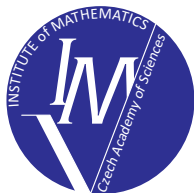


Rigorous and fully computable a posteriori error bounds for eigenfunctions

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Laplace eigenvalue problem

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

Two-sided bounds on eigenvalues:

$$\underline{\lambda}_j \leq \lambda_j \leq \bar{\lambda}_j$$

[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], [Plum 1990, 1991], [Šebestová, V. 2014], [V. 2018], [Luo, Lin, Xie 2012], [Li, Lin, Xie 2013] and many others.



Introduction

Laplace eigenvalue problem

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

Two-sided bounds on eigenvalues:

$$\underline{\lambda}_j \leq \lambda_j \leq \bar{\lambda}_j$$

Approximate eigenfunctions: \hat{u}_j

Goal: fully computable error bound for eigenfunctions

$$\|\nabla u_j - \nabla \hat{u}_j\| \leq \eta(\underline{\lambda}_j, \bar{\lambda}_j, \hat{u}_j)$$

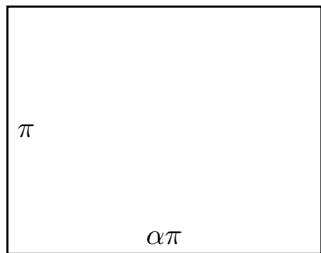
Laplace eigenvalue problem in a rectangle



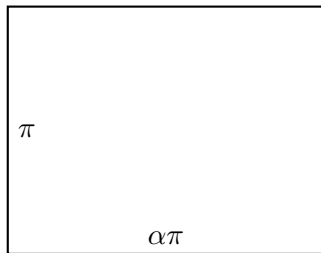
Laplace eigenvalue problem in a rectangle



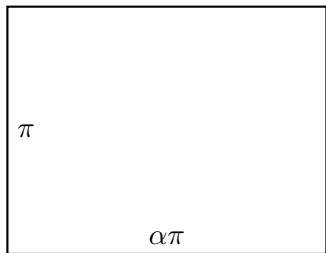
$$\alpha = 1.27$$



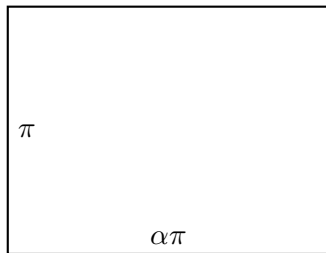
$$\alpha = 1.28$$



$$\alpha = 1.29$$



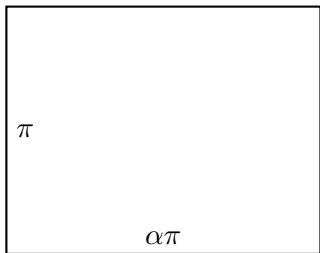
$$\alpha = 1.30$$



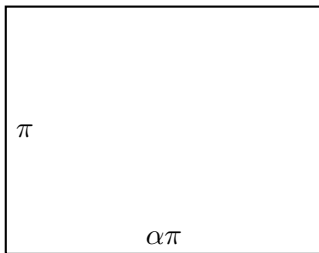


Laplace eigenvalue problem in a rectangle

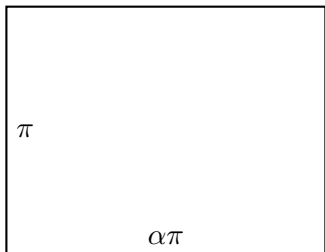
$$\alpha = 1.27, \lambda_4 = 6.4800$$



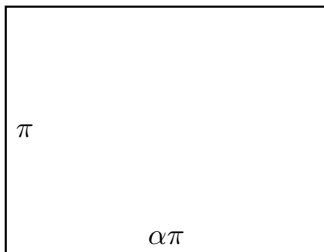
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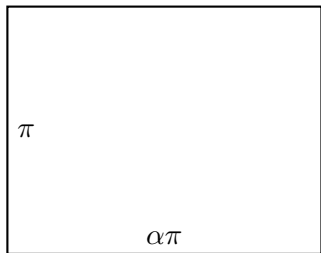
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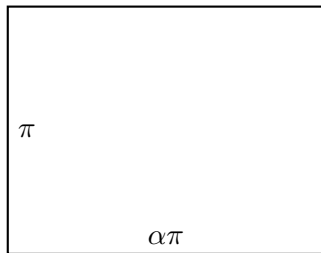


