A Priori Convergence Analysis for Krylov Subspace Eigensolvers

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1 Introduction

"Reviewing what you have learned and learning anew, you are fit to be a teacher." Similarly to this famous Confucius quote, the present habilitation thesis is devoted to reviewing and deepening the convergence theory of Krylov subspace eigensolvers. The main thematic area is the convergence analysis for modern and efficient numerical methods for solving discretized eigenvalue problems of second-order self-adjoint elliptic partial differential operators. These eigenvalue problems are of great significance for numerous scientific applications such as the computation of stationary states in the electronic structure theory [117, 10, 31, 116, 103, 14, 101, 25].

The discretization matrices of the differential operators within this topic are large and sparse, and only a small subset of the spectrum is of practical interest. Therefore one prefers to use vector iterations and subspace iterations instead of matrix transformations for the numerical solution. The basis of almost all vector iterations for solving such matrix eigenvalue problems is the power method. Proper shifts and preconditioning techniques can accelerate the convergence toward an eigenvector associated with one of the target eigenvalues. The block implementation of vector iterations enables the simultaneous approximation of several eigenvectors which span an invariant subspace associated with the target eigenvalues. The resulting subspace iterations can prevent convergence deterioration in the case of clustered eigenvalues by setting a sufficiently large block size. Furthermore, extending vector iterations by previous iterates yields another type of subspace iterations. The corresponding subspaces can provide more accurate approximate eigenpairs according to the Courant-Fischer principles.

Many popular eigensolvers are related to Krylov subspaces or block-Krylov subspaces [6]. The origin is the Lanczos method [59] which deals with eigenvalue problems of real symmetric matrices and theoretically generates orthonormal basis vectors of a growing Krylov subspace by means of a three-term recurrence. This classical method is a direct extension of the power method and usually serves to compute extreme eigenvalues. The numerical stability can be improved by additional orthogonalization [93]. A special implementation of the Lanczos method for computing arbitrary eigenvalues has been presented by Cullum and Willoughby in [22, 23]. Therein a three-term recurrence without additional orthogonalization results in an oversized tridiagonal matrix, from whose spectrum some acceptable approximate eigenvalues of the original matrix can be found by subsequent checking. Moreover, applying the Lanczos method to a shifted and inverted matrix [96] leads to more efficient eigensolvers for computing interior eigenvalues [103]. In general, the performance of the Lanczos method can be improved significantly by proper modifications with restarting [43, 19, 127, 128, 118], block implementation [21, 33, 65, 48] and preconditioning [68, 44, 46, 35]; see also some recent eigensolvers in [30, 66, 63, 69, 120, 64, 119].

In contrast to the active development of Krylov subspace eigensolvers, the corresponding convergence theory remains limited. The Chebyshev type estimates by Kaniel [42], Paige [90], Saad [98] and Parlett [94] are still state of the art. Partial or indirect improvements have been presented inter alia in [112, 105, 121, 57, 58, 61, 62], but cannot overcome certain major drawbacks such as the lengthy forms of several bounds and their dependence on the current (block-)Krylov subspace. These drawbacks are troublesome for applying the concerned estimates to modern variants of the Lanczos method, particularly to those restarted iterations which only use low-dimensional subspaces. Fortunately, some concise estimates by Knyazev [44, 45] about the power method for an abstract matrix function can be reformulated for basic Krylov subspace eigensolvers and provide reasonable bounds for restarted iterations. This inspires us to deepen the convergence theory of Krylov subspace eigensolvers by generalizing Knyazev's analysis. Some results have been presented in [83, 125, 122]. A motivation for these previous works is to extend the geometry-flavored convergence theory of preconditioned gradient-type eigensolvers [72, 73, 50, 52, 79, 2] to more efficient variants such as the generalized Davidson method [68] and the locally optimal block preconditioned conjugate gradient (LOBPCG) method [48]. In this context, the results of the present habilitation thesis for investigating Krylov subspace eigensolvers are expected to be combined with a proper interpretation of preconditioning; cf. the recent work [126] on the cluster robustness of block gradient-type eigensolvers.

1.1 Overview

This thesis aims at analyzing the convergence behavior of four types of Krylov subspace eigensolvers for real symmetric matrices, namely, standard Krylov subspace iterations (SK), restarted Krylov subspace iterations (RK), block-Krylov subspace iterations (BK) and restarted block-Krylov subspace iterations (RBK). These eigensolvers are designed for generalized matrix eigenvalue problems concerning finite element discretizations of operator eigenvalue problems. However, the most classical convergence estimates for Krylov subspace eigensolvers are formulated with respect to standard matrix eigenvalue problems. Therefore we prefer to use some reciprocal representations (see Subsection 1.4.2) which allow us to simplify the notations in our analysis and directly compare the new results with the corresponding classical ones. Furthermore, the achieved estimates can easily be reformulated for generalized matrix eigenvalue problems by reverse substitutions.

A basic tool of our analysis is, as usual, the polynomial interpretation of (block-)Krylov subspaces. Most estimates make use of Chebyshev polynomials as in the classical analysis, but considerably improve the applicability for restarted iterations and the accuracy for block iterations and clustered eigenvalues. In particular, the dependence of some classical results on the current (block-)Krylov subspace is avoided by using certain low-dimensional auxiliary subspaces. This yields more practical *a priori* bounds. Moreover, an ellipsoidal interpretation of approximate eigenvectors enables sharp estimates for restarted iterations. Therein the bounds can be represented with two further types of polynomials and are attainable in some limit cases. Our analysis is accompanied by software development. The investigated Krylov subspace eigensolvers and their preconditioned variants can be integrated in our software "Adaptive-Multigrid-Preconditioned (AMP) Eigensolver" [124]; see Figure 1.1 for an application example. The theoretical results can be demonstrated and compared within various generalized matrix eigenvalue problems which are generated by adaptive finite element discretizations.

The remaining part of Chapter 1 is devoted to introducing discretized eigenvalue problems of second-order self-adjoint elliptic partial differential operators together with suitable eigensolvers including the investigated Krylov subspace eigensolvers. The main part of this thesis containing new results of our convergence analysis is organized as follows: In Chapter 2, we restate and compare several classical estimates by Saad [98] and Knyazev [44, 45] for Krylov subspace eigensolvers. Their disadvantages and limitations are subsequently discussed concerning restarted and block iterations. We also review some auxiliary vectors and supplementary arguments which are useful for overcoming these drawbacks. New estimates for standard Krylov subspace iterations are presented in Chapter 3. Therein the corresponding angle-dependent estimates from [98] are improved by avoiding certain ratio-products in the bounds, and several comparable estimates from [44, 45] are extended to further approximate eigenvalues. In Chapter 4, some angle-free estimates are presented for restarted Krylov subspace iterations. Their sharpness and the generalization to arbitrarily located initial approximate eigenvalues are discussed on the basis of the previous works [83, 125]. Chapter 5 deals with block-Krylov subspace iterations and focuses on their cluster robustness. The analysis makes use of intersections between the initial subspace and certain invariant subspaces similarly to the work [97] by Rutishauser for investigating the block power method. This allows us to skip several interior eigenvalues in the analysis so that the convergence factors are meaningful in the case of clustered eigenvalues. The resulting estimates improve the corresponding estimates from [98] by modifying the selection of interior eigenvalues and generalizing an angle-free argument from [44, 45]. Restarted block-Krylov subspace iterations are investigated in Chapter 6. Therein sharp estimates and cluster robust estimates are derived by constructing auxiliary iterations and applying the results from previous chapters after some necessary modifications. Chapter 7 includes the introduction of the software "Adaptive-Multigrid-Preconditioned (AMP) Eigensolver" and several numerical experiments for illustrating the performance of the investigated eigensolvers accompanied by applicable convergence estimates. Finally, a conclusion of our convergence analysis is given in Chapter 8 together with an outlook on future research.

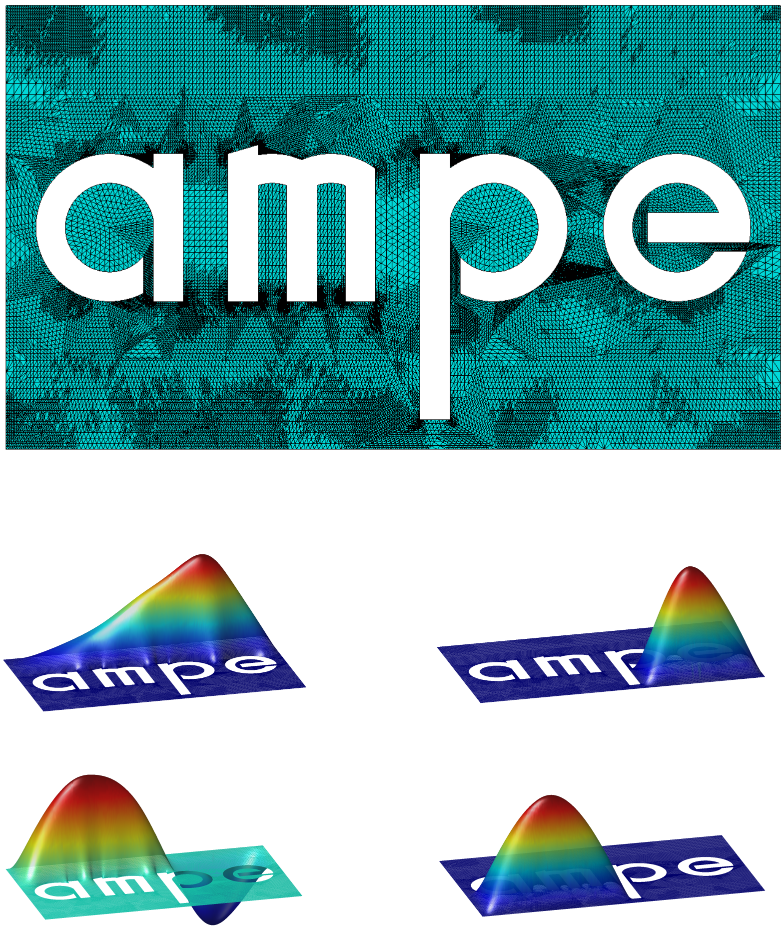

Figure 1.1: An application example of the software AMP Eigensolver. Therein the negative Laplace operator is adaptively discretized on an engraved plate with homogeneous Dirichlet boundary conditions. The adaptive grid refinement is based on the residuals of the approximate eigenfunctions associated with the four smallest eigenvalues.

1.2 Discretized operator eigenvalue problems

We start with the eigenvalue problem $\mathcal{L}\mathsf{u} = \lambda\mathsf{u}$ of a second-order self-adjoint elliptic partial differential operator $\mathcal{L}$ on a bounded domain $\Omega \subset \mathbb{R}^{\mathsf{d}}$, $\mathsf{d} \in \{2, 3\}$. Therein homogeneous Dirichlet or Neumann boundary conditions are stated on disjoint subsets of the boundary $\partial\Omega$. Usually a moderate number of eigenvalues and the associated eigenfunctions need to be determined for describing e.g. important energy levels of a quantum mechanical system. Analytical solutions are only known for some simple operators and domains [32]. Numerical methods are thus recommended in general, whereby an operator eigenvalue problem is typically discretized by the finite element method. The resulting matrix eigenvalue problems can be treated by appropriate methods from numerical linear algebra.

First, we shortly introduce the finite difference method for discretizing an operator eigenvalue problem since this method is easy to implement and still finds application in some recent works on Krylov subspace eigensolvers such as [63, 120, 64]. Therein the differential operator $\mathcal{L}$ is approximated by a symmetric difference operator L. Setting up the corresponding approximate equation $\mathsf{Lu} = \lambda \mathsf{u}$ at suitable mesh points results in a standard matrix eigenvalue problem $Cu = \lambda u$. The eigenvector u contains values of the approximate eigenfunction u at the mesh points, and the matrix C stores the coefficients of L, preferably in a sparse form. However, the finite difference method is mostly applied to simple domains. Nonequidistant mesh points could occur in the case of irregular boundaries so that asymmetric and lower-order difference operators have to be used additionally. The matrix C is thus not always symmetric. Nevertheless, the consideration of this type of discretized operator eigenvalue problems is usually restricted to the ideal case that C is a real symmetric matrix.

The finite element method is much more flexible. It has a sound theoretical basis in functional analysis and can deal with adaptively generated meshes [16]. Therein the approximation of $\mathcal{L}$ is based on a variational formulation

$$\mathsf{a}(\mathsf{u},\mathsf{v}) = \lambda \langle \mathsf{u},\mathsf{v} \rangle \qquad \forall \;\; \mathsf{v} \in \mathsf{V}$$

with the bilinear form $\mathsf{a}(\cdot,\cdot)$ associated with $\mathcal{L}$, the L^2-inner product $\langle \cdot,\cdot \rangle$ and the Hilbert space V spanned by suitable trial functions. The approximate eigenfunction u can be represented by a linear combination $\sum_{j=1}^{n} \xi_j \mathsf{v}_j$ of trial functions $\mathsf{v}_1, \ldots, \mathsf{v}_n$ which are assigned to certain mesh vertices and whose supports consist of the corresponding neighbored subdomains. Substituting u by $\sum_{j=1}^{n} \xi_j \mathsf{v}_j$ in the equations

$$\mathsf{a}(\mathsf{u},\mathsf{v}_i) = \lambda \langle \mathsf{u},\mathsf{v}_i \rangle, \qquad i = 1, \ldots, n$$

(called Ritz projection) yields a generalized matrix eigenvalue problem $Ax = \lambda Mx$. Therein the stiffness matrix A, the mass matrix M and the eigenvector x are given by

$$(A)_{ij} = \mathsf{a}(\mathsf{v}_j,\mathsf{v}_i), \qquad (M)_{ij} = \langle \mathsf{v}_j,\mathsf{v}_i \rangle \qquad \text{and} \qquad (x)_j = \xi_j,$$

respectively. The approximation errors in terms of eigenvalues and eigenfunctions have already been thoroughly analyzed in various classical works; see [3, 4, 109]. The matrices A and M are symmetric in the real case due to the self-adjointness of $\mathcal{L}$ and the symmetry of $\mathsf{a}(\cdot,\cdot)$ and $\langle \cdot,\cdot \rangle$. Moreover, the coercivity of $\langle \cdot,\cdot \rangle$ ensures that M is positive definite. From an algorithmic point of view, the matrix entries can be evaluated partially in subdomains and then assigned to mesh vertices and edges. This enables matrix-free routines for computing matrix-vector products.

The essential task in the discretized operator eigenvalue problems $Cu = \lambda u$ and $Ax = \lambda Mx$ is to compute a moderate number of eigenvalues and the associated eigenvectors of the matrix C or the matrix pair (A, M). For introducing suitable matrix eigensolvers, we only consider the problem of (A, M) since it is of more practical value and formally includes the problem of a real symmetric C by setting M to be an identity matrix. A sufficiently fine discretization can produce very large and sparse matrices. Classical diagonalization methods such as the QR algorithm usually cannot maintain the sparsity pattern of the matrices. The storage requirement would be dramatically increased by dense intermediate matrices. In addition, a complete diagonalization is rather superfluous as only a subset of the spectrum is of practical interest. Vector iterations and subspace iterations are much more appropriate since they avoid transformations of large matrices and focus on the computation of target eigenvalues.

For instance, in order to compute an arbitrary target eigenvalue of (A, M), one can use an invertible shifted matrix $A_\sigma = A - \sigma M$ with an initial approximate eigenvalue σ as shift and apply the power method to the matrix product $A_\sigma^{-1}M$. This generates a sequence of approximate eigenvectors for the closest eigenvalue to σ provided that σ does not equal the arithmetic mean of two neighboring eigenvalues. The convergence rate can be described by $|\lambda - \sigma|/|\widetilde{\lambda} - \sigma|$ with the two closest eigenvalues λ and $\widetilde{\lambda}$ to σ and can thus be bounded away from 1 by selecting a proper σ. In comparison to this, the convergence rate of some inverse free eigensolvers depends on the largest eigenvalue in magnitude [53, 35] and has the form $1 - \mathcal{O}(h^2)$ with the discretization parameter h.

Consequently, we prefer to use inverse or preconditioned eigensolvers such as the above-mentioned inverse power method for solving discretized operator eigenvalue problems. Therein matrix-vector products with $A_\sigma^{-1}M$ can be computed practically by solving linear systems of the form $A_\sigma w = Mv$. In particular, one can apply the conjugate gradient method to positive definite A_σ together with multigrid or multilevel preconditioning [38, 24, 11], e.g., based on a mesh hierarchy stemming from an adaptive finite element discretization. The positive definiteness of A_σ means that the shift σ is located on the left-hand side of the spectrum of (A, M) so that the smallest eigenvalues are target eigenvalues. Moreover, the corresponding task is equivalent to the computation of the reciprocally largest eigenvalues of (A_σ, M) where the associated eigenvectors remain the same. Next, negative definite A_σ can be excluded for discretized operator eigenvalue problems since the largest eigenvalues of the operator are not of practical interest. In the case that A_σ is indefinite, i.e., for computing some interior eigenvalues of (A, M), the generalized minimal residual method can be applied together with preconditioning of A_σ by incomplete factorizations [12]. Moreover, the corresponding task can be reformulated as the computation of the reciprocally largest eigenvalues of the matrix pairs $(A_\sigma M^{-1} A_\sigma,\ A_\sigma)$ and $(A_\sigma M^{-1} A_\sigma,\ -A_\sigma)$. Therein the first matrix $A_\sigma M^{-1} A_\sigma$ is positive definite and the associated eigenvectors remain the same. Another reformulation concerns computing the reciprocally largest eigenvalues of the matrix pair $(A_\sigma M^{-1} A_\sigma,\ M)$ whose spectrum consists of the squared eigenvalues of (A_σ, M). In addition, the eigenvectors of (A_σ, M) or (A, M) can be extracted from the invariant subspaces of $(A_\sigma M^{-1} A_\sigma,\ M)$. These reformulations with more complex matrix pairs do not lead to considerably higher computational costs for inverse eigensolvers since the corresponding linear systems $A_\sigma M^{-1} A_\sigma w = \pm A_\sigma v$ and $A_\sigma M^{-1} A_\sigma w = Mv$ can be simplified as systems $A_\sigma w = \pm Mv$ and a system sequence $A_\sigma u = Mv$, $A_\sigma w = Mu$.

