Rigorous and fully computable a posteriori error bounds for eigenfunctions

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Abstract

Guaranteed *a posteriori* estimates on the error of approximate eigenfunctions in both energy and L^2 norms are derived for the Laplace eigenvalue problem. The problem of ill-conditioning of eigenfunctions in case of tight clusters and multiple eigenvalues is solved by estimating the directed distance between the spaces of exact and approximate eigenfunctions. The error estimates for approximate eigenfunctions are based on rigorous lower and upper bounds on eigenvalues. Such eigenvalue bounds can be computed for example by the finite element method along with the recently developed explicit error estimation [24] and the Lehmann–Goerisch method. The efficiency of the derived error bounds for eigenfunctions is illustrated by numerical examples.

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1 Introduction

This paper derives rigorous and fully computable *a posteriori* error bounds for eigenfunctions of the Laplace eigenvalue problem: find eigenvalues $\lambda_i \in \mathbb{R}$ and corresponding eigenfunctions $u_i \neq 0$ such that

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega, \qquad u_i = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded d-dimensional domain. The weak formulation of this problem and specific assumptions are provided in Section 3.

The problem to determine eigenvalues λ_i is well posed in the sense that small perturbations of the data lead to small perturbations of eigenvalues. However, the variation of eigenfunctions u_i upon the perturbation of the data is not necessary small, and can even be discontinuous. For example, if two close and simple eigenvalues merge to one multiple eigenvalue then the two corresponding orthogonal eigenfunctions abruptly change into a two dimensional eigenspace. Thus, eigenfunction determination in case of tightly clustered or multiple eigenvalues is an ill-conditioned problem.

Any attempt to estimate the error of approximate eigenfunctions has to take into the account this ill-conditioning. Our approach is to consider the space spanned by eigenfunctions corresponding to all eigenvalues within a cluster. This space is well conditioned provided the cluster is well separated from the rest of the spectrum. We propose error estimators that bound the *directed distance* [29, §5.15] between the approximate and the exact space of eigenfunctions in both the energy and L^2 norms. The proposed estimators generalize the idea from [4]; see Remark 5.2 below. The quality of these estimators depends on the width of clusters and spectral gaps between them.

The two-sided bounds on individual eigenvalues play an important role in the estimation of eigenfunctions. Computing eigenvalue bounds, especially the lower bounds, is not an easy task. We use the recently developed method based on the finite element method with explicit error estimation [24] (see

also, [26, 9, 10]) for the lower bounds on eigenvalues and the Lehmann–Goerisch method [21, 22, 15] for their high-precision improvements. Note that the Lehmann–Goerisch method should be attributed to T. Kato as well, because his independently developed method [19], gives essentially the same bounds as Lehmann's method. In the current paper, we focus on the estimation of eigenfunctions and the two-sided bounds of eigenvalues are assumed to be known.

Error estimates for symmetric elliptic eigenvalue problems are widely studied in the literature. We refer to classical works [11, 2, 5] for the fundamental theories about eigenvalue problems. Most existing literature concerns error estimates valid asymptotically or containing unknown constants; see, e.g., [13, 1, 36, 28, 12, 14, 18, 17]. Recently, fully computable (containing no unknown constants) and guaranteed (bounding the error from above on all meshes, not only asymptotically) error estimates for eigenvalue problems appeared. Papers [9, 10, 24, 26, 32, 33, 34] concern the eigenvalues. Particularly, as a general framework, the method proposed in [24] has been applied to eigenvalue problems of various differential operators, including the Stokes operator [35], the Steklov operator [37], and biharmonic operators related to the quadratic interpolation error constants [27, 23]. Concerning eigenfunctions, papers [6, 7] provide guaranteed, robust, and optimally convergent *a posteriori* bounds for simple eigenvalues and corresponding eigenfunctions for both conforming and nonconforming approximations, under the assumption of *a priori* information about bounds of eigenvalues. Very recent work [8] generalizes these results to the case of clustered and multiple eigenvalues using a different approach than we present below. In [16] an attempt to bound the error of the first eigenfunction is presented.

Properties of error bounds derived below can be summarized as follows.

- Without any *a priori* information about the approximate eigenfunctions, the proposed error estimator provides a rigorous upper bound on the distance between the exact and approximate eigenspace both in the energy and L^2 norms; see estimates (4.4) and (5.1) below. The bound in the energy norm converges with the optimal rate, while the L^2 bound with a suboptimal rate.

- For finite element approximate eigenfunctions, an optimal rate estimate in the L^2 norm is derived in (6.8). This further leads to the improved bound (7.1) in the energy norm.

The rest of the paper is organized as follows. Section 2 overviews the directed distance of spaces and its properties. Section 3 briefly recalls the Laplace eigenvalue problem. Section 4 presents the *a posteriori* error bound for eigenfunctions in the energy norm. An analogous bound in the L^2 norm is provided in Section 5. Section 6 derives optimal order bound for finite element eigenfunctions in the L^2 norm. Section 7 introduces energy norm estimates computed from L^2 bounds. Section 8 presents the results of two numerical examples and Section 9 draws the conclusions.

2 Directed distance of spaces

To measure the error of spaces of eigenfunctions, the *directed distance* of spaces is employed. Its definition comes from [29, pp. 452–453]; see also [3]. Let E and $\widehat{E}$ be two subspaces of a normed linear space V with a norm $\|\cdot\|_V$ then

$$\delta(E,\widehat{E}) = \max_{\substack{v\in E\\ \|v\|_V=1}} \min_{\hat{v}\in\widehat{E}} \|v-\hat{v}\|_V \tag{2.1}$$

is called the directed distance of spaces E and $\widehat{E}$.

The directed distance is not symmetric in general. However,

$$\text{if } \dim E = \dim \widehat{E} \quad \text{then} \quad \delta(E,\widehat{E}) = \delta(\widehat{E},E).$$

It is always $\delta(E,\widehat{E}) \le 1$ and if $\dim E = \dim \widehat{E}$ and $E^\perp \cap \widehat{E} \neq \{0\}$ (or $E \cap \widehat{E}^\perp \neq \{0\}$) then $\delta(E,\widehat{E}) = 1$. If $\dim E = \dim \widehat{E}$ then the directed distance coincides with the gap between subspaces defined as

$$\operatorname{gap}(E,\widehat{E}) = \max\{\delta(E,\widehat{E}),\delta(\widehat{E},E)\}.$$

Notice that if $\dim E \neq \dim \widehat{E}$ then $\operatorname{gap}(E,\widehat{E}) = 1$. All these properties can be found in [29, p. 454].

If V is a Hilbert space with inner product $(\cdot,\cdot)_V$ and the corresponding norm $\|\cdot\|_V$ and E and $\widehat{E}$ are closed subspaces of V, then further characterizations of the directed distance are available. Recall the orthogonal projector $\widehat{\Pi} : E \to \widehat{E}$ defined by the relation

$$(v-\widehat{\Pi}v,\hat{v})_V = 0 \quad \forall \hat{v}\in\widehat{E}. \tag{2.2}$$

The projection $\widehat{\Pi}v \in \widehat{E}$ is the closest element in $\widehat{E}$ to $v \in E$, i.e.,

$$\min_{\hat{v}\in\widehat{E}} \|v - \hat{v}\|_V = \|v - \widehat{\Pi}v\|_V \quad \forall v \in E.$$

A consequence of this fact is that the directed distance can be expressed as

$$\delta(E, \widehat{E}) = \max_{\substack{v\in E \\ \|v\|_V=1}} \|v - \widehat{\Pi}v\|_V. \tag{2.3}$$

The directed distance can also be expressed using the inner product.

Lemma 2.1. *Let E and $\widehat{E}$ be two closed subspaces of a Hilbert space V with inner product $(\cdot,\cdot)_V$, then*

$$\delta^2(E, \widehat{E}) = 1 - \min_{\substack{v\in E \\ \|v\|_V=1}} \max_{\substack{\hat{v}\in\widehat{E} \\ \|\hat{v}\|_V=1}} |(v, \hat{v})_V|^2. \tag{2.4}$$

Proof. Given $v \in V$, definition (2.2) of the orthogonal projector $\widehat{\Pi}$ yields identity

$$\max_{\substack{\hat{v}\in\widehat{E} \\ \|\hat{v}\|_V=1}} (v, \hat{v})_V = \max_{\substack{\hat{v}\in\widehat{E} \\ \|\hat{v}\|_V=1}} (\widehat{\Pi}v, \hat{v})_V = \|\widehat{\Pi}v\|_V.$$

Consequently,

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

where we used the fact that $\|\widehat{\Pi}v\|_V^2 + \|v - \widehat{\Pi}v\|_V^2 = \|v\|_V^2$ for all $v \in E$ and identity (2.3). □

The directed distance of one dimensional subspaces equals to the sine of the angle between them. Indeed, if $E = \text{span}\{u\}$, $\widehat{E} = \text{span}\{\hat{u}\}$, and α denotes the angle between u and $\hat{u}$ then identity (2.4) immediately gives

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

Consequently, if $(u, \hat{u})_V \geq 0$ then the distance between u and $\hat{u}$ can be expressed as

$$\|u - \hat{u}\|_V^2 = \|u\|_V^2 + \|\hat{u}\|_V^2 - 2\|u\|_V\|\hat{u}\|_V\sqrt{1 - \delta^2(E, \widehat{E})}. \tag{2.5}$$

Moreover, if u and $\hat{u}$ are normalized such that $\|u\|_V = \|\hat{u}\|_V = 1$ then

$$\|u - \hat{u}\|_V^2 = 2\left(1 - \sqrt{1 - \delta^2(E, \widehat{E})}\right) = \delta^2(E, \widehat{E}) + \mathcal{O}\left(\delta^4(E, \widehat{E})\right),$$

where the Taylor series $\sqrt{1 - x^2} = 1 - x^2/2 + \mathcal{O}(x^4)$ is used. In this sense, the directed distance of subspaces generalizes the usual distance induced by the norm.

