.

CONVERGENCE ANALYSIS OF RESTARTED KRYLOV SUBSPACE EIGENSOLVERS

KLAUS NEYMEYR* AND MING ZHOU*

Abstract. The A-gradient minimization of the Rayleigh quotient allows to construct robust and fast-convergent eigensolvers for the generalized eigenvalue problem for (A, M) with symmetric and positive definite matrices. The A-gradient steepest descent iteration is the simplest case of more general restarted Krylov subspace iterations for the special case that all step-wise generated Krylov subspaces are two-dimensional.

This paper contains a convergence analysis of restarted Krylov subspace iterations for the minimization of the Rayleigh quotient with Krylov subspaces of arbitrary dimensions. The eigenpair approximations, namely the Ritz vector and the Ritz value, are extracted in each step of the iteration by the Rayleigh-Ritz procedure. The new convergence analysis provides a sharp Ritz vector estimate together with a Ritz value estimate. These results improve the classical estimates by Kaniel and Saad (1966, 1980) and Parlett (1980) and generalize a result from Knyazev (1987).

Key words. Krylov subspace, Rayleigh quotient, Rayleigh-Ritz procedure, multigrid, elliptic eigenvalue problem.

1. Introduction. The computation of a limited number of the smallest eigenvalues of the generalized matrix eigenvalue problem

$$Ax = \lambda Mx, \qquad A, M \in \mathbb{R}^{n\times n} \tag{1.1}$$

for very high-dimensional, symmetric and positive definite matrices A and M is still a challenging problem. A typical source of (1.1) is the finite element discretization of an operator eigenvalue problem for a self-adjoint and elliptic partial differential operator. Then A is called the stiffness matrix and M the mass matrix. The numerical eigensolver should exploit the underlying structure of the operator eigenproblem and also of its mesh discretization. These structures justify the desire for near-optimal-complexity eigensolvers which allow to compute a fixed number of the smallest eigenvalues together with the eigenvectors with computational costs which, in the best case, linearly increase with the matrix dimension n. These requirements rule out any classical eigensolvers which are based on matrix transformations (like Jacobi, QR) with their above-linear growth of the computation times and memory requirements [1, 5, 23]. Vector iterations or subspace iterations are a better basis for the construction of efficient eigensolvers.

1.1. Gradient iterations for the Rayleigh quotient and Krylov subspace iterations. The main idea for the numerical computation of the smallest eigenvalues is to find some of the smallest stationary of Rayleigh quotient

$$\rho(x) = (x, Ax)/(x, Mx), \qquad x \in \mathbb{R}^n\backslash\{0\} \tag{1.2}$$

by means of a gradient type minimization of the form $x^{(\ell+1)} = x^{(\ell)} - \omega\nabla\rho\big(x^{(\ell)}\big)$. However, the gradient direction $\nabla\rho(\cdot)$ is well known to be a poor correction direction for the minimization of (1.2), see [11, 14], as the associated convergence factor tends to 1 for n increasing to infinity.

If the gradient vector is taken with respect to the A-geometry [3], then the correction direction is $A^{-1}\nabla\rho(\cdot)$. The iterative scheme based on A-gradients reads

$$x^{(\ell+1)} = x^{(\ell)} - \omega A^{-1}\nabla\rho\big(x^{(\ell)}\big). \tag{1.3}$$

Therein ω is a step-size parameter. Optimally, the step size is determined in a way that the Rayleigh quotient is minimized in the affine space $x^{(\ell)} + \mathrm{span}\big\{A^{-1}\nabla\rho\big(x^{(\ell)}\big)\big\}$.

*Universität Rostock, Institut für Mathematik, Ulmenstraße 69, 18055 Rostock, Germany,
April 29, 2016.

Computationally, this minimization problem is solved by the Rayleigh-Ritz procedure applied to the two-dimensional subspace

$$\operatorname{span}\{x^{(\ell)}, A^{-1}\nabla\rho(x^{(\ell)})\} = \operatorname{span}\{x^{(\ell)}, A^{-1}Mx^{(\ell)}\} \tag{1.4}$$

since $\nabla\rho(x) = (2/(x, Mx))(Ax - \rho(x)Mx)$. Then $x^{(\ell+1)}$ is the Ritz vector associated with the smallest Ritz value.

Next, we discuss a natural extension of the basic gradient iteration (1.3). The idea is to extend the subspace (1.4) to k-dimensional Krylov subspaces

$$\mathcal{K}^k(x^{(\ell)}) = \operatorname{span}\{x^{(\ell)}, A^{-1}Mx^{(\ell)}, \ldots, (A^{-1}M)^{k-1}x^{(\ell)}\}, \quad k \ll n.$$

For a fixed k, the minimization of the Rayleigh quotient in $\mathcal{K}^k(x^{(\ell)})$ results in the restarted Krylov subspace iteration scheme

$$x^{(\ell+1)} \quad \leftarrow \quad \mathrm{RR}_{\min}\big(\mathcal{K}^k(x^{(\ell)})\big). \tag{1.5}$$

Therein $\mathrm{RR}_{\min}(\mathcal{K})$ provides a Ritz vector which corresponds to the smallest Ritz value of (A, M) in $\mathcal{K}$.

The iteration (1.5) can be modified in various ways. For instance, the vector iterates $x^{(\ell)}$ can be substituted by subspaces $\mathcal{X}^{(\ell)}$ in order to compute not only a single eigenpair, but an invariant subspace which is associated with the smallest eigenvalues. Alternatively, the Krylov subspace $\mathcal{K}^k(x^{(\ell)})$ can be augmented with m previous iterates $x^{(\ell-1)}, x^{(\ell-2)}, \ldots, x^{(\ell-m)}$ in order to accelerate the convergence of the Rayleigh-Ritz procedure towards the smallest eigenvalue, see [2, 4, 22]. The usage of A^{-1} in the construction of the Krylov subspace amounts to the exact solution of linear systems in A which can result in high computational costs for a very large A. For mesh discretized operator eigenvalue problems, the discretization matrix A can be very large. Finite elements codes typically do not compute or store A explicitly. Instead, only a routine exists which computes for given x the vector Ax. The random access memory (RAM) of the computer is mainly used to store the grid information and local element matrices. A factorization of A is way too expensive and has an unmanageable storage requirement due to the fill-in. However, the linear systems can be solved approximately by using proper preconditioners [9, 14, 10]. Obviously, approximate linear solvers can reduce the computational costs significantly without a disproportionate deterioration of the convergence rate.

The convergence analysis of general *preconditioned* gradient type eigensolvers is considerably complicated by the spectral assumptions on the quality of the preconditioner. The extreme case that the preconditioner is substituted by the inverse A^{-1} is easier to analyze, see iteration (1.3) and the general scheme (1.5). In this paper, we derive sharp convergence estimates for the restarted Krylov iteration scheme (1.5). The Ritz value estimate improves the classical estimates for Ritz values in Krylov subspaces of arbitrary dimensions by Kaniel, Saad and Parlett [6, 22, 21]. It also generalizes a result for the Lanczos algorithm from Knyazev [8], Section 1.4 (the estimate is based on a similar estimate for an abstract vector iteration and is indirectly mentioned without explicit proof). The Ritz vector estimate extends our previous works [18, 17] on (preconditioned) steepest descent eigensolvers. Therefore, our results improve the basis for an analytic understanding of general preconditioned gradient eigensolvers.

1.2. The restarted Krylov iteration scheme (1.5) **for** $k = 2$**.** In order to discuss the convergence behavior of the iteration (1.5), we start with the basic case $k = 2$. For this case sharp convergence estimates have been presented in [18]. Next the main result from [18] is restated in a form which applies to the generalized eigenvalue problem $Ax = \lambda Mx$.

THEOREM 1.1. *Let $\lambda_1 < \lambda_2 < \ldots < \lambda_m$ $(m \le n)$ be the distinct eigenvalues (with arbitrary multiplicity) of the matrix pair (A, M) with symmetric and positive definite matrices $A, M \in \mathbb{R}^{n\times n}$. If the Rayleigh quotient $\rho(x)$ of a vector $x \in \mathbb{R}^n\backslash\{0\}$ belongs to* *the interval* $(\lambda_i, \lambda_{i+1})$ *and if* x' *is a Ritz vector associated with the smallest Ritz value of* (A, M) *in* $\operatorname{span}\{x, A^{-1}Mx\}$, *then it holds that*

$$\frac{\rho(x') - \lambda_i}{\lambda_{i+1} - \rho(x')} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \frac{\rho(x) - \lambda_i}{\lambda_{i+1} - \rho(x)} \quad \text{with} \quad \kappa = \frac{\lambda_i(\lambda_m - \lambda_{i+1})}{\lambda_{i+1}(\lambda_m - \lambda_i)}.$$

Further, if x *is not* M*-orthogonal to the eigenspace* $\mathcal{E}_1$ *of* (A, M) *associated with the eigenvalue* λ_1, *then it holds that*

$$\tan \angle_M(x', \mathcal{E}_1) \leq \frac{\lambda_1(\lambda_m - \lambda_2)}{\lambda_2(\lambda_m - \lambda_1)} \tan \angle_M(x, \mathcal{E}_1).$$

Therein $\angle_M$ *denotes angles with respect to the* M *inner product, i.e.*

$$\angle_M(x, y) = \arccos \frac{(x, y)_M}{\|x\|_M \, \|y\|_M} \quad \text{with} \quad (x, y)_M = x^T M y, \quad \|x\|_M = (x, x)_M^{1/2}$$

for nonzero vectors $x, y \in \mathbb{R}^n$, *and* $\angle_M(x, \mathcal{U}) = \angle_M(x, \widetilde{x})$ *with the* M*-orthogonal projection* $\widetilde{x}$ *of* x *to* $\mathcal{U}$ *for a given subspace* $\mathcal{U} \subseteq \mathbb{R}^n$.

The two convergence factors in Theorem 1.1 depend on eigenvalue gap ratios. Particularly, the $\tan \angle_M(x', \mathcal{E}_1)$ estimate can be written by recursive application in the form of the a priori estimate

$$\tan \angle_M(x^{(\ell)}, \mathcal{E}_1) \leq \left(\frac{\lambda_1(\lambda_m - \lambda_2)}{\lambda_2(\lambda_m - \lambda_1)}\right)^{\ell} \tan \angle_M(x^{(0)}, \mathcal{E}_1). \tag{1.6}$$

1.3. Reduction to the standard eigenvalue problem. In order to simplify the following analysis, we transform the generalized eigenvalue problem to a standard one by means of the substitutions

$$y := A^{1/2}x, \quad H := A^{-1/2}MA^{-1/2}, \quad \mathcal{W}_1 := A^{1/2}\mathcal{E}_1 \text{ and } \mu(y) := \frac{y^T H y}{y^T y}.$$

These replacements imply that

$$\operatorname{span}\{y, Hy\} = A^{1/2}\operatorname{span}\{x, A^{-1}Mx\}, \quad \angle_H(y, \mathcal{W}_1) = \angle_M(x, \mathcal{E}_1), \text{ and } \mu(y) = \frac{1}{\rho(x)}.$$

Further, we denote the eigenvalues of H by μ_i. Thus $\mu_i = 1/\lambda_i$. Theorem 1.1 for the standard eigenvalue problem for H with the eigenvalues μ_i reads:

THEOREM 1.2. *Let* $\mu_1 > \mu_2 > \ldots > \mu_m$ *be the distinct eigenvalues of the symmetric and positive definite matrix* $H \in \mathbb{R}^{n \times n}$. *Let* $y \in \mathbb{R}^n \backslash \{0\}$ *satisfy*

$$\mu(y) = \frac{y^T H y}{y^T y} \in (\mu_{i+1}, \mu_i),$$

and let y' *be a Ritz vector associated with the largest Ritz value of* H *in* $\operatorname{span}\{y, Hy\}$, *then*

$$\frac{\mu_i - \mu(y')}{\mu(y') - \mu_{i+1}} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \frac{\mu_i - \mu(y)}{\mu(y) - \mu_{i+1}} \quad \text{with} \quad \kappa = \frac{\mu_{i+1} - \mu_m}{\mu_i - \mu_m}. \tag{1.7}$$

If y *is not* H*-orthogonal to the eigenspace* $\mathcal{W}_1$ *with respect to* μ_1, *then it holds that*

$$\tan \angle_H(y', \mathcal{W}_1) \leq \frac{\mu_2 - \mu_m}{\mu_1 - \mu_m} \tan \angle_H(y, \mathcal{W}_1). \tag{1.8}$$

1.4. Aim and overview of the paper. The goal of this paper is to generalize the estimates for the A-gradient iteration of Theorem 1.1 to the general case of the restarted Krylov subspace iteration (1.5) for any $k \geq 2$. Error estimates for Ritz values and Ritz vectors in $\operatorname{span}\{y, Hy\}$ are generalized to their counterparts with respect to the Krylov subspace $\operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ for $k \geq 2$.

