A GEOMETRIC CONVERGENCE THEORY FOR THE
PRECONDITIONED STEEPEST DESCENT ITERATION

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Abstract. Preconditioned gradient iterations for very large eigenva-

lue problems are efficient solvers with growing popularity. However, only for the simplest precon-
ditioned eigensolver, namely the precondi-
tioned gradient iteration (or preconditioned inverse iteration) with fixed step size, sharp non-asymptotic
convergence estimates are known and these estimates require an ideally scaled preconditioner. In this
paper a new sharp convergence estimate is derived for the precondi-
tioned steepest descent iteration which
combines the preconditioned gradient iteration with the Rayleigh-Ritz procedure for optimal line search
convergence acceleration. The new estimate always improves that of the fixed step size iteration. The
practical importance of this new estimate is that arbitrarily scaled preconditioners can be used. The
Rayleigh-Ritz procedure implicitly computes the optimal scaling.

Key words. eigenvalue computation; Rayleigh quotient; gradient iteration; steepest descent; pre-
conditioner.

1. Introduction. The topic of this paper is a convergence analysis of a precondi-
tioned gradient iteration with optimal step-length scaling in order to compute the smallest
eigenvalue of the generalized eigenvalue problem

\[ Ax_i = \lambda_i Bx_i \]

for symmetric positive definite matrices \( A, B \in \mathbb{R}^{n \times n} \). A typical source of \((1.1)\) is an
eigenvproblem for a self-adjoint and elliptic partial differential operator whose weak form
reads

\[ a(u, v) = \lambda \langle u, v \rangle, \quad \forall v \in H(\Omega). \]

The bilinear form \( a(\cdot, \cdot) \) is associated with the partial differential operator and an \( L^2(\Omega) \)
inner product \( \langle \cdot, \cdot \rangle \) appears on the right side. Further \( u \) is an eigenfunction and \( \lambda \) an
eigenvalue if \((1.2)\) is satisfied for all \( v \) in an appropriate Hilbert space \( H(\Omega) \). A finite

The eigenvalues of \( (1.1) \) are enumerated in increasing order \( 0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \). The
smallest eigenvalue \( \lambda_1 \) and an associated eigenvector can be computed by means of an
iterative minimization of the Rayleigh quotient

\[ \rho(x) = \frac{\langle x, Ax \rangle}{\langle x, Bx \rangle}, \]

where \( \langle \cdot, \cdot \rangle \) denotes the Euclidean inner product. To this end the simplest preconditioned
gradient iteration corrects a current iterate \( x \) in the direction of the negative preconditioned gradient of the Rayleigh quotient to form the next iterate \( x' \)

\[ x' = x - T(Ax - \rho(x)Bx). \]

Therein \( T \) is a symmetric positive definite matrix and is called the preconditioner. This
fixed-step-length preconditioned iteration is analyzed in \([2, 6, 5, 8]\); see also the references
in \([3]\).

Appropriate preconditioners \( T \) are available in various ways; especially for the operator
eigenproblem \((1.2)\) multi-grid or multi-level preconditioners are available. In this context
the quality of the preconditioner is typically controlled in terms of a real parameter \( \gamma \in [0,1) \) in a way that

\[(1 - \gamma)(z, T^{-1}z) \leq (z, Az) \leq (1 + \gamma)(z, T^{-1}z), \quad \forall z \in \mathbb{R}^n,\]

or equivalently, that the spectral radius of the error propagation matrix \( I - TA \) is bounded by \( \gamma \).

The following result for the convergence of (1.4) is known from [6, 8]; the convergence analysis interprets this preconditioned iteration as a preconditioned inverse iteration and makes use of the underlying geometry.

**Theorem 1.1.** If \( \lambda_i \leq \rho(x) < \lambda_{i+1} \) then for \( x' \) given by (1.4) and assuming (1.5) it holds that \( \rho(x') \leq \rho(x) \) and either \( \rho(x') \leq \lambda_i \) or

\[
\frac{\rho(x') - \lambda_i}{\lambda_{i+1} - \rho(x')} \leq \sigma^2 \frac{\rho(x) - \lambda_i}{\lambda_{i+1} - \rho(x)}, \quad \sigma = \gamma + (1 - \gamma) \frac{\lambda_i}{\lambda_{i+1}}.
\]

Thm. 1.1 is up to now the only known sharp estimate for this and various improved and faster converging preconditioned gradient type eigensolvers. The most popular of these improved solvers are the preconditioned steepest descent iteration (PSD) and the locally optimal preconditioned conjugate gradients (LOPCG) iteration (and also their block variants) [5]. All these eigensolvers apply the Rayleigh-Ritz procedure to proper subspaces of iterates for convergence acceleration, see [7]. A systematic hierarchy of these preconditioned gradient iterations and their variants for exact inverse preconditioning (which amounts to certain Invert-Lanczos processes [15]) has been suggested in [13]. The aim of this paper is to prove a new sharp convergence estimate for the preconditioned steepest descent iteration (PSD).

**1.1. Assumptions on the preconditioner.** A drawback of Thm. 1.1 is its assumption (1.5) on the preconditioner \( T \). The existence of constants \( 1 \pm \gamma \) with \( \gamma < 1 \) is not guaranteed for arbitrary (multigrid) preconditioners, but can always be ensured after a proper scaling of the preconditioner. To make this clear, take an arbitrary pair of symmetric positive definite matrices \( A, T \in \mathbb{R}^{n \times n} \). Then constants \( \gamma_1, \gamma_2 > 0 \) exist, so that the spectral equivalence

\[(1.7) \quad \gamma_1(z, T^{-1}z) \leq (z, Az) \leq \gamma_2(z, T^{-1}z), \quad \forall z \in \mathbb{R}^n\]

holds. If a preconditioner \( T \) satisfies (1.7), then the scaled preconditioner \( (2/(\gamma_1 + \gamma_2))T \) fulfills (1.5) with

\[(1.8) \quad \gamma = \frac{\gamma_2 - \gamma_1}{\gamma_1 + \gamma_2}.
\]

A clear benefit of the preconditioned steepest descent iteration is, that by computing the optimal step length parameter \( \vartheta_{opt} \), see Eq. (1.9), the scaling parameter \( 2/(\gamma_1 + \gamma_2) \) is determined implicitly. Therefore, we can use the assumption (1.7) or alternatively the more convenient form (1.5). This guarantees the practical applicability of the preconditioned steepest descent iteration for any preconditioner satisfying (1.7) or in its scaled form satisfying (1.8).

**1.2. The optimal-step-length iteration:** Preconditioned steepest descent.

A disadvantage of the gradient iteration (1.4) is its fixed step length resulting in a non-optimal new iterate \( x' \). An obvious improvement is to compute \( x' \) as the minimizer of the Rayleigh quotient (1.3) in the affine space \( \{x - \vartheta T(Ax - \rho(x)Bx); \vartheta \in \mathbb{R}\} \). That means we consider the optimally scaled iteration

\[(1.9) \quad x' = x - \vartheta_{opt} T(Ax - \rho(x)Bx)\]
with the optimal step length
\[ \vartheta_{\text{opt}} = \arg \min_{\vartheta \in \mathbb{R}} \rho(x - \vartheta T(Ax - \rho(x) Bx)) \]
is considered. This iteration is called the \textit{preconditioned steepest descent iteration} (PSD), \cite{2,14,18}. Computationally one gets \( x' \) and its Rayleigh quotient \( \rho(x') \) by the Rayleigh-Ritz procedure. If \( T(Ax - \rho(x) Bx) \) is not an eigenvector then \( (x', \rho(x')) \) is a Ritz pair of \((A,B)\) with respect to the column space of \([x, T(Ax - \rho(x) Bx)]\). As \eqref{eq:1.9} aims at a minimization of the Rayleigh quotient, \( \rho(x') \) is the smaller Ritz value and \( x' \) is an associated Ritz vector. The Rayleigh-Ritz procedure computes the optimal step length implicitly; the step length is determined by the components of the associated eigenvector of Rayleigh-Ritz projection matrices. Consequently the preconditioned steepest descent iteration converges faster than the fixed-step-length scheme \eqref{eq:1.4} since
\begin{equation}
\rho(x - \vartheta_{\text{opt}} T(Ax - \rho(x) Bx)) \leq \rho(x - T(Ax - \rho(x) Bx)).
\end{equation}
Therefore Thm. \ref{thm:1.1} serves as a trivial upper estimate for the accelerated iteration \eqref{eq:1.10}.