3 Laplace eigenvalue problem

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain and $H_0^1(\Omega)$ be the usual Sobolev space of square integrable functions with the square integrable gradients and with zero traces on the boundary $\partial\Omega$. The weak formulation of eigenvalue problem (1.1) then reads: find $\lambda_i \in \mathbb{R}$ and $u_i \in H_0^1(\Omega) \setminus \{0\}$ such that

$$(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \quad \forall v \in H_0^1(\Omega), \tag{3.1}$$

where $(\cdot, \cdot)$ stands for the $L^2(\Omega)$ inner product.

This problem is well studied in [2, 5]. There exists a countable sequence of eigenvalues

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots,$$

where we repeat each eigenvalue according to its multiplicity. The corresponding eigenfunctions $u_i \in H_0^1(\Omega)$ are assumed to be normalized such that

$$(u_i, u_j) = \delta_{ij}, \quad i, j = 1, 2, \ldots.$$

From the spectral theory of compact selfadjoint operators, these eigenfunctions form an orthonormal and complete sequence in both $L^2(\Omega)$ and $H_0^1(\Omega)$. Therefore, the $L^2(\Omega)$ norm $\|v\|$ satisfies Parseval identity

$$\|v\|^2 = \sum_{i=1}^{\infty} |(v, u_i)|^2 \quad \forall v \in L^2(\Omega) \tag{3.2}$$

and a similar expression for the energy norm

$$\|\nabla v\|^2 = \sum_{i=1}^{\infty} \lambda_i |(v, u_i)|^2 \quad \forall v \in H_0^1(\Omega). \tag{3.3}$$

In order to formulate the bound on eigenfunctions, a notation for clusters of eigenvalues has to be introduced. Let us focus on the leading K clusters. Let n_k and N_k stand for indices of the first and the last eigenvalue in the k-th cluster, $k = 1, 2, \ldots, K$, respectively. In particular, $n_1 = 1$, $n_{k+1} = N_k + 1$, and the k-th cluster is formed of $N_k - n_k + 1$ eigenvalues λ_{n_k}, λ_{n_k+1}, $\ldots$, λ_{N_k}; see Figure 1. Notice that the eigenvalues in a cluster do not necessarily equal to each other. To simplify the notation, we set $n = n_K$ and $N = N_K$.

Each cluster is associated with the space $E_k = \mathrm{span}\{u_{n_k}, u_{n_k+1}, \ldots, u_{N_k}\}$ of exact eigenfunctions. Similarly, arbitrary approximations $\hat{u}_i \in H_0^1(\Omega)$ of exact eigenfunctions u_i, $i = 1, 2, \ldots, N_K$, form the corresponding approximate spaces $\widehat{E}_k = \mathrm{span}\{\hat{u}_{n_k}, \hat{u}_{n_k+1}, \ldots, \hat{u}_{N_k}\}$. Spaces $\widehat{E}_k$, $k = 1, 2, \ldots, K$, of approximate eigenfunctions need not be orthogonal to each other.

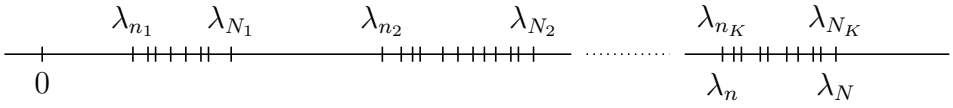

Figure 1: Clusters of eigenvalues on the real axis.

4 *A posteriori* error bound for eigenfunctions

The goal of this section is to derive an estimate of the directed distance between spaces E_K and $\widehat{E}_K$ of exact and approximate eigenfunctions for the K-th cluster. This directed distance is measured in the energy norm and it is given by (2.1) with $V = H_0^1(\Omega)$ and $\|v\|_V = \|\nabla v\|$ as

$$\Delta(E_K, \widehat{E}_K) = \max_{\substack{v \in E_K \\ \|\nabla v\| = 1}} \min_{\hat{v} \in \widehat{E}_K} \|\nabla v - \nabla \hat{v}\|. \tag{4.1}$$

In order to formulate the main result of this section (see Theorem 4.3 below), we introduce an energy measure of the non-orthogonality between spaces $\widehat{E}_k$ and $\widehat{E}_{k'}$ for $k, k' = 1, 2, \ldots, K$ as

$$\hat{\zeta}(\widehat{E}_k, \widehat{E}_{k'}) = \max_{\substack{v \in \widehat{E}_k \\ \|\nabla v\| = 1}} \max_{\substack{w \in \widehat{E}_{k'} \\ \|\nabla w\| = 1}} \langle v, w \rangle, \tag{4.2}$$

where the energy inner product is denoted by

$$\langle v, w\rangle = (\nabla v, \nabla w) \quad \forall v, w \in H_0^1(\Omega).$$

The measure of non-orthogonality $\hat{\zeta}(\widehat{E}_k, \widehat{E}_K)$ can be easily computed or estimated by using the following lemma with $E = \widehat{E}_k$, $E' = \widehat{E}_K$, $V = H_0^1(\Omega)$, and $(\cdot,\cdot)_V = \langle\cdot,\cdot\rangle$.

Lemma 4.1. *Let $v_1, v_2, \ldots, v_m$ and $v'_1, v'_2, \ldots, v'_{m'}$ form bases of finite dimensional subspaces E and E' of a Hilbert space V, respectively. Let*

$$\hat{\epsilon}^2(E, E') = \max_{\substack{v\in E \\ \|v\|_V=1}} \max_{\substack{v'\in E' \\ \|v'\|_V=1}} (v, v')_V. \tag{4.3}$$

Define matrices F, G, H as follows,

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

Then, we have

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

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

Further, suppose $\|F^T F\|_2 \le \eta_F$, $\|I - G\|_2 \le \eta_G$, $\|I - H\|_2 \le \eta_H$. If $\eta_G, \eta_H < 1$, then

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

Proof. Expand $v \in E$ and $v' \in E'$ as $v = \sum_{i=1}^m c_i v_i$ and $v' = \sum_{j=1}^{m'} c'_j v'_j$. Then

$$(v, v')_V = \boldsymbol{c}^T F \boldsymbol{c'}, \quad \|v\|_V^2 = \boldsymbol{c}^T G \boldsymbol{c}, \quad \text{and} \quad \|v'\|_V^2 = (\boldsymbol{c'})^T H \boldsymbol{c'},$$

where vectors $\boldsymbol{c} \in \mathbb{R}^m$ and $\boldsymbol{c'} \in \mathbb{R}^{m'}$ consist of coefficients c_i and c'_j, respectively. Thus, definition (4.3) gives

$$\hat{\epsilon}(E, E') = \max_{\boldsymbol{c}^T G \boldsymbol{c}=1} \max_{(\boldsymbol{c'})^T H \boldsymbol{c'}=1} \boldsymbol{c}^T F \boldsymbol{c'} = \max_{\boldsymbol{c}^T G \boldsymbol{c}=1} \max_{|\tilde{\boldsymbol{c}}'|=1} \boldsymbol{c}^T F L^{-T} \tilde{\boldsymbol{c}}' = \max_{\boldsymbol{c}^T G \boldsymbol{c}=1} |\boldsymbol{c}^T F L^{-T}|,$$

where $\tilde{\boldsymbol{c}}' = L^T \boldsymbol{c'}$, $H = LL^T$ is the Cholesky decomposition of matrix H, and $|\cdot|$ stands for the Euclidean norm. Consequently,

$$\hat{\epsilon}^2(E, E') = \max_{0\neq \boldsymbol{c}\in\mathbb{R}^m} \frac{\boldsymbol{c}^T F L^{-T} L^{-1} F^T \boldsymbol{c}}{\boldsymbol{c}^T G \boldsymbol{c}} = \lambda_{max}(F H^{-1} F^T, G).$$

Expression $\hat{\epsilon}^2(E, E') = \lambda_{max}(F^T G^{-1} F, H)$ can be proved analogously.

To prove the upper bound on $\hat{\epsilon}$, we use decomposition $G = QQ^T$. Noticing that $\|A\|_2 = \|A^T\|_2 = \sqrt{\|A^T A\|_2}$ holds for a general matrix A, we have

$$\lambda_{max}(FH^{-1}F^T, G) = \|Q^{-1}FH^{-1}F^TQ^{-T}\|_2 \le \|G^{-1}\|_2 \|H^{-1}\|_2 \|F^TF\|_2.$$

Finally, we estimate $\|G^{-1}\|_2$ and $\|H^{-1}\|_2$. If $\eta_G < 1$, then

$$\|G^{-1}\|_2 = \frac{1}{\lambda_{min}(G)} = \frac{1}{1 - \lambda_{max}(I - G)} \le \frac{1}{1 - \|I - G\|_2} \le \frac{1}{1 - \eta_G}.$$

With the same argument for H^{-1}, we easily draw the conclusion. □

Remark 4.2. Matrices F, G, and H are available in practical computations and $\lambda_{max}(F^T G^{-1} F, H)$ as well as $\lambda_{max}(FH^{-1}F^T, G)$ can be computed. Alternatively, guaranteed estimates η_F, η_H, and η_G can be obtained by the Gershgorin circle theorem. These estimates are expected to be good for $\hat{\epsilon}(\widehat{E}_k, \widehat{E}_{k'})$ with $k \neq k'$, because if the approximate eigenfunctions in $\widehat{E}_k$ and the ones in $\widehat{E}_{k'}$ are appropriately orthonormalized, then $F^TF \approx 0$, $G \approx I_m$, and $H \approx I_{m'}$.

