.

ITERATIVE MINIMIZATION OF THE RAYLEIGH QUOTIENT BY BLOCK STEEPEST DESCENT ITERATIONS

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Abstract. The topic of this paper is the convergence analysis of subspace gradient iterations for the simultaneous computation of a few of the smallest eigenvalues plus eigenvectors of a symmetric and positive definite matrix pair (A, M). The methods are based on subspace iterations for $A^{-1}M$ and use the Rayleigh-Ritz procedure for convergence acceleration. New sharp convergence estimates are proved by generalizing estimates which have been presented for vectorial steepest descent iterations (see SIAM J. Matrix Anal. Appl., 32(2):443-456, 2011).

Key words. Subspace iteration, steepest descent/ascent, Rayleigh-Ritz procedure, elliptic eigenvalue problem.

1. Introduction.

The generalized matrix eigenvalue problem

$$Ax_i = \lambda_i M x_i \tag{1.1}$$

is of fundamental importance for numerous applications. An exemplary application is the molecular electronic structure theory, where the computation of stationary states of atoms and molecules requires the solution of such matrix eigenvalue problems. Some references on the numerical solution of (1.1) in the context of the molecular quantum theory are [3, 4, 5, 8, 30, 21].

Typically, A and M are large and sparse matrices and only a few of the smallest eigenvalues together with the eigenvectors are to be determined. If (1.1) results from a finite element discretization of an operator eigenvalue problem, then A is called the discretization matrix and M the mass matrix. Here we assume that A and M are symmetric and positive definite matrices. If in a more general case A is an indefinite and symmetric matrix, then the eigenvalue problem can be transformed to one with positive definite matrices by means of a proper shift.

Our aim is a fast, storage-efficient and stable numerical computation of the smallest eigenvalues of (1.1). If these matrices are not too large, then the Lanczos and the block-Lanczos procedures [2, 10, 29] may be considered as proper numerical eigensolvers. Here we assume that n is so large that computer storage is available only for a very small number of n-vectors. Then the m-step Lanczos process may be used as a storage-efficient alternative; this method can be interpreted as a gradient iteration for the Rayleigh quotient.

1.1. Gradient type minimization of the Rayleigh quotient.

Golub and van Loan in Sec. 9.1.1 of [10] introduce the Lanczos iteration by an optimization for the Rayleigh quotient for a symmetric matrix A

$$\rho_A(x) = (x, Ax)/(x, x), \qquad x \neq 0,\ A = A^T \in \mathbb{R}^{n\times n}.$$

Consecutive corrections in the directions of negative gradients of $\rho_A(\cdot)$ result in iterates which span the Krylov subspace underlying the Lanczos algorithm.

For the generalized eigenvalue problem (1.1) the Rayleigh quotient reads

$$\rho_{A,M}(x) = (x, Ax)/(x, Mx), \qquad x \neq 0. \tag{1.2}$$

Here we are interested in various gradient iterations for the minimization of $\rho_{A,M}$.

We denote the eigenpairs of (A, M) by (λ_i, x_i) and assume all eigenvalues to be simple. The enumeration is $0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n$. Multiple eigenvalues do not add difficulties to the analysis of gradient eigensolvers as the case of multiple eigenvalues can be reduced

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to that of only simple eigenvalues by a proper projection of the eigenvalue problem. Alternatively, a continuity argument can be used to show that colliding eigenvalues do not change the structure of the convergence estimates, cf. Lemma 2.1 in [24].

The iterative minimization of (1.2) results in the smallest eigenvalue λ_1 and the minimum is attained in an associated eigenvector. A correction of a current iterate x in the direction of the negative gradient

$$-\nabla \rho_{A,M}(x) = -2(Ax - \rho_{A,M}(x)Mx)/(x, Mx)$$

allows to construct a new iterate $x' = x - \omega \nabla \rho_{A,M}(x)$ with $\rho_{A,M}(x') < \rho_{A,M}(x)$ if x is not an eigenvector. Therein $\omega \in \mathbb{R}$ is the step length. The optimal step length ω^* minimizes $\rho_{A,M}(x')$ with respect to $\omega \in \mathbb{R}$. Formally, ω^* may be infinite if $\nabla \rho_{A,M}(x)$ is a Ritz vector corresponding to the smallest Ritz value in the 2D subspace $\mathrm{span}\{x, \nabla \rho_{A,M}(x)\}$. This problem disappears if the Rayleigh-Ritz procedure is applied to $\mathrm{span}\{x, \nabla \rho_{A,M}(x)\}$.

For the case $M = I$ such a gradient iteration using the Euclidean gradient vector of (1.2) converges poorly if the largest eigenvalue λ_n is very large. For convergence estimates see [12, 13, 14, 27, 32, 17, 19]; convergence estimates for general M are given in [11, 20]. A typical example is the eigenvalue problem for a second order elliptic partial differential operator (like the Laplacian) for which the largest discrete eigenvalue λ_n behaves like $\mathcal{O}(h^{-2})$ in the discretization parameter h. As D'yakonov pointed out in [7], Chap. 9, §4.1, the Euclidean gradient iteration can be accelerated considerably by using *modified gradient methods*, see also the early work of Samokish [28]. D'yakonov stated for a symmetric and positive definite model operator B that the use of B-gradients $\nabla_B \rho_{A,M}(x) := B^{-1} \nabla \rho_{A,M}(x)$ can be interpreted as a change of the underlying geometry. The A-gradient is of special importance since using A-gradients can result in grid-independent convergence behavior. Further, A-gradients constitute the limit case of exact "preconditioning" with the inverse A^{-1}. Using approximate inverses of A represents the general case of preconditioning.

The *A-gradient steepest descent iteration* works with the optimal step length ω^*

$$x' = x - \omega^* A^{-1} \nabla \rho_{A,M}(x) \tag{1.3}$$

in a way that x' attains in ω^* the smallest possible Rayleigh quotient with respect to a variation of the step length. Then x' is a Ritz vector of (A, M) in the two-dimensional subspace $\mathrm{span}\{x, A^{-1}Mx\}$ corresponding to the smallest Ritz value. Computationally x' is determined by the Rayleigh-Ritz procedure.