The remaining part of the paper is organized as follows: First, Section 2 contains a review and comparison of known error estimates on Ritz values and Ritz vectors in Krylov subspaces. The new convergence estimates on the iteration (1.5) are presented in Section 3. Finally, Section 4 is devoted to numerical experiments with the iteration (1.5) for various mesh discretizations of an elliptic operator eigenvalue problem. The sharpness of the new estimates is demonstrated.

2. Error estimates on Ritz pairs in Krylov subspaces. Next, we review Ritz value estimates and Ritz vector estimates as presented by Kaniel and Saad [6, 22] and in their revised form by Parlett in Theorem 12.4.1 in [21]. This latter result is now reproduced in the same notation as used in Theorem 1.2.

THEOREM 2.1. *Let $\mu_1 > \mu_2 > \ldots > \mu_m$ be the distinct eigenvalues (with arbitrary multiplicity) of the symmetric matrix $H \in \mathbb{R}^{n\times n}$. Let w_i be the orthogonal projection of a vector $y \in \mathbb{R}^n\backslash\{0\}$ to the eigenspace $\mathcal{W}_i$ associated with μ_i, $i = 1, \ldots, m$. Let $w_i \neq 0$ and $z_i = w_i/\|w_i\|$ so that z_i is a normalized eigenvector associated with μ_i.*

If the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ is not H-invariant, then it holds that

$$\mu_i - \theta_i \leq (\mu_i - \mu_m)\left(\frac{\sin\angle(y, \mathcal{Z}_i)}{\cos\angle(y, z_i)}\,\frac{\prod_{j=1}^{i-1}\frac{\theta_j-\mu_m}{\theta_j-\mu_i}}{T_{k-i}(1+2\gamma_i)}\right)^2, \quad i = 1, \ldots, k, \tag{2.1}$$

for the Ritz values $\theta_1 \geq \cdots \geq \theta_k$ of H in $\mathcal{K}$. Therein $\mathcal{Z}_i = \operatorname{span}\{z_1, \ldots, z_i\}$. Additionally, it holds that

$$\tan\angle(z_i, \mathcal{K}) \leq \frac{\sin\angle(y, \mathcal{Z}_i)}{\cos\angle(y, z_i)}\,\frac{\prod_{j=1}^{i-1}\frac{\mu_j-\mu_m}{\mu_j-\mu_i}}{T_{k-i}(1+2\gamma_i)}, \quad i = 1, \ldots, k. \tag{2.2}$$

Therein T_{k-i} are the Chebyshev polynomials with respect to $[-1, 1]$ and gap ratios are given by $\gamma_i = (\mu_i - \mu_{i+1})/(\mu_{i+1} - \mu_m)$.

The analysis in [21], and thus the bounds (2.1) and (2.2), make use of the subspace angle $\angle(y, \mathcal{Z}_i)$. This analysis results in slightly tighter bounds compared to the analysis in [22], which uses $\angle(y, z_i)$. It should be mentioned that the estimate (2.1) requires the additional assumption $\theta_i > \mu_{i+1}$, $i = 1, \ldots, k$, which is missing in Theorem 12.4.1 in [21] but is included in Theorem 2 in [22]. Estimates which are similar to those in Theorem 2.1 have also been published in [16] in the context of an Invert-Lanczos process.

The estimates (2.1) and (2.2) show that one can achieve more accurate approximations of the largest eigenvalues and the associated eigenvectors by enlarging the dimension of the Krylov subspace. The reason for this is that $T_{k-i}(1 + 2\gamma_i)$ increases considerably in k, whereas the terms in the numerator of the upper bounds in (2.1) and (2.2) for a fixed i do not depend on k.

The estimates of Theorem 2.1 are not direct generalizations of the estimates in Theorem 1.2 with regard to restarted Krylov iterations. The Ritz value estimate (2.1) additionally contains angle terms compared to (1.7). For $i = 1$ the angle estimate (2.2) can be rewritten as

$$\tan\angle(z_1, \mathcal{K}) \leq T_{k-1}^{-1}(1 + 2\gamma_1)\tan\angle(y, \mathcal{W}_1)$$

by using $\angle(y, \mathcal{Z}_1) = \angle(y, w_1) = \angle(y, \mathcal{W}_1)$ as far as $w_1 \neq 0$. This form is similar to (1.8). In general, these two estimates cannot be combined recursively to derive a priori estimates as in (1.6).

In contrast to this, the convergence measure $(\mu_i - \cdot)/(\cdot - \mu_{i+1})$ in (1.7) has obvious benefits; it has been used in [8] by Knyazev for deriving convergence estimates for various basic eigensolvers and in many further papers, e.g., [20, 19, 17, 18]. In [8], fundamental estimates for restarted Krylov iterations have been derived by exploiting basic properties of Chebyshev polynomials (e.g. their boundedness), which proves again the importance of the Chebyshev polynomial analysis of iterative eigensolvers complementary to the famous Chebyshev-based analysis of the conjugate gradient method for linear systems. A further application is the analysis in Theorem 2.1 on approximations from Krylov subspaces with increasing dimensions. We restate a central estimate from [8] with the notation as used in Theorem 2.1: If $\mu(y) \in (\mu_2, \mu_1)$, then

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2} \le T_{k-1}^{-2}(1 + 2\gamma_1)\, \frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}. \tag{2.3}$$

We note that for the case $k = 2$, the estimate (2.3) coincides with the estimate (1.7) in Theorem 1.2 for the special case $i = 1$. In other words, (2.3) provides a partial generalization of (1.7), namely for the fixed interval (μ_2, μ_1). The following example shows that the bound in (2.3) is even tighter than that in the Kaniel and Paige estimate (2.1).

2.1. Numerical comparison of convergence factors. For a comparison of the bounds in (2.1) and (2.3), we consider the finite difference standard 7-point-discretization in 3D of the Laplacian on the domain $[0, \pi]^3$ with 100^3 interior nodes. The matrix H is taken as the inverse of this discretization matrix. We consider the case of three-dimensional Krylov spaces with $k = 3$. A number of 98 equidistant points α is taken in the interval $(\mu_2, \mu_1) \approx (1/6, 1/3)$. For each α we consider 1000 random vectors y in the level set $\{\widetilde{y} \in \mathbb{R}^n \ :\ \mu(\widetilde{y}) = \alpha\}$. Then for each y the resulting largest Ritz value $\theta_1 = \theta_1(y)$ of H in $\operatorname{span}\{y, Hy, H^2 y\}$ is computed. The minimum of these $\theta_1(y)$ represents the case of slowest convergence and results in the maximal ratio

$$\left(\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2}\right)\left(\frac{\mu_1 - \alpha}{\alpha - \mu_2}\right)^{-1}. \tag{2.4}$$

In Figure 2.1 these maxima are plotted versus α; see the curve "Numerically slowest convergence". The classical estimate (2.1) is represented by the maximum of

$$\left(\frac{\mu_1 - \widetilde{\theta}_1}{\widetilde{\theta}_1 - \mu_2}\right)\left(\frac{\mu_1 - \alpha}{\alpha - \mu_2}\right)^{-1} \quad \text{with} \quad \widetilde{\theta}_1 = \mu_1 - (\mu_1 - \mu_m)\,\frac{\tan^2 \angle(y, z_1)}{T_2^2(1 + 2\gamma_1)}, \tag{2.5}$$

and the bound of the estimate (2.3) reads $T_2^{-2}(1 + 2\gamma_1)$. We notice that the estimate by (2.3) is much stronger. A possible explanation is an overestimation due to the factor $\tan \angle(y, z_1)$. This comparison encourages us to derive a generalization of the Ritz value estimate (2.3) which holds for arbitrary intervals (μ_{i+1}, μ_i).

3. The new sharp estimates for the restarted Krylov iteration scheme. The following new Theorem 3.1 is on Ritz value estimates and Ritz vector estimates for the restarted Krylov type iteration (1.5). The theorem uses the settings and the notation of Theorem 1.2. For its proof, we use techniques which are similar to those used in [7, 8, 12, 18]. In order to estimate the closeness of Ritz values towards the nearest eigenvalues, we generalize the estimate (2.3) so that it applies to any interval (μ_{i+1}, μ_i) and not only to (μ_2, μ_1). In order to derive convergence estimates for the Ritz vector towards an eigenvector, we extend the 2D ellipse-analysis in [18] to a k-dimensional ellipsoid-analysis. The main result is as follows:

THEOREM 3.1. *Let $\mu_1 > \mu_2 > \cdots > \mu_m$ be the distinct eigenvalues (with arbitrary multiplicity) of the symmetric and positive definite matrix $H \in \mathbb{R}^{n \times n}$, and let $\mu(\cdot)$ be the*

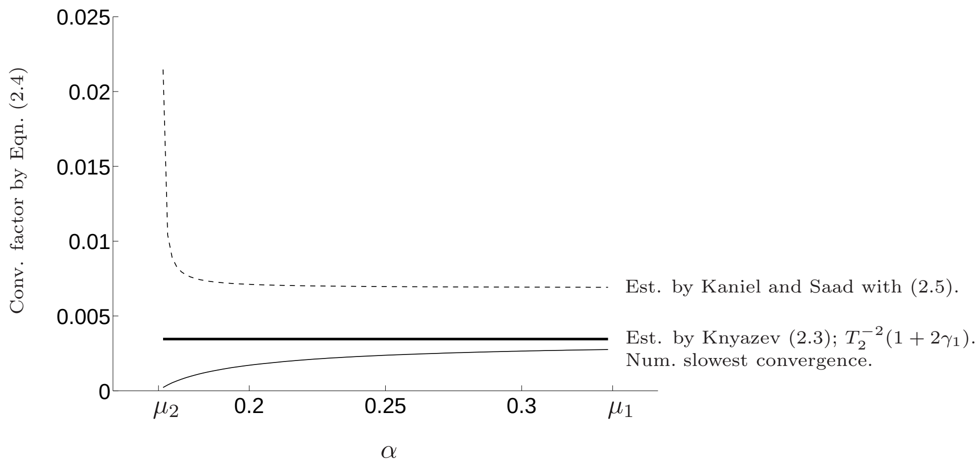

FIG. 2.1. *Numerical comparison of the convergence factors for the 3D Laplacian. We have plotted the numerically computed maximal values of* (2.4) *and the upper estimates for* (2.4)*. Lowermost curve: Numerically observed maximal values of* (2.4) *which represent the slowest convergence. An equidistant subdivision of $\alpha \in (\mu_2, \mu_1)$ is used. For each α on this grid, 1000 random initial vectors are considered whose Rayleigh quotients equal α and the slowest convergence is recorded. Middle curve: Convergence estimate* (2.3) *by Knyazev, i.e. $T_2^{-2}(1+2\gamma_1)$ is plotted. Uppermost curve: The estimate* (2.1) *by Kaniel and Saad is reformulated according to* (2.5) *and is plotted.*

Rayleigh quotient with respect to H. Consider a Ritz vector y' associated with the largest Ritz value of H in the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \dots, H^{k-1}y\}$ with $y \in \mathbb{R}^n \setminus \{0\}$ and $k \geq 2$.