**Theorem 1.2.** Let \( x \in \mathbb{R}^n \) and \( x' \) be the PSD iterate given by \eqref{eq:1.9}. The preconditioner \( T \) is assumed to satisfy \eqref{eq:1.7}. If \( \lambda_i \leq \rho(x) < \lambda_{i+1}, \ i = 1, \ldots, n-1, \) then \( \rho(x') \leq \rho(x) \) and either \( \rho(x') \leq \lambda_i \) or
\begin{equation}
\frac{\rho(x') - \lambda_i}{\lambda_{i+1} - \rho(x')} \leq \sigma^2 \frac{\rho(x) - \lambda_i}{\lambda_{i+1} - \rho(x)}.
\end{equation}
with \( \sigma = \frac{\kappa + \gamma (2 - \kappa)}{(2 - \kappa) + \gamma \kappa}, \ \kappa = \frac{\lambda_i (\lambda_n - \lambda_{i+1})}{\lambda_{i+1} (\lambda_n - \lambda_i)} \)
and \( \gamma := (\gamma_2 - \gamma_1)/(\gamma_1 + \gamma_2) \). If \( \gamma_1 = 1 - \gamma \) and \( \gamma_2 = 1 + \gamma \) as in \eqref{eq:1.3}, then \((\gamma_2 - \gamma_2)/(\gamma_1 + \gamma_2) = \gamma \). The estimate is sharp and can be attained for \( \rho(x) \rightarrow \lambda_i \) in the 3D invariant subspace associated with the eigenvalues \( \lambda_i, \ \lambda_{i+1} \) and \( \lambda_n, \ i + 1 \neq n \).

The limit case \( \gamma = 0 \) of Thm. \ref{thm:1.2} is an estimate for the convergence of the steepest descent iteration which minimizes the Rayleigh quotient in the space \( \text{span}\{x, A^{-1} B x\} \). Then the convergence estimate \eqref{eq:1.11} reads
\begin{equation}
\frac{\rho(x') - \lambda_i}{\lambda_{i+1} - \rho(x')} \leq \left( \frac{\kappa}{2 - \kappa} \right)^2 \frac{\rho(x) - \lambda_i}{\lambda_{i+1} - \rho(x)}
\end{equation}
with \( \kappa \) given by \eqref{eq:1.11}. A proof of this result (in the general setup of steepest ascent and steepest descent for \( A \) and \( A^{-1} \)) has recently been given in \cite{16}; for the smallest eigenvalue (that is for \( i = 1 \)) the estimate was proved in \cite{9}. This paper generalizes this result on steepest decent for \( A^{-1} M \) to the preconditioned variant of this iteration. For the following analysis we always assume a properly scaled preconditioner satisfying \eqref{eq:1.5}. If \( T \) fulfills \eqref{eq:2.23} we use \((2/(\gamma_1 + \gamma_2)) T \) (and call the scaled preconditioner once again \( T \)) so that \( \gamma \) is given by \eqref{eq:1.3} and \eqref{eq:1.5} is fulfilled. This substitution does not restrict the generality of the approach since the scaling constant is implicitly computed with \( \vartheta_{\text{opt}} \) in the Rayleigh-Ritz procedure. We prefer to work with \eqref{eq:1.5} since this allows to set up the proper geometry for the following proof.

Only few convergence estimates for PSD have been published. Of major importance are the work of Samokish \cite{19}, the results of Knyazev given in Thm. 3.3 together with Eq. (3.3) in \cite{4} and further the results of Ovtchinnikov \cite{15}. Knyazev uses similar assumptions and applies Chebyshev polynomials to derive the convergence estimate. Ovtchinnikov in \cite{15} derives an asymptotic convergence factor which represents the average error.
reduction per iteration; further non-asymptotic estimates are proved under specific assumptions on the preconditioner. The result of Samokish (only available in Russian) is reproduced in a finite-dimensional non-asymptotic form as Thm. 2.1 in [18]; see also Cor. 6.4 and the following paragraph in [18] for a critical discussion and comparison of these estimates. Due to different assumptions and a different form of the convergence estimates these results are not easy to compare with (1.11); an important difference is that in Thm. 1.2 the restrictive assumption \( \rho(x) < \lambda \) is not needed.

1.3. Overview. This paper is organized as follows. In Sec. 2 the geometry of PSD is introduced. Further the problem is reformulated in terms of reciprocals of the eigenvalues which makes the geometry of PSD accessible within the Euclidean space. Sec. 3 gives a proof that PSD attains its poorest convergence in a three-dimensional invariant subspace of the \( \mathbb{R}^n \). Sec. 4 contains a mini-dimensional analysis of PSD. Finally the three-dimensional convergence estimates are embedded into the full \( \mathbb{R}^n \) which completes the convergence analysis.

2. The geometry of the preconditioned steepest descent iteration. For the analysis of the preconditioned steepest descent iteration it is convenient to work with the linear pencil \( B - \mu A \) (instead of \( A - \lambda B \)). The advantage is that the \( A \)-norm by a proper basis transformation turns into the Euclidean norm, see below. A further benefit of this representation is that a generalization to a symmetric positive semidefinite or even only a symmetric \( B \) is possible (cf. the analysis of (1.4) in [8]). Hence for the pencil \( B - \mu A \) the eigenvalues \( \mu_i \) are given by

\[
Bx_i = \mu_i Ax_i \quad \text{with} \quad \mu_i = 1/\lambda_i, \quad i = 1, \ldots, n.
\]

Therefore the problem is to compute the largest eigenvalue \( \mu_1 \) by maximizing the inverse of the Rayleigh quotient (1.3)

\[
\mu(x) := \frac{(x, Bx)}{(x, Ax)} = \frac{1}{\rho(x)}.
\]

Lemma 2.1. Without loss of generality we can assume that \( A = I \) and that \( B = \text{diag}(\mu_1, \ldots, \mu_n) \) with simple eigenvalues \( \mu_1 > \mu_2 > \ldots > \mu_n > 0 \). This transforms (1.3) (after multiplication with \( \mu(x) = 1/\rho(x) \) and by denoting the transformed preconditioner again by \( T \)) in the form

\[
\mu(x)x' = \mu(x)x + \vartheta_{\text{opt}} T(Bx - \mu(x)x)
\]

with the optimal step length

\[
\vartheta_{\text{opt}} = \arg \max_{\vartheta \in \mathbb{R}} \mu(\mu(x)x + \vartheta T(Bx - \mu(x)x)).
\]

The quality constraint (1.5) on the preconditioner \( T \in \mathbb{R}^{n\times n} \) turns into a bound for the spectral norm \( \| \cdot \| \) of the symmetric matrix \( I - T \) which reads

\[
\| I - T \| \leq \gamma.
\]

Proof. The generalized eigenvalue problem (1.1) is first transformed into a standard eigenvalue problem \( C^{-1}B^{-T}y = \mu y \) using the Cholesky factorization \( A = CCT \), \( y = C^T x \) and \( \mu = 1/\lambda \). The symmetric matrix \( C^{-1}B^{-T} \) can be diagonalized by means of an orthogonal similarity transformation. Then all transformations are applied to (1.3). For convenience we denote the transformed system matrix by \( B \). Further the transformed preconditioner is denoted, once again, by \( T \), since (1.5) still holds with \( A = I \). All this results in (2.2) and (2.3).
To show that the proof of Thm. 1.2 can be restricted to the simple eigenvalue case we apply the same continuity argument which has been used in Theorem 2.1 in [8]. The argument is based on a perturbation $B_\epsilon$ of $B$ having only simple eigenvalues. Then the perturbation $\epsilon$ is reduced to 0. The continuous dependence of $x'$ and $\mu(x')$ on the perturbation completes the proof. This reasoning can be transferred to PSD since the Rayleigh-Ritz procedure preserves the continuity of the eigenvalue approximations.

Next the reformulation of Thm. 1.2 in terms of the $\mu$-notation is stated.