For the vectorial A-gradient iteration (1.3) in the case $M = I$ a sharp convergence estimate has recently been proved by Theorem 4.1 in [25], which generalizes the convergence estimate of Knyazev and Skorokhodov in [19] where only the final eigenvalue interval is considered, i.e. (λ_1, λ_2) for steepest descent and $(\lambda_{n-1}, \lambda_n)$ for steepest ascent. Here we analyze the general case of intervals $(\lambda_i, \lambda_{i+1})$ with $i \in \{1, \ldots, n-1\}$. The estimate in [19] provides the analytical ground for the formulation of four Ritz value estimates, which read as follows (see also Theorem 4.1 in [25]):

THEOREM 1.1. *Consider a symmetric matrix A with eigenpairs (λ_i, x_i), $\lambda_1 < \lambda_2 < \ldots < \lambda_n$. Let $x \in \mathbb{R}^n$ with the Rayleigh quotient $\lambda := \rho_A(x) \in (\lambda_i, \lambda_{i+1})$ for a certain index $i \in \{1, \ldots, n-1\}$. Further let $\Delta_{p,q}(\theta) := (\theta - \lambda_p)/(\lambda_q - \theta)$, and denote by $\mathcal{E}_{j,k,l}$ the invariant subspace spanned by the eigenvectors being associated with the eigenvalues $\lambda_j < \lambda_k < \lambda_l$.*

1. *Steepest descent iteration:*

   1a) Let x' be the new iterate of the Euclidean gradient steepest descent iteration so that x' is a Ritz vector of A in $\mathrm{span}\{x, Ax\}$ and $\lambda' := \rho_A(x')$ is the associated Ritz value. Then either $\lambda' < \lambda_i$ or λ' is bounded from above as follows

$$0 \leq \frac{\Delta_{i,i+1}(\lambda')}{\Delta_{i,i+1}(\lambda)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_n - \lambda_{i+1}}{\lambda_n - \lambda_i}.$$

1b) Let A additionally be a positive definite matrix and let x' be the new iterate of the A-gradient steepest descent iteration so that x' is a Ritz vector of A in $\operatorname{span}\{x, A^{-1}x\}$ *and $\lambda' := \rho_A(x')$ is the associated Ritz value. Then either $\lambda' < \lambda_i$ or λ' is bounded from above as follows*

$$0 \leq \frac{\Delta_{i,i+1}(\lambda')}{\Delta_{i,i+1}(\lambda)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \textit{with} \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}.$$

The bounds cannot be improved in the eigenvalues λ_i, λ_{i+1} and λ_n and can be attained for $\lambda \to \lambda_i$ in $\mathcal{E}_{i,i+1,n}$.

2. *Steepest ascent iteration:*
2a) Let x' be the new iterate of the Euclidean gradient steepest ascent iteration so that x' is a Ritz vector of A in $\operatorname{span}\{x, Ax\}$ *and $\lambda' := \rho_A(x')$ is the associated Ritz value. Then either $\lambda' > \lambda_{i+1}$ or λ' is bounded from below as follows*

$$0 \leq \frac{\Delta_{i+1,i}(\lambda')}{\Delta_{i+1,i}(\lambda)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \textit{with} \quad \kappa = \frac{\lambda_i - \lambda_1}{\lambda_{i+1} - \lambda_1}.$$

2b) Let A additionally be a positive definite matrix and let x' be the new iterate of the A-gradient steepest ascent iteration so that x' is a Ritz vector of A in $\operatorname{span}\{x, A^{-1}x\}$ *and $\lambda' := \rho_A(x')$ is the associated Ritz value. Then either $\lambda' > \lambda_{i+1}$ or λ' is bounded from below as follows*

$$0 \leq \frac{\Delta_{i+1,i}(\lambda')}{\Delta_{i+1,i}(\lambda)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \textit{with} \quad \kappa = \frac{\lambda_{i+1}(\lambda_i - \lambda_1)}{\lambda_i(\lambda_{i+1} - \lambda_1)}.$$

The bounds cannot be improved in the eigenvalues λ_1, λ_i and λ_{i+1} and can be attained for $\lambda \to \lambda_{i+1}$ in $\mathcal{E}_{1,i,i+1}$.

There are close relations between these four estimates. Essentially, only one estimate has to be proved from scratch, and the remaining estimates follow by simple transformations. For the details see the proof of Theorem 4.1 in [25]. See also [19, 25] for the tangent estimates for these gradient iterations. Furthermore, the estimate 1b can easily be reformulated into an estimate for the vectorial A-gradient iteration (1.3) with a general symmetric and positive definite mass matrix M, cf. section 3.1.

1.2. Aim of this paper. The aim of this paper is to analyze A-gradient and Euclidean-gradient subspace iterations and to prove subspace convergence estimates which generalize the vectorial convergence estimates given in Theorem 1.1.

In all the eigensolvers an initial s-dimensional subspace is iteratively corrected so that the sequence of subspaces converges to the invariant subspace which is spanned by the eigenvectors corresponding to the s smallest eigenvalues. The Rayleigh-Ritz procedure is used in each step to extract the Ritz values and Ritz vectors as proper eigenpair approximations. We consider the standard as well as the generalized eigenvalue problem.

The central Theorem 3.1 of this paper contributes new sharp subspace estimates to the hierarchy of non-preconditioned and preconditioned vector and subspace solvers for eigenproblems. All these convergence estimates have the standardized form

$$\Delta_{i,i+1}(\lambda') \leq \sigma^2 \Delta_{i,i+1}(\lambda)$$

with $\Delta_{i,i+1}(\xi) = (\xi - \lambda_i)/(\lambda_{i+1} - \xi)$. For the non-preconditioned gradient iteration with fixed step-length the convergence factor is $\sigma = \lambda_i/\lambda_{i+1}$, see [23], while for the preconditioned inverse iteration, also called preconditioned gradient iteration, the convergence factor reads $\sigma = \gamma + (1-\gamma)\lambda_i/\lambda_{i+1}$, see [18]. The latter estimate also applies to the corresponding subspace iteration; a discussion follows in Section 3.1. The convergence of non-preconditioned gradient iterations with optimal step-length is analyzed in [25], cf. Theorem 1.1. Estimates for the preconditioned optimal step-length gradient iterations are given in [24].

1.3. Notation and overview. We use the following notation for subspaces: Calligraphic capital letters denote subspaces; the column space of a matrix Z is $\mathcal{Z} = \mathrm{span}\{Z\}$. Similarly, $\mathrm{span}\{Z, Y\}$ is the smallest vector space which contains the column spaces of Z and of Y.

The paper is structured as follows: The subspace iterations and their relations to the truncated block-Lanczos iteration are introduced in Section 2. The new convergence estimates on A-gradient and Euclidean gradient block steepest descent/ascent are presented in Section 3; Theorem 3.1 provides new sharp convergence estimates for the Ritz values. Some numerical experiments presenting the sharpness of the estimates and the cluster-robustness of the A-gradient subspace iteration are presented in Section 4.

2. Subspace iteration with Rayleigh-Ritz projections. We generalize the vector iteration (1.3) to a subspace iteration. The starting point is an s-dimensional subspace $\mathcal{V}$ of the $\mathbb{R}^n$ which is given by the column space of the M-orthonormal matrix $V \in \mathbb{R}^{n\times s}$. The columns of V are assumed to be the M-normalized Ritz vectors of (A, M) in $\mathcal{V}$. Further $\Theta = \mathrm{diag}(\theta_1, \ldots, \theta_s)$ is the $s \times s$ diagonal matrix of the corresponding Ritz values. The matrix residual

$$AV - MV\Theta \in \mathbb{R}^{n\times s}$$

contains columnwise the residuals of the Ritz vectors. By solving s linear systems in A one gets the subspace correction term $A^{-1}(AV - MV\Theta)$ of an A-gradient subspace iteration. Optimal eigenpair approximations are to be determined in

$$\mathrm{span}\{V,\, A^{-1}(AV - MV\Theta)\} = \mathrm{span}\{V,\, A^{-1}MV\}.$$

The desired optimal eigenpair approximations are just the s smallest Ritz values and the associated Ritz vectors. These can be computed by applying the Rayleigh-Ritz procedure for (A, M) to the subspace $\mathrm{span}\{V,\, A^{-1}MV\}$.

