MAJORIZATION-TYPE CONVERGENCE RATE BOUNDS OF SUBSPACE ITERATIONS∗
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Abstract. We revisit the classical subject of convergence of subspace iterations for Hermitian eigenvalue problems. We reestablish convergence rate bounds with a new twist—using majorization. Our novel majorization-type bounds are sharp, compact, and supersede the traditional results. The Rayleigh-Ritz (RR) method is typically used in subspace iterations to extract approximations to individual eigenvectors from the iterative trial subspace. We combine our majorization-type convergence rate bounds for subspace iterations with RR error bounds to estimate the convergence speed of the block Lanczos method.

Key words. Majorization, angles, subspaces, Ritz values, Rayleigh-Ritz, eigenvalue, subspace iterations.block Lanczos method.


(Place for Digital Object Identifier, to get an idea of the final spacing.)

1. Introduction.

2. Convergence Rate Bounds of Subspace Iterations. Our final application of the Rayleigh-Ritz error bounds of section 2 to estimate the convergence rate of subspace iterations. In this application, we consider a specific context, where our space $H$ is the standard complex $n$-dimensional space $\mathbb{C}^n$ of column-vectors with $n$ complex components. The real case can be also covered with trivial modifications.

We proceed in two main steps. First, we prove new majorization-type convergence rate bounds for subspace iterations in terms of the principal angles between subspaces. Second, we assume that the Rayleigh-Ritz method is applied to subspace iterations, so we combine subspace iterations convergence rate bounds for angles with our error bounds of section 2 for eigenvalues using the Rayleigh-Ritz method. In the latter, we deal with the case of a general $A$-invariant subspace and then we derive an improved bound for the case of the contiguous set of several largest eigenvalues of $A$.

In abstract subspace iterations, ones starts with a subspace $\mathcal{Y}$ of $H$ as an initial approximation to an $A$-invariant subspace $\mathcal{X}$ of the same dimension and for a given operator $F$ in $H$ (called the iterative transition operator) one introduces the subspace $FY$ as a possibly improved approximation of $\mathcal{X}$. Then the Rayleigh-Ritz method is applied to the trial subspace $FY$ and the Ritz pairs are considered as approximations to the corresponding eigenpairs of $A$. In typical practical examples of subspace iterations, $F$ is a suitably chosen function of the operator $A$, e.g., $F$ is a family of monomials of $A$ in the classical power method. We use the same notation $F$ both for the transition operator and for the corresponding $\mathbb{C}^{n \times n}$ matrix.

We first derive majorization-type convergence rate bounds for subspace iterations. We bound the principal angles between $FY$ and $\mathcal{X}$ in terms of the principal angles between $\mathcal{Y}$ and $\mathcal{X}$ and some values describing the quality of $F$, which we do not assume to be Hermitian. The bound below is multiplicative, involving the log function. In

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contrast to our previous use of the log in majorization-type bounds, here we may have a situation where there are zero values in the log vector argument, in which case we must use the interpretation of the majorization statement with the logs based on the products as described in subsection ??.

AKQuestion 2.1. I vaguely recollect that we have had once a bit stronger formulation with the assumption \( \dim \mathcal{Y} \leq \dim \mathcal{X} \). We should use it here, just in case.

Theorem 2.1. Let \( \dim \mathcal{Y} = \dim \mathcal{X} \) and assume \( \Theta(\mathcal{Y}, \mathcal{X}) < \pi/2 \). Let \( F \) be invariant on both \( \mathcal{X} \) and on its orthogonal complement \( \mathcal{X}^\perp \), and assume that \( (P_X F) |_{\mathcal{X}} \) is invertible. Then \( \dim(F\mathcal{Y}) = \dim \mathcal{Y} \) and

\[
\log \left( \frac{\tan \Theta(F\mathcal{Y}, \mathcal{X})}{\tan \Theta(\mathcal{Y}, \mathcal{X})} \right) < \log \left( S \left( (P_X F) |_{\mathcal{X}} \right)^{-1} \right) S \left( (P_{X^\perp} F) |_{X^\perp} \right). 
\]

We add zeros to the vector \( S((P_X F) |_{X^\perp}) \) if \( \dim \mathcal{X}^\perp < \dim \mathcal{X} \) to match the sizes.

