Guaranteed error bounds for eigenfunctions

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics
Czech Academy of Sciences

Joint work with Xuefeng Liu (Niigata University, Japan)

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Introduction

Eigenvalue problem for linear elliptic operators (e.g. Laplace):

$$\lambda_i > 0,\ u_i \in V \setminus \{0\}: \quad a(u_i, v) = \lambda_i b(\gamma u_i, \gamma v) \quad \forall v \in V$$

Guaranteed a posteriori error bounds on
(a) eigenvalues

$$|\lambda_i - \hat{\lambda}_i| \leq \eta_{\mathrm{ev}} \qquad \Leftrightarrow \qquad \lambda_i^{\mathrm{low}} \leq \lambda_i \leq \lambda_i^{\mathrm{up}}$$

[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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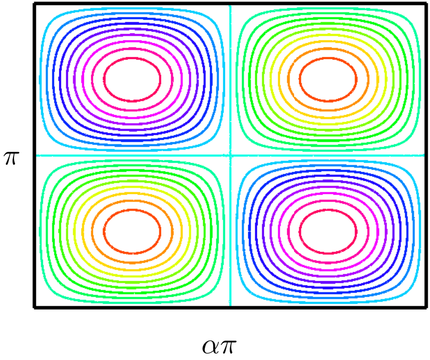
(b) eigenfunctions

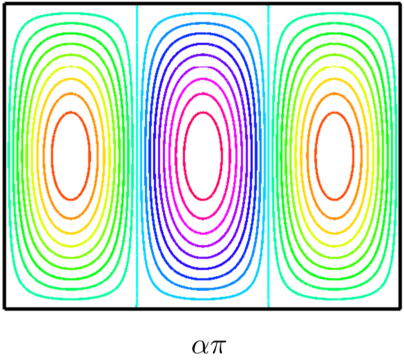
$$\|u_i - \hat{u}_i\|_a \leq \eta(\lambda_i^{\mathrm{low}}, \lambda_i^{\mathrm{up}}, \hat{u}_i)$$

Laplace eigenvalue problem in a rectangle

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



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



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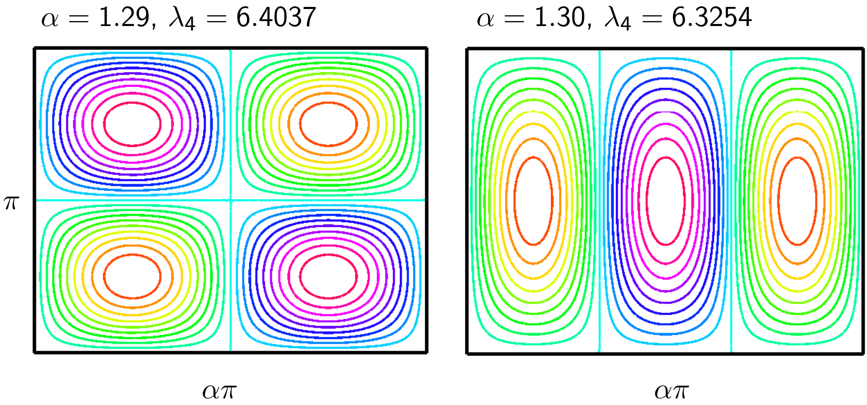

Double eigenvalue: $\alpha = \sqrt{5/3} \approx 1.2910 \quad \Rightarrow \quad \lambda_4 = \lambda_5$

Error bounds on eigenfunctions

Spaces of eigenfunctions

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

Directed distance of spaces

- $\delta(E, \widehat{E}) \leq \eta(\lambda_i^{\text{low}}, \lambda_i^{\text{up}}, \hat{u}_i)$ [Meyer 2000]

Eigenvalue problem for a compact self-adjoint operator

- V, W ... Hilbert spaces with inner products $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$
- $\gamma : V \to W$ ... a compact operator

Eigenvalue problem

$$\lambda_i > 0,\ u_i \in V \setminus \{0\} : \quad a(u_i, v) = \lambda_i b(\gamma u_i, \gamma v) \quad \forall v \in V$$

