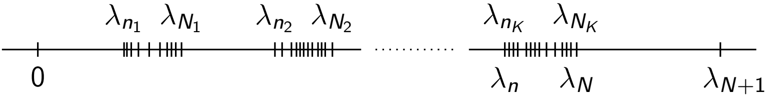
Nonorthogonality

$$\hat{\zeta}(\widehat{E}_k, \widehat{E}_K) = \max_{\substack{v \in \widehat{E}_k \\ \|\nabla v\|=1}} \max_{\substack{w \in \widehat{E}_K \\ \|\nabla w\|=1}} (\nabla v, \nabla w) = \lambda_{max}(FG^{-1}F^T, H)$$

where $F = [(\nabla \hat{u}_i, \nabla \hat{u}_j)]_{j=n,\dots,N}^{i=n_k,\dots,N_k}$, $\quad G = [(\nabla \hat{u}_i, \nabla \hat{u}_j)]_{i,j=n_k,\dots,N_k}, \dots$

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



Theorem 2. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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

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

Errors in previous clusters:

$$\theta^{(K)} = \sum_{k=1}^{K-1} (\rho - \lambda_{n_k}) \left[\hat{\varepsilon}(\widehat{E}_k, \widehat{E}_K) + \delta(E_k, \widehat{E}_k) \right]^2.$$

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

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

Conforming finite element method:

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

Error constant for elliptic projection P_h:

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

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

Theorem 3

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

where $\mathcal{C}(k) = \{n_k, n_k+1, \ldots, N_k\}$, $|\mathcal{C}(k)| = N_k - n_k + 1$, 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 $E = \mathrm{span}\{u_n, \dots, u_N\}$ be a space of exact eigenfunctions.
- Let $\widehat{E} = \mathrm{span}\{\hat{u}_n, \dots, \hat{u}_N\} \subset H_0^1(\Omega)$ have dimension $N - n + 1$.

Then

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

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

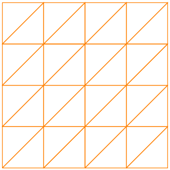
Iterativelyimproved bounds

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

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

Example 1: Square

Laplace eigenvalue problem



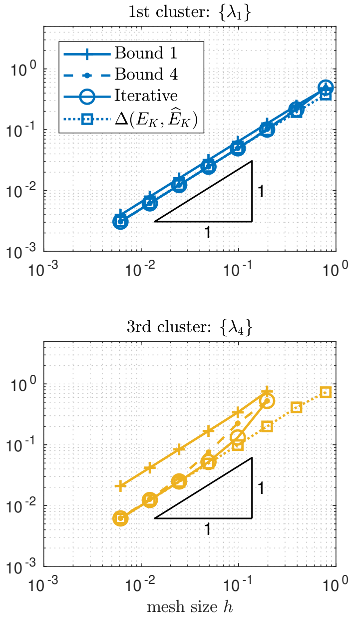
$$
\begin{aligned}
-\Delta u_i &= \lambda_i u_i \quad && \text{in } \Omega = (0,1)^2 \\
u_i &= 0 && \text{on } \partial\Omega
\end{aligned}
$$

Exact eigenvalues:

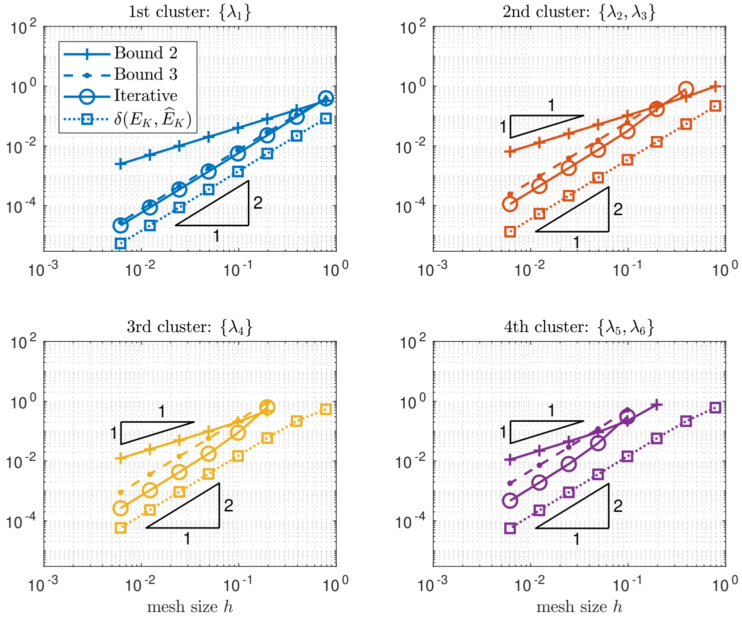
$$
\underbrace{2\pi^2}_{\text{cluster 1}}, \quad \underbrace{5\pi^2,\ 5\pi^2}_{\text{cluster 2}}, \quad \underbrace{8\pi^2}_{\text{cluster 3}}, \quad \underbrace{9\pi^2,\ 9\pi^2}_{\text{cluster 4}}, \ldots .
$$