This subspace iteration can be understood as a *2-step block-invert-Lanczos process* with respect to the matrices $\tilde{A} = M^{-1/2}AM^{-1/2}$, $\tilde{V} = M^{1/2}V$. To explain this let us first consider a one-dimensional subspace: An m-step vectorial Lanczos iteration starts with an initial vector $\tilde{v}^{(0)}$ from which the Krylov subspace

$$\mathcal{K}_m(\tilde{A}, \tilde{v}^{(0)}) = \mathrm{span}\{\tilde{v}^{(0)}, \tilde{A}\tilde{v}^{(0)}, \ldots, \tilde{A}^{m-1}\tilde{v}^{(0)}\}$$

is built. A Ritz vector corresponding to the smallest Ritz value of $\tilde{A}$ in this Krylov space constitutes the next iterate $\tilde{v}^{(1)}$. Such a Ritz pair corresponds to a Ritz pair of (A, M) in the Krylov subspace $\mathcal{K}_m(M^{-1}A, v^{(0)})$ with $M^{1/2}v^{(0)} = \tilde{v}^{(0)}$ because of $\rho_{\tilde{A}}(M^{1/2}v) = \rho_{A,M}(v)$ and

$$\mathrm{span}\{\tilde{v}^{(0)}, \tilde{A}\tilde{v}^{(0)}, \ldots, \tilde{A}^{m-1}\tilde{v}^{(0)}\} = M^{1/2}\mathrm{span}\{v^{(0)}, (M^{-1}A)v^{(0)}, \ldots, (M^{-1}A)^{m-1}v^{(0)}\}.$$

The memory requirements for the m-step Lanczos scheme is foreseeable and relatively small whereas for the classical Lanczos scheme in each step a further n-vector is to be stored. Some references on the m-step Lanczos iteration are [6, 15, 32, 31].

The block variant of an m-step iteration substitutes the initial vector $v^{(0)}$ by an initial subspace $\mathcal{V}^{(0)}$ with the Ritz basis $V^{(0)} \in \mathbb{R}^{n\times s}$ which leads to the block-Krylov subspace

$$\mathcal{K}_m(M^{-1}A, V^{(0)}) = \mathrm{span}\{V^{(0)}, (M^{-1}A)V^{(0)}, \ldots, (M^{-1}A)^{m-1}V^{(0)}\}. \tag{2.1}$$

The Rayleigh-Ritz procedure for (A, M) is used to extract from $\mathcal{K}_m(M^{-1}A, V^{(0)})$ the next subspace $\mathcal{V}^{(1)}$. This space is spanned by the s Ritz vectors of (A, M) which correspond to the s smallest Ritz values. See [9, 10] for block-Lanczos iterations. For $m = 2$ the invert-Lanczos process uses

$$\mathcal{K}_2(A^{-1}M, V^{(0)}) = \mathrm{span}\{V^{(0)}, A^{-1}MV^{(0)}\}$$

with constant and minimal memory requirements throughout the iteration. Hence the block steepest descent iteration has the following form:

Algorithm 1 A-gradient steepest descent subspace iteration:

Require: $A, M \in \mathbb{R}^{n\times n}$ s.p.d.

1. **Initialization**: *Generate a random initial s-dimensional subspace $\mathcal{V}^{(0)}$ being the column space of $V^{(0)} \in \mathbb{R}^{n\times s}$. $\mathcal{V}^{(0)}$ satisfies $\angle_M(\mathcal{V}^{(0)}, \mathcal{E}_{1:s}) < \pi/2$ where $\mathcal{E}_{1:s}$ is the invariant subspace associated with the s smallest eigenvalues of (A, M) and the angle $\angle_M$ is induced by the inner product w.r.t. the matrix M.*
2. **Iteration**: *For $i \geq 0$ (until the termination condition is satisfied) apply the Rayleigh-Ritz procedure to* $\mathrm{span}\{V^{(i)}, A^{-1}MV^{(i)}\}$ *and let $V^{(i+1)} = [v_1^{(i+1)}, \dots v_s^{(i+1)}]$ be the Ritz vectors of (A, M) corresponding to the s smallest Ritz values $\theta_1^{(i+1)}, \dots, \theta_s^{(i+1)}$. Further let $\Theta^{(i+1)} = \mathrm{diag}(\theta_1^{(i+1)}, \dots, \theta_s^{(i+1)})$.*
3. **Termination**: *If $\|R^{(i+1)}\| := \|AV^{(i+1)} - MV^{(i+1)}\Theta^{(i+1)}\| \leq \epsilon$ for an appropriate accuracy ϵ, then stop the iteration.*

Algorithm 1 can easily be modified to a block steepest ascent iteration and can be reformulated to block steepest descent/ascent iterations in $\mathrm{span}\{V, M^{-1}AV\}$. All these subspace iterations are analyzed in Section 3.

3. Convergence analysis. In our convergence analysis we first discuss the case $M = I$ and refer to section 3.1 for the general case. Now Theorem 1.1 is generalized to subspace iterations. Convergence estimates for the Ritz values are presented for block steepest descent/ascent iterations in $\mathrm{span}\{V, A^{-1}V\}$ and $\mathrm{span}\{V, AV\}$. Symmetry is always assumed for A; positive definiteness is required if the iteration involves A^{-1}.

THEOREM 3.1. *Consider a symmetric matrix A with eigenpairs (λ_i, x_i), $\lambda_1 < \lambda_2 < \dots < \lambda_n$. Let $\mathcal{V}$ be an s-dimensional subspace of the $\mathbb{R}^n$ and let $V := [v_1, \dots, v_s]$ whose columns are the Ritz vectors v_i, $i = 1, \dots, s$ of A in $\mathcal{V}$. The associated Ritz values are $\theta_i = \rho_A(v_i)$. Indexes k_i are given so that $\theta_i \in (\lambda_{k_i}, \lambda_{k_i+1})$. Moreover, the subspace $\mathcal{V}$ is assumed to contain no eigenvector of A (which otherwise could easily be split off within the Rayleigh-Ritz procedure). Let $\Delta_{p,q}(\theta) := (\theta - \lambda_p)/(\lambda_q - \theta)$ and let $\mathcal{E}_{j,k,l}$ be the invariant subspace spanned by the eigenvectors for the eigenvalues $\lambda_j < \lambda_k < \lambda_l$.*

1. Block steepest descent iteration: The Ritz values of A in $\mathcal{V}$ are enumerated in increasing order $\theta_1 \leq \dots \leq \theta_s$.