Proof. Let our Euclidean space be already mapped into a space of vectors, so that we give a matrix proof here. Let us consider a matrix \( X \) with \( \dim \mathcal{X} \) columns, which form an orthonormal basis for \( \mathcal{X} \), and arbitrarily complete \( X \) to a unitary matrix \([X, X_\perp]\). The \( F \)-invariance of \( \mathcal{X} \) and \( \mathcal{X}^\perp \) assumption is equivalent to assuming that the matrix of the operator \( F \) is block-diagonal in the basis given by the columns of the unitary matrix \([X, X_\perp]\).

We choose any matrix \( Y \) with \( \dim \mathcal{Y} \) columns which span \( \mathcal{Y} \). The matrix \( Y \) has full rank by construction, so \( Y^H Y \) is nonsingular, the columns of \( Y(Y^H Y)^{-1/2} \) are orthonormal and span \( \mathcal{Y} \), and thus \( S\left( Y^H Y(Y^H Y)^{-1/2} \right) = \cos \Theta(\mathcal{Y}, \mathcal{X}) > 0 \) by the definition of the angles and using the theorem’s assumption that \( \Theta(\mathcal{Y}, \mathcal{X}) < \pi/2 \). So the matrix \( X^H Y \) has full rank, the assumptions of Theorem 2.7 are satisfied and for \( T = X^H Y (X^H Y)^{-1} \) we have \( \tan \Theta(\mathcal{Y}, \mathcal{X}) = [s(T), 0, \ldots, 0] \).

We now show that the matrix \( F \mathcal{Y} \) has full rank and so \( \dim(F\mathcal{Y}) = \dim \mathcal{Y} \). We have \( F = P_X F P_X + P_{X^\perp} F P_{X^\perp} = XX^H FX X^H + X_\perp X^H F X_\perp X^H \) by the \( F \)-invariance of \( \mathcal{X} \) and \( \mathcal{X}^\perp \) assumption, which implies that \( X^H F = X^H F X X^H \). The operator \((P_X F)|_{\mathcal{X}} \) and its matrix representation \( X^H F X \) are invertible by the theorem’s assumption, thus the ranks of \( X^H F Y = X^H F X X^H Y \) and \( X^H Y \) are equal, so \( F \mathcal{Y} \) has full rank.

Since \( X^H F Y \) is invertible, we define \( T_F = X^H F Y (X^H F Y)^{-1} \) to be used in Theorem 2.7 for the pair of matrices \( X \) and \( F Y \). By the \( F \)-invariance assumption,

\[
T_F = X^H F Y (X^H F Y)^{-1} = X^H F X_\perp X^H Y (X^H F X X^H Y)^{-1} = X^H F X_\perp X^H Y (X^H Y)^{-1} (X^H F X)^{-1} = X^H F X_\perp T (X^H F X)^{-1}.
\]

We apply Theorem ?? with \( A := X^H F X_\perp \), \( B := T \), and \( C := (X^H F X)^{-1} \), and notice that \( [S(T_F), 0, \ldots, 0] = \tan(\Theta(\mathcal{Y}, \mathcal{X})) \) and \( [S(T), 0, \ldots, 0] = \tan(\Theta(\mathcal{Y}, \mathcal{X})) \) each with the same number of zeros by Theorem 2.7. □

AKQuestion 2.2. I suspect that the statement using \( \Theta(\mathcal{X}, \mathcal{Y}) \) fails under the assumption \( \dim \mathcal{Y} > \dim \mathcal{X} \). If so, I would like to have a counterexample here.

AKQuestion 2.3. We need a practical example of \( F \), which is not a function of \( A \), satisfying the assumptions of the theorem.

Traditional subspace iterations for computing eigenpairs of \( A \) use transition operators \( F \) that are functions of \( A \), most commonly polynomials. Let a scalar function
f of a scalar variable be defined on the spectrum of A so that the operator f(A) is well-defined using the spectral decomposition of the Hermitian operator A. The eigenvectors of A are also the eigenvectors of f(A) corresponding to the eigenvalues f(λ) of A(λ)). Since A is Hermitian, the operator f(A) is in general normal (Hermitian if f is real-valued) and S(F) = |f(A)|₁. Noticing that the A-invariance of a subspace X implies the f(A)-invariance of subspaces X and X⁺, and using the spectral decomposition of A, we can trivially derive specific formulas for the singular values that appear as multipliers in the convergence rate bound of Theorem 2.1.