The following theorem provides the desired estimate of the directed distance $\Delta(E_K, \widehat{E}_K)$ defined in (4.1).

Theorem 4.3. *Let the above specified partition of the spectrum into K clusters be arbitrary. Let $\hat{u}_i \in H_0^1(\Omega)$, $i = 1, 2, \ldots, N$, be such that* $\dim \widehat{E}_k = N_k - n_k + 1$ *for all $k = 1, 2, \ldots, K$. Let $\lambda_n < \rho \le \lambda_{N+1}$. Then*

$$\Delta^2(E_K, \widehat{E}_K) \le \frac{\rho(\hat{\lambda}_N^{(K)} - \lambda_n) + \lambda_n \hat{\lambda}_N^{(K)} \vartheta^{(K)}}{\hat{\lambda}_N^{(K)}(\rho - \lambda_n)} \tag{4.4}$$

where

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

Proof. Let $\hat{u} \in \widehat{E}_K$, $\|\nabla \hat{u}\| = 1$, be arbitrary and fixed. The proof is based on estimates of $\|\nabla P_k \hat{u}\|$ for all $k = 1, 2, \ldots, K$, where energy projectors $P_k : H_0^1(\Omega) \to E_k$ are defined by

$$\langle \hat{u} - P_k \hat{u}, v \rangle = 0 \quad \forall v \in E_k.$$

Using eigenfunctions $w_i = u_i/\|\nabla u_i\|$ normalized in the energy norm, these energy projections clearly satisfy identities

$$P_k\hat{u} = \sum_{i=n_k}^{N_k} \langle \hat{u}, w_i\rangle w_i,\ \ \|\nabla P_k\hat{u}\|^2 = \sum_{i=n_k}^{N_k} \langle \hat{u}, w_i\rangle^2,\ \ \|P_k\hat{u}\|^2 = \sum_{i=n_k}^{N_k} \frac{1}{\lambda_i}\langle \hat{u}, w_i\rangle^2. \tag{4.5}$$

The first step is to bound $\|\nabla P_k\hat{u}\|$ for $k = 1, 2, \ldots, K-1$. Introduce $z_k = P_k\hat{u}/\|\nabla P_k\hat{u}\| \in E_k$ and the energy projector $\widehat{P}_k : H_0^1(\Omega) \to \widehat{E}_k$ that maps z_k to $\widehat{P}_k z_k \in \widehat{E}_k$. Since $P_k\hat{u} = \langle \hat{u}, z_k\rangle z_k$ and $\|\nabla \widehat{P}_k z_k\| \le \|\nabla z_k\| = 1$, definition (4.2) and relation (2.3) imply

$$|\langle \hat{u}, \widehat{P}_k z_k\rangle| \le \hat{\zeta}(\widehat{E}_k, \widehat{E}_K) \quad \text{and} \quad \|\nabla(z_k - \widehat{P}_k z_k)\| \le \Delta(E_k, \widehat{E}_k).$$

These estimates then provide the bound

$$\|\nabla P_k\hat{u}\| = |\langle \hat{u}, z_k\rangle| \le |\langle \hat{u}, \widehat{P}_k z_k\rangle| + |\langle \hat{u}, z_k - \widehat{P}_k z_k\rangle| \le \hat{\zeta}(\widehat{E}_k, \widehat{E}_K) + \Delta(E_k, \widehat{E}_k). \tag{4.6}$$

The second step is to estimate $\|\nabla P_K\hat{u}\|$ from below. Using $(\hat{u}, u_i)^2 = \langle \hat{u}, w_i\rangle^2/\lambda_i$ in (3.2) and (3.3), we derive identity

$$\rho\|\hat{u}\|^2 - \|\nabla\hat{u}\|^2 = \sum_{i=1}^{\infty}\Big(\frac{\rho}{\lambda_i} - 1\Big)\langle \hat{u}, w_i\rangle^2 = \vartheta(\hat{u}) + \sum_{i=n}^{\infty}\Big(\frac{\rho}{\lambda_i} - 1\Big)\langle \hat{u}, w_i\rangle^2, \tag{4.7}$$

where

$$\vartheta(\hat{u}) = \sum_{i=1}^{n-1}\Big(\frac{\rho}{\lambda_i} - 1\Big)\langle \hat{u}, w_i\rangle^2 = \sum_{k=1}^{K-1}\sum_{i=n_k}^{N_k}\Big(\frac{\rho}{\lambda_i} - 1\Big)\langle \hat{u}, w_i\rangle^2. \tag{4.8}$$

Since $\lambda_n \le \lambda_i$ for $i = n, \ldots, N$ and $\rho \le \lambda_i$ for $i = N+1, N+2, \ldots$, identity (4.7) yields estimate

$$\begin{aligned}\rho\|\hat{u}\|^2 - \|\nabla\hat{u}\|^2 - \vartheta(\hat{u}) &= \sum_{i=n}^{\infty}\left(\frac{\rho}{\lambda_i} - 1\right)\langle \hat{u}, w_i\rangle^2 \\ &\le \left(\frac{\rho}{\lambda_n} - 1\right)\sum_{i=n}^{N}\langle \hat{u}, w_i\rangle^2 = \left(\frac{\rho}{\lambda_n} - 1\right)\|\nabla P_K\hat{u}\|^2. \end{aligned} \tag{4.9}$$

It remains to bound $\vartheta(\hat{u})$ from above. Using definition (4.8), the fact that $\lambda_{n_k} \le \lambda_i$ for $i = n_k, \dots, N_k$, and the second identity in (4.5), we obtain

$$\vartheta(\hat{u}) \le \sum_{k=1}^{K-1} \left(\frac{\rho}{\lambda_{n_k}} - 1 \right) \sum_{i=n_k}^{N_k} \langle \hat{u}, w_i \rangle^2 = \sum_{k=1}^{K-1} \left(\frac{\rho}{\lambda_{n_k}} - 1 \right) \|\nabla P_k \hat{u}\|^2.$$

Estimate (4.6) then yields

$$\vartheta(\hat{u}) \le \sum_{k=1}^{K-1} \left(\frac{\rho}{\lambda_{n_k}} - 1 \right) \left[\hat{\zeta}(\widehat{E}_k, \widehat{E}_K) + \Delta(E_k, \widehat{E}_k) \right]^2 = \vartheta^{(K)}. \tag{4.10}$$

The desired estimate of $\|\nabla P_K \hat{u}\|$ from below then follows from (4.9) and (4.10):

$$\|\nabla P_K \hat{u}\|^2 \ge \lambda_n \frac{\rho \|\hat{u}\|^2 - \|\nabla \hat{u}\|^2 - \vartheta^{(K)}}{\rho - \lambda_n}. \tag{4.11}$$

The final step is to express the directed distance $\Delta^2(\widehat{E}_K, E_K)$ using (2.4) as follows

$$\Delta^2(\widehat{E}_K, E_K) = 1 - \min_{\substack{\hat{u} \in \widehat{E}_K \\ \|\nabla \hat{u}\| = 1}} \max_{\substack{u \in E_K \\ \|\nabla u\| = 1}} \langle \hat{u}, u \rangle^2 = 1 - \min_{\substack{\hat{u} \in \widehat{E}_K \\ \|\nabla \hat{u}\| = 1}} \|\nabla P_K \hat{u}\|^2. \tag{4.12}$$

Estimate (4.11) and the definition of $\hat{\lambda}_N^{(K)}$ then provide the statement (4.4). Note that $\Delta(E_K, \widehat{E}_K) = \Delta(\widehat{E}_K, E_K)$, because $\dim E_K = \dim \widehat{E}_K = N - n + 1$. □

The quality of bound (4.4) depends on $\hat{\lambda}_N^{(K)} - \lambda_n$, $\rho - \lambda_n$, and $\vartheta^{(K)}$. Quantity $\hat{\lambda}_N^{(K)} - \lambda_n$ corresponds to the width of the last cluster, the difference $\rho - \lambda_n$ is determined by the spectral gap between the last cluster and the following eigenvalues, and the value of $\vartheta^{(K)}$ measures errors in all previous clusters. Notice that quantity $\vartheta^{(K)}$ depends on $\Delta(E_k, \widehat{E}_k)$, i.e., on errors in spaces of eigenfunctions for previous clusters, and on $\hat{\zeta}(\widehat{E}_k, \widehat{E}_K)$ which accounts for possible non-orthogonality of approximate eigenfunctions.

Approximations $\hat{u}_i \in H_0^1(\Omega)$ of eigenfunctions can be arbitrary. The only assumption is that the dimension of $\widehat{E}_k$ equals to the number of approximate eigenfunctions forming this space, i.e., that eigenfunctions forming $\widehat{E}_k$ are linearly independent. Consequently, the approximate eigenfunctions in Theorem 4.3 can be computed by arbitrary conforming numerical method. On

top of that result (4.4) estimates the total error, meaning that approximate eigenfunctions can be polluted by iteration, quadrature, round-off, and any other errors and the statement of Theorem 4.3 still applies as long as the approximate eigenfunctions are conforming in $H_0^1(\Omega)$ and linearly independent within each cluster.

Bound (4.4) is naturally computed iteratively starting from the first cluster. Accuracy of this procedure is illustrated on numerical examples below in Section 8.