1a) If $\theta'_1 \leq \dots \leq \theta'_s$ are the s smallest Ritz values of A in $\mathrm{span}\{V, AV\}$*, then for each $i \in \{1, \dots, s\}$ it holds that $\theta'_i \leq \theta_i$ and either $\theta'_i < \lambda_{k_i}$ or*

$$0 \leq \frac{\Delta_{k_i,k_i+1}(\theta'_i)}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_n - \lambda_{k_i+1}}{\lambda_n - \lambda_{k_i}}. \tag{3.1}$$

1b) Let A additionally be a positive definite matrix. If $\theta'_1 \leq \dots \leq \theta'_s$ are the s smallest Ritz values of A in $\mathrm{span}\{V, A^{-1}V\}$*, then for each $i \in \{1, \dots, s\}$ it holds that $\theta'_i \leq \theta_i$ and either $\theta'_i < \lambda_{k_i}$ or*

$$0 \leq \frac{\Delta_{k_i,k_i+1}(\theta'_i)}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_{k_i}(\lambda_n - \lambda_{k_i+1})}{\lambda_{k_i+1}(\lambda_n - \lambda_{k_i})}. \tag{3.2}$$

The bounds in (3.1) and (3.2) cannot be improved in terms of the eigenvalues of A and can be attained for $\theta_i \to \lambda_{k_i}$ in $\mathcal{E}_{k_i,k_i+1,n}$.

2. Block steepest ascent iteration: The Ritz values of A in $\mathcal{V}$ are enumerated in decreasing order $\theta_1 \geq \ldots \geq \theta_s$. This enumeration allows to state the estimates in a form which is most similar to the cases 1a and 1b.

2a) If $\theta'_1 \geq \ldots \geq \theta'_s$ are the s largest Ritz values of A in $\operatorname{span}\{V, AV\}$, then for each $i \in \{1, \ldots, s\}$ it holds that $\theta'_i \geq \theta_i$ and either $\theta'_i > \lambda_{k_i+1}$ or

$$0 \leq \frac{\Delta_{k_i+1,k_i}(\theta'_i)}{\Delta_{k_i+1,k_i}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_{k_i} - \lambda_1}{\lambda_{k_i+1} - \lambda_1}. \tag{3.3}$$

2b) Let A additionally be a positive definite matrix. If $\theta'_1 \geq \ldots \geq \theta'_s$ are the s largest Ritz values of A in $\operatorname{span}\{V, A^{-1}V\}$, then for each $i \in \{1, \ldots, s\}$ it holds that $\theta'_i \geq \theta_i$ and either $\theta'_i > \lambda_{k_i+1}$ or

$$0 \leq \frac{\Delta_{k_i+1,k_i}(\theta'_i)}{\Delta_{k_i+1,k_i}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_{k_i+1}(\lambda_{k_i} - \lambda_1)}{\lambda_{k_i}(\lambda_{k_i+1} - \lambda_1)}. \tag{3.4}$$

The bounds in (3.3) and (3.4) cannot be improved in terms of the eigenvalues of A and can be attained for $\theta_i \to \lambda_{k_i+1}$ in $\mathcal{E}_{1,k_i,k_i+1}$.

Theorem 3.1 generalizes Theorem 2.5 in [17] (see also its original version [16] in Russian). In [17] all the Ritz values are restricted to the final intervals, which means that in our notation $k_i = i$ is assumed. In [17] the case 2a is considered explicitly as a particular case of a general theory. We start proving the assertion for the case 1a. The remaining estimates can then be shown by applying proper transformations. A first step towards the proof for the case 1a is to show that a vector $v \in \mathcal{V} \setminus \{0\}$ of poor convergence exists so that the s-th Ritz value θ'_s is bounded by the *vector-wise attainable* Ritz value if the vector iteration is applied to v.

Theorem 3.2. *On the assumption and notation of the case 1a of Theorem 3.1 a vector (of relatively poor convergence) $v \in \mathcal{V} = \operatorname{span}\{V\}$, $v \neq 0$, exists so that*

$$\theta'_s \leq \min_{u \in \operatorname{span}\{v, Av\}} \rho_A(u).$$

Proof. Let the columns of $U \in \mathbb{R}^{n \times \tilde{s}}$ (with $\tilde{s} \leq 2s$) be a Euclidean orthonormal basis of $\operatorname{span}\{V, AV\}$. Then the Ritz values $\theta'_1 \leq \ldots \leq \theta'_{\tilde{s}}$ of A in $\operatorname{span}\{V, AV\}$ are identical with the eigenvalues of the matrix $B := U^T AU \in \mathbb{R}^{\tilde{s} \times \tilde{s}}$. Let $\mathcal{S}$ be the invariant subspace of B spanned by the eigenvectors with the indexes $s, \ldots, \tilde{s}$ and let $\mathcal{Y} := U^T \mathcal{V}$ be the representing subspace of $\mathcal{V}$ w.r.t. the basis U. Summing up the dimensions of $\mathcal{S}$ and $\mathcal{Y}$ shows that

$$\dim \mathcal{S} + \dim \mathcal{Y} = (\tilde{s} - s + 1) + s = \tilde{s} + 1.$$

Since each $\mathcal{S}$ and $\mathcal{Y}$ are subspaces of the $\tilde{s}$-dimensional space $\operatorname{span}\{U^T\}$ we conclude that a nonzero vector y exists with $y \in \mathcal{S} \cap \mathcal{Y}$. Next we discuss two representations of y.

First, $y \in \mathcal{S}$ together with the B-invariance of $\mathcal{S}$ proves that $\operatorname{span}\{y, By\} \subseteq \mathcal{S}$. Thus

$$\min_{z \in \operatorname{span}\{y, By\}} \frac{z^T Bz}{z^T z} \geq \min_{z \in \mathcal{S}} \frac{z^T Bz}{z^T z} = \theta'_s.$$

Second, $y \in \mathcal{Y}$ implies $v := Uy \in U\mathcal{Y} = UU^T \mathcal{V} = \mathcal{V}$, since UU^T is the Euclidean orthogonal projector on $\operatorname{span}\{U\}$ and $\mathcal{V} \subseteq \operatorname{span}\{U\}$. Analogously, since also $A\mathcal{V} \subseteq \operatorname{span}\{U\}$, we get from $v \in \mathcal{V}$ that

$$Av = (UU^T)(Av) = UU^T AUy = UBy$$

and further

$$\operatorname{span}\{v, Av\} = \operatorname{span}\{Uy, UBy\} = U\operatorname{span}\{y, By\} = \big\{Uz\ ;\ z \in \operatorname{span}\{y, By\}\big\}.$$

Combining these results we get

$$\min_{u \in \operatorname{span}\{v,Av\}} \rho_A(u) = \min_{z \in \operatorname{span}\{y,By\}} \rho_A(Uz) = \min_{z \in \operatorname{span}\{y,By\}} \frac{z^T B z}{z^T z} \geq \theta'_s$$

and the existence of v. □

Theorem 3.2 serves to prove the case 1a of Theorem 3.1 for the largest Ritz value with $i = s$.

COROLLARY 3.1. *The convergence estimate (3.1) of Theorem 3.1 holds for $i = s$.*

Proof. If $k_s = n-1$, then the first alternative $\theta'_s < \lambda_{k_s}$ applies since the s-th Ritz value of A in an $\tilde{s}$-dimensional subspace with $\tilde{s} > s$ is always less than λ_{n-1}. Next let $k_s < n-1$ and let $\lambda_{k_s} \leq \theta'_s$ (for which (3.1) is to be proved).

