CLUSTER ROBUST ESTIMATES FOR BLOCK GRADIENT-TYPE EIGENSOLVERS

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Abstract. Sharp convergence estimates have been derived in recent years for gradient-type eigensolvers for large and sparse symmetric matrices or matrix pairs. An extension of these estimates to the corresponding block iterative methods can be achieved by applying a similar analysis to an embedded vector iteration. Although the resulting estimates are also sharp in the sense that they are not improvable without further assumptions, they cannot reflect the well-known cluster robustness of block eigensolvers. In the present paper, we analyze the cluster robustness of the preconditioned inverse subspace iteration. The main estimate has a weaker assumption and a simpler form compared to some known cluster robust estimates. In addition, it is applicable to further block gradient-type eigensolvers such as LOBPCG. The analysis is based on an orthogonal splitting for the block power method and a geometric interpretation of preconditioning. As a by-product, a cluster robust Ritz value estimate for the block power method is improved.

1. Introduction

For large and sparse symmetric matrices or matrix pairs arising from the discretization of a self-adjoint and elliptic partial differential operator, gradient iterations with respect to the corresponding Rayleigh quotient can be applied with a proper preconditioning. These iterations can efficiently solve partial eigenvalue problems, i.e., the approximate computation of small subsets of the spectrum and the associated invariant subspaces. We consider the generalized eigenvalue problem for the pair (A, M) of symmetric and positive definite matrices $A, M \in \mathbb{R}^{n\times n}$ with the eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. The computation of its smallest eigenvalue amounts to a minimization of the Rayleigh quotient

$$\rho : \mathbb{R}^n \backslash \{0\} \to \mathbb{R}, \quad \rho(x) = \frac{x^T A x}{x^T M x}. \tag{1.1}$$

A straightforward method for this minimization is the gradient iteration

$$x^{(\ell+1)} = x^{(\ell)} - \omega \nabla \rho(x^{(\ell)}).$$

In order to make the gradient iteration more efficient, approximate inverses $T \approx A^{-1}$, called preconditioners, can be used to form an improved descent direction $-T\,\nabla\rho(x^{(\ell)})$ [4]. A simple example is the preconditioned inverse iteration [9]

$$x^{(\ell+1)} = x^{(\ell)} - Tr^{(\ell)} \quad \text{with} \quad r^{(\ell)} = Ax^{(\ell)} - \rho(x^{(\ell)})Mx^{(\ell)} \tag{1.2}$$

since the gradient $\nabla\rho(x^{(\ell)})$ is collinear to the residual $r^{(\ell)}$. Although the step size in (1.2) is constant, the convergence of (1.2) can be guaranteed if the constraint $\|I - TA\|_A \leq \gamma < 1$ (with the identity matrix $I \in \mathbb{R}^{n\times n}$) is satisfied. In the case that $\rho(x^{(\ell)})$ belongs to an eigenvalue

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interval $(\lambda_i, \lambda_{i+1})$, the estimate

$$\frac{\rho(x^{(\ell+1)}) - \lambda_i}{\lambda_{i+1} - \rho(x^{(\ell+1)})} \le \sigma_i^2 \frac{\rho(x^{(\ell)}) - \lambda_i}{\lambda_{i+1} - \rho(x^{(\ell)})} \quad \text{with} \quad \sigma_i = \gamma + (1-\gamma)\frac{\lambda_i}{\lambda_{i+1}} \tag{1.3}$$

from [9, Theorems 1 and 4] is applicable. Convergence estimates with the structure of (1.3) have been derived in the analyses of various gradient-type eigensolvers with individual convergence factors σ_i; see [7, 14, 13]. The inequality in such estimates turns into an equality in certain limit cases, which means that the estimates cannot be improved without further assumptions. Therefore these estimates are considered to be sharp.

In practice, these gradient-type eigensolvers are often implemented in a block form which allows a simultaneous approximation of several of the smallest eigenvalues [2]. For example, the vector iterates in (1.2) can be replaced by s-dimensional subspace iterates. The resulting block iteration is the preconditioned inverse subspace iteration

$$\operatorname{span}\{X^{(\ell+1)}\} = \operatorname{span}\{X^{(\ell)} - TR^{(\ell)}\} \quad \text{with} \quad R^{(\ell)} = AX^{(\ell)} - MX^{(\ell)}\widehat{\Theta}^{(\ell)}. \tag{1.4}$$

Therein the diagonal entries of the diagonal matrix $\widehat{\Theta}^{(\ell)}$ are the Ritz values of (A, M) in the current subspace $\operatorname{span}\{X^{(\ell)}\}$. The columns of the basis matrix $X^{(\ell)}$ are given by the corresponding M-orthonormal Ritz vectors, i.e., $(X^{(\ell)})^T MX^{(\ell)} = I_s \in \mathbb{R}^{s\times s}$ (identity matrix) and $(X^{(\ell)})^T AX^{(\ell)} = \widehat{\Theta}^{(\ell)}$. From another point of view, the columns of $X^{(\ell)} - TR^{(\ell)}$ are just the one-step results of (1.2) applied to the Ritz vectors in $\operatorname{span}\{X^{(\ell)}\}$. However, this argument only allows us to analyze the change of the smallest Ritz value by a direct application of (1.3). For the other Ritz values, one can start with the Ritz vectors in $\operatorname{span}\{X^{(\ell+1)}\}$ and combine them with certain auxiliary vectors from $\operatorname{span}\{X^{(\ell)}\}$ within an iteration similar to (1.2); cf. the block extension of a strictly sharp variant of (1.3) in [11, Section 3]. The results from [11] can be modified in order to generalize (1.3). Denoting the j-th Ritz values (in ascending order) in the consecutive subspace iterates $\operatorname{span}\{X^{(\ell)}\}$, $\operatorname{span}\{X^{(\ell+1)}\}$ by $\vartheta_j^{(\ell)}$, $\vartheta_j^{(\ell+1)}$, it holds in the case $\vartheta_j^{(\ell)} \in (\lambda_i, \lambda_{i+1})$ that

$$\frac{\vartheta_j^{(\ell+1)} - \lambda_i}{\lambda_{i+1} - \vartheta_j^{(\ell+1)}} \le \sigma_i^2 \frac{\vartheta_j^{(\ell)} - \lambda_i}{\lambda_{i+1} - \vartheta_j^{(\ell)}} \quad \text{with} \quad \sigma_i = \gamma + (1-\gamma)\frac{\lambda_i}{\lambda_{i+1}}. \tag{1.5}$$

The estimate (1.5) preserves the sharpness of (1.3). In the corresponding limit case, the Ritz values in $\operatorname{span}\{X^{(\ell)}\}$ other than $\vartheta_j^{(\ell)}$ can be set equal to eigenvalues, without contradicting the assumption $\vartheta_j^{(\ell)} \in (\lambda_i, \lambda_{i+1})$. An evident drawback of (1.5) is that it is not suitable for interpreting the well-known cluster robustness of block eigensolvers (also called subspace eigensolvers). If the eigenvalues λ_i, λ_{i+1} belong to a cluster (e.g. due to the approximation of a multiple eigenvalue of the underlying operator eigenproblem), the convergence factor σ_i in (1.5) is close to 1 and thus cannot predict a fast minimization of the j-th Ritz value. Nevertheless, a fast minimization can practically be realized by setting the dimension of subspace iterates larger than the number of clustered eigenvalues.

An older and improvable estimate of the block iteration (1.4) (in an equivalent form for standard eigenvalue problems) in [3, Theorem 2.1] succeeds in describing the cluster robustness with the convergence factor $\gamma + (1-\gamma)\lambda_j/\lambda_{s+1}$ for the j-th Ritz value. However, this estimate has a more complex form than (1.5) and requires a strong assumption on angles between the initial subspace and the target eigenvectors. The suggested tolerance in the assumption contains the factor $\left(\max_{i=1,\dots,s}\left((\lambda_{i+1}+\lambda_i)/(\lambda_{i+1}-\lambda_i)\right)\right)^{-2}$ which is very small if the first s eigenvalues are clustered. Thus the initial subspace needs to be a very accurate approximation of the target invariant subspace. In other words, this estimate is applicable only if (1.4) is very close to its convergence. Cluster robust estimates for (1.4) under the weaker assumption $\vartheta_s^{(0)} < \lambda_{s+1}$ can be derived by using [18, Theorems 2 and 3] and have the form $\sum_{j=1}^{s}\left(\lambda_j^{-1} - (\vartheta_j^{(\ell+1)})^{-1}\right) \le$

$\tau \sum_{j=1}^{s} \big(\lambda_j^{-1} - (\vartheta_j^{(\ell)})^{-1}\big)$ according to a reciprocal representation of the eigenvalue problem. Therein the convergence factor τ has to be defined in a complicated form requiring the Ritz value $\vartheta_s^{(\ell)}$ together with certain angles between $\operatorname{span}\{X^{(\ell)}\}$ and the target invariant subspace. In contrast to this, the convergence factor σ_i in (1.5) only depends on two eigenvalues λ_i, λ_{i+1} and the quality parameter γ of the preconditioner. Moreover, the estimates based on [18] do not reflect the possibly distinct convergence rates of the Ritz values such as λ_j/λ_{s+1}.

1.1. **New cluster robust estimates.** These considerations lead us to the idea of developing a new estimate for (1.4) which can interpret the cluster robustness under a suitable assumption and in a simple form. For this purpose, we consider first the special version of (1.4) with $T = A^{-1}$, i.e. the inverse subspace iteration

$$\operatorname{span}\{X^{(\ell+1)}\} = \operatorname{span}\{A^{-1}MX^{(\ell)}\widehat{\Theta}^{(\ell)}\} = \operatorname{span}\{A^{-1}MX^{(\ell)}\}, \tag{1.6}$$

for the matrix pair (A, M). By using a reciprocal representation, (1.6) corresponds to the block power method for which some cluster robust estimates on the angle between a target eigenvector and the subspace iterate are presented by Rutishauser [20, Section 2] and Parlett [19, Section 14.4]. These estimates can be applied to (1.6) after simple reformulation:

$$\angle_A\big(w_j, X^{(\ell)}\big) = \mathcal{O}\big((\lambda_j/\lambda_{s+1})^{\ell}\big) \quad \text{and} \quad \tan\angle_A\big(w_j, X^{(\ell)}\big) \le \left(\frac{\lambda_j}{\lambda_{s+1}}\right)^{\ell} \tan\angle_A\big(W, X^{(0)}\big)$$

for an eigenvector w_j associated with the j-th eigenvalue λ_j, $j \in \{1, \ldots, s\}$ and the invariant subspace $\operatorname{span}\{W\}$ associated with the first s eigenvalues. The angles denoted by $\angle_A$ are defined with respect to the inner product induced by A. However, the angle $\angle_A(w_j, X^{(\ell)})$ generally differs from the angle between w_j and a Ritz vector so that these traditional estimates cannot directly imply estimates on Ritz vectors or Ritz values. An improvement has been made by Andrew Knyazev within the convergence analysis of an abstract block iteration in [6, 7]. The improvement includes a cluster robust Ritz value estimate which can be reformulated as

$$\frac{\vartheta_j^{(\ell)} - \lambda_j}{\lambda_n - \vartheta_j^{(\ell)}} \le \frac{\lambda_j}{\lambda_n}\left(\frac{\lambda_j}{\lambda_{s+1}}\right)^{2\ell} \tan^2\angle_A\big(W, X^{(0)}\big).$$

In addition, combining this with the estimate [7, (2.7)] on the relation between Ritz vectors and Ritz values implies a Ritz vector estimate. We aim to achieve a further improvement by deriving intermediate estimates in terms of Ritz values instead of angles. The improved estimate can be modified in the general case $T \approx A^{-1}$ by using an alternative quality parameter $\widetilde{\gamma}$ of the preconditioner based on the geometric arguments from [10, 1]. Therein we consider an embedded vector iteration within the orthogonal complement of an invariant subspace associated with certain interior eigenvalues. The parameter $\widetilde{\gamma}$ is introduced in an assumption depending on auxiliary vectors concerning the inverse subspace iteration. This approach is inspired by the work [17] of Yvan Notay on an inexact Rayleigh quotient iteration and leads to an intermediate estimate for the embedded vector iteration. The estimate is similar to (1.3), namely, for estimating the j-th Ritz values, one obtains

$$\frac{\rho(x^{(\ell+1)}) - \lambda_{i-s+j}}{\lambda_{i+1} - \rho(x^{(\ell+1)})} \le \left(\widetilde{\gamma} + (1-\widetilde{\gamma})\frac{\lambda_{i-s+j}}{\lambda_{i+1}}\right)^2 \frac{\rho(x^{(\ell)}) - \lambda_{i-s+j}}{\lambda_{i+1} - \rho(x^{(\ell)})}$$

for auxiliary vectors $x^{(\ell)}$ and $x^{(\ell+1)}$ provided that $\rho(x^{(\ell)})$ is located between λ_{i-s+j} and λ_{i+1} for a certain $i \in \{s, \ldots, n-1\}$. The interior eigenvalues between λ_{i-s+j} and λ_{i+1} are skipped. (In the special case $i = s$, these eigenvalues are between λ_j and λ_{s+1}.) We prove this intermediate estimate in an equivalent form in Lemma 3.1. Furthermore, a multistep estimate

$$\frac{\vartheta_j^{(\ell)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_j^{(\ell)}} \le \left(\widetilde{\gamma} + (1-\widetilde{\gamma})\frac{\lambda_{i-s+j}}{\lambda_{i+1}}\right)^{2\ell} \frac{\vartheta_s^{(0)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_s^{(0)}}$$

without auxiliary vectors is achieved in Theorem 3.5. The bound uses the s-th Ritz value $\vartheta_s^{(0)}$ and can thus be looser than that from the multistep form of (1.5) in the first several steps, but it is significantly better in total because of the possibly much smaller convergence factor based on the ratio $\lambda_{i-s+j}/\lambda_{i+1}$ compared to λ_i/λ_{i+1}; see the numerical experiments in section 4.