**Theorem 2.2.** If $\mu_{i+1} < \mu(x) \leq \mu_i$ then $\mu(x') \geq \mu(x)$ and either $\mu(x') \geq \mu_i$ or

$$
\frac{\mu_i - \mu(x')}{\mu(x') - \mu_{i+1}} \leq \frac{\mu_i - \mu(x)}{\mu(x) - \mu_{i+1}},
$$

with $\sigma = \frac{\kappa + \gamma(2-\kappa)}{(2-\kappa) + \gamma\kappa}$ and $\kappa = \frac{\mu_{i+1} - \mu_n}{\mu_i - \mu_n}$.

The estimate is sharp and can be attained for $\mu(x) \to \mu_i$ in the 3D invariant subspace associated with the eigenvalues $\mu_i$, $\mu_{i+1}$ and $\mu_n$, $i+1 \neq n$.

**2.1. The cone of PSD iterates.** The starting point of the geometric description of PSD is the *non-scaled* preconditioned gradient iteration (1.4) whose $\mu$-representation reads

$$
\mu(x)x' = \mu(x)x + T(Bx - \mu(x)x) = Bx - (I - T)(Bx - \mu(x)x).
$$

A central idea of its convergence analysis in [11, 12, 6] is to treat the preconditioners on the whole. This means that all admissible preconditioners satisfying the spectral equivalence (2.3) are inserted to (2.5) with $x$ being fixed. This results in a set $B_\gamma(x)$ of all possible iterates

$$
B_\gamma(x) := \{Bx - (I - T)(Bx - \mu(x)x); \ T \text{ s.p.d. with } \|I - T\| \leq \gamma\}.
$$

The set $B_\gamma(x)$ is a full ball with the center $Bx$ and the radius $\gamma\|Bx - \mu(x)x\|$. The subject of the convergence analysis of (2.5) in [11, 12] is to localize a vector of poorest convergence (i.e. with the smallest Rayleigh quotient) in $B_\gamma(x)$ and to derive an estimate for its Rayleigh quotient.

In contrast to (2.5) the PSD iteration (2.2) works with an optimal step length parameter $\vartheta_{opt}$ in order to maximize the Rayleigh quotient in the one-dimensional affine space

$$
\mu(x)x + \vartheta T(Bx - \mu(x)x), \quad \vartheta \in \mathbb{R}.
$$
The union of all these affine spaces for all the preconditioners satisfying (2.3) is the smallest circular cone with its vertex in \( \mu(x)x \) which encloses \( B_\gamma(x) \). This cone is denoted by \( \mathcal{F}_\gamma(x) \), see Fig. 2.1 and it holds that

\[
\mathcal{F}_\gamma(x) := \{ \mu(x)x + \vartheta(y - \mu(x)x); \ y \in B_\gamma(x); \ \vartheta \in \mathbb{R} \} \\
= \{ \mu(x)x + \vartheta d; \ \| Bx - (\mu(x)x + d) \| \leq \gamma \| Bx - \mu(x)x \|; \ \vartheta \in \mathbb{R} \}.
\]

2.2. The geometric convergence analysis as a two-level optimization. The geometric convergence analysis of preconditioned steepest descent consists of estimating the poorest convergence behavior. Therefore a two-level optimization problem is to be solved. On the one hand one has to determine this affine space (2.7) in the cone \( \mathcal{F}_\gamma(x) \) in which the maximum of the Rayleigh quotient (i.e. the largest Ritz value in this space) takes its smallest value; this vector is associated with the poorest convergence due to the choice of the preconditioner. On the other hand the cone \( \mathcal{F}_\gamma(x) \) depends on \( x \); hence one can analyze the dependence of this vector of poorest convergence on all vectors in the \( \mathbb{R}^n \) having the same Rayleigh quotient as \( x \). This amounts to considering the level set of the Rayleigh quotient of vectors having a fixed Rayleigh quotient \( \mu_0 \), i.e.

\[
\mathcal{L}(\mu_0) := \{ x \in \mathbb{R}^n; \ \mu(x) = \mu_0 \}.
\]

Let \( x^* \in \mathcal{L}(\mu_0) \) be the minimizer representing the poorest convergence and let \( d^* \in \mathcal{F}_\gamma(x) - \mu(x)x \) be the search direction of poorest convergence. So the two-level optimization is

\[
\mu := \min_{x \in \mathcal{L}(\mu_0)} \min_{d \in \mathcal{F}_\gamma(x) - \mu_0x} \mu(\mu_0x + \vartheta_{\text{opt}}[x,d]d).
\]

Therein \( \mu(x)x + \vartheta_{\text{opt}}[x,d]d \) is the Ritz vector which is associated with the larger Ritz value \( \mu(x + \vartheta_{\text{opt}}[x,d]d) \) in \( \text{span}\{x,d\} \). The factor \( \vartheta_{\text{opt}} = \vartheta_{\text{opt}}[x,d] \) depends on \( x \) and \( d \). The minimum \( \mu \) is now to be estimated from below.

3. The level set optimization - a reduction to 3D. The aim of this section is to show that the poorest convergence of PSD with respect to the admissible preconditioners and with respect to all vectors \( x \in \mathcal{L}(\mu_0) \) is attained in a three-dimensional \( B \)-invariant subspace of the \( \mathbb{R}^n \).

The representation (2.7) of the PSD iteration applies the line search to \( d \in \mathcal{F}_\gamma(x) - \mu(x)x \). This may result in an unbounded step length. To see this let \( d = e_1 = (1,0,\ldots,0)^T \) which is an eigenvector of \( B \). If \( \gamma \) is close to 1, then \( e_1 \in \mathcal{F}_\gamma(x) - \mu(x)x \) can be attained since \( \lim_{\gamma \to 1} \mathcal{F}_\gamma(x) = \mathbb{R}^n \). The unboundedness is a consequence of \( \lim_{\vartheta \to \pm \infty} \mu(\mu(x)x + \vartheta e_1) = \mu_1 \). The potential unboundedness of the step length has already been pointed out by Knystazev [10].

Next we want to avoid this singularity. Therefore let \( x' = \vartheta x + d \). Due to \( \mu(x') > \mu(x) \) (which is guaranteed by Thm. [10]) \( \vartheta \) is bounded. So the minimization problem is reformulated as

\[
\mu := \min_{x \in \mathcal{L}(\mu_0)} \min_{d \in \mathcal{F}_\gamma(x) - \mu_0x} \mu(\vartheta_{\text{opt}}[x,d]x + d).
\]

In the next theorem a necessary condition characterizing this minimum is derived by means of the Kuhn-Tucker conditions [17]. The application of the Kuhn-Tucker conditions in the context of the convergence analysis of the fixed-step size preconditioned gradient iteration has been suggested by R. Argentati, see [1].

**Theorem 3.1.** The minimum (3.1) is attained in a three-dimensional \( B \)-invariant subspace of the \( \mathbb{R}^n \).
If PSD does not terminate in an eigenvector, then the associated Ritz vector $w$ of poorest convergence is also contained in the same three-dimensional $B$-invariant subspace of the $\mathbb{R}^n$, i.e.
\[(B + a)w = c(B + b)x\]
with $a, b, c \in \mathbb{R}$ and $B + a$ being a regular matrix.

**Proof.** The minimization problem (3.1) reads as follows:

Minimize
\[\mu(\vartheta_{\text{opt}}x + d)\]
with respect to $x, d \in \mathbb{R}^n$ satisfying the two constraints:

1. The cone inequality constraint $d \in \mathcal{F}_c(x) - \mu_0x$
\[g(x, d) = \|Bx - (\mu_0x + d)\|^2 - \gamma^2\|Bx - \mu_0x\|^2\]
\[= (1 - \gamma^2)\|Bx - \mu_0x\|^2 - 2(Bx - \mu_0x, d) + \|d\|^2 \leq 0.

2. The level set constraint $x \in \mathcal{L}(\mu_0)$
\[h(x, d) = (x, Bx) - \mu_0(x, x) = 0.

Therein $\vartheta_{\text{opt}} = \vartheta_{\text{opt}}[x, d] \in \mathbb{R}$ is a functional depending on $x$ and $d$ which maximizes the Rayleigh quotient in the two-dimensional subspace $\text{span}\{x, d\}$. Equivalently $w := \vartheta_{\text{opt}}x + d$ is a Ritz vector corresponding to the larger Ritz value in just this two-dimensional subspace. The first constraint guarantees that $d$ is an admissible search direction, i.e. the distance of $\mu_0x + d$ to the center $Bx$ of the ball $B_c(x)$ is bounded by its radius $\gamma\|Bx - \mu_0x\|$.