Laplace eigenvalue problem in a rectangle

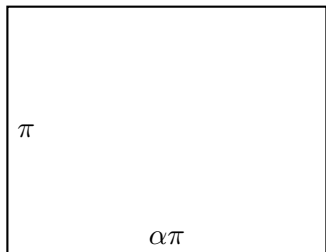
$$\alpha = 1.27, \lambda_4 = 6.4800$$



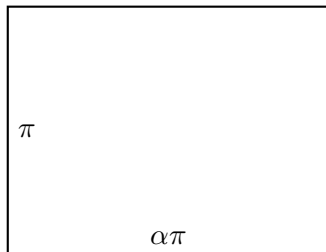
$$\alpha = 1.28, \lambda_4 = 6.4414$$



$$\alpha = 1.29$$



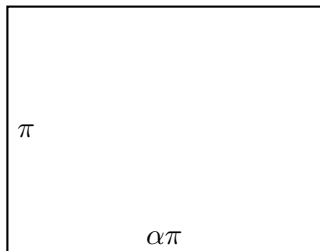
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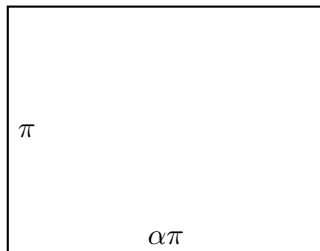
Laplace eigenvalue problem in a rectangle



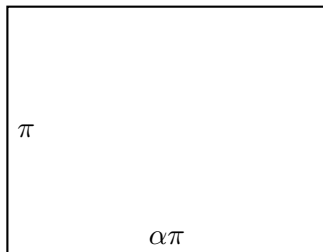
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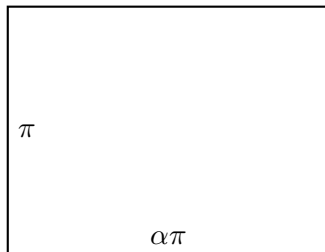
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



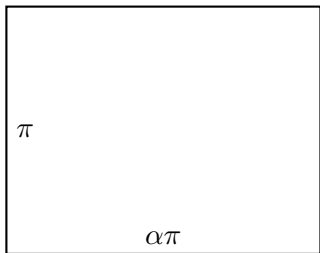
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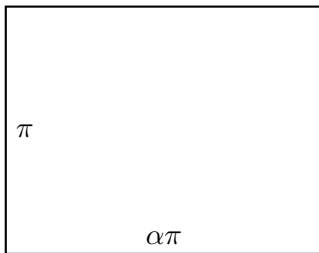
Laplace eigenvalue problem in a rectangle



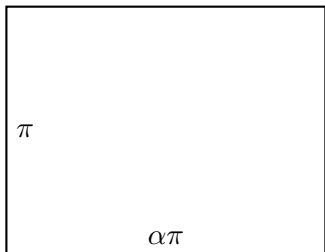
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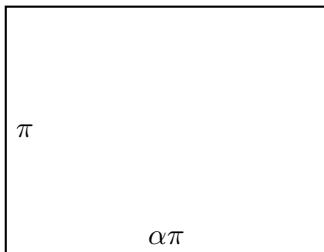
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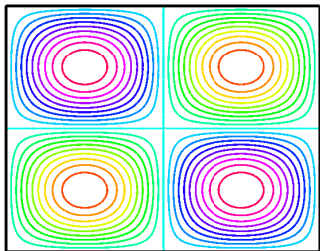
$$\alpha = 1.30, \lambda_4 = 6.3254$$