We first prove that $\theta'_s \leq \theta_s$ by applying the variational principles

$$\theta'_s = \min_{\substack{\mathcal{U} \subseteq \operatorname{span}\{V,AV\} \\ \dim(\mathcal{U})=s}} \max_{y \in \mathcal{U}\setminus\{0\}} \rho_A(y) \leq \min_{\substack{\mathcal{U} \subseteq \mathcal{V} \\ \dim(\mathcal{U})=s}} \max_{y \in \mathcal{U}\setminus\{0\}} \rho_A(y) = \theta_s.$$

Theorem 3.2 shows the existence of a vector $v \in \mathcal{V}$ so that

$$\theta'_s \leq \min_{u \in \operatorname{span}\{v,Av\}} \rho_A(v) =: \widehat{\theta}_s.$$

Since $\Delta_{k_s,k_s+1}(\theta) = (\theta - \lambda_{k_s})/(\lambda_{k_s+1} - \theta)$ is for $\theta \in [\lambda_{k_s}, \lambda_{k_s+1})$ a monotone increasing function we get that $\Delta_{k_s,k_s+1}(\theta'_s) \leq \Delta_{k_s,k_s+1}(\widehat{\theta}_s)$; for completeness one has to check that $\widehat{\theta}_s \leq \lambda_{k_s+1}$ by using the variational principles. Further, the vectorial estimate for steepest descent (case 1a in Theorem 1.1) is applied to this particular v. This results the rightmost inequality in

$$\Delta_{k_s,k_s+1}(\theta'_s) \leq \Delta_{k_s,k_s+1}(\widehat{\theta}_s) \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \Delta_{k_s,k_s+1}(\rho_A(v)).$$

The proof is completed by recognizing that $\rho_A(v)$ is bounded by the largest Ritz value θ_s of A in $\mathcal{V}$, i.e. $\Delta_{k_s,k_s+1}(\rho_A(v)) \leq \Delta_{k_s,k_s+1}(\theta_s)$. □

The convergence estimate for the remaining Ritz values θ'_i, $i = 1, \ldots, s-1$, follows from Corollary 3.1 by induction. Further, the convergence estimates for the remaining cases follow by proper substitutions.

Proof. (of Theorem 3.1)

1a) The proof is given by induction on the subspace dimension s. For the case of a 1D subspace $\mathcal{V} = \operatorname{span}\{x\}$ with $x \in \mathbb{R}^n \setminus \{0\}$ the smallest Ritz value of A in $\operatorname{span}\{x, Ax\}$ is to be determined. Theorem 1.1 can be applied, which proves the Ritz value estimate (3.1) with $\rho_A(x') = \theta'_1$.

Next we consider an s-dimensional subspace $\mathcal{V}$ being the column space of $V = [v_1, \ldots, v_s]$. Let $\mathcal{V}^{(s-1)}$ be the column space of the submatrix $V^{(s-1)} := [v_1, \ldots, v_{s-1}]$. We denote the $s-1$ smallest Ritz values of A in $\operatorname{span}\{V^{(s-1)}, AV^{(s-1)}\}$ by $\theta'_1(\mathcal{V}^{(s-1)}) \leq \ldots \leq \theta'_{s-1}(\mathcal{V}^{(s-1)})$. The induction hypothesis in the $(s-1)$-dimensional space says that either $\theta'_i(\mathcal{V}^{(s-1)}) < \lambda_{k_i}$ or

$$0 \leq \frac{\Delta_{k_i,k_i+1}(\theta'_i(\mathcal{V}^{(s-1)}))}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_n - \lambda_{k_i+1}}{\lambda_n - \lambda_{k_i}}.$$

These first $s-1$ Ritz values $\theta_i'(\mathcal{V}^{(s-1)})$ decrease while expanding the $\mathcal{V}^{(s-1)}$ to $\mathcal{V}$ due to the variational characterization of the Ritz values, i.e.

$$\begin{aligned}\theta_i'(\mathcal{V}^{(s-1)}) &= \min_{\substack{\mathcal{U}\subseteq \mathrm{span}\{V^{(s-1)},AV^{(s-1)}\}\\ \dim(\mathcal{U})=i}} \max_{y\in\mathcal{U}\setminus\{0\}} \rho_A(y)\\ &\geq \min_{\substack{\mathcal{U}\subseteq \mathrm{span}\{V,AV\}\\ \dim(\mathcal{U})=i}} \max_{y\in\mathcal{U}\setminus\{0\}} \rho_A(y) = \theta_i'.\end{aligned}$$

Further $\Delta_{k_i,k_i+1}(\theta)$ is a monotone increasing function for $\theta \in [\lambda_{k_s},\lambda_{k_s+1})$ so that either $\theta_i' < \lambda_{k_i}$ or

$$0 \leq \frac{\Delta_{k_i,k_i+1}(\theta_i')}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \frac{\Delta_{k_i,k_i+1}(\theta_i'(\mathcal{V}^{(s-1)}))}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2,$$

which proves the proposition for the $s-1$ smallest Ritz values. For the Ritz value θ_s Corollary 3.1 proves the proposition.

In order to show that the estimate (3.1) cannot be improved in terms of the eigenvalues, let v_i be a normalized vector in the invariant subspace $\mathcal{E}_{k_i,k_i+1,n}$ with $\rho_A(v_i)=\theta_i$. The further columns of V are filled with pairwise different eigenvectors of A which are Euclidean orthogonal to $\mathcal{E}_{k_i,k_i+1,n}$; the subspace spanned by these eigenvectors is denoted by $\overline{\mathcal{E}}$. Then a step of the block steepest descent iteration lets all the eigenvectors invariant and the convergence of the ith column v_i behaves exactly like a vector iteration as the Rayleigh-Ritz projection to $\mathrm{span}\{V,AV\}$ decays to isolated blocks. Within the 2×2 block for $\mathrm{span}\{v_i,Av_i\} \subset \mathcal{E}_{k_i,k_i+1,n}$ the poorest convergence as described by Theorem 1.1 can be attained.

2a) Estimate 1a can be applied to the matrix $-A$. The s smallest Ritz values of $-A$ in $\mathrm{span}\{V\}$ or $\mathrm{span}\{V,-AV\}$ are just the s largest Ritz values of A in $\mathrm{span}\{V\}$ or $\mathrm{span}\{V,AV\}$ multiplied by -1 because of

$$\rho_{-A}(x) = -\rho_A(x) \quad \text{and} \quad \mathrm{span}\{V,-AV\} = \mathrm{span}\{V,AV\}.$$

The associated substitution

$$(\lambda_{k_i},\theta_i',\theta_i,\lambda_{k_i+1},\lambda_n) \;\to\; (-\lambda_{k_i+1},-\theta_i',-\theta_i,-\lambda_{k_i},-\lambda_1)$$

results in the estimate for the case 2a. Therein the meaning of θ_i and θ_i' on the left- and right-hand side is also transformed. To show that the estimate (3.3) cannot be improved in terms of the eigenvalues, all these transformations are applied to the arguments in the last paragraph of the proof for 1a.