5 Analogous estimate in the L^2 norm

While the previous section presents error bounds in the energy norm, this section derives analogous bounds in the $L^2(\Omega)$ norm. The directed distance between subspaces E and $\widehat{E}$ measured in the $L^2(\Omega)$ norm is given by (2.1) with $V = L^2(\Omega)$ and $\|v\|_V = \|v\|$. Hence, with a slight abuse of notation, we set

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

Analogously to (4.2), the non-orthogonality of subspaces $\widehat{E}_k$ and $\widehat{E}_K$ is measured in the $L^2(\Omega)$ inner product by the quantity

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

This quantity can be computed or bounded by using Lemma 4.1 with $E = \widehat{E}_k$, $E' = \widehat{E}_K$, $V = L^2(\Omega)$, and $(\cdot,\cdot)_V = (\cdot,\cdot)$. Similarly to Theorem 4.3 we formulate a bound on $\delta(E_K, \widehat{E}_K)$.

Theorem 5.1. *Consider an arbitrary partition of the spectrum into K clusters as in Theorem 4.3. Let $\hat{u}_i \in H_0^1(\Omega)$, $i = 1, 2, \ldots, N$, be such that $\dim \widehat{E}_k = N_k - n_k + 1$ for all $k = 1, 2, \ldots, K$. Let $\lambda_n < \rho \le \lambda_{N+1}$. Then*

$$\delta^2(E_K, \widehat{E}_K) \le \frac{\hat{\lambda}_N^{(K)} - \lambda_n + \theta^{(K)}}{\rho - \lambda_n}, \tag{5.1}$$

where

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

Proof. The proof is analogous to the proof of Theorem 4.3. Therefore, we only sketch the main steps. Consider $\hat{u} \in \widehat{E}_K$, $\|\hat{u}\| = 1$, and the $L^2(\Omega)$ orthogonal projector $\Pi_k : H_0^1(\Omega) \to E_k$. Similar to (4.5), we have

$$\Pi_k \hat{u} = \sum_{i=n_k}^{N_k} (\hat{u}, u_i) u_i, \quad \|\Pi_k \hat{u}\|^2 = \sum_{i=n_k}^{N_k} (\hat{u}, u_i)^2, \quad \|\nabla(\Pi_k \hat{u})\|^2 = \sum_{i=n_k}^{N_k} \lambda_i (\hat{u}, u_i)^2.$$

Analogous argument as for (4.6) yields

$$\|\Pi_k \hat{u}\| \leq \hat{\varepsilon}(\widehat{E}_k, \widehat{E}_K) + \delta(E_k, \widehat{E}_k).$$

Identities (3.2) and (3.3) imply

$$\rho\|\hat{u}\|^2 - \|\nabla \hat{u}\|^2 = \sum_{i=1}^{\infty} (\rho - \lambda_i)(\hat{u}, u_i)^2 = \theta(\hat{u}) + \sum_{i=n}^{\infty} (\rho - \lambda_i)(\hat{u}, u_i)^2, \tag{5.2}$$

where, cf. (4.7) and (4.8),

$$\theta(\hat{u}) = \sum_{k=1}^{K-1} \sum_{i=n_k}^{N_k} (\rho - \lambda_i)(\hat{u}, u_i)^2 \,.$$

Expressing $\theta(\hat{u})$ as in (4.8), we obtain a bound similar to (4.10):

$$\theta(\hat{u}) \leq \sum_{k=1}^{K-1} (\rho - \lambda_{n_k}) \|\Pi_k \hat{u}\|^2 \leq \theta^{(K)}. \tag{5.3}$$

Since $\rho \leq \lambda_{N+1}$, we have

$$\sum_{i=n}^{\infty} (\rho - \lambda_i)(\hat{u}, u_i)^2 \leq \sum_{i=n}^{N} (\rho - \lambda_i)(\hat{u}, u_i)^2 \leq (\rho - \lambda_n) \|\Pi_K \hat{u}\|^2. \tag{5.4}$$

Finally, a combination of (5.2), (5.3) and (5.4) provides the lower bound

$$\|\Pi_K \hat{u}\|^2 \geq \frac{\rho\|\hat{u}\|^2 - \|\nabla \hat{u}\|^2 - \theta^{(K)}}{\rho - \lambda_n} \geq \frac{\rho\|\hat{u}\|^2 - \hat{\lambda}_N^K - \theta^{(K)}}{\rho - \lambda_n}. \tag{5.5}$$

The directed distance $\delta(\widehat{E}_K, E_K)$ can be expressed analogously to (4.12) as

$$\delta^2(\widehat{E}_K, E_K) = 1 - \min_{\substack{\hat{u} \in \widehat{E}_K \\ \|\hat{u}\|=1}} \max_{\substack{u \in E_K \\ \|u\|=1}} (\hat{u}, u)^2 = 1 - \min_{\substack{\hat{u} \in \widehat{E}_K \\ \|\hat{u}\|=1}} \|\Pi_K \hat{u}\|^2$$

and the proof is finished by applying (5.5). □

Remark 5.2. Bound (5.1) is a direct and nontrivial generalization of [4, Corollary 1]. Indeed, if all eigenvalues are simple and well separated (forming clusters of size one) and the corresponding approximate eigenfunctions $\{\hat{u}_i\}$ are mutually orthogonal, then the bound (5.1) coincides with the estimate

$$(\lambda_{i+1} - \lambda_i)\sigma_i^2 \leq (\mu_i - \lambda_i) + \sum_{j=1}^{i-1}[\lambda_{i+1} - \lambda_j]\sigma_j^2 \quad \text{for } i = 1, 2, 3, \ldots,$$

where $\sigma_i = \sqrt{1 - (u_i, \hat{u}_i)^2}$, $\mu_i = \|\nabla \hat{u}_i\|^2 / \|\hat{u}_i\|^2$, and ρ was chosen as λ_{i+1}. This is exactly the statement of [4, Corollary 1].

However, bound (5.1) has a smaller rate of convergence than $\delta(\widehat{E}_K, E_K)$ for approximate eigenfunctions obtained by the finite element method; see examples in Section 8 for an illustration. Therefore, the following section derives optimal order estimates for the special case of finite element approximations. Note that in case $\lambda_N > \lambda_n$ bounds (4.4) and (5.1) do not converge to zero due to the difference $\hat{\lambda}_N^{(K)} - \lambda_n$. However, such clusters can be (theoretically) split into smaller clusters consisting of a single or a multiple eigenvalue and for these clusters bounds (4.4) and (5.1) do converge. Therefore, the notion of convergence is understood in this sense throughout the paper.

6 Optimal order estimate in L^2 norm for finite element eigenfunctions

Error estimates in the L^2 norm with the optimal speed of convergence can be achieved in the context of the finite element method by using Aubin–Nitsche technique, an idea from [5], and the explicitly known value of the constant in the *a priori* error estimate for the energy projection [26].

For simplicity, assume Ω to be a polytope. Consider the usual conforming simplicial mesh $\mathcal{T}_h$ in Ω and define the finite element space V_h of piece-wise polynomial and continuous functions over the mesh $\mathcal{T}_h$ satisfying the Dirichlet boundary conditions as

$$V_h = \{v_h \in H_0^1(\Omega) : v_h|_K \in \mathbb{P}_p(K) \text{ for all } K \in \mathcal{T}_h\},$$

where $\mathbb{P}_p(K)$ stands for the space of polynomials of degree at most p defined in K.

The finite element eigenvalue problem reads: find $\lambda_{h,i} \in \mathbb{R}$ and $u_{h,i} \in V_h \setminus \{0\}$ such that

$$(\nabla u_{h,i}, \nabla v_h) = \lambda_{h,i}(u_{h,i}, v_h) \quad \forall v_h \in V_h, \tag{6.1}$$

where $i = 1, 2, \ldots, \dim V_h$. Discrete eigenfunctions are assumed to be normalized such that $(u_{h,i}, u_{h,j}) = \delta_{ij}$ and $(\nabla u_{h,i}, \nabla u_{h,j}) = \lambda_{h,i}\delta_{ij}$.

Remark 6.1. Generally $u_{h,i}$ is not available in practical computation, because it is a result of a generalized matrix eigenvalue solver polluted typically by rounding errors and truncation errors of iterative algorithms. In principle, we can consider a general approximation $\hat{u}_i$ instead of $u_{h,i}$ in what follows and then estimate the difference $\hat{u}_i - u_{h,i}$ by applying results of Section 5. Such argument would make the paper lengthy and not easy to read. Therefore, the estimates in this sub-section remain as a theoretical analysis of the discretization error $u_{h,i} - u_i$.

We first recall several results about the *a priori* error estimates for finite element solutions of the Poisson equation. These *a priori* error estimates will play an important role in subsequent error bounds for eigenfunctions.

Given $f \in L^2(\Omega)$, let $u \in H_0^1(\Omega)$ be the weak solution of the Poisson problem satisfying

$$(\nabla u, \nabla v) = (f, v) \quad \forall v \in H_0^1(\Omega).$$

The corresponding Galerkin approximation $u_h \in V_h$ is determined by the identity

$$(\nabla u_h, \nabla v_h) = (f, v_h) \quad \forall v_h \in V_h.$$

The energy projector $P_h : H_0^1(\Omega) \to V_h$ is defined by equality $(\nabla u - \nabla P_h u, \nabla v_h) = 0$ for all $v_h \in V_h$. Clearly, $u_h = P_h u$.

In [26], Liu and Oishi proposed the following constructive *a priori* error estimate with a computable constant C_h:

$$\|\nabla(u - P_h u)\| \le C_h \|f\|, \quad \|u - P_h u\| \le C_h \|\nabla(u - P_h u)\| \le C_h^2 \|f\|. \tag{6.2}$$

In case of non-convex domains, the value of C_h can be computed by solving a dual saddle-point problem based on the hypercircle method; see [26, Sections 3.2–3.3]. In case of convex domains, the value of C_h can be easily computed by considering the Lagrange interpolation error constant; see [26, Theorem 3.1]. The specific value of C_h is provided below in Section 8 for the considered examples.