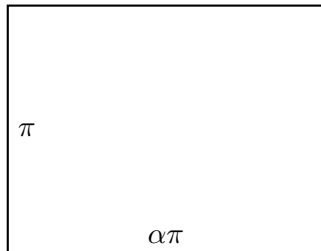


Laplace eigenvalue problem in a rectangle

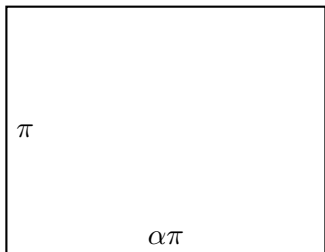
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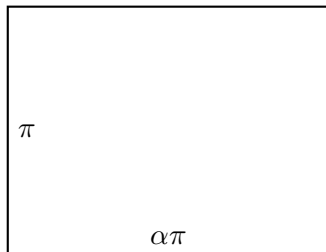
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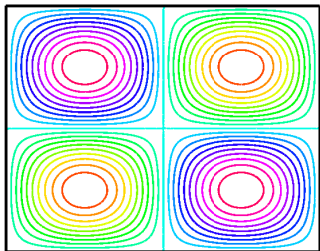
$$\alpha = 1.30, \lambda_4 = 6.3254$$



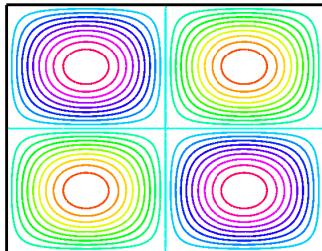


Laplace eigenvalue problem in a rectangle

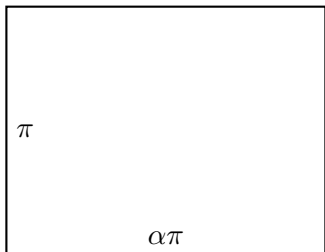
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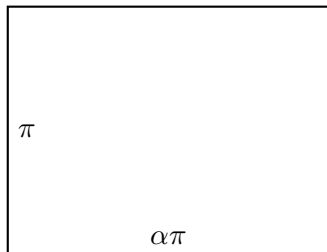
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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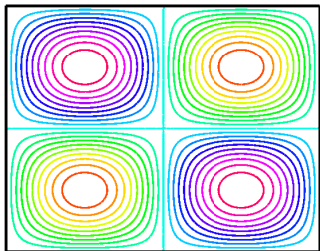
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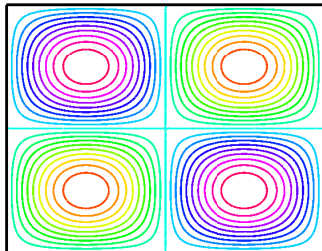


Laplace eigenvalue problem in a rectangle

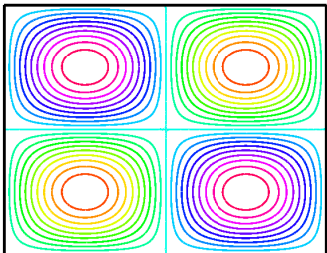
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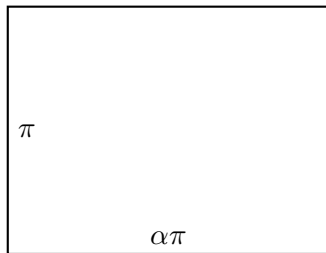
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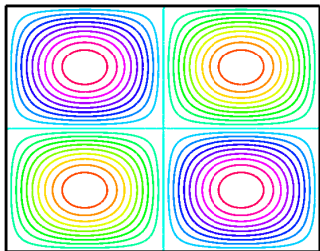
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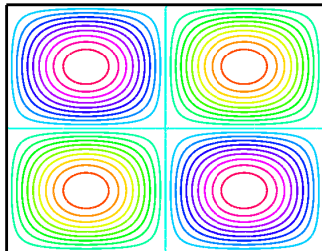


