

THE BLOCK PRECONDITIONED STEEPEST DESCENT ITERATION FOR ELLIPTIC OPERATOR EIGENVALUE PROBLEMS

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Abstract. The block preconditioned steepest descent iteration is an iterative eigensolver for subspace eigenvalue and eigenvector computations. An important area of application of the method is the approximate solution of mesh eigenproblems for self-adjoint and elliptic partial differential operators. The subspace iteration allows to compute some of the smallest eigenvalues together with the associated invariant subspaces simultaneously. The building blocks of the iteration are the computation of the preconditioned residual subspace for the current iteration subspace and the application of the Rayleigh-Ritz method in order to extract an improved subspace iterate.

The convergence analysis of this iteration provides new sharp estimates for the Ritz values. It is based on the analysis of the vectorial preconditioned steepest descent iteration which appeared in SIAM J. Numer. Anal., 50(6):3188-3207, 2012. Numerical experiments using a finite element discretization of the Laplacian with up to $5 \cdot 10^7$ degrees of freedom and with multigrid preconditioning demonstrate the near-optimal complexity of the method.

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

1. Introduction. Let Ω be a bounded polygonal region in the \mathbb{R}^d , often $d = 2$ or $d = 3$, and let the boundary $\partial\Omega$ be the disjoint union of $\partial\Omega_1$ and $\partial\Omega_2$. We consider the self-adjoint elliptic eigenvalue problem

$$(1.1) \quad \begin{aligned} -\nabla \cdot (c(x)\nabla u) + q(x)u &= \lambda u && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega_1, \\ \underline{n} \cdot c(x)\nabla u &= 0 && \text{on } \partial\Omega_2. \end{aligned}$$

Therein $c(x)$ is a symmetric and positive definite matrix valued function, $q(x)$ a nonnegative real function and \underline{n} denotes the normal vector on the boundary $\partial\Omega_2$. The coefficient functions are assumed piecewise continuous. We are interested in the numerical approximation of some of the smallest eigenvalues λ and the corresponding eigenfunctions u .

The finite element discretization of (1.1) is the generalized matrix eigenvalue problem

$$(1.2) \quad Ax_i = \lambda_i Mx_i.$$

The discretization matrix A and the mass matrix M are symmetric, positive definite $n \times n$ matrices. Typically, these matrices are very large and sparse.

Our aim is to compute a fixed number of the smallest eigenvalues of (1.2) together with the associated eigenvectors. The numerical algorithm should exploit the structure of the mesh eigenproblem, and its computational costs should increase almost linearly in dimension n . The demand for a near-optimal-complexity method rules out all eigensolvers which are usually used for small and dense matrices. See [4, 21, 2] for getting an overview on the wide variety of numerical eigensolvers primarily for small and dense matrices.

A conceptually easy approach to the desired near-optimal-complexity eigensolvers is based on gradient iterations for the Rayleigh quotient; cf. Dyakonov's monograph on optimization for elliptic problems [3] and its Chapter 9 on the Rayleigh-Ritz method for spectral problems. The starting point is the generalized Rayleigh quotient for (1.2)

$$(1.3) \quad \rho(x) = (x, Ax)/(x, Mx), \quad x \neq 0.$$

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As $\rho(\cdot)$ attains its minimum λ_1 in an associated eigenvector, the minimization of (1.3) can be implemented by means of a gradient iteration. The negative gradient of (1.3) reads

$$-\nabla\rho(x) = -2(Ax - \rho(x)Mx)/(x, Mx)$$

and allows to construct a new iterate $x' = x - \omega\nabla\rho(x)$ with $\rho(x') < \rho(x)$ whenever x is not an eigenvector and $\omega \in \mathbb{R}$ is a proper step length. The optimal step length ω^* minimizes $\rho(x')$ with respect to $\omega \in \mathbb{R}$. These optimal x' and $\rho(x')$ can be computed by applying the Rayleigh-Ritz procedure to the 2D space spanned by x and $\nabla\rho(x)$. The gradient iteration does not change A and M and does not need these matrices explicitly. It is a so-called matrix-free method in the sense that its implementation only requires routines $z \mapsto Az$ and $z \mapsto Mz$. The sparsity of A and M allows to implement these matrix-vector products with computational costs which only increase linearly in the number of unknowns.

1.1. Preconditioning of gradient iterations. Gradient iterations for the Rayleigh quotient which use the Euclidean gradient $\nabla\rho(x)$ are well known to converge poorly if the condition number of A is large [5, 6, 7, 23, 28, 8, 12]. This is particularly the case for a finite element discretization of (1.1) since the condition number of A increases as $\mathcal{O}(h^{-2})$ in the discretization parameter h .

The key ingredient to make a gradient iteration an efficient solver for the operator eigenvalue problem (1.1) is multigrid preconditioning. If a symmetric and positive definite matrix T is an approximate inverse of A , then T is called a preconditioner for A . The preconditioned gradient iteration uses

$$-T\nabla\rho(x)$$

as the descent direction for the Rayleigh quotient. The usage of the T -gradient can be interpreted as a change of the underlying geometry which makes ellipsoidal level sets of $\rho(\cdot)$ more spherical [25, 3]. Proper preconditioning, for instance by multigrid or multilevel preconditioning, can accelerate the convergence considerably. In the best case this can result in grid-independent convergence behavior [10, 11].

The *T-gradient steepest descent iteration* optimizes the step length ω

$$(1.4) \quad x' = x - \omega T\nabla\rho(x) = x - 2\omega T(Ax - \rho(x)Mx)/(x, Mx)$$

in a way that x' attains the smallest possible Rayleigh quotient for all $\omega \in \mathbb{R}$. If $T(Ax - \rho(x)Mx)$ is a Ritz vector, then ω may be infinite. Computationally x' is determined by the Rayleigh-Ritz procedure since x' is a Ritz vector of (A, M) in the two-dimensional subspace $\text{span}\{x, T(Ax - \rho(x)Mx)\}$ corresponding to the smaller Ritz value. The resulting iteration has some similarities with the Davidson method [24, 20] if the iteration is restarted after each step so that the dimension of the truncated search subspace always equals 2. Stathopoulos [27] calls such an iteration with constant memory requirement a Generalized Davidson method.

The eigenpairs of (1.2) are denoted by (λ_i, x_i) . The enumeration is $0 < \lambda_1 < \lambda_2 < \dots < \lambda_n$. We assume simple eigenvalues. The case of multiple eigenvalues can simply be reduced 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 [17].

For the vectorial Preconditioned Steepest Descent (PSD) iteration (1.4) sharp convergence estimates have recently been proved in [17]. The central theorem reads as follows:

THEOREM 1.1. *Let $x \in \mathbb{R}^n$ so that the Rayleigh quotient $\rho(x)$ satisfies $\lambda_i < \rho(x) < \lambda_{i+1}$ for some $i \in \{1, \dots, n-1\}$. Let x' be the Ritz vector of (A, M) in $\text{span}\{x, T(Ax - \rho(x)Mx)\}$ which corresponds to the smaller Ritz value. The Ritz value is $\rho(x')$. The preconditioner satisfies*

$$(1.5) \quad \gamma_1(x, T^{-1}x) \leq (x, Ax) \leq \gamma_2(x, T^{-1}x) \quad \forall x \in \mathbb{R}^n$$

with constants $\gamma_1, \gamma_2 \geq 0$. Let $\gamma := (\gamma_2 - \gamma_1)/(\gamma_2 + \gamma_1)$.

Then either $\rho(x') \leq \lambda_i$ or $\rho(x') \in (\lambda_i, \lambda_{i+1})$ is bounded from above as follows

$$(1.6) \quad 0 < \frac{\Delta_{i,i+1}(\rho(x'))}{\Delta_{i,i+1}(\rho(x))} \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}.$$

Therein $\Delta_{p,q}(\theta) := (\theta - \lambda_p)/(\lambda_q - \theta)$.