(i) Strictly monotone convergence: If $\mathcal{K}$ is not H-invariant, then

$$\mu(y') > \mu(y). \tag{3.1}$$

(ii) Ritz value estimate: If $\mu(y) \in (\mu_{i+1}, \mu_i)$, then

$$\frac{\mu_i - \mu(y')}{\mu(y') - \mu_{i+1}} \leq T_{k-1}^{-2}(1+2\gamma_i)\,\frac{\mu_i - \mu(y)}{\mu(y) - \mu_{i+1}} \tag{3.2}$$

with the Chebyshev polynomial T_{k-1} with respect to $[-1,1]$ and the gap ratio $\gamma_i = (\mu_i - \mu_{i+1})/(\mu_{i+1} - \mu_m)$.

(iii) Ritz vector estimate: If y is not H-orthogonal to the eigenspace $\mathcal{W}_1$ with respect to μ_1, then

$$\tan \angle_H(y', \mathcal{W}_1) \leq \prod_{j=1}^{k-1} \frac{\mu_2 - \mu_{m+1-j}}{\mu_1 - \mu_{m+1-j}} \tan \angle_H(y, \mathcal{W}_1). \tag{3.3}$$

This bound cannot be improved in the eigenvalues. Equality can be attained in a limit case with y belonging to the invariant subspace associated with the relevant eigenvalues.

Remark. The estimate (3.2) includes the favorable case of very fast convergence. In this case the Rayleigh quotient starts from a value equal to $\mu(y) \in (\mu_{i+1}, \mu_i)$ and the Rayleigh quotient of the next iterate y' has left this interval so that $\mu(y') \geq \mu_i$. In this case the left-hand side of (3.2) is non-positive whereas the right-hand side is always positive. Thus (3.2) holds trivially. We note that the estimate (3.2) can even be proved without assuming the positive definiteness of H. The same holds for the estimate (3.3) if the H-angles are substituted by angles with respect to the Euclidean geometry for the same vectors.

The proof of Theorem 3.1 is given in three steps in the following three subsections 3.1–3.3.

3.1. Proof of the strictly monotone convergence of the Ritz values (3.1)**.**

Proof. Since $\mu(y')$ is the maximal Ritz value in $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots\}$, the inequality $\mu(y') \geq \mu(y)$ holds. In the case of equality, y maximizes $\mu(\cdot)$ in $\mathcal{K}$. Then y is a Ritz vector and its residual $r = Hy - \mu(y)y$ is orthogonal to $\mathcal{K}$ and also to itself, since $r \in \mathcal{K}$ as $k \geq 2$. Hence $r = 0$, which means that y is an eigenvector of H. Thus it holds that $\mathcal{K} = \operatorname{span}\{y\}$. This contradicts the premise that $\mathcal{K}$ is not H-invariant. □

3.2. Analysis of the Ritz value estimate (3.2)**.** In this section we give a proof of the Ritz value estimate (3.2). We treat the two cases:

If $\mathcal{K}$ is H-invariant, then the Ritz vector y' is an eigenvector (see the argument given in Section 3.1) so that $\mu(y')$ is an eigenvalue of H. Then $\mu(y') \geq \mu(y)$ and $\mu(y) \in (\mu_{i+1}, \mu_i)$ imply that $\mu(y') \geq \mu_i$. In this case (3.2) holds trivially.

If $\mathcal{K}$ is not H-invariant, then (i) shows $\mu(y') > \mu(y)$. We only have to consider the nontrivial case $\mu_i > \mu(y') > \mu(y) > \mu_{i+1}$. The key point of the proof is to define an intermediate vector by means of the Chebyshev polynomial T_{k-1}. Here, we use some ideas from the proof of Theorem 2.3.1 in [7] (where the p-th Ritz value from an abstract iteration of p-dimensional subspaces $\mathcal{S}^{(\ell)} = F_l(H)\mathcal{S}^{(0)}$ is similarly analyzed). First, we prove estimates for changes of the Rayleigh quotient under re-weighting of the expansion coefficients in its argument, cf. Lemma 2.3.2 in [7] and Lemma A.1 in [13]. The proof of the estimate (3.2) follows after Lemma 3.2.

Lemma 3.2. *With the settings from Theorem 3.1 let* $\widetilde{y} \in \mathbb{R}^n \backslash \{0\}$ *with* $\widetilde{y} = \sum_{j=1}^m \widetilde{w}_j$ *be the expansion of* $\widetilde{y}$ *in its orthogonal projections* $\widetilde{w}_j$ *to the eigenspaces of* H *for the* m *distinct eigenvalues* μ_j*. If* $\mu(\widetilde{y}) \in [\mu_{i+1}, \mu_i]$*, then the re-weighted vector* $\widetilde{z} = \sum_{j=1}^m \alpha_j \widetilde{w}_j$ *satisfies:*

(a) If $|\alpha_j| \geq 1 \ \forall\ j \leq i$ *and* $|\alpha_j| \leq 1 \ \forall\ j > i$*, then* $\mu(\widetilde{z}) \geq \mu(\widetilde{y})$*.*

(b) If $|\alpha_j| \leq 1 \ \forall\ j \leq i$ *and* $|\alpha_j| \geq 1 \ \forall\ j > i$*, then* $\mu(\widetilde{z}) \leq \mu(\widetilde{y})$*.*

Proof. For the proof we drop the tilde superscripts. Then $y = \sum_{j=1}^m w_j = \sum_{j=1}^m \omega_j z_j$ is the expansion of y in terms of the orthonormal eigenvectors z_j with the expansion coefficients ω_j. The derivative of $\mu(y) = \sum_{k=1}^m \omega_k^2 \mu_k / \sum_{k=1}^m \omega_k^2$ with respect to ω_ℓ^2 reads

$$\frac{d}{d\omega_\ell^2}\mu(y) = \frac{\mu_\ell \sum_{k=1}^m \omega_k^2 - \sum_{k=1}^m \omega_k^2 \mu_k}{(\sum_{k=1}^m \omega_k^2)^2} = \frac{1}{\sum_{k=1}^m \omega_k^2}(\mu_\ell - \mu(y)). \tag{3.4}$$

For $\mu_\ell \geq \mu(y)$ the derivative is nonnegative so that the Rayleigh quotient $\mu(y)$ increases or decreases together with ω_ℓ^2. If $\mu_\ell \leq \mu(y)$, then $\mu(y)$ and ω_ℓ^2 have a reverse growth characteristic.

The proof is completed by applying these arguments inductively first for all indexes j with $|\alpha_j| \geq 1$ and then for the indexes with $|\alpha_j| \leq 1$. The starting point is $\mu(y) \in [\mu_{i+1}, \mu_i]$, then the absolute value of the expansion coefficient is increased (in the second cycle decreased) for an eigenvalue μ_ℓ, $\ell = i, i-1, \ldots, 1$ for the case (a) and $\ell = i+1, i+2, \ldots, m$ for the case (b). The Rayleigh quotient of the vector $\widehat{y}$ resulting from the substitution $w_\ell \to \alpha_\ell w_\ell$ is contained in the interval $[\min(\mu_\ell, \mu_{i+1}), \max(\mu_\ell, \mu_i)]$ as $\mu(y) \in [\mu_{i+1}, \mu_i]$ and $\lim_{|\alpha_\ell| \to \infty} \mu(\widehat{y}) = \mu_\ell$. Then this argument can be applied for the next index whereby $\mu(\widehat{y})$ replaces $\mu(y)$ in (3.4). □

Lemma 3.2 is the central ingredient for the proof of the Ritz value estimate (3.2) for the nontrivial case $\mu_i > \mu(y') > \mu(y) > \mu_{i+1}$.

Proof. [of the Ritz value estimate (3.2)] We define the auxiliary polynomial

$$p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha - \mu_{i+1}}{\mu_{i+1} - \mu_m}\right). \tag{3.5}$$

Thus $p^{-2}(\mu_i) = T_{k-1}^{-2}(1+2\gamma_i)$ is the convergence factor in (3.2). For $k \geq 2$, the properties of the Chebyshev polynomial T_{k-1}

$$T_{k-1}(1) = 1, \quad \frac{d}{dt}T_{k-1}(t) > 0 \text{ for } t \geq 1, \quad \text{and} \quad |T_{k-1}(t)| \leq 1 \;\Leftrightarrow\; |t| \leq 1$$

imply that

$$\min_{j=1,\ldots,i} |p(\mu_j)| = p(\mu_i) > 1, \quad \text{and} \quad \max_{j=i+1,\ldots,m} |p(\mu_j)| = 1. \tag{3.6}$$

According to (3.6) and Lemma 3.2, we use the representation $y = \sum_{j=1}^{m} w_j$ of y with its orthogonal projections w_j to the eigenspaces of H, and define the three auxiliary vectors

$$y_1 := \sum_{j=1}^{i} w_j, \quad y_2 := \sum_{j=i+1}^{m} w_j, \quad \text{and} \quad z := p(\mu_i)y_1 + y_2. \tag{3.7}$$

Next we prove the chain of inequalities $\mu(y') \geq \mu(z) \geq \mu(y)$:

First, we show $\mu(z) \geq \mu(y)$ by applying Lemma 3.2 (a) to $\widetilde{y} = y$ and $\widetilde{z} = z$: Then (3.6) guarantees that $|\alpha_j| \geq 1 \;\forall\, j \leq i$ and $|\alpha_j| \leq 1 \;\forall\, j > i$ are satisfied for an index i with $\mu(y) \in (\mu_{i+1}, \mu_i)$. This yields $\mu(z) \geq \mu(y)$.

Second, we show $\mu(y') \geq \mu(z)$: We use the auxiliary vector $p(H)y$ with the polynomial $p(\cdot)$ given in (3.5). Since p has a degree of $k-1$, the vector $p(H)y$ belongs to the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$. By definition y' maximizes the Rayleigh quotient $\mu(\cdot)$ in $\mathcal{K}$. Hence $\mu(y') \geq \mu\big(p(H)y\big)$. Moreover, Lemma 3.2 applied to $\widetilde{y} = y$ and $\widetilde{z} = p(H)y$ guarantees with (3.6) that

$$\mu(p(H)y) = \mu(\sum_{j=1}^{m} p(\mu_j)w_j) \geq \mu(y).$$

Therefore, $\mu\big(p(H)y\big) \in [\mu(y), \mu(y')] \subseteq (\mu_{i+1}, \mu_i)$, which allows us to apply Lemma 3.2 for the case (b) to $\widetilde{y} = p(H)y$ and $\widetilde{z} = z$. By using (3.6) again, one gets $\mu(z) \leq \mu\big(p(H)y\big) \leq \mu(y')$.