Laplace eigenvalue problem in a rectangle

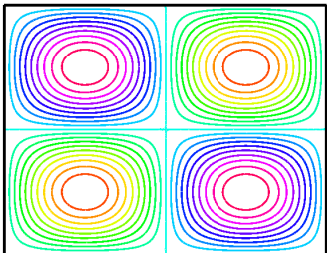
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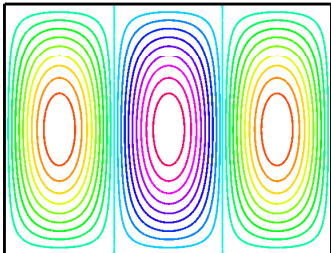
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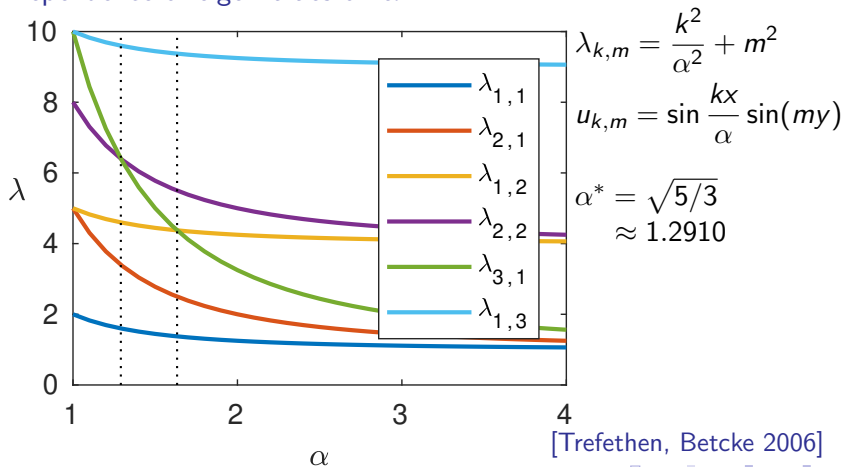


Laplace eigenvalue problem in a rectangle



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

Dependence of eigenvalues on α



[Trefethen, Betcke 2006]

Error bounds on eigenfunctions



Problem: Eigenfunctions may be ill-posed.

Solution:

(a) consider spaces of eigenfunctions

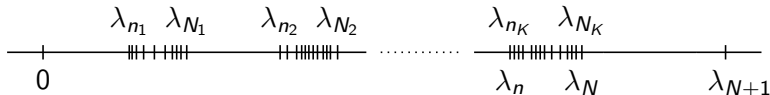
- ▶ $\lambda_n, \lambda_{n+1}, \dots, \lambda_N$ (cluster)
- ▶ $E = \text{span}\{u_n, u_{n+1}, \dots, u_N\}$ (space of eigenfunctions)
- ▶ $\hat{E} = \text{span}\{\hat{u}_n, \hat{u}_{n+1}, \dots, \hat{u}_N\}$ (its approximation)

(b) bound the directed distance of spaces

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



Error bounds on eigenfunctions in the energy norm

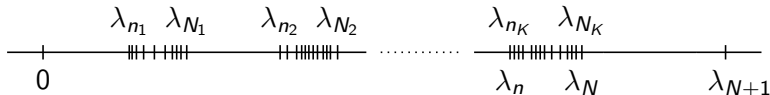


Theorem 1. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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



Error bounds on eigenfunctions in the energy norm



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

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

Space of exact eigenfunctions

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

Notation

$$n = n_K \text{ and } N = N_K$$

Space of approximate eigenfunctions

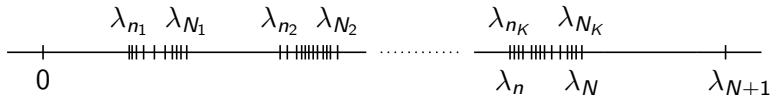
$$\hat{E}_K = \text{span}\{\hat{u}_n, \hat{u}_{n+1}, \dots, \hat{u}_N\}$$

Assumption

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



Error bounds on eigenfunctions in the energy norm



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

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

Directed distance

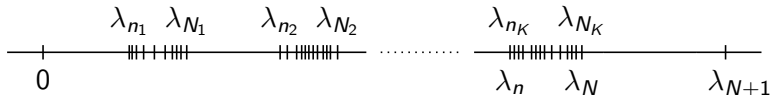
$$\Delta(E_K, \hat{E}_K) = \max_{\substack{v \in E_K \\ \|\nabla v\|=1}} \min_{\hat{v} \in \hat{E}_K} \|\nabla v - \nabla \hat{v}\|$$