**Lemma 2.2.** Let A be Hermitian and X be A-invariant. If f = f(A) then

\[
S \left( \left( (P_X A) |X \right)^{-1} \right) = \left| 1 / f (\Lambda ((P_X A) |X)) \right|₁,
\]

\[
S \left( (P_{X⁺} A) |X⁺ \right) = \left| f (\Lambda ((P_{X⁺} A) |X⁺)) \right|₁.
\]

In the case \( F = f(A) \), combining Theorem 2.1 and Lemma 2.2 is not ideal. If \( f(λ_i) \) is relatively large for an eigenvalue λᵢ, which is one of the components of the vector \( Λ ((P_X A) |X) \), then the corresponding eigenvector \( x_i \in X \) is well approximated by the subspace \( FY \). However, Theorem 2.1 only tells us in this case that some angle in a weak majorization, see [17, Prop. 4.B.2, p. 109], multiplying both sides by the vector \( \tan(θ(X, FY)) \) for the eigenvector \( x_i \). Having one small angle in the vector \( θ(X, FY) \) does not imply that one of the eigenvectors is well approximated, even though it actually is in this case.

Next, we want to analyze the Rayleigh-Ritz method applied in subspace iterations, by combining our earlier tangent-based Rayleigh-Ritz error bounds with the results of Theorem 2.1 and Lemma 2.2. Specifically, we want to obtain bounds for the approximation error of eigenvalues of A corresponding to the A-invariant subspace X by the Ritz values on the trial subspace FY generated by subspace iterations with the transition operator \( F = f(A) \) in terms of the tangent of the angles between X and the initial subspace Y and the values of f(·) from Lemma 2.2.

We cannot take advantage of the multiplicative result of Theorem 2.1 directly, so we first transform it into the following additive bound

\[
\tan^2(θ(X, FY)) \lesssim \cdot \cdot S^2 \left( \left( (P_X F) |X \right)^{-1} \right) \cdot \cdot S^2 \left( (P_{X⁺} F) |X⁺ \right) \cdot \cdot \tan^2(θ(X, Y))
\]

by applying a convex increasing function \( e^t \), which preserves the weak majorization, see [17, Prop. 4.B.2, p. 109], multiplying both sides by the vector \( \tan(θ(X, Y)) \), and taking the square of both sides as the function \( t^2 \) is convex increasing for \( t ≥ 0 \).

The following subspace iteration convergence rate bound is rather general as it makes no assumptions on the A-invariant subspace X, and thus can be used e.g., for internal eigenvalues \( Λ ((P_X A) |X) \) and for rational functions f.

**Theorem 2.3.** Let \( X \) and \( Y \) be subspaces of \( H \) such that \( \dim X = \dim Y \) and \( θ(X, Y) < π/2 \). Let the operator A be Hermitian, and let X be an A-invariant subspace. Let \( F = f(A) \) and \( f (\Lambda ((P_X A) |X)) \) \( \neq 0 \). Then \( \dim(FY) = \dim Y \) and

\[
\left| Λ ((P_X A) |X) - Λ ((P_{FY} A) |FY) \right| \lesssim \left( λ_{max(X+Y)} - λ_{min(X+Y)} \right) \cdot \cdot \left( \frac{|f (\Lambda ((P_{X⁺} A) |X⁺))|}{|f (\Lambda ((P_{X} A) |X))|} \right)^2 \cdot \cdot \tan^2(θ(X, Y)).
\]

**Proof.** The assumptions of Theorem 2.1 are satisfied, so \( \dim Y = \dim FY \). The statement of the theorem—bound (2.2)—is simply our Rayleigh-Ritz error bound (??)
applied to the pair of subspaces $X$ and $F\gamma$, where we replace $\sin^2$ with $\tan^2$, which is larger, and use (2.1) to bound the vector $\tan^2 \Theta(X,F\gamma)$. □

It is intuitively clear that one wants to choose the function $f$ such that it is as large as possible on $\Lambda ((P_X A)|_X)$ and at the same time as small as possible on $\Lambda ((P_{X^\perp} A)|_{X^\perp})$. Our new Theorem 2.1, Lemma 2.2, and Theorem 2.3 support this intuition with rigorous bounds.