Let $\mathcal{C}(k) = \{n_k, n_k + 1, \ldots, N_k\}$ denote the set of indices of eigenvalues in the kth cluster and $\mathcal{C} = \{1, 2, \ldots, \dim V_h\}$ the set of all indices. The number of indices in $\mathcal{C}(k)$ is denoted by $|\mathcal{C}(k)| = N_k - n_k + 1$. The space of finite element eigenfunctions corresponding to the kth clusters is $E_{h,k} = \operatorname{span}\{u_{h,n_k}, u_{h,n_k+1}, \ldots, u_{h,N_k}\}$. The $L^2(\Omega)$ orthogonal projector from $L^2(\Omega)$ to $E_{h,k}$ is denoted by $\Pi_{h,k}$.

The quantity

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

to appear in Lemma 6.2 extends the one in [5, pages 53, 57] and has its origin in [31]. The following result bounds the error of the $L^2(\Omega)$ orthogonal projection $\Pi_{h,k} : H_0^1(\Omega) \to E_{h,k}$ by the error of the energy projection $P_h : H_0^1(\Omega) \to V_h$.

Lemma 6.2. *Consider an arbitrary partition of the spectrum into K clusters as described above. Then the estimate*

$$\max_{\substack{u \in E_k \\ \|u\|=1}} \|u - \Pi_{h,k} u\| \leq \left(1 + \tau_k \sqrt{|\mathcal{C}(k)|}\right) \max_{\substack{u \in E_k \\ \|u\|=1}} \|u - P_h u\| \tag{6.3}$$

holds for all clusters $k = 1, 2, \ldots, K$.

Proof. Since the orthogonal projection $\Pi_{h,k} u$ is the closest element in $E_{h,k}$ to u and due to the triangle inequality, we have

$$\|u - \Pi_{h,k} u\| \leq \|u - \Pi_{h,k} P_h u\| \leq \|u - P_h u\| + \|P_h u - \Pi_{h,k} P_h u\|. \tag{6.4}$$

First, let us consider a single eigenfunction $u_j \in E_k$. Notice that the equality

$$P_h u_j - \Pi_{h,k} P_h u_j = \sum_{i \in \mathcal{C} \setminus \mathcal{C}(k)} (P_h u_j, u_{h,i}) u_{h,i} \in V_h,$$

leads to

$$\|(I - \Pi_{h,k}) P_h u_j\|^2 = \sum_{i \in \mathcal{C} \setminus \mathcal{C}(k)} (P_h u_j, u_{h,i})^2 \,. \tag{6.5}$$

In equality

$$\lambda_{h,i}(P_h u_j, u_{h,i}) = (\nabla P_h u_j, \nabla u_{h,i}) = (\nabla u_j, \nabla u_{h,i}) = \lambda_j (u_j, u_{h,i}),$$

we subtract $\lambda_j(P_h u_j, u_{h,i})$ on both sides and obtain

$$(P_h u_j, u_{h,i}) = \frac{\lambda_j}{(\lambda_{h,i} - \lambda_j)}(u_j - P_h u_j, u_{h,i}).$$

Summation over $i \notin \mathcal{C}(k)$ gives

$$\sum_{i \in \mathcal{C} \setminus \mathcal{C}(k)} (P_h u_j, u_{h,i})^2 \leq \tau_k^2 \sum_{i \in \mathcal{C} \setminus \mathcal{C}(k)} (u_j - P_h u_j, u_{h,i})^2 \leq \tau_k^2 \|u_j - P_h u_j\|^2,$$

where the last inequality follows form the identity $\sum_{i \in \mathcal{C}} (u_j - P_h u_j, u_{h,i})^2 = \|\pi_h(u_j - P_h u_j)\|^2$ with $\pi_h : H_0^1(\Omega) \to V_h$ denoting the $L^2(\Omega)$ orthogonal projector. Using this in (6.5), we finally derive

$$\|(I - \Pi_{h,k}) P_h u_j\| \leq \tau_k \|(I - P_h) u_j\|. \tag{6.6}$$

Second, let us consider a general $u = \sum_{j \in \mathcal{C}(k)} c_j u_j \in E_k$ with $\|u\| = 1$. Clearly, $\sum_{j \in \mathcal{C}(k)} c_j^2 = 1$. Denoting the linear operator $(I - \Pi_{h,k}) P_h$ by L, the estimate (6.6) leads to

$$\|Lu\|^2 = \left\| \sum_{j \in \mathcal{C}(k)} c_j L u_j \right\|^2 \leq \sum_{j \in \mathcal{C}(k)} \|L u_j\|^2 \leq \tau_k^2 \sum_{j \in \mathcal{C}(k)} \|(I - P_h) u_j\|^2.$$

Thus, we can estimate $\|(I - \Pi_{h,k}) P_h u\|$ as

$$\|(I - \Pi_{h,k}) P_h u\| \leq \tau_k \sqrt{|\mathcal{C}(k)|} \max_{\substack{u \in E_k \\ \|u\| = 1}} \|u - P_h u\|. \tag{6.7}$$

Statement (6.3) then easily follows from (6.4) and (6.7). □

Now, we formulate and prove the main result of this section.

Theorem 6.3. *The following estimate*

$$\delta(E_k, E_{h,k}) \leq \sqrt{\lambda_{N_k}} C_h \left(1 + \tau_k \sqrt{|\mathcal{C}(k)|}\right) \Delta(E_k, E_{h,k}) \tag{6.8}$$

holds for all $k = 1, 2, \ldots, K$.

Proof. Consider the energy orthogonal projector $P_{h,k} : H_0^1(\Omega) \to E_{h,k}$. For $u \in E_k$, $\|\nabla u\| = 1$, expression (2.3) implies

$$\|\nabla(u - P_{h,k}u)\| \leq \Delta(E_k, E_{h,k}).$$

The *a priori* error estimate (6.2) and the fact that $P_h u$ is the closest element to u in V_h yield

$$\|u - P_h u\| \leq C_h \|\nabla(u - P_h u)\| \leq C_h \|\nabla(u - P_{h,k}u)\| \leq C_h \Delta(E_k, E_{h,k}). \quad (6.9)$$

Identity (2.3) and bound (6.3) give

$$\delta(E_k, E_{h,k}) = \max_{\substack{u \in E_k \\ \|u\|=1}} \|u - \Pi_{h,k}u\| \leq (1 + \tau_k \sqrt{|\mathcal{C}(k)|}) \max_{\substack{u \in E_k \\ \|u\|=1}} \|u - P_h u\|. \quad (6.10)$$

Since inequality $\|\nabla u\|/\|u\| \leq \sqrt{\lambda_{N_k}}$ holds for all $u \in E_k$, we easily obtain bound

$$\max_{\substack{u \in E_k \\ \|u\|=1}} \|u - P_h u\| = \max_{\substack{u \in E_k \\ \|\nabla u\|=1}} \frac{1}{\|u\|} \|u - P_h u\| \leq \sqrt{\lambda_{N_k}} \max_{\substack{u \in E_k \\ \|\nabla u\|=1}} \|u - P_h u\|. \quad (6.11)$$

Combination of (6.10), (6.11), and (6.9) finishes the proof.

□

7 Sharp energy norm estimates based on L^2 bounds

This section provides an estimate of the energy distance Δ by utilizing the L^2 distance δ. The idea is motivated by the following well known formula (see e.g. [5, page 55])

$$\|\nabla(u_i - u_{h,i})\|^2 = \lambda_i \|u_i - u_{h,i}\|^2 - (\lambda_i - \lambda_{h,i}).$$

This identity essentially tells that the error $\|\nabla(u_i - u_{h,i})\|$ is dominated by the error of the approximate eigenvalue itself, because the term $\|u_i - u_{h,i}\|$ has a higher order of convergence.

The following estimate is theoretically independent of the partition of eigenvalues into clusters, but its natural usage is to bound $\Delta(E_k, \widehat{E}_k)$ by $\delta(E_k, \widehat{E}_k)$, where k is the index of a cluster as it is introduced at the end of Section 3.