1.2. **Notation.** The generalized eigenvalue problem $Ax = \lambda Mx$ can be represented by a reciprocal form, namely, by the standard eigenvalue problem $Hy = \lambda^{-1}y$ with $H = A^{-1/2}MA^{-1/2}$ and $y = A^{1/2}x$. This representation can considerably simplify the convergence analysis; cf. [16, Section 1.3]. We remark that the auxiliary matrices $A^{-1/2}$ and $A^{1/2}$ do not occur in our convergence estimates and are thus not required in the corresponding numerical experiments. Additionally, it holds for the Rayleigh quotient (1.1) and the Rayleigh quotient

$$\mu : \mathbb{R}^n \backslash \{0\} \to \mathbb{R}, \quad \mu(y) = \frac{y^T H y}{y^T y} \tag{1.7}$$

that $\rho(x) = \big(\mu(y)\big)^{-1}$. For the preconditioned inverse iteration (1.2), the reformulation

$$A^{1/2}x^{(\ell+1)} = A^{1/2}x^{(\ell)} - A^{1/2}TA^{1/2}\big(A^{1/2}x^{(\ell)} - \rho(x^{(\ell)})A^{-1/2}MA^{-1/2}A^{1/2}x^{(\ell)}\big)$$

together with $N = A^{1/2}TA^{1/2}$ results in the representation

$$y^{(\ell+1)} = y^{(\ell)} - N\big(y^{(\ell)} - \big(\mu(y^{(\ell)})\big)^{-1}Hy^{(\ell)}\big). \tag{1.8}$$

Similarly, the preconditioned inverse subspace iteration (1.4) can be represented by

$$\operatorname{span}\{Y^{(\ell+1)}\} = \operatorname{span}\{Y^{(\ell)} - N\big(Y^{(\ell)} - HY^{(\ell)}(\Theta^{(\ell)})^{-1}\big)\} \tag{1.9}$$

with $Y^{(\ell)} = A^{1/2}X^{(\ell)}(\widehat{\Theta}^{(\ell)})^{-1/2}$ and $\Theta^{(\ell)} = (\widehat{\Theta}^{(\ell)})^{-1}$. Therein the columns of $Y^{(\ell)}$ are orthonormal Ritz vectors of H since $(Y^{(\ell)})^TY^{(\ell)}$ is the identity matrix I_s and $(Y^{(\ell)})^THY^{(\ell)}$ is a diagonal matrix:

$$(Y^{(\ell)})^TY^{(\ell)} = (\widehat{\Theta}^{(\ell)})^{-1/2}\underbrace{(X^{(\ell)})^TAX^{(\ell)}}_{=\widehat{\Theta}^{(\ell)}}(\widehat{\Theta}^{(\ell)})^{-1/2} = I_s,$$

$$(Y^{(\ell)})^THY^{(\ell)} = (\widehat{\Theta}^{(\ell)})^{-1/2}\underbrace{(X^{(\ell)})^TMX^{(\ell)}}_{=I_s}(\widehat{\Theta}^{(\ell)})^{-1/2} = (\widehat{\Theta}^{(\ell)})^{-1} = \Theta^{(\ell)}.$$

Correspondingly, $\Theta^{(\ell)}$ is a diagonal matrix with the Ritz values of H as the diagonal entries. The matrix N in (1.8) and (1.9) represents the preconditioner T and is assumed to satisfy the constraint $\|I - N\|_2 \le \gamma < 1$ according to

$$\|I - TA\|_A = \|A^{1/2}(I - TA)A^{-1/2}\|_2 = \|I - A^{1/2}TA^{1/2}\|_2 = \|I - N\|_2.$$

This allows us to reformulate the estimates (1.3), (1.5) in the following lemma.

Lemma 1.1. *Let $\mu_1 \ge \cdots \ge \mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H \in \mathbb{R}^{n\times n}$. The corresponding Rayleigh quotient is defined by* (1.7). *Let the matrix N in the iterations* (1.8) *and* (1.9) *satisfy $\|I - N\|_2 \le \gamma < 1$.*

(a) *For* (1.8), *it holds in the case $\mu(y^{(\ell)}) \in (\mu_{i+1}, \mu_i)$ that*

$$\frac{\mu_i - \mu(y^{(\ell+1)})}{\mu(y^{(\ell+1)}) - \mu_{i+1}} \le \sigma_i^2 \frac{\mu_i - \mu(y^{(\ell)})}{\mu(y^{(\ell)}) - \mu_{i+1}} \quad \textit{with} \quad \sigma_i = \gamma + (1-\gamma)\frac{\mu_{i+1}}{\mu_i}. \tag{1.10}$$

(b) *Let $\theta_j^{(\ell)}$, $\theta_j^{(\ell+1)}$ be the j-th Ritz values in descending order of H in $\operatorname{span}\{Y^{(\ell)}\}$, $\operatorname{span}\{Y^{(\ell+1)}\}$. Then it holds for* (1.9) *in the case $\theta_j^{(\ell)} \in (\mu_{i+1}, \mu_i)$ that*

$$\frac{\mu_i - \theta_j^{(\ell+1)}}{\theta_j^{(\ell+1)} - \mu_{i+1}} \le \sigma_i^2 \frac{\mu_i - \theta_j^{(\ell)}}{\theta_j^{(\ell)} - \mu_{i+1}} \quad \textit{with} \quad \sigma_i = \gamma + (1-\gamma)\frac{\mu_{i+1}}{\mu_i}. \tag{1.11}$$

The reformulation simply uses the fact that the eigenvalues and the Ritz values of (A, M) are the reciprocals of those of H. For a self-contained proof of (1.10) one can use the succinct analysis from [1] after a simple conversion of the eigenvalue notation $\mu_1 > \cdots > \mu_m$ in [1] (i.e., the multiple eigenvalues are counted only once) to that in Lemma 1.1. Some arguments from [11, 1] can be combined and applied to a self-contained proof of (1.11). Furthermore, these arguments are used below in subsection 3.1 for deriving the new estimate.

1.3. **Aim and overview.** In this paper, we analyze the cluster robustness of block gradient-type eigensolvers. New estimates are derived for the preconditioned inverse subspace iteration (1.4) by combing an orthogonal splitting for the block power method and a geometric interpretation of preconditioning. These two tools are implemented concerning the symmetric and positive definite matrix H with eigenvalues $\mu_1 \geq \cdots \geq \mu_n$ introduced in subsection 1.2. The orthogonal splitting makes use of the intersection of the initial subspace and the invariant subspace associated with the eigenvalues $\mu_1, \ldots, \mu_{i-s+j}$, $\mu_{i+1}, \ldots, \mu_n$ for a certain index $i \in \{s, \ldots, n-1\}$. The orthogonality of this intersection to the eigenvectors associated with the interior eigenvalues $\mu_{i-s+j+1}, \ldots, \mu_i$ is preserved while we multiply it by H. These eigenvalues are thus skipped in the further analysis so that the cluster robust convergence factor μ_{i+1}/μ_{i-s+j} is achieved; see subsection 2.2 for more details. The geometric interpretation of preconditioning compares the preconditioned inverse iteration with the power method $y_{\text{new}} = Hy$. The new iterates can be analyzed within a ball centred at Hy or within a cone around span$\{Hy\}$; cf. [10, 1]. We utilize these tools in order to modify a description of (1.4) from [11] as an important step of our new analysis; see subsection 3.1 for more details. The resulting main estimate has a similar simple form as (1.5) but is much more accurate in the case of clustered eigenvalues. Additionally, the new results serve as a supplement to the convergence analysis of further block gradient-type eigensolvers.

The remaining part of the paper is organized as follows. In section 2, we consider the inverse subspace iteration (1.6). This is a special version of (1.4) with $T = A^{-1}$ and corresponds to the block power method by using the reciprocal representation in subsection 1.2. The convergence analysis of an abstract block iteration by Knyazev [6, 7] is directly applicable and results in typical cluster robust estimates. However, the central part of this analysis works with angles between subspaces and cannot easily be applied to the case of inexact preconditioning. Thus we derive a further cluster robust estimate in terms of Ritz values and generalize it in section 3 to preconditioned iterations. Therein the perturbation of some auxiliary vectors caused by inexact preconditioning is described with an alternative quality parameter so that the proof techniques from [10, 1] can be used. The main result is a multistep estimate for the preconditioned inverse subspace iteration (1.4) under a proper assumption and can easily be compared with the multistep form of (1.5). In section 4, numerical experiments with large scale matrices from an adaptive finite element discretization of the Laplacian eigenvalue problem demonstrate the benefit of the new results.

2. Cluster robustness of the block power method

We start with a special version of the preconditioned inverse subspace iteration (1.4). By setting $N = I$ in its reciprocal representation (1.9), we obtain span$\{Y^{(\ell+1)}\} = $ span$\{HY^{(\ell)}(\Theta^{(\ell)})^{-1}\}$ $=$ span$\{HY^{(\ell)}\}$, i.e. the block power method for the standard eigenvalue problem of H, or the reciprocal representation of the inverse subspace iteration (1.6).

2.1. **Convergence estimates by Andrew Knyazev.** The block power method is also a special version of an abstract block iteration which has been thoroughly analyzed by Knyazev [6, 7]. We select two typical cluster robust estimates [7, (2.18), (2.20)] and reformulate them with respect to the block power method.

Lemma 2.1. *Let $\mu_1 \geq \cdots \geq \mu_s > \mu_{s+1} \geq \cdots \geq \mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H \in \mathbb{R}^{n\times n}$ and let $z_1, \ldots, z_s, z_{s+1}, \ldots, z_n$ be the associated orthonormal eigenvectors. We consider the block power method* $\operatorname{span}\{Y^{(\ell+1)}\} = \operatorname{span}\{HY^{(\ell)}\}$ *with* $\dim(\operatorname{span}\{Y^{(0)}\}) = s$ *and denote by $\angle(U, V)$ the Euclidean angle between two subspaces* $\operatorname{span}\{U\}$, $\operatorname{span}\{V\}$*. If $\angle\big(Y^{(0)}, Z\big) < \pi/2$ for $Z = [z_1, \ldots, z_s]$, then it holds that*

$$\tan \angle\big(Y^{(\ell)}, Z\big) \leq \left(\frac{\mu_{s+1}}{\mu_s}\right)^{\ell} \tan \angle\big(Y^{(0)}, Z\big). \tag{2.1}$$

Furthermore, denoting by $\theta_j^{(\ell)}$ the j-th Ritz value in descending order of H in $\operatorname{span}\{Y^{(\ell)}\}$*, it holds that*

$$\frac{\mu_j - \theta_j^{(\ell)}}{\theta_j^{(\ell)} - \mu_n} \leq \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell} \tan^2 \angle\big(Y^{(0)}, Z\big). \tag{2.2}$$

Remark 2.2. In [6, 7], a generalized eigenvalue problem is considered and the angles are defined with respect to the inner product induced by a symmetric and positive definite matrix. The target eigenvalues are taken to be simple. In spite of these different settings, the analysis in [6, 7] is applicable to the proof of Lemma 2.1 after slight reformulation. The probably more natural setting with only one strict inequality $\mu_s > \mu_{s+1}$ dates back to the analysis of the inverse subspace iteration by Parlett [19, Section 14.4].

2.2. **Auxiliary vectors.** The estimates [7, (2.18), (2.20)] can be proved by combining several valuable arguments from [6] (in Russian). Next, we recapitulate two arguments in equivalent forms together with some auxiliary vectors which are also used for deriving our new estimates. For the reader's convenience, we prove these arguments in a more direct and elementary way.

Lemma 2.3. *With the settings from Lemma 2.1 there exist unique vectors $y_k \in \operatorname{span}\{Y^{(0)}\}$, $k \in \{1, \ldots, s\}$ satisfying $z_i^T y_k = \delta_{ik}$ for $i \in \{1, \ldots, s\}$. Furthermore, the matrix $Y_j = [y_1, \ldots, y_j]$, $j \in \{1, \ldots, s\}$ has the rank j, and it holds for $Z_j = [z_1, \ldots, z_j]$ that (cf.* [6, (2.3.11)]*)*

$$\tan \angle\big(H^\ell Y_j,\, Z_j\big) \leq \left(\frac{\mu_{s+1}}{\mu_j}\right)^{\ell} \tan \angle\big(Y_j,\, Z_j\big). \tag{2.3}$$

Proof. The condition $z_i^T y_k = \delta_{ik}$ together with the representation $y_k = Y^{(0)} g_k$ leads to the linear system $Z^T Y^{(0)} g_k = e_k$ with $Z = [z_1, \ldots, z_s]$ and the k-th standard basis vector e_k in $\mathbb{R}^s$. The assumption $\angle\big(Y^{(0)}, Z\big) < \pi/2$ from Lemma 2.1 ensures that $Z^T Y^{(0)}$ is invertible $\big($since otherwise there exists a nonzero vector $g \in \mathbb{R}^s$ with $Z^T Y^{(0)} g = 0$, i.e., $\operatorname{span}\{Y^{(0)}\}$ contains an vector $Y^{(0)} g$ which is orthogonal to $\operatorname{span}\{Z\}\big)$. Thus the solution g_k is unique as well as y_k. These auxiliary vectors have already been suggested by Rutishauser in [20].

The resulting representation $y_k = Y^{(0)}(Z^T Y^{(0)})^{-1} e_k$ shows that

$$Y_j = Y^{(0)}(Z^T Y^{(0)})^{-1}[e_1, \ldots, e_j]$$

and thus Y_j evidently has the rank j. In order to prove (2.3), we use the fact $\operatorname{span}\{H^\ell Y_j\} = H^\ell \operatorname{span}\{Y_j\}$ so that

$$\tan \angle\big(H^\ell Y_j,\, Z_j\big) = \max_{w \in \operatorname{span}\{H^\ell Y_j\}} \tan \angle\big(w,\, Z_j\big) = \max_{y \in \operatorname{span}\{Y_j\}} \tan \angle\big(H^\ell y,\, Z_j\big).$$

Then we consider a (nonunique) $y^* \in \operatorname{span}\{Y_j\}$ which maximizes $\tan \angle\big(H^\ell y,\, Z_j\big)$. The condition $z_i^T y_k = \delta_{ik}$ implies that y^* is orthogonal to the eigenvectors $z_{j+1}, \ldots, z_s$ in the case $j < s$. Thus y^* can be represented by $y^* = \sum_{i=1}^{j} \alpha_i z_i + \sum_{i=s+1}^{n} \alpha_i z_i$ with certain coefficients $\alpha_i \in \mathbb{R}$, also in the case $j = s$. Consequently, it holds that $H^\ell y^* = \sum_{i=1}^{j} \mu_i^\ell \alpha_i z_i + \sum_{i=s+1}^{n} \mu_i^\ell \alpha_i z_i$ and

$$\tan^2 \angle\big(H^\ell y^*,\, Z_j\big) = \frac{\sum_{i=s+1}^{n} \mu_i^{2\ell} \alpha_i^2}{\sum_{i=1}^{j} \mu_i^{2\ell} \alpha_i^2} \leq \frac{\mu_{s+1}^{2\ell} \sum_{i=s+1}^{n} \alpha_i^2}{\mu_j^{2\ell} \sum_{i=1}^{j} \alpha_i^2} = \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell} \tan^2 \angle\big(y^*,\, Z_j\big).$$

Combining this with

$$\tan\angle\big(H^\ell y^*,\, Z_j\big) = \tan\angle\big(H^\ell Y_j,\, Z_j\big), \quad \tan\angle\big(y^*,\, Z_j\big) \le \tan\angle\big(Y_j,\, Z_j\big)$$

and using the positivity of the concerned tangent values and eigenvalues yield (2.3). □

The special version of (2.3) for $j = s$ coincides with the estimate (2.1) in Lemma 2.1. Additionally, (2.3) can be extended to the estimate (2.2) by using the following argument.