Practical choices of the classes of functions $f$ are normally limited to polynomials and rational functions. The polynomials are easier to implement, since the only required operation is multiplication of a vector or a block of vectors by $A$. Implementation of rational functions requires linear solves and thus is more computationally expensive, but rational functions may lead to a much faster convergence of subspace iterations. In the rest of the section, we only consider polynomials for $f$.

Let $f$ be a real polynomial of degree $k$. Ideally, we want to choose $f$ a priori in an optimal way in order to minimize the $f$ dependent ratio in estimate (2.2). With few exceptions, where specific distributions of eigenvalues in $\Lambda ((P_X A)|_X)$ are known, such an optimization problem is too challenging, so we follow the standard approach to simplify it. First, we assume that the $A$-invariant subspace $X$ corresponds to the contiguous set of the $p$ largest eigenvalues of $A$, i.e., $\Lambda ((P_X A)|_X) = \{\lambda_1, \ldots, \lambda_p\}$, and thus the $A$-invariant subspace $X^\perp$ corresponds to the contiguous set of the $n-p$ (counting the multiplicities) smallest eigenvalues of $A$, i.e. $\Lambda ((P_{X^\perp} A)|_{X^\perp}) = \{\lambda_{p+1}, \ldots, \lambda_{\min}\}$.

Second, we bound the $f$ dependent ratio as follows:

\[
\left( \frac{|f([\lambda_{p+1}, \ldots, \lambda_{\min}])|}{|f([\lambda_1, \ldots, \lambda_p])|} \right)^2 \leq \left( \frac{\max_{t : \lambda_{p+1} \geq t \geq \lambda_{\min}} |f(t)|}{|f([\lambda_1, \ldots, \lambda_p])|} \right)^2. \tag{2.3}
\]

We note that the upper bound in (2.3) is a vector, since it is a ratio of a scalar and a vector. Which component of the vector do we want to minimize by choosing the optimal polynomial $f$? Luckily, the optimal polynomial simultaneously minimize all the components as we see in the next theorem, inspired by [?, Lemma 2.4.1].

**Theorem 2.4.** Every component of the vector on the right-hand side of (2.3) is minimized in the class of real polynomials $f$ of degree $k$ on

\[
f(t) = T_k \left( \frac{2t - \lambda_{p+1} - \lambda_{\min}}{\lambda_{p+1} - \lambda_{\min}} \right),
\]

where $T_k$ is the Chebyshev polynomial of the first kind defined by $T_k(\cos \theta) = \cos(k\theta)$. With this choice of $f$, the vector on the right-hand side of (2.3) is

\[
[\sigma_p^*, \ldots, \sigma_1^*], \quad \text{where } \sigma_i^* = \left| T_k \left( \frac{1 + \xi_i}{1 - \xi_i} \right) \right|^{-2}, \quad \xi_i = \frac{\lambda_{i} - \lambda_{p+1}}{\lambda_{i} - \lambda_{\min}}, \quad i = 1, \ldots, p.
\]

**Proof.** The optimal polynomial (2.4), which solves the problem of minimizing $\sigma_i(f)$, does not depend on $i$, i.e., each (unordered or ordered) component of the vector on the right-hand side of (2.3) is minimized by the same polynomial (2.4). We finally note that the absolute value of the Chebyshev polynomial is monotonically increasing outside of the interval $(-1, 1)$, so the vector $[\sigma_p^*, \ldots, \sigma_1^*]$ is decreasing. □

Several implementations of subspace iterations based on Chebyshev polynomials are available, see, e.g., [?] for the three-term recurrence and [?] for the two-term recurrence iterative formulas. Reasonable quality bounds of $\lambda_{p+1}$ and $\lambda_{\min}$ are normally
required for standard implementations. In the past two–three decades in most practical calculations the block Lanczos methods have replaced the subspace iterations using Chebyshev polynomials. Nevertheless, the theory of convergence rate bounds for subspace iterations using Chebyshev polynomials is traditionally used to derive the convergence rate bounds for the block Lanczos method. We follow this tradition here in the next subsection to establish our final result.