Theorem 7.1. *Let $u_n, \dots, u_N$ be the exact eigenfunctions of (3.1) and $0 < n \le N$ the corresponding indices. Let $\hat{u}_n, \dots, \hat{u}_N \in H_0^1(\Omega)$ be linearly independent. Let $E = \operatorname{span}\{u_n, \dots, u_N\}$ and $\widehat{E} = \operatorname{span}\{\hat{u}_n, \dots, \hat{u}_N\}$. Then*

$$\Delta^2(E, \widehat{E}) \le 2 - 2\lambda_n \left(\frac{1 - \delta^2(E, \widehat{E})}{\lambda_N \hat{\lambda}_N} \right)^{1/2} \tag{7.1}$$

where λ_n and λ_N are exact eigenfunctions corresponding to u_n and u_N and

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

Proof. Consider the linear mapping $\tau : E \to E$ defined by

$$\tau(u) = \sum_{i=n}^{N} c_i \lambda_i u_i, \quad \text{where } u = \sum_{i=n}^{N} c_i u_i.$$

Since $\lambda_i > 0$ for all $i = n, \dots, N$, τ is a bijection. Given arbitrary $u \in E$ and $\hat{u} \in \widehat{E}$, we clearly have

$$(\nabla u, \nabla \hat{u}) = \sum_{i=n}^{N} c_i (\nabla u_i, \nabla \hat{u}) = \sum_{i=n}^{N} c_i \lambda_i (u_i, \hat{u}) = (\tau(u), \hat{u}).$$

This enables us to estimate the distance between E and $\widehat{E}$ as follows

$$\begin{aligned} \Delta^2(E, \widehat{E}) &= \max_{\substack{u \in E \\ \|\nabla u\| = 1}} \min_{\hat{u} \in \widehat{E}} \|\nabla u - \nabla \hat{u}\|^2 \le \max_{\substack{u \in E \\ \|\nabla u\| = 1}} \min_{\substack{\hat{u} \in \widehat{E} \\ \|\nabla \hat{u}\| = 1}} \|\nabla u - \nabla \hat{u}\|^2 \\ &= \max_{\substack{u \in E \\ \|\nabla u\| = 1}} \min_{\substack{\hat{u} \in \widehat{E} \\ \|\nabla \hat{u}\| = 1}} \left[2 - 2\left(\tau(u), \hat{u}\right) \right] \le 2 - 2\lambda_n \min_{\substack{u \in E \\ \|\nabla u\| = 1}} \max_{\substack{\hat{u} \in \widehat{E} \\ \|\nabla \hat{u}\| = 1}} \left(\frac{\tau(u)}{\|\nabla \tau(u)\|}, \hat{u} \right), \end{aligned} \tag{7.2}$$

where the last inequality follows from the fact that

$$\|\nabla \tau(u)\|^2 = \sum_{i=n}^{N} \lambda_i^3 c_i^2 \ge \lambda_n^2 \sum_{i=n}^{N} \lambda_i c_i^2 = \lambda_n^2 \|\nabla u\|^2 = \lambda_n^2 \quad \forall u \in E,\ \|\nabla u\| = 1.$$

Since τ is a bijection, it is easy to show that

$$\left\{ \frac{\tau(u)}{\|\nabla \tau(u)\|} : u \in E,\ \|\nabla u\| = 1 \right\} = \left\{ u \in E : \|\nabla u\| = 1 \right\}.$$

This equality together with bounds $\|\nabla u\|^2 \le \lambda_N \|u\|^2$ for all $u \in E$ and $\|\nabla \hat{u}\|^2 \le \hat{\lambda}_N \|\hat{u}\|^2$ for all $\hat{u} \in \widehat{E}$ imply

$$\min_{\substack{u\in E\\ \|\nabla u\|=1}} \max_{\substack{\hat{u}\in\widehat{E}\\ \|\nabla\hat{u}\|=1}} \left(\frac{\tau(u)}{\|\nabla\tau(u)\|}, \hat{u}\right) = \min_{\substack{u\in E\\ \|\nabla u\|=1}} \max_{\substack{\hat{u}\in\widehat{E}\\ \|\nabla\hat{u}\|=1}} (u,\hat{u})$$

$$= \min_{\substack{u\in E\\ u\neq 0}} \max_{\substack{\hat{u}\in\widehat{E}\\ \hat{u}\neq 0}} \left(\frac{u}{\|\nabla u\|}, \frac{\hat{u}}{\|\nabla\hat{u}\|}\right) = \min_{\substack{u\in E\\ \|u\|=1}} \max_{\substack{\hat{u}\in\widehat{E}\\ \|\hat{u}\|=1}} \left(\frac{u}{\|\nabla u\|}, \frac{\hat{u}}{\|\nabla\hat{u}\|}\right)$$

$$\ge \frac{1}{\left(\lambda_N\hat{\lambda}_N\right)^{1/2}} \min_{\substack{u\in E\\ \|u\|=1}} \max_{\substack{\hat{u}\in\widehat{E}\\ \|\hat{u}\|=1}} (u,\hat{u}) = \left(\frac{1-\delta^2(E,\widehat{E})}{\lambda_N\hat{\lambda}_N}\right)^{1/2}, \quad (7.3)$$

where we note that $\max_{\hat{u}\in\widehat{E},\ \|\hat{u}\|=1}(u,\hat{u})$ is non-negative and the last equality follows from (2.4). The proof is finished by substituting (7.3) to (7.2). □

Let us mention that in the context of the finite element method, the directed distance $\delta(E,\widehat{E})$ measured in the $L^2(\Omega)$ sense is of higher order than the directed distance $\Delta(E,\widehat{E})$ measured in the energy sense. Therefore, the influence of $\delta(E,\widehat{E})$ is negligible for sufficiently fine meshes and the accuracy of the bound (7.1) is then dominated by the width of the cluster, i.e. $\hat{\lambda}_N - \lambda_n$, and by the error of the approximate eigenvalue, i.e. $\hat{\lambda}_N - \lambda_N$. For this reason the bound (7.1) has the potential to be of high accuracy.

In numerical examples below, we first compute the bound (4.4) on $\Delta(E_K,\widehat{E}_K)$ and use it in (6.8) to estimate $\delta(E_K,\widehat{E}_K)$. This estimate is then substituted to (7.1) to obtain a new bound on $\Delta(E_K,\widehat{E}_K)$. As soon as the new bound improves the original one, estimates (6.8) and (7.1) can be iterated. The accuracy of this approach is illustrated on numerical examples in Section 8.

Remark 7.2. A similar bound as (7.1) can be obtained for the quantity

$$\widetilde{\Delta}(E,\widehat{E}) = \max_{\substack{u\in E\\ \|u\|=1}} \min_{\hat{u}\in\widehat{E}} \|\nabla(u-\hat{u})\|^2.$$

Note that this quantity is not the directed distance (2.1), because the distance between u and $\hat{u}$ is measured by the energy norm, while functions u are normalized in the $L^2(\Omega)$ norm. Under the assumptions of Theorem 7.1 and using the same steps as in its proof, we can derive bound

$$\widetilde{\Delta}(E,\widehat{E}) \le \lambda_N + \hat{\lambda}_N - 2\lambda_n\sqrt{1-\delta^2(E,\widehat{E})}.$$

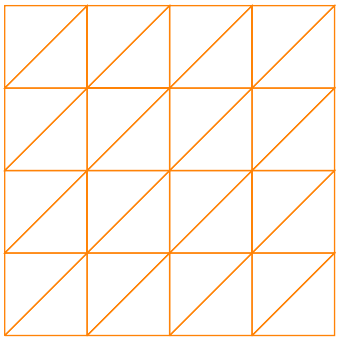

Figure 2: The uniform mesh in the unit square with mesh size $h = 1/4$.

Cluster	Eigenvalues
1	$\lambda_1 = 2\pi^2$
2	$\lambda_2 = \lambda_3 = 5\pi^2$
3	$\lambda_4 = 8\pi^2$
4	$\lambda_5 = \lambda_6 = 10\pi^2$

Table 1: The four leading clusters for the square.

Remark 7.3. Theorem 8.1 of [5] proves the estimate

$$\Delta(\widehat{E}_K, E_K) \leq C(K) \sup_{v \in E_1 \cup \cdots \cup E_K, \|v\|=1} \|\nabla(v - P_h v)\|,$$

where we use the notation of the current paper. Although the explicit bound on $\Delta(\widehat{E}_K, E_K)$ is not given in [5], we believe that using the constant C_h from (6.2), we can provide an explicit bound on $C(K)$ and $\|\nabla(v - P_h v)\|$ and, thus, an estimate for $\Delta(\widehat{E}_K, E_K)$. In our future work, we will derive this estimate and compare it with bounds derived in the current paper.

8 Numerical examples

This section numerically illustrates the accuracy of proposed bounds on the directed distances of spaces of exact and approximate eigenfunctions. The first example is the Laplace eigenvalue problem (1.1) in a square, where the exact solution is known. The second example is the same problem considered

in a dumbbell shaped domain. This domain is not convex, eigenfunctions have singularities, and eigenvalues form tight clusters.

Both examples are computed in the floating point arithmetic and the influence of rounding errors is not taken into account. However, if needed, mathematically rigorous estimates could be obtained by employing the interval arithmetic [30].

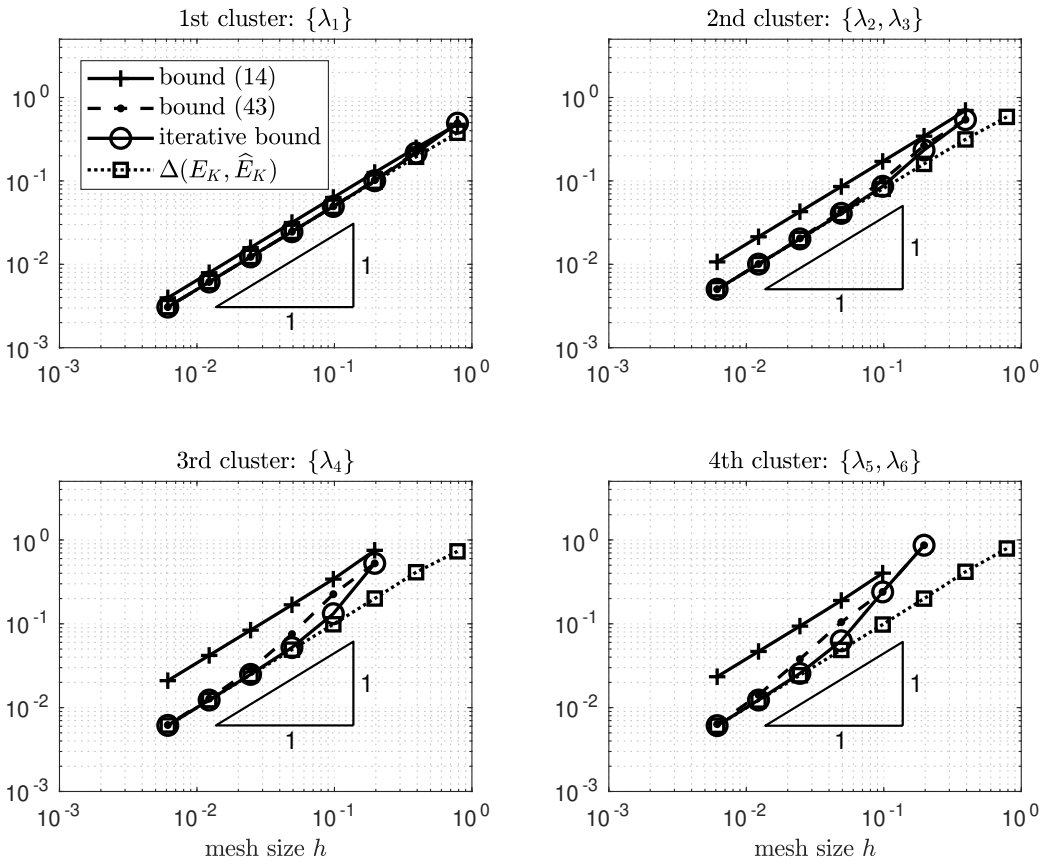

Figure 3: Bounds on the error of spaces of eigenfunctions in the energy norm for the square domain and the first four clusters. The exact value of $\Delta(E_K, \widehat{E}_K)$ for $K = 1, 2, 3, 4$ is plotted by the dotted line.