Lemma 2.4. *With the settings from Lemma 2.1 and Lemma 2.3 it holds that (cf.* [6, (2.2.42)] *in terms of tangent values)*

$$\cos^2\angle\big(H^\ell Y_j,\, Z_j\big) \le \frac{\theta_j^{(\ell)} - \mu_n}{\mu_j - \mu_n}. \tag{2.4}$$

Proof. We denote by β the smallest Ritz value of H in $\operatorname{span}\{H^\ell Y_j\}$. Since Y_j is a submatrix of $Y^{(0)}$ with the rank j (and H has full rank), $\operatorname{span}\{H^\ell Y_j\}$ is a j-dimensional subspace within $\operatorname{span}\{H^\ell Y^{(0)}\} = \operatorname{span}\{Y^{(\ell)}\}$. Then we have $\mu_j \ge \theta_j^{(\ell)} \ge \beta$ by using the Courant-Fischer principles. Thus (2.4) can be derived from the intermediate estimate

$$\cos^2\angle\big(H^\ell Y_j,\, Z_j\big) \le \frac{\beta - \mu_n}{\mu_j - \mu_n}. \tag{2.5}$$

Evidently, (2.5) is trivial in the case $\cos^2\angle\big(H^\ell Y_j,\, Z_j\big) = 0$. In the nontrivial case, we use a Ritz vector w in $\operatorname{span}\{H^\ell Y_j\}$ associated with β. Then $\mu(w) = \beta$, and $0 < \cos^2\angle\big(H^\ell Y_j,\, Z_j\big) \le \cos^2\angle\big(w,\, Z_j\big)$ so that w is not orthogonal to $\operatorname{span}\{Z_j\}$ and thus has a nonzero orthogonal projection z to $\operatorname{span}\{Z_j\}$. In addition, it holds that

$$\cos^2\angle\big(H^\ell Y_j,\, Z_j\big) \le \cos^2\angle\big(w,\, Z_j\big) = \cos^2\angle\big(w,\, z\big).$$

Since $z \in \operatorname{span}\{Z_j\}$, and $\operatorname{span}\{Z_j\}$ is an invariant subspace with respect to H, we have $Hz \in \operatorname{span}\{Z_j\}$. Thus the orthogonality $w - z \perp \operatorname{span}\{Z_j\}$ implies that

$$(w-z)^T z = 0, \qquad (w-z)^T Hz = 0 \qquad \text{and} \qquad (w-z)^T(H - \mu_n I)z = 0.$$

Consequently, it holds that $w^T z = \|z\|_2^2$ and

$$w^T(H-\mu_n I)w = z^T(H-\mu_n I)z + (w-z)^T(H-\mu_n I)(w-z) \ge z^T(H-\mu_n I)z > 0.$$

Therein the first inequality follows from the positive semidefiniteness of $H - \mu_n I$, and the second inequality is based on the fact that z is not an eigenvector associated with μ_n because of $z \in \operatorname{span}\{Z_j\}$ and $\mu_j \ge \mu_s > \mu_{s+1} \ge \mu_n$. Summarizing the above gives

$$\begin{aligned}
\cos^2\angle\big(H^\ell Y_j,\, Z_j\big) \le \cos^2\angle\big(w,\, z\big) &= \left(\frac{w^T z}{\|w\|_2\|z\|_2}\right)^2 = \frac{\|z\|_2^2}{\|w\|_2^2} \\
&\le \frac{\|z\|_2^2}{z^T(H-\mu_n I)z}\,\frac{w^T(H-\mu_n I)w}{\|w\|_2^2} = \big(\mu(z)-\mu_n\big)^{-1}\big(\mu(w)-\mu_n\big)
\end{aligned}$$

which shows (2.5) by using $\mu(w) = \beta$ and $\mu(z) \ge \mu_j$ (according to $z \in \operatorname{span}\{Z_j\}$). □

Remark 2.5. Two equivalent versions of (2.4) can immediately be derived by trigonometric conversions:

$$\sin^2\angle\big(H^\ell Y_j,\, Z_j\big) \ge \frac{\mu_j - \theta_j^{(\ell)}}{\mu_j - \mu_n}, \qquad \tan^2\angle\big(H^\ell Y_j,\, Z_j\big) \ge \frac{\mu_j - \theta_j^{(\ell)}}{\theta_j^{(\ell)} - \mu_n}. \tag{2.6}$$

Additionally, for each $y \in \operatorname{span}\{Y_j\}$ and its orthogonal projection $\tilde{y}$ to $\operatorname{span}\{Z_j\}$, we have

$$y - \tilde{y} \perp \operatorname{span}\{Z_j\}, \quad y \perp \operatorname{span}\{z_{j+1}, \dots, z_s\}, \quad \tilde{y} \perp \operatorname{span}\{z_{j+1}, \dots, z_s\}$$

so that $y-\tilde{y}$ is orthogonal to $\operatorname{span}\{Z_j\}+\operatorname{span}\{z_{j+1},\ldots,z_s\}=\operatorname{span}\{Z\}$. Thus $\tilde{y}$ is also the orthogonal projection of y to $\operatorname{span}\{Z\}$, and

$$\begin{aligned}\tan\angle\big(Y_j,\,Z_j\big)&=\max_{y\in\operatorname{span}\{Y_j\}}\tan\angle\big(y,\,Z_j\big)=\max_{y\in\operatorname{span}\{Y_j\}}\tan\angle\big(y,\,Z\big)\\&\le\max_{y\in\operatorname{span}\{Y^{(0)}\}}\tan\angle\big(y,\,Z\big)=\tan\angle\big(Y^{(0)},Z\big).\end{aligned}$$

Combining this with (2.3) and the tangent estimate in (2.6) (cf. [6, (2.3.12)]) yields the estimate (2.2) in Lemma 2.1. Similarly, the sine estimate in (2.6) can be extended to $(\mu_j-\theta_j^{(\ell)})/(\mu_j-\mu_n)\le\sin^2\angle\big(Y^{(\ell)},Z\big)$. This corresponds in the special case $\ell=0$ to a well-known relationship between Ritz values and subspace angles where no iterative methods are considered; see [5, Theorem 1] or its slightly weaker variant [3, Lemma 3.1].

2.3. **New estimates.** As seen in the previous subsection, the central part of the derivation of the cluster robust estimates in Lemma 2.1 or [7, (2.18), (2.20)] is a tangent estimate like (2.3). For the purpose of a generalized analysis for preconditioned iterations, however, (2.3) and the underlying proof technique cannot easily be used since the orthogonality between the auxiliary vectors and the eigenvectors $z_{j+1},\ldots,z_s$ does not need to be preserved under preconditioning. Indeed, the known sharp estimates for preconditioned iterations from [11, 9] are not in terms of angles but in terms of Ritz values. This consideration leads to the following new cluster robust estimates in Theorems 2.6, 2.8.

Theorem 2.6. *Let $\mu_1\ge\cdots\ge\mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H\in\mathbb{R}^{n\times n}$. We consider the block power method* $\operatorname{span}\{Y^{(\ell+1)}\}=\operatorname{span}\{HY^{(\ell)}\}$ *with* $\dim(\operatorname{span}\{Y^{(0)}\})=s$ *and denote by $\theta_j^{(\ell)}$ the j-th Ritz value in descending order of H in the subspace iterate* $\operatorname{span}\{Y^{(\ell)}\}$. *If $\theta_s^{(0)}>\mu_{s+1}$, then it holds that*

$$\frac{\mu_j-\theta_j^{(\ell)}}{\theta_j^{(\ell)}-\mu_{s+1}}\le\left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell}\frac{\mu_j-\theta_s^{(0)}}{\theta_s^{(0)}-\mu_{s+1}}.\tag{2.7}$$

In comparison to Lemma 2.1, Theorem 2.6 does not depend on the invariant subspace $Z=[z_1,\ldots,z_s]$. The assumption $\theta_s^{(0)}>\mu_{s+1}$ ensures $\mu_s>\mu_{s+1}$ because of $\mu_s\ge\theta_s^{(0)}$ by the Courant-Fischer principles. The estimate (2.7) contains only eigenvalues and Ritz values. It is not a direct improvement of (2.2) due to their different convergence measures. However, a coarser variant of (2.7) can be proved by extracting an upper bound of $(\mu_j-\theta_s^{(0)})/(\theta_s^{(0)}-\mu_{s+1})$ from the trivial version of (2.2) with $\ell=0$ and $j=s$. The essential advantage of using (2.7) is that its extension to the preconditioned case can preserve the orthogonality between auxiliary vectors and eigenvectors. In the derivation of (2.7) we use the auxiliary vectors introduced in subsection 2.2, and prove first a similar estimate concerning Ritz values in subspaces $\operatorname{span}\{Y_j\}\subseteq\operatorname{span}\{Y^{(0)}\}$.

Lemma 2.7. *With the settings from Lemma 2.1 and Lemma 2.3 let $\tilde{\theta}_j$ be the smallest Ritz value of H in* $\operatorname{span}\{Y_j\}$. *Then $\tilde{\theta}_j\ge\theta_s^{(0)}$, and, if $\theta_s^{(0)}>\mu_{s+1}$, it holds that*

$$\frac{\mu_j-\theta_j^{(\ell)}}{\theta_j^{(\ell)}-\mu_{s+1}}\le\left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell}\frac{\mu_j-\tilde{\theta}_j}{\tilde{\theta}_j-\mu_{s+1}}.\tag{2.8}$$

Proof. The inequality $\tilde{\theta}_j\ge\theta_s^{(0)}$ follows from the relation $\operatorname{span}\{Y_j\}\subseteq\operatorname{span}\{Y^{(0)}\}$ and the fact that $\tilde{\theta}_j$, $\theta_s^{(0)}$ are the smallest Ritz values in $\operatorname{span}\{Y_j\}$, $\operatorname{span}\{Y^{(0)}\}$, respectively.

For the proof of (2.8) we use, similarly to the proof of Lemma 2.4, the smallest Ritz value β of H in $\operatorname{span}\{H^\ell Y_j\}$. Then the inequality $\theta_j^{(\ell)}\ge\beta$ (based on the Courant-Fischer principles) and the monotonicity of the function $\big(\mu_j-*\big)/\big(*-\mu_{s+1}\big)$ on the interval $\big(\mu_{s+1},\,\mu_j\big]$ allow us to derive (2.8) from the intermediate estimate

$$\frac{\mu_j - \beta}{\beta - \mu_{s+1}} \le \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell} \frac{\mu_j - \tilde{\theta}_j}{\tilde{\theta}_j - \mu_{s+1}}. \tag{2.9}$$

We prove (2.9) by using a Ritz vector of H in $\operatorname{span}\{H^\ell Y_j\}$ associated with β. This vector can be represented by $H^\ell Y_j c$ with a coefficient vector $c \in \mathbb{R}^j \backslash \{0\}$. We consider further the vector $Y_j c$ and denote it by y so that

$$y \in \operatorname{span}\{Y_j\}, \qquad \mu(y) \ge \tilde{\theta}_j \ge \theta_s^{(0)} > \mu_{s+1}, \qquad \beta = \mu(H^\ell Y_j c) = \mu(H^\ell y). \tag{2.10}$$

Because of $y \in \operatorname{span}\{Y_j\} = \operatorname{span}\{y_1, \dots, y_j\}$ and the condition $z_i^T y_k = \delta_{ik}$ from Lemma 2.3, the vector y is orthogonal to the eigenvectors $z_{j+1}, \dots, z_s$ in the case $j < s$. Thus y can be represented by

$$y = u + v \qquad \text{with} \qquad u = \sum_{i=1}^{j} w_i, \quad v = \sum_{i=s+1}^{n} w_i, \quad w_i \in \operatorname{span}\{z_i\},$$

also in the case $j = s$. Therein u and v are the orthogonal projections of y to the invariant subspaces $\operatorname{span}\{z_1, \dots, z_j\}$ and $\operatorname{span}\{z_{s+1}, \dots, z_n\}$ so that $u^T H v = u^T v = 0$ and

$$\mu(y) = \frac{(u+v)^T H (u+v)}{(u+v)^T (u+v)} = \frac{u^T H u + v^T H v}{u^T u + v^T v} = \frac{\mu(u)\, u^T u + \mu(v)\, v^T v}{u^T u + v^T v}.$$

The vector u cannot be zero, since otherwise y belongs to $\operatorname{span}\{z_{s+1}, \dots, z_n\}$ so that $\mu(y) \le \mu_{s+1}$ which contradicts the inequalities in (2.10). Then we have

$$\frac{\mu(u) - \mu(y)}{\mu(y) - \mu(v)} = \frac{v^T v}{u^T u} = \frac{\|v\|_2^2}{\|u\|_2^2}.$$

In addition, an analogous equation for the partially scaled vector $\tilde{y} = \mu_j^\ell u + \mu_{s+1}^\ell v$ yields

$$\frac{\mu(u) - \mu(\tilde{y})}{\mu(\tilde{y}) - \mu(v)} = \frac{\mu(\mu_j^\ell u) - \mu(\tilde{y})}{\mu(\tilde{y}) - \mu(\mu_{s+1}^\ell v)} = \frac{\|\mu_{s+1}^\ell v\|_2^2}{\|\mu_j^\ell u\|_2^2} = \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell} \frac{\mu(u) - \mu(y)}{\mu(y) - \mu(v)}. \tag{2.11}$$

Furthermore, the inequality $\mu(H^\ell y) \ge \mu(\tilde{y})$ follows from the coefficient comparison

$$H^\ell y = H^\ell u + H^\ell v = \sum_{i=1}^{j} \underbrace{\mu_i^\ell}_{\ge \mu_j^\ell} w_i + \sum_{i=s+1}^{n} \underbrace{\mu_i^\ell}_{\le \mu_{s+1}^\ell} w_i$$

analogously to [6, Lemma 2.3.2] and [16, Lemma 3.2]. Combining $\mu(H^\ell y) \ge \mu(\tilde{y})$ with the known relations

$$\mu(u) \ge \mu_j \ge \theta_j^{(\ell)} \ge \beta = \mu(H^\ell y), \qquad \mu(y) \ge \tilde{\theta}_j \ge \theta_s^{(0)} > \mu_{s+1} \ge \mu(v)$$

and (2.11) yields $\mu(u) \ge \mu_j \ge \beta \ge \mu(\tilde{y}) \ge \mu(y) \ge \tilde{\theta}_j > \mu_{s+1} \ge \mu(v)$. More precisely,

$$\frac{\mu(u) - \beta}{\beta - \mu(v)} \le \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell} \frac{\mu(u) - \tilde{\theta}_j}{\tilde{\theta}_j - \mu(v)}$$

follows from (2.11) by using the monotonicity of the function $\big(\mu(u) - *\big)/\big(* - \mu(v)\big)$ on the interval $\big(\mu(v), \mu(u)\big]$. The subsequent extension

$$\left(\frac{\mu_j - \beta}{\beta - \mu_{s+1}}\right)\left(\frac{\mu_j - \tilde{\theta}_j}{\tilde{\theta}_j - \mu_{s+1}}\right)^{-1} = \left(\frac{\mu_j - \beta}{\mu_j - \tilde{\theta}_j}\right)\left(\frac{\tilde{\theta}_j - \mu_{s+1}}{\beta - \mu_{s+1}}\right)$$

$$\le \left(\frac{\mu(u) - \beta}{\mu(u) - \tilde{\theta}_j}\right)\left(\frac{\tilde{\theta}_j - \mu(v)}{\beta - \mu(v)}\right) = \left(\frac{\mu(u) - \beta}{\beta - \mu(v)}\right)\left(\frac{\mu(u) - \tilde{\theta}_j}{\tilde{\theta}_j - \mu(v)}\right)^{-1} \le \left(\frac{\mu_{s+1}}{\mu_j}\right)^{2\ell}$$

results in (2.9). □

The proof of Theorem 2.6 follows immediately from Lemma 2.7 and is given next.