Furthermore, the reformulated tasks can be gathered under a common roof concerning an abstract problem, namely computing the reciprocally largest eigenvalues and the associated eigenvectors of a matrix pair of real symmetric matrices where the first matrix is positive definite; cf. similar problem settings in [37] on a modification of the Lanczos method. In order to simplify the notation, (A, M) denotes from now on the matrix pair in this abstract problem, i.e., we consider the eigenvalue equation

$$Ax = \lambda M x \quad \text{with symmetric } A, M \in \mathbb{R}^{n \times n} \text{ where } A \text{ is positive definite.} \tag{1.1}$$

Some gradient-type eigensolvers and Krylov subspace eigensolvers aiming at the reciprocally largest eigenvalues of (A, M) from (1.1) are introduced in the following sections. It is remarkable that the reciprocally largest eigenvalues are just the smallest positive eigenvalues if the spectrum has sufficiently many positive elements.

1.3 Gradient-type eigensolvers

We first consider the generalized matrix eigenvalue problem (1.1) in the case that M is also positive definite. Then all eigenvalues of (A, M) are positive so that the reciprocally largest eigenvalues are simply the smallest eigenvalues. The smallest one can be approximated iteratively by applying the power method to the matrix product $A^{-1}M$ and evaluating the Rayleigh quotient

$$\rho : \mathbb{R}^n \backslash \{0\} \to \mathbb{R}, \qquad \rho(x) = \frac{x^T A x}{x^T M x} \tag{1.2}$$

at the iterates. Another fundamental method is the gradient iteration for minimizing the Rayleigh quotient $\rho(\cdot)$. The minimum of $\rho(\cdot)$ coincides with the smallest eigenvalue of (A, M) and can be approximated by

$$x^{(\ell+1)} = x^{(\ell)} - \omega^{(\ell)} r^{(\ell)} \qquad \text{with} \qquad r^{(\ell)} = Ax^{(\ell)} - \rho(x^{(\ell)}) M x^{(\ell)}. \tag{1.3}$$

Therein the residual $r^{(\ell)}$ of the iterate $x^{(\ell)}$ is collinear with the Euclidean gradient $\nabla\rho(\cdot)$ of the Rayleigh quotient at $x^{(\ell)}$, namely,

$$\nabla\rho(x^{(\ell)}) = \frac{2}{(x^{(\ell)})^T M x^{(\ell)}}\, r^{(\ell)}.$$

An optimal step size $\omega^{(\ell)}$ can implicitly be determined by minimizing $\rho(\cdot)$ in the subspace $\text{span}\{x^{(\ell)}, r^{(\ell)}\}$. This local minimization problem is typically solved by the Rayleigh-Ritz procedure which restricts the matrix pair (A, M) to $\text{span}\{x^{(\ell)}, r^{(\ell)}\}$. Solving the corresponding eigenvalue problem $(V^T AV)g = \vartheta(V^T MV)g$ with respect to a basis matrix V yields approximate eigenpairs (ϑ, Vg), called Ritz pairs. Subsequently, the next iterate $x^{(\ell+1)}$ is given by a Ritz vector associated with the smallest Ritz value.

However, the gradient iteration (1.3) is not recommended for solving discretized operator eigenvalue problems since its convergence rate would tend to 1 with increasing dimension of the matrices [51, 75]. In order to accelerate the convergence, one can use a preconditioner $T \approx A^{-1}$ and modify (1.3) as the preconditioned gradient iteration

$$x^{(\ell+1)} = x^{(\ell)} - \omega^{(\ell)} T r^{(\ell)} \qquad \text{with} \qquad r^{(\ell)} = Ax^{(\ell)} - \rho(x^{(\ell)}) M x^{(\ell)} \tag{1.4}$$

which can be interpreted as a gradient iteration with respect to a proper geometry [27]. In addition, one can implement (1.4) in a block form for computing a number of the smallest eigenvalues. The preconditioner T is not always needed in an explicit form. The formal matrix-vector product $Tr^{(\ell)}$ can be constructed by an approximate solution of the linear system $Aw = r^{(\ell)}$. The convergence of the iteration (1.4) for $\omega^{(\ell)} = 1$ or an optimal $\omega^{(\ell)}$ determined by the Rayleigh-Ritz procedure can be guaranteed by the quality condition

$$\|I - TA\|_A \leq \gamma \qquad \text{with} \qquad 0 \leq \gamma < 1. \tag{1.5}$$

Therein the matrix norm is defined with respect to the A-inner product, and I denotes the $(n \times n)$-identity matrix. The matrix T is not necessarily symmetric [2, 15]. For symmetric T, the norm $\|I - TA\|_A$ coincides with the spectral radius of $I - TA$. Moreover, some symmetric and positive definite preconditioners of the form $T = B^{-1}$ satisfying the condition

$$\alpha\, x^T B x \leq x^T A x \leq \beta\, x^T B x \qquad \forall\, x \in \mathbb{R}^n$$

do not always fulfill (1.5). Instead, one can use

$$T \;=\; \frac{2}{\beta + \alpha}\, B^{-1}$$

which fulfills (1.5) with $\gamma = (\beta - \alpha)/(\beta + \alpha)$. Indeed, this scaling is only required in the convergence analysis and can be skipped in the implementation since the factor $2/(\beta + \alpha)$ can be merged into the step size.

In the case that M is not necessarily positive definite, the computation of the reciprocally largest eigenvalues of (A, M) can be reformulated as a maximization problem of the Rayleigh quotient

$$\widetilde{\rho} : \mathbb{R}^n \backslash \{0\} \to \mathbb{R}, \qquad \widetilde{\rho}(x) = \frac{x^T M x}{x^T A x} \tag{1.6}$$

with respect to the reverse matrix pair (M, A). A suitable preconditioned gradient iteration is

$$x^{(\ell+1)} = x^{(\ell)} + \widetilde{\omega}^{(\ell)} T \widetilde{r}^{(\ell)} \qquad \text{with} \qquad \widetilde{r}^{(\ell)} = M x^{(\ell)} - \widetilde{\rho}(x^{(\ell)}) A x^{(\ell)}. \tag{1.7}$$

For positive definite M, (1.7) coincides with (1.4) in the sense that the associated correction directions are collinear, namely,

$$T\widetilde{r}^{(\ell)} = TMx^{(\ell)} - \frac{1}{\rho(x^{(\ell)})} TAx^{(\ell)} = \frac{1}{\rho(x^{(\ell)})} \big(\rho(x^{(\ell)}) TMx^{(\ell)} - TAx^{(\ell)}\big) = \frac{-1}{\rho(x^{(\ell)})} Tr^{(\ell)}.$$

Further gradient-type eigensolvers related to (1.4) and (1.7) can systematically be introduced in a methodical hierarchy.

1.3.1 A methodical hierarchy

A hierarchy of preconditioned iterations for solving discretized operator eigenvalue problems is suggested in [75] for extending the geometric convergence analysis of a simple eigensolver from [72, 73, 50] to further eigensolvers such as the gradient iteration (1.4) and the LOBPCG method [48]. The original formulation [75] starts with a reduction of the generalized matrix eigenvalue problem (1.1) for positive definite M to the corresponding standard matrix eigenvalue problem with respect to the M-inner product. We drop this reduction in the following review in order to highlight the practical forms of the eigensolvers. We prefer to use a similar notational simplification with respect to the A-inner product in our convergence analysis; cf. the previous works [81, 82].

The methodical hierarchy from [75] is called "PINVIT" which is the abbreviation for the simple eigensolver "preconditioned inverse iteration"

$$x^{(\ell+1)} = x^{(\ell)} - Tr^{(\ell)} \qquad \text{with} \qquad r^{(\ell)} = Ax^{(\ell)} - \rho(x^{(\ell)}) M x^{(\ell)}. \tag{1.8}$$

Evidently, the iteration (1.8) coincides with the gradient iteration (1.4) if the fixed step size $\omega^{(\ell)} = 1$ is used. For a systematic review of the PINVIT hierarchy, we denote (1.8) by $\mathscr{P}_1$. The next method $\mathscr{P}_2$ improves $\mathscr{P}_1$ by minimizing the Rayleigh quotient (1.2) in the subspace $\operatorname{span}\{x^{(\ell)},\, x^{(\ell)} - Tr^{(\ell)}\}$ spanned by the current iterate and the one-step result of $\mathscr{P}_1$. This subspace is identical with $\operatorname{span}\{x^{(\ell)},\, Tr^{(\ell)}\}$ so that $\mathscr{P}_2$ coincides with the optimized version of the gradient iteration (1.4), also known as the preconditioned steepest descent iteration. In the further methods $\mathscr{P}_k$ with $k \geq 3$, the subspace for the local minimization of the Rayleigh quotient is extended as $\operatorname{span}\{x^{(\ell-k+2)}, \ldots, x^{(\ell-1)}, x^{(\ell)}, x^{(\ell)} - Tr^{(\ell)}\}$ or equivalently

$$\operatorname{span}\{x^{(\ell-k+2)}, \ldots, x^{(\ell-1)}, x^{(\ell)}, Tr^{(\ell)}\}$$

by using $k-2$ previous iterates. The initialization of $\mathscr{P}_k$ requires the iterates $x^{(1)}, \ldots, x^{(k-2)}$ which can be computed successively by $\mathscr{P}_2, \ldots, \mathscr{P}_{k-1}$. Then $\mathscr{P}_k$ with $k \geq 3$ is implemented as

$$\left\{\begin{array}{l} V^{(0)} = x^{(0)}\,; \\ \text{for} \quad \ell = 0, 1, 2, \ldots \\ \quad \text{(a) compute the Ritz pairs of } (A, M) \text{ in } \operatorname{span}\{V^{(\ell)}\} \text{ and the residual } r^{(\ell)} \\ \qquad \text{of a Ritz vector } x^{(\ell)} \text{ associated with the smallest Ritz value,} \\ \qquad \text{then check for convergence}\,; \\ \quad \text{(b) compute } Tr^{(\ell)} \text{ by approximately solving the linear system } Aw = r^{(\ell)}\,; \\ \quad \text{(c) set } \; V^{(\ell+1)} = [x^{(0)}, \ldots, x^{(\ell)}, Tr^{(\ell)}] \;\text{ for }\; \ell < k-2 \\ \qquad \text{or } \; V^{(\ell+1)} = [x^{(\ell-k+2)}, \ldots, x^{(\ell-1)}, x^{(\ell)}, Tr^{(\ell)}] \;\text{ for }\; \ell \geq k-2\,; \\ \text{end} \end{array}\right. \tag{1.9}$$

where orthonormalizing the columns of $V^{(\ell+1)}$ can improve the stability. The Rayleigh-Ritz procedure for computing the Ritz pairs refers to the (usually small) projected eigenvalue problem $\big((V^{(\ell)})^T A V^{(\ell)}\big) w = \vartheta \big((V^{(\ell)})^T M V^{(\ell)}\big) w$ which can be solved by using the LAPACK routine `DSYGV` (depending on further LAPACK routines for Cholesky factorization, Householder tridiagonalization and QR algorithm).

Indeed, the implementation (1.9) of $\mathscr{P}_k$ turns into a basic version of the generalized Davidson method [68] by setting $V^{(\ell+1)} = [x^{(0)}, \ldots, x^{(\ell)}, Tr^{(\ell)}]$ for each ℓ. In exact arithmetic, $\mathscr{P}_3$ coincides with the locally optimal preconditioned conjugate gradient (LOPCG) method, i.e., the single-vector version of the LOBPCG method [48]. Their implementations can be stabilized by orthonormalizing basis vectors; cf. [40]. The LOPCG method is a practical variant of the preconditioned conjugate gradient iteration for solving the linear system $(A - \lambda_{\min} M)x = 0$, or in other words, for computing an eigenvector associated with the smallest eigenvalue $\lambda_{\min}$. Since $\lambda_{\min}$ and the associated eigenvectors are usually not computed separately, one has to use an approximate eigenvalue instead of $\lambda_{\min}$, e.g., $\rho(x^{(\ell)})$ as in LOPCG. A remarkable convergence behavior of $\mathscr{P}_3$ is that it cannot be accelerated significantly by $\mathscr{P}_k$ with $k > 3$ (even with respect to the number of outer steps) for typical discretized operator eigenvalue problems such as the Laplacian eigenvalue problem on a square domain. An acceleration by larger k can be observed in the case of clustered eigenvalues; cf. the numerical experiments in [123].

The PINVIT hierarchy also includes the block versions of $\mathscr{P}_k$. These are denoted by $\mathscr{P}_{k,s}$ with the block size s which means that the vector iterates in $\mathscr{P}_k$ are generalized as s-dimensional subspace iterates. The simplest block method $\mathscr{P}_{1,s}$, also called the preconditioned inverse subspace iteration, has the form

$$\operatorname{span}\{X^{(\ell+1)}\} = \operatorname{span}\{X^{(\ell)} - TR^{(\ell)}\} \quad \text{with} \quad R^{(\ell)} = AX^{(\ell)} - MX^{(\ell)}\big((X^{(\ell)})^T A X^{(\ell)}\big).$$

Therein the columns of the basis matrix $X^{(\ell)}$ of the current subspace iterate are given by M-orthonormal Ritz vectors, i.e., $(X^{(\ell)})^T M X^{(\ell)}$ is the identity matrix $I_s \in \mathbb{R}^{s\times s}$, and $(X^{(\ell)})^T A X^{(\ell)}$ is a diagonal matrix whose diagonal entries are the corresponding Ritz values. In the next method $\mathscr{P}_{2,s}$, the subspace $\operatorname{span}\{X^{(\ell)} - TR^{(\ell)}\}$ is extended as $\operatorname{span}\{X^{(\ell)}, TR^{(\ell)}\}$ where the Ritz vectors associated with the s smallest Ritz values are utilized to build the next subspace iterate. The same approach applied to $\operatorname{span}\{X^{(\ell-k+2)}, \ldots, X^{(\ell-1)}, X^{(\ell)}, TR^{(\ell)}\}$ leads to further methods $\mathscr{P}_{k,s}$ with $k \geq 3$. A practical implementation is

$$\left\{\begin{array}{l}
V^{(0)} = X^{(0)}\,; \\
\text{for} \quad \ell = 0, 1, 2, \ldots \\
\qquad \text{(a) compute the Ritz pairs of } (A, M) \text{ in } \operatorname{span}\{V^{(\ell)}\} \text{ and the residuals} \\
\qquad\quad r_1^{(\ell)}, \ldots, r_s^{(\ell)} \text{ of } M\text{-orthonormal Ritz vectors } x_1^{(\ell)}, \ldots, x_s^{(\ell)} \\
\qquad\quad \text{associated with the } s \text{ smallest Ritz values, then check for convergence}\,; \\
\qquad \text{(b) compute } Tr_j^{(\ell)} \text{ by approximately solving the linear systems} \\
\qquad\quad Aw = r_j^{(\ell)}, \quad j = 1, \ldots, s, \quad \text{then set } X^{(\ell)} = [x_1^{(\ell)}, \ldots, x_s^{(\ell)}]\,, \\
\qquad\quad TR^{(\ell)} = [Tr_1^{(\ell)}, \ldots, Tr_s^{(\ell)}]\,; \\
\qquad \text{(c) set } V^{(\ell+1)} = [X^{(0)}, \ldots, X^{(\ell)}, TR^{(\ell)}] \text{ for } \ell < k-2 \\
\qquad\quad \text{or } V^{(\ell+1)} = [X^{(\ell-k+2)}, \ldots, X^{(\ell-1)}, X^{(\ell)}, TR^{(\ell)}] \text{ for } \ell \geq k-2\,; \\
\text{end}
\end{array}\right. \tag{1.10}$$

which turns into a block variant of the generalized Davidson method [68] if one always sets $V^{(\ell+1)} = [X^{(0)}, \ldots, X^{(\ell)}, TR^{(\ell)}]$. Moreover, $\mathscr{P}_{3,s}$ coincides with the LOBPCG method [48].

The above-mentioned eigensolvers from the PINVIT hierarchy are applicable to the generalized matrix eigenvalue problem (1.1) for positive definite M. If M is not necessarily positive definite, one can easily reformulate these eigensolvers with respect to the reverse matrix pair (M, A). For instance, the block method $\mathscr{P}_{k,s}$ with $k \geq 3$ implemented by (1.10) can be reformulated as

$$\left\{\begin{array}{l} V^{(0)} = X^{(0)}\,; \\ \text{for} \quad \ell = 0,\, 1,\, 2,\, \ldots \\ \qquad \text{(a) compute the Ritz pairs of } (M,A) \text{ in } \operatorname{span}\{V^{(\ell)}\} \text{ and the residuals} \\ \qquad\quad \widetilde{r}_1^{(\ell)}, \ldots, \widetilde{r}_s^{(\ell)} \text{ of } A\text{-orthonormal Ritz vectors } x_1^{(\ell)}, \ldots, x_s^{(\ell)} \\ \qquad\quad \text{associated with the } s \text{ largest Ritz values, then check for convergence}\,; \\ \qquad \text{(b) compute } T\widetilde{r}_j^{(\ell)} \text{ by approximately solving the linear systems} \\ \qquad\quad Aw = \widetilde{r}_j^{(\ell)}, \quad j = 1, \ldots, s, \quad \text{then set } \; X^{(\ell)} = [x_1^{(\ell)},\, \ldots,\, x_s^{(\ell)}]\,, \\ \qquad\quad T\widetilde{R}^{(\ell)} = [T\widetilde{r}_1^{(\ell)},\, \ldots,\, T\widetilde{r}_s^{(\ell)}]\,; \\ \qquad \text{(c) set } \; V^{(\ell+1)} = [X^{(0)},\, \ldots,\, X^{(\ell)},\, T\widetilde{R}^{(\ell)}] \; \text{ for } \; \ell < k-2 \\ \qquad\quad \text{or } \; V^{(\ell+1)} = [X^{(\ell-k+2)},\, \ldots,\, X^{(\ell-1)},\, X^{(\ell)},\, T\widetilde{R}^{(\ell)}] \; \text{ for } \; \ell \geq k-2\,; \\ \text{end} \end{array}\right. \tag{1.11}$$

where the residuals $\widetilde{r}_j^{(\ell)}$ are generally defined in (1.7) and the Ritz pairs correspond to the projected eigenvalue problem $\big((V^{(\ell)})^T M V^{(\ell)}\big)w = \theta\big((V^{(\ell)})^T A V^{(\ell)}\big)w$. It is remarkable that the reformulation of the simplest method $\mathscr{P}_1$ and its block form $\mathscr{P}_{1,s}$ requires a modification of the fixed step size in order to compute the largest eigenvalues of (M, A); cf. [50]. For $\mathscr{P}_k$ and $\mathscr{P}_{k,s}$ with $k \geq 2$ one can skip this modification since the associated step sizes are optimized implicitly by the Rayleigh-Ritz procedure.

