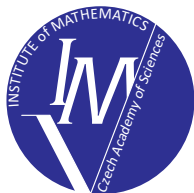


Fully computable error bounds for eigenfunctions

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics
Czech Academy of Sciences



Joint work with Xuefeng Liu (Niigata University, Japan)

Eigenvalue Day, Berlin, April 15, 2019



Laplace eigenvalue problem

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

Two-sided bounds on eigenvalues:

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

Approximate eigenfunctions: \hat{u}_i

Goal: fully computable error bound for eigenfunctions

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

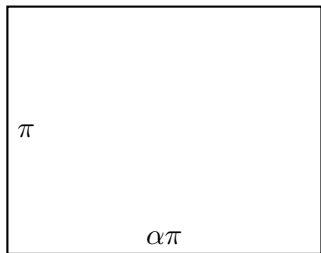
Laplace eigenvalue problem in a rectangle



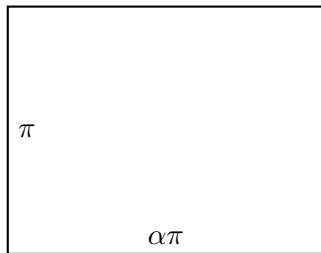
Laplace eigenvalue problem in a rectangle



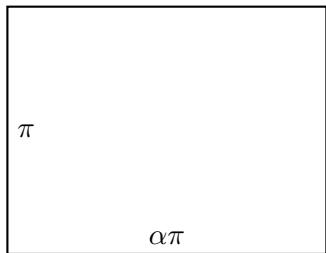
$$\alpha = 1.27$$



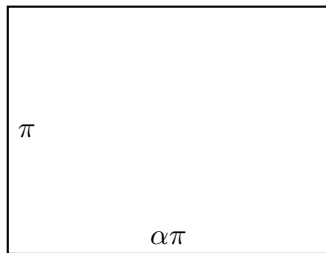
$$\alpha = 1.28$$



$$\alpha = 1.29$$



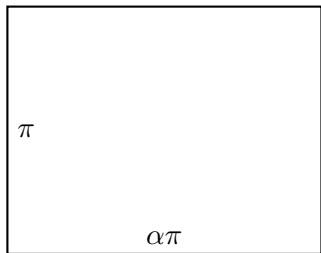
$$\alpha = 1.30$$



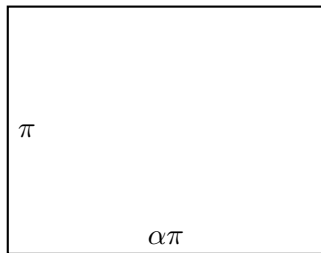


Laplace eigenvalue problem in a rectangle

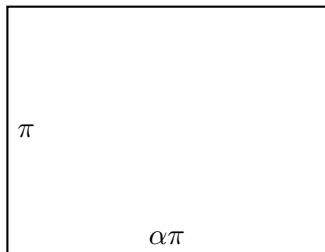
$$\alpha = 1.27, \lambda_4 = 6.4800$$



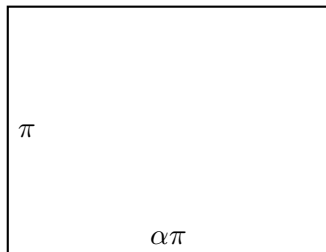
$$\alpha = 1.28$$



$$\alpha = 1.29$$



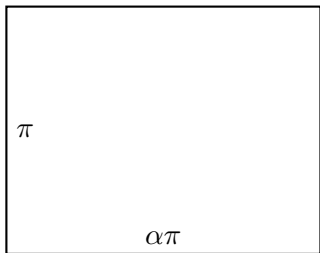
$$\alpha = 1.30$$