2.1. Convergence Rate Bounds for the Block Lanczos Method. The block Lanczos method applies the Rayleigh-Ritz procedure on the so-called block Krylov subspace \( K_{k+1}(A, \mathcal{X}_0) \equiv \mathcal{X}_0 + \mathcal{A} \mathcal{X}_0 + \cdots + A^k \mathcal{X}_0 \), where the subspace \( \mathcal{X}_0 \) is an initial approximation to the \( A \)-invariant subspace \( \mathcal{X} \). In nontrivial cases we have that \( \dim K_{k+1}(A, \mathcal{X}_0) > \dim \mathcal{X}_0 = \dim \mathcal{X} \), so we need Corollary ??.

**Theorem 2.5.** Let \( \dim \mathcal{X} = \dim \mathcal{X}_0 = p \), operator \( A \) be Hermitian, and let the \( A \)-invariant subspace \( \mathcal{X} \) correspond to the contiguous set of the largest eigenvalues of \( A \). Let \( \mathcal{Y} = \mathcal{X}_0 + A \mathcal{X}_0 + \cdots + A^k \mathcal{X}_0 \) and \( \sigma^*_i \) defined by (2.5), then

\[
0 \leq \frac{\Lambda ((P_X A)|_X) - \Lambda_{\dim \mathcal{X}} ((P_Y A)|_Y)}{\Lambda_{\dim \mathcal{X}} ((P_Y A)|_Y) - \lambda_{\min (\mathcal{X} + \mathcal{Y})}} \leq [\sigma^*_1, \ldots, \sigma^*_p] \tan^2 \Theta(\mathcal{X}, \mathcal{X}_0).
\]

**Proof.** For any polynomial \( f \) of degree \( k \) we have \( f(A) \mathcal{X}_0 \subseteq \mathcal{Y} \) by the definition of \( \mathcal{Y} \), so we can bound the term \( \tan^2 \Theta(\mathcal{X}, \mathcal{Y}) \) using \( \tan^2 \Theta(\mathcal{X}, f(A) \mathcal{X}_0) \). We choose \( f \) as in (2.4), so \( \tan^2 \Theta(\mathcal{X}, f(A) \mathcal{X}_0) \leq [\sigma^*_1, \ldots, \sigma^*_p] \tan^2 \Theta(\mathcal{X}, \mathcal{X}_0) \) by (2.1), Lemma 2.2 with (2.3), and using Theorem 2.4 that gives (2.5). Finally, we apply the tangent bound of Corollary ?? to the pair of subspaces \( \mathcal{X} \) and \( f(A) \mathcal{X}_0 \). \[\Box\]

We conclude this section with a comparison of the bound of Theorem 2.5 with one of the known results that we reproduce here.

**Theorem 2.6.** [?], Formulas (2.3.5), (2.4.7), Section 2.6] Under the assumptions of Theorem 2.5, we have

\[
0 \leq \frac{\Lambda ((P_X A)|_X) - \Lambda_{\dim \mathcal{X}} ((P_Y A)|_Y)}{\Lambda_{\dim \mathcal{X}} ((P_Y A)|_Y) - \lambda_{\min (\mathcal{X} + \mathcal{Y})}} \leq [\sigma^*_1, \ldots, \sigma^*_p] \max \{ \tan^2 \Theta(\mathcal{X}, \mathcal{X}_0) \}.
\]

Since \( \Lambda_{\dim \mathcal{X}} ((P_Y A)|_Y) - \lambda_{\min (\mathcal{X} + \mathcal{Y})} \leq \Lambda ((P_X A)|_X) - \lambda_{\min (\mathcal{X} + \mathcal{Y})} \leq \lambda_1 - \lambda_{\min} \) the bound of Theorem 2.6 is a slight but aesthetically pleasing improvement of the classical bound of [?], also reproduced in [?, Theorem 9.2.2].