The estimate (1.6) cannot be improved in terms of the eigenvalues λ_i, λ_{i+1} and λ_n . The bound can be attained for $\lambda \rightarrow \lambda_i$ in the three-dimensional invariant subspace $\mathcal{E}_{i,i+1,n}$, which is spanned by the eigenvectors corresponding to λ_i, λ_{i+1} and λ_n .

Theorem 1.1 guarantees monotone convergence of the Ritz values $\rho(x')$ towards an eigenvalue. If the Rayleigh quotient $\rho(x)$ has reached the final interval $[\lambda_1, \lambda_2)$, then (1.6) proves linear convergence of the Ritz values towards the smallest eigenvalue λ_1 .

1.2. Aim of this paper. This paper aims at generalizing the preconditioned gradient iteration (1.4) to a subspace iteration for the simultaneous computation of s smallest eigenvalues of (1.2). New and sharp convergence estimates on the Ritz values of (A, M) in the iteration subspaces are presented, which generalize Theorem 1.1.

The effectiveness of the method is demonstrated for the Laplacian eigenvalue problem on the sliced unit circle with mixed homogeneous Dirichlet and Neumann boundary conditions. The operator eigenvalue problem is discretized with linear and quadratic (only for error estimation) finite elements. Our finite element code AMPE, see Section 4, is demonstrated to work with up to $5 \cdot 10^7$ degrees of freedom. AMPE uses a multigrid preconditioner with Jacobi smoothing.

1.3. Notation and overview. Subspaces are denoted by capital calligraphic letters, e.g., the column space of a matrix Z is $\mathcal{Z} = \text{span}\{Z\}$. Similarly, $\text{span}\{Z, Y\}$ is the smallest vector space which contains the column spaces of Z and of Y . All eigenvalues and Ritz values are enumerated in order of increasing magnitude. Further, $\mathcal{E}_{\text{index-set}}$ denotes the invariant subspace of (A, M) which is spanned by the eigenvectors of (A, M) whose indexes are contained in the index set.

The paper is structured as follows: The preconditioned gradient subspace iteration is introduced in Section 2. The new convergence estimates are presented in Section 3; Theorem 3.2 is the central new estimate on the convergence of the Ritz values. In Section 4 numerical experiments illustrate the sharpness of the estimates and the cluster-robustness of the preconditioned gradient subspace iteration.

2. The block preconditioned iteration with Rayleigh-Ritz projections. The preconditioned subspace/block iteration is a straightforward generalization of the vector iteration (1.4). The iteration (1.4) is just applied to each column of the matrix which columnwise contains the Ritz vectors of the current subspace. Each subspace correction step is followed by the Rayleigh-Ritz procedure in order to extract the Ritz approximations.

The starting point is an s -dimensional subspace \mathcal{V} of the \mathbb{R}^n which is given by the column space of $V \in \mathbb{R}^{n \times s}$. The columns of V are assumed to be the M -normalized Ritz vectors of (A, M) in \mathcal{V} . Further, $\Theta = \text{diag}(\theta_1, \dots, \theta_s)$ 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. Left multiplication with the preconditioner $T \approx A^{-1}$ coincides with the approximate solution of s linear systems in A . This yields the correction-subspace $\text{span}\{T(AV - MV\Theta)\}$ of the preconditioned subspace

iteration. The Rayleigh-Ritz procedure is used to extract the s smallest Ritz values and the associated Ritz vectors of (A, M) in $\text{span}\{V, T(AV - MV\Theta)\}$, see Algorithm 1.

Algorithm 1 Block preconditioned steepest descent iteration:

Require: Symmetric and positive definite matrices $A, M \in \mathbb{R}^{n \times n}$, a preconditioner T satisfying (1.5) and an initial (random) s -dimensional subspace $\mathcal{V}^{(0)}$ with $\angle_M(\mathcal{V}^{(0)}, \mathcal{E}_{1:s}) < \pi/2$ where $\mathcal{E}_{1:s}$ is the invariant subspace of (A, M) associated with the s smallest eigenvalues.

1. **Initialization:** Apply the Rayleigh-Ritz procedure to $\mathcal{V}^{(0)}$. The $n \times s$ matrix $V^{(0)} = [v_1^{(0)}, \dots, v_s^{(0)}]$ contains the Ritz vectors of (A, M) corresponding to the s Ritz values $\theta_1^{(0)}, \dots, \theta_s^{(0)}$. Let $\Theta^{(0)} = \text{diag}(\theta_1^{(0)}, \dots, \theta_s^{(0)})$ and $R^{(0)} = AV^{(0)} - MV^{(0)}\Theta^{(0)}$.
 2. **Iteration, $i \geq 0$:** The Rayleigh-Ritz procedure is applied to $\text{span}\{V^{(i)}, TR^{(i)}\}$. The columns of $V^{(i+1)} = [v_1^{(i+1)}, \dots, v_s^{(i+1)}]$ are the Ritz vectors of (A, M) corresponding to the s smallest Ritz values $\theta_1^{(i+1)}, \dots, \theta_s^{(i+1)}$. Let $\Theta^{(i+1)} = \text{diag}(\theta_1^{(i+1)}, \dots, \theta_s^{(i+1)})$ and $R^{(i+1)} = AV^{(i+1)} - MV^{(i+1)}\Theta^{(i+1)}$.
 3. **Termination:** The iteration is stopped if $\|R^{(i+1)}\|$ drops below a final accuracy.
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2.1. The block steepest descent iteration. The block steepest descent iteration as given by Algorithm 1 has already been analyzed for the special case $T = A^{-1}$ (preconditioning with the exact inverse of the discretization matrix A) in [19]. If in the central convergence estimates of this paper, see Corollary 3.2 and Theorem 3.2, $\gamma = 0$ is inserted, then the convergence factor

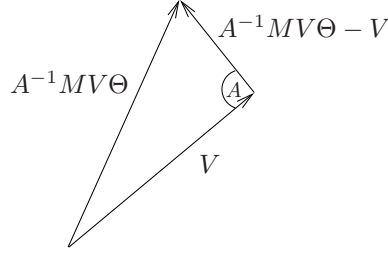
$$\frac{\kappa_i + \gamma(2 - \kappa_i)}{(2 - \kappa_i) + \gamma\kappa_i} \quad \text{with} \quad \kappa_i = \frac{\lambda_{k_i}(\lambda_n - \lambda_{k_{i+1}})}{\lambda_{k_{i+1}}(\lambda_n - \lambda_{k_i})}$$

simplifies to $\kappa_i/(2 - \kappa_i)$. This bound has been proved in case 1b of Theorem 1.1 in [19].

However, the convergence analysis for the block steepest descent iteration with a general preconditioner does not rest upon the analysis in [19]. In fact, the analysis of the current paper uses the convergence analysis for the vectorial preconditioned steepest descent iteration from [17]. By starting with the result from [17] some of the proof techniques from [19] can be adapted to the block iteration with general preconditioning. One important modification is that the argument using the subspace dimensions from Theorem 3.2 of [19] cannot be transferred to the case of general preconditioning. Instead, we use here Sion's theorem for the proof of Theorem 3.1. The proof structure of the present paper has also some similarities with the chain of arguments in [14] wherein a convergence analysis of the subspace variant of the preconditioned inverse iteration is contained. References to similar results and similar proof techniques are given prior to Lemma 3.1, Theorem 3.1 and Theorem 3.2.

3. Convergence analysis. Next convergence estimates on the convergence of the Ritz values $\theta_j^{(i+1)}$ with $j = 1, \dots, s$ and $i \geq 0$, see Algorithm 1, towards the eigenvalues of (A, M) are proved. In Theorem 3.1 together with Corollary 3.2 the convergence of the largest of these Ritz values, namely $\theta'_s := \theta_s^{(i+1)}$, is analyzed. It is shown that the Ritz value θ'_s of (A, M) in $\text{span}\{V, T(AV - MV\Theta)\}$ is bounded from above by the largest Ritz value which can be attained by the *vector* iteration PSD (1.4) if applied elementwise to the column space of V . Theorem 3.2 proves sharp estimates for the remaining Ritz values by induction.