The Karush-Kuhn-Tucker stationarity condition for a local minimizer $(x^*, d^*)$ reads
\[\nabla_{(x,d)} \mu(\vartheta_{\text{opt}}x^* + d^*) + \alpha \nabla_{(x,d)} g(x^*, d^*) + \beta \nabla_{(x,d)} h(x^*, d^*) = 0\]
with the multipliers $\alpha$ and $\beta$. In order to simplify the notation, the asterisks are omitted from now on.

Next we derive the gradients of these functions $\mu$, $g$ and $h$ with respect to $x$ and $d$.
The chain rule gives (for column vectors)
\[\nabla_x \left( \mu(\vartheta_{\text{opt}}x + d) \right) = (D_x(\vartheta_{\text{opt}}x + d))^T (\nabla \mu)(\vartheta_{\text{opt}}x + d).
\]
It holds that
\[\left((D_x(\vartheta_{\text{opt}}x + d))_{ij}\right) = (x(\nabla_x \vartheta_{\text{opt}})^T + \vartheta_{\text{opt}} I)_{ij}.
\]
With $w := \vartheta_{\text{opt}}x + d$ we get
\[\nabla_x (\mu(\vartheta_{\text{opt}}x + d)) = \vartheta_{\text{opt}}(\nabla \mu)(w) + (\nabla_x \vartheta_{\text{opt}})(x, (\nabla \mu)(w))\]
\[= \vartheta_{\text{opt}}(\nabla \mu)(w) = \vartheta_{\text{opt}} \frac{2}{(w, w)}(Bw - \mu(w)w).
\]
Therein, $(x, (\nabla \mu)(w)) = 0$ has been used which holds since $(\nabla \mu)(w)$ is collinear to the residual of the Ritz vector and further, by definition of a Ritz vector, its residual is orthogonal to the approximating subspace $\text{span}\{x, d\}$. For the $d$-gradient it holds that
\[\nabla_d (\mu(\vartheta_{\text{opt}}x + d)) = (\nabla \mu)(w) = \frac{2}{(w, w)}(Bw - \mu(w)w).
\]
The gradients of the constraining functions $g$ and $h$ with $r = Bx - \mu_0x$ are
\[\nabla_x g(x, d) = (1 - \gamma^2)2(B - \mu_0)r - 2(B - \mu_0)d, \quad \nabla_x h(x, d) = 2r, \quad \nabla_d g(x, d) = -2(B - \mu_0)x + 2d = 2(d - r), \quad \nabla_d h(x, d) = 0.
\]
Hence the $x$-components of the Karush-Kuhn-Tucker stationarity condition are

\begin{equation}
(3.2) \quad \frac{\partial_{opt}}{w,w} (B - \mu(w))w + \alpha \left\{ (1 - \gamma^2)(B - \mu_0)^2 x - (B - \mu_0)(w - \partial_{opt}x) \right\} + \beta r = 0
\end{equation}

and the $d$-components read \((Bw - \mu(w))w + \alpha(w, w)(d - r) = 0\). The equation for the $d$-components can be reformulated as

\begin{equation}
(3.3) \quad (B + a)w = \alpha(w, w)(B + b)x
\end{equation}

with \(a = \alpha(w, w) - \mu(w)\) and \(b = \partial_{opt} - \mu_0\). Multiplication of (3.2) with \(B + a\) and insertion of (3.3) results in

\[
\alpha \left\{ (1 - \gamma^2)(B - \mu_0)^2(B + a)x - (B - \mu_0)\left[ \alpha(w, w)(B + b)x - \partial_{opt}(B + a)x \right] \right\} \\
+ \alpha \partial_{opt}(B - \mu(w))(B + b)x + \beta(B + a)(B - \mu_0)x = 0.
\]

This can be expressed as

\begin{equation}
(3.4) \quad p_3(B)x = 0
\end{equation}

with a third order polynomial \(p_3\). Due to the basis assumptions \(B\) is a diagonal matrix and so \(p_3(B)\) is diagonal. As \(p_3\) has at most three different zeros, (3.4) can only hold if \(x\) has at most three non-zero components, which proves the first assertion.

Hence \(x \in \text{span}\{e_j, e_k, e_l\}\) for proper indexes \(j, k\) and \(l\). For that \(x\) Eq. (3.3) shows that \(w\) has not more than four non-zero components; four non-zero components are only possible if \(a = -\mu_s\) for \(s \neq j, k, l\). Then (3.2) can be written as \(p_1(B)w = p_2(B)x \in \text{span}\{e_j, e_k, e_l\}\) with a first order polynomial \(p_1\) and a second order polynomial \(p_2\). The latter equation implies that \(p_1(\mu_s) = p_1(-a) = 0\). The \(s\)-th component of the polynomial identity results in \(a = (\alpha \mu_0(w, w) - \mu(w)\partial_{opt})/(\partial_{opt} - \alpha(w, w))\). Together with the known form \(a = \alpha(w, w) - \mu(w)\) we get by direct computation that \(a = b\). Insertion of this result to (3.3) shows that \(w = \alpha(w, w)x + Ce_x\) for a real constant \(C\). Then \(x \perp e_x\) and \(x\) and \(e_x\) are the Ritz vectors. PSD terminates in \(e_x\) and \(w\) with not more than three non-zero components is the normal case.

4. The cone optimization - a mini-dimensional geometric analysis. Next the convergence behavior with respect to the cone \(F_\gamma(x)\) is analyzed. Some of the following arguments are valid in the \(\mathbb{R}^n\); however we need these properties only for \(n = 3\).

The (half) opening angle \(\varphi\) of the cone \(F_\gamma(x)\) is given by \(\sin \varphi = \gamma\), since \(\gamma\) is the ratio of the radius \(\gamma\|Bx - \mu(x)x\|\) of the ball \(B_\gamma(x)\), see (2.6), and its (maximal) radius \(\|Bx - \mu(x)x\|\) for \(\gamma \rightarrow 1\). With \(\cos \varphi = \sqrt{1 - \gamma^2}\) the cone \(F_\gamma(x)\) can be written as

\[
F_\gamma(x) := \mu(x)x + \{z \in \mathbb{R}^n; \quad \left( \frac{z}{\|z\|} \frac{Bx - \mu(x)x}{\|Bx - \mu(x)x\|} \right) \geq \sqrt{1 - \gamma^2} \}.
\]

4.1. Restriction to non-negative vectors. The analysis of PSD can be restricted to component-wise non-negative vectors \(x \in \mathbb{R}^n\). The justification is as follows. Consider the Householder reflections \(H_i = I - 2e_i e_i^T\) for which \(x \mapsto H_i x\) changes the sign of the \(i\)-th component of \(x\). The Rayleigh quotient is invariant under \(H_i\), i.e. \(\mu(x) = \mu(H_i x)\). If \(v\) is an admissible search direction, i.e. \(v \in F_\gamma(x) - \mu(x)x\), then

\[
\cos \angle(v, Bx - \mu(x)x) = \left( \frac{v}{\|v\|} \frac{Bx - \mu(x)x}{\|Bx - \mu(x)x\|} \right) = \left( \frac{H_i v}{\|H_i v\|} \frac{B H_i x - \mu(H_i x) H_i x}{\|B H_i x - \mu(H_i x) H_i x\|} \right) = \cos \angle(H_i v, B H_i x - \mu(H_i x) H_i x),
\]

search directions, see Fig. 2.2. Next we work with the disc $S$ with $x\rangle $. Thus the analysis can be restricted to any Rayleigh quotient in the cone $F$ which means that $H_i v$ encloses the same angle with the residual vector associated with $H_i x$. As for all $\alpha \in \mathbb{R}$

$$
\mu (\mu (H_i x) H_i x + \alpha H_i v) = \mu (H_i (\mu (x) x + \alpha v)) = \mu (\mu (x) x + \alpha v)
$$

any Rayleigh quotient in the cone $F_\gamma (x)$ can be reproduced in the cone $F_\gamma (H_i x)$ and vice versa. Thus the analysis can be restricted to $x \geq 0$.