Note

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



Error bounds on eigenfunctions in the energy norm



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

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

Directed distance

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

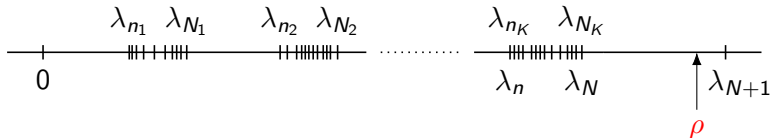
Example

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

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



Error bounds on eigenfunctions in the energy norm

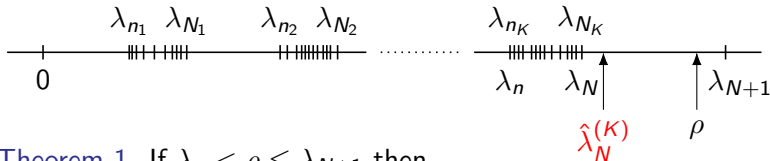


Theorem 1. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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



Error bounds on eigenfunctions in the energy norm



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

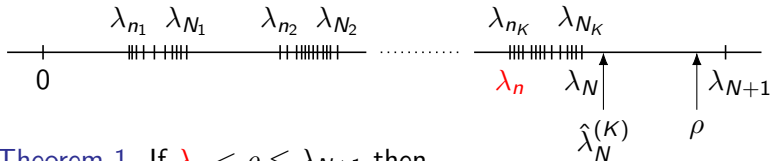
$$\Delta^2(E_K, \hat{E}_K) \leq \frac{\rho \left(\hat{\lambda}_N^{(K)} - \lambda_n \right) + \lambda_n \hat{\lambda}_N^{(K)} \vartheta^{(K)}}{\hat{\lambda}_N^{(K)} (\rho - \lambda_n)}.$$

Approximation of λ_N

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



Error bounds on eigenfunctions in the energy norm

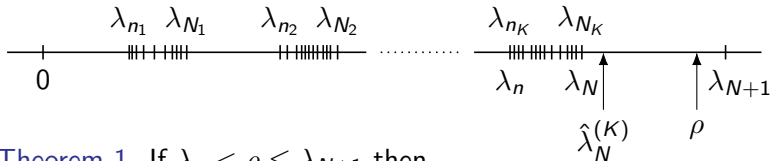


Theorem 1. If $\lambda_n < \rho \leq \lambda_{N+1}$ then

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Error bounds on eigenfunctions in the energy norm



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

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Errors in previous clusters

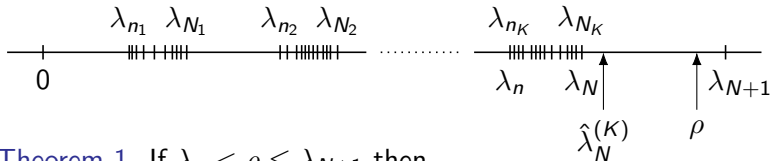
$$\vartheta^{(K)} = \sum_{k=1}^{K-1} \frac{\rho - \lambda_{n_k}}{\lambda_{n_k}} \left[\hat{\zeta}(\hat{E}_k, \hat{E}_K) + \Delta(E_k, \hat{E}_k) \right]^2$$

Nonorthogonality

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



Error bounds on eigenfunctions in the energy norm



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

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

Errors in previous clusters

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

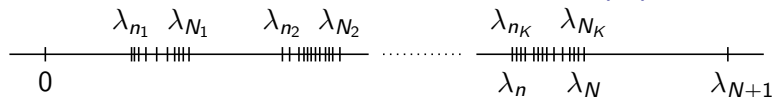
Nonorthogonality

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

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



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



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

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

Directed distance: $\delta(E_K, \hat{E}_K) = \max_{\substack{v \in E_K \\ \|v\|=1}} \min_{\hat{v} \in \hat{E}_K} \|v - \hat{v}\|$

Errors in previous clusters:

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

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



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

Conforming finite element method:

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

Error constant for elliptic projection P_h :

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

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



Theorem 4

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

Then

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

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



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

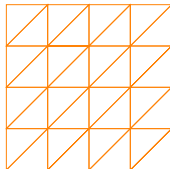
1. Compute the original bound on $\Delta(E_K, \hat{E}_K)$ by Thm 1
2. Compute the analogous bound on $\delta(E_K, \hat{E}_K)$ by Thm 2
3. Compute the optimal order bound on $\delta(E_K, \hat{E}_K)$ by Thm 3, using $\Delta(E_K, \hat{E}_K)$
4. Compute asymptotically sharp bound on $\Delta(E_K, \hat{E}_K)$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