In the following analysis we assume that the preconditioner satisfies the inequality $\|I - TA\|_A \leq \gamma < 1$. This assumption is equivalent to (1.5) with $\gamma := (\gamma_2 - \gamma_1)/(\gamma_2 + \gamma_1)$

FIG. 3.1. A -orthogonal decomposition in the $\mathbb{R}^{n \times s}$

if the preconditioner is optimally scaled. The PSD iteration implicitly determines this optimal scaling by the Rayleigh-Ritz procedure.

The next lemma generalizes Lemma 3.1 from [14].

LEMMA 3.1. *Let the columns of $V \in \mathbb{R}^{n \times s}$ form a Ritz basis of $\text{span}\{V\}$, and let T be a symmetric and positive definite matrix with $\|I - TA\|_A \leq \gamma < 1$.*

i) *For any $a \in \mathbb{R}^s \setminus \{0\}$ and any $c \in \mathbb{R}^s$ it holds that*

$$(3.1) \quad \|A^{-1}MV\Theta a - Va\|_A \leq \|A^{-1}MV\Theta a - Vc\|_A.$$

ii) *The matrix $\omega V\Theta + (V - T(AV - MV\Theta))$ preserves for all $\omega \in \mathbb{R}$ the full rank s of the matrix V .*

iii) *Let x be given as in Theorem 1.1, and let $\tilde{x} \in \mathbb{R}^n$ satisfy*

$$(3.2) \quad \|A^{-1}Mx - \tilde{x}\|_A \leq \gamma \|A^{-1}Mx - x/\rho(x)\|_A.$$

If

$$(3.3) \quad x' \in \arg \min_{v \in \text{span}\{x, \tilde{x}\}} \rho(v),$$

then the PSD estimate (1.6) applies to the Ritz vector x' given by (3.3) and its Rayleigh quotient $\rho(x')$.

Proof. i) The A -orthogonality, see Fig. 3.1,

$$(Vz, (A^{-1}MV\Theta - V)a)_A = z^T V^T (MV\Theta - AV)a = z^T (\Theta - \Theta)a = 0 \quad \forall z \in \mathbb{R}^s$$

shows that Va is the A -orthogonal projection of $A^{-1}MV\Theta a$ on $\text{span}\{V\}$. This guarantees that

$$\|A^{-1}MV\Theta a - Va\|_A \leq \|A^{-1}MV\Theta a - Vc\|_A$$

for all $c \in \mathbb{R}^s$.

ii) Direct computation shows that for $a \in \mathbb{R}^s \setminus \{0\}$

$$\begin{aligned} & \|\omega V\Theta a + (V - T(AV - MV\Theta))a\|_A \\ &= \|\omega V\Theta a + A^{-1}MV\Theta a + (I - TA)(V - A^{-1}MV\Theta)a\|_A \\ &\geq \|\omega V\Theta a + A^{-1}MV\Theta a\|_A - \|(I - TA)(V - A^{-1}MV\Theta)a\|_A \\ &> \|A^{-1}MV\Theta a - \underbrace{(-\omega\Theta a)}_{=:c}\|_A - \|(V - A^{-1}MV\Theta)a\|_A \geq 0. \end{aligned}$$

The last inequality holds with $c = -\omega\Theta a$ due to (3.1). The fact $\|\omega V\Theta a + (V - T(AV - MV\Theta))a\|_A > 0$ for all $a \neq 0$ proves that the matrix $\omega V\Theta + (V - T(AV - MV\Theta))$ has the full rank.

iii) Inequality (3.2) is equivalent to $\|\rho(x)A^{-1}Mx - \rho(x)\tilde{x}\|_A \leq \gamma\|\rho(x)A^{-1}Mx - x\|_A$. This means that $\rho(x)\tilde{x}$ is contained in a ball with the center $\rho(x)A^{-1}Mx$ and the radius $\gamma\|\rho(x)A^{-1}Mx - x\|_A$. The geometry of the fixed-step-length preconditioned gradient iteration [10, 17] shows that $\rho(x)\tilde{x}$ is representable by a symmetric and positive definite \tilde{T} with $\|I - \tilde{T}A\|_A \leq \gamma$ in the form

$$\rho(x)\tilde{x} = x - \tilde{T}(Ax - \rho(x)Mx).$$

The preconditioned steepest descent iteration accelerates the convergence of this fixed-step-length iteration by applying the Rayleigh-Ritz procedure to

$$\text{span}\{x, \tilde{T}(Ax - \rho(x)Mx)\} = \text{span}\{x, \tilde{x}\}.$$

Thus the smallest Ritz value $\rho(x')$ in this space is bounded from above by the estimate (1.6). \square

The next theorem proves the desired convergence behavior for the largest Ritz value θ'_s . Comparable estimates on the largest Ritz values, but with respect to different spaces, have been used in Theorem 3.2 in [14] on the subspace analysis of the preconditioned inverse iteration and in Theorem 3.2 in [19] on the block steepest descent iteration.

THEOREM 3.1. *Let $\text{span}\{V\}$ contain no eigenvector of A , which otherwise could easily be split off within the Rayleigh-Ritz procedure. Then the s -th Ritz value θ'_s of (A, M) in $\mathcal{W} := \text{span}\{V, T(AV - MV\Theta)\}$, which is given by*

$$(3.4) \quad \theta'_s = \min_{\substack{\mathcal{Z} \subseteq \mathcal{W} \\ \dim \mathcal{Z} = s}} \max_{z \in \mathcal{Z} \setminus \{0\}} \rho(z),$$

satisfies

$$(3.5) \quad \theta'_s \leq \max_{a \in \mathbb{R}^s \setminus \{0\}} \min_{\omega \in \mathbb{R}} \rho(\omega V\Theta a + (V - T(AV - MV\Theta))a) =: \hat{\theta}_s.$$

Proof. Let $a^* \in \mathbb{R}^s \setminus \{0\}$ and $\omega^* \in \mathbb{R}$ be given in a way so that the max-min in (3.5) is attained

$$(3.6) \quad \hat{\theta}_s = \rho(\underbrace{\omega^* V\Theta a^*}_{=: W_1} + \underbrace{(V - T(AV - MV\Theta))a^*}_{=: W_2}).$$

Hence (a^*, ω^*) is a saddle point of the Rayleigh quotient. In a sufficiently small neighborhood $Q \times \Omega$ of (a^*, ω^*) the Rayleigh quotient $\rho(\cdot)$ is a smooth function which is concave in a and convex in ω . Sion's-minimax theorem [26, 22] provides the justification to swap the order of the minimization and the maximization, i.e.

$$\hat{\theta}_s = \rho(\omega^* W_1 a^* + W_2 a^*) = \max_{a \in Q} \min_{\omega \in \Omega} \rho(\omega W_1 a + W_2 a) = \min_{\omega \in \Omega} \max_{a \in Q} \rho(\omega W_1 a + W_2 a).$$

Thus $\rho(\omega W_1 a + W_2 a)$ is the Rayleigh quotient of a with respect to the projected matrix-pair $(W^T A W, W^T M W)$ with $W = \omega W_1 + W_2$. The local maximum in $a \in Q$ coincides with the global maximum of $\rho(\cdot)$ in the column space of W (because the maximum is taken in the interior of Q and because the Hessian of the Rayleigh quotient shows that there is only one local extremum which is a maximum). We conclude that

$$\min_{\omega \in \Omega} \max_{a \in Q} \rho(\omega W_1 a + W_2 a) = \min_{\omega \in \Omega} \theta_{\max}(\omega W_1 + W_2).$$

We denote the minimum point with respect to $\omega \in \Omega$ by $\bar{\omega}$ so that $\hat{\theta}_s = \theta_{\max}(\bar{\omega} W_1 + W_2)$. Therefore $\hat{\theta}_s$ is the largest Ritz value of (A, M) in the column space $\bar{\mathcal{Z}}$ of $\bar{\omega} W_1 + W_2 \in \mathbb{R}^{n \times s}$.