1.3.2 Sharp convergence estimates

An innovative feature of the PINVIT hierarchy is the following geometric interpretation of $\mathscr{P}_1$ concerning the formula (1.8) for positive definite M. In the case of exact preconditioning $T = A^{-1}$, (1.8) turns into a scaled inverse iteration (inverse power method), namely,

$$x^{(\ell+1)} = x^{(\ell)} - A^{-1}r^{(\ell)} = x^{(\ell)} - A^{-1}\big(Ax^{(\ell)} - \rho(x^{(\ell)})Mx^{(\ell)}\big) = \rho(x^{(\ell)})A^{-1}Mx^{(\ell)}.$$

This consideration motivates the error propagation formula

$$x^{(\ell+1)} - \rho(x^{(\ell)})A^{-1}Mx^{(\ell)} = (I - TA)\big(x^{(\ell)} - \rho(x^{(\ell)})A^{-1}Mx^{(\ell)}\big) \tag{1.12}$$

for investigating (1.8) in the case of inexact preconditioning $T \approx A^{-1}$. Combining (1.12) with the quality condition (1.5) of T results in the inequality

$$\|x^{(\ell+1)} - \rho(x^{(\ell)})A^{-1}Mx^{(\ell)}\|_A \leq \gamma\, \|x^{(\ell)} - \rho(x^{(\ell)})A^{-1}Mx^{(\ell)}\|_A \tag{1.13}$$

which means that the next iterate $x^{(\ell+1)}$ belongs to a ball centred at $\rho(x^{(\ell)})A^{-1}Mx^{(\ell)}$ with respect to the A-norm. This geometric interpretation is fundamental for the derivation of sharp convergence estimates for (1.8) in [72, 73, 50, 74]. In the case that $\rho(x^{(\ell)})$ is located in the interval $(\lambda_j, \lambda_{j+1})$ between two neighboring eigenvalues arranged in ascending order, a concise estimate based on [50, Theorems 1 and 4] reads

$$\frac{\rho(x^{(\ell+1)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell+1)})} \leq \left(\gamma + (1-\gamma)\frac{\lambda_j}{\lambda_{j+1}}\right)^2 \frac{\rho(x^{(\ell)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell)})}. \tag{1.14}$$

Some special $x^{(\ell)}$ can be constructed in a two-dimensional invariant subspace associated with λ_j and λ_{j+1}, with which the inequality in (1.14) turns into an equality in the limit case $\rho(x^{(\ell)}) \to \lambda_j$. In this sense, (1.14) is a sharp estimate. An earlier and somewhat cumbersome variant of (1.14) is strictly sharp in the sense that the equality is attainable without considering any limit cases. It is worthwhile to note that in earlier works such as [75] the words "asymptotically sharp" and "nonasymptotically sharp" are used instead of "sharp" and "strictly sharp". Moreover, the convergence measure $(\cdot - \lambda_j)/(\lambda_{j+1} - \cdot)$ in (1.14) has been applied to various gradient-type eigensolvers, occasionally in the form $(\lambda_j - \cdot)/(\cdot - \lambda_{j+1})$ if the eigenvalues are arranged in descending order; cf. [45, 80, 79]. In particular, [45, Theorem 3.3] concerning an abstract two-stage method is applicable to $\mathscr{P}_1$. The corresponding estimate has been improved and extended by (1.14) regarding the sharpness and the arbitrary eigenvalue interval.

A further geometric interpretation using a cone associated with the ball arising from (1.13) is suggested for $\mathscr{P}_2$ in [75, Section 6.3]. In addition, a conjecture on the convergence rate is presented based on the sharp estimate

$$\frac{\rho(x^{(\ell+1)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell+1)})} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \frac{\rho(x^{(\ell)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell)})} \quad \text{with} \quad \kappa = \frac{\lambda_j(\lambda_{\max} - \lambda_{j+1})}{\lambda_{j+1}(\lambda_{\max} - \lambda_j)} \tag{1.15}$$

for the special version of $\mathscr{P}_2$ with $T = A^{-1}$. Therein $x^{(\ell+1)}$ is a Ritz vector associated with the smallest Ritz value in the subspace

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

(the second equality holds since the positive definiteness of A and M guarantees that $\rho(x^{(\ell)})$ is nonzero). This is a small Krylov subspace with respect to $A^{-1}M$. Indeed, the estimate (1.15) for $j=1$ has already been introduced in an equivalent form in [44, 45] where similar estimates concerning larger Krylov subspaces are derived by means of Chebyshev polynomials. The sharpness of (1.15) for $j=1$ is verified in [75] by solving a parameterized optimization problem stemming from [53]. The proof of (1.15) for arbitrary $j \in \{1, \ldots, n-1\}$ is completed in [80]. Moreover, some arguments from [80] inspire a breakthrough in the convergence theory of $\mathscr{P}_2$ so that the following sharp estimate is achieved in [79]:

$$\frac{\rho(x^{(\ell+1)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell+1)})} \leq \left(\frac{\kappa + \gamma(2-\kappa)}{(2-\kappa) + \gamma\kappa}\right)^2 \frac{\rho(x^{(\ell)}) - \lambda_j}{\lambda_{j+1} - \rho(x^{(\ell)})} \quad \text{with} \quad \kappa = \frac{\lambda_j(\lambda_{\max} - \lambda_{j+1})}{\lambda_{j+1}(\lambda_{\max} - \lambda_j)}. \tag{1.16}$$

It is remarkable that the first convergence estimate of $\mathscr{P}_2$ under its common name "preconditioned steepest descent iteration" has been presented by Samokish in [102], and restated in an alternative form in [89]. The main results in [89] are several improved estimates where the convergence factors depend on the current approximate eigenvalue. For instance, the estimate [89, (6.4)] can be reformulated as

$$\frac{\rho(x^{(\ell+1)}) - \lambda_1}{\lambda_2 - \rho(x^{(\ell+1)})} \leq \left(\frac{\widetilde{\kappa} + \gamma(2-\widetilde{\kappa})}{(2-\widetilde{\kappa}) + \gamma\widetilde{\kappa}}\right)^2 \frac{\rho(x^{(\ell)}) - \lambda_1}{\lambda_2 - \rho(x^{(\ell)})} \quad \text{with} \quad \widetilde{\kappa} = \frac{\rho(x^{(\ell)})(\lambda_{\max} - \lambda_2)}{\lambda_2(\lambda_{\max} - \rho(x^{(\ell)}))}. \tag{1.17}$$

The estimate (1.17) concerns the case that $\rho(x^{(\ell)})$ is located in the interval (λ_1, λ_2), and can easily be compared with (1.16) for $j = 1$. By considering the fact $\widetilde{\kappa} > \kappa$, (1.16) is more accurate than (1.17). However, they provide the same bound in the limit case $\rho(x^{(\ell)}) \to \lambda_1$ and improve a comparable estimate from [85].

It is challenging to extend the geometric interpretation of $\mathscr{P}_1$ to $\mathscr{P}_k$ with $k \geq 3$, since the required previous iterates have to be described together with the current iterate. Moreover, even the extension of the estimate (1.15) to $\mathscr{P}_k$ with exact preconditioning $T = A^{-1}$, called "inverse iteration" (INVIT) $\mathscr{I}_k$ [76], is complicated. In [78], $\mathscr{I}_k$ is interpreted as a truncated Krylov subspace iteration. Therein the relation $Tr^{(\ell)} = A^{-1}r^{(\ell)} = x^{(\ell)} - \rho(x^{(\ell)})A^{-1}Mx^{(\ell)}$ implies that

$$x^{(\ell+1)} \in \operatorname{span}\{x^{(0)}, \ldots, x^{(\ell)}, Tr^{(\ell)}\} = \operatorname{span}\{x^{(0)}, \ldots, x^{(\ell)}, A^{-1}Mx^{(\ell)}\} \quad \text{for} \quad \ell < k-2,$$

$$x^{(\ell+1)} \in \operatorname{span}\{x^{(\ell-k+2)}, \ldots, x^{(\ell)}, Tr^{(\ell)}\} \subseteq \operatorname{span}\{x^{(0)}, \ldots, x^{(\ell)}, A^{-1}Mx^{(\ell)}\} \quad \text{for} \quad \ell \geq k-2.$$

In addition, denoting by $\mathcal{K}^j$ the Krylov subspace of degree j with respect to the matrix $A^{-1}M$ and the initial vector $x^{(0)}$, we have

$$x^{(1)} \in \operatorname{span}\{x^{(0)},\, A^{-1}Mx^{(0)}\} = \mathcal{K}^2$$

and, inductively,

$$\begin{aligned} x^{(\ell+1)} &\in \operatorname{span}\{\underbrace{x^{(0)},\,\ldots,\,x^{(\ell)}}_{\in\mathcal{K}^{\ell+1}},\, A^{-1}M\,\underbrace{x^{(\ell)}}_{\in\mathcal{K}^{\ell+1}}\} \\ &\subseteq \operatorname{span}\{x^{(0)},\, A^{-1}Mx^{(0)},\,\ldots,\,(A^{-1}M)^{\ell}x^{(0)},\,(A^{-1}M)^{\ell+1}x^{(0)}\} = \mathcal{K}^{\ell+2}. \end{aligned}$$

Thus the smallest Ritz value $\vartheta_{\min}$ in $\mathcal{K}^{\ell+2}$ is a better approximation of the smallest eigenvalue in comparison to $\rho(x^{(\ell+1)})$. Due to the empirical argument that $\mathscr{I}_k$ with $k \geq 3$ cannot be accelerated significantly by increasing k, one can assume that $\rho(x^{(\ell+1)})$ is almost as good as $\vartheta_{\min}$ so that the estimates on $\vartheta_{\min}$ are asymptotically applicable to $\rho(x^{(\ell+1)})$. In this sense, some Chebyshev type estimates have been derived in [78] based on classical results from [98, 94] and serve as indirect estimates on $\rho(x^{(\ell+1)})$. However, these estimates are less meaningful in the case of clustered eigenvalues where $\vartheta_{\min}$ could be considerably better than $\rho(x^{(\ell+1)})$. Therefore we prefer to investigate certain iterations which extract, similarly to $\mathscr{I}_k$ with $k \geq 3$, approximate eigenvalues from a series of k-dimensional subspaces within $\mathcal{K}^{\ell+2}$. In particular, we are interested in the convergence behavior of restarted Krylov subspace iterations, and have derived sharp estimates on Ritz vectors and Ritz values in [83, 125] toward the completion of the convergence analysis of $\mathscr{P}_k$.

Furthermore, the convergence behavior of the block method $\mathscr{P}_{k,s}$ can be analyzed by observing certain auxiliary vector iterations which are similar to $\mathscr{P}_k$ [71]. Such an analysis applied to $\mathscr{P}_{1,s}$ generalizes the estimate (1.14) for $\mathscr{P}_1$ as

$$\frac{\vartheta_i^{(\ell+1)} - \lambda_j}{\lambda_{j+1} - \vartheta_i^{(\ell+1)}} \leq \left(\gamma + (1-\gamma)\frac{\lambda_j}{\lambda_{j+1}}\right)^2 \frac{\vartheta_i^{(\ell)} - \lambda_j}{\lambda_{j+1} - \vartheta_i^{(\ell)}}. \tag{1.18}$$

Therein $\vartheta_i^{(\ell)}$, $\vartheta_i^{(\ell+1)}$ denote the ith Ritz values in ascending order in the consecutive subspace iterates $\operatorname{span}\{X^{(\ell)}\}$, $\operatorname{span}\{X^{(\ell+1)}\}$, and $\vartheta_i^{(\ell)}$ is assumed to be located in the interval $(\lambda_j, \lambda_{j+1})$. In [82], we have generalized the estimate (1.16) for $\mathscr{P}_2$ to the block method $\mathscr{P}_{2,s}$ by using a minimax theorem [104, 95]. However, these generalized estimates are not suitable for interpreting the well-known cluster robustness of block eigensolvers. For instance, if the eigenvalues λ_j and λ_{j+1} are very close to each other, (1.18) only shows a slight reduction of the Ritz value. In [126], we have derived a cluster robust estimate for $\mathscr{P}_{1,s}$ based on an alternative interpretation of preconditioning similarly to [84]. This estimate possesses a simpler form and requires a weaker assumption in comparison to the corresponding estimates from [17, 86]. In order to complete the convergence analysis of $\mathscr{P}_{k,s}$, we prefer to begin with some relevant Krylov subspace eigensolvers; cf. [81, 122].

Additionally, the above-mentioned convergence estimates can easily be modified in the case that M is not necessarily positive definite, i.e., for the reformulated $\mathscr{P}_{k,s}$ which computes the largest eigenvalues of the reverse matrix pair (M, A) as in (1.11). For instance, the modification of (1.18) reads

$$\frac{\widetilde{\lambda}_j - \widetilde{\vartheta}_i^{(\ell+1)}}{\widetilde{\vartheta}_i^{(\ell+1)} - \widetilde{\lambda}_{j+1}} \leq \left(\gamma + (1-\gamma)\,\frac{\widetilde{\lambda}_{j+1} - \widetilde{\lambda}_{\min}}{\widetilde{\lambda}_j - \widetilde{\lambda}_{\min}}\right)^2 \frac{\widetilde{\lambda}_j - \widetilde{\vartheta}_i^{(\ell)}}{\widetilde{\vartheta}_i^{(\ell)} - \widetilde{\lambda}_{j+1}}.$$

Therein the eigenvalues and the Ritz values of (M, A) are arranged in descending order.

1.4 Krylov subspace eigensolvers

There is a wide range of Krylov subspace methods for solving matrix eigenvalue problems and the related linear systems; see [59, 28, 99, 113, 36, 92, 60, 5, 29, 8, 9, 1, 41, 55, 13, 26]. We aim at investigating several methods concerning the convergence analysis of the PINVIT hierarchy for solving the generalized matrix eigenvalue problem (1.1). These eigensolvers serve to compute a moderate number of the reciprocally largest eigenvalues (or the smallest positive eigenvalues where appropriate; cf. the end of Section 1.2) of (A, M) and the associated eigenvectors. They generate Krylov subspaces or block-Krylov subspaces with respect to the matrix product $A^{-1}M$ which can be denoted by

$$\mathcal{K}^k(x) = \text{span}\{x,\, A^{-1}Mx,\, \dots,\, (A^{-1}M)^{k-1}x\} \tag{1.19}$$

with the initial vector x, or

$$\mathcal{K}^k(X) = \text{span}\{X,\, A^{-1}MX,\, \dots,\, (A^{-1}M)^{k-1}X\} \tag{1.20}$$

with a basis matrix X of the initial subspace $\mathcal{X}$. The Krylov subspace (1.19) can be built up successively by an invert-Lanczos process

$$\left\{\begin{array}{l} v_1 = x/\|x\|_A\,; \quad w = Mv_1\,; \quad \alpha_1 = v_1^T w\,; \\ w = A^{-1}w - \alpha_1 v_1\,; \quad \beta_1 = \|w\|_A\,; \quad i = 1\,; \\ \text{while} \quad |\beta_i| > \varepsilon \quad \text{and} \quad i < k \\ \qquad v_{i+1} = w/\beta_i\,; \quad i = i+1\,; \quad w = Mv_i\,; \quad \alpha_i = v_i^T w\,; \\ \qquad w = A^{-1}w - \alpha_i v_i - \beta_{i-1}v_{i-1}\,; \quad \beta_i = \|w\|_A\,; \\ \text{end} \end{array}\right. \tag{1.21}$$

where $A^{-1}w$ is computed by solving the corresponding linear system. The process (1.21) determines a basis matrix V consisting of A-orthonormal basis vectors $v_1, \dots, v_{i_{\max}}$. Moreover, V^TMV is a symmetric tridiagonal matrix with $\alpha_1, \dots \alpha_{i_{\max}}$ as diagonal entries and $\beta_1, \dots \beta_{i_{\max}-1}$ as subdiagonal and superdiagonal entries. Thus the projected eigenvalue problem $\big(V^TMV\big)w = \widetilde{\vartheta}\big(V^TAV\big)w$ from the Rayleigh-Ritz procedure applied to the reverse matrix pair (M, A) has an ideal form and can be handled directly by a shifted QR algorithm. The resulting Ritz vectors of (M, A) associated with Ritz values $\widetilde{\vartheta}$ can be extracted as Ritz vectors of (A, M) associated with Ritz values $\widetilde{\vartheta}^{-1}$ (including infinity). Similarly, the block-Krylov subspace (1.20) can be constructed by a block invert-Lanczos process. Therein A-orthonormal basis vectors are determined together with a block-tridiagonal matrix. However, the theoretical orthogonality is often destroyed due to rounding errors [91]. Additional orthogonalization can stabilize the process. Alternatively, one can construct (block-)Krylov subspaces by using residuals of Ritz vectors; cf. variants of the Davidson method [68, 67, 70, 20, 107, 87, 88] and the implementation (1.11) of a reformulated $\mathscr{P}_{k,s}$.

1.4.1 Classification

In order to classify typical Krylov subspace eigensolvers for computing the reciprocally largest eigenvalues of the matrix pair (A, M) from (1.1), we denote by $\text{RR}\,(\mathcal{K}, s)$ the Rayleigh-Ritz procedure which extracts A-orthonormal Ritz vectors of (A, M) in a given subspace $\mathcal{K} \subseteq \mathbb{R}^n$ associated with the s reciprocally largest Ritz values. We consider the following four types based on an overview from [6]:

Standard Krylov subspace iterations (SK)

$$\text{RR}\,\big(\mathcal{K}^k(x^{(0)}), s\big) \quad \text{with increasing } k > s, \tag{1.22}$$

Restarted Krylov subspace iterations (RK)

$$\mathcal{K}^c(x^{(\ell+1)}) \quad \leftarrow \quad \mathrm{RR}\left(\mathcal{K}^k(x^{(\ell)}), c\right) \quad \text{with fixed } k > s \text{ and fixed } c \in [s, k), \tag{1.23}$$

Block-Krylov subspace iterations (BK)

$$\mathrm{RR}\left(\mathcal{K}^k(X^{(0)}), s\right) \quad \text{with increasing } k, \tag{1.24}$$

Restarted block-Krylov subspace iterations (RBK)

$$X^{(\ell+1)} \quad \leftarrow \quad \mathrm{RR}\left(\mathcal{K}^k(X^{(\ell)}), c\right) \quad \text{with fixed } k \text{ and fixed } c \geq s. \tag{1.25}$$

The type SK uses a Krylov subspace $\mathcal{K}^k(x^{(0)})$ of increasing degree $k > s$. The s reciprocally largest Ritz values $\vartheta_1^{(k)}, \dots, \vartheta_s^{(k)}$ in $\mathcal{K}^k(x^{(0)})$ form the sequences $(\vartheta_i^{(k)})_{k\in\mathbb{N}}$, $i = 1, \dots, s$, which are reciprocally nondecreasing according to the Courant-Fischer principles applied to the reverse matrix pair (M, A). Moreover, the limits of $(\vartheta_i^{(k)})_{k\in\mathbb{N}}$ are the s reciprocally largest of all those distinct eigenvalues for which the eigenprojections of the initial vector $x^{(0)}$ are nonzero. A pseudorandom $x^{(0)}$ usually has no zero eigenprojections so that the limits are simply the s reciprocally largest distinct eigenvalues.