Example 1: Square



Laplace eigenvalue problem

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



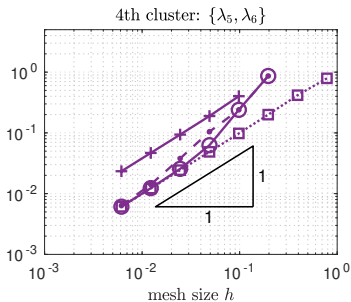
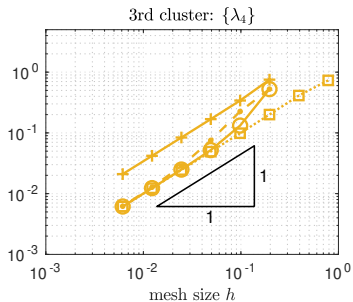
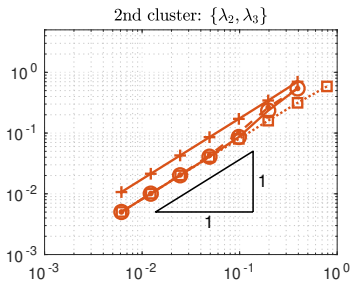
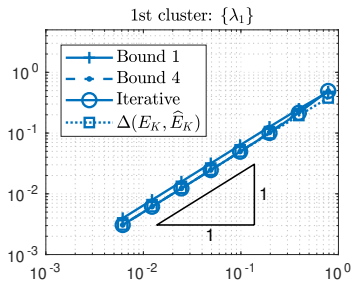
Exact eigenvalues:

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

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

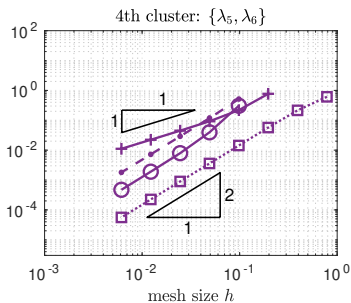
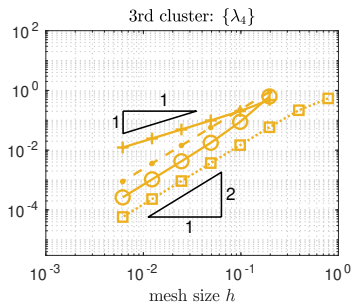
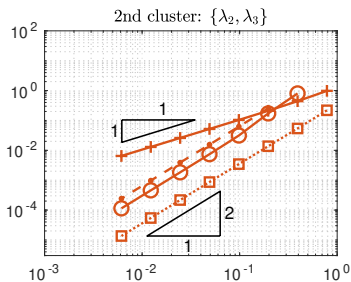
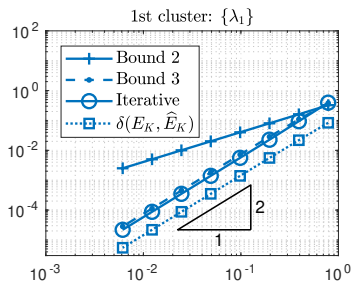


Example 1: Square – bounds in the energy norm





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

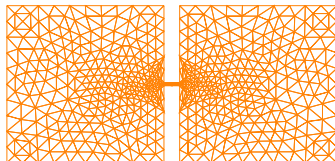




Example 2: Dumbbell

Laplace eigenvalue problem

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

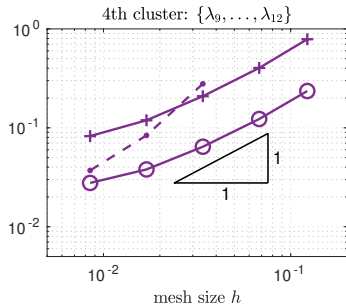
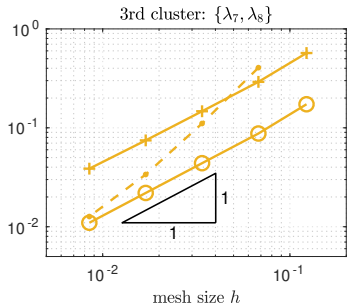
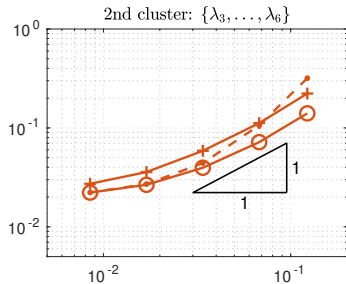
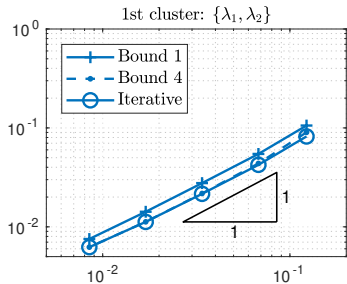