Additionally, the vectors y_1 and y_2 defined in (3.7) satisfy $\mu(y_1) \geq \mu_i$ and $\mu(y_2) \leq \mu_{i+1}$. The combination of all these inequalities reads

$$\mu(y_1) \geq \mu_i > \mu(y') \geq \mu(z) \geq \mu(y) > \mu_{i+1} \geq \mu(y_2).$$

Then monotonicity arguments are used to prove that

$$\begin{aligned}
&\left(\frac{\mu_i - \mu(y')}{\mu(y') - \mu_{i+1}}\right)\left(\frac{\mu_i - \mu(y)}{\mu(y) - \mu_{i+1}}\right)^{-1} \\
&\leq \left(\frac{\mu_i - \mu(z)}{\mu(z) - \mu_{i+1}}\right)\left(\frac{\mu_i - \mu(y)}{\mu(y) - \mu_{i+1}}\right)^{-1} = \left(\frac{\mu_i - \mu(z)}{\mu_i - \mu(y)}\right)\left(\frac{\mu(y) - \mu_{i+1}}{\mu(z) - \mu_{i+1}}\right) \\
&\leq \left(\frac{\mu(y_1) - \mu(z)}{\mu(y_1) - \mu(y)}\right)\left(\frac{\mu(y) - \mu(y_2)}{\mu(z) - \mu(y_2)}\right) = \left(\frac{\mu(y_1) - \mu(z)}{\mu(z) - \mu(y_2)}\right)\left(\frac{\mu(y_1) - \mu(y)}{\mu(y) - \mu(y_2)}\right)^{-1}.
\end{aligned}$$

In the final step we show that the last term equals $p^{-2}(\mu_i) = T_{k-1}^{-2}(1+2\gamma_i)$. To prove this, we use the representation (3.7) of z which implies that $y_1^T y_2 = y_1^T H y_2 = 0$. Thus we get

$$\mu(z) = \frac{\mu(y_1)\|y_1\|_2^2 p^2(\mu_i) + \mu(y_2)\|y_2\|_2^2}{\|y_1\|_2^2 p^2(\mu_i) + \|y_2\|_2^2} \quad \Rightarrow \quad \frac{\mu(y_1)-\mu(z)}{\mu(z)-\mu(y_2)} = p^{-2}(\mu_i)\frac{\|y_2\|_2^2}{\|y_1\|_2^2}.$$

Similarly, the decomposition $y = y_1 + y_2$ implies that $\big(\mu(y_1)-\mu(y)\big)/\big(\mu(y)-\mu(y_2)\big) = \|y_2\|_2^2/\|y_1\|_2^2$. A combination of these two results completes the proof. □

3.3. Analysis of the Ritz vector estimate (3.3)**.** This section contains the proof of the Ritz vector estimate (3.3). We start with an eigenvector expansion of y. By assumption, y is not H-orthogonal to $\mathcal{W}_1$ so that the H-projection w_1 of y to $\mathcal{W}_1$ is nonzero. Thus (μ_1, w_1) is an eigenpair of H. Moreover, y can be represented in the form $y = w_1 + \sum_{i=1}^{\ell} w_{\sigma(i)}$ with ℓ further nonzero projections on the eigenspaces with indices $\sigma(i) \in \{2, \dots, m\}$. We consider the following two cases:

If $\mathcal{K} = \mathrm{span}\{y, Hy, \dots, H^{k-1}y\}$ is H-invariant, then a $j \le k$ exists so that $H^j y$ linearly depends on the linearly independent vectors $(y, Hy, \dots, H^{j-1}y)$. Then for the eigenvector expansion $y = w_1 + \sum_{i=1}^{\ell} w_{\sigma(i)}$ it holds that $\ell \le j-1$, since otherwise w.l.o.g. for $\ell = j$ the equality

$$\big[y, Hy, \dots, H^{j-1}y, H^j y\big] = \big[w_1, w_{\sigma(1)}, \dots, w_{\sigma(j)}\big] \begin{pmatrix} 1 & \mu_1 & \cdots & \mu_1^j \\ 1 & \mu_{\sigma(1)} & \cdots & \mu_{\sigma(1)}^j \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \mu_{\sigma(j)} & \cdots & \mu_{\sigma(j)}^j \end{pmatrix}$$

with the regular $(j+1)\times(j+1)$ Vandermonde matrix would prove that $y, Hy, \dots, H^j y$ are linearly independent vectors. This contradicts the assumption.

The H-invariant subspace $\mathcal{W} = \mathrm{span}\{w_1, w_{\sigma(1)}, \dots, w_{\sigma(\ell)}\}$ contains the vector y. It holds that $\mathcal{K} \subseteq \mathcal{W}$. Further, $\ell \le j-1$ implies that $\dim \mathcal{W} = \ell + 1 \le j = \dim \mathcal{K}$ so that $\mathcal{K} = \mathcal{W}$ together with $\ell = j-1$. Therefore, the eigenvectors $w_1, w_{\sigma(1)}, \dots, w_{\sigma(\ell)}$ are also the Ritz vectors associated with the distinct Ritz values $\mu_1, \mu_{\sigma(1)}, \dots, \mu_{\sigma(\ell)}$ of H in $\mathcal{K}$. Consequently, the desired Ritz vector y' is collinear to w_1 and is associated with the largest Ritz value μ_1. This leads to $\angle_H(y', \mathcal{W}_1) = \angle_H(w_1, \mathcal{W}_1) = 0$. Thus, (3.3) holds trivially.

If $\mathcal{K}$ is not H-invariant, we consider the auxiliary subspace

$$\mathcal{U} = \mathrm{span}\{w_1, \mathcal{K}\} = \mathrm{span}\{w_1, y, Hy, \dots, H^{k-1}y\}. \tag{3.8}$$

First we analyze properties of the Krylov subspace $\mathcal{K}$ in $\mathcal{U}$ with regard to the Ritz values of H in $\mathcal{U}$. In [12] this technique has been used for the case $k = 2$. For the general case $k \ge 2$, we first have to verify some properties of the subspace $\mathcal{U}$ and of the associated Ritz values. We work out the key arguments in two lemmata:

1. Lemma 3.3 shows that the Krylov subspace $\mathcal{K}$ can be represented by a second k-dimensional Krylov subspace in $\mathbb{R}^{k+1}$. This allows a so-called mini-dimensional analysis. Furthermore, strict interlacing properties of the Ritz values of H in $\mathcal{K}$ related to the Ritz values of H in $\mathcal{U}$ ensure that all these Ritz values are simple. Then this property is used in order to determine a polynomial which results in an intermediate estimate.
2. In Lemma 3.4 we prove an estimate similar to (3.3) with respect to the Ritz values of H in $\mathcal{U}$. In its proof, the angles $\angle_H(y', \mathcal{W}_1)$ and $\angle_H(y, \mathcal{W}_1)$ are represented by certain coefficient ratios with respect to a Ritz vector basis of $\mathcal{U}$. Finally, we prove the main estimate (3.3) by using Lemma 3.4 and monotonicity arguments on page 14.

LEMMA 3.3. *With the settings from Theorem 3.1 let U be an orthonormal matrix whose column space equals $\mathcal{U}$ by (3.8). Further, let $\widehat{H} = U^T H U$ and $\widehat{y} = U^T y$. If $\mathcal{K}$ is not H-invariant, then the following statements hold:*

(a) $\mathcal{U}$ has the dimension $k+1$.

(b) Left multiplication of $\mathcal{K}$ with U^T results in the Krylov subspace

$$\widehat{\mathcal{K}} = \operatorname{span}\{\widehat{y}, \widehat{H}\widehat{y}, \ldots, \widehat{H}^{k-1}\widehat{y}\}.$$

The pair (θ, v) is a Ritz pair of H in $\mathcal{K}$, if and only if $(\theta, \widehat{v})$ with $\widehat{v} = U^T v$ is a Ritz pair of $\widehat{H}$ in $\widehat{\mathcal{K}}$.

(c) Let $\alpha_1 \geq \cdots \geq \alpha_{k+1}$ be the $k+1$ Ritz values of H in the $(k+1)$-dimensional space $\mathcal{U}$, which are the eigenvalues of $\widehat{H}$. Let $\theta_1 \geq \cdots \geq \theta_k$ be the Ritz values of H in $\mathcal{K}$. Then the following interlacing properties hold

$$\mu_1 = \alpha_1 > \theta_1 > \alpha_2 > \cdots > \alpha_k > \theta_k > \alpha_{k+1}.$$

Further, the eigenspace of $\widehat{H}$ associated with α_1 is the column space of $U^T w_1$.

Proof.

(a) Since $\mathcal{K}$ is not H-invariant, the vectors $y, Hy, \ldots, H^{k-1}y$ are linearly independent. Hence $\dim\mathcal{U} \in \{k, k+1\}$. It remains to show that the assumption $\dim\mathcal{U} = k$ results in a contradiction. If $\dim\mathcal{U} = k$, then w_1 can be represented by a linear combination $\sum_{i=0}^{k-1} \beta_i H^i y$, and the eigenvalue equation $Hw_1 = \mu_1 w_1$ turns into

$$\sum_{i=0}^{k-1} \beta_i H^{i+1} y = \sum_{i=0}^{k-1} \mu_1 \beta_i H^i y$$

so that $\beta_{k-1} H^k y$ belongs to $\mathcal{K}$. As $\mathcal{K}$ is not H-invariant, i.e. $H^k y \notin \mathcal{K}$, we conclude that $\beta_{k-1} = 0$. These arguments can be applied recursively for the smaller spaces and the remaining β_i. This proves that $\beta_i = 0 \; \forall\, i \in \{0, \ldots, k-1\}$. Thus $w_1 = 0$, which contradicts our assumption in Theorem 3.1 that y is not H-orthogonal to $\mathcal{W}_1$. Consequently, only $\dim\mathcal{U} = k+1$ can hold.

(b) The matrix UU^T is an orthogonal projection operator to $\mathcal{U}$. Thus $\mathcal{K} \subset \mathcal{U}$ proves that $UU^T v = v$ for all $v \in \mathcal{K}$. Direct computation shows that

$$\begin{aligned} U^T\mathcal{K} &= U^T \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\} \\ &= \operatorname{span}\{U^T y, U^T H U U^T y, \ldots, (U^T H U)^{k-1} U^T y\} \\ &= \operatorname{span}\{\widehat{y}, \widehat{H}\widehat{y}, \ldots, \widehat{H}^{k-1}\widehat{y}\} = \widehat{\mathcal{K}}. \end{aligned}$$

For any $\theta \in \mathbb{R}$ it holds that

$$(Hv - \theta v)^T \mathcal{K} = (HUU^T v - \theta U U^T v)^T U U^T \mathcal{K} = (\widehat{H}\widehat{v} - \theta\widehat{v})^T \widehat{\mathcal{K}}.$$

Thus, (θ, v) satisfies $Hv - \theta v \perp \mathcal{K}$ if and only if $(\theta, \widehat{v})$ satisfies $\widehat{H}\widehat{v} - \theta\widehat{v} \perp \widehat{\mathcal{K}}$.

(c) By (a), the matrix H has exactly $k+1$ Ritz values in $\mathcal{U}$. The equality $\alpha_1 = \mu_1$ holds because the global maximum of $\mu(\cdot)$ is also attained in $\mathcal{U}$, namely $w_1 \in \mathcal{U}$ results in $\alpha_1 = \mu(w_1) = \mu_1$.

The Courant-Fischer principles for the subspace $\mathcal{K}$ of $\mathcal{U}$ together with $\dim\mathcal{U} = k + 1 = 1 + \dim\mathcal{K}$ guarantee that

$$\alpha_1 \geq \theta_1 \geq \alpha_2 \geq \cdots \geq \alpha_k \geq \theta_k \geq \alpha_{k+1}.$$

For each of the "$\geq$" relations in this chain of inequalities, an equality can be ruled out by the following arguments.