Proof of Theorem 2.6. The settings from Theorem 2.6 are compatible with those used in Lemma 2.7. In particular, the assumption $\theta_s^{(0)} > \mu_{s+1}$ ensures $\angle\big(Y^{(0)}, Z\big) < \pi/2$, since otherwise $\mathrm{span}\{Y^{(0)}\}$ contains a nonzero vector y which is orthogonal to $\mathrm{span}\{Z\}$ so that $\theta_s^{(0)} \leq \mu(y) \leq \mu_{s+1}$. Thus the results of Lemma 2.7 are applicable. The inequality $\tilde{\theta}_j \geq \theta_s^{(0)}$ and the monotonicity of $\big(\mu_j - *\big)/\big(* - \mu_{s+1}\big)$ on $\big(\mu_{s+1}, \mu_j\big]$ show that $\big(\mu_j - \tilde{\theta}_j\big)/\big(\tilde{\theta}_j - \mu_{s+1}\big) \leq \big(\mu_j - \theta_s^{(0)}\big)/\big(\theta_s^{(0)} - \mu_{s+1}\big)$. Combining this with (2.8) yields (2.7). □

We remark that our analysis in Lemma 2.7 and Theorem 2.6 can be applied to the abstract block iteration from [6, 7] after slight reformulation. The resulting pendant of (2.7) generalizes the estimate [7, (2.22)] which corresponds to the special case $j = s$. However, the Ritz value $\theta_s^{(0)}$ in the bound in such a generalization cannot be replaced by $\theta_j^{(0)}$ for the purpose of a tighter bound; cf. the numerical example concerning the restarted block-Lanczos method in [22, Section 3, Figure 1].

Furthermore, the estimate (2.7) can be generalized to arbitrarily located $\theta_s^{(0)}$ where the auxiliary subspaces like $\mathrm{span}\{Y_j\}$ can be constructed by subspace intersections.

Theorem 2.8. *Let $\mu_1 \geq \cdots \geq \mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H \in \mathbb{R}^{n\times n}$. We consider the block power method $\mathrm{span}\{Y^{(\ell+1)}\} = \mathrm{span}\{HY^{(\ell)}\}$ with $\dim(\mathrm{span}\{Y^{(0)}\}) = s$ and denote by $\theta_j^{(\ell)}$ the j-th Ritz value in descending order of H in the subspace iterate $\mathrm{span}\{Y^{(\ell)}\}$. If $\mu_i \geq \theta_s^{(0)} > \mu_{i+1}$ for a certain $i \in \{s, \ldots, n-1\}$, then it holds that*

$$\frac{\mu_{i-s+j} - \theta_j^{(\ell)}}{\theta_j^{(\ell)} - \mu_{i+1}} \leq \left(\frac{\mu_{i+1}}{\mu_{i-s+j}}\right)^{2\ell} \frac{\mu_{i-s+j} - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{i+1}}. \tag{2.12}$$

Proof. The estimate (2.12) is trivial in the case $\theta_j^{(\ell)} \geq \mu_{i-s+j}$ (since the left-hand side is then nonpositive). In the nontrivial case $\theta_j^{(\ell)} < \mu_{i-s+j}$, we use orthonormal eigenvectors $z_1, \ldots, z_n$ of H associated with the eigenvalues $\mu_1 \geq \cdots \geq \mu_n$. Then the intersection of $\mathcal{Y}^{(0)} = \mathrm{span}\{Y^{(0)}\}$ and the invariant subspace $\widetilde{\mathcal{Z}} = \mathrm{span}\{z_1, \ldots, z_{i-s+j}, z_{i+1}, \ldots, z_n\}$ has at least the dimension j because of

$$\dim\big(\mathcal{Y}^{(0)} \cap \widetilde{\mathcal{Z}}\big) = \dim \mathcal{Y}^{(0)} + \dim \widetilde{\mathcal{Z}} - \underbrace{\dim\big(\mathcal{Y}^{(0)} + \widetilde{\mathcal{Z}}\big)}_{\leq \dim \mathbb{R}^n = n} \geq s + (n - s + j) - n = j. \tag{2.13}$$

Thus there exists a j-dimensional subspace $\widetilde{\mathcal{Y}} \subseteq \big(\mathcal{Y}^{(0)} \cap \widetilde{\mathcal{Z}}\big)$. We denote by $\tilde{\theta}$, $\tilde{\beta}$ the smallest Ritz values of H in $\widetilde{\mathcal{Y}}$, $H^\ell \widetilde{\mathcal{Y}}$, respectively. Then the Courant-Fischer principles yield

$$\tilde{\theta} \geq \theta_s^{(0)} > \mu_{i+1} \quad \text{and} \quad \tilde{\beta} \leq \theta_j^{(\ell)} < \mu_{i-s+j}$$

because of $\widetilde{\mathcal{Y}} \subseteq \mathcal{Y}^{(0)} = \mathrm{span}\{Y^{(0)}\}$ and $H^\ell \widetilde{\mathcal{Y}} \subseteq \mathrm{span}\{H^\ell Y^{(0)}\} = \mathrm{span}\{Y^{(\ell)}\}$. Therein we consider $\tilde{\theta}$, $\theta_s^{(0)}$ as the smallest Ritz values and $\tilde{\beta}$, $\theta_j^{(\ell)}$ as the j-th Ritz values in descending order. Subsequently, the estimate (2.12) follows from the intermediate estimate

$$\frac{\mu_{i-s+j} - \tilde{\beta}}{\tilde{\beta} - \mu_{i+1}} \leq \left(\frac{\mu_{i+1}}{\mu_{i-s+j}}\right)^{2\ell} \frac{\mu_{i-s+j} - \tilde{\theta}}{\tilde{\theta} - \mu_{i+1}}, \tag{2.14}$$

which can be shown analogously to the proof of (2.9), i.e., by using an auxiliary vector $y \in \widetilde{\mathcal{Y}}$ and its orthogonal projections to $\mathrm{span}\{z_1, \ldots, z_{i-s+j}\}$ and $\mathrm{span}\{z_{i+1}, \ldots, z_n\}$. □

The estimate (2.12) is independent of angles and can provide a tighter bound compared to the estimate (2.2); cf. Experiment I in section 4. Moreover, (2.12) is only sharp in the case $j = s$ where it corresponds to the special version of a sharp estimate from [11] for the preconditioned inverse subspace iteration. Nevertheless, (2.12) provides an important cluster robust supplement to the estimates from [11] in the case $j < s$. We aim to improve (2.12) in future work concerning sharpness for $j < s$.

Additionally, we reformulate Theorem 2.8 for analyzing the inverse subspace iteration (1.6) with respect to the generalized eigenvalue problem $Ax = \lambda Mx$. The reformulation is based on the substitutions introduced in subsection 1.2.

Theorem 2.9. *Let $\lambda_1 \leq \cdots \leq \lambda_n$ be the eigenvalues of the pair (A, M) of symmetric and positive definite matrices $A, M \in \mathbb{R}^{n\times n}$. We consider the inverse subspace iteration* (1.6) *with* $\dim(\operatorname{span}\{X^{(0)}\}) = s$ *and denote by $\vartheta_j^{(\ell)}$ the j-th Ritz value in ascending order of (A, M) in the subspace iterate* $\operatorname{span}\{X^{(\ell)}\}$. *If $\lambda_i \leq \vartheta_s^{(0)} < \lambda_{i+1}$ for a certain $i \in \{s, \ldots, n-1\}$, then it holds that*

$$\frac{\vartheta_j^{(\ell)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_j^{(\ell)}} \leq \left(\frac{\lambda_{i-s+j}}{\lambda_{i+1}}\right)^{2\ell} \frac{\vartheta_s^{(0)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_s^{(0)}}. \tag{2.15}$$

3. Cluster robustness of the preconditioned inverse subspace iteration

The goal of this section is to generalize the new estimates from Theorem 2.6 and Theorem 2.8 to the preconditioned case. We consider the preconditioned inverse subspace iteration (1.4) with respect to its reciprocal representation (1.9).

3.1. Preconditioning.

The generalization of the new estimates is partially known, namely, for $j = s$, the estimate

$$\frac{\mu_i - \theta_s^{(\ell)}}{\theta_s^{(\ell)} - \mu_{i+1}} \leq \left(\gamma + (1-\gamma)\frac{\mu_{i+1}}{\mu_i}\right)^{2\ell} \frac{\mu_i - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{i+1}}. \tag{3.1}$$

can be derived by recursively applying (1.11) with $j = s$.

For the full generalization, we first review a proof sketch of (1.11) based on the analysis from [11, 1]. For convenience, we use the simplified formula

$$Y' = Y - N(Y - HY\Theta^{-1}) \tag{3.2}$$

of (1.9) where $Y = Y^{(\ell)}$ so that $\operatorname{span}\{Y'\} = \operatorname{span}\{Y^{(\ell+1)}\}$. Correspondingly, (1.11) with $j = s$ has the simplified form

$$\frac{\mu_i - \theta_s'}{\theta_s' - \mu_{i+1}} \leq \left(\gamma + (1-\gamma)\frac{\mu_{i+1}}{\mu_i}\right)^{2} \frac{\mu_i - \theta_s}{\theta_s - \mu_{i+1}} \tag{3.3}$$

where θ_s, θ_s' are the smallest Ritz values in $\operatorname{span}\{Y\}$, $\operatorname{span}\{Y'\}$ and γ comes from the condition $\|I - N\|_2 \leq \gamma < 1$. In the proof one can first show that Y' has the full rank s and is thus a basis matrix. Then a Ritz vector associated with θ_s' can be represented by $Y'c$ with $c \in \mathbb{R}^s \backslash \{0\}$. By using (3.2), one obtains the vector iteration

$$Y'c = Yc - N(Yc - HY\Theta^{-1}c).$$

A further reformulation

$$HY\Theta^{-1}c - Y'c = (I - N)(HY\Theta^{-1}c - Yc)$$

is necessary in order to apply known estimates for vector iterations such as (1.10). This leads to

$$\|Hy - Y'c\|_2 \leq \gamma \, \|Hy - \mu(y)y\|_2 \quad \text{with} \quad y = Y\Theta^{-1}c, \tag{3.4}$$

i.e., $Y'c$ is contained in a ball corresponding to one step of the iteration (1.8) with $y^{(\ell)} = y = Y\Theta^{-1}c$. Thus (1.10) is applicable and implies (3.3) by using $\mu(Y'c) = \theta_s'$ and $\mu(Y\Theta^{-1}c) \geq \theta_s$. In the case $j < s$, the same proof technique is applied to a j-dimensional subspace within $\operatorname{span}\{Y\}$. The resulting intermediate estimate can be combined with the Courant-Fischer principles so that (1.11) is shown.

Now we aim to formulate an argument which is similar to (3.4) and allows us to restrict the analysis from [11, 1] to the orthogonal complement of $\operatorname{span}\{z_{j+1}, \dots, z_s\}$. Therein one has to overcome the obstacle that the three vectors $Y'c$, $Y\Theta^{-1}c$ and $HY\Theta^{-1}c$ generally cannot be orthogonal to $z_{j+1}, \dots, z_s$ at the same time. With this aim in mind, we consider a scaling-invariant alternative of (3.4), namely,

$$\sin\angle(HY\Theta^{-1}c,\, Y'c) \leq \gamma \sin\angle(HY\Theta^{-1}c,\, Y\Theta^{-1}c)$$

which means that $Y'c$ belongs to a cone around $\operatorname{span}\{HY\Theta^{-1}c\}$; cf. [10, Theorem 2.2]. Moreover, this alternative is compatible with the analysis from [11, 1]. Further, we use the fact that $\operatorname{span}\{Y'\}$ would coincide with $\operatorname{span}\{HY\Theta^{-1}\} = \operatorname{span}\{HY\}$ in the special case $N = I$ (correspondingly, the new iterate in (1.4) is an approximate solution of a block linear system and coincides with the exact solution if $T = A^{-1}$). Thus, if $Y'c$ is a Ritz vector in $\operatorname{span}\{Y'\}$ associated with the smallest Ritz value, then $\operatorname{span}\{Y'c\}$ can be regarded as a perturbation of $\operatorname{span}\{HYd\}$ where HYd is a Ritz vector in $\operatorname{span}\{HY\}$ associated with the smallest Ritz value. Consequently, the quality of the preconditioner can be measured by

$$\sin\angle(HYd,\, Y'c) \leq \widetilde{\gamma} \sin\angle(HYd,\, Yd), \qquad \widetilde{\gamma} \in [0,\, 1). \tag{3.5}$$

Therein $\widetilde{\gamma} = 0$ corresponds to $N = I$. Based on the condition (3.5), we can analyze $Y'c$ within a cone corresponding to one step of the iteration (1.8) with $y^{(\ell)} = Yd$. Then an alternative of the estimate (3.3) with $\widetilde{\gamma}$ instead of γ can be derived. We remark that the condition (3.5) is inspired by the measure [17, (3.3)] for preconditioners of (slightly) indefinite matrices within an inexact Rayleigh quotient iteration. The parameter $\widetilde{\gamma}$ cannot simply be replaced by γ in the following estimates. The replacement is allowed in the special case that the eigenvectors of H are invariant with respect to N so that $Y'c$, $Y\Theta^{-1}c$ and $HY\Theta^{-1}c$ can belong to a same invariant subspace. Indeed, $\widetilde{\gamma}$ is slightly larger than γ within the numerical examples in section 4. A theoretical description of the relation between $\widetilde{\gamma}$ and γ possibly requires a generic constant for representing the angle between Yd and $Y\Theta^{-1}c$ so that the corresponding estimates would be asymptotic.

3.2. **An intermediate one-step estimate.** By setting similar conditions as (3.5) for certain subspaces which are orthogonal to $z_{j+1}, \dots, z_s$, an intermediate one-step estimate for the generalization of Theorem 2.6 has the following form.