Lemma 3.1 guarantees that the dimension of $\overline{\mathcal{Z}}$ equals s . Since $\overline{\mathcal{Z}}$ is a subspace of \mathcal{W} one gets with (3.4) that $\theta'_s \leq \max_{z \in \overline{\mathcal{Z}} \setminus \{0\}} \rho(z) = \widehat{\theta}_s$. \square

COROLLARY 3.2. *If the s -th Ritz value θ_s of (A, M) in \mathcal{V} is contained in $(\lambda_q, \lambda_{q+1})$, $q \in \{1, \dots, n-1\}$, then for the s -th Ritz value θ'_s of (A, M) in $\text{span}\{V, T(AV - MV\Theta)\}$ it holds that either $\theta'_s \leq \lambda_q$ or*

$$(3.7) \quad 0 < \frac{\Delta_{q,q+1}(\theta'_s)}{\Delta_{q,q+1}(\theta_s)} \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2 \quad \text{with} \quad \kappa = \frac{\lambda_q(\lambda_n - \lambda_{q+1})}{\lambda_{q+1}(\lambda_n - \lambda_q)}.$$

Proof. If $q = n-1$, then the first alternative $\theta'_s \leq \lambda_{n-1}$ applies since the s -th Ritz value of (A, M) in the at least $(s+1)$ -dimensional subspace $\text{span}\{V, T(AV - MV\Theta)\}$ is smaller than or equal to λ_{n-1} (due to the min-max principles).

Next let $q < n-1$ and assume $\lambda_q < \theta'_s$ for which (3.7) is to be proved. For $\lambda_q \leq \theta < \lambda_r$ the function $\Delta_{q,r}(\theta) = (\theta - \lambda_q)/(\lambda_r - \theta)$ is monotone increasing in θ . Theorem 3.1 shows that $\theta'_s \leq \widehat{\theta}_s$ so that

$$(3.8) \quad \Delta_{q,q+1}(\theta'_s) \leq \Delta_{q,q+1}(\widehat{\theta}_s).$$

In order to apply Lemma 3.1, case iii, to $x = V\Theta a^*$ and $\tilde{x} = (V - T(AV - MV\Theta))a^*$ we show that

$$\begin{aligned} \|A^{-1}Mx - \tilde{x}\|_A &= \|A^{-1}MV\Theta a^* - Va^* + T(AV - MV\Theta)a^*\|_A \\ &= \|(I - TA)(A^{-1}MV\Theta a^* - Va^*)\|_A \\ &\leq \gamma \|A^{-1}MV\Theta a^* - Va^*\|_A \\ &\leq \gamma \|A^{-1}MV\Theta a^* - \underbrace{V\Theta a^* / \rho(x)}_c\|_A = \gamma \|A^{-1}Mx - x/\rho(x)\|_A \end{aligned}$$

Therein the last inequality is proved with (3.1). Thus part iii in Lemma 3.1 guarantees that the PSD estimate (1.6) can be applied to the smallest Ritz value of (A, M) in $\text{span}\{x, \tilde{x}\}$. By (3.6) this Ritz vector is $\omega^*x + \tilde{x}$ with the Ritz value $\widehat{\theta}_s$. Hence the vectorial PSD estimate (1.6) results in

$$(3.9) \quad \Delta_{q,q+1}(\widehat{\theta}_s) \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2 \Delta_{q,q+1}(\rho(x)).$$

This concludes the proof since $\rho(x)$, $x \in \text{span}\{V\}$, is bounded by the largest Ritz value θ_s of (A, M) in $\text{span}\{V\}$, i.e.

$$(3.10) \quad \Delta_{q,q+1}(\rho(x)) \leq \Delta_{q,q+1}(\theta_s).$$

The chain of inequalities (3.8)–(3.10) proves the proposition. \square

The convergence estimates for the remaining Ritz values θ'_i , $i = 1, \dots, s-1$, follow from Corollary 3.2 by induction. Comparable estimates on the remaining $s-1$ Ritz values, but with respect to different spaces, have been used in Theorem 3.3 in [14] on the subspace analysis of the preconditioned inverse iteration and in Theorem 3.1 in [19] on the block steepest descent iteration.

THEOREM 3.2. *Let \mathcal{V} be an s -dimensional subspace of the \mathbb{R}^n . The Ritz vectors of (A, M) in \mathcal{V} are denoted by v_1, \dots, v_s and let $V := [v_1, \dots, v_s] \in \mathbb{R}^{n \times s}$. The associated Ritz values are $\theta_i = \rho(v_i)$ with $\theta_1 \leq \dots \leq \theta_s$. Indexes k_i are given so that $\theta_i \in (\lambda_{k_i}, \lambda_{k_i+1})$.*

The s smallest Ritz values of (A, M) in $\text{span}\{V, T(AV - MV\Theta)\}$ are denoted by θ'_i with $\theta'_1 \leq \dots \leq \theta'_s$. Then for each $i \in \{1, \dots, s\}$ it holds that $\theta'_i \leq \theta_i$ and either $\theta'_i \leq \lambda_{k_i}$ or

$$(3.11) \quad 0 < \frac{\Delta_{k_i, k_i+1}(\theta'_i)}{\Delta_{k_i, k_i+1}(\theta_i)} \leq \left(\frac{\kappa_i + \gamma(2 - \kappa_i)}{(2 - \kappa_i) + \gamma\kappa_i} \right)^2 \quad \text{with} \quad \kappa_i = \frac{\lambda_{k_i}(\lambda_n - \lambda_{k_i+1})}{\lambda_{k_i+1}(\lambda_n - \lambda_{k_i})}.$$

Therein $\Delta_{p,q}(\theta) := (\theta - \lambda_p)/(\lambda_q - \theta)$.

The bound (3.11) cannot be improved in terms of the eigenvalues of (A, M) as for each i the upper bound is attained for $\theta_i \rightarrow \lambda_{k_i}$ in the 3D invariant subspace associated with the eigenvalues λ_{k_i} , λ_{k_i+1} and λ_n .

Proof. The proof is given by induction on the subspace dimension s . For a one-dimensional subspace $\mathcal{V} = \text{span}\{x\}$ Theorem 1.1 proves the Ritz value estimate (3.11) with $\rho(x') = \theta'_1$.

For an s -dimensional subspace the Ritz vectors v_i of (A, M) are arranged in the columns of $V = [v_1, \dots, v_s] =: [V^{(s-1)}, v_s] \in \mathbb{R}^{n \times s}$. Let $\theta'_i(V^{(s-1)})$ be the $s-1$ smallest Ritz values of (A, M) in

$$\text{span}\{V^{(s-1)}, T(AV^{(s-1)} - MV^{(s-1)}\Theta^{(s-1)})\}, \quad \Theta^{(s-1)} := \text{diag}(\theta_1, \dots, \theta_{s-1}),$$

with $\theta'_1(V^{(s-1)}) \leq \dots \leq \theta'_{s-1}(V^{(s-1)})$. The induction hypothesis with respect to the $(s-1)$ -dimensional space reads

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

The Courant-Fischer variational principles show that these $s-1$ smallest Ritz values $\theta'_i(V^{(s-1)})$ decrease when $\text{span}\{V^{(s-1)}\}$ is enlarged to \mathcal{V} , i.e.

$$\begin{aligned} \theta'_i(V^{(s-1)}) &= \min_{\substack{\mathcal{U} \subseteq \text{span}\{V^{(s-1)}, T(AV^{(s-1)} - MV^{(s-1)}\Theta^{(s-1)})\} \\ \dim(\mathcal{U})=i}} \max_{y \in \mathcal{U} \setminus \{0\}} \rho(y) \\ &\geq \min_{\substack{\mathcal{U} \subseteq \text{span}\{V, T(AV - MV\Theta)\} \\ \dim(\mathcal{U})=i}} \max_{y \in \mathcal{U} \setminus \{0\}} \rho(y) = \theta'_i. \end{aligned}$$

Finally, $\Delta_{k_i, k_i+1}(\theta)$ is a monotone increasing function in θ so that

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

which proves the proposition for the first $s-1$ smallest Ritz values. For the Ritz value θ_s Corollary 3.2 completes the proof.