4.2. The poorest convergence in the three-dimensional cone $F_\gamma (x)$. Any circular cross section $S_\gamma ^c$ (with non-zero radius) of $F_\gamma (x)$ can serve to represent the admissible search directions, see Fig. 2.2. Next we work with the disc

$$
S_\gamma ^c (x) := \mu (x) x + (1 - \gamma ^2) r + \{ f y; y \in \mathbb{R}^3, \| y \| \leq 1, y \perp r \}
$$

with $r := B x - \mu (x) x$. Its radius $f$, see Fig. 4.1 is given by

$$
f = \gamma \sqrt{1 - \gamma ^2 \| r \|}.
$$

Further we use only search directions $d \in S_\gamma ^c (x) - \mu (x) x$ which are orthogonalized against $x$; this is justified since the Rayleigh-Ritz approximations (and so the PSD iterate $x'$) only depend on the subspace. So the set of relevant search directions forms a line segment. By using the vector $v = x \times r / \| x \times r \| = x \times r / (\| x \| \| r \|)$ one can construct the intersection of this line segment with the surface of the cone. The points of intersection are $d_{1/2}$ with

$$
\begin{align*}
(1 - \gamma ^2) r + \gamma \sqrt{1 - \gamma ^2 \| r \|} v, \\
\end{align*}

\begin{align*}
(1 - \gamma ^2) r - \gamma \sqrt{1 - \gamma ^2 \| r \|} v,
\end{align*}
$$

Therefore the line segment has the form (see Fig. 4.2)

$$
S_\gamma (x) := \{ d(t) := td_1 + (1 - t)d_2; t \in [0, 1] \}.
$$

Lemma 4.1. The poorest convergence of PSD in 3D (aside from the singular cases that PSD terminates in an eigenvector) is attained in $d_1$ or $d_2$ as given by (4.3) and (4.4).

Proof. The line segment $S_\gamma$ has the form $d(t)$ with $t \in [0, 1]$ by (4.5). The PSD iteration maps $S_\gamma$ into a curve $w(t)$, $t \in [0, 1]$, where $w(t)$ is the Ritz vector $w(t) = \mu (x) x + \partial_{\text{opt}}(t) d(t)$ corresponding to the larger Ritz value in span$\{ x, d(t) \}$. (A singularity like that mentioned at the beginning of Sec. 3 has not to be considered since otherwise
the first alternative $\mu(x') \geq \mu_i$ in Thm. \ref{thm:Ritz-eigenvalues} applies and nothing is to be proved.) Along $w(t)$ we are looking for a vector $w^* = w(t^*)$ so that
\[
\mu(w(t^*)) \leq \mu(w(t)) \quad \forall t \in [0,1].
\]
Since $w(t)$ is a Ritz vector its residual $Bw(t) - \mu(w(t))w(t)$ is orthogonal to the subspace spanned by $x$ and $d(t)$. As the residual is collinear to the gradient vector $\nabla \mu(w(t))$ we get
\[
(\nabla \mu(w(t))), \text{span}\{x, d(t)\} = 0.
\]
A stationary point of the Rayleigh quotient in a $t \in (0,1)$ is attained if
\[
0 = \frac{d}{dt} \mu(w(t)) = (\nabla \mu(w(t)), w'(t)) = (\nabla \mu(w(t)), \vartheta^{\text{opt}}_t d(t) + \vartheta_\text{opt}(t)d'(t)) = (\nabla \mu(w(t)), \vartheta_\text{opt}(t)d'(t))
\]
where (1.0) has been used for the last identity. As $d'(t)$ is collinear to $x \times r$ we get from \[
(\nabla \mu(w(t)), d'(t)) = 0
\]
together with (1.0) that $\nabla \mu(w) = 0$ (since $x$, $d$, and $d'$ span the $\mathbb{R}^3$).
So any interior stationary point must be an eigenvector and hence $\mu(w(t))$ take the other extrema on the surface for $t = 0$ or $t = 1$ in $d_1$ or $d_2$.

Next we apply the Rayleigh-Ritz procedure to the two-dimensional subspaces $[x, d_i - \mu(x)x], i = 1, 2$, in order to determine whether the poorest convergence is attained in $d_1$ or $d_2$. First the Euclidean norm of $d_i - \mu(x)x$ is determined
\[
\|d_i - \mu(x)x\|^2 = (1 - \gamma^2)^2(r, r) + (1 - \gamma^2)\gamma\sqrt{1 - \gamma^2(r, x \times r)}/\|x\| + \gamma^2(1 - \gamma^2)\|x \times r\|^2/\|x\|^2
\]
\[
= (1 - \gamma^2)^2\|r\|^2 + \gamma^2(1 - \gamma^2)\|r\|^2 = (1 - \gamma^2)\|r\|^2.
\]
Hence the normalized search directions $(d_i - \mu(x)x)/\|d_i - \mu(x)x\|$ are
\[
\tilde{d}_{1/2} := \frac{d_{1/2} - \mu(x)x}{\sqrt{1 - \gamma^2}\|x\|} = \sqrt{1 - \gamma^2} \frac{r}{\|r\|} \pm \gamma \frac{x \times r}{\|x\| \|r\|}
\]
and therefore $V_1 = [x, \tilde{d}_1]$ and $V_2 = [x, \tilde{d}_2] \in \mathbb{R}^{3 \times 2}$ are orthonormal matrices. The Ritz values of $B$ in the column space of $V_i$ are the eigenvalues of the projection
\[
B_i := V_i^T BV_i = \begin{pmatrix} \mu(x) & \langle d_i, Bx \rangle \\ \langle d_i, Bx \rangle & \mu(\tilde{d}_i) \end{pmatrix}.
\]
The larger Ritz value (that is the larger eigenvalue of $B_i$) reads
\[
\theta_{2,i} = \frac{\mu(x) + \mu(\tilde{d}_i)}{2} + \sqrt{\frac{(\mu(x) - \mu(\tilde{d}_i))^2}{4} + \langle \tilde{d}_i, Bx \rangle^2}.
\]
In order to decide whether in $d_1$ or in $d_2$ poorest convergence is taken, we show that the non-diagonal elements of $B_i$ do not depend on $i$ since
\[
\langle \tilde{d}_i, Bx \rangle = \langle \tilde{d}_i, Bx - \mu(x)x \rangle = \|r\| \langle \tilde{d}_i, \frac{r}{\|r\|} \rangle = \|r\| \cos \angle(\tilde{d}_i, r) = \sqrt{1 - \gamma^2}\|r\|.
\]
Hence only the $(2,2)$ element of $B_i$ depends on $i$. As further
\[
\frac{d\theta_{2,i}}{d\mu(\tilde{d}_i)} = \frac{1}{2} \left( 1 - \frac{1}{1 + \left( \frac{2\langle \tilde{d}_i, Bx \rangle}{\mu(x) - \mu(\tilde{d}_i)} \right)^{1/2}} \right) > 0
\]
Preconditioned steepest descent

shows that $\theta_{2,i}$ is a monotone increasing function of $\mu(\vec{d}_i)$ we still have to find the $\vec{d}_i$ with the smaller Rayleigh quotient in order to find the search direction which is associated with the poorer PSD convergence.

**Lemma 4.2.** PSD in 3D takes its poorest convergence, i.e. the smallest value of $\theta_{2,i}$, in

$$d = \mu(x)x + (1 - \gamma^2)r + \gamma \sqrt{1 - \gamma^2} x \times r,$$

if $x \in \mathbb{R}^n$ is a component-wise non-negative vector (cf. Sec. 4.1). The associated Ritz value is accessible from (4.7).