Lemma 3.1. *Let $\mu_1 \geq \cdots \geq \mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H \in \mathbb{R}^{n\times n}$ with the associated orthonormal eigenvectors $z_1, \dots, z_n$. Furthermore, let $\theta_1 \geq \cdots \geq \theta_s$ be the Ritz values of H in the subspace $\operatorname{span}\{Y\}$ where the columns of Y are the associated orthonormal Ritz vectors. We consider the subspace iteration $Y' = Y - N(Y - HY\Theta^{-1})$ with $\Theta = \operatorname{diag}(\theta_1, \dots, \theta_s)$ and $N \in \mathbb{R}^{n\times n}$ satisfying $\|I - N\|_2 < 1$. Then the following hold:*

- (a) *Y' has full rank. Denoting by $\theta'_1 \geq \cdots \geq \theta'_s$ the Ritz values of H in $\operatorname{span}\{Y'\}$, it holds that $\theta'_j \geq \theta_j$, $j \in \{1, \dots, s\}$. If $\operatorname{span}\{Y\}$ contains no eigenvectors, then $\theta'_j > \theta_j$.*
- (b) *If $\theta_s > \mu_{s+1}$, then there exist unique vectors $y_k \in \operatorname{span}\{Y\}$, $y'_k \in \operatorname{span}\{Y'\}$ satisfying $z_i^T y_k = z_i^T y'_k = \delta_{ik}$ for $i, k \in \{1, \dots, s\}$. Furthermore, the matrices $Y_j = [y_1, \dots, y_j]$, $Y'_j = [y'_1, \dots, y'_j]$, $j \in \{1, \dots, s\}$ have the rank j.*
- (c) *Additionally, we denote by $\tilde{\theta}_j$, $\tilde{\theta}'_j$ the smallest Ritz values in $\operatorname{span}\{Y_j\}$, $\operatorname{span}\{Y'_j\}$, respectively. In the special case $N = I$, $\operatorname{span}\{Y'_j\}$ coincides with $\operatorname{span}\{HY_j\}$ so that a Ritz vector $Y'_j c_j$ associated with $\tilde{\theta}'_j$ can be represented by $HY_j d_j$. In the general case $N \approx I$, $Y'_j c_j$ can be regarded as a perturbation of $HY_j d_j$. If*

$$\sin\angle(HY_j d_j,\, Y'_j c_j) \leq \widetilde{\gamma} \sin\angle(HY_j d_j,\, Y_j d_j) \tag{3.6}$$

with $\widetilde{\gamma} \in [0, 1)$*, then it holds that*

$$\frac{\mu_j - \tilde{\theta}'_j}{\tilde{\theta}'_j - \mu_{s+1}} \leq \left(\widetilde{\gamma} + (1 - \widetilde{\gamma})\frac{\mu_{s+1}}{\mu_j}\right)^2 \frac{\mu_j - \tilde{\theta}_j}{\tilde{\theta}_j - \mu_{s+1}}. \tag{3.7}$$

Proof. (a) Since Y consists of s orthonormal Ritz vectors, Y has full rank. If Y' does not have full rank, then there exists a nonzero vector $c \in \mathbb{R}^s$ with $0 = Y'c = Yc - N(Yc - HY\Theta^{-1}c)$ so that $HY\Theta^{-1}c = (I - N)(HY\Theta^{-1}c - Yc)$ and

$$\|HY\Theta^{-1}c\|_2 \leq \|I - N\|_2 \|HY\Theta^{-1}c - Yc\|_2 < \|HY\Theta^{-1}c - Yc\|_2.$$

Therein $\|HY\Theta^{-1}c - Yc\|_2 \neq 0$ since otherwise $\|HY\Theta^{-1}c\|_2 = 0$ and thus $c = 0$. This inequality contradicts the fact

$$\|HY\Theta^{-1}c\|_2^2 = \|HY\Theta^{-1}c - Yc\|_2^2 + \|Yc\|_2^2 \geq \|HY\Theta^{-1}c - Yc\|_2^2$$

which follows from the orthogonality

$$(Yc)^T(HY\Theta^{-1}c - Yc) = c^TY^THY\Theta^{-1}c - c^TY^TYc = c^T\Theta\Theta^{-1}c - c^Tc = 0.$$

Thus Y' has full rank, and there are s Ritz values $\theta'_1 \geq \cdots \geq \theta'_s$ in $\operatorname{span}\{Y'\}$.

We consider further the subspaces $\operatorname{span}\{Y'E_j\}$, $j \in \{1, \ldots, s\}$ where $E_j \in \mathbb{R}^{s \times j}$ consists of the first j columns of the identity matrix $I_s \in \mathbb{R}^{s \times s}$. Therein $Y'E_j$ also has full rank, and it holds that

$$Y'E_j = YE_j - N(YE_j - HY\Theta^{-1}E_j) = YE_j - N(YE_j - HYE_j\Theta_j^{-1})$$

with $\Theta_j = \operatorname{diag}(\theta_1, \ldots, \theta_j)$. We denote by y' a Ritz vector in $\operatorname{span}\{Y'E_j\}$ associated with the smallest Ritz value, i.e. the j-th Ritz value in descending order because of $\dim(\operatorname{span}\{Y'E_j\}) = j$. Then $\operatorname{span}\{Y'E_j\} \subseteq \operatorname{span}\{Y'\}$ and the Courant-Fischer principles yield $\mu(y') \leq \theta'_j$. Furthermore, y' can be represented by $y' = Y'E_jc$ with a coefficient vector $c \in \mathbb{R}^j \backslash \{0\}$, and $Y'E_jc = YE_jc - N(YE_jc - HYE_j\Theta_j^{-1}c)$ implies

$$\|HYE_j\Theta_j^{-1}c - y'\|_2 \leq \|I - N\|_2 \|HYE_j\Theta_j^{-1}c - YE_jc\|_2. \tag{3.8}$$

Moreover, YE_jc is the orthogonal projection of $HYE_j\Theta_j^{-1}c$ to $\operatorname{span}\{YE_j\}$: the projection matrix is $P = (YE_j)(YE_j)^T$ according to $(YE_j)^T(YE_j) = E_j^TY^TYE_j = E_j^TE_j = I_j$ (identity matrix) so that

$$P\,(HYE_j\Theta_j^{-1}c) = YE_j\big(E_j^T(Y^THY)E_j\big)\Theta_j^{-1}c = YE_j\Theta_j\Theta_j^{-1}c = YE_jc.$$

Thus $\|HYE_j\Theta_j^{-1}c - YE_jc\|_2$ is the minimum of $\|HYE_j\Theta_j^{-1}c - YE_jd\|_2$ for $d \in \mathbb{R}^j$. We denote $YE_j\Theta_j^{-1}c$ by y and select $d = \mu(y)\,\Theta_j^{-1}c$, then it follows from (3.8) that

$$\|Hy - y'\|_2 \leq \|I - N\|_2 \|Hy - \mu(y)y\|_2 \leq \|Hy - \mu(y)y\|_2. \tag{3.9}$$

Next, $\|Hy - y'\|_2^2 \leq \|Hy - \mu(y)y\|_2^2$ implies

$$\begin{aligned}
&\|y'\|_2^2 - 2(Hy)^Ty' \leq \|\mu(y)y\|_2^2 - 2(Hy)^T\big(\mu(y)y\big) = -\mu(y)\,\|y\|_H^2 \\
\Rightarrow\quad &\mu(y)\,\|y'\|_2^2 \leq 2\big(\mu(y)y\big)^THy' - \|\mu(y)y\|_H^2 = \|y'\|_H^2 - \|y' - \mu(y)y\|_H^2 \leq \|y'\|_H^2 \\
\Rightarrow\quad &\mu(y) \leq \frac{\|y'\|_H^2}{\|y'\|_2^2} = \mu(y').
\end{aligned}$$

Furthermore, $y = YE_j\Theta_j^{-1}c$ belongs to $\operatorname{span}\{YE_j\}$, and the columns of YE_j are Ritz vectors associated with $\theta_1 \geq \cdots \geq \theta_j$. Thus $\theta_j \leq \mu(y) \leq \mu(y') \leq \theta'_j$. If $\operatorname{span}\{Y\}$ contains no eigenvectors, then the residual $Hy - \mu(y)y$ of $y \in \operatorname{span}\{YE_j\} \subseteq \operatorname{span}\{Y\}$ is nonzero so that the second inequality in (3.9) is strict. Hence $\|Hy - y'\|_2^2 < \|Hy - \mu(y)y\|_2^2$, which implies $\theta_j \leq \mu(y) < \mu(y') \leq \theta'_j$ analogously.

(b) If $\theta_s > \mu_{s+1}$, then also $\theta'_s > \mu_{s+1}$ according to (a). This ensures that $\angle(Y, Z)$ and $\angle(Y', Z)$ for $Z = [z_1, \dots, z_s]$ are both smaller than $\pi/2$; cf. the proof of Theorem 2.6. Consequently, (b) follows from the first part of the proof of Lemma 2.3.

(c) For $N = I$, we have $Y' = HY\Theta^{-1}$ so that $\operatorname{span}\{Y'\} = \operatorname{span}\{HY\}$. Then HY can be used as a basis matrix of $\operatorname{span}\{Y'\}$ in order to represent the unique vectors y'_k, $k \in \{1, \dots, s\}$ mentioned in (b). Therein (cf. the proof of Lemma 2.3)

$$y'_k = HYg'_k \;\Rightarrow\; e_k = Z^T y'_k = Z^T HY g'_k = (HZ)^T Y g'_k = (ZD)^T Y g'_k = D(Z^T Y) g'_k$$

with $D = \operatorname{diag}(\mu_1, \dots, \mu_s)$. Thus

$$g'_k = (Z^T Y)^{-1} D^{-1} e_k = (Z^T Y)^{-1} \mu_k^{-1} e_k \quad\Rightarrow\quad y'_k = \mu_k^{-1} HY (Z^T Y)^{-1} e_k.$$

Moreover, y_k has the representation $Y(Z^T Y)^{-1} e_k$ so that $y'_k = \mu_k^{-1} H y_k$. Correspondingly, it holds that

$$\operatorname{span}\{Y'_j\} = \operatorname{span}\{y'_1, \dots, y'_j\} = \operatorname{span}\{\mu_1^{-1} H y_1, \dots, \mu_j^{-1} H y_j\} = \operatorname{span}\{HY_j\}.$$

Then $Y'_j c_j$ belongs to $\operatorname{span}\{HY_j\}$ and has the representation $HY_j d_j$.

For $N \approx I$, the assumption (3.6) means that $Y'_j c_j$ is contained in a cone around the axis $\operatorname{span}\{HY_j d_j\}$. By considering a sphere centred at a point on the axis and tangent to the cone, the inequality

$$\|Hy - y'\|_2 \le \widetilde{\gamma} \|Hy - \mu(y) y\|_2 \tag{3.10}$$

holds for some y, y' which are collinear to $Y_j d_j$, $Y'_j c_j$, respectively. By construction, $\operatorname{span}\{Y_j\}$ and $\operatorname{span}\{Y'_j\}$ are orthogonal to the eigenvectors $z_{j+1}, \dots, z_s$. Thus the further analysis can be restricted to the orthogonal complement of $\operatorname{span}\{z_{j+1}, \dots, z_s\}$. Therein it can be shown that two auxiliary vectors $\widetilde{y}$, $\widetilde{y}'$ exist in a two-dimensional invariant subspace and satisfy

$$\mu(\widetilde{y}) = \mu(y), \quad \mu(\widetilde{y}') \le \mu(y'), \quad \sin\angle(H\widetilde{y}, \widetilde{y}') = \widetilde{\gamma} \sin\angle(H\widetilde{y}, \widetilde{y}),$$

analogously to [1, Lemma 4.1]. Next, the mini-dimensional analysis in [1, Lemma 4.2] is applicable and implies $\mu(\widetilde{y}') \ge \mu(\widetilde{y})$. More precisely, it holds that

$$\left(\frac{\mu_{k_1} - \mu(\widetilde{y}')}{\mu(\widetilde{y}') - \mu_{k_2}}\right)\left(\frac{\mu_{k_1} - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{k_2}}\right)^{-1} \le \left(\widetilde{\gamma} + (1 - \widetilde{\gamma})\frac{\mu_{k_2}}{\mu_{k_1}}\right)^2 \tag{3.11}$$

with the eigenvalues $\mu_{k_2} < \mu_{k_1}$ corresponding to the invariant subspace. Furthermore, y' is collinear to $Y'_j c_j$ so that $\mu(y')$ coincides with the Ritz value $\tilde{\theta}'_j$. Then $\mu(y') = \tilde{\theta}'_j \le \mu_j$ by using the Courant-Fischer principles. The estimate (3.7) holds trivially if $\tilde{\theta}'_j = \mu_j$. In the nontrivial case $\tilde{\theta}'_j < \mu_j$, we sum up the known relations

$$\mu_{k_2} \le \mu_{s+1} < \theta_s \le \tilde{\theta}_j \le \mu(y) = \mu(\widetilde{y}) \le \mu(\widetilde{y}') \le \mu(y') = \tilde{\theta}'_j < \mu_j \le \mu_{k_1} \tag{3.12}$$

where the first and the last inequalities are based on the fact that μ_j and μ_{s+1} are neighboring eigenvalues in the restricted analysis. Combining this with monotonicity arguments extends

(3.11) to

$$
\begin{aligned}
&\left(\frac{\mu_j-\tilde\theta'_j}{\tilde\theta'_j-\mu_{s+1}}\right)\left(\frac{\mu_j-\tilde\theta_j}{\tilde\theta_j-\mu_{s+1}}\right)^{-1}\le\left(\frac{\mu_j-\mu(\widetilde{y}\,')}{\mu(\widetilde{y}\,')-\mu_{s+1}}\right)\left(\frac{\mu_j-\mu(\widetilde{y})}{\mu(\widetilde{y})-\mu_{s+1}}\right)^{-1}\\
=&\left(\frac{\mu_j-\mu(\widetilde{y}\,')}{\mu_j-\mu(\widetilde{y})}\right)\left(\frac{\mu(\widetilde{y})-\mu_{s+1}}{\mu(\widetilde{y}\,')-\mu_{s+1}}\right)\le\left(\frac{\mu_{k_1}-\mu(\widetilde{y}\,')}{\mu_{k_1}-\mu(\widetilde{y})}\right)\left(\frac{\mu(\widetilde{y})-\mu_{k_2}}{\mu(\widetilde{y}\,')-\mu_{k_2}}\right)\\
=&\left(\frac{\mu_{k_1}-\mu(\widetilde{y}\,')}{\mu(\widetilde{y}\,')-\mu_{k_2}}\right)\left(\frac{\mu_{k_1}-\mu(\widetilde{y})}{\mu(\widetilde{y})-\mu_{k_2}}\right)^{-1}\\
\overset{(3.11)}{\le}&\left(\widetilde\gamma+(1-\widetilde\gamma)\frac{\mu_{k_2}}{\mu_{k_1}}\right)^2\le\left(\widetilde\gamma+(1-\widetilde\gamma)\frac{\mu_{s+1}}{\mu_j}\right)^2
\end{aligned}
$$

and yields (3.7). □

3.3. **Multistep estimates.** The intermediate estimate (3.7) can easily be extended to a one-step estimate concerning the Ritz values in the subspace iterates $\operatorname{span}\{Y\}$, $\operatorname{span}\{Y'\}$. However, the Ritz value in the extended bound is not the j-th Ritz value in descending order but the smallest Ritz value. Thus the bound is somewhat loose. Instead, a multistep extension is much more meaningful.