The type RK uses a series of Krylov subspaces of fixed degree $k > s$ in order to reduce the storage requirement. The construction of the next Krylov subspace $\mathcal{K}^k(x^{(\ell+1)})$ depends on the c reciprocally largest Ritz values in the current Krylov subspace $\mathcal{K}^k(x^{(\ell)})$. A properly selected $c \in [s, k)$ can ensure a sufficiently large distance between the sth and the $(c+1)$ th reciprocally largest eigenvalues so that the iterations are cluster robust. The next initial vector $x^{(\ell+1)}$ does not need to be determined explicitly. Instead, one can first construct the Krylov subspace $\mathcal{K}^c(x^{(\ell+1)})$ of degree c and subsequently extend it as $\mathcal{K}^k(x^{(\ell+1)})$. For constructing $\mathcal{K}^c(x^{(\ell+1)})$, one can utilize Ritz vectors in $\mathcal{K}^k(x^{(\ell)})$ associated with the c reciprocally largest Ritz values or implement a shifted QR algorithm with the remaining Ritz values as shifts; cf. the thick-restart Lanczos method [118] and the implicitly restarted Lanczos method [19] related to [106].

The types BK and RBK analogously generate a growing block-Krylov subspace or a series of block-Krylov subspaces. A benefit of BK and RBK is that they can determine entire eigenspaces associated with multiple eigenvalues provided that the dimension of the initial subspace is sufficiently large. In contrast to this, SK and NK can only determine the nonzero eigenprojections of the initial vector which correspond to one-dimensional subspaces within the eigenspaces. Moreover, the block implementation generally improves the cluster robustness; cf. the analysis of the block power method in [97].

For analyzing the convergence behavior of these Krylov subspace eigensolvers, we prefer to denote the eigenvalues of (A, M) together with the associated eigenspaces or eigenvectors in two different ways.

Notation 1.1. *Consider a matrix pair (A, M) of symmetric matrices $A, M \in \mathbb{R}^{n\times n}$ where A is positive definite. Its distinct eigenvalues $\lambda_1, \dots, \lambda_m$ are arranged in reciprocally descending order, i.e., $\lambda_1^{-1} > \cdots > \lambda_m^{-1}$. Let $\mathcal{W}_1, \dots, \mathcal{W}_m$ be the associated eigenspaces, and denote by P_i the eigenprojector on $\mathcal{W}_i$ for $i = 1, \dots, m$.*

Notation 1.2. *Consider a matrix pair (A, M) of symmetric matrices $A, M \in \mathbb{R}^{n\times n}$ where A is positive definite. Its eigenvalues $\lambda_1, \dots, \lambda_n$ are arranged in reciprocally descending order, i.e., $\lambda_1^{-1} \geq \cdots \geq \lambda_n^{-1}$. Let $w_1, \dots, w_n$ be A-orthonormal eigenvectors associated with $\lambda_1, \dots, \lambda_n$, and denote by P_i the eigenprojector on* $\mathrm{span}\{w_i\}$ *for $i = 1, \dots, n$.*

The eigenprojector P_i in Notations 1.1 and 1.2 is an A-orthogonal projector and can be constructed by using an arbitrary basis W_i of $\mathcal{W}_i$ or $\mathrm{span}\{w_i\}$ in the form

$$P_i = W_i(W_i^T A W_i)^{-1}(A W_i)^T.$$

If M is positive definite, P_i is also an M-orthogonal projector, namely,

$$P_i = W_i(W_i^T AW_i)^{-1}(AW_i)^T = W_i(W_i^T \lambda_i MW_i)^{-1}(\lambda_i MW_i)^T = W_i(W_i^T MW_i)^{-1}(MW_i)^T.$$

Notation 1.1 is particularly suitable for SK and NK since therein the iterates belong to an invariant subspace spanned by the eigenprojections $P_i x^{(0)}$ of the initial vector $x^{(0)}$ to the eigenspaces $\mathcal{W}_i$. A similar description "eigenprojections of the initial subspace $\mathcal{X}^{(0)}$" for BK and RBK is not always meaningful since $\mathcal{X}^{(0)}$ can have a higher dimension than some eigenspaces. Instead, A-orthogonal projections of $\mathcal{X}^{(0)}$ to invariant subspaces can easily be defined by using Notation 1.2, e.g., $(P_1 + \cdots + P_c)\,\mathcal{X}^{(0)}$ with $c \geq \dim \mathcal{X}^{(0)}$.

1.4.2 Reciprocal representations

In order to simplify our convergence analysis, we represent the generalized matrix eigenvalue problem (1.1) by a standard matrix eigenvalue problem $Hy = \lambda^{-1}y$ based on the substitution

$$H = A^{-1/2}MA^{-1/2}, \qquad y = A^{1/2}x \tag{1.26}$$

as in our previous works [83, 125, 122]. Therein the square roots $A^{-1/2}$ and $A^{1/2}$ of the symmetric and positive definite matrices A^{-1} and A only serve as auxiliary matrices in the substitution. They are not required in our convergence estimates or for the numerical implementation of the considered eigensolvers. Moreover, H is evidently real symmetric, and possesses the positive definiteness in the case that M is positive definite, namely,

$$w \in \mathbb{R}^n \backslash \{0\} \quad \Rightarrow \quad A^{-1/2}w \in \mathbb{R}^n \backslash \{0\} \quad \Rightarrow \quad w^T Hw = (A^{-1/2}w)^T M(A^{-1/2}w) > 0.$$

We call the affiliated representations of vectors and subspaces reciprocal representations by considering the fact that the eigenvalues of H are reciprocals of the eigenvalues of (A, M). We first introduce the reciprocal representations of Krylov subspaces and block-Krylov subspaces. Based on the reformulation

$$A^{1/2}(A^{-1}M)^i x = (A^{-1/2}MA^{-1/2})^i(A^{1/2}x) = H^i y, \qquad i = 0, 1, \ldots, k-1,$$

the Krylov subspaces from (1.19) are represented by

$$A^{1/2}\mathcal{K}^k(x) = A^{1/2}\text{span}\{x, A^{-1}Mx, \ldots, (A^{-1}M)^{k-1}x\} = \text{span}\{y, Hy, \ldots, H^{k-1}y\},$$

i.e., by Krylov subspaces with respect to the matrix H. We denote them by

$$\widehat{\mathcal{K}}^k(y) = \text{span}\{y, Hy, \ldots, H^{k-1}y\} = A^{1/2}\mathcal{K}^k(x). \tag{1.27}$$

Analogously, by using $Y = A^{1/2}X$, the block-Krylov subspaces from (1.20) are represented by

$$\widehat{\mathcal{K}}^k(Y) = \text{span}\{Y, HY, \ldots, H^{k-1}Y\} = A^{1/2}\mathcal{K}^k(X). \tag{1.28}$$

The reciprocal representations of the Ritz vectors in $\mathcal{K}^k(x)$ and $\mathcal{K}^k(X)$ can be described together in the following more general form.

Remark 1.3. *With the substitution* (1.26)*, the Rayleigh-Ritz procedure with respect to* (A, M) *and the basis matrix* V *of a given subspace* $\mathcal{K} \subseteq \mathbb{R}^n$ *corresponds to the Rayleigh-Ritz procedure with respect to* H *and the basis matrix* $U = A^{1/2}V$ *of the subspace* $\widehat{\mathcal{K}} = A^{1/2}\mathcal{K}$*. The projected eigenvalue problem* $\big(V^T AV\big)w = \vartheta\big(V^T MV\big)w$ *has the representation* $\big(U^T U\big)w = \vartheta\big(U^T HU\big)w$*, or equivalently,* $\big(U^T HU\big)w = \vartheta^{-1}\big(U^T U\big)w$*. Thus a Ritz pair* (ϑ, v) *of* (A, M) *in* $\mathcal{K}$ *corresponds to a Ritz pair* (θ, u) *of* H *in* $\widehat{\mathcal{K}}$ *by setting* $\theta = \vartheta^{-1}$ *and* $u = A^{1/2}v$*.*

Consequently, the four types of Krylov subspace iterations introduced in Subsection 1.4.1 can be represented by using the Rayleigh-Ritz procedure $\widehat{\mathrm{RR}}\,(\widehat{\mathcal{K}}, s)$ which extracts orthonormal Ritz vectors of H in a given subspace $\widehat{\mathcal{K}} \subseteq \mathbb{R}^n$ associated with the s largest Ritz values. The resulting representations are the following Krylov subspace iterations concerning H:

$$\widehat{\mathrm{RR}}\left(\widehat{\mathcal{K}}^k(y^{(0)}), s\right) \quad \text{with increasing } k > s, \tag{1.29a}$$

$$\widehat{\mathcal{K}}^c(y^{(\ell+1)}) \quad \leftarrow \quad \widehat{\mathrm{RR}}\left(\widehat{\mathcal{K}}^k(y^{(\ell)}), c\right) \quad \text{with fixed } k > s \text{ and fixed } c \in [s, k), \tag{1.29b}$$

$$\widehat{\mathrm{RR}}\left(\widehat{\mathcal{K}}^k(Y^{(0)}), s\right) \quad \text{with increasing } k, \tag{1.29c}$$

$$Y^{(\ell+1)} \quad \leftarrow \quad \widehat{\mathrm{RR}}\left(\widehat{\mathcal{K}}^k(Y^{(\ell)}), c\right) \quad \text{with fixed } k \text{ and fixed } c \geq s. \tag{1.29d}$$

Furthermore, we reformulate Notations 1.1 and 1.2 with respect to H. The eigenvalues of H can be denoted by $\mu_i = \lambda_i^{-1}$ with eigenvalues λ_i of (A, M). The associated eigenspaces and eigenvectors of H are given by

$$\mathcal{Z}_i = A^{1/2}\mathcal{W}_i \qquad \text{and} \qquad z_i = A^{1/2}w_i \tag{1.30}$$

with eigenspaces $\mathcal{W}_i$ and eigenvectors w_i of (A, M).

Notation 1.4. *Consider a symmetric matrix $H \in \mathbb{R}^{n\times n}$ together with its distinct eigenvalues $\mu_1 > \cdots > \mu_m$ and the associated eigenspaces $\mathcal{Z}_1, \ldots, \mathcal{Z}_m$. Denote by Q_i the eigenprojector on $\mathcal{Z}_i$ for $i = 1, \ldots, m$.*

Notation 1.5. *Consider a symmetric matrix $H \in \mathbb{R}^{n\times n}$ together with its eigenvalues $\mu_1 \geq \cdots \geq \mu_n$. Let $z_1, \ldots, z_n$ be orthonormal eigenvectors associated with $\mu_1, \ldots, \mu_n$, and denote by Q_i the eigenprojector on* $\mathrm{span}\{z_i\}$ *for $i = 1, \ldots, n$.*

The eigenprojector Q_i in Notations 1.4 and 1.5 is an orthogonal projector and can be constructed by using an arbitrary basis Z_i of $\mathcal{Z}_i$ or $\mathrm{span}\{z_i\}$ in the form

$$Q_i = Z_i(Z_i^T Z_i)^{-1} Z_i^T.$$

If H is positive definite, Q_i is also an H-orthogonal projector, namely,

$$Q_i = Z_i(Z_i^T Z_i)^{-1} Z_i^T = Z_i(Z_i^T \mu_i^{-1} H Z_i)^{-1}(\mu_i^{-1} H Z_i)^T = Z_i(Z_i^T H Z_i)^{-1}(H Z_i)^T.$$

1.4.3 Convergence measures and basic properties

Our convergence analysis focuses on the four types of Krylov subspace iterations introduced in Subsection 1.4.1 concerning the matrix pair (A, M) with Notations 1.1 and 1.2. The central estimates are formulated for their reciprocal representations listed in (1.29) concerning the matrix H with Notations 1.4 and 1.5 so that these estimates can easily be compared with some classical estimates. The associated convergence measures and some basic properties are introduced below.

With Notation 1.1, the initial vector x of a Krylov subspace $\mathcal{K}^k(x)$ defined in (1.19) can be represented by $x = \sum_{i=1}^m P_i x$ with its eigenprojections $P_i x$. Then $\mathcal{K}^k(x)$ is a subset of the invariant subspace spanned by all those nonzero $P_i x$. Each nonzero $P_i x$ is an eigenvector associated with the eigenvalue λ_i, and can be approximated by a Ritz vector in $\mathcal{K}^k(x)$. With Notation 1.2, the invariant subspace $\mathrm{span}\{w_1, \ldots, w_s\}$ can be approximated by an s-dimensional subspace within a block-Krylov subspace $\mathcal{K}^k(\mathcal{X})$ defined in (1.20) in the case that the projection $(P_1 + \cdots + P_s)\,x$ of each $x \in \mathcal{X}\backslash\{0\}$ is nonzero.

The approximation of such eigenvectors and invariant subspaces can be measured in terms of trigonometric values of A-angles or Euclidean angles. A general definition is as follows:

Definition 1.6. *Let $\Psi \in \mathbb{R}^{n\times n}$ be a symmetric and positive definite matrix. Denote by $(\cdot\,,\cdot)_\Psi$ and $\|\cdot\|_\Psi$ the corresponding Ψ-inner product and Ψ-norm, i.e.,*

$$(u,v)_\Psi = u^T\Psi\, v = v^T\Psi\, u \qquad \text{and} \qquad \|u\|_\Psi = (u,u)_\Psi^{1/2} \qquad \text{for} \quad u,\, v \in \mathbb{R}^n.$$

Then, concerning arbitrary nonzero vectors $u, v \in \mathbb{R}^n$ and subspaces $\mathcal{U}, \mathcal{V} \subseteq \mathbb{R}^n$ with $1 \le \dim\mathcal{U} \le \dim\mathcal{V}$, the following Ψ-angles are defined:

$$\begin{aligned} \angle_\Psi(u,v) &= \arccos\left(\frac{(u,v)_\Psi}{\|u\|_\Psi\,\|v\|_\Psi}\right), \qquad \angle_\Psi(u,\mathcal{V}) = \min_{v\in\mathcal{V}\backslash\{0\}} \angle_\Psi(u,v), \\ \angle_\Psi(\mathcal{U},\mathcal{V}) &= \max_{u\in\mathcal{U}\backslash\{0\}} \angle_\Psi(u,\mathcal{V}) = \max_{u\in\mathcal{U}\backslash\{0\}}\ \min_{v\in\mathcal{V}\backslash\{0\}} \angle_\Psi(u,v). \end{aligned} \tag{1.31}$$

These angles have the ranges $\angle_\Psi(u,v) \in [0,\pi]$, $\angle_\Psi(u,\mathcal{V}) \in [0,\frac{1}{2}\pi]$, $\angle_\Psi(\mathcal{U},\mathcal{V}) \in [0,\frac{1}{2}\pi]$ and the relations

$$\begin{aligned} \sin\angle_\Psi(u,\mathcal{V}) &= \min_{v\in\mathcal{V}\backslash\{0\}} \sin\angle_\Psi(u,v), & \sin\angle_\Psi(\mathcal{U},\mathcal{V}) &= \max_{u\in\mathcal{U}\backslash\{0\}} \sin\angle_\Psi(u,\mathcal{V}), \\ \cos\angle_\Psi(u,\mathcal{V}) &= \max_{v\in\mathcal{V}\backslash\{0\}} \big|\cos\angle_\Psi(u,v)\big|, & \cos\angle_\Psi(\mathcal{U},\mathcal{V}) &= \min_{u\in\mathcal{U}\backslash\{0\}} \cos\angle_\Psi(u,\mathcal{V}), \\ \tan\angle_\Psi(u,\mathcal{V}) &= \min_{v\in\mathcal{V}\backslash\{0\}} \big|\tan\angle_\Psi(u,v)\big|, & \tan\angle_\Psi(\mathcal{U},\mathcal{V}) &= \max_{u\in\mathcal{U}\backslash\{0\}} \tan\angle_\Psi(u,\mathcal{V}), \\ \angle_\Psi(v,u) = \angle_\Psi(u,v), & & \angle_\Psi(\mathcal{V},\mathcal{U}) = \angle_\Psi(\mathcal{U},\mathcal{V}) & \quad \text{if} \quad \dim\mathcal{U} = \dim\mathcal{V}. \end{aligned} \tag{1.32}$$

Moreover, an alternative definition of $\angle_\Psi(u,\mathcal{V})$ by using the Ψ-orthogonal projector P on $\mathcal{V}$ reads

$$\angle_\Psi(u,\mathcal{V}) = \arcsin\left(\frac{\|u-Pu\|_\Psi}{\|u\|_\Psi}\right) = \arccos\left(\frac{\|Pu\|_\Psi}{\|u\|_\Psi}\right) = \arctan\left(\frac{\|u-Pu\|_\Psi}{\|Pu\|_\Psi}\right) \tag{1.33}$$

where $\arctan(\infty) = \frac{1}{2}\pi$ is added for completeness. If Ψ is the identity matrix $I \in \mathbb{R}^{n\times n}$, the above Ψ-terms are Euclidean terms, and are thus denoted by $(\cdot\,,\cdot)_2$, $\|\cdot\|_2$, $\angle_2(\cdot\,,\cdot)$, respectively.