**Proof.** We show that $\theta_{2,1}$ is the smaller Ritz value by showing (we use the monotonicity of $\theta_{2,i}[\mu(\vec{d}_i)]$) that $\mu(\vec{d}_1) \leq \mu(\vec{d}_2)$. This inequality is true if $(r, B(x \times r)) \leq 0$. By using $\text{span}\{x, r\} \perp x \times r$ and $r \perp x$ direct computation results in

$$(r, B(x \times r)) = (B(Bx - \mu(x)x), x \times r) = (B^2x, x \times r) - \mu(x)(Bx, x \times r)$$

$$= (B^2x, x \times r) - \mu(x)(r + \mu(x)x, x \times r)$$

$$= (B^2x, x \times r) = (r, B^2x \times x) = (Bx, B^2x \times x)$$

$$= -x_1x_2x_3(\mu_1 - \mu_2)(\mu_1 - \mu_3)(\mu_2 - \mu_3) \leq 0.$$

The last inequality holds since $x \geq 0$ and $\mu_1 > \mu_2 > \mu_3$. $\Box$

**4.3. A mini-dimensional convergence analysis of PSD.** Due to Thm. 4.1 the “mini-dimensional” convergence analysis can be restricted to three-dimensional $B$-invariant subspaces of the $\mathbb{R}^n$. With respect to the basis of eigenvectors these subspaces have the form $\text{span}\{e_j, e_k, e_l\}$ where $e_*$ is the $*$-th unit vector. The associated eigenvalues are indexed so that $\mu_j > \mu_k > \mu_l$.

Lemma 4.2 delivers for any $x \in \mathcal{L}(\mu)$ in 3D the vector of $B, \langle x \rangle$-poorest PSD convergence. Next we have to analyze the $\mathcal{L}(\mu)$-dependence of the poorest convergence case.

**Theorem 4.3.** In the three-dimensional space $\text{span}\{e_j, e_k, e_l\}$ the following sharp estimate for PSD holds

$$\frac{\Delta_j,k(\mu')}{\Delta_j,k(\mu)} \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{2 - \kappa + \gamma \kappa}\right)^2$$

with

$$\Delta_j,k(\xi) = \frac{\mu_j - \xi}{\xi - \mu_k} \text{ and } \kappa = \frac{\mu_k - \mu_l}{\mu_j - \mu_l}.$$
Proof. The starting point of the following analysis are the vectors $x$ and

$$d = \mu(x)x + (1 - \gamma^2)r + \gamma \sqrt{1 - \gamma^2} \frac{x \times r}{\|x\|}.$$  

Without loss of generality $x$ can be normalized in a way that

$$x = e_j + \alpha_0 e_k + \beta_0 e_l;$$

hence $x$ is an element of the affine space $E_j := e_j + \text{span}\{e_k, e_l\}$. The coordinate form of $x$ in 3D then is $x = (1, \alpha_0, \beta_0)^T$. Further let $\tilde{d} = (1, \tilde{\alpha}, \tilde{\beta})^T \in E_j$ the corresponding multiple of $d$. Since $\text{span}\{x, d\}$ is a tangential plane of the ball $B_r(x)$ in $d$ and $Bx - d$ is a radius vector of the ball it holds that

$$(4.10) \quad Bx - d \perp \text{span}\{x, d\} = \text{span}\{x, \tilde{d}\}.$$  

Hence $Bx - d$ is collinear to

$$x \times \tilde{d} = (\alpha_0 \tilde{\beta} - \tilde{\alpha} \beta_0, \beta_0 - \tilde{\beta}, \tilde{\alpha} - \alpha_0)^T.$$  

By $S_1 = (1, c_k, 0)^T$ and $S_2 = (1, 0, c_l)^T$ with $S_1, S_2 \in E_j$ we denote the points of intersection of $\text{span}\{x, d\}$ with $e_j + \text{span}\{e_k\}$ and $e_j + \text{span}\{e_l\}$, see Fig. 4.3. Due to (4.10) it holds that $(Bx - d, S_i) = 0, i = 1, 2$. Since

$$Bx - d = \gamma^2 r - \gamma \sqrt{1 - \gamma^2} \frac{x \times r}{\|x\|}$$

we get with

$$r = \begin{pmatrix} \mu_j - \mu \\ (\mu_k - \mu) \alpha_0 \\ (\mu - \mu) \beta_0 \end{pmatrix}, \quad x \times r = \begin{pmatrix} \alpha_0 \beta_0 (\mu_j - \mu_k) \\ \beta_0 (\mu_j - \mu_l) \\ \alpha_0 (\mu_k - \mu_l) \end{pmatrix}$$

from $(Bx - d, S_1) = 0$ that

$$(4.11) \quad c_k = \frac{(Bx - d)_{|1}}{(Bx - d)_{|2}} = \frac{\|x\|(\mu_j - \mu) + \Gamma \alpha_0 \beta_0 (\mu_k - \mu_l)}{\|x\| \alpha_0 (\mu - \mu_k) + \Gamma \beta_0 (\mu_j - \mu_l)}.$$  

Analogously $(Bx - d, S_2) = 0$ results in

$$(4.12) \quad c_l = \frac{(Bx - d)_{|1}}{(Bx - d)_{|3}} = \frac{\|x\|(\mu_j - \mu) + \Gamma \alpha_0 \beta_0 (\mu_k - \mu_l)}{\|x\| \beta_0 (\mu - \mu_l) + \Gamma \alpha_0 (\mu_k - \mu_j)}.$$  

with $\Gamma = \sqrt{1 - \gamma^2}/\gamma$.

Any $x \in E_j \cap L(\mu)$ is an element of the ellipse $(x_k/a)^2 + (x_l/b)^2 = 1$ with

$$a = \sqrt{\frac{\mu_j - \mu}{\mu - \mu_k}}, \quad b = \sqrt{\frac{\mu_j - \mu}{\mu - \mu_l}}.$$  

As justified in Sec. 4.1 the analysis can be restricted to componentwise non-negative $x = (1, \alpha_0, \beta_0)^T$ so that its components $\alpha_0$ and $\beta_0$ can be represented in terms of $\psi \in (0, \pi/2)$ and $t = \tan \psi$

$$(4.13) \quad \alpha_0 = a \cos(\psi) = a \sqrt{\frac{1}{1 + t^2}}, \quad \beta_0 = b \sin(\psi) = b \sqrt{\frac{t^2}{1 + t^2}}.$$
Two further ellipses in $E_j$ are relevant for the subsequent analysis. These ellipses are very similar, each centered in $c_j$ (the origin of $E_j$) and each tangential to the line through $S_1$ and $S_2$. The first ellipse is $E_j \cap L(\mu')$ with $\mu' = \mu(x')$ and has the semi-axes

$$a' = \sqrt{\frac{\mu_j - \mu'}{\mu' - \mu_k}}, \quad b' = \sqrt{\frac{\mu_j - \mu'}{\mu' - \mu_i}}.$$ 

This ellipse is tangential to the line through $S_1$ and $S_2$ since $\mu(x')$ is associated with the poorest convergence on the cone $F_\gamma(x)$ projected to $E_j$. Direct computation shows that $a'/b' < a/b$.

The second ellipse $E$, see Fig. [4.13] has the semi-axes $\tilde{a}$ and $\tilde{b}$ so that the ratio of its semi-axes equals that of $E_j \cap L(\mu)$. This means that $\tilde{a}/\tilde{b} = a/b$. It holds that $\tilde{a} \geq a'$, since otherwise a contradiction can be derived. Assuming $\tilde{a} < a'$ for any point $(\alpha, \beta)$ on the ellipse $E$ it holds that (by using $a'/b' < a/b$)

$$\alpha^2 + \frac{a'^2}{b'^2} \beta^2 < \alpha^2 + \frac{a^2}{b^2} \beta^2 = \alpha^2 + \frac{\tilde{a}^2}{\tilde{b}^2} \beta^2 = \tilde{a}^2 < a'^2$$

so that $a^2/a'^2 + \beta^2/b'^2 < 1$. The latter inequality means that the ellipse $E$ is completely surrounded by the ellipse $L(\mu') \cap E_j$, which contradicts its tangentiality to the line through $S_1$ and $S_2$. Hence

$$\Delta(\mu') = \frac{\mu_j - \mu'}{\mu' - \mu_k} = a'^2 \leq \tilde{a}^2$$

and an upper limit for $\tilde{a}^2/\Delta(\mu) = \tilde{a}^2/a^2$ remains to be determined. Next we show that (the case $c_1 \to \infty$ is to be treated separately by analyzing the limits of $c_k$ and $c_l$)

$$\frac{\tilde{a}^2}{a^2} = \frac{c_k^2 c_l^2}{b^2 c_k^2 + a^2 c_l^2}.$$ 

To prove this we determine the point of contact of the line through $S_1$ and $S_2$ and the ellipse $E$. The semi-axes of $E$ are $\tilde{a}$ and $\tilde{b} = b\tilde{a}/a$. By a rescaling of the second semi-axis with the factor $a/b$ the ellipse becomes a circle with the radius $\tilde{a}$ and the point of contact does not change. Further the line segment connecting $S_1$ and $S_2$ is transformed

$$s(\sigma) = \left( \begin{array}{c} 0 \\ \frac{\sigma}{c_l} \end{array} \right) + \sigma \left( \begin{array}{c} c_k \\ -\frac{a}{b} c_l \end{array} \right), \quad \sigma \in [0, 1].$$