1b) Now A is assumed to be a positive definite matrix. This allows to form A^{-1} and the subspace $A^{1/2}V$ to which the estimate 2a can be applied. Because of

$$\rho_{A^{-1}}(A^{1/2}x) = \frac{x^Tx}{x^TAx} = \frac{1}{\rho_A(x)} \quad \text{and} \quad \mathrm{span}\{A^{1/2}V, A^{-1}A^{1/2}V\} = A^{1/2}\mathrm{span}\{V,A^{-1}V\}$$

the s largest Ritz values of A^{-1} in $\mathrm{span}\{A^{1/2}V\}$ or $\mathrm{span}\{A^{1/2}V,A^{-1}A^{1/2}V\}$ are just the reciprocals of the s smallest Ritz values of A in $\mathrm{span}\{V\}$ or $\mathrm{span}\{V,A^{-1}V\}$. Further we get with the substitution

$$(\lambda_1,\lambda_{k_i},\theta_i,\theta_i',\lambda_{k_i+1}) \;\to\; (\lambda_n^{-1},\lambda_{k_i+1}^{-1},\theta_i^{-1},\theta_i'^{-1},\lambda_{k_i}^{-1})$$

that

$$\frac{\Delta_{k_i+1,k_i}(\theta_i')}{\Delta_{k_i+1,k_i}(\theta_i)} \;\to\; \left(\frac{\theta_i'^{-1}-\lambda_{k_i}^{-1}}{\lambda_{k_i+1}^{-1}-\theta_i'^{-1}}\right)\left(\frac{\theta_i^{-1}-\lambda_{k_i}^{-1}}{\lambda_{k_i+1}^{-1}-\theta_i^{-1}}\right)^{-1} = \frac{\Delta_{k_i,k_i+1}(\theta_i')}{\Delta_{k_i,k_i+1}(\theta_i)},$$

$$\frac{\lambda_{k_i}-\lambda_1}{\lambda_{k_i+1}-\lambda_1} \;\rightarrow\; \frac{\lambda_{k_i+1}^{-1}-\lambda_n^{-1}}{\lambda_{k_i}^{-1}-\lambda_n^{-1}} = \frac{\lambda_{k_i}(\lambda_n-\lambda_{k_i+1})}{\lambda_{k_i+1}(\lambda_n-\lambda_{k_i})}.$$

This proves the estimate for the case 1b.

2b) The estimate follows from the estimate in case 1a by applying the argument which has been used for the proof of case 1b. □

The Ritz value convergence estimates in Theorem 3.1 cannot be improved in terms of the eigenvalues without further assumptions on the subspace $\mathcal{V}$. Therefore cluster robust convergence estimates, which should depend in some way on the ratio λ_i/λ_{s+1}, are not provable in terms of the convergence measure used in Theorem 3.1. Nevertheless, the block steepest descent iteration is a cluster robust iteration, see the numerical experiments in Section 4.

3.1. Steepest descent A-gradient iteration for generalized eigenproblems. In order to apply the important estimate 1b in Theorem 3.1 to the generalized eigenvalue problem for (A, M) the substitution

$$A \rightarrow M^{-1/2}AM^{-1/2}, \quad V \rightarrow M^{1/2}V$$

can be used. The conversion of the associated Rayleigh quotients

$$\rho_{M^{-1/2}AM^{-1/2}}(M^{1/2}v) = \frac{v^TAv}{v^TMv} = \rho_{A,M}(v),$$

shows that the Ritz values of $M^{-1/2}AM^{-1/2}$ in $\operatorname{span}\{M^{1/2}V, (M^{1/2}A^{-1}M^{1/2})(M^{1/2}V)\}$, or equivalently in $M^{1/2}\operatorname{span}\{V, A^{-1}MV\}$, are equal to the corresponding Ritz values of (A, M) in $\operatorname{span}\{V, A^{-1}MV\}$. As the convergence estimates in Theorem 3.1 are formulated only in terms of eigenvalues and Ritz values, one can apply Theorem 3.1 to $M^{-1/2}AM^{-1/2}$ and to $M^{1/2}\mathcal{V}$. The eigenvalues and Ritz values are the same, which proves the following result.

Theorem 3.3. *The assumptions and notations of Theorem 3.1 are assumed to hold mutatis mutandis for the pair (A, M) of positive definite matrices. The Ritz values of (A, M) in $\mathcal{V}$ are enumerated in increasing order $\theta_1 \leq \ldots \leq \theta_s$. The s smallest Ritz values of (A, M) in $\operatorname{span}\{V, A^{-1}MV\}$ are θ'_i with $\theta'_1 \leq \ldots \leq \theta'_s$. Then for each $i \in \{1, \ldots, s\}$ it holds that $\theta'_i \leq \theta_i$ and either $\theta'_i < \lambda_{k_i}$ or*

$$0 \leq \frac{\Delta_{k_i,k_i+1}(\theta'_i)}{\Delta_{k_i,k_i+1}(\theta_i)} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_{k_i}(\lambda_n-\lambda_{k_i+1})}{\lambda_{k_i+1}(\lambda_n-\lambda_{k_i})}. \tag{3.5}$$

The bound cannot be improved in terms of the eigenvalues λ_i of (A, M) and is attained for $\theta_i \rightarrow \lambda_{k_i}$ in $\mathcal{E}_{k_i,k_i+1,n}$.

The other estimates of Theorem 3.1 can also be reformulated for the generalized eigenvalue problem in this way.

The convergence estimate (3.5) for the A-gradient subspace iteration constitutes an estimate for the case of exact preconditioning (with the inverse of the discretization matrix) for the preconditioned inverse subspace iteration with fixed step-length, see [22] and Theorem 13 in [18]. If the estimate (29) in [18] is evaluated for $\gamma = 0$, then the resulting convergence factor $\lambda_{k_i}/\lambda_{k_i+1}$ is clearly improved by the current estimate (3.5). The accelerating influence of the Rayleigh-Ritz procedure can be seen in the factor $(\lambda_n - \lambda_{k_i+1})/(\lambda_n - \lambda_{k_i}) < 1$ together with the ratio $\kappa/(2-\kappa) < \kappa$.

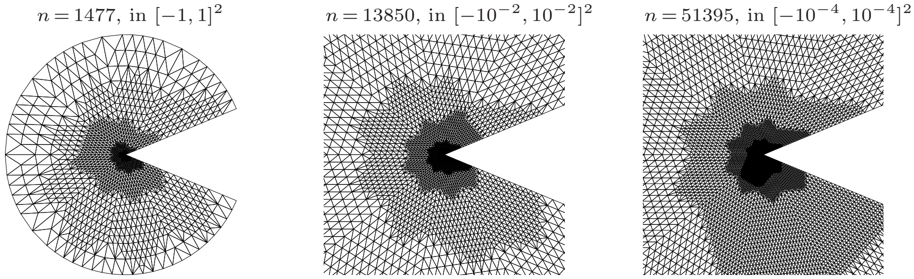

FIG. 4.1. *Adaptively generated triangulations with* $n \in \{1477, 13850, 51395\}$ *nodes; the corresponding depths of the triangulations are* 12*,* 26 *and* 40*.*

4. Numerical experiments. The test problem is the Laplacian eigenproblem

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

on

$$\Omega := \Big\{ \big(r\cos(\varphi), r\sin(\varphi) \big) \ ; \ r \in [0,1], \ \varphi \in \Big[\frac{1}{8}\pi, \ \frac{15}{8}\pi\Big] \Big\}.$$

Homogeneous Dirichlet boundary conditions are assumed for boundary points with $r = 1$ and on $\{(r, \varphi); \ r \in [0,1], \ \varphi = \frac{1}{8}\pi\}$. Homogeneous Neumann boundary conditions are used for $\varphi = \frac{15}{8}\pi$ with $r \in (0,1)$. The numerical results can be compared with the exact eigenvalues and eigenfunctions. The eigenfunctions are

$$\sin\big(\alpha_k(\varphi - \pi/8)\big) J_{\alpha_k}(\xi_{k,l} r)$$

with $\alpha_k := \frac{4}{7}k + \frac{2}{7}$ and the Bessel functions J_{α_k} of first kind and fractional order [1]. The eigenvalues are $\xi_{k,l}^2$ with the positive zeros $\xi_{k,l}$ of J_{α_k}.