(I) *It holds that $\alpha_1 \neq \theta_1$:* Otherwise, it would hold that $\alpha_1 = \theta_1 = \mu_1$ with the largest eigenvalue μ_1 of H. Then $\mathcal{K}$ would contain an eigenvector associated with μ_1. The same arguments as applied to w_1 in part (a) of this proof can be used for this eigenvector. The resulting contradiction proves that $\alpha_1 \neq \theta_1$.

(II) *The Krylov subspace $\widehat{\mathcal{K}}$ contains no eigenvectors of $\widehat{H}$:* First we prove that $\widehat{\mathcal{K}}$ cannot be an $\widehat{H}$-invariant space. Then the arguments of part (a) of this proof can be adapted and re-used in order to show that the assumption of an eigenvector of $\widehat{H}$ in the space $\widehat{\mathcal{K}}$ results in a contradiction.
So we assume $\widehat{\mathcal{K}}$ to be $\widehat{H}$-invariant and derive a contradiction: Due to (b) the Ritz values $\theta_1 \geq \cdots \geq \theta_k$ of H in $\mathcal{K}$ are also Ritz values of $\widehat{H}$ in $\widehat{\mathcal{K}}$. The $\widehat{H}$-invariance of $\widehat{\mathcal{K}}$ implies that all these θ_i turn into eigenvalues of $\widehat{H}$. This is true since for a Ritz pair $(\widehat{\mu}(\widehat{v}), \widehat{v})$ of $\widehat{H}$ in $\widehat{\mathcal{K}}$ the orthogonality

$$z := \widehat{H}\widehat{v} - \widehat{\mu}(\widehat{v})\widehat{v} \perp \widehat{\mathcal{K}}$$

implies that $z = 0$ as $z \in \widehat{\mathcal{K}}$ by the $\widehat{H}$-invariance.
All these Ritz values or eigenvalues must be different from α_1 due to (I). Thus $\widehat{\mathcal{K}}$ is orthogonal to the eigenvectors associated with α_1. Furthermore, $U^T w_1$ is an eigenvector associated with α_1 since

$$\widehat{H}(U^T w_1) = U^T H U U^T w_1 = U^T H w_1 = U^T(\alpha_1 w_1) = \alpha_1(U^T w_1).$$

In particular $\widehat{\mathcal{K}}$ is orthogonal to the eigenvector $U^T w_1$, i.e. for $U^T y \in \widehat{\mathcal{K}}$ it holds that $U^T y \perp U^T w_1$. Hence

$$y^T(Hw_1) = (UU^T y)^T(\mu_1 w_1) = \mu_1 (U^T y)^T (U^T w_1) = 0.$$

This contradicts our assumption that y is not H-orthogonal to $\mathcal{W}_1$.

(III) *An orthogonality argument:* We show that the 1D-subspace spanned by $r = \left(\prod_{i=1}^k (\widehat{H} - \theta_i I)\right)\widehat{y}$ is the orthogonal complement of the k-dimensional space $\widehat{\mathcal{K}}$ in the $\mathbb{R}^{k+1}$. First, the vector r is nonzero, since otherwise the eigenvalue equation $\widehat{H}\widehat{v} = \theta_j \widehat{v}$ with $\widehat{v} = \left(\prod_{i=j+1}^k (\widehat{H} - \theta_i I)\right)\widehat{y} \neq 0$ would hold. This would contradict (II) since $\widehat{v} \in \widehat{\mathcal{K}}$.
Furthermore, for each Ritz pair $(\theta_j, \widehat{v}_j)$, $j = 1, \ldots, k$ of $\widehat{H}$ in $\widehat{\mathcal{K}}$, it holds that

$$\widehat{v}_j^T r = \widehat{v}_j^T \left(\prod_{i=1}^k (\widehat{H} - \theta_i I)\right)\widehat{y} = \big(\underbrace{(\widehat{H} - \theta_j I)\widehat{v}_j}_{\in \widehat{\mathcal{K}}^\perp}\big)^T \underbrace{\left(\prod_{i=1, i\neq j}^k (\widehat{H} - \theta_i I)\right)\widehat{y}}_{\in \widehat{\mathcal{K}}} = 0.$$

All these Ritz vectors $\widehat{v}_j$ span $\widehat{\mathcal{K}}$. Hence r is orthogonal to $\widehat{\mathcal{K}}$. A dimension argument shows that $\widehat{\mathcal{K}}^\perp$ is one-dimensional so that $\widehat{\mathcal{K}}^\perp = \operatorname{span}\{r\}$.

If a certain θ_j would be equal to an eigenvalue of $\widehat{H}$, then the associated eigenvector $\widehat{u}$ would satisfy

$$\widehat{u}^T r = \widehat{u}^T \left(\prod_{i=1}^k (\widehat{H} - \theta_i I)\right)\widehat{y} = \big(\underbrace{(\widehat{H} - \theta_j I)\widehat{u}}_{=0}\big)^T \left(\prod_{i=1, i\neq j}^k (\widehat{H} - \theta_i I)\right)\widehat{y} = 0.$$

Thus (III) implies that $\widehat{u} \in \widehat{\mathcal{K}}$. This contradicts (II). Hence, none of the Ritz values θ_j equals an eigenvalue of $\widehat{H}$. This proves the strict interlacing property.

Counting the pairwise different eigenvalues of $\widehat{H}$ shows that all eigenvalues are simple so that the associated eigenspaces are one-dimensional. The eigenspace which corresponds to α_1 is $\operatorname{span}\{U^T w_1\}$.

∎

Lemma 3.3 allows to derive an intermediate error estimate on the Ritz vectors which uses the Ritz values α_i of H in $\mathcal{U}$.

LEMMA 3.4. *With the settings and notation from Theorem 3.1 and from Lemma 3.3 it holds that*

$$\tan\angle_H(y',\mathcal{W}_1) \le \prod_{j=3}^{k+1} \frac{\alpha_2-\alpha_j}{\alpha_1-\alpha_j}\,\tan\angle_H(y,\mathcal{W}_1). \tag{3.9}$$

Proof. First, we represent the H-angles by the corresponding angles in $\mathcal{U}$. Since w_1 is the H-projection of y to $\mathcal{W}_1$, it holds that $\angle_H(y,\mathcal{W}_1)=\angle_H(y,w_1)$. Further, since y' belongs to the Krylov subspace generated by y and H, the H-projection of y' to $\mathcal{W}_1$ is collinear with w_1 so that $\angle_H(y',\mathcal{W}_1)=|\angle_H(y',w_1)|$. In order to derive a representation of these angles with respect to $\mathcal{U}$, we use an orthonormal basis of $\mathcal{U}$ consisting of eigenvectors $\widehat{u}_1,\dots,\widehat{u}_{k+1}$ of $\widehat{H}$ associated with the eigenvalues $\alpha_1\ge\cdots\ge\alpha_{k+1}$. According to Lemma 3.3 (c), these eigenvalues are simple, and $\widehat{u}_1=\beta\,U^T w_1$ with $\beta\in\mathbb{R}\backslash\{0\}$. Then it holds for $\widehat{y}=U^T y\in\mathbb{R}^{k+1}$ that

$$(\widehat{y},\,\widehat{u}_1)_{\widehat{H}}=(U^Ty)^T(U^THU)(\beta\,U^Tw_1)=\beta(UU^Ty)^TH(UU^Tw_1)=\beta y^THw_1=\beta(y,w_1)_H,$$

since $y\in\mathcal{U}$ and $w_1\in\mathcal{U}$. Similarly, it holds that $\|\widehat{y}\|_{\widehat{H}}=\|y\|_H$, $\|\widehat{u}_1\|_{\widehat{H}}=|\beta|\,\|w_1\|_H$. Thus,

$$\cos^2\angle_{\widehat{H}}(\widehat{y},\,\widehat{u}_1)=\frac{(\widehat{y},\,\widehat{u}_1)^2_{\widehat{H}}}{\|\widehat{y}\|^2_{\widehat{H}}\|\widehat{u}_1\|^2_{\widehat{H}}}=\frac{\beta^2(y,w_1)^2_H}{\|y\|^2_H\beta^2\|w_1\|^2_H}=\cos^2\angle_H(y,w_1)$$

so that $\tan^2\angle_{\widehat{H}}(\widehat{y},\,\widehat{u}_1)=\tan^2\angle_H(y,w_1)$. Analogously, $\tan^2\angle_{\widehat{H}}(\widehat{y}\,',\,\widehat{u}_1)=\tan^2\angle_H(y',w_1)$ can be shown for $\widehat{y}\,'=U^Ty'$. Each angle in (3.9) is an angle between a vector and a subspace. Hence all these angles are bounded by $\pi/2$. The tangent values are nonnegative so that (3.9) is equivalent to

$$\tan^2\angle_{\widehat{H}}(\widehat{y}\,',\,\widehat{u}_1)\le\left(\prod_{j=3}^{k+1}\frac{\alpha_2-\alpha_j}{\alpha_1-\alpha_j}\right)^2\tan^2\angle_{\widehat{H}}(\widehat{y},\,\widehat{u}_1). \tag{3.10}$$

In order to reformulate these tangent values in terms of the coefficients with respect to the basis vectors $\widehat{u}_j$, we use Lemma 3.3 again. We begin with the representation $\widehat{y}=\sum_{j=1}^{k+1}\widehat{u}_j(\widehat{u}_j^T\widehat{y})$ with the orthonormal eigenvectors $\widehat{u}_j$ introduced in the first part of the proof. If at least one of the coefficients $(\widehat{u}_j^T\widehat{y})$ is equal to zero, then the Krylov subspace $\widehat{\mathcal{K}}$ would be a subspace of an $\widehat{H}$-invariant subspace whose dimension is at most k. The property (b) in Lemma 3.3 shows that $\widehat{\mathcal{K}}=U^T\mathcal{K}$ has the same dimension as $\mathcal{K}$, namely the dimension k, since $\mathcal{K}$ is not H-invariant. Hence, $\widehat{\mathcal{K}}$ would be an $\widehat{H}$-invariant subspace, and the Ritz values of $\widehat{H}$ in $\widehat{\mathcal{K}}$, which are also Ritz values of H in $\mathcal{K}$ according to (b), would be eigenvalues of $\widehat{H}$. This contradicts the strict interlacing in (c) and shows that all the coefficients $(\widehat{u}_j^T\widehat{y})$ are nonzero. Then $\widehat{y}$ can be normalized with respect to $\widehat{u}_1$. The normalized vector has the representation $\widetilde{y}=\widehat{u}_1+\sum_{j=2}^{k+1}\beta_j\widehat{u}_j$ with $\beta_j\ne0$ and satisfies

$$\tan^2\angle_{\widehat{H}}(\widehat{y},\,\widehat{u}_1)=\tan^2\angle_{\widehat{H}}(\widetilde{y},\,\widehat{u}_1)=\frac{\sum_{j=2}^{k+1}\|\beta_j\widehat{u}_j\|^2_{\widehat{H}}}{\|\widehat{u}_1\|^2_{\widehat{H}}}=\alpha_1^{-1}\sum_{j=2}^{k+1}\alpha_j\beta_j^2 \tag{3.11}$$

since the eigenvectors are pairwise $\widehat{H}$-orthogonal. Additionally, we use the affine subspace

$$\widehat{\mathcal{U}} = \widehat{u}_1 + \operatorname{span}\{\widehat{u}_2, \ldots, \widehat{u}_{k+1}\}$$

and the Rayleigh quotient $\widehat{\mu}(\cdot)$ with respect to $\widehat{H}$. Each $\widehat{u} \in \widehat{\mathcal{U}}$ can be represented by a coefficient vector in $\mathbb{R}^k$ with respect to the basis vectors $\widehat{u}_2, \ldots, \widehat{u}_{k+1}$. Then the level set $\{\widehat{u} \in \widehat{\mathcal{U}} \ : \ \widehat{\mu}(\widehat{u}) = \theta_1\}$ can be represented by an ellipsoid. (Therein, θ_1 is the largest Ritz value of H in $\mathcal{K}$, see Lemma 3.3.) Namely, the defining equation for the ellipsoid with $\widehat{u} = \widehat{u}_1 + \sum_{j=2}^{k+1} \widehat{\beta}_j \widehat{u}_j$ reads as follows

$$\theta_1 = \widehat{\mu}(\widehat{u}) = \frac{\alpha_1 + \sum_{j=2}^{k+1} \alpha_j \widehat{\beta}_j^2}{1 + \sum_{j=2}^{k+1} \widehat{\beta}_j^2} \quad \text{or equivalently} \quad \sum_{j=2}^{k+1} \frac{\widehat{\beta}_j^2}{\dfrac{\alpha_1 - \theta_1}{\theta_1 - \alpha_j}} = 1. \tag{3.12}$$