Based on Definition 1.6, certain coefficient ratios of approximate eigenvectors can be interpreted as trigonometric values. For instance, we consider an arbitrary nonzero vector $\widetilde{x}$ from the Krylov subspace $\mathcal{K}^k(x)$ and denote by τ the index set of all nonzero eigenprojections $P_i x$ of the initial vector x. Normalizing these nonzero eigenprojections with respect to $\|\cdot\|_A$ yields A-orthonormal eigenvectors $w_i = P_i x/\|P_i x\|_A$. Then $\mathcal{K}^k(x)$ is a subset of $\operatorname{span}\{w_j\,;\, j\in\tau\}$ so that $\widetilde{x}$ belongs to $\operatorname{span}\{w_j\,;\, j\in\tau\}$ and can be represented by $\widetilde{x} = \sum_{j\in\tau}\alpha_j w_j$ with coefficients $\alpha_j \in \mathbb{R}$. Then, by using (1.31), the cosine squared of the A-angle between w_i and $\widetilde{x}$ has the form

$$\cos^2\angle_A(w_i,\widetilde{x}) = \frac{(w_i,\widetilde{x})_A^2}{\|w_i\|_A^2\,\|\widetilde{x}\|_A^2} = \frac{(w_i^T A\,\widetilde{x})^2}{\|\widetilde{x}\|_A^2} = \frac{\big(\sum_{j\in\tau}\alpha_j w_i^T A w_j\big)^2}{\sum_{j\in\tau}\alpha_j^2} = \frac{\alpha_i^2}{\sum_{j\in\tau}\alpha_j^2}.$$

In addition, Definition 1.6 can be applied to the conversion of A-angles concerning the matrix pair (A,M) into Euclidean angles concerning the matrix H and vice versa. The conversion makes use of the equivalence

$$(u,v)_A = u^T A v = \big(A^{1/2}u\big)^T\big(A^{1/2}v\big) = (\widehat{u},\widehat{v})_2$$

for arbitrary nonzero vectors $u, v \in \mathbb{R}^n$ and their reciprocal representations $\widehat{u} = A^{1/2}u$, $\widehat{v} = A^{1/2}v$ based on the substitution (1.26). Consequently, the A-angles between two objects with Notation 1.1 coincide with the Euclidean angles between the corresponding reciprocal representations with Notation 1.4. For instance, we consider an arbitrary basis W_i of the eigenspace $\mathcal{W}_i$ from Notation

1.1 together with its reciprocal representation $Z_i = A^{1/2}W_i$ which is a basis of the eigenspace $\mathcal{Z}_i = A^{1/2}\mathcal{W}_i$ from Notation 1.4 due to (1.30). Then the corresponding eigenprojectors P_i and Q_i have the relation

$$Q_i = Z_i(Z_i^T Z_i)^{-1}Z_i^T = (A^{1/2}W_i)(W_i^T AW_i)^{-1}(A^{1/2}W_i)^T = A^{1/2}P_iA^{-1/2}.$$

Combining this with the substitution (1.26) implies that

$$Q_iy = (A^{1/2}P_iA^{-1/2})(A^{1/2}x) = A^{1/2}(P_ix),$$

i.e., Q_iy is the reciprocal representation of P_ix. Moreover, $\widehat{\mathcal{K}}^k(y)$ is the reciprocal representation of $\mathcal{K}^k(x)$ due to (1.27) so that

$$\angle_2\big(Q_iy,\, \widehat{\mathcal{K}}^k(y)\big) = \angle_A\big(P_ix,\, \mathcal{K}^k(x)\big)$$

holds. In the case that M is positive definite, Definition 1.6 is also applicable to the conversion between M-angles and H-angles based on the equivalence

$$(u,v)_M = u^T Mv = \big(A^{1/2}u\big)^T(A^{-1/2}MA^{-1/2})\big(A^{1/2}v\big) = (\widehat{u},\widehat{v})_H.$$

Furthermore, the approximation of eigenvalues can be measured in terms of relative positions in eigenvalue intervals. As an example, we consider the convergence measure $(\mu_i - \cdot\,)/(\,\cdot - \mu_{i+1})$ concerning the interval (μ_{i+1}, μ_i) which is compatible with Notations 1.4 and 1.5. Typically, we apply this measure to a Ritz pair (θ, u) of H in a subspace $\widehat{\mathcal{K}} \subseteq \mathbb{R}^n$. As mentioned in Remark 1.3, (θ, u) can be used as the reciprocal representation of a Ritz pair (ϑ, v) of (A, M) in a subspace $\mathcal{K} \subseteq \mathbb{R}^n$ based on the relations $\widehat{\mathcal{K}} = A^{1/2}\mathcal{K}$, $\theta = \vartheta^{-1}$ and $u = A^{1/2}v$. Then, by considering that μ_i and μ_{i+1} correspond to reciprocals of the eigenvalues λ_i and λ_{i+1} of (A, M) in Notations 1.1 and 1.2, it holds that

$$\frac{\mu_i - \theta}{\theta - \mu_{i+1}} = \frac{\lambda_i^{-1} - \vartheta^{-1}}{\vartheta^{-1} - \lambda_{i+1}^{-1}} = \left(\frac{\lambda_{i+1}}{\lambda_i}\right)\left(\frac{\vartheta - \lambda_i}{\lambda_{i+1} - \vartheta}\right)$$

for $\theta \in (\mu_{i+1}, \mu_i)$. This suggests equivalent convergence measures for a Ritz value ϑ of (A, M). Additionally, in order to compare ϑ with an improved Ritz value ϑ', we can use the corresponding reciprocal representation $\theta' = \vartheta'^{-1}$ and consider the ratio

$$\left(\frac{\mu_i - \theta'}{\theta' - \mu_{i+1}}\right)\left(\frac{\mu_i - \theta}{\theta - \mu_{i+1}}\right)^{-1} = \left(\frac{\vartheta' - \lambda_i}{\lambda_{i+1} - \vartheta'}\right)\left(\frac{\vartheta - \lambda_i}{\lambda_{i+1} - \vartheta}\right)^{-1}.$$

Moreover, we prefer to use the convergence measure $(\,\cdot - \lambda_i)/(\lambda_{i+1} - \cdot\,)$ in the case that M is positive definite; cf. the estimate (1.14) for the PINVIT method $\mathscr{P}_1$. Therein one can denote the Ritz values ϑ, ϑ' of (A, M) by $\rho(v)$, $\rho(v')$ with the associated Ritz vectors v, v' and the Rayleigh quotient $\rho(\cdot)$ defined in (1.2). Then, by using the reciprocal representations $u = A^{1/2}v$, $u' = A^{1/2}v'$ and the Rayleigh quotient

$$\mu : \mathbb{R}^n\backslash\{0\} \to \mathbb{R}, \qquad \mu(y) = \frac{y^T Hy}{y^T y}, \tag{1.34}$$

it holds that

$$\mu(u) = \frac{(A^{1/2}v)^T(A^{-1/2}MA^{-1/2})(A^{1/2}v)}{(A^{1/2}v)^T(A^{1/2}v)} = \frac{v^T Mv}{v^T Av} = \big(\rho(v)\big)^{-1} = \vartheta^{-1} = \theta,$$

and analogously $\mu(u') = \big(\rho(v')\big)^{-1} = \vartheta'^{-1} = \theta'$. This yields the ratio transformation

$$\left(\frac{\mu_i - \mu(u')}{\mu(u') - \mu_{i+1}}\right)\left(\frac{\mu_i - \mu(u)}{\mu(u) - \mu_{i+1}}\right)^{-1} = \left(\frac{\rho(v') - \lambda_i}{\lambda_{i+1} - \rho(v')}\right)\left(\frac{\rho(v) - \lambda_i}{\lambda_{i+1} - \rho(v)}\right)^{-1}.$$

Finally, we introduce the Chebyshev polynomials (of the first kind) which are frequently used in the convergence theory of Krylov subspace eigensolvers. They are defined by

$$T_t(\xi) = \begin{cases} \cos\big(t \arccos \xi\big) & \text{for } \xi \in [-1,1] \\ \frac{1}{2}\Big(\big(\xi - \sqrt{\xi^2-1}\big)^t + \big(\xi + \sqrt{\xi^2-1}\big)^t\Big) & \text{for } \xi \in (-\infty,-1) \cup (1,\infty) \end{cases} \tag{1.35}$$

and possess the properties

$$T_t(1) = 1, \qquad \frac{d}{d\xi}\,T_t(\xi) > 0 \;\text{ for }\; \xi \geq 1 \qquad \text{and} \qquad |T_t(\xi)| \leq 1 \;\Leftrightarrow\; |\xi| \leq 1. \tag{1.36}$$

For investigating Krylov subspace eigensolvers, one can define a type of shifted Chebyshev polynomials concerning nontarget eigenvalues in order to construct certain auxiliary vectors. For instance, if $\mu_{s+1}, \dots, \mu_m$ are nontarget eigenvalues of the matrix H with Notation 1.4, we can use the shifted Chebyshev polynomial

$$p(\alpha) = T_t\left(1 + 2\,\frac{\alpha - \mu_{s+1}}{\mu_{s+1} - \mu_m}\right)$$

for which the properties from (1.36) yield

$$p(\mu_{s+1}) = 1, \qquad \frac{d}{d\alpha}\,p(\alpha) > 0 \;\text{ for }\; \alpha \geq \mu_{s+1} \qquad \text{and} \qquad |p(\alpha)| \leq 1 \;\Leftrightarrow\; \mu_{s+1} \geq \alpha \geq \mu_m.$$

In particular, it holds that

$$p(\mu_l) \geq p(\mu_s) > 1 \quad \forall\, l \in \{1,\dots,s\}, \qquad \text{and} \qquad |p(\mu_l)| \leq 1 \quad \forall\, l \in \{s+1,\dots,m\}$$

so that the ratio $\big(\max_{l>s} |p(\mu_l)|\big) \,/\, \big(\min_{l\leq s} |p(\mu_l)|\big)$ concerning the eigenexpansion

$$p(H)w \;=\; p(H)\textstyle\sum_{l=1}^m Q_l w \;=\; \textstyle\sum_{l=1}^m p(\mu_l) Q_l w$$

of an auxiliary vector $p(H)w$ results in the Chebyshev factor

$$\frac{1}{p(\mu_s)} = \left[T_t\left(1 + 2\,\frac{\mu_s - \mu_{s+1}}{\mu_{s+1} - \mu_m}\right)\right]^{-1}.$$

2 Classical convergence estimates for Krylov subspace eigensolvers

The research on the convergence analysis for Krylov subspace eigensolvers began more than six decades ago. In 1951, Hestenes and Karush analyzed in their work [39] the convergence behavior of several variants of the Rayleigh quotient gradient iteration for computing some eigenpairs of a real symmetric matrix. An extended iteration corresponding to the Lanczos method [59] was investigated in [39, Sections IX, X, XI]. The resulting asymptotic convergence estimate is somewhat suboptimal since it requires an assumption on the fixed step size of an auxiliary gradient iteration.

As the nowadays common ingredients for analyzing the convergence behavior of Krylov subspace eigensolvers, the Chebyshev polynomials were first suggested by Kaniel [42] in 1966, partially based on Stiefel's work [108]. A collection of classical Chebyshev type estimates for standard Krylov subspace iterations was presented by Parlett [94, Section 12.4]. Therein Kaniel's estimates from [42] with corrections by Paige [90] were compared with similar estimates from Saad's work [98, Section 2]. Parlett preferred Saad's estimates on the basis of the numerical tests in [94, Section 12.5]. The central part of these classical estimates is the Chebyshev factor $[T_{k-i}(1+2\gamma_i)]^{-1}$ with a Chebyshev polynomial $T_{k-i}(\cdot)$ defined in (1.35) and an eigenvalue gap ratio $\gamma_i > 0$, depending on the degree k of the corresponding Krylov subspace and the index i of the considered eigenpair. This factor decreases rapidly with k provided that γ_i is bounded away from zero. However, γ_i is close to zero for clustered eigenvalues. In this case, a refined Chebyshev factor $[T_{k-i-t}(1+2\widetilde{\gamma}_i)]^{-1}$ with $\widetilde{\gamma}_i \gg 0$ can be constructed by using an auxiliary vector which is orthogonal to an invariant subspace associated with t clustered eigenvalues; cf. [98, Theorem 4]. Nevertheless, some further and possibly large factors in the estimates cannot be refined in this way. Thus these classical estimates can only provide meaningful bounds for sufficiently large k, and are less suitable for low-dimensional Krylov subspaces arising from restarted Krylov subspace iterations. Furthermore, these classical estimates can be generalized to block-Krylov subspace iterations; cf. Saad's work [98, Section 3]. The resulting estimates also have the drawback that some possibly large factors prevent a reasonable application to restarted iterations. It is worth mentioning that some Chebyshev type estimates presented by Knyazev [44, 45] do not require any factors other than the Chebyshev factors, and provide significantly better bounds in certain cases. This inspires us to improve Saad's estimates by generalizing Knyazev's analysis.

This chapter is devoted to reviewing the classical Chebyshev type estimates and showing the necessity of improving them. We focus on the standard matrix eigenvalue problem $Hy = \mu y$ with Notations 1.4 and 1.5. In the case that H is positive definite, one can additionally derive estimates in terms of H-angles.

In Section 2.1, we restate and compare the classical estimates by Saad [98] and Knyazev [44, 45]. Their disadvantages and limitations are discussed concerning restarted and block iterations. Some auxiliary vectors are reviewed in Section 2.2 based on the analysis from [98] in order to discover the causes of suboptimal bounds. Moreover, in Section 2.3, several supplementary arguments from [44, 45] which serve as tools for deriving new estimates in further chapters are formulated in lemmas with more direct and elementary proofs. In addition, an overview of some improvements of the classical estimates is given concerning the four types of Krylov subspace eigensolvers introduced in Subsection 1.4.1.

2.1 Classical estimates by Saad and Knyazev

We review and reformulate the classical estimates from [98, 44, 45] with Notations 1.4 and 1.5. For the sake of simplicity, the Krylov subspaces $\widehat{\mathcal{K}}^k(y)$ and the block-Krylov subspaces $\widehat{\mathcal{K}}^k(Y)$ defined in (1.27) and (1.28) are denoted by $\mathcal{K}$ within the associated theorems. We slightly modify Saad's estimates from [98] concerning the trigonometric representation of some coefficient ratios; cf. [94, Theorem 12.4.1] by Parlett. Furthermore, Knyazev's estimates from [44, 45] were not directly formulated for Krylov subspace eigensolvers, but for some abstract iterations which can be regarded as slower variants of the corresponding Krylov subspace eigensolvers. For the reader's convenience, we provide a direct formulation.

2.1.1 Saad's estimates

We start with the analysis of standard Krylov subspace iterations and summarize the estimates from [98, Theorems 1, 3 and 2] in the following theorem.

Theorem 2.1. *With Notation 1.4, consider a Krylov subspace*

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

with the initial vector $y \in \mathbb{R}^n \backslash \{0\}$, and assume that the eigenprojection $Q_i y$ is nonzero for an index $i < k$. Then it holds, in terms of the normalized eigenprojection $z_i = Q_i y / \|Q_i y\|_2$, the invariant subspace $\mathcal{Z} = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_i$, the gap ratio $\gamma_i = (\mu_i - \mu_{i+1})/(\mu_{i+1} - \mu_m)$ (where μ_m is the smallest eigenvalue), and the Chebyshev polynomial $T_{k-i}(\cdot)$, that

$$\tan \angle_2\big(z_i, \mathcal{K}\big) \leq \frac{\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}}{T_{k-i}(1 + 2\gamma_i)} \, \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)}. \tag{2.1}$$

Moreover, let $u_1, \ldots, u_k$ be orthonormal Ritz vectors of H in $\mathcal{K}$ associated with the Ritz values $\theta_1 \geq \cdots \geq \theta_k$, and denote by P the orthogonal projector on $\mathcal{K}$. Assume that the distance $\delta_i = \min_{j \in \{1,\ldots,k\} \backslash \{i\}} |\mu_i - \theta_j|$ is nonzero. Then it holds that

$$\sin^2 \angle_2(z_i, u_i) \leq \Big(1 + \delta_i^{-2} \big\|(I - P)HP\big\|_2^2\Big) \sin^2 \angle_2\big(z_i, \mathcal{K}\big). \tag{2.2}$$

Combining (2.2) *with* (2.1) *yields a Chebyshev type estimate on the Ritz vector u_i. In addition, a Chebyshev type estimate on the Ritz value θ_i reads*

$$\mu_i - \theta_i \leq (\mu_i - \mu_m) \left(\frac{\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}}{T_{k-i}(1 + 2\gamma_i)} \, \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \right)^2 \tag{2.3}$$

where $\theta_{i-1} > \mu_i$ is assumed in the case $i > 1$.

The estimates in Theorem 2.1, although can be formulated for arbitrary i up to $k-1$, are of practical interest only for $i \ll k$. The trigonometric ratio $\sin \angle_2(y, \mathcal{Z}) / \cos \angle_2(y, z_i)$ represents the coefficient ratio $\big(\sum_{j=i+1}^{m} \|Q_j y\|_2^2 / \|Q_i y\|_2^2\big)^{1/2}$ which was overestimated by

$$\big(\textstyle\sum_{j \in \{1,\ldots,m\} \backslash \{i\}} \|Q_j y\|_2^2 / \|Q_i y\|_2^2\big)^{1/2} = \tan \angle_2(y, z_i)$$

in [98]. The Chebyshev factor $[T_{k-i}(1 + 2\gamma_i)]^{-1}$ depends on the degree k of the Krylov subspace $\mathcal{K}$, and decreases rapidly with k for $\gamma_i \gg 0$. However, if μ_i and μ_{i+1} belong to a cluster of eigenvalues, γ_i is close to zero so that $[T_{k-i}(1 + 2\gamma_i)]^{-1}$ results in weak bounds. For this reason, Saad suggested a refinement in [98, Theorem 4, Corollary 3] which can be reformulated as follows.