Eigenvalue problem for a compact self-adjoint operator

- V, W ... Hilbert spaces with inner products $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$
- $\gamma : V \to W$ ... a compact operator

Eigenvalue problem

$$\lambda_i > 0,\ u_i \in V \setminus \{0\} : \quad \begin{aligned} a(u_i, v) &= \lambda_i b(\gamma u_i, \gamma v) \quad \forall v \in V \\ &= \lambda_i a(T\gamma u_i, v) \quad \forall v \in V \end{aligned}$$

Solution operator

$$T : W \to V \text{ such that } \quad a(Tf, v) = b(f, \gamma v) \quad \forall v \in V, f \in W$$

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Equivalent to

$$u_i = \lambda_i T\gamma u_i \quad \Leftrightarrow \quad T\gamma u_i = \frac{1}{\lambda_i} u_i$$

Solution operator

$$T : W \to V \text{ such that } \quad a(Tf, v) = b(f, \gamma v) \quad \forall v \in V, f \in W$$

Example 1: Laplace eigenvalue problem

Eigenvalue problem

$$\lambda_i > 0,\ u_i \in V \setminus \{0\} : \quad a(u_i, v) = \lambda_i b(\gamma u_i, \gamma v) \quad \forall v \in V$$

Laplace eigenvalue problem

- $V = H_0^1(\Omega), \quad a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x$
- $W = L^2(\Omega), \quad b(u,v) = \int_\Omega uv \, \mathrm{d}x$
- $\gamma =$ identity

Weak formulation

$$\int_\Omega \nabla u_i \cdot \nabla v \, \mathrm{d}x = \lambda_i \int_\Omega u_i v \, \mathrm{d}x \quad \forall v \in H_0^1(\Omega)$$

Classical formulation

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

Example 2: Steklov eigenvalue problem

Eigenvalue problem

$$\lambda_i > 0,\ u_i \in V \setminus \{0\} : \quad a(u_i, v) = \lambda_i b(\gamma u_i, \gamma v) \quad \forall v \in V$$

Steklov eigenvalue problem

- $V = H^1(\Omega), \quad a(u, v) = \int_\Omega (\nabla u \cdot \nabla v + uv)\,\mathrm{d}x$
- $W = L^2(\partial\Omega), \quad b(u, v) = \int_{\partial\Omega} uv\,\mathrm{d}s$
- $\gamma =$ trace operator

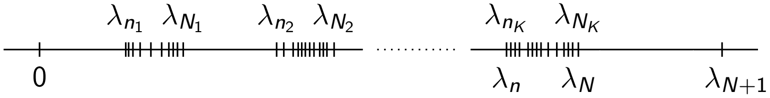
Weak formulation

$$\int_\Omega (\nabla u_i \cdot \nabla v + u_i v)\,\mathrm{d}x = \lambda_i \int_{\partial\Omega} u_i v\,\mathrm{d}s \quad \forall v \in H^1(\Omega)$$

Classical formulation

$$\begin{aligned} -\Delta u_i + u_i &= 0 && \text{in } \Omega \\ \frac{\partial u_i}{\partial \boldsymbol{n}} &= \lambda_i u_i && \text{on } \partial\Omega \end{aligned}$$

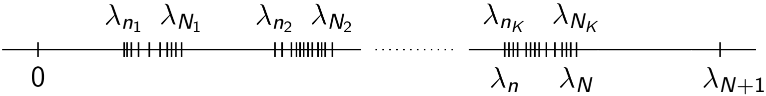
Error bounds on eigenfunctions in the a-norm



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

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

Error bounds on eigenfunctions in the a-norm



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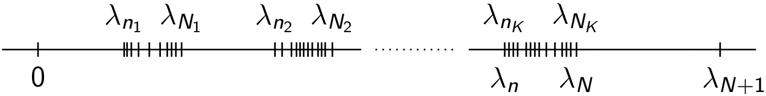
Space of exact eigenfunctions
$E_K = \operatorname{span}\{u_n, u_{n+1}, \dots, u_N\}$

Notation
$n = n_K$ and $N = N_K$

Space of approximate eigenfunctions
$\widehat{E}_K = \operatorname{span}\{\hat{u}_n, \hat{u}_{n+1}, \dots, \hat{u}_N\}$