The sharpness of the estimate (3.11) is a consequence of Theorem 1.1 since for $\theta_i \in (\lambda_{k_i}, \lambda_{k_i+1})$ the columns of V can be formed by the vector of poorest convergence in $\mathcal{E}_{k_i, k_i+1, n}$ and all other columns are taken as eigenvectors with indexes different from k_i , k_i+1 and n . Then the subspace iteration behaves like the vectorial preconditioned steepest descent iteration due to stationarity of the iteration in the eigenvectors. \square

Corollary 3.3 shows that the convergence estimate (3.11) cannot be improved in terms of the eigenvalues without further assumptions on the subspace \mathcal{V} . Hence 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 $\Delta_{q,q+1}$ as used in Theorem 3.2. The numerical experiments in Section 4 illustrate that the block preconditioned steepest descent

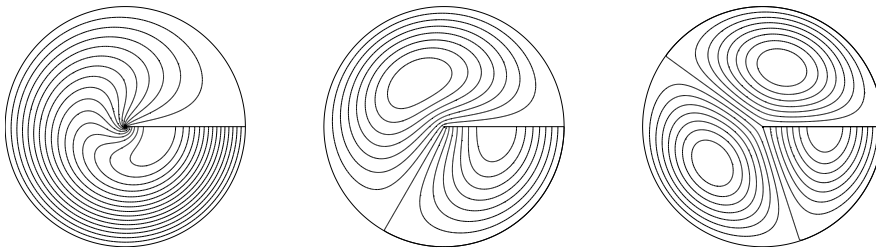


FIG. 4.1. Contour lines of the three eigenfunctions of (4.1) corresponding to the three smallest eigenvalues.

iteration behaves as a cluster robust iteration. In order to derive cluster robust convergence estimates, additional assumptions are to be made: For instance the angle between the iteration subspace and the invariant subspace has to be bounded.

COROLLARY 3.3. *The Ritz value convergence estimate (3.11) cannot be improved in terms of the eigenvalues λ_{k_i} , λ_{k_i+1} and λ_n and is attainable for $\theta_i \rightarrow \lambda_{k_i}$ in $\mathcal{E}_{k_i, k_i+1, n}$.*

Proof. For $\theta_i \in (\lambda_{k_i}, \lambda_{k_i+1})$ let v_i be an M -normalized vector in the invariant subspace $\mathcal{E}_{k_i, k_i+1, n}$ with $\rho(v_i) = \theta_i$. The remaining columns of V are filled with pairwise different eigenvectors of (A, M) which are M -orthogonal to $\mathcal{E}_{k_i, k_i+1, n}$. Then a step of the block steepest descent iteration, Algorithm 1, lets all the eigenvectors invariant. The convergence of the i th column v_i is exactly that of the *vectorial* preconditioned steepest descent iteration as treated in Theorem 1.1 because the iteration is stationary in all eigenvectors. The non-improvability of the convergence estimate in terms of the eigenvalues has already been treated in Theorem 1.1. \square

4. Numerical experiments. The block preconditioned steepest descent iteration is applied to the Laplacian eigenvalue problem

$$(4.1) \quad -\Delta u(x) = \lambda u(x), \quad x \in \Omega := \{(r \cos(\varphi), r \sin(\varphi)) : r \in [0, 1], \varphi \in [0, 2\pi]\}$$

on the unit circle with a slit along the positive abscissa. Homogeneous Dirichlet boundary conditions are given on the boundary for $r = 1$ and on the upper side of the slit $\{(r, \varphi) : r \in [0, 1], \varphi = 0\}$. Homogeneous Neumann boundary conditions are used on the lower side of the slit. The numerical approximations of the eigenvalues and eigenfunctions can be compared with the exact solutions of (4.1). The eigenfunctions are $\sin(\alpha_k \varphi) J_{\alpha_k}(\xi_{k,l} r)$; see Fig. 4.1. Therein J_{α_k} is a Bessel function of first kind and fractional order [1] and $\alpha_k := \frac{1}{2}k + \frac{1}{4}$. The eigenvalues are the squares of the positive zeros $\xi_{k,l}$ of J_{α_k} .

The operator eigenvalue problem is discretized by linear finite elements on a triangle mesh. Our program code AMPE (Adaptive Multigrid Preconditioned Eigensolver) in FORTRAN is an adaptive multigrid finite element code with an edge oriented error estimator which uses linear and quadratic finite elements. All test computations have been executed on a personal computer with an Intel Xeon 3.2GHz CPU and with a RAM of 31.4GiB. Our finite element code on this computer can solve eigenvalue problems that exceed $50 \cdot 10^6$ degrees of freedom. The program includes multigrid preconditioning with Jacobi smoothing. The FORTRAN code is embedded in a Matlab GUI which allows an easy and convenient usage of the program and the graphical presentation of its output.

Experiment I: In this first experiment the block preconditioned steepest descent iteration is applied in a 3-dimensional subspace; we refer to this algorithm as PSD($s = 3$). Further, the eigenvalue problem is discretized on a series of uniform triangle meshes to

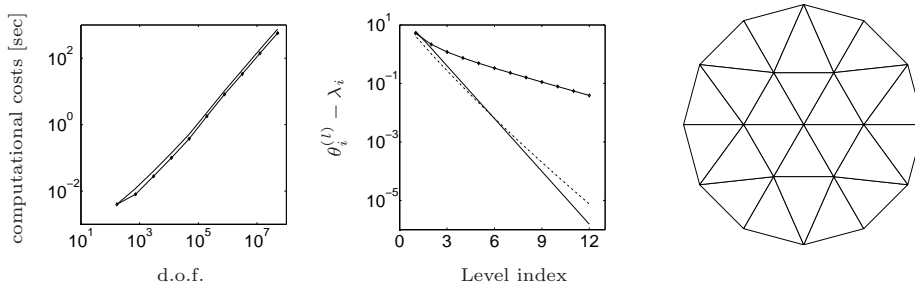


FIG. 4.2. $PSD(s = 3)$ nested iteration on uniform triangle meshes. Left: Computational costs until a level is reached and finished (solid line); computation time on the current level (markers). Center: Error of the eigenvalue approximations, $i = 1$ by a line with markers, $i = 2$ by a broken line and $i = 3$ by a solid line. Right: The initial triangulation.

which nested iteration is applied. The first grid level comprises 21 nodes from which 15 are located on the Dirichlet boundary. This gives 6 initial degrees of freedom. On this coarsest level the eigenvalue problem is solved exactly (aside from rounding errors). Piecewise linear interpolation is used to prolongate the approximate eigenfunctions from one grid level to the next refined level. The multigrid preconditioner is a V-cycle multigrid solver with damped Jacobi-smoothing; the damping constant is $\omega = 2/3$ and two pre-smoothing and post-smoothing iterations are applied on each level.

The quality of the preconditioner is controlled by a stopping condition for the linear system solver. For each Ritz vector the bound $\|A(Tr) - r\|_2 < 10/n$ is tested. Therein r denotes the residual of a Ritz vector, Tr is the preconditioned residual and n is the dimension of the discrete problem on the current level. In most cases only one V-cycle is required to reach this accuracy since the initial solution on a refined grid is the prolongation of the solution from the coarser grid.