Theorem 2.2. *With the settings from Theorem 2.1, consider the case that the interior eigenvalues* $\mu_i, \ldots, \mu_{i+t}$ *are clustered for* $i+t<k$*, but bounded away from* μ_{i+t+1}*. Then it holds, in terms of the auxiliary vector*

$$\widetilde{y} = \left(\prod_{j=i+1}^{i+t} (H - \mu_j I) \right) y$$

which is nonzero, and the gap ratio $\widetilde{\gamma}_i = (\mu_i - \mu_{i+t+1})/(\mu_{i+t+1} - \mu_m)$*, that*

$$\begin{aligned} \tan \angle_2(z_i, \mathcal{K}) &\leq \frac{\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}}{T_{k-i-t}(1+2\widetilde{\gamma}_i)} \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)} \\ &\leq \frac{\left(\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}\right)\left(\prod_{j=i+1}^{i+t} \frac{\mu_j - \mu_m}{\mu_i - \mu_j}\right)}{T_{k-i-t}(1+2\widetilde{\gamma}_i)} \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)}, \end{aligned} \tag{2.4}$$

$$\begin{aligned} \mu_i - \theta_i &\leq (\mu_i - \mu_m) \left(\frac{\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}}{T_{k-i-t}(1+2\widetilde{\gamma}_i)} \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)} \right)^2 \\ &\leq (\mu_i - \mu_m) \left(\frac{\left(\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}\right)\left(\prod_{j=i+1}^{i+t} \frac{\mu_j - \mu_m}{\mu_i - \mu_j}\right)}{T_{k-i-t}(1+2\widetilde{\gamma}_i)} \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \right)^2. \end{aligned} \tag{2.5}$$

In comparison to the formulation in [98], we emphasize the property $\widetilde{y} \neq 0$ concerning the definition of the angles $\angle_2(\widetilde{y}, \mathcal{Z})$ and $\angle_2(\widetilde{y}, z_i)$. This property is ensured by the assumption $Q_i y \neq 0$, namely, the eigenprojection $Q_i \widetilde{y}$ reads $Q_i\big(\prod_{j=i+1}^{i+t}(H-\mu_j I)\big)\, y = \big(\prod_{j=i+1}^{i+t}(\mu_i - \mu_j)\big)\, Q_i y$. It is nonzero because of $Q_i y \neq 0$ and the fact that the concerned eigenvalues are distinct. The estimates (2.4) and (2.5) are refined forms of the estimates (2.1) and (2.3). The auxiliary vector $\widetilde{y}$ is orthogonal to the eigenspaces associated with the t clustered eigenvalues $\mu_{i+1}, \ldots, \mu_{i+t}$. Thus these eigenvalues can be skipped in the derivation of the estimates, and a better Chebyshev factor with $\widetilde{\gamma}_i \gg 0$ is achieved. The trigonometric ratio $\sin \angle_2(\widetilde{y}, \mathcal{Z})/\cos \angle_2(\widetilde{y}, z_i)$ coincides with the tangent value in the estimate [98, (2.24)] which concerns the angle between z_i and the orthogonal projection of $\widetilde{y}$ to $\mathcal{Z}_i \oplus \cdots \oplus \mathcal{Z}_m$. Nevertheless, the estimates (2.4) and (2.5) still contain some ratio-products which are large if μ_{i-1} or θ_{i-1} is close to μ_i. Thus meaningful bounds could only be achieved for sufficiently large k, and one has to use other approaches for deriving suitable estimates for low-dimensional Krylov subspaces arising from restarted Krylov subspace eigensolvers.

Next, we discuss the estimates from [98, Theorems 5 and 6] for investigating block-Krylov subspace iterations.

Theorem 2.3. *With Notation 1.5, consider a block-Krylov subspace*

$$\mathcal{K} = \operatorname{span}\{Y, HY, \ldots, H^{k-1}Y\}$$

with a basis matrix $Y \in \mathbb{R}^{n \times s}$ *of the initial subspace* $\mathcal{Y}$*, and assume that the multiplicity of each eigenvalue of* H *does not exceed* s*. If the orthogonal projections of the eigenvectors* $z_i, \ldots, z_{i+s-1}$ *to* $\mathcal{Y}$ *are linearly independent for an index* $i<k$*, then there exists a unique vector* $\widetilde{y} \in \mathcal{Y}$ *satisfying* $\widetilde{y}^T z_i = 1$ *and* $\widetilde{y}^T z_j = 0$ *for each* $j \in \{i+1, \ldots, i+s-1\}$*. By using* $\widetilde{y}$ *as an auxiliary vector, it holds, in terms of the set* σ_i *of all distinct eigenvalues larger than* μ_i*, the cardinality* $\#\sigma_i$ *of* σ_i*, the invariant subspace* $\mathcal{Z} = \operatorname{span}\{z_1, \ldots, z_i\}$*, the gap ratio* $\gamma_i = (\mu_i - \mu_{i+s})/(\mu_{i+s} - \mu_n)$*, and the Chebyshev polynomial* $T_{k-1-\#\sigma_i}(\cdot)$*, that*

$$\tan \angle_2(z_i, \mathcal{K}) \leq \frac{\prod_{\mu \in \sigma_i} \frac{\mu - \mu_n}{\mu - \mu_i}}{T_{k-1-\#\sigma_i}(1+2\gamma_i)} \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)}. \tag{2.6}$$

Moreover, let $u_1, \ldots, u_{\widehat{k}}$ *be orthonormal Ritz vectors of* H *in* $\mathcal{K}$ *associated with the Ritz values* $\theta_1 \geq \cdots \geq \theta_{\widehat{k}}$ *with* $\widehat{k} = \dim \mathcal{K}$*. Denote by* τ *the index set of all eigenvalues of* H *which are equal to* μ_i*, and by* P *the orthogonal projector on* $\mathcal{K}$*. Assume that the distance* $\delta_i = \min_{j\in\{1,\ldots,\widehat{k}\}\setminus\tau} |\mu_i - \theta_j|$ *is nonzero. Then it holds that*

$$\sin^2 \angle_2\big(z_i, \operatorname{span}\{u_j \,;\, j \in \tau\}\big) \leq \Big(1 + \delta_i^{-2} \big\|(I-P)HP\big\|_2^2\Big) \sin^2 \angle_2\big(z_i, \mathcal{K}\big). \tag{2.7}$$

Combining (2.7) *with* (2.6) *yields a Chebyshev type estimate on Ritz vectors which approximate eigenvectors associated with* μ_i*, or associated with a multiple eigenvalue equal to* μ_i*. In addition, it holds, in terms of the set* $\widetilde{\sigma}_i$ *of all distinct Ritz values larger than* θ_i*, and the cardinality* $\#\widetilde{\sigma}_i$ *of* $\widetilde{\sigma}_i$*, that*

$$\mu_i - \theta_i \leq (\mu_i - \mu_n) \left(\frac{\prod_{\theta\in\widetilde{\sigma}_i} \frac{\theta-\mu_n}{\theta-\mu_i}}{T_{k-1-\#\widetilde{\sigma}_i}(1+2\gamma_i)} \, \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)} \right)^2 \tag{2.8}$$

where $\theta_{i-1} > \mu_i$ *is assumed in the case* $i > 1$*.*

The auxiliary vector $\widetilde{y}$ in Theorem 2.3 plays a similar role as the $\widetilde{y}$ in Theorem 2.2, namely, it allows us to select a sufficiently large gap ratio so that the corresponding Chebyshev factor is reasonable. The sets σ_i and $\widetilde{\sigma}_i$ were described in [98] as sets of the first $i-1$ distinct eigenvalues or Ritz values. However, if these first $i-1$ distinct values are not all simple, then some elements in σ_i and $\widetilde{\sigma}_i$ would be not larger than μ_i, and the ratio-products in (2.6) and (2.8) would be meaningless, e.g., $\prod_{\mu\in\sigma_i} \frac{\mu-\mu_n}{\mu-\mu_i}$ could be infinite or negative. This description is corrected in Theorem 2.3 by omitting the number of distinct values. In the case that $\#\sigma_i = \#\widetilde{\sigma}_i = i-1$, i.e., the included distinct values are all simple, the ratio-products in (2.6) and (2.8) turn into $\prod_{j=1}^{i-1} \frac{\mu_j-\mu_n}{\mu_j-\mu_i}$ and $\prod_{j=1}^{i-1} \frac{\theta_j-\mu_n}{\theta_j-\mu_i}$, respectively, which are similar to those in Theorems 2.1 and 2.2. Moreover, if μ_i is close to some elements of σ_i or $\widetilde{\sigma}_i$, then the ratio-products become large. Thus meaningful bounds demand sufficiently large k, and low-dimensional block-Krylov subspaces have to be analyzed in another way.

2.1.2 Knyazev's estimates

In [44, 45], Knyazev provided several elegant convergence estimates for two abstract iterations where the power method and the block power method are applied to a matrix function. Some estimates are indirectly applicable to Krylov subspace iterations by using the Courant-Fischer principles; cf. [45, Sections 1.4, 2.4]. In particular, the estimates [45, (1.10), (1.9), (1.3)] can be applied to standard Krylov subspace iterations. We reformulate these estimates in comparison to Saad's estimates from Theorem 2.1.

Theorem 2.4. *With the settings from Theorem 2.1, it holds that*

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_m} \leq [\,T_{k-1}(1+2\gamma_1)\,]^{-2} \tan^2 \angle_2(y, z_1). \tag{2.9}$$

In addition, if $\mu(y) > \mu_2$*, then*

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2} \leq [\,T_{k-1}(1+2\gamma_1)\,]^{-2} \, \frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}, \tag{2.10}$$

$$\sin^2 \angle_2(u_1, z_1) \leq \frac{\mu_1 - \theta_1}{\mu_1 - \mu_2}. \tag{2.11}$$

Combining (2.11) *with* (2.9) *or* (2.10) *yields a Chebyshev type estimate on the Ritz vector* u_1*.*

Theorem 2.4 only deals with the index $i=1$ which is of interest for a simply restarted Krylov subspace iteration. The estimate (2.9) slightly improves the special form

$$\frac{\mu_1-\theta_1}{\mu_1-\mu_m} \le \left(\frac{\prod_{j=1}^{0} \frac{\theta_j-\mu_m}{\theta_j-\mu_1}}{T_{k-1}(1+2\gamma_1)} \frac{\sin\angle_2(y,z_1)}{\cos\angle_2(y,z_1)} \right)^2 = [\,T_{k-1}(1+2\gamma_1)\,]^{-2} \tan^2\angle_2(y,z_1)$$

of (2.3) because of $\frac{\mu_1-\theta_1}{\mu_1-\mu_m} \le \frac{\mu_1-\theta_1}{\theta_1-\mu_m}$. A significant improvement can be made by (2.10) provided that $\tan^2\angle_2(y,z_1)$ is large. For further restarted Krylov subspace iterations, it is desirable to generalize Theorem 2.4 to arbitrary indices and to refine the Chebyshev factors similarly to Theorem 2.2.

Next, for block-Krylov subspace iterations, we summarize the estimates [45, (2.20), (2.22), (2.9), (2.7)] in the following theorem.

Theorem 2.5. *With the settings from Theorem 2.3, consider the case that the s largest eigenvalues are distinct. Then it holds, in terms of the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1,\dots,z_s\}$, the gap ratio $\gamma_i = (\mu_i-\mu_{s+1})/(\mu_{s+1}-\mu_n)$, and the Chebyshev polynomial $T_{k-1}(\cdot)$, that*

$$\frac{\mu_i-\theta_i}{\theta_i-\mu_n} \le [\,T_{k-1}(1+2\gamma_i)\,]^{-2} \tan^2\angle_2(\mathcal{Y},\mathcal{Z}), \qquad i=1,\dots,s. \tag{2.12}$$

In addition, denote by $\eta_1 \ge \dots \ge \eta_s$ the Ritz values of H in $\mathcal{Y}$. If $\eta_s > \mu_{s+1}$, then

$$\frac{\mu_s-\theta_s}{\theta_s-\mu_{s+1}} \le [\,T_{k-1}(1+2\gamma_s)\,]^{-2} \frac{\mu_s-\eta_s}{\eta_s-\mu_{s+1}}. \tag{2.13}$$

Moreover, if $\theta_1 \ge \mu_2$, then $\sin^2\angle_2(u_1,z_1) \le (\mu_1-\theta_1)/(\mu_1-\mu_2)$ holds which is denotationally identical with (2.11). If $\theta_{i-1} \ge \mu_i$, $\theta_i \ge \mu_{i+1}$, and $\theta_{i-1} > \theta_i$ for a certain $i \in \{2,\dots,s\}$, then

$$\sin^2\angle_2(u_i,z_i) \le 1 - \frac{(\mu_1-\theta_i)(\theta_i-\mu_{i+1})(\theta_{i-1}-\mu_i)}{(\mu_1-\mu_i)(\mu_i-\mu_{i+1})(\theta_{i-1}-\theta_i)}. \tag{2.14}$$

Combining this with (2.12) yields a Chebyshev type estimate on Ritz vectors.

Theorem 2.5 does not require the ratio-products $\prod_{\mu\in\sigma_i} \frac{\mu-\mu_n}{\mu-\mu_i}$ and $\prod_{\theta\in\widetilde{\sigma}_i} \frac{\theta-\mu_n}{\theta-\mu_i}$ in comparison to Theorem 2.3, and can thus provide meaningful bounds in the case that the i largest eigenvalues are clustered. A further advantage of Theorem 2.5 is that the auxiliary vectors in its proof are eliminated in the estimates by means of slight overestimation. This improves the readability. The assumption that the s largest eigenvalues are distinct avoids some singular cases, e.g., $\gamma_i = 0$ in the Chebyshev factor and $\mu_i - \mu_{i+1} = 0$ in the estimate (2.14). Indeed, the estimates (2.12) and (2.13) only require $\mu_s > \mu_{s+1}$, and the estimate (2.14) can be generalized as

$$\sin^2\angle_2\big(\operatorname{span}\{u_i,\dots,u_{i+t}\},\operatorname{span}\{z_i,\dots,z_{i+t}\}\big) \le 1 - \frac{(\mu_1-\theta_{i+t})(\theta_{i+t}-\mu_{i+t+1})(\theta_{i-1}-\mu_i)}{(\mu_1-\mu_i)(\mu_i-\mu_{i+t+1})(\theta_{i-1}-\theta_{i+t})}$$

which is applicable in the case $\mu_{i-1} > \mu_i = \dots = \mu_{i+t} > \mu_{i+t+1}$ with a multiple eigenvalue. As motivations for improving and extending Theorem 2.5, we note that the estimate (2.12) is not very accurate for large $\tan^2\angle_2(\mathcal{Y},\mathcal{Z})$ and relatively small k, and that the estimate (2.13) only treats the sth Ritz value.

2.2 Auxiliary vectors

In order to overcome the drawbacks of the classical Chebyshev type estimates, we reformulate the proof techniques from [98] in a concise manner and discuss which ingredients cause suboptimal bounds. In particular, we review those auxiliary vectors which produce the Chebyshev factors in the main estimates.

The most auxiliary vectors for deriving the classical Chebyshev type estimates are based on the well-known polynomial representations for Krylov subspaces. For instance, the convergence analysis in [98] begins with the polynomial representation of an arbitrary vector in the considered Krylov subspace. By minimizing the bounds of certain intermediate estimates, a shifted Chebyshev polynomial is constructed. The resulting estimates are optimal for the first index in the sense that the associated Chebyshev bounds can be attained for certain special matrices and initial vectors; cf. the third remark at the end of [98, Section 2.2]. However, by regarding arbitrary symmetric matrices, these Chebyshev bounds are only attainable for Krylov subspaces of degree 2. Instead, sharp bounds can be provided by two further types of polynomials; see Chapter 4. Because of this "weak sharpness" of the Chebyshev bounds, we drop the bound-minimization and directly introduce the shifted Chebyshev polynomial. The reformulated analysis includes the following topics:

(i) Construction and properties of auxiliary vectors concerning Theorem 2.1.

(ii) Derivation of main estimates for standard Krylov subspace iterations.

(iii) Refinement and extension concerning clustered eigenvalues, block-Krylov subspace iterations and estimates on Ritz vectors.

2.2.1 Construction and properties

We first consider Theorem 2.1 for standard Krylov subspace iterations. Therein the estimates (2.1) and (2.3) can be derived by using two auxiliary vectors $p(H)y$ and $q(H)y$ depending on the polynomials $p(\cdot)$ and $q(\cdot)$ defined by

$$p(\alpha) = \left(\prod_{j=1}^{i-1}(\alpha-\mu_j)\right) f(\alpha), \qquad q(\alpha) = \left(\prod_{j=1}^{i-1}(\alpha-\theta_j)\right) f(\alpha)$$

with the common factor

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

which is a shifted Chebyshev polynomial of degree $k-i$. Thus $p(\cdot)$ and $q(\cdot)$ have degree $k-1$ so that $p(H)y$ and $q(H)y$ belong to the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$. The linear factors in the definitions of $p(\cdot)$ and $q(\cdot)$ ensure that $p(H)y$ is orthogonal to the eigenvectors associated with $\mu_1, \ldots, \mu_{i-1}$ and that $q(H)y$ is orthogonal to the Ritz vectors associated with $\theta_1, \ldots, \theta_{i-1}$.

Moreover, for each eigenvalue $\mu_l \in \{\mu_{i+1}, \ldots, \mu_m\}$, it holds that

$$\mu_m \le \mu_l \le \mu_{i+1} \quad \Rightarrow \quad \left|1 + 2\,\frac{\mu_l-\mu_{i+1}}{\mu_{i+1}-\mu_m}\right| \le 1 \quad \Rightarrow \quad |f(\mu_l)| = \left|T_{k-i}\left(1 + 2\,\frac{\mu_l-\mu_{i+1}}{\mu_{i+1}-\mu_m}\right)\right| \le 1$$

according to the properties in (1.36). Subsequently, $|f(\mu_l)| \le 1$ implies

$$|p(\mu_l)| \le \prod_{j=1}^{i-1}|\mu_l-\mu_j| \le \prod_{j=1}^{i-1}(\mu_j-\mu_m), \qquad |q(\mu_l)| \le \prod_{j=1}^{i-1}|\mu_l-\theta_j| \le \prod_{j=1}^{i-1}(\theta_j-\mu_m) \tag{2.15}$$

where the second inequality for $|q(\mu_l)|$ uses the assumption $\theta_{i-1} > \mu_i$ from Theorem 2.1.

Next, we extend the eigenvector $z_i = Q_i y/\|Q_i y\|_2$ to an orthonormal system

$$\{z_1, \ldots, z_m\} \qquad \text{with} \qquad z_l = \begin{cases} \text{arbitrary normalized } z_l \in \mathcal{Z}_l & \text{if} \quad Q_l y = 0\,, \\ Q_l y/\|Q_l y\|_2 & \text{if} \quad Q_l y \ne 0\,. \end{cases} \tag{2.16}$$

Then y can be expanded as $y = \sum_{l=1}^{m} \alpha_l\, z_l$ with the coefficients $\alpha_l = \|Q_l y\|_2$, and $\alpha_l\, z_l = Q_l y$ holds for each index l. The corresponding expansions of $p(H)y$ and $q(H)y$ are

$$p(H)y = \sum_{l=1}^{m} p(\mu_l)\, \alpha_l\, z_l = \sum_{l=i}^{m} p(\mu_l)\, \alpha_l\, z_l, \qquad q(H)y = \sum_{l=1}^{m} q(\mu_l)\, \alpha_l\, z_l$$

where the second equality for $p(H)y$ uses the fact that $p(\mu_l) = 0$ holds for each $l \in \{1, \ldots, i-1\}$. In addition, (1.36) implies $f(\mu_i) > 1$ because of $\mu_i > \mu_{i+1}$. Thus

$$p(\mu_i) = \left(\prod_{j=1}^{i-1} (\mu_i - \mu_j) \right) f(\mu_i) \neq 0, \qquad q(\mu_i) = \left(\prod_{j=1}^{i-1} (\mu_i - \theta_j) \right) f(\mu_i) \neq 0$$

where the products are nonzero since the eigenvalues are distinct and $\theta_1 \geq \cdots \geq \theta_{i-1} > \mu_i$ holds. Consequently, the terms $p(\mu_i)\, \alpha_i\, z_i$ and $q(\mu_i)\, \alpha_i\, z_i$ in the expansions of $p(H)y$ and $q(H)y$ are nonzero so that $p(H)y$ and $q(H)y$ are nonzero.