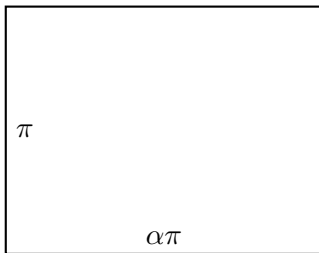


Laplace eigenvalue problem in a rectangle

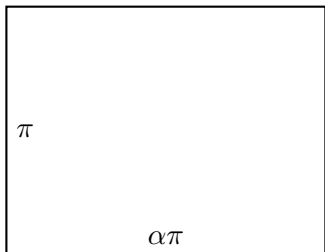
$$\alpha = 1.27, \lambda_4 = 6.4800$$



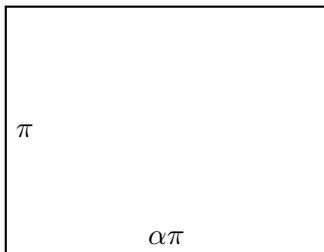
$$\alpha = 1.28, \lambda_4 = 6.4414$$



$$\alpha = 1.29$$



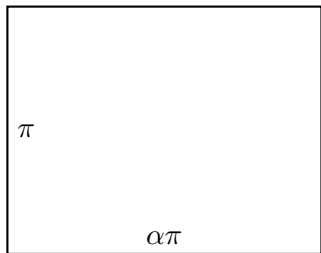
$$\alpha = 1.30$$



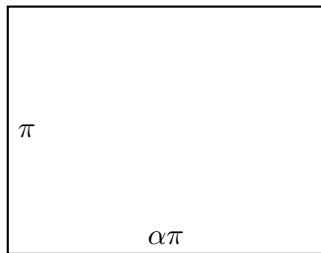
Laplace eigenvalue problem in a rectangle



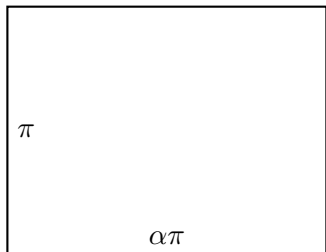
$$\alpha = 1.27, \lambda_4 = 6.4800$$



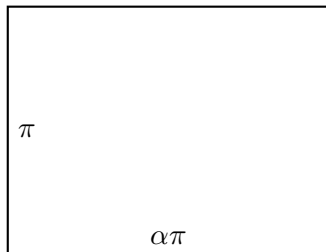
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



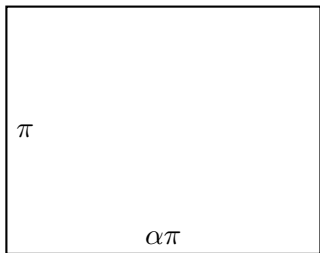
$$\alpha = 1.30$$



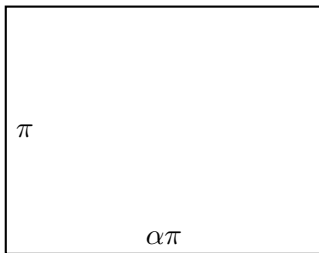
Laplace eigenvalue problem in a rectangle



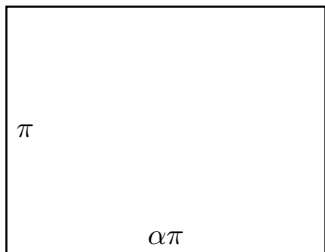
$$\alpha = 1.27, \lambda_4 = 6.4800$$



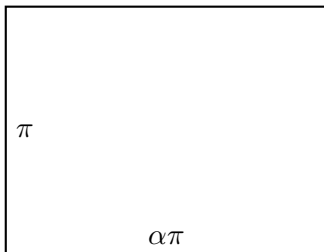
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



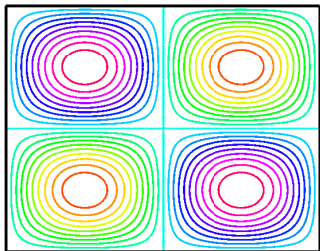
$$\alpha = 1.30, \lambda_4 = 6.3254$$



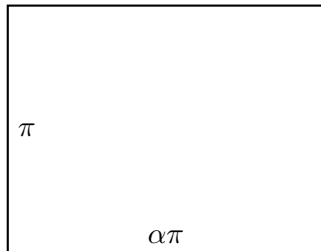


Laplace eigenvalue problem in a rectangle

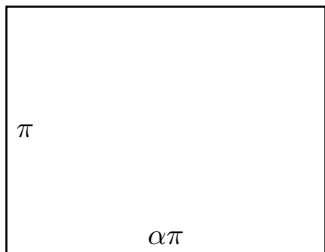
$$\alpha = 1.27, \lambda_4 = 6.4800$$



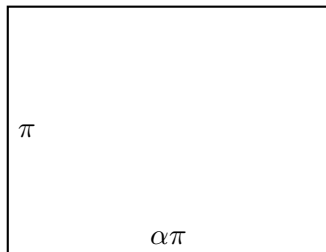
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