Assumption: $\widehat{E}_K \subset V$
$\dim \widehat{E}_k = \dim E_k = N_k - n_k + 1$ for all $k = 1, 2, \dots, K$

Error bounds on eigenfunctions in the a-norm



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Directed distance

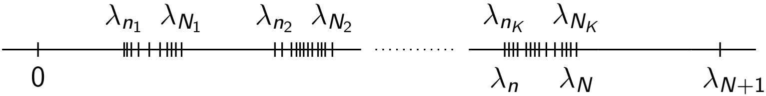
$$\delta_a(E_K, \widehat{E}_K) = \max_{\substack{v \in E_K \\ \|v\|_a = 1}} \min_{\hat{v} \in \widehat{E}_K} \|v - \hat{v}\|_a$$

Note

If $\dim E_K = \dim \widehat{E}_K$ then

$$\delta_a(E_K, \widehat{E}_K) = \delta_a(\widehat{E}_K, E_K) = \operatorname{gap}(E_K, \widehat{E}_K).$$

Error bounds on eigenfunctions in the a-norm



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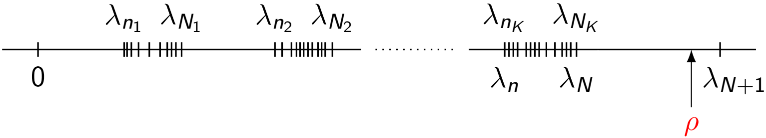
Example

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

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

Error bounds on eigenfunctions in the a-norm



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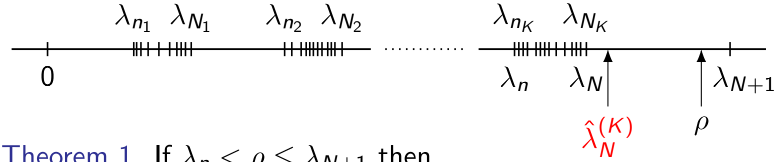
Set

$\rho = \lambda_{N+1}^{\text{low}}$

Error bounds on eigenfunctions in the a-norm



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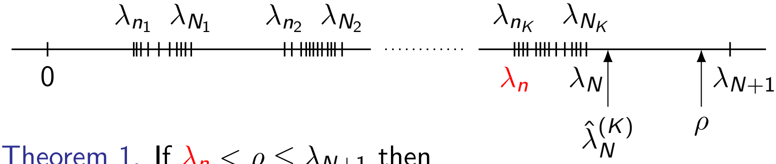
Approximation of λ_N

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

Error bounds on eigenfunctions in the a-norm



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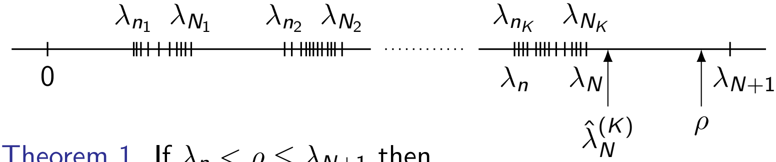
Use

$\lambda_n^{\text{low}} \leq \lambda_n \leq \lambda_n^{\text{up}}$

Error bounds on eigenfunctions in the a-norm



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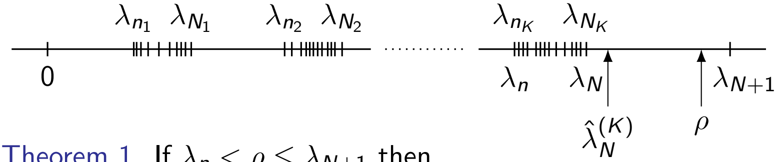
Errors in previous clusters

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

Nonorthogonality

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

Error bounds on eigenfunctions in the a-norm



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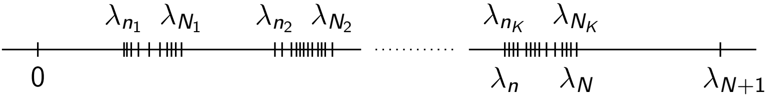
Nonorthogonality

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

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

Analogous bound on eigenfunctions in b-norm



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

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

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

Errors in previous clusters:

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

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

Sharp a-norm estimates based on the b-norm bounds

Theorem 3

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

Then

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

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

Note:

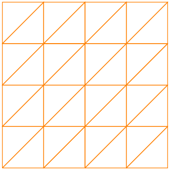
$\|u_i - \hat{u}_i\|_a^2 = \lambda_i \|\gamma(u_i - \hat{u}_i)\|_b^2 - (\lambda_i - \hat{\lambda}_i)\|\gamma \hat{u}_i\|_b^2$

where $\hat{u}_i \in V$ is arbitrary and $\hat{\lambda}_i = \|\hat{u}_i\|_a^2 / \|\gamma \hat{u}_i\|_b^2$

Example 1: Square

Laplace eigenvalue problem

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

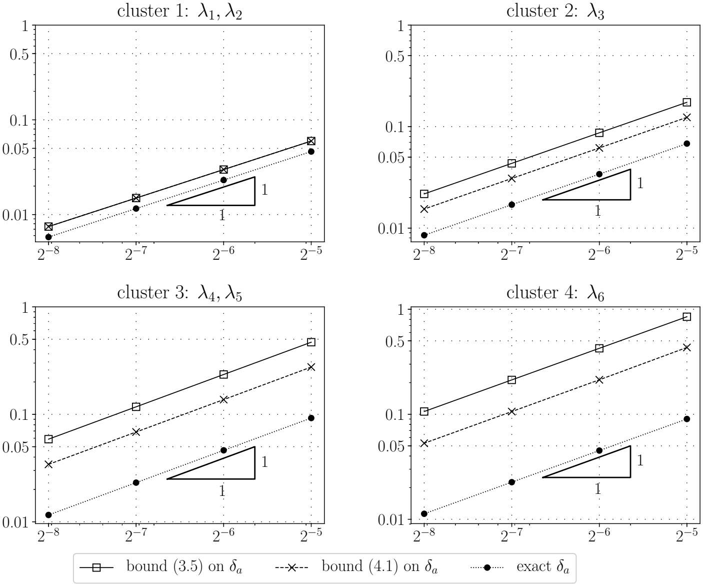


Exact eigenvalues:

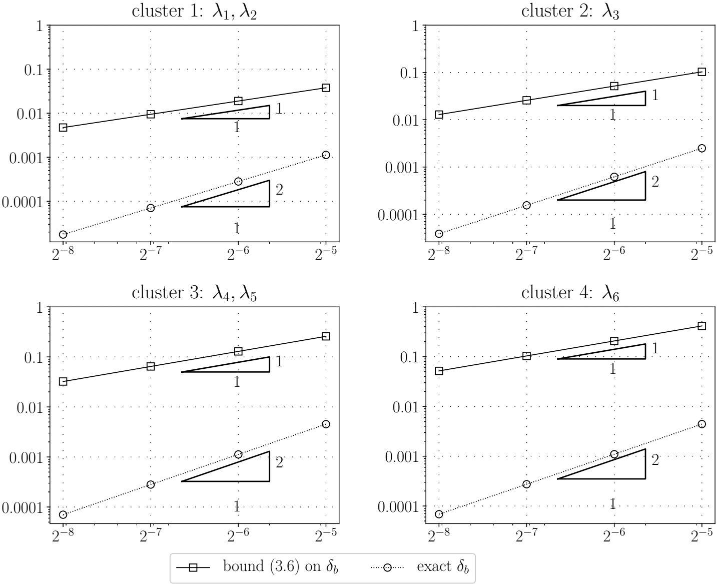
$$\underbrace{2\pi^2}_{\text{cluster 1}}, \underbrace{5\pi^2, 5\pi^2}_{\text{cluster 2}}, \underbrace{8\pi^2}_{\text{cluster 3}}, \underbrace{9\pi^2, 9\pi^2}_{\text{cluster 4}}, \ldots.$$

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

Example 1: Square – bounds in the energy norm



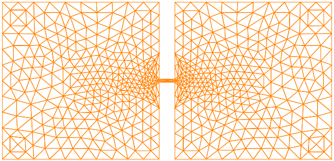
Example 1: Square – bounds in the $L^2(\Omega)$ norm