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

Example 1: Square – bounds in the energy norm



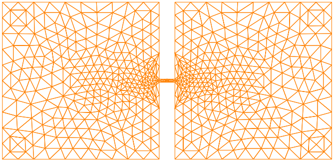
Example 1: Square – bounds in the $L^2(\Omega)$ norm



Example 2: Dumbbell

Laplace eigenvalue problem

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

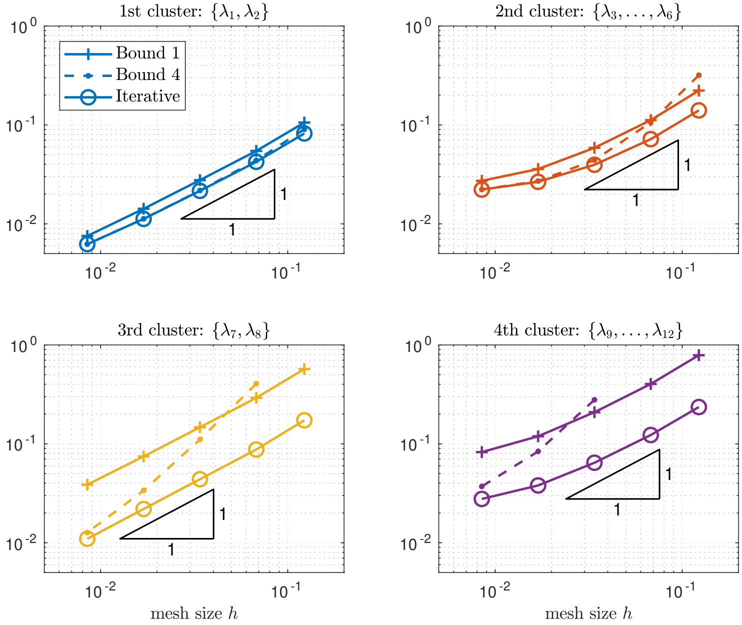


Exact eigenvalues – unknown, but close to

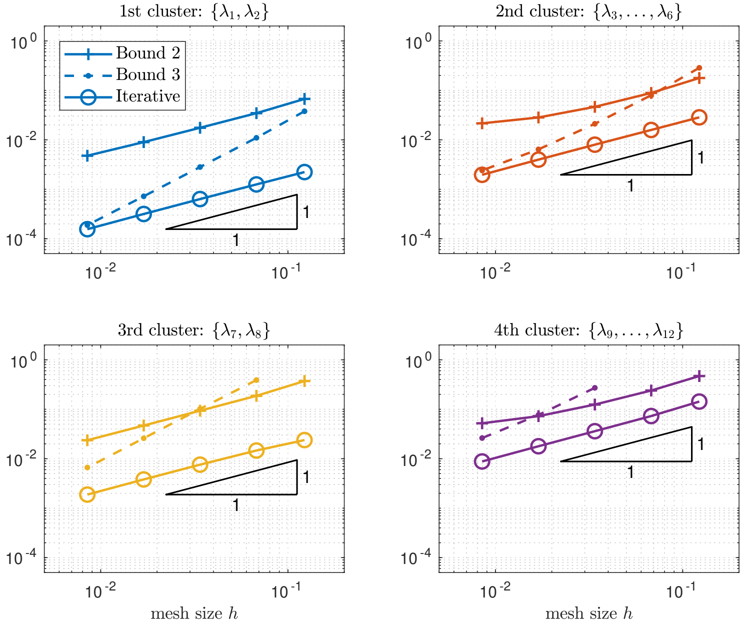
$$\underbrace{2\pi^2,\ 2\pi^2}_{\text{cluster 1}},\ \underbrace{5\pi^2,\ 5\pi^2,\ 5\pi^2,\ 5\pi^2}_{\text{cluster 2}},\ \underbrace{8\pi^2,\ 8\pi^2}_{\text{cluster 3}},\ \underbrace{9\pi^2,\ 9\pi^2, 9\pi^2,\ 9\pi^2}_{\text{cluster 4}},\ \ldots$$

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	$\lambda_9 = 98.6^{71154}_{69041},\ \lambda_{10} = 98.6^{71154}_{69041},\ \lambda_{11} = 98.69604^{41}_{39},\ \lambda_{12} = 98.69604^{41}_{39}$

Example 2: Dumbbell – bounds in the energy norm

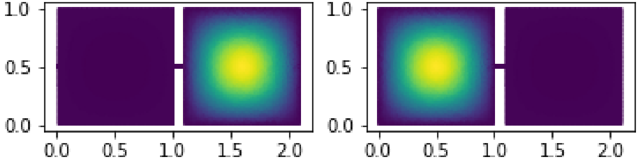


Example 2: Dumbbell – bounds in the $L^2(\Omega)$ norm

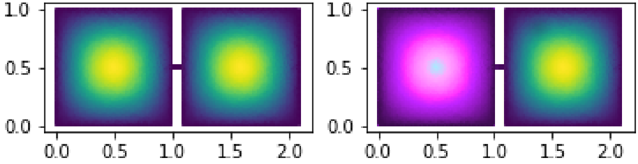


Are the computed eigenfunctions wrong?

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

Work in progress:
To derive bounds independent of errors in previous clusters

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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