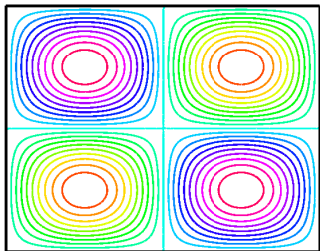
$$\alpha = 1.30, \lambda_4 = 6.3254$$



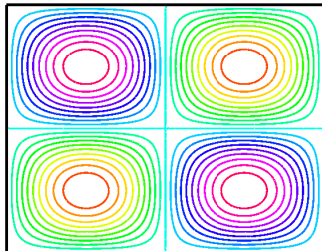


Laplace eigenvalue problem in a rectangle

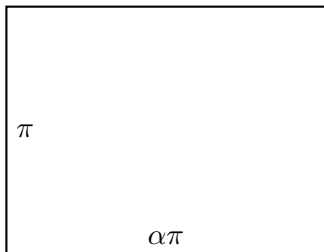
$$\alpha = 1.27, \lambda_4 = 6.4800$$



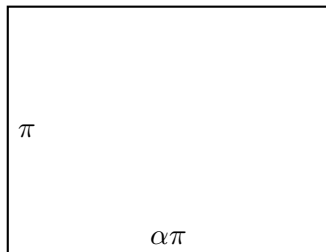
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



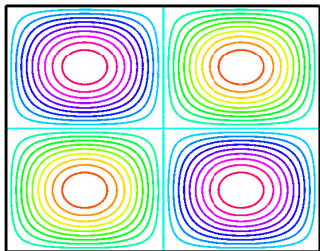
$$\alpha = 1.30, \lambda_4 = 6.3254$$



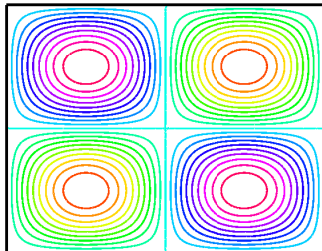


Laplace eigenvalue problem in a rectangle

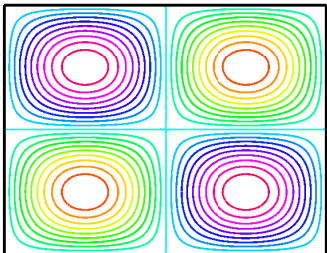
$$\alpha = 1.27, \lambda_4 = 6.4800$$



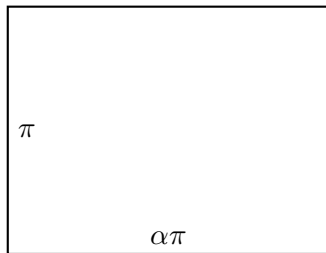
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