The problem is discretized by linear finite elements on an adaptively generated triangle mesh. The error estimation is based on local estimates of the discretization error. A triangle is marked for a further regular subdivision (red-refinement) if some error barrier is exceeded between the linear interpolant of the eigenfunction approximation on the father triangle and the eigenfunction approximation of the current grid. Here, we only use the eigenfunction corresponding to the smallest eigenvalue in order to steer the refinement process. The grid consistency is ensured if regular (red) refinements are followed by irregular (green) refinements to avoid hanging nodes.

The origin at $r = 0$ is a critical point since the partial derivative $(\partial/\partial r)J_{\alpha_k}$ is unbounded for certain k. Thus the adaptive grid refinement procedure results in a highly non-uniform triangulation. Figure 4.1 shows three different grids with sectional enlargements to regions close to the origin.

A triangulation with 56332 nodes is used for the numerical computations. The associated generalized matrix eigenvalue problem $Ax = \lambda Mx$ for the inner nodes and the nodes on the Neumann boundary has the dimension 55655. The 15 smallest eigenvalues of (4.1) are listed in Table 1 together with the numerical approximations from the block A-gradient steepest descent method with a 20-dimensional subspace.

Experiment I - Poorest convergence of the block steepest descent iteration: We consider subspaces which contain a nonzero vector from the invariant subspace $\mathcal{E}_{i,i+1,n}$ since Theorem 1.1 shows that the poorest convergence of the vector variant of the block steepest descent iteration attains its poorest convergence in certain vectors from $\mathcal{E}_{i,i+1,n}$. All the other basis vectors of the subspace are eigenvectors of (A, M) with indexes different from

k \ l	1	2	3
0	8.02725	35.52780	82.76227
1	13.23485	46.36149	
2	19.36200	58.14138	
3	26.37462	70.85000	
4	34.24802	84.47130	
5	42.96336		
6	52.50562		
7	62.86257		
8	74.02394		

k \ l	1	2	3
0	8.0294	35.5390	82.8033
1	13.2359	46.3720	
2	19.3640	58.1577	
3	26.3784	70.8744	
4	34.2547	84.5067	
5	42.9742		
6	52.5221		
7	62.8864		
8	74.0574		

TABLE 1

The 15 smallest eigenvalues $\xi_{k,l}^2$ of (4.1) (left) and the numerical approximations (right) by the block A-gradient steepest descent iteration with $s = 20$ for a FE-discretization with $n = 55655$ degrees of freedom.

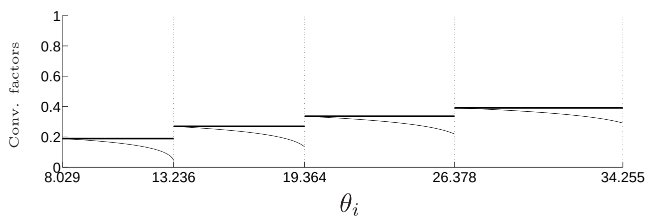

FIG. 4.2. *Poorest convergence of block steepest descent iteration. Abscissa: Five smallest eigenvalues according to Table 1. Bold lines in the intervals $(\lambda_i, \lambda_{i+1}]$ are the upper bounds $\kappa^2/(2-\kappa)^2$ and the curves are the largest ratios $\Delta_{i,i+1}(\theta_i')/\Delta_{i,i+1}(\theta_i)$ over 1000 equispaced test vectors in $\mathcal{E}_{i,i+1,n}$ whose Rayleigh quotients equal θ_i.*

i, $i+1$ and n. Then the subspace iteration behaves like a vectorial A-gradient iteration since the iteration is stationary in the eigenvectors. Theorem 1.1 provides a convergence estimate for the single vector from $\mathcal{E}_{i,i+1,n}$. Figure 4.2 shows the upper bounds $\kappa^2/(2-\kappa)^2$ (bold lines) and the largest ratios $\Delta_{i,i+1}(\theta_i')/\Delta_{i,i+1}(\theta_i)$ in the intervals $(\lambda_i, \lambda_{i+1})$ for 1000 equispaced normalized test vectors in $\mathcal{E}_{i,i+1,n}$ whose Rayleigh quotients equal θ_i. All this is done for equidistant $\theta_i \in (\lambda_i, \lambda_{i+1})$. In each interval $(\lambda_i, \lambda_{i+1})$ the estimate (3.5) is sharp (see Theorem 3.3) and is attained for $\theta_i \to \lambda_i$.

Experiment II - Convergence of the Ritz vectors: The convergence of the sequence of subspaces $\mathcal{V}^{(k)}$ towards the eigenvectors x_i is measured in terms of the tangent values $\tan\angle_M(x_i, \mathcal{V}^{(k)})$ where $\angle_M$ denotes an angle with respect to the M-geometry. The *simple subspace iteration* [26] for $A^{-1}M$ differs from the block steepest descent iteration in which the Rayleigh-Ritz procedure is applied to the s-dimensional subspace $A^{-1}M\mathcal{V}$ and not to the larger space $\operatorname{span}\{\mathcal{V}, A^{-1}M\mathcal{V}\}$. It holds that, see [26],

$$(4.2)\qquad \tan\angle_M(x_i, \mathcal{V}^{(k)}) \le \left(\frac{\lambda_i}{\lambda_{s+1}}\right)^k \tan\angle_M(\operatorname{span}\{x_1,\dots,x_s\}, \mathcal{V}^{(0)}), \qquad i = 1,\dots,s.$$

The ratio λ_i/λ_{s+1} expresses the cluster robustness of this subspace iteration. The initial space $\mathcal{V}^{(0)}$ should only contain (nonzero) vectors which are not orthogonal to the desired invariant subspace $\operatorname{span}\{x_1,\dots,x_s\}$.

The block steepest descent iteration is the faster convergent iteration compared to the subspace iteration for $A^{-1}M$ since the Courant-Fischer variational principles show that the kth Ritz value, $k = 1,\dots,s$, of (A,M) in $\operatorname{span}\{\mathcal{V}, A^{-1}M\mathcal{V}\}$ is less or equal to the kth Ritz value in $\operatorname{span}\{A^{-1}M\mathcal{V}\}$. Hence the block steepest descent iteration can result in improved eigenvalue approximations and therefore is a cluster robust iteration.