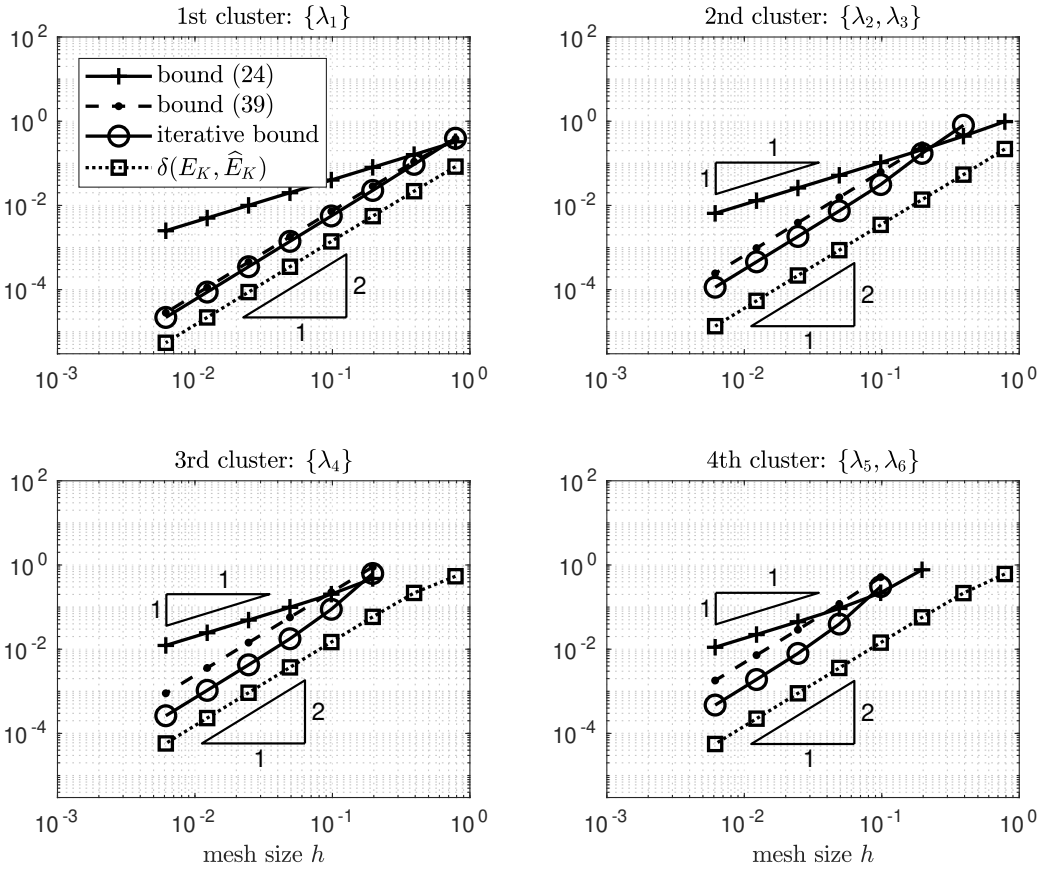

Figure 4: Bounds on the error of spaces of eigenfunctions in the L^2 norm for the square domain and the first four clusters. The exact value of $\delta(E_K, \widehat{E}_K)$ for $K = 1, 2, 3, 4$ is plotted by the dotted line.

8.1 The unit square domain

Consider the Laplace eigenvalue problem (1.1) in the unit square $\Omega = (0, 1)^2$. The exact eigenpairs are known analytically to be

$$\lambda_{ij} = (i^2 + j^2)\pi^2, \quad u_{ij} = \sin(i\pi x)\sin(j\pi y), \quad i, j = 1, 2, 3, \ldots.$$

These eigenvalues are either simple or double and we clustered them according to the multiplicity. The first four clusters are listed in Table 1. Since the exact eigenvalues are known, we do not need to compute their two-sided bounds and evaluate error bounds (4.4), (5.1), (6.8), and (7.1) using the analytically known eigenvalues.

This problem is solved by the finite element method (6.1) of the first order ($p = 1$). The finite element mesh $\mathcal{T}_h$ is chosen as the uniform triangulation consisting of isosceles right triangles; see Figure 2. For this mesh, the explicit value of C_h in the *a priori* error estimates (6.2) is known to be $C_h = 0.493h$ for conforming piece-wise linear finite elements [20, 25]. Here, h denotes the length of the leg of right triangles in the mesh $\mathcal{T}_h$. Note that explicit values of C_h are also available for non-uniform triangulations of general convex domains [20, 25] and for quadratic finite elements [27].

The quantity ρ needed to evaluate bounds (4.4) and (5.1) is chosen as $\rho = \lambda_{N+1}$, where we take advantage of the knowledge of exact eigenvalues. If the exact eigenvalues are not known, their two-sided bounds have to be employed as we show in the subsequent example.

In general, the computed eigenfunctions $\hat{u}_i$ differ from the exact Galerkin approximations $u_{h,i}$ given by (6.1) due to rounding errors and errors in the solver of the generalized matrix eigenvalue problem. However, for the purpose of this numerical illustration, we ignore this difference and evaluate bounds (6.8) and consequently (7.1) as if $\hat{u}_i = u_{h,i}$.

For each cluster $K = 1, 2, 3, 4$, we compute the following estimates:

(i) bound (4.4) on $\Delta(E_K, \widehat{E}_K)$;

(ii) the analogous bound (5.1) on $\delta(E_K, \widehat{E}_K)$;

(iii) the optimal order bound (6.8) on $\delta(E_K, \widehat{E}_K)$ using $\Delta(E_K, \widehat{E}_K)$;

(iv) the sharp bound (7.1) on $\Delta(E_K, \widehat{E}_K)$ using the smallest available value of $\delta(E_K, \widehat{E}_K)$;

(v) the improved bounds by repeating steps (iii) and (iv) five times using the best bounds on $\Delta(E_K, \widehat{E}_K)$ and $\delta(E_K, \widehat{E}_K)$ available.

Figure 3 presents the results for the directed distance measured in the energy norm. It compares bounds (i), (iv), and (v) with the exact directed distance $\Delta(E_K, \widehat{E}_K)$ for the first four clusters on a sequence of uniformly refined meshes. The results confirm the optimal convergence rate of the bound (4.4) and show high accuracy of the iteratively improved bounds on sufficiently fine meshes. Figure 4 presents similar results for the L^2 norm, in particular bounds (ii), (iii), and (v). The suboptimal convergence rate of (5.1) and the optimal rate of (6.8) and the iteratively improved bound are observed.

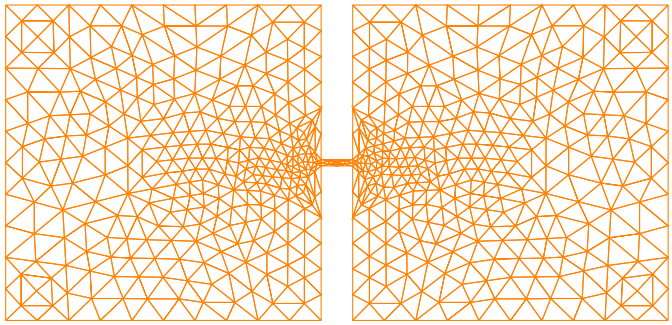

Figure 5: Dumbbell-shaped domain and the initial mesh

Cluster	lower and upper bounds
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	$\lambda_9 = 98.6^{71154}_{69041},\ \lambda_{10} = 98.6^{71154}_{69041},\ \lambda_{11} = 98.69604^{41}_{39},\ \lambda_{12} = 98.69604^{41}_{39}$

Table 2: Lower and upper bounds of eigenvalues for the dumbbell shaped domain. Two times refined initial mesh and third order finite element spaces were used.

8.2 The 2D dumbbell shaped domain

In this example, we again consider the Laplace eigenvalue problem (1.1), but now in a dumbbell shaped domain consisting of two unit squares connected by a bar of width 0.02 and length 0.1, see Figure 5, where also the initial mesh is depicted.

The exact solution of this eigenvalue problem is not known, but the eigenvalues are expected to be close to eigenvalues for a union of two squares, i.e., two eigenvalues close to $2\pi^2 \approx 19.739$, four eigenvalues close to $5\pi^2 \approx 49.348$, etc. In order to compute high precision two-sided bounds for these eigenvalues, we combine the Crouzeix–Raviart nonconforming finite elements and the Lehmann–Goerisch method as proposed in [24]. The resulting two-sided

bounds obtained on a fine mesh and finite element spaces of the third order are presented in Table 2.