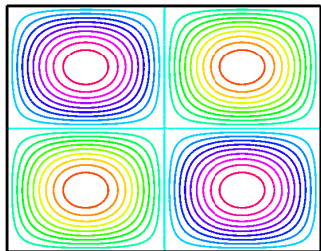
$$\alpha = 1.30, \lambda_4 = 6.3254$$



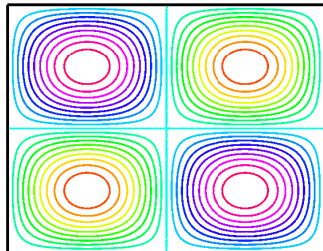


Laplace eigenvalue problem in a rectangle

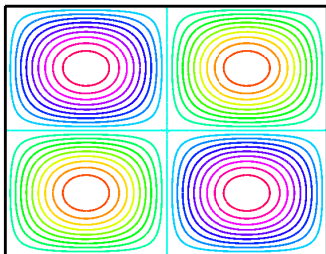
$$\alpha = 1.27, \lambda_4 = 6.4800$$



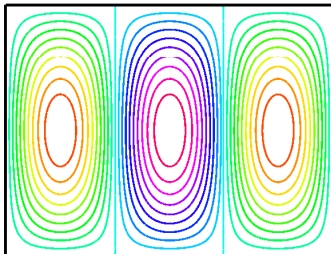
$$\alpha = 1.28, \lambda_4 = 6.4414$$



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



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

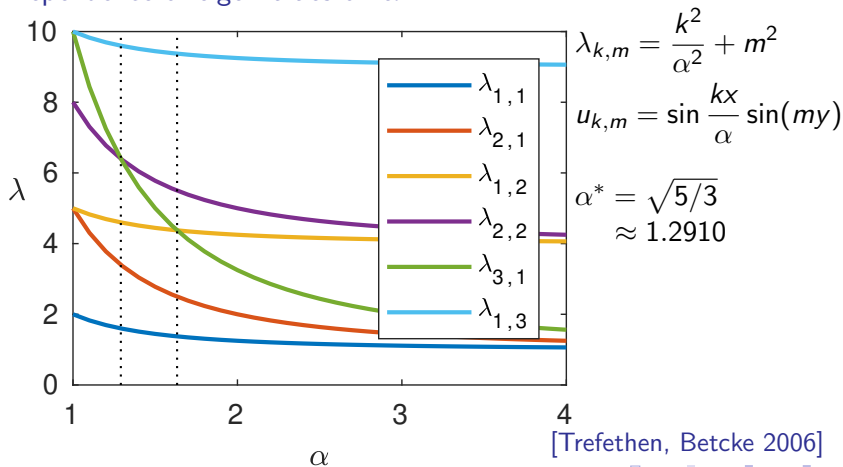


Laplace eigenvalue problem in a rectangle



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

Dependence of eigenvalues on α





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

▶ $\delta(E, \hat{E}) \leq \eta$ [Meyer 2000]

Assume two-sided bounds on eigenvalues:

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



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 ???]

Many recent relevant works:

[Carstensen, Gedicke 2014], [Carstensen, Gallistl 2014],

[Hu, Huang, Lin 2014], [Liu 2015], [Liu, Oishi 2013],

[Šebestová, V. 2014], [V. 2018], and many others.

Classics:

[Goerisch, Haunhorst 1985], [Kato 1949], [Lehmann 1949, 1950],
and many others.



1. Directed distance of spaces
2. Clusters of eigenvalues
3. Measure of nonorthogonality
4. The error bound in the energy norm
5. Analogous bound in the L^2 norm
6. Optimal order bound in the L^2 norm
7. Asymptotically sharp bound in the energy norm
8. Iteratively improved bounds
9. Numerical examples



Directed distance of spaces

Definition

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

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

Properties

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

Example

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

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

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



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

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

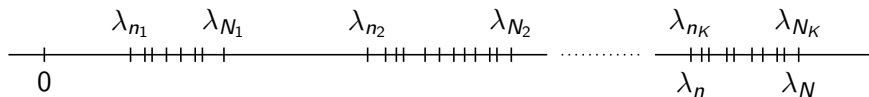
Then

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

where $\lambda_{\max}(A, B)$ denotes the maximum eigenvalue of $Ax = \lambda Bx$.
Further, suppose $\|F^T F\|_2 \leq \eta_F$, $\|I - G\|_2 \leq \eta_G$, $\|I - H\|_2 \leq \eta_H$.
If $\eta_G, \eta_H < 1$, then

$$\hat{\epsilon}^2(E, E') \leq \frac{\eta_F}{(1 - \eta_G)(1 - \eta_H)}.$$

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

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

Notation:

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



The bound on eigenfunctions in energy norm

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

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

Theorem

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

Let $\lambda_n < \rho \leq \lambda_{N+1}$. Then

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

where

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

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



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

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

Theorem

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

Let $\lambda_n < \rho \leq \lambda_{N+1}$. Then

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

where

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



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

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

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

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

Iteratively improved bounds



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

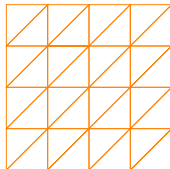
1. Compute the original bound on $\Delta(E_K, \hat{E}_K)$
2. Compute the analogous bound on $\delta(E_K, \hat{E}_K)$
3. Compute the optimal order bound on $\delta(E_K, \hat{E}_K)$ using $\Delta(E_K, \hat{E}_K)$
4. Compute asymptotically sharp bound on $\Delta(E_K, \hat{E}_K)$ using $\delta(E_K, \hat{E}_K)$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