Theorem 3.2. *Let $\mu_1\ge\cdots\ge\mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H\in\mathbb{R}^{n\times n}$ with the associated orthonormal eigenvectors $z_1,\dots,z_n$. We consider the subspace iteration* (1.9) *with* $\dim(\operatorname{span}\{Y^{(0)}\})=s$ *and* $\|I-N\|_2<1$. *Then the following hold:*

(a) *Each* $\operatorname{span}\{Y^{(\ell)}\}$ *has the dimension s. Denoting by $\theta_1^{(\ell)}\ge\cdots\ge\theta_s^{(\ell)}$ the Ritz values of H in* $\operatorname{span}\{Y^{(\ell)}\}$, *it holds that $\theta_j^{(\ell+1)}\ge\theta_j^{(\ell)}$, $j\in\{1,\dots,s\}$. If* $\operatorname{span}\{Y^{(\ell)}\}$ *contains no eigenvectors, then $\theta_j^{(\ell+1)}>\theta_j^{(\ell)}$.*

(b) *If $\theta_s^{(0)}>\mu_{s+1}$, then each* $\operatorname{span}\{Y^{(\ell)}\}$ *contains unique vectors $y_k^{(\ell)}$ satisfying $z_i^Ty_k^{(\ell)}=\delta_{ik}$ for $i,\,k\in\{1,\dots,s\}$. Furthermore, the matrix $Y_j^{(\ell)}=[y_1^{(\ell)},\dots,y_j^{(\ell)}]$, $j\in\{1,\dots,s\}$ has the rank j.*

(c) *Additionally, we denote by $Y_j^{(\ell+1)}c^{(\ell)}$ a Ritz vector in* $\operatorname{span}\{Y_j^{(\ell+1)}\}$ *associated with the smallest Ritz value. In the special case $N=I$,* $\operatorname{span}\{Y_j^{(\ell+1)}\}$ *coincides with* $\operatorname{span}\{HY_j^{(\ell)}\}$ *so that the vector $Y_j^{(\ell+1)}c^{(\ell)}$ can be represented by $HY_j^{(\ell)}d^{(\ell)}$. In the general case $N\approx I$, $Y_j^{(\ell+1)}c^{(\ell)}$ can be regarded as a perturbation of $HY_j^{(\ell)}d^{(\ell)}$. If*

$$\sin\angle\big(HY_j^{(\ell)}d^{(\ell)},\,Y_j^{(\ell+1)}c^{(\ell)}\big)\le\widetilde\gamma\sin\angle\big(HY_j^{(\ell)}d^{(\ell)},\,Y_j^{(\ell)}d^{(\ell)}\big)$$

with $\widetilde\gamma\in[0,\,1)$ for each $\ell<L$, then it holds that

$$\frac{\mu_j-\theta_j^{(L)}}{\theta_j^{(L)}-\mu_{s+1}}\le\left(\widetilde\gamma+(1-\widetilde\gamma)\frac{\mu_{s+1}}{\mu_j}\right)^{2L}\frac{\mu_j-\theta_s^{(0)}}{\theta_s^{(0)}-\mu_{s+1}}. \tag{3.13}$$

Proof. (a) and (b) follow trivially from the corresponding parts of Lemma 3.1. For (c), we denote by $\tilde\theta_j^{(\ell)}$ the smallest Ritz value in $\operatorname{span}\{Y_j^{(\ell)}\}$ for each ℓ. Then recursively applying the estimate (3.7) from Lemma 3.1 implies

$$\frac{\mu_j-\tilde\theta_j^{(L)}}{\tilde\theta_j^{(L)}-\mu_{s+1}}\le\left(\widetilde\gamma+(1-\widetilde\gamma)\frac{\mu_{s+1}}{\mu_j}\right)^{2L}\frac{\mu_j-\tilde\theta_j^{(0)}}{\tilde\theta_j^{(0)}-\mu_{s+1}}.$$

Combining this with $\theta_j^{(L)}\ge\tilde\theta_j^{(L)}$ and $\tilde\theta_j^{(0)}\ge\theta_s^{(0)}$ (based on $\operatorname{span}\{Y_j^{(\ell)}\}\subseteq\operatorname{span}\{Y^{(\ell)}\}$ for each ℓ and the Courant-Fischer principles) yields (3.13). □

Analogously to Theorem 2.8, a multistep estimate for arbitrarily located $\theta_s^{(0)}$ can also be derived. Therein we construct auxiliary subspaces by subspace intersections and apply some arguments from the proof of Lemma 3.1.

Theorem 3.3. *Let $\mu_1 \geq \cdots \geq \mu_n$ be the eigenvalues of the symmetric and positive definite matrix $H \in \mathbb{R}^{n\times n}$ with the associated orthonormal eigenvectors $z_1,\ldots,z_n$. We consider the subspace iteration* (1.9) *with* $\dim(\operatorname{span}\{Y^{(0)}\}) = s$ *and* $\|I-N\|_2 < 1$*, and denote (according to (a) from Theorem 3.2) by $\theta_1^{(\ell)} \geq \cdots \geq \theta_s^{(\ell)}$ the Ritz values of H in* $\operatorname{span}\{Y^{(\ell)}\}$*. Let $\mathcal{Y}_j^{(\ell)}$ be the intersection* $\operatorname{span}\{Y^{(\ell)}\} \cap \operatorname{span}\{z_1,\ldots,z_{i-s+j},z_{i+1},\ldots,z_n\}$ *for $j \in \{1,\ldots,s\}$ and $i \in \{s,\ldots,n-1\}$. Then each $\mathcal{Y}_j^{(\ell)}$ has at least the dimension j. Additionally, we denote by $y_j^{(\ell)}$ a Ritz vector in $\mathcal{Y}_j^{(\ell)}$ associated with the smallest Ritz value. In the special case $N=I$, $\mathcal{Y}_j^{(\ell+1)}$ coincides with $H\mathcal{Y}_j^{(\ell)}$ so that $y_j^{(\ell+1)}$ can be represented by Hy with a certain $y \in \mathcal{Y}_j^{(\ell)}\backslash\{0\}$. In the general case $N \approx I$, $y_j^{(\ell+1)}$ can be regarded as a perturbation of Hy. If $\mu_i \geq \theta_s^{(0)} > \mu_{i+1}$ and*

$$\sin\angle\big(Hy,\, y_j^{(\ell+1)}\big) \leq \widetilde{\gamma}\sin\angle\big(Hy,\, y\big)$$

with $\widetilde{\gamma} \in [0,\,1)$ for each $y_j^{(\ell+1)}$, $\ell < L$ and the corresponding y, then it holds that

$$\frac{\mu_{i-s+j}-\theta_j^{(L)}}{\theta_j^{(L)}-\mu_{i+1}} \leq \left(\widetilde{\gamma}+(1-\widetilde{\gamma})\frac{\mu_{i+1}}{\mu_{i-s+j}}\right)^{2L} \frac{\mu_{i-s+j}-\theta_s^{(0)}}{\theta_s^{(0)}-\mu_{i+1}}. \tag{3.14}$$

Proof. According to (a) from Theorem 3.2, each $\operatorname{span}\{Y^{(\ell)}\}$ has the dimension s. Analogously to (2.13), a dimension comparison shows that each $\mathcal{Y}_j^{(\ell)}$ has at least the dimension j. For $N=I$, we have $\operatorname{span}\{Y^{(\ell+1)}\} = \operatorname{span}\{HY^{(\ell)}\} = H\operatorname{span}\{Y^{(\ell)}\}$ so that

$$\begin{aligned}\mathcal{Y}_j^{(\ell+1)} &= \operatorname{span}\{Y^{(\ell+1)}\} \cap \operatorname{span}\{z_1,\ldots,z_{i-s+j},z_{i+1},\ldots,z_n\}\\ &= \big(H\operatorname{span}\{Y^{(\ell)}\}\big) \cap \big(H\operatorname{span}\{z_1,\ldots,z_{i-s+j},z_{i+1},\ldots,z_n\}\big) = H\mathcal{Y}_j^{(\ell)}\end{aligned}$$

and there exists a $y \in \mathcal{Y}_j^{(\ell)}\backslash\{0\}$ with $y_j^{(\ell+1)} = Hy$. For $N \approx I$, the estimate (3.14) holds trivially if $\theta_j^{(L)} \geq \mu_{i-s+j}$. In the nontrivial case $\theta_j^{(L)} < \mu_{i-s+j}$, we have $\theta_j^{(\ell+1)} < \mu_{i-s+j}$ for $\ell < L$ since the sequence $(\theta_j^{(\ell)})_{\ell\in\mathbb{N}}$ is nondecreasing according to (a) from Theorem 3.2. The smallest Ritz value in $\mathcal{Y}_j^{(\ell+1)}$, i.e. $\mu(y_j^{(\ell+1)})$, is not larger than the j-th Ritz value (in descending order) in $\mathcal{Y}_j^{(\ell+1)}$ because of $\dim\mathcal{Y}_j^{(\ell+1)} \geq j$. Then $\mu(y_j^{(\ell+1)}) \leq \theta_j^{(\ell+1)}$ by using $\mathcal{Y}_j^{(\ell+1)} \subseteq \operatorname{span}\{Y^{(\ell+1)}\}$ and the Courant-Fischer principles. Furthermore, the arguments (for $N \approx I$) in the part (c) of the proof of Lemma 3.1 are applicable after slight reformulation. In particular, the sine assumption formally leads to (3.10) and (3.11), and the relations in (3.12) correspond to

$$\begin{aligned}\mu_{k_2} \leq \mu_{i+1} < \theta_s^{(0)} &\leq \mu(y_j^{(\ell)}) \leq \mu(y) = \mu(\widetilde{y})\\ &\leq \mu(\widetilde{y}') \leq \mu(y') = \mu(y_j^{(\ell+1)}) < \mu_{i-s+j} \leq \mu_{k_1}.\end{aligned}$$

Subsequently, an extension of (3.11) implies

$$\left(\frac{\mu_{i-s+j}-\mu(y_j^{(\ell+1)})}{\mu(y_j^{(\ell+1)})-\mu_{i+1}}\right) \leq \left(\widetilde{\gamma}+(1-\widetilde{\gamma})\frac{\mu_{i+1}}{\mu_{i-s+j}}\right)^{2} \left(\frac{\mu_{i-s+j}-\mu(y_j^{(\ell)})}{\mu(y_j^{(\ell)})-\mu_{i+1}}\right)$$

and further

$$\left(\frac{\mu_{i-s+j}-\mu(y_j^{(L)})}{\mu(y_j^{(L)})-\mu_{i+1}}\right) \leq \left(\widetilde{\gamma}+(1-\widetilde{\gamma})\frac{\mu_{i+1}}{\mu_{i-s+j}}\right)^{2L} \left(\frac{\mu_{i-s+j}-\mu(y_j^{(0)})}{\mu(y_j^{(0)})-\mu_{i+1}}\right).$$

Combining this with $\theta_j^{(L)} \geq \mu(y_j^{(L)})$ and $\mu(y_j^{(0)}) \geq \theta_s^{(0)}$ yields (3.14). $\square$

Remark 3.4. The parts (b) and (c) of Theorem 3.2 can be included in Theorem 3.3 as a special case, because the intersection $\mathcal{Y}_j^{(\ell)}$ in the case $i = s$, i.e.

$$\mathcal{Y}_j^{(\ell)} = \operatorname{span}\{Y^{(\ell)}\} \cap \operatorname{span}\{z_1, \ldots, z_j, z_{s+1}, \ldots, z_n\},$$

coincides with the subspace $\operatorname{span}\{Y_j^{(\ell)}\} \subseteq \operatorname{span}\{Y^{(\ell)}\}$ from Theorem 3.2. This can be proved as follows: By definition, the orthogonality between $\operatorname{span}\{Y_j^{(\ell)}\}$ and $\operatorname{span}\{z_{j+1}, \ldots, z_s\}$ holds and implies $\operatorname{span}\{Y_j^{(\ell)}\} \subseteq \operatorname{span}\{z_1, \ldots, z_j, z_{s+1}, \ldots, z_n\}$ so that $\operatorname{span}\{Y_j^{(\ell)}\} \subseteq \mathcal{Y}_j^{(\ell)}$. Furthermore, for $i = s$, the assumption on $\theta_s^{(0)}$ reads $\mu_s \geq \theta_s^{(0)} > \mu_{s+1}$. Then $\theta_s^{(\ell)} > \mu_{s+1}$ for each ℓ since the sequence $(\theta_s^{(\ell)})_{\ell \in \mathbb{N}}$ is nondecreasing according to (a) from Theorem 3.2. Consequently, the dimension of $\mathcal{Y}_j^{(\ell)}$ cannot exceed j, since otherwise the smallest Ritz value of H in $\mathcal{Y}_j^{(\ell)}$ can be interpreted as the k-th Ritz value $\tilde{\theta}_k$ in descending order with $k \geq j+1$. Since $\mathcal{Y}_j^{(\ell)}$ is a subset of the invariant subspace $\operatorname{span}\{z_1, \ldots, z_j, z_{s+1}, \ldots, z_n\}$, the Courant-Fischer principles imply the relation $\mu_{s+(k-j)} \geq \tilde{\theta}_k$ so that $\theta_s^{(\ell)} > \mu_{s+1} \geq \mu_{s+(k-j)} \geq \tilde{\theta}_k$. This contradicts $\theta_s^{(\ell)} \leq \tilde{\theta}_k$ which is based on the fact that $\theta_s^{(\ell)}$ is the smallest Ritz value of H in $\operatorname{span}\{Y^{(\ell)}\}$ and $\mathcal{Y}_j^{(\ell)} \subseteq \operatorname{span}\{Y^{(\ell)}\}$. Thus $\dim(\mathcal{Y}_j^{(\ell)}) \leq j$, and $j = \dim(\operatorname{span}\{Y_j^{(\ell)}\}) \leq \dim(\mathcal{Y}_j^{(\ell)}) \leq j$ because of $\operatorname{span}\{Y_j^{(\ell)}\} \subseteq \mathcal{Y}_j^{(\ell)}$. Then the dimension inequalities turn into equalities so that $\operatorname{span}\{Y_j^{(\ell)}\}$ and $\mathcal{Y}_j^{(\ell)}$ coincide.

3.4. **Multistep estimates with respect to $Ax = \lambda Mx$.** We reformulate the new multistep estimates from Theorems 3.2, 3.3 for the generalized eigenvalue problem $Ax = \lambda Mx$. Therein we merge Theorem 3.3 with only the part (a) of Theorem 3.2, since the other two parts correspond to a special case of Theorem 3.3.

Theorem 3.5. *Let $\lambda_1 \leq \cdots \leq \lambda_n$ be the eigenvalues of the pair (A, M) of symmetric and positive definite matrices $A, M \in \mathbb{R}^{n \times n}$ with the associated A-orthonormal eigenvectors $v_1, \ldots, v_n$. We consider the preconditioned inverse subspace iteration* (1.4) *with* $\dim(\operatorname{span}\{X^{(0)}\}) = s$ *and* $\|I - TA\|_A < 1$. *Then the following hold:*

(a) *Each* $\operatorname{span}\{X^{(\ell)}\}$ *has the dimension s. Denoting by $\vartheta_1^{(\ell)} \leq \cdots \leq \vartheta_s^{(\ell)}$ the Ritz values of (A, M) in* $\operatorname{span}\{X^{(\ell)}\}$, *it holds that $\vartheta_j^{(\ell+1)} \leq \vartheta_j^{(\ell)}$, $j \in \{1, \ldots, s\}$. If* $\operatorname{span}\{X^{(\ell)}\}$ *contains no eigenvectors, then $\vartheta_j^{(\ell+1)} < \vartheta_j^{(\ell)}$.*

(b) *Let $\mathcal{X}_j^{(\ell)}$ be the intersection* $\operatorname{span}\{X^{(\ell)}\} \cap \operatorname{span}\{v_1, \ldots, v_{i-s+j}, v_{i+1}, \ldots, v_n\}$ *for $j \in \{1, \ldots, s\}$ and $i \in \{s, \ldots, n-1\}$. Then each $\mathcal{X}_j^{(\ell)}$ has at least the dimension j. Additionally, we denote by $x_j^{(\ell)}$ a Ritz vector in $\mathcal{X}_j^{(\ell)}$ associated with the largest Ritz value. In the special case $T = A^{-1}$, $\mathcal{X}_j^{(\ell+1)}$ coincides with $A^{-1}M\mathcal{X}_j^{(\ell)}$ so that $x_j^{(\ell+1)}$ can be represented by $A^{-1}Mx$ with a certain $x \in \mathcal{X}_j^{(\ell)} \backslash \{0\}$. In the general case $T \approx A^{-1}$, $x_j^{(\ell+1)}$ can be regarded as a perturbation of $A^{-1}Mx$. If $\lambda_i \leq \vartheta_s^{(0)} < \lambda_{i+1}$ and*

$$\sin \angle_A\big(A^{-1}Mx,\, x_j^{(\ell+1)}\big) \leq \widetilde{\gamma} \sin \angle_A\big(A^{-1}Mx,\, x\big)$$

with $\widetilde{\gamma} \in [0,\, 1)$ for each $x_j^{(\ell+1)}$, $\ell < L$ and the corresponding x, then it holds that

$$\frac{\vartheta_j^{(L)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_j^{(L)}} \leq \left(\widetilde{\gamma} + (1 - \widetilde{\gamma})\frac{\lambda_{i-s+j}}{\lambda_{i+1}}\right)^{2L} \frac{\vartheta_s^{(0)} - \lambda_{i-s+j}}{\lambda_{i+1} - \vartheta_s^{(0)}}. \tag{3.15}$$

In addition, the estimates in Theorem 3.5 can be applied to the accelerated versions of the preconditioned inverse subspace iteration (1.4) such as the block preconditioned steepest descent iteration [15] and the locally optimal block preconditioned conjugate gradient method (LOBPCG) [8]. We note that the estimate (3.15) is only sharp in the case $j = s$ where it coincides with a sharp estimate from [11] for the preconditioned inverse subspace iteration. Nevertheless, (3.15) serves as a cluster robust supplement to the known estimates. It is still improvable concerning sharpness and extendable for advanced methods.