The stopping criterion for $PSD(s = 3)$ is $\|r\|_T = (r^T Tr)^{1/2} < 10^{-10}$ where r runs through the residuals $Av_i - \rho(v_i)Mv_i$ for the Ritz vectors v_1, v_2 and v_3 . This stopping criterion is justified by the generalized Temple inequality (see Lemma 3 in Chapter 11 of [3]), which is the first inequality in

$$\frac{\rho(x)(\rho(x) - \lambda_i)(\lambda_{i+1} - \rho(x))}{\lambda_i \lambda_{i+1}} \leq \|r\|_{A^{-1}}^2 \leq \frac{1}{1 - \gamma} \|r\|_T^2 \quad \text{if } \rho(x) \in [\lambda_i, \lambda_{i+1}].$$

The second inequality follows with $\|I - TA\|_A \leq \gamma < 1$. Hence $\|r\|_T^2$ is an upper bound for the product of the relative distances of $\rho(x)$ to the enclosing eigenvalues λ_i and λ_{i+1} .

The nested iteration is stopped on the level $l = 12$ with 50348033 nodes and 50319360 degrees of freedom. Figure 4.2 (left) shows that the computational costs increase more or less linearly in the dimension of the problem which indicated the near optimal complexity of the $PSD(s = 3)$ solver. Figure 4.2 also shows the errors $\theta_i^{(k)} - \lambda_i$, $i = 1, 2, 3$, for the three smallest eigenvalues

$$\lambda_1 = \xi_{0,1}^2 \approx 7.733337, \quad \lambda_2 = \xi_{1,1}^2 \approx 12.18714, \quad \lambda_3 = \xi_{2,1}^2 \approx 17.35078.$$

The error $\theta_1^{(k)} - \lambda_1$ is relatively large since the associated eigenfunction has an unbounded derivative at the origin. The next experiment shows that the approximation of this eigenfunction clearly profits from an adaptively generated grid.

Experiment II: Next we show that adaptive mesh generation with *a posteriori* edge oriented error estimation similar to that in [15] results in much better approximations.

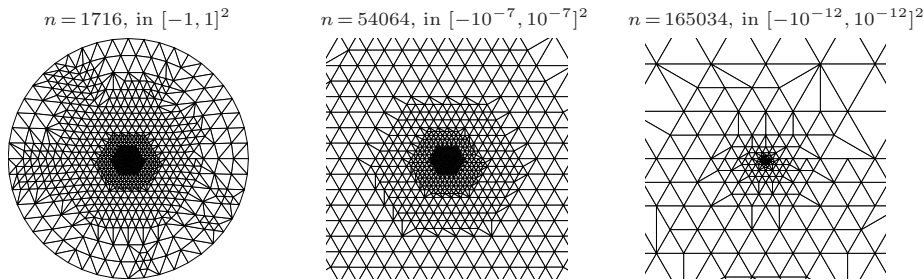


FIG. 4.3. Triangle meshes and enlargements around the origin with 1716, 54064 and 165034 nodes (with 1628, 53387 and 163772 inner nodes). The associated depths of the triangulations are 17, 39 and 46. The positive axis $r \geq 0$ and $\varphi = 0$ belongs to the boundary.

The error estimator computes the eigenvector residuals with respect to quadratic finite elements for Ritz vectors which are represented by linear finite elements. The largest (in modulus) components of the residual are used to select those edges which belong to triangles that are to be refined.

Once again, the PSD($s = 3$) solver is used. In order to compute a grid which allows an optimal approximation of the eigenfunction associated with the smallest eigenvalue, the error estimation and grid refinement aims at an optimal approximation of just this eigenfunction. Figure 4.3 shows a relatively coarse triangulation of the unit circle and sectional enlargements of finer triangulations around the origin, where the depth of the triangulations takes its largest values due to the unbounded derivative $(\partial/\partial r)J_{\alpha_k}$ around $r = 0$. The adaptive process generates highly non-uniform triangulations. Further details of the adaptive process and its more or less linearly increasing costs (as a function of the d.o.f) are shown in Figure 4.4. The resulting smallest Ritz values θ_1 , which approximate the smallest eigenvalue $\lambda_1 \approx 7.733337$, are as follows:

Depth of triang.	1	30	43	57	68	73
Nodes	21	10709	108693	1185777	10961756	34157092
D.o.f.	6	10409	107630	1182184	10951337	34137627
θ_1	12.95561	7.738704	7.733789	7.733379	7.733341	7.733338

In contrast to this, a uniform refinement results with a final depth 12 with 50348033 nodes only in a poor approximation $\theta_1 = 7.772233$; a comparable quality of approximation can be gained by the adaptive process on level 19 with 2377 nodes and $\theta_1 = 7.762841$.

Finally, the results of the PSD iteration to approximate the 15 smallest eigenvalues in a 20-dimensional subspace are listed in Table 1.

Experiment III: Next the case of poorest convergence of the block preconditioned steepest descent iteration is explored. Therefore, we use the final grid from Experiment II with about $34.1 \cdot 10^6$ d.o.f. and apply the PSD($s = 3$) iteration. According to Theorem 1.1 poorest convergence of the vectorial iteration PSD($s = 1$) is attained in the invariant subspace $\mathcal{E}_{i,i+1,n}$. The subspace iteration behaves similarly. To show this we consider subspaces which are spanned by a single nonzero vector from $\mathcal{E}_{i,i+1,n}$ whereas all the other basis vectors are eigenvectors of (A, M) with indexes different from $i, i + 1$ and n . Then block-PSD behaves like a vectorial iteration due to the stationarity in the eigenvectors. Theorem 1.1 provides the convergence estimate for the single vector from $\mathcal{E}_{i,i+1,n}$. Figure 4.5 shows in the intervals $(\lambda_i, \lambda_{i+1})$ the upper bounds $(\kappa + \gamma(2 - \kappa))^2 / ((2 - \kappa) + \gamma\kappa)^2$ (dashed lines) and the largest ratios $\Delta_{i,i+1}(\theta'_i) / \Delta_{i,i+1}(\theta_i)$ 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 (3.11) is sharp, cf. Theorem 3.2,

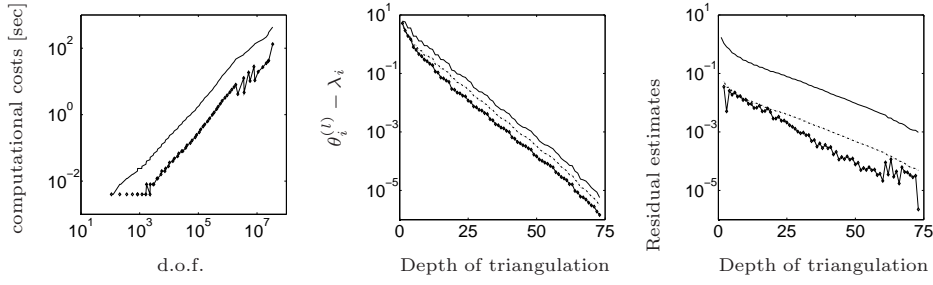


FIG. 4.4. Result of PSD($s = 3$) adaptive eigensolver. Left: Computational costs: Total computation time until # d.o.f. has been reached by solid line. Line with markers shows the computation time on the current level. Center: Errors $\theta_i^{(l)} - \lambda_i$ for $i = 1$ by line with markers, $i = 2$ by broken line and $i = 3$ by solid line. Right: Estimated residual norm for θ_1 by solid line, estimate used for the stopping criterion by broken line and actual residual norm $\|r\|_T^2 / \|Tr\|_A$ w.r.t. linear elements by line with markers.

k \ l	1	2	k \ l	1	2	k \ l	1	2
0	7.733389	34.88339	0	7.733342	34.88260	0	7.733337	34.88252
1	12.18725	44.25893	1	12.18715	44.25768	1	12.18714	44.25756
2	17.35102	54.36164	2	17.35080	54.35978	2	17.35078	54.35960
3	23.19983	65.17971	3	23.19943	65.17704	3	23.19939	65.17677
4	29.71530	76.70204	4	29.71460	76.69829	4	29.71453	76.69790
5	36.88311		5	36.88199		5	36.88189	
6	44.69164		6	44.69009		6	44.68994	
7	53.13167		7	53.12939		7	53.12918	
8	62.19503		8	62.19189		8	62.19159	
9	71.87493		9	71.87073		9	71.87033	

TABLE 1

The 15 smallest eigenvalues $\xi_{k,i}^2$ of (4.1). Left: Ritz values in a 1047534-dimensional linear finite element space. Center: Ritz values in a 10052735-dimensional linear finite element space. Right: “Exact” eigenvalues of (4.1).

and can be attained for $\theta_i \rightarrow \lambda_i$.