Exact eigenvalues – unknown, but close to

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

| Cluster | lower and upper bound |
|---------|---|
| 1 | $\lambda_1 = 19.736_{634}^{729}, \lambda_2 = 19.736_{635}^{729}$ |
| 2 | $\lambda_3 = 49.33_{761}^{809}, \lambda_4 = 49.33_{761}^{809}, \lambda_5 = 49.348020_5^8, \lambda_6 = 49.348020_5^8$ |
| 3 | $\lambda_7 = 78.9568_{290}^{301}, \lambda_8 = 78.9568_{290}^{301}$ |
| 4 | $\lambda_9 = 98.6_{69041}^{71154}, \lambda_{10} = 98.6_{69041}^{71154}, \lambda_{11} = 98.69604_{39}^{41}, \lambda_{12} = 98.69604_{39}^{41}$ |

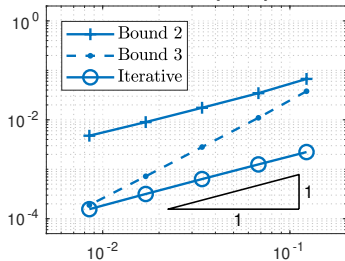
Example 2: Dumbbell – bounds in the energy norm



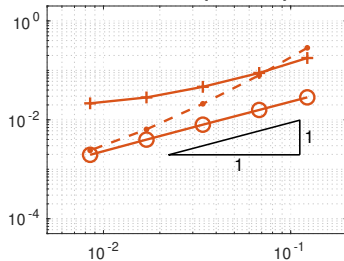
Example 2: Dumbbell – bounds in the $L^2(\Omega)$ norm



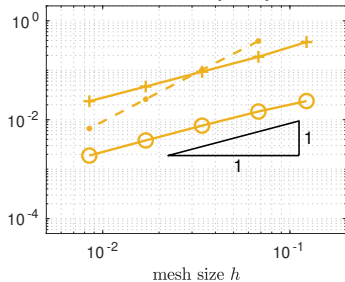
1st cluster: $\{\lambda_1, \lambda_2\}$



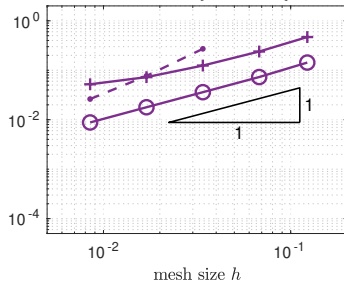
2nd cluster: $\{\lambda_3, \dots, \lambda_6\}$



3rd cluster: $\{\lambda_7, \lambda_8\}$



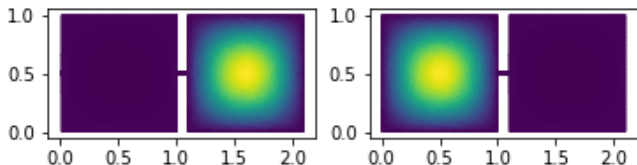
4th cluster: $\{\lambda_9, \dots, \lambda_{12}\}$



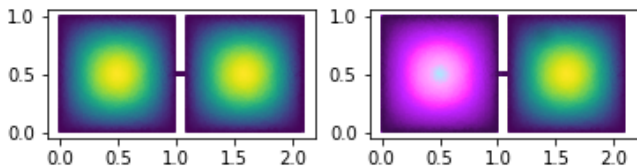


Are the computed eigenfunctions wrong?

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 $E_{h,1} = \text{span}\{u_{h,1}, u_{h,2}\}$.



- ▶ 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



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]

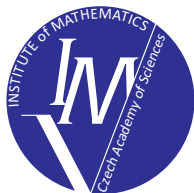
[Cancès, Dusson, Maday, Stamm, Vohralík, 2018]

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

Thank you for your attention

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