4. Numerical Experiments

We demonstrate the benefit of the new results by three numerical experiments. In Experiment I, we consider the block power method for a simple standard eigenvalue problem and compare the new estimate (2.12) with the known estimates (1.11) and (2.2). In Experiments II and III, the preconditioned inverse subspace iteration is tested within the AMP Eigensolver software [21]. Two generalized eigenvalue problems are derived from the finite element discretization of the Laplacian eigenvalue problem and used for the comparison of the new estimate (3.15) with the known estimate (1.5).

Experiment I. We use the diagonal matrix $H = \mathrm{diag}(\mu_1, \ldots, \mu_{6000})$ with six clustered eigenvalues close to 10 and 5994 equidistant eigenvalues in the interval $[1, 9]$, namely, $\mu_i = 10+(7-i)/100$ for $i \in \{1, \ldots, 6\}$ and $\mu_i = 9 - 8(i-7)/5993$ for $i \in \{7, \ldots, 6000\}$. The block power method $\mathrm{span}\{Y^{(\ell+1)}\} = \mathrm{span}\{HY^{(\ell)}\}$ is implemented for 1000 random initial subspaces $\mathrm{span}\{Y^{(0)}\}$ of dimension $s = 6$. We document the Ritz values $\theta_1^{(\ell)} \geq \cdots \geq \theta_6^{(\ell)}$ of each $\mathrm{span}\{Y^{(\ell)}\}$, $\ell \in \{0, \ldots, 156\}$. The numerical maxima of the distances $\mu_j - \theta_j^{(\ell)}$, $j \in \{1, \ldots, 6\}$ (over the 1000 samples) are illustrated by solid curves in Figure 1. Subsequently, we determine a lower bound of $\theta_j^{(\ell)}$ by using the estimate (2.12). Therein $\theta_s^{(0)}$ and the index will be implicitly updated if the current smallest Ritz value leaves the interval $(\mu_{i+1}, \mu_i]$. The numerical maxima of the distance between μ_j and this lower bound are plotted by bold curves. Similarly, we compute the numerical maxima of distances corresponding to the multistep form

$$\frac{\mu_i - \theta_j^{(\ell)}}{\theta_j^{(\ell)} - \mu_{i+1}} \leq \left(\frac{\mu_{i+1}}{\mu_i}\right)^{2\ell} \frac{\mu_i - \theta_j^{(0)}}{\theta_j^{(0)} - \mu_{i+1}} \tag{4.1}$$

of the classical sharp estimate (1.11) (for $\gamma = 0$) and the classical cluster robust estimate (2.2) (special form of [7, (2.20)]). These are displayed by dashed and dotted curves, respectively. Since the first six eigenvalues build a cluster, the convergence factor μ_{i+1}/μ_i from (4.1) is close to 1 in the final phase of the approximation of the first five eigenvalues. Thus the resulting dashed curves cannot reflect the cluster robustness. Each of (2.2) and (2.12) does not suffer this drawback, as the convergence factors μ_{s+1}/μ_j and μ_{i+1}/μ_{i-s+j} are sufficiently small in spite of the eigenvalue cluster. Furthermore, (2.12) provides a tighter bound. The overestimation of (2.2) might be caused by the extension of the intermediate estimate (2.3) in the derivation and by the possibly large tangent values similarly to the numerical example in [16, Section 2.1] for a Krylov subspace iteration. For $j = 6$, (4.1) coincides with (2.12) so that the dashed curve is covered by the bold curve. We also note that the actual convergence rates for approximating clustered eigenvalues are not always monotone with respect to the indices. In this experiment, the corresponding number of the required steps is minimal at $j = 3$ instead of $j = 1$.

Experiment II. We consider a generalized eigenvalue problem $Ax = \lambda Mx$ derived from an adaptive finite element discretization of the Laplacian eigenvalue problem introduced in Appendix I. We select the matrices from the 62nd grid with 1,567,785 degrees of freedom, and compare the estimates (3.15) and (1.5). Similarly to Experiment I, we implement the preconditioned inverse subspace iteration (1.4) for 1000 random initial subspaces $\mathrm{span}\{X^{(0)}\}$ of dimension $s = 6$. In contrast to the multigrid preconditioning used for solving matrix eigenvalue problems on a series of grids with up to 22,201,036 degrees of freedom during the adaptive finite element discretization, the preconditioning for the selected moderate-sized test problem is generated by the incomplete Cholesky factorization `C = ichol(A,struct('type','ict','droptol',1e-6))` in Matlab. This allows us to utilize a unique preconditioner for the 1000 tests. More precisely, the

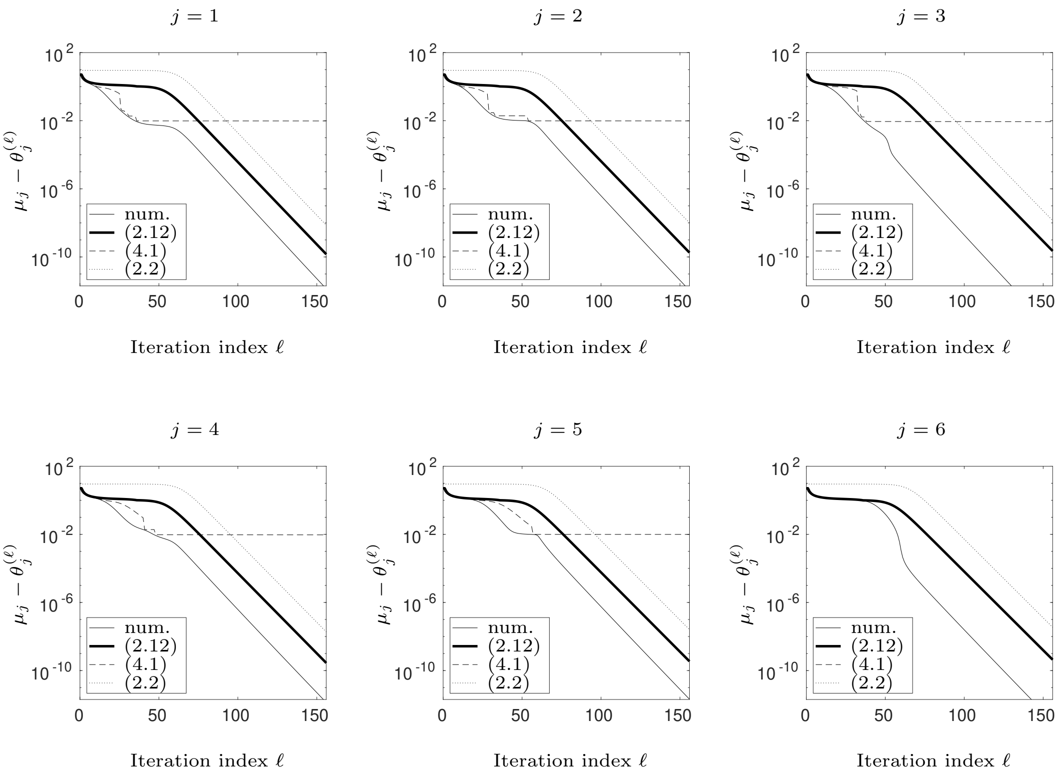

FIGURE 1. Comparison between the estimates (2.12), (4.1) and (2.2). Solid curves: numerical maxima of the distances $\mu_j - \theta_j^{(\ell)}$ over 1000 random initial subspaces. Bold curves: bounds based on (2.12). Dashed curves: bounds based on (4.1). Dotted curves: bounds based on (2.2).

product $B = CC^T$ yields an approximate of A and satisfies the traditional condition

$$\alpha(x^T Bx) \leq x^T Ax \leq \beta(x^T Bx) \quad \forall\, x \in \mathbb{R}^n$$

with $\alpha \approx 0.40$ and $\beta \approx 1.01$. The preconditioner T is then defined by $\big(2/(\beta+\alpha)\big)B^{-1}$ (but implemented by solving linear systems of matrices C, C^T) and satisfies the condition $\|I - TA\|_A \leq \gamma$ with $\gamma = (\beta-\alpha)/(\beta+\alpha) \approx 0.43$. The Ritz values $\vartheta_1^{(\ell)} \leq \cdots \leq \vartheta_6^{(\ell)}$ of $\operatorname{span}\{X^{(\ell)}\}$ are documented for $\ell \in \{0,\dots,60\}$. In Figure 2, we draw first the numerical maxima of the distances $\vartheta_j^{(\ell)} - \lambda_j$, $j \in \{1,\dots,6\}$ by solid curves. Subsequently, two upper bounds of $\vartheta_j^{(\ell)}$ are computed by using (3.15) and (1.5). Therein we rewrite the index L in (3.15) as ℓ so that (3.15) can easily be compared with the multistep form

$$\frac{\vartheta_j^{(\ell)} - \lambda_i}{\lambda_{i+1} - \vartheta_j^{(\ell)}} \leq \left(\gamma + (1-\gamma)\frac{\lambda_i}{\lambda_{i+1}}\right)^{2\ell} \frac{\vartheta_j^{(0)} - \lambda_i}{\lambda_{i+1} - \vartheta_j^{(0)}} \tag{4.2}$$

of (1.5). The quality parameter $\widetilde{\gamma} \approx 0.46$ required for (3.15) is determined by maximizing the sine quotient $\sin\angle_A\big(A^{-1}Mx,\, x_j^{(\ell+1)}\big)/\sin\angle_A\big(A^{-1}Mx,\, x\big)$ for the auxiliary vectors introduced in Theorem 3.5 over the computed iterates. Analogously, we can determine the quality parameter $\gamma \approx 0.43$ for (4.2) by maximizing the quotient $\|\widetilde{w}_j\|_A/\|w_j\|_A$ for the j-th column $\widetilde{w}_j$ of $(X^{(\ell)} - TR^{(\ell)}) - A^{-1}MX^{(\ell)}\widehat{\Theta}^{(\ell)}$ and the j-th column w_j of $X^{(\ell)} - A^{-1}MX^{(\ell)}\widehat{\Theta}^{(\ell)}$ according to (1.4) and the relation

$$(X^{(\ell)} - TR^{(\ell)}) - A^{-1}MX^{(\ell)}\widehat{\Theta}^{(\ell)} = (I - TA)\big(X^{(\ell)} - A^{-1}MX^{(\ell)}\widehat{\Theta}^{(\ell)}\big).$$

For (3.15), an implicit update of $\vartheta_s^{(0)}$ and the index is made if the current largest Ritz value leaves the interval $[\lambda_i, \lambda_{i+1})$. The numerical maxima of the distances between λ_j and each of the upper bounds by (3.15) and (4.2) are plotted by bold and dashed curves. For $j \in \{1, \ldots, 5\}$, the bold curves give looser bounds than the dashed curves in the first several steps since the s-th Ritz value $\vartheta_s^{(0)}$ is used, but they are much steeper because of $\lambda_{i-s+j}/\lambda_{i+1} < \lambda_i/\lambda_{i+1}$ so that the bounds are tighter in total. Nevertheless, the dashed curves are clearly decreasing, since the smallest eigenvalues are well separated:

$$\lambda_1 \approx 8.895089, \quad \lambda_2 \approx 13.77993, \quad \lambda_3 \approx 21.63029, \quad \lambda_4 \approx 25.08266,$$

$$\lambda_5 \approx 29.64299, \quad \lambda_6 \approx 35.76182, \quad \lambda_7 \approx 44.90599, \quad \lambda_8 \approx 47.47379,$$

and the convergence factor in (4.2) is thus not close to 1. For $j = 6$, (3.15) and (4.2) have the same form except for the difference between $\widetilde{\gamma}$ and γ. Therefore the dashed curve is slightly better because of $\gamma < \widetilde{\gamma}$. Moreover, the observed actual convergence rates are monotone with respect to the indices. This corresponds to the strict monotonicity of the convergence factors $\lambda_{i-s+j}/\lambda_{i+1}$ since the relevant eigenvalues are well separated. In contrast to this, the weaker monotonicity caused by clustered eigenvalues in Experiment I can be disturbed by numerical errors.

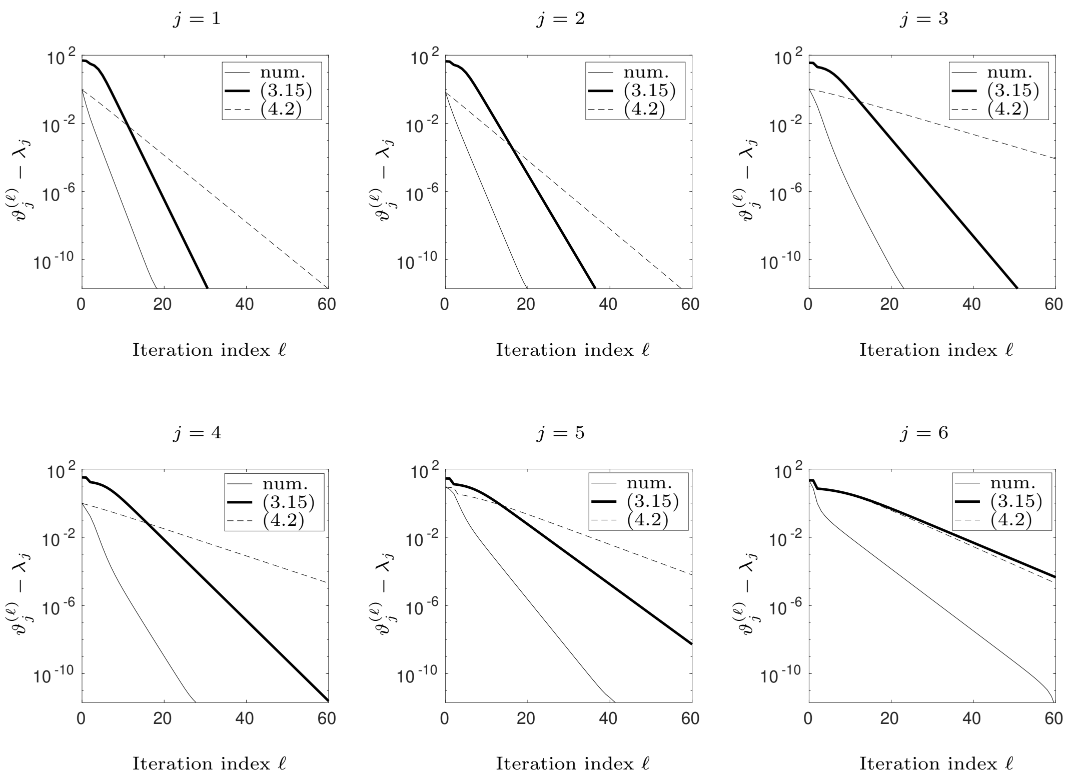

FIGURE 2. Comparison between the estimates (3.15) and (4.2) in Experiment II. Solid curves: numerical maxima of the distances $\vartheta_j^{(\ell)} - \lambda_j$ over 1000 random initial subspaces. Bold curves: bounds based on (3.15). Dashed curves: bounds based on (4.2).