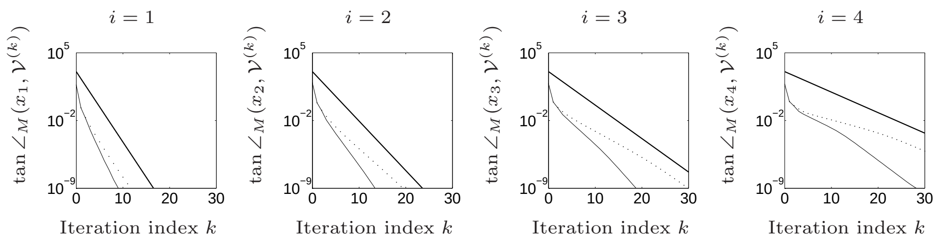

FIG. 4.3. *Convergence of the eigenvector approximations in terms of subspace angles* $\tan\angle_M(x_i,\mathcal{V}^{(k)})$ *for* $i=1,\ldots,4$. *Bold line: Estimate (4.2) on the simple subspace iteration. Dotted line: Poorest convergence of the simple subspace iteration for 1000 random initial spaces. Thin solid line: The faster convergent block steepest descent iteration.*

Figure 4.3 displays the convergence of the subspaces $\mathcal{V}^{(k)}$, $\dim\mathcal{V}^{(k)}=6$, towards the eigenvectors x_i for $i=1,\ldots,4$. The bold lines represent the theoretical bound (4.2). The dotted lines illustrate the convergence of the subspace iteration for $A^{-1}M$ and the thin solid lines stand for the faster convergent block steepest descent. All curves are plotted for the case of poorest convergence, which has been observed for 1000 random initial subspaces $\mathcal{V}^{(0)}$. For all computations a symmetric approximate minimum degree permutation has been used in order to factorize the stiffness matrix A and to compute $A^{-1}M\mathcal{V}$.

Experiment III - Sharp single-step estimates vs. multistep estimates: If the ith Ritz value $\theta_i =: \theta_i^{(0)}$ has reached its "destination interval", i.e. $\theta_i^{(0)}\in(\lambda_i,\lambda_{i+1})$, then (3.5) can be applied recursively resulting in the k-step estimate

$$\frac{\theta_i^{(k)}-\lambda_i}{\lambda_{i+1}-\theta_i^{(k)}} \le \left(\frac{\kappa}{2-\kappa}\right)^{2k}\frac{\theta_i^{(0)}-\lambda_i}{\lambda_{i+1}-\theta_i^{(0)}}, \qquad k=1,2,\ldots. \tag{4.3}$$

In contrast to this we consider 1-step estimates in the form

$$\frac{\theta_i^{(l+1)}-\lambda_i}{\lambda_{i+1}-\theta_i^{(l+1)}} \le \left(\frac{\kappa}{2-\kappa}\right)^{2}\frac{\theta_i^{(l)}-\lambda_i}{\lambda_{i+1}-\theta_i^{(l)}}, \qquad l=1,2,\ldots,$$

where in each step the actual numerical value $\theta_i^{(l)}$ is inserted in the right hand side of the estimate. Figure 4.4 shows the multistep bound (4.3) as a bold line, the 1-step bound as a dotted line and the numerical worst-case result as a thin solid line. For this experiment initial subspaces $\mathcal{V}^{(0)}$ with $\dim(\mathcal{V}^{(0)})=6$ are used for which the six Ritz values satisfy $\theta_i(\mathcal{V}^{(0)})\in(\lambda_i,\lambda_{i+1})$ for $i=1,\ldots,6$. The last condition holds if the subspace $\mathcal{V}^{(0)}$ properly approximates the invariant subspace corresponding to the six smallest eigenvalues.

For these computations 1000 random initial subspaces are used and the cases of slowest convergence are plotted. The 1-step estimate is a good upper estimate and the multistep estimate (bold line) is a relatively poor estimate especially for small $i\ll s$. For $i=1,2$ a convergence factor depending on the cluster robust ratio λ_i/λ_{s+1} appears to be more suitable. However, such a cluster robustness cannot be expressed in terms of the estimate (3.5) whose feature is just its 1-step sharpness. In any case cluster robustness is already guaranteed as illustrated in experiment II.

5. Conclusion. Block gradient iterations for the Rayleigh quotient are simple, storage-efficient and potentially fast solvers for symmetric and positive definite eigenvalue problems. They allow the simultaneous computation of some of the smallest eigenvalues together with the associated eigenvectors.

In this paper sharp estimates have been proved on the convergence of block A-gradient and Euclidean gradient iterations. A benefit of an A-gradient iteration is its fast conver-

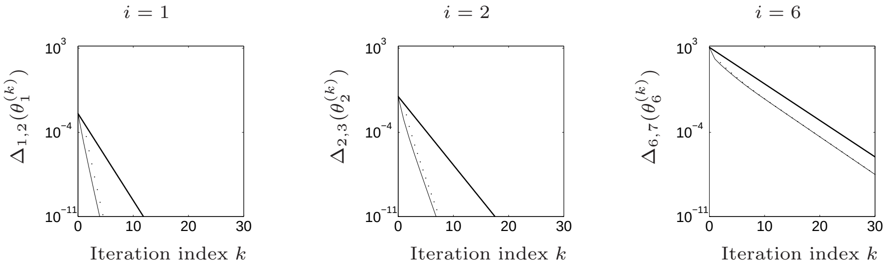

FIG. 4.4. *Error of the eigenvalue approximations* $\Delta_{i,i+1}(\theta_i^{(k)}) = (\theta_i^{(k)} - \lambda_i)/(\lambda_{i+1} - \theta_i^{(k)})$ *for* $i = 1, 2, 6$ *for subspaces with the dimension* $s = 6$*. The multistep estimate* (4.3) *(bold lines) is a relatively poor estimate for* $i = 1, 2$*. The* 1*-step estimate (dotted line) is good estimate for the numerical worst-case results (thin solid line); the data representing the case of poorest convergence for 1000 random initial subspaces is plotted.*

gence compared to a Euclidean gradient iteration. Especially, if (A, M) are the discretization matrix and the mass matrix of an eigenvalue problem for an elliptic and self-adjoint partial differential operator, then A and M are typically very large and sparse matrices. For such a problem the convergence factor of an A-gradient iteration can be bounded away from 1 independently on the mesh size of the discretization. This guarantees a grid-independent convergence factor. In contrast to this, the convergence factor of a Euclidean gradient iteration tends to 1 if the mesh size decreases towards 0, see Equation (3.1). However, an A-gradient iteration requires the solution of linear systems in A, which may appear as a computationally expensive step. Once again, in the context of operator eigenvalue problems this solution of linear systems in A can be implemented in terms of multigrid or multilevel iterations. These very efficient solvers allow to solve such linear systems with costs that, in the best case, increase only linearly in the number of variables. Further, even an approximate solution of these linear systems can result in a convergent eigensolver. Then the A-gradient iteration turns into a B-gradient iteration where B approximates A. The inverse B^{-1} is called a preconditioner or approximate inverse for A and the resulting eigensolver is a block B-gradient subspace iteration. The convergence analysis of such B-gradient subspace iterations is the topic of a forthcoming paper - for the limit case $B \to A$ the current paper makes available a closed convergence analysis.

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