Therein all the quotients $(\alpha_1 - \theta_1)/(\theta_1 - \alpha_j)$ are positive due to (c) in Lemma 3.3. Further, the intersection $\widehat{\mathcal{U}} \cap \widehat{\mathcal{K}}$ can be represented by an affine hyperplane in $\mathbb{R}^k$, which is a tangential hyperplane of the ellipsoid defined in (3.12) according to the convexity of the ellipsoid and the fact that θ_1 is the maximum of $\widehat{\mu}(\cdot)$ in $\widehat{\mathcal{K}}$. The point of tangency corresponds to a certain Ritz vector $\widetilde{y}'$ associated with θ_1. By (c) in Lemma 3.3, θ_1 is a simple Ritz value so that all the associated Ritz vectors are collinear. Moreover, (b) in Lemma 3.3 shows that $\widehat{y}' = U^T y'$ is a further Ritz vector associated with θ_1. Since the normalized vector $\widetilde{y}'$ is collinear to $\widehat{y}'$ it holds with the representation $\widetilde{y}' = \widehat{u}_1 + \sum_{j=2}^{k+1} \beta_j' \widehat{u}_j$ that

$$\tan^2 \angle_{\widehat{H}}(\widehat{y}', \widehat{u}_1) = \tan^2 \angle_{\widehat{H}}(\widetilde{y}', \widehat{u}_1) = \frac{\sum_{j=2}^{k+1} \|\beta_j' \widehat{u}_j\|_{\widehat{H}}^2}{\|\widehat{u}_1\|_{\widehat{H}}^2} = \alpha_1^{-1} \sum_{j=2}^{k+1} \alpha_j {\beta_j'}^2. \tag{3.13}$$

With (3.11) and (3.13) the assertion (3.10) can be written as

$$\sum_{j=2}^{k+1} \alpha_j \beta_j'^2 \leq \left(\prod_{j=3}^{k+1} \frac{\alpha_2 - \alpha_j}{\alpha_1 - \alpha_j} \right)^2 \sum_{j=2}^{k+1} \alpha_j \beta_j^2. \tag{3.14}$$

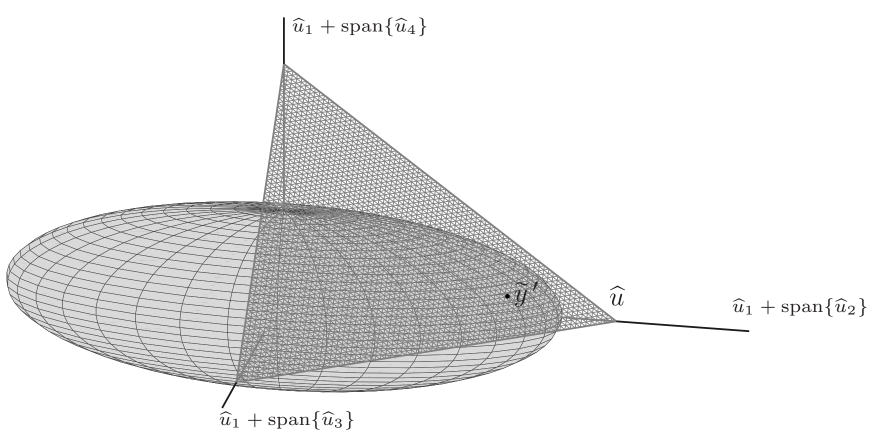

FIG. 3.1. *Geometry in the affine subspace $\widehat{\mathcal{U}}$ for the case $k = 3$.*

Next, the proof is completed by deriving (3.14). In Figure 3.1 the geometry of the ellipsoid and its tangent plane is illustrated for the case $k = 3$. (This figure is the counterpart of Figure 3.2 in [18] where the case $k = 2$ is analyzed.) Since the $\widehat{\mathcal{U}}$-representation $b_{\widetilde{y}'} = (\beta_2', \ldots, \beta_{k+1}')^T$ of $\widetilde{y}'$ is a point of tangency on the ellipsoid defined in (3.12), the Euclidean norm $\|b_{\widetilde{y}'}\|_2$ is not larger than the length of the semi-major axis of the ellipsoid, i.e., $\|b_{\widetilde{y}'}\|_2 \le a = \sqrt{(\alpha_1 - \theta_1)/(\theta_1 - \alpha_2)}$. Additionally, the $\widehat{\mathcal{U}}$-representation $b_{\widehat{u}}$ of the intersection $\widehat{u} = \widehat{\mathcal{K}} \cap (\widehat{u}_1 + \operatorname{span}\{\widehat{u}_2\})$ defines a point on the line containing the major axis, and the point is outside the ellipsoid because of the tangential property of $\widehat{\mathcal{K}}$, see Figure 3.1. Thus, $\|b_{\widetilde{y}'}\|_2 \le a \le \|b_{\widehat{u}}\|_2$. Further, $\widehat{u}$ can be represented by $p(\widehat{H})\widehat{y}$ with a polynomial p whose degree is not larger than $k-1$ because of $\widehat{u} \in \widehat{\mathcal{K}}$. We write $\widehat{y}$ in the form $\widetilde{y}(\widehat{u}_1^T\widehat{y})$ with the normalized vector $\widetilde{y} = \widehat{u}_1 + \sum_{j=2}^{k+1} \beta_j \widehat{u}_j$. Then the vector $\widehat{u} = p(\widehat{H})\widehat{y}$ has the representation

$$\widehat{u} = p(\widehat{H}) \left(\widehat{u}_1 + \sum_{j=2}^{k+1} \beta_j \widehat{u}_j \right) (\widehat{u}_1^T \widehat{y}) = \left(p(\alpha_1)\widehat{u}_1 + \sum_{j=2}^{k+1} \beta_j p(\alpha_j) \widehat{u}_j \right) (\widehat{u}_1^T \widehat{y}).$$

Because of $\widehat{u} \in \widehat{u}_1 + \operatorname{span}\{\widehat{u}_2\}$, $\widehat{u}_1^T\widehat{y} \ne 0$ and $\beta_j \ne 0$, we have

$$p(\alpha_1) = (\widehat{u}_1^T\widehat{y})^{-1}, \quad p(\alpha_j) = 0 \quad \text{for} \quad j = 3, \ldots, k+1.$$

Due to (c) in Lemma 3.3, the eigenvalues α_j are pairwise different so that the polynomial p has $k-1$ isolated zeros. Hence p is a multiple of the polynomial $\prod_{j=3}^{k+1}(\alpha - \alpha_j)$. Combining this with $p(\alpha_1) = (\widehat{u}_1^T\widehat{y})^{-1}$ implies that p has the form

$$p(\alpha) = (\widehat{u}_1^T\widehat{y})^{-1} \prod_{j=3}^{k+1} \frac{\alpha - \alpha_j}{\alpha_1 - \alpha_j}$$

so that

$$\widehat{u} = \widehat{u}_1 + \beta_2 p(\alpha_2)\widehat{u}_2(\widehat{u}_1^T\widehat{y}) = \widehat{u}_1 + \beta_2 \prod_{j=3}^{k+1} \frac{\alpha_2 - \alpha_j}{\alpha_1 - \alpha_j} \widehat{u}_2.$$

Thus, the coefficient vector $b_{\widehat{u}}$ is given by $(\beta_2\kappa, 0, \ldots, 0)^T$ with $\kappa = \prod_{j=3}^{k+1}(\alpha_2 - \alpha_j)/(\alpha_1 - \alpha_j)$, and $\|b_{\widetilde{y}'}\|_2^2 \le \|b_{\widehat{u}}\|_2^2 = \beta_2^2\kappa^2$. This leads to (3.14), namely

$$\sum_{j=2}^{k+1} \alpha_j \beta_j'^2 \le \sum_{j=2}^{k+1} \alpha_2 \beta_j'^2 = \alpha_2 \|b_{\widetilde{y}'}\|_2^2 \le \alpha_2 \beta_2^2 \kappa^2 \le \kappa^2 \sum_{j=2}^{k+1} \alpha_j \beta_j^2. \tag{3.15}$$

The two inequalities are equalities in the limit case $\beta_2^2 \to \infty$, which implies to ${\beta_2'}^2 \to \infty$. ∎

Next, we use Lemma 3.4 together with monotonicity arguments in order to complete the proof of the Ritz vector estimate (3.3) for the nontrivial case that $\mathcal{K}$ is not H-invariant.

Proof. [of the Ritz vector estimate (3.3)] For the Ritz values $\alpha_1, \ldots, \alpha_{k+1}$ defined in Lemma 3.3 (c), the Courant-Fischer principles guarantee the following inequalities to hold

$$\mu_1 = \alpha_1 > \mu_2 \ge \alpha_2, \quad \text{and} \quad \alpha_j \ge \mu_{m-(k+1)+j} \quad \text{for} \quad j = 3, \ldots, k+1.$$

The monotonicity of $(\alpha_2 - \alpha_j)/(\alpha_1 - \alpha_j)$ with respect to α_2 or α_j proves that

$$\frac{\alpha_2 - \alpha_j}{\alpha_1 - \alpha_j} \le \frac{\mu_2 - \mu_{m-(k+1)+j}}{\mu_1 - \mu_{m-(k+1)+j}} \quad \text{for} \quad j = 3, \ldots, k+1.$$

This proves by means of the intermediate estimate (3.9) in Lemma 3.4 the desired inequality (3.3). The estimate (3.3) is sharp, since the same analysis applied to an H-invariant subspace associated with the eigenvalues $\mu_1, \mu_2, \mu_{m-k+2}, \ldots, \mu_m$ results in an equality in the limit case that y tends to an eigenvector associated with μ_2. ∎

3.4. Restatement of Theorem 3.1 for the generalized eigenvalue problem $Ax = \lambda Mx$. The restarted Krylov subspace iteration eigensolver (1.5) can be applied to the generalized matrix eigenvalue problem $Ax = \lambda Mx$. We use the same substitutions which join Theorem 1.1 with Theorem 1.2 in order to restate the central theorem 3.1 for the generalized eigenvalue problem.

THEOREM 3.5. *Let $\lambda_1 < \lambda_2 < \ldots < \lambda_m$ be the distinct eigenvalues of the generalized eigenvalue problem $Ax = \lambda Mx$ with symmetric and positive definite matrices $A, M \in \mathbb{R}^{n\times n}$. Further, let $\rho(\cdot)$ be the Rayleigh quotient (1.2). Consider a Ritz vector x' associated with the smallest Ritz value of (A, M) in the Krylov subspace $\mathcal{K} = \mathrm{span}\{x, A^{-1}Mx, \ldots, (A^{-1}M)^{k-1}x\}$ with $x \in \mathbb{R}^n\backslash\{0\}$ and $k \geq 2$.*

(i) If $\mathcal{K}$ is not $(A^{-1}M)$-invariant, then $\rho(x') < \rho(x)$.