Experiment III. We consider a generalized eigenvalue problem $Ax = \lambda Mx$ with clustered eigenvalues from Appendix II. We use the matrices from the 36th grid with 1,509,276 degrees of freedom for the comparison of the new estimate (3.15) with the multistep form (4.2) of the known estimate (1.5). The preconditioned inverse subspace iteration (1.4) is implemented for 1000 random initial subspaces span$\{X^{(0)}\}$ of dimension $s = 9$. The preconditioner for A is generated by `C = ichol(A,struct('type','ict','droptol',3e-6))` in Matlab. The resulting approximate $B = CC^T$ satisfies the traditional condition $\alpha(x^T Bx) \le x^T Ax \le \beta(x^T Bx)\ \forall\ x \in \mathbb{R}^n$ with $\alpha \approx 0.41$ and $\beta \approx 1.27$, whereas the preconditioner $T = \big(2/(\beta+\alpha)\big)B^{-1}$ satisfies $\|I - TA\|_A \le \gamma$ with the quality parameter $\gamma = (\beta-\alpha)/(\beta+\alpha) \approx 0.51$ for (4.2). Moreover, the quality parameter for (3.15) has the value $\widetilde{\gamma} \approx 0.53$. In Figure 3, the numerical maxima of the distances $\vartheta_j^{(\ell)} - \lambda_j$, $j \in \{1,\dots,9\}$ between Ritz values and eigenvalues are displayed by solid curves. Additionally, two upper bounds for $\vartheta_j^{(\ell)}$ are determined by (3.15) and (4.2). Their distances to λ_j are illustrated by bold and dashed curves. Since the nine smallest eigenvalues build two clusters, namely,

$$\lambda_1, \lambda_2, \lambda_3 \in (2.559876,\ 2.559941), \qquad \lambda_4, \dots, \lambda_9 \in (6.495853,\ 6.500676)$$

(whereas $\lambda_{10} \approx 11.62294$), the convergence factor in (4.2) is close to 1 for $i = j$ and $j \in \{1,2\} \cup \{4,\dots,8\}$ so that the dashed curves turn into nearly horizontal lines in the final phase and cannot predict the actual convergence. In contrast to this, (3.15) and the bold curves reflect the convergence behavior correctly. For $j \in \{3,9\}$, the dashed curves are appropriate because the two relevant eigenvalues in (4.2) belong to different clusters so that the convergence factor is bounded away from 1. The bold curves are slightly looser because of $\widetilde{\gamma} > \gamma$. On the whole, the estimate (3.15) is suitable for interpreting the cluster robustness of the preconditioned inverse subspace iteration.

5. Conclusion

The block implementation of gradient-type eigensolvers allows the simultaneous approximation of eigenpairs and prevents convergence deteriorations in the case of clustered eigenvalues. The cluster robustness can be explained by using an accompanying sequence of vectors which are orthogonal to the eigenspaces associated with certain interior eigenvalues. Typical examples are the classical estimates of the block power method [20] and the abstract block iteration [7]. Therein the orthogonality to the interior eigenspaces enables one to restrict the convergence analysis to a subspace in order to skip the most of the clustered eigenvalues. However, it is difficult to generalize these estimates directly to the corresponding preconditioned eigensolvers because the preconditioning disturbs the orthogonality.

In the present paper, we combine the above orthogonal splitting with the geometric interpretation of preconditioning from [10, 1]. This results in cluster robust estimates for the preconditioned inverse subspace iteration. In the special case with exact preconditioning, a reciprocal representation of this iteration corresponds to the block power method. Therein we provide a new estimate in terms of Ritz values which improves an estimate from [7] with angle-type bounds. In the general case with inexact preconditioning, we use an assumption concerning perturbations of Ritz vectors from the special case. Then the resulting intermediate estimate in terms of Ritz values is applied recursively and leads to a cluster robust estimate. In comparison to the previous cluster robust estimates from [3, 18], our estimate has a weaker assumption and a simpler form. Its benefit compared to the one-step sharp estimate from [11] can easily be demonstrated by numerical experiments. Although the new results are also applicable to further preconditioned gradient-type eigensolvers, it seems possible and interesting to derive individual and more accurate estimates for each eigensolver in future work.

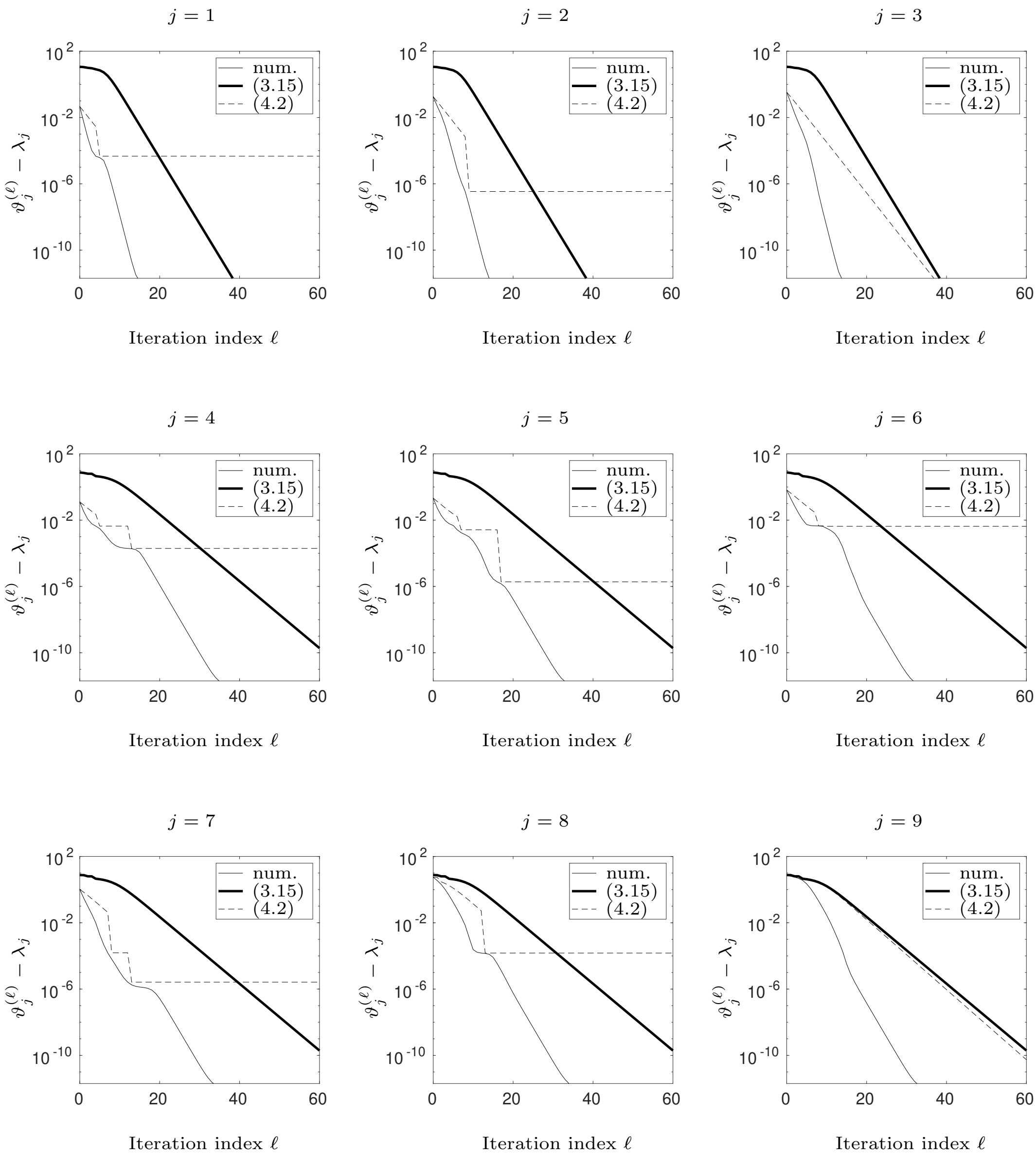

FIGURE 3. Comparison between the estimates (3.15) and (4.2) in Experiment III. Solid curves: numerical maxima of the distances $\vartheta_j^{(\ell)} - \lambda_j$ over 1000 random initial subspaces. Bold curves: bounds based on (3.15). Dashed curves: bounds based on (4.2).

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Appendix: Laplacian eigenvalue problem

I. For Experiment II in section 4, we consider the Laplacian eigenvalue problem $-\Delta u = \lambda u$ on a 2D mushroom-shaped domain shown in Figure 4. The boundary $\Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ is defined by

$$\Gamma_1 = \left\{ \left(\cos(t)+\tfrac{1}{3}\cos(3t),\, \sin(t)+\tfrac{1}{4}\sin(4t) \right)^T;\ t \in [0,\, 2\pi) \right\},$$

$$\Gamma_2 = \left\{ \left(\tfrac{4}{3}(1-t),\, 0 \right)^T;\ t \in (0,\, 1] \right\}, \qquad \Gamma_3 = \left\{ \left(\tfrac{4}{3}t,\, 0 \right)^T;\ t \in (0,\, 1) \right\}$$

where Γ_2 and Γ_3 correspond to the two sides of a slit along the horizontal axis. We set homogeneous Dirichlet boundary conditions on $\Gamma_1 \cup \Gamma_2$ and homogeneous Neumann boundary conditions on Γ_3. We combine an adaptive finite element discretization and the LOBPCG method [8] within the AMP Eigensolver software [21]. The initial grid leads to a matrix eigenvalue problem $Ax = \lambda Mx$ of dimension 5 which can easily be solved by matrix transformations. For the matrix pairs (A, M) from further grids, we compute the three smallest eigenvalues by using the LOBPCG method with the block size 3. In addition, the residual-based error estimator from [12] is applied to the computed eigenfunction approximations associated with the smallest eigenvalue in order to control the adaptive grid refinement. Since the corresponding eigenfunction has an unbounded derivative at the origin, the refinement depths increase rapidly near the origin; see Figure 4. Moreover, the preconditioners for the matrix eigenvalue problem are generated by multigrid iterations with the adaptively refined grids. The smallest matrix eigenvalues $\lambda_1^{(A,M)}$ from six grids are listed in Table 1.

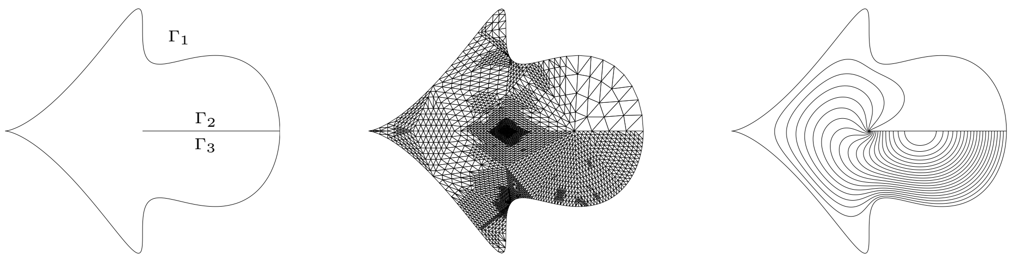

Figure 4. Model problem for Experiment II in section 4. Left: the $2D$ domain for the Laplacian eigenvalue problem $-\Delta u = \lambda u$ and its boundary in three parts. Center: the 23rd grid from the adaptive grid refinement. Right: the contour lines of an eigenfunction associated with the smallest eigenvalue.

Table 1. The smallest matrix eigenvalues $\lambda_1^{(A,M)}$ of the model problem for Experiment II in section 4 computed by using LOBPCG within AMP Eigensolver. These converge to the smallest operator eigenvalue $\lambda_1^{(-\Delta)} \approx 8.895049$.

level	1	23	36	51	62	78
nodes	27	3810	31504	390322	1572517	17712651
d.o.f.	5	3582	30838	387963	1567785	17696832
$\lambda_1^{(A,M)}$	12.33746	8.913402	8.897231	8.895217	8.895089	8.895050

II. For Experiment III in section 4, we need a model problem with clustered eigenvalues. For this purpose, we connect three circle domains by a thin annulus; see Figure 5. The circles have the same radius $r = 1.5$ and are centred at $(-\sqrt{3}, -1)^T$, $(\sqrt{3}, -1)^T$, $(0, 2)^T$, respectively. The annulus is centred at the origin with the radii $r_1 = 1.2$, $r_2 = 1.5$. We consider again the Laplacian eigenvalue problem $-\Delta u = \lambda u$ and set only homogeneous Dirichlet boundary conditions. Similarly to Appendix I, the AMP Eigensolver derives a sequence of matrix eigenvalue problems on 63 adaptively refined grids. The refinement is based on the residuals of the computed eigenfunction approximations associated with the three smallest eigenvalues. The eigenfunctions are partially similar to the well-known peak eigenfunction on the unit circle.

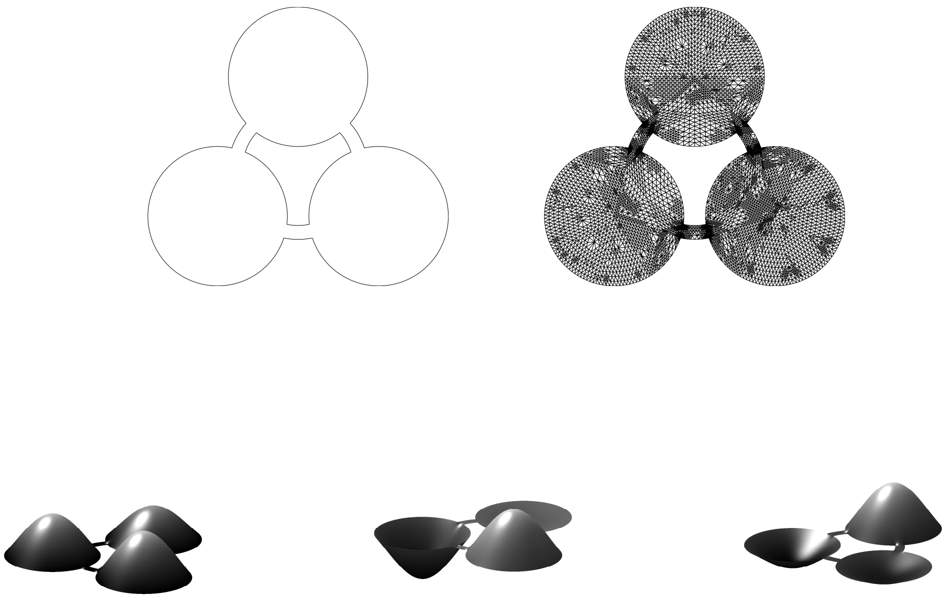

FIGURE 5. Model problem for Experiment III in section 4. Top left: the $2D$ domain for the Laplacian eigenvalue problem $-\Delta u = \lambda u$. Top right: the 12th grid from the adaptive grid refinement. Bottom: three eigenfunctions associated with the three smallest eigenvalues.

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