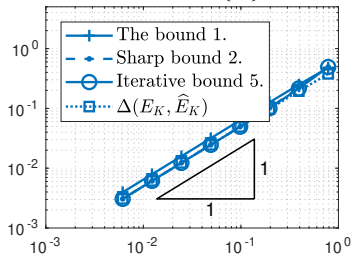
$$\underbrace{2\pi^2}_{\text{cluster 1}}, \quad \underbrace{5\pi^2, 5\pi^2}_{\text{cluster 2}}, \quad \underbrace{8\pi^2}_{\text{cluster 3}}, \quad \underbrace{9\pi^2, 9\pi^2}_{\text{cluster 4}}, \dots$$

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

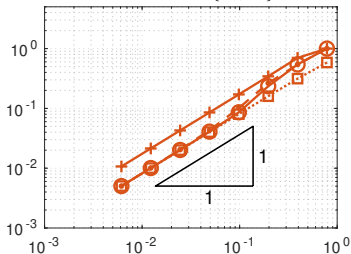


Example 1: Square – bounds in the energy norm

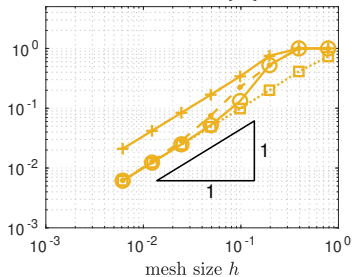
1st cluster: $\{\lambda_1\}$



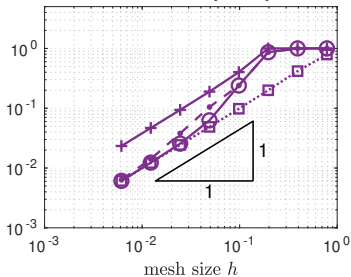
2nd cluster: $\{\lambda_2, \lambda_3\}$



3rd cluster: $\{\lambda_4\}$

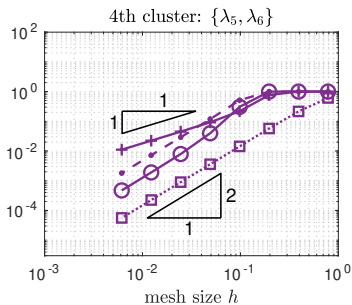
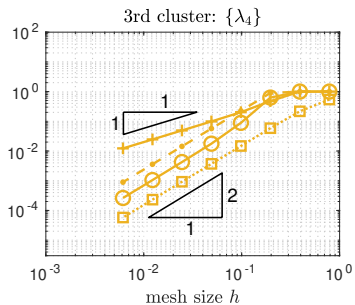
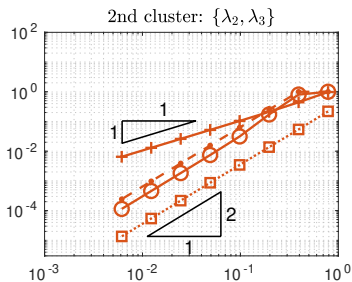
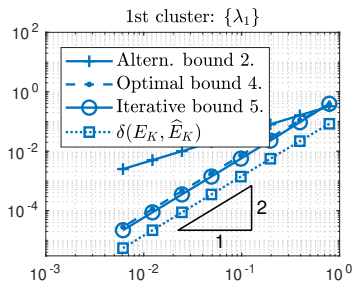