(ii) If $\rho(x) \in (\lambda_i, \lambda_{i+1})$, then

$$\frac{\rho(x') - \lambda_i}{\lambda_{i+1} - \rho(x')} \leq T_{k-1}^{-2}(1 + 2\gamma_i)\,\frac{\rho(x) - \lambda_i}{\lambda_{i+1} - \rho(x)}$$

with the Chebyshev polynomial T_{k-1} and the gap ratio $\gamma_i = (\lambda_i^{-1} - \lambda_{i+1}^{-1})/(\lambda_{i+1}^{-1} - \lambda_m^{-1})$.

(iii) If x is not M-orthogonal to the eigenspace $\mathcal{E}_1$ with respect to λ_1, then

$$\tan\angle_M(x', \mathcal{E}_1) \leq \prod_{j=1}^{k-1} \frac{\lambda_2^{-1} - \lambda_{m+1-j}^{-1}}{\lambda_1^{-1} - \lambda_{m+1-j}^{-1}}\,\tan\angle_M(x, \mathcal{E}_1).$$

The bound cannot be improved in the eigenvalues. Equality can be attained in a limit case that y belongs to the invariant subspace associated with the relevant eigenvalues.

4. Numerical experiments. Next we study the numerical convergence behavior of the restarted Krylov subspace eigensolver. We compare the numerical results with the various estimates as derived in this paper. For these experiments we consider the operator eigenvalue problem for the Laplacian

$$-\Delta u = \lambda u \tag{4.1}$$

on a 2D domain with the boundary $\Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ with

$$\begin{aligned}
\Gamma_1 &= \big\{\big(\cos(t)\big(1+\sin(t)\big),\, \sin(t)\big(1+\cos(t)\big)\big)^T \;;\; t = [0, 2\pi)\big\},\\
\Gamma_2 &= \big\{\big(\alpha(1-t) + 0.25\,t\big)(1,\,1)^T \;;\; t = (0,1)\big\},\\
\Gamma_3 &= \big\{\big(0.25(1-t) + \alpha\,t\big)(1,\,1)^T \;;\; t = [0,1)\big\}
\end{aligned}$$

and $\alpha = \cos(\frac{5}{4}\pi)\big(1+\sin(\frac{5}{4}\pi)\big)$, see Figure 4.1. Homogeneous Dirichlet boundary conditions are imposed on $\Gamma_1 \cup \Gamma_3$ and homogeneous Neumann boundary conditions on Γ_2.

The eigenfunction corresponding to the smallest eigenvalue has an unbounded derivative at the boundary point $(0.25,\, 0.25)^T$, see Figure 4.1. We use the Adaptive-Multigrid-Preconditioned (AMP) Eigensolver software in order to generate an adaptive finite element grid. The homepage of this software is

`http://www.math.uni-rostock.de/ampe` .

The adaptive scheme is based on linear finite elements. It uses quadratic elements only for the residual based error estimator. The components of the residual vector of a current eigenpair approximation are taken as local error estimates for the grid refinement. We consider the iteration of the blockwise restarted Krylov subspace iteration (1.5) with $k = 3$. The triangle mesh with 1736 nodes is shown in Figure 4.2 together with two sectional enlargements of triangle meshes with 31795 and 217221 nodes around the critical point $(0.25, 0.25)^T$. In Figure 4.3, the left subfigure shows the computational costs (on a personal computer using only a single core of an Intel Xeon 3.2GHz CPU and 31.4GiB RAM) versus the degrees of freedom. The solid curve denotes the total cumulative computation times on the full level hierarchy and the oscillatory lower curve denotes the computation times on the current level. The centered subfigure shows the convergence history on the approximation error for the smallest eigenvalues with the uppermost curve for $i = 1$, the middle curve for $i = 2$ and the lowermost curve for $i = 3$. The final values of λ_i refer to an approximation from a grid with a number of 14927142 nodes. The right subfigure shows error indicators of the residual-based error estimator associated with the smallest eigenvalue λ_1. The uppermost solid curve shows the values of the residual-based error estimator using quadratic elements. The components of this vector are used as error indicators for the adaptive grid refinement. The middle (broken) curve represents a modified residual based error estimator, see Section 4 in [15]. This estimator is used for the stopping criterion of the restarted Krylov subspace iteration. The lowermost oscillatory curve shows the actual values of the residual with respect to linear finite elements. The resulting numerical approximations θ_1 of the smallest eigenvalue are listed in Table 1.

level	1	16	34	45	56	67
nodes	54	1736	31795	217294	1446646	10126530
d.o.f.	20	1610	31105	215432	1441718	10113303
θ_1	13.66037	9.836651	9.774950	9.772454	9.772125	9.772076

TABLE 1

Ritz approximations θ_1 of the smallest eigenvalue $\lambda_1 \approx 9.772073$ computed by the iteration (1.5) with $k = 3$ by means of the AMP Eigensolver software. For the finest grid with the level index 67 more then 10 million degrees of freedom (d.o.f.) have been used.

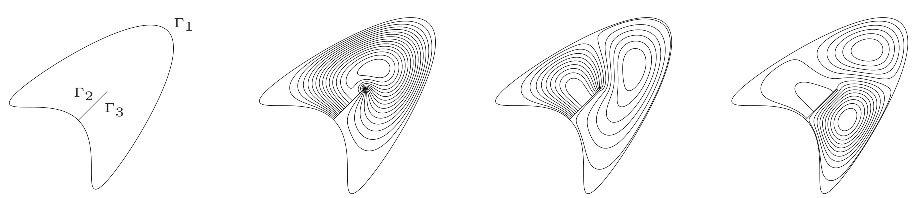

FIG. 4.1. *The 2D domain for the operator eigenvalue problem (4.1) and the contour lines of three eigenfunctions corresponding to the three smallest eigenvalues.*

Experiment I: We consider the generalized eigenvalue problem for the discretization matrix and the mass matrix with respect to the refinement level 56 with about 1.4 million degrees of freedom. We compare the slowest convergence of the Krylov subspace iteration with the estimated convergence rate from Theorem 3.5 for $k \in \{2, 3\}$. The largest ratios $\Delta_{i,i+1}(\rho(x'))/\Delta_{i,i+1}(\rho(x))$ with $\Delta_{i,i+1}(\theta) = \big(\theta - \lambda_i\big)/\big(\lambda_{i+1} - \theta\big)$ over 1000 random test vectors with a fixed value of the Rayleigh quotient are documented. The results are shown in Figure 4.4. The bold lines in the three intervals $(\lambda_i, \lambda_{i+1})$ are the upper bounds by Theorem 3.5. The three curves are the largest numerically observed ratios $\Delta_{i,i+1}(\rho(x'))/\Delta_{i,i+1}(\rho(x))$ for each 1000 test vectors with fixed Rayleigh quotients equal

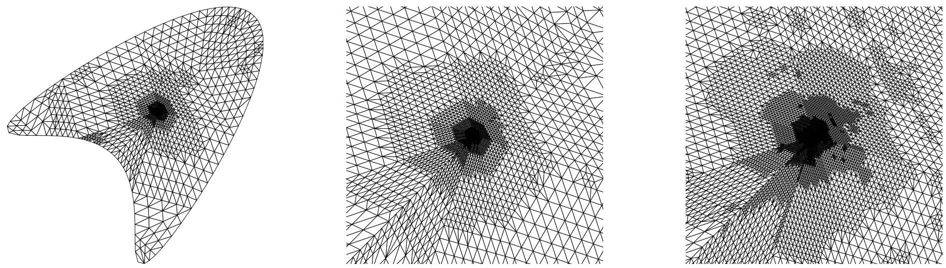

FIG. 4.2. *Triangle meshes with* 1736, 31795 *and* 217221 *nodes and associated numbers of* 1610, 31105 *and* 215359 *inner nodes. The associated depths of the triangulations are* 16, 34 *and* 45. *Sectional enlargements are drawn for the latter two finer meshes with a center in the critical point* $(0.25, 0.25)^T$. *The side lengths of these enlargements are either* $2 \cdot 10^{-3}$ *or* $2 \cdot 10^{-5}$.

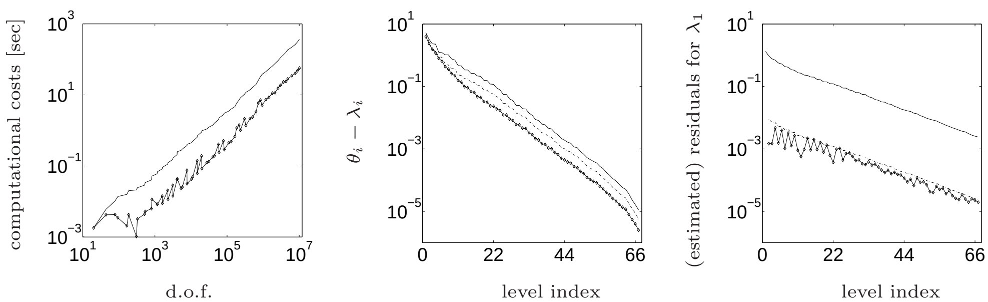

FIG. 4.3. *Computational information of the AMPEigensolver with the residual-based error estimator associated with the smallest eigenvalue* λ_1.

to 98 equidistant values in these intervals. For $k = 2$ the Ritz value estimate in Theorem 3.5 is equal to the sharp Ritz value estimate in Theorem 1.1 for the steepest descent method. These bounds are by theory attained for $\theta_i \to \lambda_i$, $i = 1, 2, 3$. The numerical data clearly confirm this property because each of the three curves tend to the limit values at the left end-points of the three intervals.

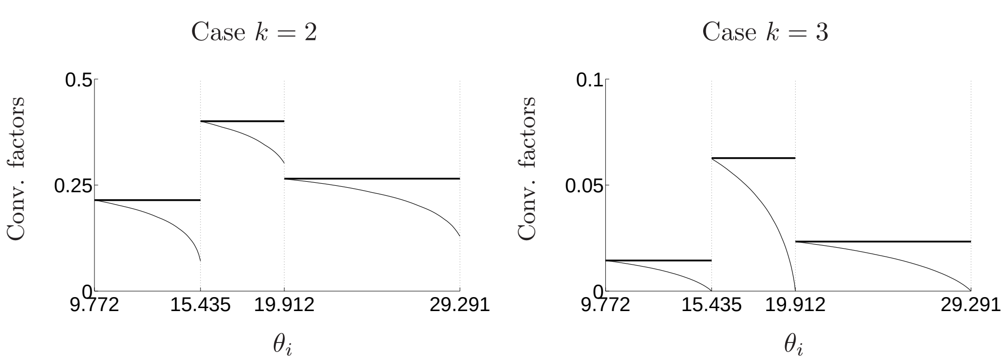

FIG. 4.4. *Poorest convergence of the Ritz values* θ_i *for* $i = 1, 2, 3$ *for the two Krylov subspace iterations with* $k = 2$ *(left subplot) and* $k = 3$ *(right subplot). Abscissa: The four smallest eigenvalues are marked.*

Experiment II: The convergence of the Ritz values is tested for the case $i = 1$ according to estimate (ii) of Theorem 3.1, respectively for its pendant in Theorem 3.5. The convergence of the eigenvalue approximations $\rho(x^{(\ell)})$ towards λ_1 is measured in terms of

$$\Delta_{1,2}\big(\rho(x^{(\ell)})\big) := \big(\rho(x^{(\ell)}) - \lambda_1\big)/\big(\lambda_2 - \rho(x^{(\ell)})\big)$$

and compared with the one-step bound $T_{k-1}^{-2}(1+2\gamma_1)\Delta_{1,2}\big(\rho(x^{(\ell-1)})\big)$ and the multi-step bound $T_{k-1}^{-2\ell}(1+2\gamma_1)\Delta_{1,2}\big(\rho(x^{(0)})\big)$. Figure 4.5 displays the convergence of the Krylov subspace iteration for $k \in \{2,3,6\}$. All curves are plotted for the case of poorest convergence, which has been observed for 1000 random initial vectors $x^{(0)}$ which all have the Rayleigh quotient $\rho(x^{(0)}) = 12$. The comparison coincides with the fact that the convergence rate $T_{k-1}^{-2}(1+2\gamma_1)$ decreases rapidly for $\lambda_1 \approx 9.77 \ll 15.44 \approx \lambda_2$ (therefore $\gamma_1 \gg 0$) and increasing k. The obvious rule is as follows: The larger the subspace index k the smaller the number of iterations until a final accuracy is reached.