Based on these expansions, some relevant coefficient ratios for proving the estimates (2.1) and (2.3) can be represented by trigonometric terms. In particular, it holds that

$$\frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} = \frac{\sqrt{\sum_{l=i+1}^{m} \alpha_l^2}}{\alpha_i}. \tag{2.17}$$

In (2.17), the coefficient ratio is positive since $\alpha_i = \|Q_i y\|_2 > 0$. The equality can be verified by using Definition 1.6 as follows. Since $Q = Q_1 + \cdots + Q_i$ is the orthogonal projector on $\mathcal{Z} = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_i$, we have

$$\sin \angle_2(y, \mathcal{Z}) \overset{(1.33)}{=} \frac{\|y - Qy\|_2}{\|y\|_2} = \frac{\| \sum_{l=i+1}^{m} Q_l y\|_2}{\|y\|_2} = \frac{\| \sum_{l=i+1}^{m} \alpha_l\, z_l\|_2}{\|y\|_2} = \frac{\sqrt{\sum_{l=i+1}^{m} \alpha_l^2}}{\|y\|_2}.$$

Combining this with

$$\cos \angle_2(y, z_i) \overset{(1.32)}{=} \cos \angle_2(z_i, y) \overset{(1.31)}{=} \frac{(z_i, y)_2}{\|z_i\|_2\, \|y\|_2} = \frac{z_i^T y}{\|y\|_2} = \frac{\sum_{l=1}^{m} \alpha_l\, z_i^T z_l}{\|y\|_2} = \frac{\alpha_i}{\|y\|_2} \tag{2.18}$$

yields (2.17). A further relevant coefficient ratio is represented by $\tan^2 \angle_2\big(z_i, p(H)y\big)$ with the auxiliary vector $p(H)y$, namely, analogously to (2.18), it holds that

$$\cos^2 \angle_2\big(z_i, p(H)y\big) = \frac{\big(z_i^T p(H)y\big)^2}{\big\|p(H)y\big\|_2^2} = \frac{\big(\sum_{l=i}^{m} p(\mu_l)\, \alpha_l\, z_i^T z_l\big)^2}{\sum_{l=i}^{m} \big\|p(\mu_l)\, \alpha_l\, z_l\big\|_2^2} = \frac{p^2(\mu_i)\, \alpha_i^2}{\sum_{l=i}^{m} p^2(\mu_l)\, \alpha_l^2},$$

and consequently

$$\tan^2 \angle_2\big(z_i, p(H)y\big) \;=\; \frac{1}{\cos^2 \angle_2\big(z_i, p(H)y\big)} - 1 \;=\; \frac{\sum_{l=i+1}^{m} p^2(\mu_l)\, \alpha_l^2}{p^2(\mu_i)\, \alpha_i^2}. \tag{2.19}$$

2.2.2 Derivation of main estimates

We derive the main estimates (2.1) and (2.3) in Theorem 2.1 by using the auxiliary vectors $p(H)y$ and $q(H)y$ constructed in Subsection 2.2.1.

The estimate (2.1) can be derived based on the representations (2.17) and (2.19) together with the boundedness of $|p(\mu_l)|$ for $\mu_l \in \{\mu_{i+1}, \ldots, \mu_m\}$ by (2.15) as follows.

$$\begin{aligned}
\tan^2 \angle_2\big(z_i, p(H)y\big) &\overset{(2.19)}{=} \frac{\sum_{l=i+1}^m p^2(\mu_l)\,\alpha_l^2}{p^2(\mu_i)\,\alpha_i^2} \overset{(2.15)}{\leq} \frac{\sum_{l=i+1}^m \big(\prod_{j=1}^{i-1}(\mu_j-\mu_m)^2\big)\,\alpha_l^2}{p^2(\mu_i)\,\alpha_i^2} \\
&= \frac{\prod_{j=1}^{i-1}(\mu_j-\mu_m)^2}{\big(\prod_{j=1}^{i-1}(\mu_i-\mu_j)^2\big)\,T_{k-i}^2\Big(1+2\,\frac{\mu_i-\mu_{i+1}}{\mu_{i+1}-\mu_m}\Big)} \left(\frac{\sum_{l=i+1}^m \alpha_l^2}{\alpha_i^2}\right) \qquad (2.20)\\
&\overset{(2.17)}{=} \left(\frac{\prod_{j=1}^{i-1}\frac{\mu_j-\mu_m}{\mu_j-\mu_i}}{T_{k-i}(1+2\gamma_i)}\;\frac{\sin\angle_2(y,\mathcal{Z})}{\cos\angle_2(y,z_i)}\right)^2.
\end{aligned}$$

This implies (2.1) by using the properties

$$\tan^2\angle_2\big(z_i,\mathcal{K}\big) \leq \tan^2\angle_2\big(z_i,p(H)y\big) \qquad \text{and} \qquad \tan\angle_2\big(z_i,\mathcal{K}\big) \geq 0$$

according to (1.32) together with the fact that the expression between parentheses in the last line of (2.20) is nonnegative.

For proving the estimate (2.3), the expansion $q(H)y = \sum_{l=1}^m q(\mu_l)\,\alpha_l\,z_l$ can be applied to the reformulation of $\mu\big(q(H)y\big)$ for the Rayleigh quotient $\mu(\cdot)$ defined in (1.34), namely,

$$\mu\big(q(H)y\big) = \frac{\big(q(H)y\big)^T H\big(q(H)y\big)}{\big(q(H)y\big)^T\big(q(H)y\big)} = \frac{\sum_{l=1}^m \mu_l\,q^2(\mu_l)\,\alpha_l^2}{\sum_{l=1}^m q^2(\mu_l)\,\alpha_l^2}.$$

Then it holds that

$$\begin{aligned}
\mu_i - \mu\big(q(H)y\big) &= \frac{\sum_{l=1}^m (\mu_i-\mu_l)\,q^2(\mu_l)\,\alpha_l^2}{\sum_{l=1}^m q^2(\mu_l)\,\alpha_l^2} \leq \frac{\sum_{l=i+1}^m (\mu_i-\mu_l)\,q^2(\mu_l)\,\alpha_l^2}{\sum_{l=1}^m q^2(\mu_l)\,\alpha_l^2} \qquad (2.21)\\
&\leq (\mu_i-\mu_m)\,\frac{\sum_{l=i+1}^m q^2(\mu_l)\,\alpha_l^2}{q^2(\mu_i)\,\alpha_i^2} \leq (\mu_i-\mu_m)\left(\frac{\prod_{j=1}^{i-1}\frac{\theta_j-\mu_m}{\theta_j-\mu_i}}{T_{k-i}(1+2\gamma_i)}\;\frac{\sin\angle_2(y,\mathcal{Z})}{\cos\angle_2(y,z_i)}\right)^2
\end{aligned}$$

where the last inequality is derived analogously to (2.20). In addition, since $q(H)y$ is orthogonal to the Ritz vectors associated with those Ritz values which are larger than θ_i, we get the relation $\theta_i \geq \mu\big(q(H)y\big)$. Combining this with (2.21) yields the estimate (2.3).

Indeed, those eigenvectors in the orthonormal system (2.16) which are added in the case $Q_l y \neq 0$ can be omitted in order to slightly improve the bounds. For instance, we can denote by τ the index set of all nonzero eigenprojections $Q_l y$ so that the analysis can be restricted to the orthonormal system $\{z_l\ ;\ l \in \tau\}$ with $z_l = Q_l y/\|Q_l y\|_2$. Subsequently, we define an index $\widehat{i}$ for which μ_i is the $\widehat{i}$th largest value in the set $\{\mu_l\ ;\ l \in \tau\}$. Thus μ_i is approximated by the $\widehat{i}$th largest Ritz value $\theta_{\widehat{i}}$. Correspondingly, we construct the auxiliary vectors $p(H)y$ and $q(H)y$ by

$$p(\alpha) = \Bigg(\prod_{j\in\tau,\ j<i}(\alpha-\mu_j)\Bigg)\,f(\alpha), \qquad q(\alpha) = \Bigg(\prod_{j=1}^{\widehat{i}-1}(\alpha-\theta_j)\Bigg)\,f(\alpha)$$

with the shifted Chebyshev polynomial

$$f(\alpha) = T_{k-\widehat{i}}\left(1 + 2\,\frac{\alpha-\beta_1}{\beta_1-\beta_2}\right)$$

where $\beta_1 = \max_{j\in\tau,\ j>i}\mu_j$ and $\beta_2 = \min_{j\in\tau}\mu_j$. This leads to a better Chebyshev factor due to the higher degree $k-\widehat{i}$ and the smaller interval $[\beta_2,\beta_1]$ in comparison to $k-i$ and $[\mu_m,\mu_{i+1}]$. Nevertheless, since the eigenprojections of a pseudorandom initial vector are usually nonzero, we prefer the more flexible formulation with the complete orthonormal system (2.16).

2.2.3 Refinement and extension

The refined estimates (2.4), (2.5) in Theorem 2.2 for standard Krylov subspace iterations and the extended estimates (2.6), (2.8) in Theorem 2.3 for block-Krylov subspace iterations can be derived analogously to (2.1), (2.3). Basically, one only needs to construct some alternative auxiliary vectors.

In Theorem 2.2, starting with the auxiliary vector $\widetilde{y} = \left(\prod_{j=i+1}^{i+t} (H - \mu_j I)\right) y$ which is already suggested in the settings, two further auxiliary vectors $\widetilde{p}(H)\widetilde{y}$ and $\widetilde{q}(H)\widetilde{y}$ can be constructed with the polynomials

$$\widetilde{p}(\alpha) = \left(\prod_{j=1}^{i-1}(\alpha - \mu_j)\right) T_{k-i-t}\left(1 + 2\,\frac{\alpha - \mu_{i+t+1}}{\mu_{i+t+1} - \mu_m}\right),$$

$$\widetilde{q}(\alpha) = \left(\prod_{j=1}^{i-1}(\alpha - \theta_j)\right) T_{k-i-t}\left(1 + 2\,\frac{\alpha - \mu_{i+t+1}}{\mu_{i+t+1} - \mu_m}\right).$$

Since $\widetilde{y}$ is orthogonal to the eigenvectors associated with the eigenvalues $\mu_{i+1}, \dots, \mu_{i+t}$, one can skip these eigenvalues in the analysis so that a better Chebyshev factor is achieved.

Additionally, $\widetilde{p}(H)\widetilde{y}$, $\widetilde{q}(H)\widetilde{y}$ can be rewritten as $p(H)y$, $q(H)y$ with the polynomials

$$p(\alpha) = \left(\prod_{j=i+1}^{i+t}(\alpha - \mu_j)\right)\widetilde{p}(\alpha), \qquad q(\alpha) = \left(\prod_{j=i+1}^{i+t}(\alpha - \mu_j)\right)\widetilde{q}(\alpha)$$

in order to provide some weaker bounds which do not contain the auxiliary vector $\widetilde{y}$.

In Theorem 2.3, $\widetilde{y}$ denotes an auxiliary vector in the initial subspace $\mathcal{Y}$. The orthogonality between $\widetilde{y}$ and the eigenvectors $z_{i+1}, \dots, z_{i+s-1}$ allows us to skip the eigenvalues $\mu_{i+1}, \dots, \mu_{i+s-1}$. Then, similarly to the proof of Theorem 2.2, two auxiliary vectors $\widetilde{p}(H)\widetilde{y}$, $\widetilde{q}(H)\widetilde{y}$ can be constructed with the polynomials

$$\widetilde{p}(\alpha) = \left(\prod_{\mu\in\sigma_i}(\alpha - \mu)\right) T_{k-1-\#\sigma_i}\left(1 + 2\,\frac{\alpha - \mu_{i+s}}{\mu_{i+s} - \mu_n}\right),$$

$$\widetilde{q}(\alpha) = \left(\prod_{\theta\in\widetilde{\sigma}_i}(\alpha - \theta)\right) T_{k-1-\#\widetilde{\sigma}_i}\left(1 + 2\,\frac{\alpha - \mu_{i+s}}{\mu_{i+s} - \mu_n}\right).$$

Remark 2.6. *Summarizing the above, it is evident that the suboptimal bounds of Saad's estimates from [98] are caused by the linear factors in the polynomials for defining auxiliary vectors. In Theorem 2.1, the denominators of the ratio-products in the estimates* (2.1) *and* (2.3) *consist of the absolute values of the linear factors* $(\alpha - \mu_j)$ *and* $(\alpha - \theta_j)$ *at* μ_i*. In the case that the eigenvalues* $\mu_1, \dots, \mu_i$ *are clustered, these absolute values are close to zero so that the ratio-products are large. The refinement in Theorem 2.2 only improves the Chebyshev factor, but does not affect these linear factors. Thus the whole bounds are not significantly refined for relatively small* k*. The derivation of the estimates* (2.6) *and* (2.8) *in Theorem 2.3 is based on the same idea as in Theorem 2.2 so that similar linear factors result in possibly large ratio-products.*

Thus we need to select some other auxiliary vectors without such linear factors in order to improve Saad's estimates. We got some inspiration from Knyazev's analysis [44, 45], namely, for proving the estimates (2.12) *and* (2.13) *in Theorem 2.5, one can start with the auxiliary vectors* y_j, $j = 1, \dots, s$*, satisfying* $y_j^T z_j = 1$ *and* $y_j^T z_l = 0$ *for each* $l \in \{1, \dots, s\}\backslash\{j\}$*. Then an auxiliary subspace* $p(H)\widetilde{\mathcal{Y}}$ *can be constructed for an arbitrary index* $i \in \{1, \dots, s\}$ *by the subspace*

$\widetilde{\mathcal{Y}} = \operatorname{span}\{y_1, \ldots, y_i\}$ and the polynomial

$$p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha - \mu_{s+1}}{\mu_{s+1} - \mu_n}\right).$$

We introduce the detailed derivation with some supplementary arguments in Section 2.3.

Furthermore, the estimates (2.2) and (2.7) for providing indirect Chebyshev type estimates on Ritz vectors are special versions of the following more general estimate (2.22). Therein the arrangement of eigenvalues and eigenprojectors is irrelevant so that the estimate is applicable to both of Notations 1.4 and 1.5.

Lemma 2.7. *Consider a symmetric matrix $H \in \mathbb{R}^{n\times n}$. Let z be a normalized eigenvector of H associated with the eigenvalue μ, and let $u_1, \ldots, u_t$ be orthonormal Ritz vectors of H in a subspace $\mathcal{U}$ of dimension t associated with the Ritz values $\theta_1 \geq \cdots \geq \theta_t$. Denote by τ an arbitrary strict subset of $\{1, \ldots, t\}$, and by P the orthogonal projector on $\mathcal{U}$. Assume that the distance $\delta = \min_{j\in\{1,\ldots,t\}\setminus\tau} |\mu - \theta_j|$ is nonzero. Then it holds that*

$$\sin^2 \angle_2\big(z, \operatorname{span}\{u_j\,;\, j \in \tau\}\big) \leq \Big(1 + \delta^{-2}\big\|(I-P)HP\big\|_2^2\Big) \sin^2 \angle_2\big(z, \mathcal{U}\big). \tag{2.22}$$

Proof. The orthonormal Ritz vectors $u_1, \ldots, u_t$ form an orthonormal basis of the subspace $\mathcal{U}$ so that the orthogonal projector P can be represented by

$$P = [u_1, \ldots, u_t]\,[u_1, \ldots, u_t]^T = \textstyle\sum_{j=1}^t u_j u_j^T.$$

Then the orthogonal projection Pz of z has the representation $Pz = \sum_{j=1}^t u_j u_j^T z = \sum_{j=1}^t \beta_j u_j$ with $\beta_j = u_j^T z$. By using the formula (1.33) in Definition 1.6 for angles together with the properties $\|z\|_2 = 1$ and $(z - Pz)^T(Pz) = 0$, we have

$$\begin{aligned} \sin^2 \angle_2\big(z, \mathcal{U}\big) &\overset{(1.33)}{=} \left(\frac{\|z - Pz\|_2}{\|z\|_2}\right)^2 \;=\; \big\|z - Pz\big\|_2^2 \\ &= \big\|z\big\|_2^2 - \big\|Pz\big\|_2^2 \;=\; 1 - \Big\|\textstyle\sum_{j=1}^t \beta_j u_j\Big\|_2^2 \;=\; 1 - \textstyle\sum_{j=1}^t \beta_j^2. \end{aligned} \tag{2.23}$$

Analogously, the value $\sin^2 \angle_2\big(z, \operatorname{span}\{u_j\,;\, j \in \tau\}\big)$ can be represented in terms of the corresponding orthogonal projector $\widetilde{P} = \sum_{j\in\tau} u_j u_j^T$ and the expansion $\widetilde{P}z = \sum_{j\in\tau} \beta_j u_j$, namely,

$$\sin^2 \angle_2\big(z, \operatorname{span}\{u_j\,;\, j \in \tau\}\big) \;=\; \big\|z - \widetilde{P}z\big\|_2^2 \;=\; 1 - \textstyle\sum_{j\in\tau} \beta_j^2.$$

Combining this with (2.23) shows that

$$\sin^2 \angle_2\big(z, \operatorname{span}\{u_j\,;\, j \in \tau\}\big) - \sin^2 \angle_2\big(z, \mathcal{U}\big) \;=\; \textstyle\sum_{j\in\{1,\ldots,t\}\setminus\tau} \beta_j^2. \tag{2.24}$$

Moreover, it holds that

$$PHu_j = \textstyle\sum_{l=1}^t u_l u_l^T H u_j = u_j u_j^T H u_j = u_j \mu(u_j) = \theta_j u_j$$

which corresponds to the well-known fact that Ritz pairs are eigenpairs of the concerned projected matrix. Consequently, we have

$$\begin{aligned} Pz = \textstyle\sum_{j=1}^t \beta_j u_j \;\;&\Rightarrow\;\; PHPz \;=\; \textstyle\sum_{j=1}^t \beta_j PHu_j \;=\; \textstyle\sum_{j=1}^t \beta_j\theta_j u_j \\ &\Rightarrow\;\; PH(I-P)z \;=\; PHz - PHPz \;=\; P\mu z - PHPz \;=\; \textstyle\sum_{j=1}^t \beta_j(\mu - \theta_j)u_j \\ &\Rightarrow\;\; \big\|PH(I-P)z\big\|_2^2 \;=\; \textstyle\sum_{j=1}^t \beta_j^2\,|\mu - \theta_j|^2 \\ &\qquad\qquad \geq\; \textstyle\sum_{j\in\{1,\ldots,t\}\setminus\tau} \beta_j^2\,|\mu - \theta_j|^2 \;\geq\; \delta^2 \textstyle\sum_{j\in\{1,\ldots,t\}\setminus\tau} \beta_j^2 \end{aligned}$$

so that

$$\begin{aligned}\delta^2 \textstyle\sum_{j\in\{1,\dots,t\}\setminus\tau} \beta_j^2 \;&\le\; \big\|PH(I-P)z\big\|_2^2 \;=\; \big\|PH(I-P)(z-Pz)\big\|_2^2 \\ &\le\; \big\|PH(I-P)\big\|_2^2\,\big\|z-Pz\big\|_2^2 \;\overset{(2.23)}{=}\; \big\|PH(I-P)\big\|_2^2\,\sin^2\angle_2\big(z,\mathcal{U}\big) \\ &=\; \big\|\big(PH(I-P)\big)^T\big\|_2^2\,\sin^2\angle_2\big(z,\mathcal{U}\big) \;=\; \big\|(I-P)HP\big\|_2^2\,\sin^2\angle_2\big(z,\mathcal{U}\big).\end{aligned}$$

Combining this with (2.24) yields

$$\delta^2\Big(\sin^2\angle_2\big(z,\,\mathrm{span}\{u_j\,;\,j\in\tau\}\big)-\sin^2\angle_2\big(z,\mathcal{U}\big)\Big)\le\big\|(I-P)HP\big\|_2^2\,\sin^2\angle_2\big(z,\mathcal{U}\big)$$

which is equivalent to the estimate (2.22). □

Lemma 2.7 is an extension of [98, Theorem 3] and [100, Theorem 4.6] as it deals with several Ritz pairs $(\theta_j,\,u_j)$, $j\in\tau$ instead of a single Ritz pair. An estimate similar to (2.22) was mentioned at the end of [98, Section 3.3] without proof. In particular, (2.22) is applicable in the case that τ is an index set of multiple or clustered eigenvalues; cf. the estimate (2.7) in Theorem 2.3.