4th cluster: $\{\lambda_5, \lambda_6\}$





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

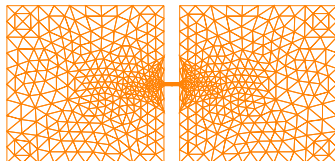




Example 2: Dumbbell

Laplace eigenvalue problem

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

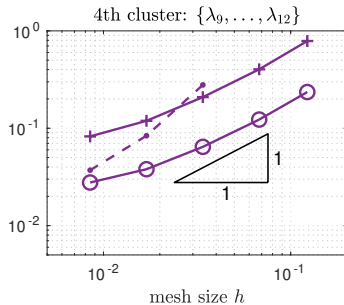
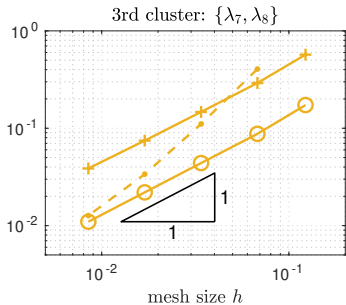
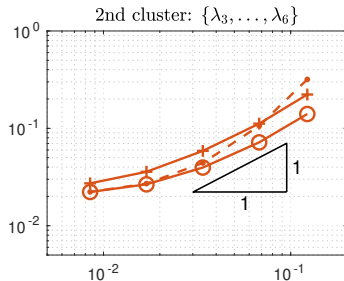
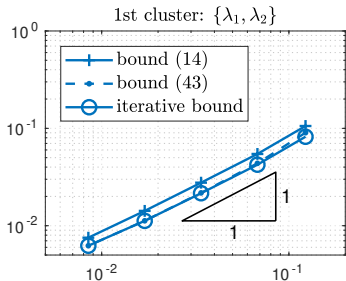


Exact eigenvalues – unknown, but close to

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

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

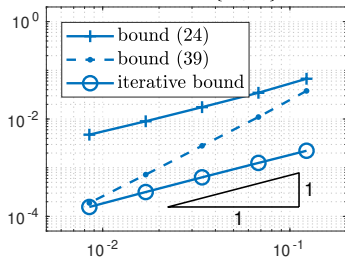
Example 2: Dumbbell – bounds in the energy norm



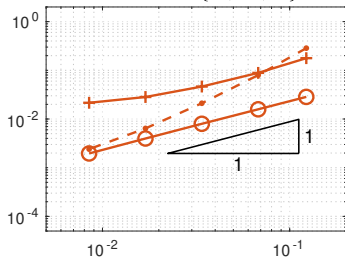
Example 2: Dumbbell – bounds in the $L^2(\Omega)$ norm



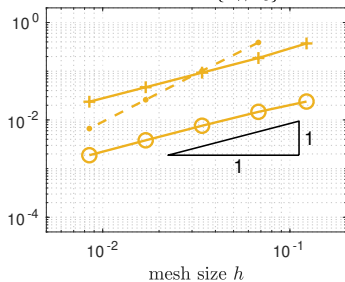
1st cluster: $\{\lambda_1, \lambda_2\}$



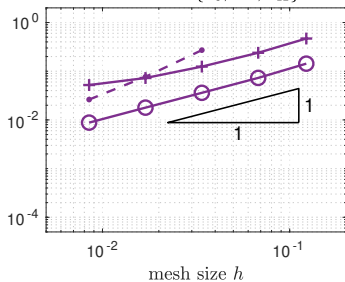
2nd cluster: $\{\lambda_3, \dots, \lambda_6\}$



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



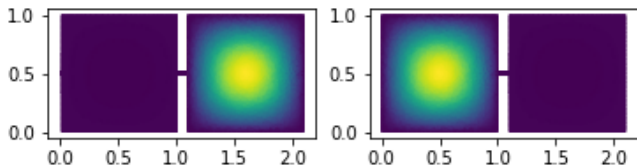
4th cluster: $\{\lambda_9, \dots, \lambda_{12}\}$



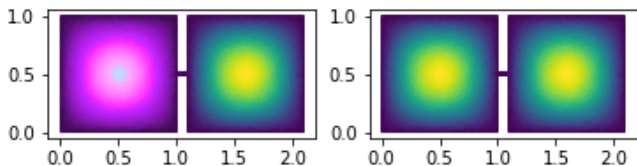
Are the computed eigenfunctions wrong?



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

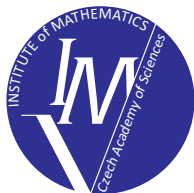


- ▶ Fully computable upper bounds on the directed distance of spaces of eigenfunctions
- ▶ The (first) bounds are good for arbitrary approximations
 - ▶ Optimal rate for the energy norm
 - ▶ Suboptimal rate for the $L^2(\Omega)$ norm
- ▶ Improved bounds for finite element approximations
 - ▶ Optimal rates even in the $L^2(\Omega)$ norm
- ▶ Further iterative improvement possible

Thank you for your attention

Tomáš Vejchodský (vejchod@math.cas.cz)

Institute of Mathematics
Czech Academy of Sciences



Joint work with Xuefeng Liu (Niigata University, Japan)

Eigenvalue Day, Berlin, April 15, 2019