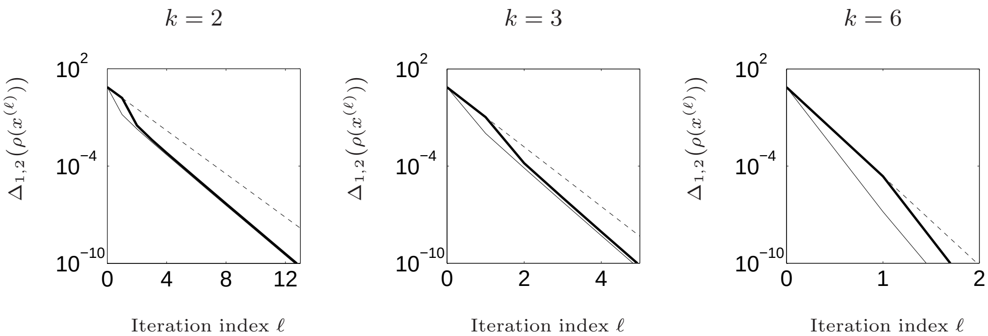

Fig. 4.5. *Convergence of the eigenvalue approximations in terms of the ratios* $\Delta_{1,2}\big(\rho(x^{(\ell)})\big) = (\rho(x^{(\ell)}) - \lambda_1)/(\lambda_2 - \rho(x^{(\ell)}))$ *for* $k \in \{2,3,6\}$. *Bold lines: One-step estimates. Dashed line: Multi-step estimates. Thin solid lines: Experimental, numerically observed data for the poorest convergence for each 1000 random initial vectors with a fixed Rayleigh quotient equal to 12.*

Experiment III: The convergence of the Ritz vectors is tested for the case $i = 1$ according to estimate (iii) of Theorem 3.1, respectively for its pendant in Theorem 3.5. The convergence of the Ritz vectors $x^{(\ell)}$ towards the eigenspace $\mathcal{E}_1$ is measured in terms of $\tan\angle_M(x^{(\ell)},\mathcal{E}_1)$ and compared with the one-step bound $\kappa\tan\angle_M(x^{(\ell-1)},\mathcal{E}_1)$ and the multi-step bound $\kappa^\ell\tan\angle_M(x^{(0)},\mathcal{E}_1)$ with $\kappa = \prod_{j=1}^{k-1}(\lambda_2^{-1} - \lambda_{m+1-j}^{-1})/(\lambda_1^{-1} - \lambda_{m+1-j}^{-1})$. Figure 4.6 displays the convergence of the Krylov subspace iterations for $k \in \{2,3,6\}$. All curves are plotted for the case of poorest convergence which has been observed for 1000 random initial vectors $x^{(0)}$ with the same initial angle $\tan\angle_M(x^{(0)},\mathcal{E}_1) = 32$. The results coincide with the fact that the convergence rate including the decisive factor $(\lambda_1/\lambda_2)^{k-1}$ decreases rapidly for $\lambda_1 \approx 9.77 \ll 15.44 \approx \lambda_2$ and increasing k. The multi-step estimates seem to be coarse. However, this does not contradict our convergence analysis as we have derived a sharp single-step estimate. The point is that the multi-step estimates simply use the one-step estimate multiple times. This does not allow to reflect an acceleration effect of multiple steps. Furthermore, the sharpness of the single-step estimate is attained in the (one-sided) limit case of decreasing $\rho(x^{(\ell)})$ towards λ_2. If $\rho(x^{(\ell)}) < \lambda_2$, then a different and smaller convergence bound exists, cf. Section 3.1 in [18] for details of a similar argument on the steepest descent iteration.

5. Conclusion. A-gradient steepest descent iterations and their generalizations in the form of restarted Krylov subspace iterations are efficient schemes in order to compute (a modest number of) the smallest eigenvalue(s) together with the invariant spectral subspace of the discretization of self-adjoint and elliptic partial differential operators. However, each step of these iterations requires the solution of a linear system of equations in A. The solution of such a linear system, which corresponds to the solution of a

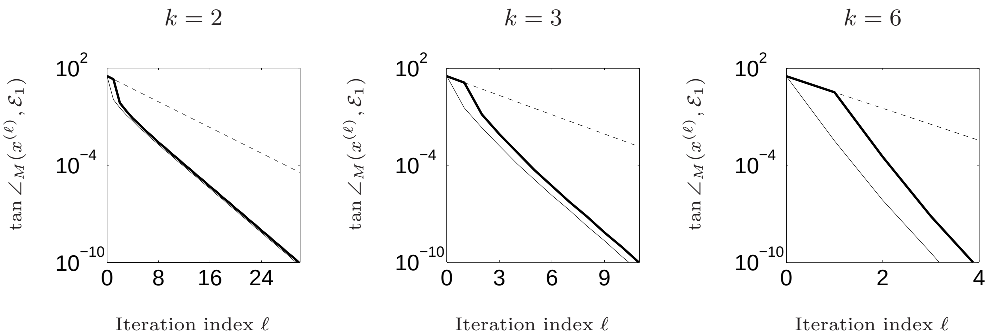

FIG. 4.6. *Convergence of the eigenvector approximations in terms of* $\tan \angle_M(x^{(\ell)}, \mathcal{E}_1)$ *for* $k \in \{2, 3, 6\}$. *Bold lines: One-step estimates. Dashed lines: Multi-step estimates. Thin solid lines: Experimental, numerically observed data for the poorest convergence for each 1000 random initial vectors with a fixed initial subspace angle* $\tan \angle_M(x^{(0)}, \mathcal{E}_1) = 32$.

boundary value problem for the given partial differential operator, can be implemented numerically by a (multigrid) preconditioned iterative scheme. This scheme can either be a pure multigrid solver or a multigrid preconditioned iterative solver which is possibly based on a conjugate gradient iteration. Instead of a precise solution of the linear system, an approximate solver can be constructed from the precise solver by using a loosened stopping condition. The approximate solver can ideally be used as a preconditioner in order to substitute the exact solver in the A-gradient scheme. The resulting iterative scheme is a preconditioned gradient iteration for the solution of eigenvalue problems.

As already mentioned in Section 1.1, the convergence analysis of preconditioned gradient type eigensolvers suffers from the complication by the spectral assumptions of the quality of the preconditioner. However, the present analysis provides convergence estimates for the limit case that an exact-inverse “preconditioning” has been used. Therefore, our analysis of restarted Krylov subspace eigensolvers with arbitrary subspace dimensions constitutes the basis for an understanding of a large class of preconditioned eigensolver iterations for the important limit case of accurate preconditioning.

REFERENCES

[1] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst, editors. *Templates for the solution of algebraic eigenvalue problems: A practical guide.* SIAM, Philadelphia, 2000.

[2] J. Cullum and W.E. Donath. A block generalization of the symmetric s-step Lanczos algorithm. IBM Research, RC 4845, Yorktown Heights, N.Y., 1974.

[3] E.G. D'yakonov. *Optimization in solving elliptic problems.* CRC Press, Boca Raton, Florida, 1996.

[4] G.H. Golub and R. Underwood. The block Lanczos method for computing eigenvalues. In *Mathematical software, III (Proc. Sympos., Math. Res. Center, Univ. Wisconsin, Madison, Wis., 1977)*, pages 361–377. Publ. Math. Res. Center, No. 39. Academic Press, New York, 1977.

[5] G.H. Golub and C.F. Van Loan. *Matrix computations.* Johns Hopkins University Press, Baltimore, MD, third edition, 1996.

[6] S. Kaniel. Estimates for some computational techniques in linear algebra. *Math. Comp.*, 20:369–378, 1966.

[7] A.V. Knyazev. *Computation of eigenvalues and eigenvectors for mesh problems: algorithms and error estimates.* Dept. Numerical Math. USSR Academy of Sciences, Moscow, 1986. (In Russian).

[8] A.V. Knyazev. Convergence rate estimates for iterative methods for a mesh symmetric eigenvalue problem. *Russian J. Numer. Anal. Math. Modelling*, 2:371–396, 1987.

[9] A.V. Knyazev. Preconditioned eigensolvers—an oxymoron? *Electron. Trans. Numer. Anal.*, 7:104–123, 1998.

[10] A.V. Knyazev and K. Neymeyr. A geometric theory for preconditioned inverse iteration. III: A short and sharp convergence estimate for generalized eigenvalue problems. *Linear Algebra Appl.*, 358:95–114, 2003.

[11] A.V. Knyazev and K. Neymeyr. Efficient solution of symmetric eigenvalue problems using multigrid preconditioners in the locally optimal block conjugate gradient method. *Electron. Trans. Numer. Anal.*, 15:38–55, 2003.

[12] A.V. Knyazev and A.L. Skorokhodov. On exact estimates of the convergence rate of the steepest ascent method in the symmetric eigenvalue problem. *Linear Algebra Appl.*, 154–156:245–257, 1991.

[13] K. Neymeyr. A geometric theory for preconditioned inverse iteration. I: Extrema of the Rayleigh quotient. *Linear Algebra Appl.*, 322:61–85, 2001.

[14] K. Neymeyr. A hierarchy of preconditioned eigensolvers for elliptic differential operators. Habilitationsschrift an der Mathematischen Fakultät, Universität Tübingen, 2001.

[15] K. Neymeyr. A posteriori error estimation for elliptic eigenproblems. *Numer. Linear Algebra Appl.*, 9:263–279, 2002.

[16] K. Neymeyr. On preconditioned eigensolvers and Invert-Lanczos processes. *Linear Algebra Appl.*, 430:1039–1056, 2009.

[17] K. Neymeyr. A geometric convergence theory for the preconditioned steepest descent iteration. *SIAM J. Numer. Anal.*, 50:3188–3207, 2012.

[18] K. Neymeyr, E. Ovtchinnikov, and M. Zhou. Convergence analysis of gradient iterations for the symmetric eigenvalue problem. *SIAM J. Matrix Anal. Appl.*, 32(2):443–456, 2011.

[19] K. Neymeyr and M. Zhou. Iterative minimization of the Rayleigh quotient by the block steepest descent iteration. *Numer. Linear Algebra Appl.*, 21:604–617, 2014.

[20] K. Neymeyr and M. Zhou. The block preconditioned steepest descent iteration for elliptic operator eigenvalue problems. *Electron. Trans. Numer. Anal.*, 41:93–108, 2014.

[21] B.N. Parlett. *The symmetric eigenvalue problem.* Prentice Hall, Englewood Cliffs New Jersey, 1980.

[22] Y. Saad. On the rates of convergence of the Lanczos and the block-Lanczos methods. *SIAM J. Numer. Anal.*, 17(5):687–706, 1980.

[23] H.A. van der Vorst. A generalized Lanczos scheme. *Math. Comp.*, 39:559–561, 1982.