Experiment IV: In this experiment the sharp single-step estimates (3.11) are compared with multi-step estimates for the PSD($s = 3$) iteration. For each grid level l with $l > 1$ the initial subspace $\mathcal{V}^{(0,l)}$, which is the prolongation of the final subspace from the level $l - 1$, is of sufficient quality so that the three Ritz values of (A_l, M_l) in $\mathcal{V}^{(0,l)}$ have reached their “destination interval”, i.e.

$$\theta_i(\mathcal{V}^{(0,l)}) \in (\lambda_i^{(l)}, \lambda_{i+1}^{(l)}), \quad i = 1, 2, 3,$$

so that the Ritz values $\theta_i^{(k,l)}$ (k is the iteration index on level l) do not leave this interval. Therein, $\lambda_i^{(l)}$ are the eigenvalues of (A_l, M_l) with respect to the grid level l . Theorem 3.2 guarantees that $\lim_{k \rightarrow \infty} \theta_i^{(k,l)} = \lambda_i^{(l)}$.

All this allows to apply the 1-step estimates

$$(4.2) \quad \frac{\theta_i^{(k+1,l)} - \lambda_i^{(l)}}{\lambda_{i+1}^{(l)} - \theta_i^{(k+1,l)}} \leq \left(\frac{\kappa^{(l)} + \gamma(2 - \kappa^{(l)})}{(2 - \kappa^{(l)}) + \gamma\kappa^{(l)}} \right)^2 \frac{\theta_i^{(k,l)} - \lambda_i^{(l)}}{\lambda_{i+1}^{(l)} - \theta_i^{(k,l)}} =: \sigma(\theta_i^{(k+1,l)}), \quad k = 0, 1, \dots,$$

recursively, which yields the multistep estimate

$$(4.3) \quad \frac{\theta_i^{(k,l)} - \lambda_i^{(l)}}{\lambda_{i+1}^{(l)} - \theta_i^{(k,l)}} \leq \left(\frac{\kappa^{(l)} + \gamma(2 - \kappa^{(l)})}{(2 - \kappa^{(l)}) + \gamma\kappa^{(l)}} \right)^{2k} \frac{\theta_i^{(0,l)} - \lambda_i^{(l)}}{\lambda_{i+1}^{(l)} - \theta_i^{(0,l)}} =: \tau(\theta_i^{(k,l)}), \quad k = 1, 2, \dots$$

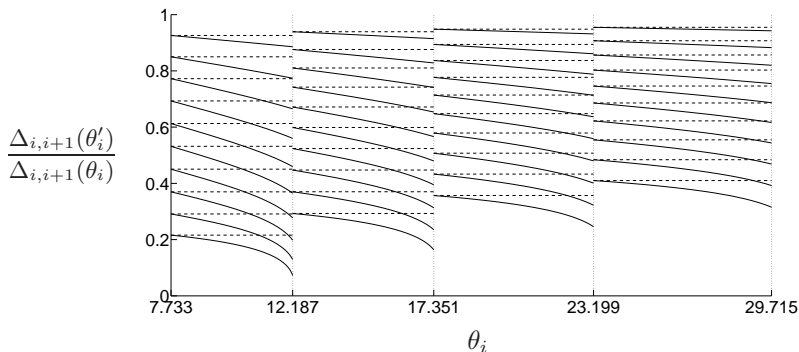


FIG. 4.5. *Poorest convergence of block preconditioned steepest descent iteration. Abscissa: Five smallest eigenvalues according to Table 1. The dashed lines in the intervals $(\lambda_i, \lambda_{i+1})$ are the upper bounds $(\kappa + \gamma(2 - \kappa))^2 / ((2 - \kappa) + \gamma\kappa)^2$ for $\gamma \in \{0, 0.1, \dots, 0.9\}$. 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 .*

Therein, $\kappa^{(l)}$ is given by (3.11) after substitution of λ_i by $\lambda_i^{(l)}$ for the relevant indexes i . The parameter $\gamma = \|I - TA\|_A$ on the quality of the preconditioner is approximated on each grid level by computing the spectral radius of $I - TA$ with the power method. For this experiment we use again two steps of pre-/post-smoothing on each level with damped ($\omega = 2/3$) Jacobi-smoothing. This results in $\gamma \approx 0.78$. The discrete eigenvalues $\lambda_i^{(l)}$ are estimated by extrapolation from the computed Ritz values.

Figure 4.6 shows the multistep bound (4.3) as a bold line, the 1-step bound as a dotted line and the numerical result as a thin solid line. The 1-step estimate (4.2) is a very good upper estimate. In all cases the multistep estimate (4.3) is a relatively rough estimate. It accumulates the over-estimation of the error from step to step and suffers from its inability to use the current $\theta_i^{(k,l)}$ on the right-hand side of the estimate in order to improve the quality of the upper bound.

The $\Delta(\theta)$ -ratio depends on the discrete eigenvalues $\lambda^{(l)}$ and decreases monotonically for the iteration on each grid level; the ratio may increase after prolongation to a refined grid level. The somewhat oscillating behavior of the $\Delta(\theta)$ -ratio for λ_2 in contrast to the smoother behavior for λ_1 reflects the fact that the error estimation and grid generation is controlled by error estimates for the first eigenfunction. The second eigenfunction also profits from the grid refinement (cf. Figure 4.4) but the $\Delta(\theta)$ -ratio shows a stronger variation for changing level index l .

5. Conclusion. This paper concludes the efforts for analyzing preconditioned gradient iterations and their subspace variants with either fixed step length (case of inverse iteration and preconditioned inverse iteration) or with with optimal step-length (case of steepest descent and preconditioned steepest descent). Within the hierarchy of preconditioned gradient iterations, as suggested in [13], these solvers are denoted as INVIT(k,s) and PINVIT(k,s) with $k = 1, 2$ and subspace dimensions $s \in \mathbb{N}$.

For all these iterative eigensolvers sharp convergence estimates have been derived which have the common form

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

with $\Delta_{i,i+1}(\xi) = (\xi - \lambda_i) / (\lambda_{i+1} - \xi)$ and convergence factors σ . The following sharp convergence estimates have been gained:

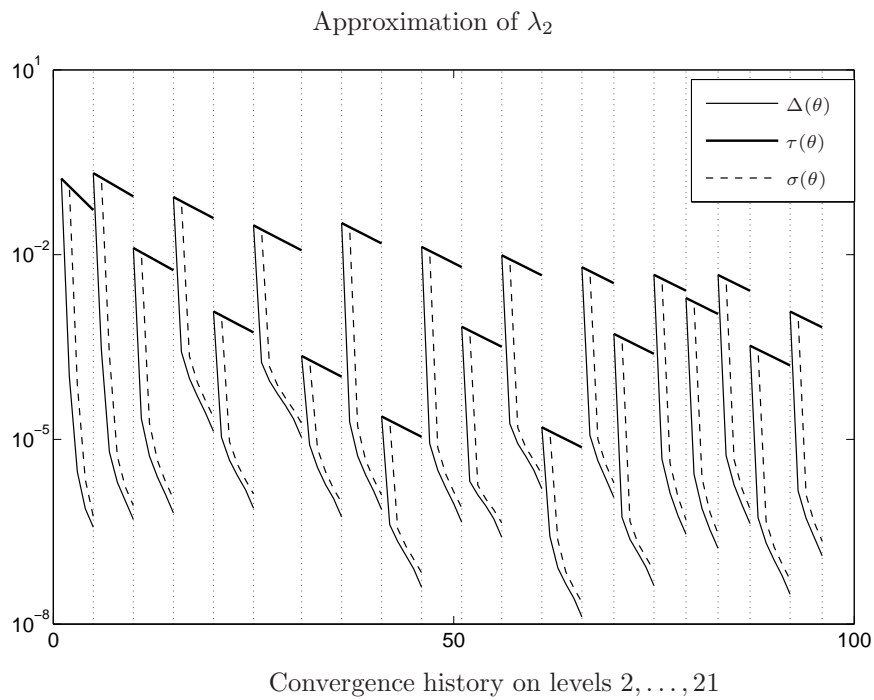
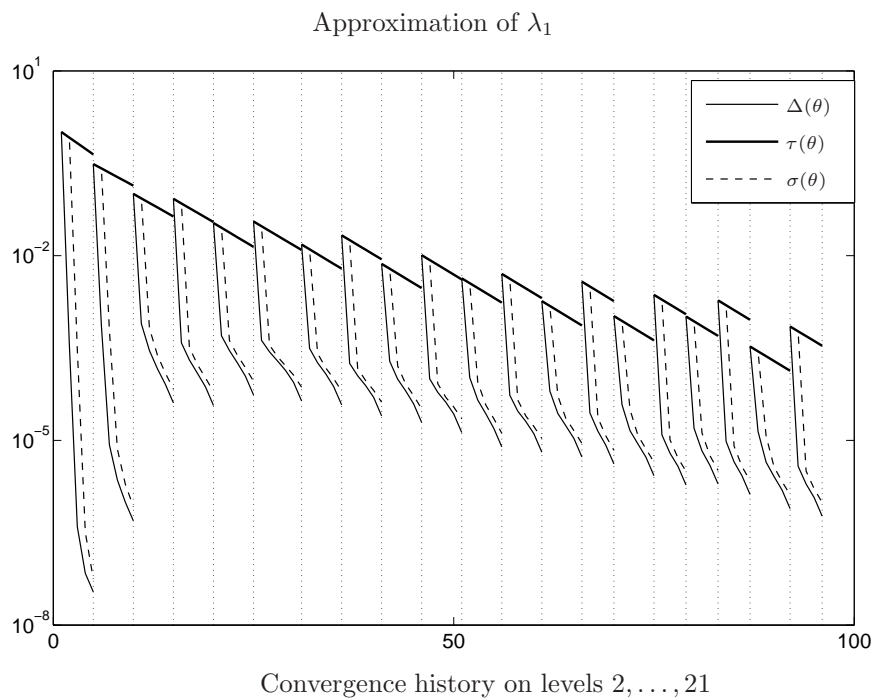


FIG. 4.6. Convergence history of the error ratios $\Delta_{i,i+1}^{(l)}(\theta_i^{(k,l)}) = (\theta_i^{(k,l)} - \lambda_i^{(l)}) / (\lambda_{i+1}^{(l)} - \theta_i^{(k,l)})$ for $i = 1, 2$ and PSD(3). The 1-step estimate (4.2) (broken line) is good estimate for the numerical worst-case results (thin solid line); the multistep estimate (4.3) (bold line) accumulates the over-estimation from step to step.

Iterative Eigensolver	Convergence factor	Ref.
Inverse iteration	$\sigma = \frac{\lambda_i}{\lambda_{i+1}}$	[16]
Preconditioned inverse iteration	$\sigma = \gamma + (1 - \gamma) \frac{\lambda_i}{\lambda_{i+1}}$	[10]
Block preconditioned inverse iteration		[14]
Steepest descent	$\sigma = \frac{\kappa}{2-\kappa}, \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}$	[18]
Precond. steepest descent	$\sigma = \frac{\kappa + \gamma(2-\kappa)}{(2-\kappa) + \gamma\kappa}, \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}$	[17]
Block preconditioned steepest descent		here

Scientific efforts for the future are aimed at a convergence analysis of the important locally optimal preconditioned conjugate gradient (LOPCG) iteration [9]. As the convergence behavior of the LOPCG eigensolver has been observed to behave similarly to the conjugate gradient iteration for linear systems, sharp convergence estimates are highly desired.

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REFERENCES

- [1] G. Arfken. *Mathematical Methods for Physicists*. Academic Press, San Diego, 1985.
- [2] 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.
- [3] E.G. D'yakonov. *Optimization in Solving Elliptic Problems*. CRC Press, Boca Raton, Florida, 1996.
- [4] G.H. Golub and C.F. Van Loan. *Matrix Computations*. Johns Hopkins University Press, Baltimore, MD, third edition, 1996.
- [5] M.R. Hestenes and W. Karush. A method of gradients for the calculation of the characteristic roots and vectors of a real symmetric matrix. *J. Res. Nat. Bureau Standards*, 47:45–61, 1951.
- [6] L.V. Kantorovich. *Functional analysis and applied mathematics*. U. S. Department of Commerce National Bureau of Standards, Los Angeles, Calif., 1952. Translated by C. D. Benster.
- [7] L.V. Kantorovich and G.P. Akilov. *Functional Analysis in Normed Spaces*. Pergamon, London, 1964.
- [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. Gradient flow approach to geometric convergence analysis of preconditioned eigensolvers. *SIAM J. Matrix Anal. Appl.*, 31:621–628, 2009.
- [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 hierarchy of preconditioned eigensolvers for elliptic differential operators. Habilitationsschrift an der Mathematischen Fakultät, Universität Tübingen, 2001.
- [14] K. Neymeyr. A geometric theory for preconditioned inverse iteration applied to a subspace. *Math. Comp.*, 71:197–216, 2002.
- [15] K. Neymeyr. A posteriori error estimation for elliptic eigenproblems. *Numer. Linear Algebra Appl.*, 9:263–279, 2002.
- [16] K. Neymeyr. A note on inverse iteration. *Numer. Linear Algebra Appl.*, 12:1–8, 2005.
- [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. Accepted for Numer. Linear Algebra Appl., DOI: 10.1002/nla.1915, 2013.

- [20] E. Ovtchinnikov. Convergence estimates for the generalized Davidson method for symmetric eigenvalue problems II: The subspace acceleration. *SIAM Journal on Numerical Analysis*, 41(1):272–286, 2003.
- [21] B.N. Parlett. *The Symmetric Eigenvalue Problem*. Prentice Hall, Englewood Cliffs New Jersey, 1980.
- [22] J. Ponstein. An extension of the min-max theorem. *SIAM Rev.*, 7:181–188, 1965.
- [23] V.G. Prikazchikov. Strict estimates of the rate of convergence of an iterative method of computing eigenvalues. *USSR J. Comput. Math. and Math. Physics*, 15:235–239, 1975.
- [24] Y. Saad. *Numerical Methods for Large Eigenvalue Problems*. Manchester University Press, Manchester, 1992.
- [25] B.A. Samokish. The steepest descent method for an eigenvalue problem with semi-bounded operators. *Izv. Vyssh. Uchebn. Zaved. Mat.*, 5:105–114, 1958. (In Russian).
- [26] M. Sion. On general minimax theorems. *Pacific J. Math.*, 8:171–176, 1958.
- [27] A. Stathopoulos. Nearly Optimal Preconditioned Methods for Hermitian Eigenproblems under Limited Memory. Part I: Seeking One Eigenvalue. *SIAM Journal on Scientific Computing*, 29(2):481–514, 2007.
- [28] P.F. Zhuk and L.N. Bondarenko. Sharp estimates for the rate of convergence of the s -step method of steepest descent in eigenvalue problems. *Ukrain. Mat. Zh.*, 49(12):1694–1699, 1997.