On the one hand, the already known Theorem 2.6 is stronger than Theorem 2.5 in the sense that the bound is an inequality where each term is individually estimated; moreover, the error bound for the \( i \)-th eigenvalue involves the \( \sigma^*_i \) multiplier. On the other hand, Theorem 2.6 uses only the largest angle, while the weak majorization statement of Theorem 2.5 uses all angles between the target subspace \( \mathcal{X} \) and the initial approximation \( \mathcal{X}_0 \). The advantage of Theorem 2.5 can be clearly seen in the situation where all \( p \) largest eigenvalues are clustered so that all \( \sigma^*_i, i = 1, \ldots, p \) are nearly the same, and where the set of angles between \( \mathcal{X} \) and \( \mathcal{X}_0 \) contains many small values, e.g., in the extreme case where \( \dim \mathcal{X} \cap \mathcal{X}_0 = p - 1 \) so that there is only one nonzero angle, \( \max \{ \Theta(\mathcal{X}, \mathcal{X}_0) \} \), in the set \( \Theta(\mathcal{X}, \mathcal{X}_0) \). In this case, all bounds in Theorem 2.6 are nearly the same as the largest bound in Theorem 2.5, while the smallest bound in Theorem 2.5 is at least \( p \) times smaller.

Let us finally note that *preconditioned* subspace iterations, e.g., [?, ?], which are gaining popularity in the last decades, do not satisfy most of the assumptions of Theorem 2.1 or Lemma 2.2. In these methods typically the operator \( F \) is nonlinear, is not a function of \( A \), and is not invariant on \( \mathcal{X} \), so their convergence theory, e.g., [?], is quite limited and much more complex.
AKQuestion 2.4. I vaguely recollect that we have had once a bit stronger formulation with the assumption \( Y \in \mathbb{C}^{n \times p} \) where \( m \geq n \). We should use it here, just in case.

Theorem 2.7. (Inspired by [?], Chapter 5, Lemma 3.11, p. 255). For integers \( n \geq p \) let the matrix \( X \in \mathbb{C}^{n \times p} \) have orthonormal columns and be arbitrarily completed to a unitary matrix \( [X, X_{\perp}] \). Let the matrix \( Y \in \mathbb{C}^{n \times p} \) be such that the matrix \( X^HY \) has full rank. Then the singular values \( S(T) \) of the matrix \( T = X_\perp^HY \) are invertible. We easily obtain by direct calculation that \( S(T) = \|X\|_2 \cdot \|X_\perp\|_2 \). Since the matrix \( X^HY \) is invertible, we immediately obtain the majorization that \( \|X\|_2 \cdot \|X_\perp\|_2 \leq \|Y\|_2 \).

Proof. Our assumption that the matrix \( X^HY \) has full rank implies that the matrix \( Y \) has full rank, i.e., \( \dim(\mathcal{R}(Y)) = p = \dim(\mathcal{R}(X)) \). We denote \( Z = X + X_\perp T \). The identities \( Y = P_X Y + P_{X_\perp}Y = XX^HY + X^HY = ZX^HY \) imply \( \mathcal{R}(Y) = \mathcal{R}(Z) \) since the matrix \( X^HY \) is invertible. We easily obtain by direct calculation that \( X^H \cdot (X + X_\perp T) = I \) and \( Z^H = (X + X_\perp T)^H = I + T^HT \), since the matrix \( [X, X_{\perp}] \) is unitary by assumption. Thus, \( X^H \cdot Z^H \cdot Z^{-1/2} = (I + T^HT)^{-1/2} \) is Hermitian positive definite. However, the matrix \( Z(\mathcal{R}(Z))^{-1/2} \) by construction has orthonormal columns that span \( \mathcal{Y} \), since \( \mathcal{R}(Y) = \mathcal{R}(Z) \), so we finally observe that \( \cos \Theta(\mathcal{Y}, X) = S^T \cdot (X^H \cdot Z^H \cdot Z^{-1/2}) = \Lambda^T \cdot ((I + T^HT)^{-1/2}) = (1 + S^2(T))^{-1/2} \).

Conclusions. Majorization is a powerful tool that gives elegant and general error bounds for eigenvalues approximated by the Rayleigh-Ritz method. We discover several new results of this kind, including multiplicative bounds for relative errors. We apply majorization, apparently for first time, in the contexts of FEM error bounds. Our initial results are promising and expected to lead to further development of the majorization technique for the theory of eigenvalue computations.

REFERENCES