The point of contact is that point on $s(\sigma)$ with the smallest Euclidean norm. From

$$\|s(\sigma)\|^2 = \sigma^2 c_k^2 + \left( \frac{a}{b} c_l \right)^2 (\sigma - 1)^2$$

direct computation shows that the minimum is attained in $\sigma^* = a^2 c_l^2/(b^2 c_k^2 + a^2 c_l^2)$. The resulting identity $\tilde{a}^2 = \|s(\sigma^*)\|^2$ yields (4.14).

Insertion of (4.11), (4.12) and (4.13) in (4.14) and using the variables $\Gamma := \sqrt{1 - \gamma^2}/\gamma \in (0, \infty]$, $\Delta = a^2$, $b^2 = \Delta(1 - \kappa)/(1 + \kappa \Delta)$ with

$$\kappa = \frac{\mu_k - \mu_l}{\mu_j - \mu_l}$$

results in a representation of $\tilde{a}^2/a^2$ as a function of $t$, $\Delta$, $\Gamma$ and $\kappa$. (The limit $\Gamma \to \infty$ needs additional care; however this limit corresponds to $\gamma = 0$. For $\gamma = 0$ Thm. [2.2] is
already proved in [10].) The details are as follows. With

\[ A = \sqrt{1 + \alpha_0^2 + \beta_0^2 (\mu_j - \mu) + \Gamma \alpha_0 \beta_0 (\mu_k - \mu_l)}, \]
\[ B = \sqrt{1 + \alpha_0^2 + \beta_0^2 \alpha_0 (\mu - \mu_k) + \Gamma \beta_0 (\mu_j - \mu_l)}, \]
\[ C = \sqrt{1 + \alpha_0^2 + \beta_0^2 \beta_0 (\mu - \mu_l) + \Gamma \alpha_0 (\mu_k - \mu_j)} \]

it holds that \( c_k = A/B \) and \( c_l = A/C \). Instead of considering \( \hat{a}^2/a^2 \) it is more convenient to estimate its reciprocal from below. From [11,13] one gets

\[ \frac{a^2}{\hat{a}^2} = \frac{\Delta(1 - \kappa)}{1 + \kappa \Delta} \left( \frac{C}{A} \right)^2 + \Delta \left( \frac{B}{A} \right)^2 \]

with

\[ C = \frac{\sqrt{1 + \alpha_0^2 + \beta_0^2 \beta_0 + \Gamma \alpha_0 \frac{\mu_k - \mu_l}{\mu_k - \mu_l}}}{\sqrt{1 + \alpha_0^2 + \beta_0^2 \beta_0 + \Gamma \alpha_0 \frac{\mu_k - \mu_l}{\mu_k - \mu_l}}}, \quad B = \frac{\sqrt{1 + \alpha_0^2 + \beta_0^2 \alpha_0 + \Gamma \beta_0 \frac{\mu_j - \mu_l}{\mu_j - \mu_l}}}{\sqrt{1 + \alpha_0^2 + \beta_0^2 \alpha_0 + \Gamma \beta_0 \frac{\mu_j - \mu_l}{\mu_j - \mu_l}}} \]

In these formula the ratios of eigenvalue differences are to be expressed in terms of \( \Delta \) and \( \kappa \). Therefore let \( U := \mu_j - \mu, V := \mu - \mu_k \) and \( W := \mu_l - \mu_l \) so that \( \mu_k - \mu_l = W - V \), \( \mu_j - \mu_l = U + W \) and \( \mu_k - \mu_j = -U - V \). Since \( \Delta = U/V \) and \( \Delta(1 - \kappa)/(1 + \kappa \Delta) = U/W \) we get that

\[ \frac{\mu_k - \mu_j}{\mu - \mu_l} = \frac{U}{W}(1 + \frac{V}{U}) = \frac{(\kappa - 1)(1 + \Delta)}{1 + \kappa \Delta}, \]
\[ \frac{\mu_k - \mu_j}{\mu - \mu_l} = 1 - \frac{V}{U} \frac{U}{W} = \frac{\kappa(1 + \Delta)}{1 + \kappa \Delta}, \]
\[ \frac{\mu_j - \mu_l}{\mu - \mu_k} = \frac{U + W}{V} = \frac{U}{V}(1 + \frac{W}{U}) = \frac{1 + \Delta}{1 - \kappa}, \]
\[ \frac{\mu_k - \mu_j}{\mu - \mu_k} = \frac{W - V}{V} = \frac{W}{U}(1 - \frac{V}{U}) = \frac{\kappa(1 + \Delta)}{1 - \kappa}. \]

Therefore we have

\[ \frac{a^2}{\hat{a}^2} = \frac{\Delta(1 - \kappa)}{1 + \kappa \Delta} \left( \frac{\sqrt{1 + \alpha_0^2 + \beta_0^2 \beta_0 + \Gamma \alpha_0 \frac{(\kappa - 1)(1 + \Delta)}{1 + \kappa \Delta}}}{\sqrt{1 + \alpha_0^2 + \beta_0^2 \Delta(1 - \kappa) + \Gamma \alpha_0 \beta_0 \frac{\kappa(1 + \Delta)}{1 + \kappa \Delta}}} \right)^2 + \Delta \left( \frac{\sqrt{1 + \alpha_0^2 + \beta_0^2 \alpha_0 + \Gamma \beta_0 \frac{\kappa(1 + \Delta)}{1 + \kappa \Delta}}}{\sqrt{1 + \alpha_0^2 + \beta_0^2 \Delta + \Gamma \alpha_0 \beta_0 \frac{\kappa(1 + \Delta)}{1 + \kappa \Delta}}} \right)^2. \]

Insertion of (1.13) yields \( f := f(\Delta, t, \kappa, \Gamma) \) with

\[ f = \frac{a^2}{\hat{a}^2} = (1 + \Delta)(\Gamma^2(1 - \kappa)^2 + \kappa(1 - \kappa)^2 + \Gamma^2 t^2) + (1 - \kappa)^2 + t^2(1 - \kappa) + 2\kappa \Gamma t \sqrt{1/(1 + t^2)} \sqrt{1 + t^2 + \kappa \Delta \sqrt{1 - \kappa} \sqrt{1 + \Delta}} / \left( \sqrt{1 - \kappa} \sqrt{1 + t^2 + \kappa \Delta} + \kappa \Gamma t \sqrt{1/(1 + t^2)} \sqrt{1 + \Delta} \right)^2. \]

This function is monotone increasing in \( \Delta \) since \( \partial f / \partial \Delta \) equals

\[ \frac{\Gamma^2 \sqrt{1 - \kappa} (1 - \kappa)^3 + 3(1 - \kappa)^2 t^2 + 3(1 - \kappa)^3 t^2 + t^6}{(1 + t^2) \sqrt{1 + t^2 + \kappa \Delta} (\sqrt{1 - \kappa} \sqrt{1 + t^2 + \kappa \Delta} + \kappa \Gamma t \sqrt{1/(1 + t^2)} \sqrt{1 + \Delta})^3} > 0. \]
Therefore $f(0, t, \kappa, \Gamma)$ is a lower bound for $\bar{a}^2/\hat{a}^2$ which reads

$$f(0, t, \kappa, \Gamma) = \frac{(1 + t^2)(1 - \kappa)^2 + (1 + t^2)(1 - \kappa) + \Gamma^2t^2 + 2\kappa\Gamma\sqrt{1 - \kappa}}{(\sqrt{1 - \kappa} + t\Gamma)^2}.$$ 