Example 2: Dumbbell

Laplace eigenvalue problem

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

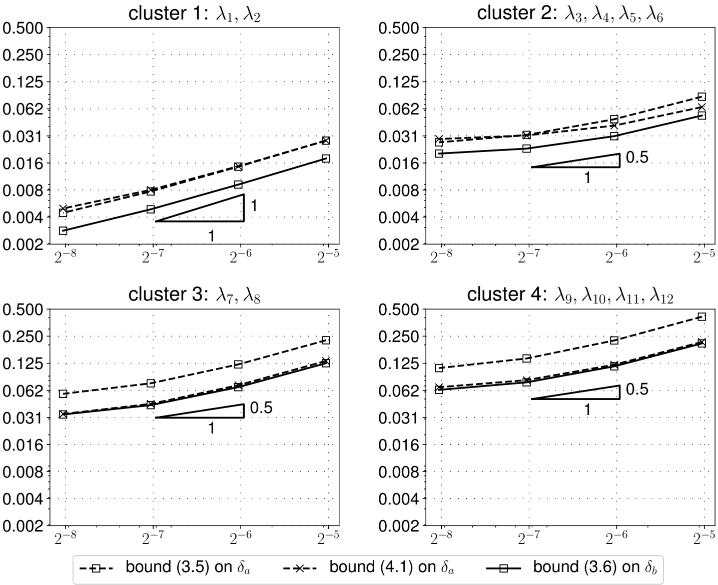


Exact eigenvalues – unknown, but close to

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

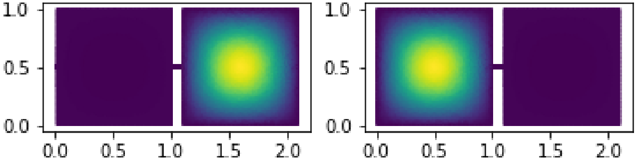
Cluster	lower and upper bound
1	$\lambda_1 = 19.736^{729}_{634},\ \lambda_2 = 19.736^{729}_{635}$
2	$\lambda_3 = 49.33^{809}_{761},\ \lambda_4 = 49.33^{809}_{761},\ \lambda_5 = 49.348020^{8}_{5},\ \lambda_6 = 49.348020^{8}_{5}$
3	$\lambda_7 = 78.9568^{301}_{290},\ \lambda_8 = 78.9568^{301}_{290}$
4	$\lambda_9 = 98.6^{71154}_{69041},\ \lambda_{10} = 98.6^{71154}_{69041},\ \lambda_{11} = 98.69604^{41}_{39},\ \lambda_{12} = 98.69604^{41}_{39}$

Example 2: Dumbbell – energy and L^2 bounds

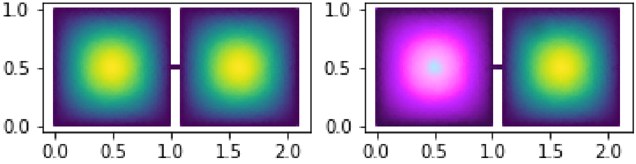


Are the computed eigenfunctions wrong?

Computed eigenfunctions



Exact eigenfunctions



- Both $\|\nabla u_1 - \nabla u_{h,1}\|$ and $\|\nabla u_2 - \nabla u_{h,2}\|$ are large,
- but $\delta_a(E_1, \widehat{E}_1)$ is small for $E_1 = \mathrm{span}\{u_1,\, u_2\}$ and $\widehat{E}_1 = \mathrm{span}\{u_{h,1},\, u_{h,2}\}$.

Conclusions

- General eigenvalue problem
- 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)

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

Literature

Preprint
X. Liu, T. V.: Fully computable a posteriori error bounds for eigenfunctions, arXiv:1904.07903v2

Generalization of:
[Birkhoff, de Boor, Swartz, Wendroff, 1966]

Related to:
[Davis, Kahan, 1970]

Alternative approach:
[Cancès, Dusson, Maday, Stamm, Vohralík, 2017]
[Cancès, Dusson, Maday, Stamm, Vohralík, 2018]
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Thank you for your attention

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics
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