Table 2 also shows the chosen division of the first twelve eigenvalues into four clusters. Note that eigenvalues λ_3 and λ_4 are strictly separated from λ_5 and λ_6. Therefore, they could be considered as two separate clusters, but then the spectral gap between them would be small and the factor $\rho - \lambda_n$ in (4.4) and (5.1) would yield large overestimation. For this reason, all four eigenvalues $\lambda_3, \ldots, \lambda_6$ are considered in one cluster.

The value of C_h in (6.2) is computed for the mesh depicted in Figure 5 and for its five successive uniform refinements by using the method from [26]. The obtained values are presented in Table 3.

Refinement times	0	1	2	3	4	5
C_h	0.0419	0.0233	0.0118	0.00588	0.00290	0.00155

Table 3: Values of C_h for the dumbbell shaped domain and linear conforming finite elements. The first row indicates the number of uniform mesh refinements of the initial mesh shown in Figure 5.

We compute the bounds on $\Delta(E_K, \widehat{E}_K)$ and $\delta(E_K, \widehat{E}_K)$ for the four clusters $K = 1, 2, 3, 4$ as we did for the square domain. Figure 6 presents the bound (4.4), (7.1), and the iteratively improved bound for the energy norm. The first and the third cluster are very tight and we observe the first order convergence. However, the convergence curves for the second and the fourth cluster bend due to the larger width of these clusters. Figure 7 shows the bound (5.1), (6.8), and its iterative improvement for the L^2 norm. The second order convergence of bound (6.8) and the first order convergence of (5.1) and of the iteratively improved bound are observed.

9 Conclusions

The derived *a posteriori* error estimates provide guaranteed upper bounds on the directed distance between spaces of exact and approximate eigenfunctions in both energy and $L^2(\Omega)$ sense. The approximate eigenfunctions can be arbitrary and estimates of their total error are easily computed by using solely the two-sided bounds on exact eigenvalues and the approximate eigenfunctions themselves. Numerical examples confirm that the estimate of the energy distance Δ converges with the optimal rate. The analogous estimate

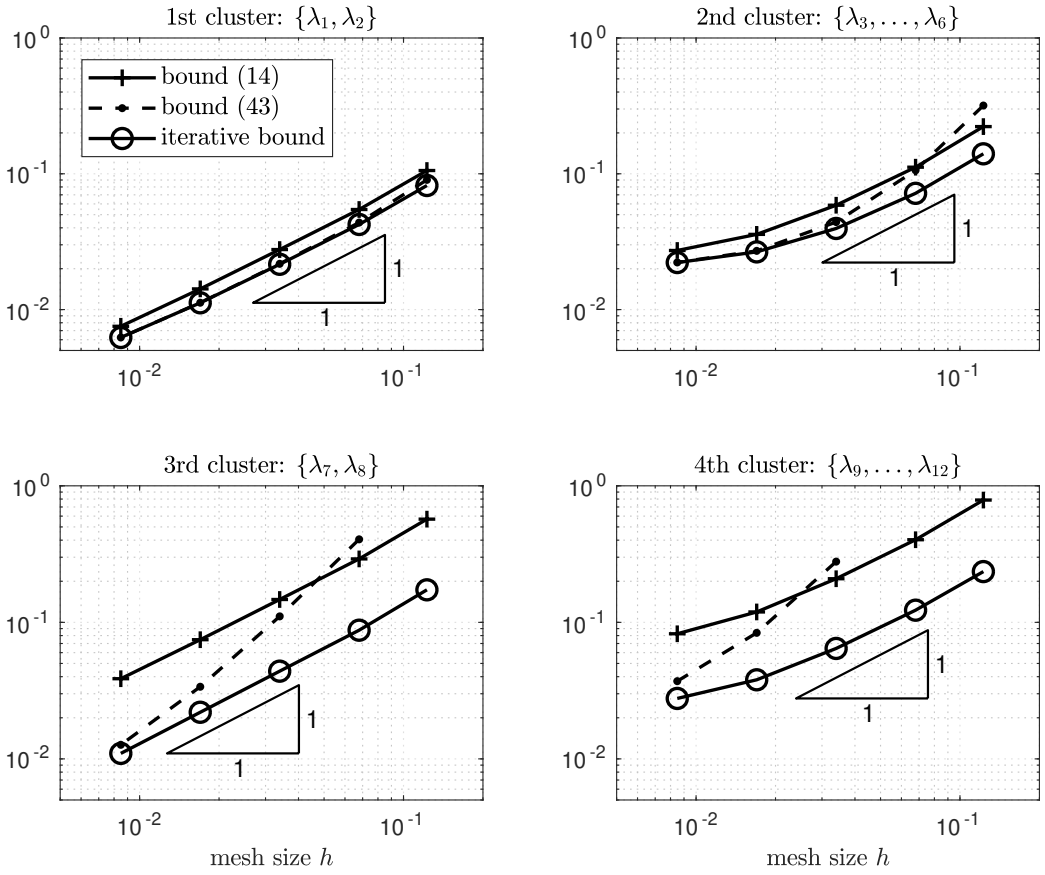

Figure 6: Bounds on the error of spaces of eigenfunctions in the energy norm for the dumbbell shaped domain.

of the $L^2(\Omega)$ distance δ converges with the same rate as Δ, which is suboptimal. For exact finite element eigenfunctions, an optimal order bound on the $L^2(\Omega)$ distance δ is derived by employing the Aubin–Nitsche technique and the explicitly known value of the constant in the *a priori* error estimate for the energy projection.

Further, the bound on the $L^2(\Omega)$ distance δ can be used to improve the bound on the energy distance Δ. The improved Δ can be used to compute improved δ leading to a simple iterative process. This process proved to be efficient in the considered numerical examples, where highly accurate bounds were computed for considered clusters on sufficiently fine meshes.

In the case of eigenfunctions corresponding to simple eigenvalues, there

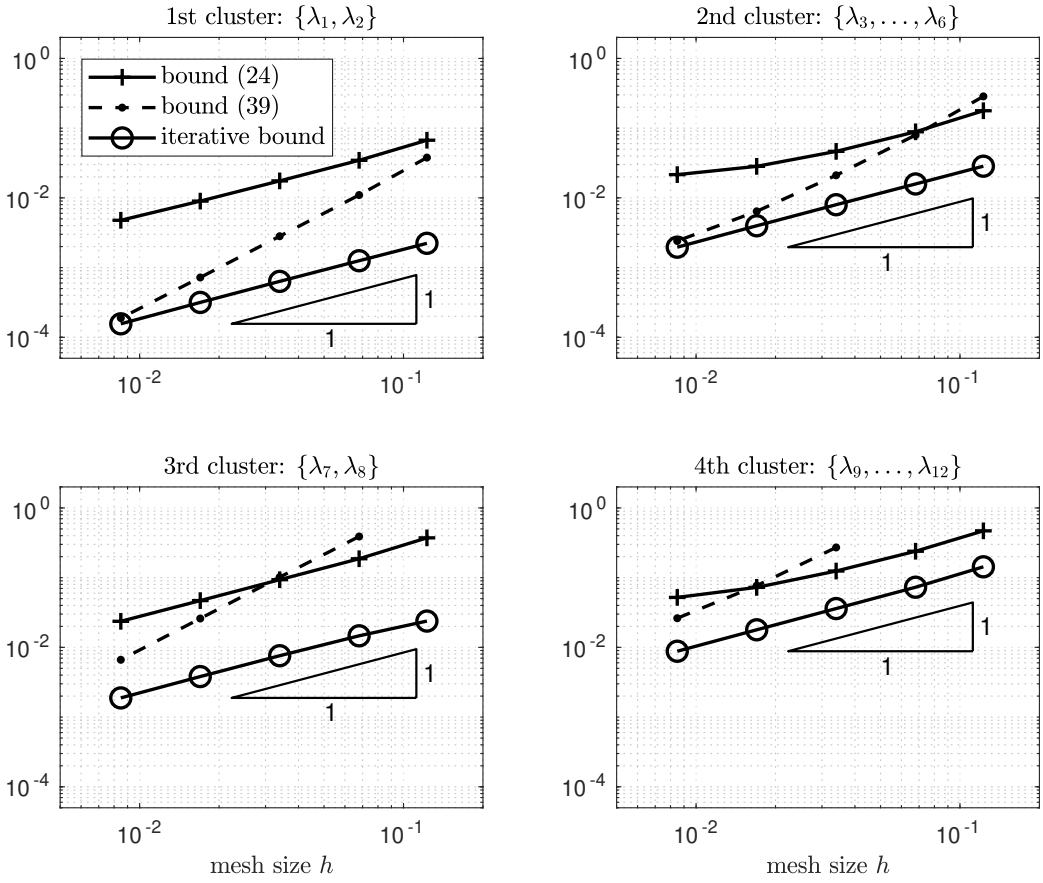

Figure 7: Bounds on the error of spaces of eigenfunctions in the L^2 norm for the dumbbell shaped domain.

is an easy formula (2.5) that links the directed distance of spaces and the usual distance induced by the standard energy or $L^2(\Omega)$ norm. Therefore, the derived estimates of the directed distance of eigenspaces can also easily bound the usual energy and $L^2(\Omega)$ norms of the error.

To simplify the exposition, the a posteriori error bounds were derived for the Dirichlet Laplacian. However, the idea and the bounds in this paper can be easily generalized to a wider class of linear symmetric elliptic operators.

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