The parameter $t$ determines the choice of $x$ in the level set $\mathcal{L}(\mu)$. The derivative with respect to $t$ reads

$$\frac{\partial}{\partial t}f(0, t, \kappa, \Gamma) = \frac{2\kappa(1 - \kappa + t^2)(1 - \kappa) + \Gamma^2t^2 - \Gamma(1 - \kappa)}{(\sqrt{1 - \kappa} + t\Gamma)^3}.$$ 

The two real zeros of this derivative are

$$t_{1, 2} = \frac{\sqrt{1 - \kappa(-1 + \sqrt{1 + \Gamma^2})}}{\Gamma}.$$ 

The global minimum is taken in

$$0 < t_1 = \frac{\sqrt{1 - \kappa(-1 + \sqrt{1 + \Gamma^2})}}{\Gamma} = \frac{\sqrt{1 - \kappa(1 - \gamma)}}{\sqrt{1 - \gamma^2}}.$$ 

Therefore the minimum is given by

$$f(0, t_1, \kappa, \Gamma) = \left( \frac{2 - \kappa + \gamma\kappa}{\kappa + \gamma(2 - \kappa)} \right)^2$$ 

and its inverse yields the desired convergence estimate

$$\frac{\Delta(\mu')}{\Delta(\mu)} \leq \left( \frac{\alpha}{\alpha} \right)^2 \leq \left( \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2.$$ 

This estimate is sharp since for $\Delta = 0$ the right inequality turns into an identity. Further $\Delta = 0$ implies $\mu(x) \to \mu_j$ and also $\mu(x') \to \mu_j$ so that $\lim_{\mu(x) \to \mu_j} \hat{a}/\hat{b} - a'/b' = 0$ and in this limit $\mathcal{L}(\mu') \cap \mathcal{E}_j$ and $\mathcal{E}$ coincide; this implies that the left inequality also turns into an identity. 

\textbf{Proof}. [of Theorem 2.2 and Theorem 1.2] Let $\mu = \mu(x) \in (\mu_{i+1}, \mu_i)$. Theorem 3.1 proves that the poorest convergence is attained in a three-dimensional invariant subspace. Theorem 4.3 proves in span$\{e_j, e_k, e_l\}$ that

$$\frac{\Delta_{j, k}(\mu')}{\Delta_{j, k}(\mu)} \leq \left( \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2.$$ 

It either holds that $\mu_i \leq \mu_{i+1} \leq \mu(x) < \mu_k \leq \mu_j$ or that $\mu_i \leq \mu_k \leq \mu_{i+1} < \mu(x) < \mu_j \leq \mu_j$. In the first case the Ritz value $\mu(x')$ in span$\{e_j, e_k, e_l\}$ satisfies that $\mu_k \leq \mu(x')$, which is the first alternative in Thm. 2.2. To analyze the second case we get that the convergence factor is a monotone increasing function in $\kappa \in (0, 1)$ since

$$\frac{\partial}{\partial \kappa} \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} = \frac{2(1 - \gamma^2)}{(2 - \kappa) + \gamma\kappa} \geq 0.$$ 

Further $\kappa = (\mu_k - \mu_i)/(\mu_j - \mu_i)$ is a monotone decreasing function in $\mu_j$ and $\mu_i$ and a monotone increasing function in $\mu_k$. Hence the poorest convergence with the maximal convergence factor is attained in $j = i$, $k = i + 1$ and $l = n$ which proves Thm. 2.2

$$\frac{\Delta_{i, i+1}(\mu')}{\Delta_{i, i+1}(\mu)} \leq \left( \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2$$ with $\kappa = \frac{\mu_{i+1} - \mu_n}{\mu_i - \mu_n}.$

Thm. 1.2 follows by inserting the reciprocals of the eigenvalues and Ritz values. 

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**Conclusions.** The new convergence bound given in Theorem 1.2 completes the efforts to find sharp convergence estimates within the hierarchy of preconditioned PINVIT\((k)\) and non-preconditioned INVIT\((k)\) eigensolvers for the index \(k = 2\); a hierarchy of these solvers has been suggested in [13]. Next the results are summarized. All these convergence estimates have the common form

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

with \(\Delta_{i,i+1}(\xi) = (\xi - \lambda_i)/(\lambda_{i+1} - \xi)\).

The convergence factor for the non-preconditioned inverse iteration INVIT\((1)\) procedure is (see [14])

\[
\sigma(\text{INVIT}(1)) = \frac{\lambda_i}{\lambda_{i+1}}.
\]

The associated preconditioned scheme, i.e. the preconditioned inverse iteration PINVIT\((1)\) or preconditioned gradient iteration, has the convergence factor (see [6])

\[
\sigma(\text{PINVIT}(1)) = \gamma + (1 - \gamma)\frac{\lambda_i}{\lambda_{i+1}}.
\]

Further the convergence factor of the non-preconditioned steepest descent iteration INVIT\((2)\) reads (see [16])

\[
\sigma(\text{INVIT}(2)) = \frac{\kappa}{2 - \kappa} \quad \text{with} \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}.
\]

The new result on PINVIT\((2)\), which is the preconditioned steepest descent iteration, is now

\[
\sigma(\text{PINVIT}(2)) = \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \quad \text{with} \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{i+1})}{\lambda_{i+1}(\lambda_n - \lambda_i)}.
\]

All these convergence factors are sharp.

Further progress in deriving convergence estimates for the hierarchy of non-preconditioned and preconditioned iteration is a matter of future work. Especially for the practically important locally optimal preconditioned conjugate gradient (LOPCG) iteration [5] sharp convergence estimates are highly desired.

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**REFERENCES**

[1] R. Argentati, A. Knyazev, K. Neymeyr, and E. Ovtchinnikov, Preconditioned eigensolver convergence theory in a nutshell, tech. rep., in preparation, 2010.

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

[3] J. Bramble, J. Pasciak, and A. Knyazev, A subspace preconditioning algorithm for eigenvector/eigenvalue computation, Adv. Comput. Math., 6 (1996), pp. 159–189.

[4] A. Knyazev, Convergence rate estimates for iterative methods for a mesh symmetric eigenvalue problem, Russian J. Numer. Anal. Math. Modelling, 2 (1987), pp. 371–396.

[5] ———, Preconditioned eigensolvers—an oxymoron?, Electron. Trans. Numer. Anal., 7 (1998), pp. 104–123.
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[6] A. 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 (2003), pp. 95–114.

[7] ———, Efficient solution of symmetric eigenvalue problems using multigrid preconditioners in the locally optimal block conjugate gradient method, Electron. Trans. Numer. Anal., 15 (2003), pp. 38–55.

[8] ———, Gradient flow approach to geometric convergence analysis of preconditioned eigensolvers, SIAM J. Matrix Analysis, 31 (2009), pp. 621–628.

[9] A. Knyazev and A. Skorokhodov, On exact estimates of the convergence rate of the steepest ascent method in the symmetric eigenvalue problem, Linear Algebra Appl., 154–156 (1991), pp. 245–257.

[10] A. V. Knyazev, Modified gradient methods for spectral problems, Differ. Uravn., 23 (1987), pp. 715–717. (In Russian).

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

[12] ———, A geometric theory for preconditioned inverse iteration. II: Convergence estimates, Linear Algebra Appl., 322 (2001), pp. 87–104.

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

[14] ———, A note on inverse iteration, Numer. Linear Algebra Appl., 12 (2005), pp. 1–8.

[15] ———, On preconditioned eigensolvers and Invert-Lanczos processes, Linear Algebra Appl., 430 (2009), pp. 1039–1056.

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

[17] J. Nocedal and S. Wright, Numerical Optimization, Springer series in optimization research, Springer, 2006.

[18] E. E. Ovtchinnikov, Sharp convergence estimates for the preconditioned steepest descent method for hermitian eigenvalue problems, SIAM J. Numer. Anal., 43 (2006), pp. 2668–2689.

[19] B. Samokish, The steepest descent method for an eigenvalue problem with semi-bounded operators, Izv. Vyssh. Uchebn. Zaved. Mat., 5 (1958), pp. 105–114. (In Russian).