2.3 Supplementary arguments

In comparison to the derivation of Saad's estimates, the derivation of Knyazev's estimates requires certain supplementary arguments in addition to the properties of the auxiliary vectors introduced in Section 2.2. For instance, the estimate (2.9) in Theorem 2.4 is an extension of the special form

$$\tan\angle_2\big(z_1,\mathcal{K}\big)\le\big[\,T_{k-1}(1+2\gamma_1)\,\big]^{-1}\,\tan\angle_2(y,z_1) \tag{2.25}$$

of Saad's estimate (2.1) for $i=1$ by applying the supplementary argument

$$\frac{\mu_1-\theta_1}{\theta_1-\mu_m}\le\tan^2\angle_2\big(z_1,\mathcal{K}\big). \tag{2.26}$$

We introduce several supplementary arguments concerning the following types of estimates:

(i) Angle-dependent estimates on Ritz values; including the estimates (2.9) and (2.12).

(ii) Angle-free estimates on Ritz values; including the estimates (2.10) and (2.13).

(iii) Additional estimates on Ritz vectors; including the estimates (2.11) and (2.14).

The most arguments were not directly given for Krylov subspace eigensolvers in [44, 45]. For the reader's convenience, we formulate several key arguments in lemmas and prove them in a more direct and elementary way.

2.3.1 Angle-dependent estimates on Ritz values

We consider the angle-dependent estimates (2.9) concerning the largest Ritz value in a Krylov subspace and (2.12) concerning the s largest Ritz values in a block-Krylov subspace.

For deriving (2.9), we introduce in Lemma 2.8 a relation between $\mu(v)$ and $\angle_2(\widetilde{z}_1,v)$ for a nonzero vector v and its normalized eigenprojection $\widetilde{z}_1$. Then the supplementary argument (2.26) is verified by this relation so that the derivation of (2.9) by extending the known estimate (2.25) with (2.26) is completed.

For deriving (2.12), we generalize another proof of (2.9) to block-Krylov subspaces. More precisely, the relation in Lemma 2.8 is generalized in Lemma 2.9 to a subspace $\mathcal{U}$ and an invariant subspace $\widetilde{\mathcal{Z}}$, and an intermediate estimate concerning the angle $\angle_2\big(\mathcal{U},\widetilde{\mathcal{Z}}\big)$ is given in Lemma 2.10.

Arguments for Krylov subspaces

Lemma 2.8. *With Notation 1.4, let v be an arbitrary nonzero vector in an arbitrary subspace $\mathcal{V} \subseteq \mathbb{R}^n$ with $\dim \mathcal{V} \geq 1$, and let θ_1 be the largest Ritz value of H in $\mathcal{V}$. If the eigenprojection $Q_1 v$ is nonzero, then it holds, in terms of the Rayleigh quotient $\mu(\cdot)$ defined in (1.34) and the normalized eigenprojection $\widetilde{z}_1 = Q_1 v / \|Q_1 v\|_2$, that*

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_m} \leq \frac{\mu_1 - \mu(v)}{\mu(v) - \mu_m} \leq \tan^2 \angle_2(\widetilde{z}_1, v). \tag{2.27}$$

Proof. The first inequality in (2.27) holds according to $\mu_1 \geq \theta_1 \geq \mu(v) \geq \mu_m$ and the monotonicity of the function $(\mu_1 - \cdot)/(\cdot - \mu_m)$. In order to prove the second inequality in (2.27), we extend the eigenvector $\widetilde{z}_1$ to an orthonormal system $\{\widetilde{z}_1, \ldots, \widetilde{z}_m\}$ analogously to (2.16). Then v can be expanded as $v = \sum_{l=1}^{m} \alpha_l \, \widetilde{z}_l$ with the coefficients $\alpha_l = \|Q_l v\|_2$ so that

$$\mu(v) = \frac{v^T H v}{v^T v} = \frac{\sum_{l=1}^{m} \mu_l \, \alpha_l^2}{\sum_{l=1}^{m} \alpha_l^2},$$

and $\cos \angle_2(\widetilde{z}_1, v) = \alpha_1 / \|v\|_2$ analogously to (2.18). Consequently, we get

$$\begin{aligned} \frac{\mu_1 - \mu(v)}{\mu(v) - \mu_m} &= \frac{\sum_{l=1}^{m} (\mu_1 - \mu_l) \, \alpha_l^2}{\sum_{l=1}^{m} (\mu_l - \mu_m) \, \alpha_l^2} = \frac{\sum_{l=2}^{m} (\mu_1 - \mu_l) \, \alpha_l^2}{\sum_{l=1}^{m-1} (\mu_l - \mu_m) \, \alpha_l^2} \leq \frac{\sum_{l=2}^{m} (\mu_1 - \mu_m) \, \alpha_l^2}{(\mu_1 - \mu_m) \, \alpha_1^2} = \frac{\sum_{l=2}^{m} \alpha_l^2}{\alpha_1^2} \\ &= \frac{\sum_{l=1}^{m} \alpha_l^2}{\alpha_1^2} - 1 = \left(\frac{\|v\|_2}{\alpha_1} \right)^2 - 1 = \frac{1}{\cos^2 \angle_2(\widetilde{z}_1, v)} - 1 = \tan^2 \angle_2(\widetilde{z}_1, v). \qquad \square \end{aligned}$$

In order to verify (2.26), we regard the Krylov subspace $\mathcal{K}$ as $\mathcal{V}$ in Lemma 2.8, and select a nonzero vector $v \in \mathcal{V} = \mathcal{K}$ satisfying $\tan^2 \angle_2(z_1, v) = \min_{w \in \mathcal{K} \setminus \{0\}} \tan^2 \angle_2(z_1, w) = \tan^2 \angle_2\big(z_1, \mathcal{K}\big)$; cf. (1.32). Since $\mathcal{K}$ is a subset of the invariant subspace spanned by all nonzero eigenprojections $Q_l y$ of the initial vector y, the eigenprojection $Q_l v$ of v is collinear with $z_l = Q_l y / \|Q_l y\|_2$ for each nonzero $Q_l y$. In particular, $Q_1 v$ and z_1 are collinear, and $Q_1 v$ is nonzero since otherwise v is orthogonal to $\mathcal{Z}_1$ so that

$$\angle_2(z_1, v) = \pi/2 \quad \Rightarrow \quad \tan^2 \angle_2(z_1, y) \geq \tan^2 \angle_2(z_1, v) = \infty \quad \Rightarrow \quad \angle_2(z_1, y) = \pi/2$$

which contradicts $z_1^T y = z_1^T (\sum_{l=1}^{m} Q_l y) = z_1^T (Q_1 y) = z_1^T z_1 \|Q_1 y\|_2 = \|Q_1 y\|_2 > 0$. Thus $\widetilde{z}_1 = Q_1 v / \|Q_1 v\|_2$ can be defined, and the collinearity of $Q_1 v$ and z_1 shows that z_1 is either $\widetilde{z}_1$ or $-\widetilde{z}_1$. Combining this with (2.27) yields (2.26), namely,

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_m} \leq \tan^2 \angle_2(\widetilde{z}_1, v) = \tan^2 \angle_2(\pm \widetilde{z}_1, v) = \tan^2 \angle_2(z_1, v) = \tan^2 \angle_2\big(z_1, \mathcal{K}\big). \tag{2.28}$$

However, the derivation of (2.9) by extending (2.25) with (2.26) cannot be generalized to the derivation of (2.12) concerning block-Krylov subspaces since the generalized form (2.6) of (2.25) or (2.1) contains ratio-products. Thus we introduce another approach for deriving (2.9). By regarding the auxiliary vector $p(H)y$ with the shifted Chebyshev polynomial

$$p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha - \mu_2}{\mu_2 - \mu_m}\right)$$

as v in Lemma 2.8, the estimate (2.27) results in

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_m} \leq \tan^2 \angle_2(z_1, v) = \tan^2 \angle_2\big(z_1, p(H)y\big)$$

analogously to (2.28). Combining this with the intermediate estimate

$$\tan^2 \angle_2\big(z_1, p(H)y\big) \overset{(2.20)}{\leq} \big[T_{k-1}(1 + 2\gamma_1)\big]^{-2} \tan^2 \angle_2(y, z_1) \tag{2.29}$$

yields the estimate (2.9). For deriving (2.12), we generalize Lemma 2.8 together with (2.29) as Lemmas 2.9 and 2.10.

Arguments for block-Krylov subspaces

Lemma 2.9. *With Notation 1.5, consider arbitrary subspaces $\mathcal{U}, \mathcal{V} \subseteq \mathbb{R}^n$ with $\mathcal{U} \subseteq \mathcal{V}$ and* $\dim \mathcal{U} = i \geq 1$. *Let $\beta_1 \geq \cdots \geq \beta_i$ be the Ritz values of H in $\mathcal{U}$, and let $\theta_1 \geq \cdots \geq \theta_i$ be the i largest Ritz values of H in $\mathcal{V}$, then it holds, in terms of the invariant subspace $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_1, \ldots, z_i\}$, that*

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_n} \leq \frac{\mu_i - \beta_i}{\beta_i - \mu_n} \leq \tan^2 \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big). \tag{2.30}$$

Proof. According to $\mathcal{U} \subseteq \mathcal{V}$ and the Courant-Fischer principles, we have $\mu_i \geq \theta_i \geq \beta_i \geq \mu_n$. Then the monotonicity of the function $(\mu_i - \cdot\,)/(\,\cdot - \mu_n)$ implies the first inequality in (2.30).

The second inequality in (2.30) is trivial in the case $\tan \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big) = \infty$. In the nontrivial case, we use a Ritz vector $u \in \mathcal{U}$ associated with β_i, then

$$\tan \angle_2\big(u, \widetilde{\mathcal{Z}}\big) \overset{(1.32)}{\leq} \tan \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big) < \infty \quad \Rightarrow \quad \angle_2\big(u, \widetilde{\mathcal{Z}}\big) \neq \pi/2.$$

Thus u is not orthogonal to $\widetilde{\mathcal{Z}}$ so that its orthogonal projection $\widetilde{z}$ to $\widetilde{\mathcal{Z}}$ is nonzero. In addition, the difference vector $w = u - \widetilde{z}$ is the orthogonal projection of u to the orthogonal complement of $\widetilde{\mathcal{Z}}$ in $\mathbb{R}^n$, i.e., to the invariant subspace $\operatorname{span}\{z_{i+1}, \ldots, z_n\}$. Consequently, it holds that $\widetilde{z}^T w = 0$, $\widetilde{z}^T H w = 0$ so that

$$\beta_i = \mu(u) = \frac{u^T H u}{u^T u} = \frac{(\widetilde{z} + w)^T H (\widetilde{z} + w)}{(\widetilde{z} + w)^T (\widetilde{z} + w)} = \frac{\widetilde{z}^T H \widetilde{z} + w^T H w}{\widetilde{z}^T \widetilde{z} + w^T w}. \tag{2.31}$$

In the subcase $w = 0$, by considering $\mu_i \geq \beta_i$ (as mentioned at the beginning of the proof), (2.31), and $\widetilde{z} \in \widetilde{\mathcal{Z}} = \operatorname{span}\{z_1, \ldots, z_i\}$, we get $\mu_i \geq \beta_i = \mu(\widetilde{z}) \geq \mu_i$. Thus $\beta_i = \mu_i$ so that the second inequality in (2.30) is trivial. In the nontrivial subcase $w \neq 0$, the value $\mu(w)$ can be defined, and

$$(2.31) \quad \Rightarrow \quad \beta_i(\widetilde{z}^T \widetilde{z}) + \beta_i(w^T w) = \widetilde{z}^T H \widetilde{z} + w^T H w \quad \Rightarrow \quad (w^T w)\big(\beta_i - \mu(w)\big) = (\widetilde{z}^T \widetilde{z})\big(\mu(\widetilde{z}) - \beta_i\big)$$

so that

$$\frac{\mu(\widetilde{z}) - \beta_i}{\beta_i - \mu(w)} = \frac{w^T w}{\widetilde{z}^T \widetilde{z}} = \left(\frac{\|w\|_2}{\|\widetilde{z}\|_2}\right)^2. \tag{2.32}$$

Moreover, in terms of the orthogonal projector $Q = Q_1 + \cdots + Q_i$ on $\widetilde{\mathcal{Z}}$, we have

$$\frac{\|w\|_2}{\|\widetilde{z}\|_2} = \frac{\|u - Qu\|_2}{\|Qu\|_2} \overset{(1.33)}{=} \tan \angle_2\big(u, \widetilde{\mathcal{Z}}\big) \overset{(1.32)}{\leq} \tan \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big). \tag{2.33}$$

Combining (2.32) and (2.33) yields

$$\frac{\mu(\widetilde{z}) - \beta_i}{\beta_i - \mu(w)} \leq \tan^2 \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big)$$

which can easily be extended as the second inequality in (2.30) by using the properties $\mu(\widetilde{z}) \geq \mu_i$ and $\mu(w) \geq \mu_n$. □

We note that the second inequality in (2.30) can be rewritten by trigonometric conversions as

$$\frac{\mu_i - \beta_i}{\mu_i - \mu_n} \leq \sin^2 \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big), \qquad \frac{\beta_i - \mu_n}{\mu_i - \mu_n} \geq \cos^2 \angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big).$$

These alternative inequalities can be proved by other means; cf. [47, Theorem 1] and [126, Lemma 2.4]. Next, the intermediate estimate (2.29) is generalized to an auxiliary subspace $p(H)\widetilde{\mathcal{Y}}$ mentioned in Remark 2.6.

Lemma 2.10. *With Notation 1.5, consider a block-Krylov subspace*

$$\mathcal{K} = \operatorname{span}\{Y, HY, \ldots, H^{k-1}Y\}$$

with a basis matrix $Y \in \mathbb{R}^{n\times s}$ *of the initial subspace* $\mathcal{Y}$*, and denote by* $\mathcal{Z}$ *the invariant subspace* $\operatorname{span}\{z_1, \ldots, z_s\}$*. If* $\angle_2\big(\mathcal{Y}, \mathcal{Z}\big) < \pi/2$*, then there exist unique vectors* $y_j \in \mathcal{Y}$*,* $j = 1, \ldots, s$*, satisfying* $y_j^T z_j = 1$ *and* $y_j^T z_l = 0$ *for each* $l \in \{1, \ldots, s\}\backslash\{j\}$*. In addition, denote by* $\widetilde{\mathcal{Y}}$ *the subspace* $\operatorname{span}\{y_1, \ldots, y_i\}$ *for an arbitrary* $i \in \{1, \ldots, s\}$*, and denote by* $\mathcal{U}$ *the subspace* $p(H)\widetilde{\mathcal{Y}}$ *where* $p(\cdot)$ *is a polynomial defined by* $p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha-\mu_{s+1}}{\mu_{s+1}-\mu_n}\right)$ *depending on the Chebyshev polynomial* $T_{k-1}(\cdot)$*, then* $\widetilde{\mathcal{Y}}$ *and* $\mathcal{U}$ *both have dimension* i*. Moreover, it holds, in terms of the gap ratio* $\gamma_i = (\mu_i - \mu_{s+1})/(\mu_{s+1} - \mu_n)$ *and the invariant subspace* $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_1, \ldots, z_i\}$*, that*

$$\tan\angle_2\big(\mathcal{U}, \widetilde{\mathcal{Z}}\big) \le [\,T_{k-1}(1 + 2\gamma_i)\,]^{-1} \tan\angle_2\big(\mathcal{Y}, \mathcal{Z}\big). \tag{2.34}$$

Proof. In order to show the existence and uniqueness of y_j, we merge the given orthogonality conditions as $y_j^T Z = e_j^T$ with the basis matrix $Z = [z_1, \ldots, z_s]$ of $\mathcal{Z}$ and the jth standard basis vector e_j in $\mathbb{R}^s$. Then, by using the representation $y_j = Y g_j$ with the basis matrix Y and the coefficient vector g_j, we get $g_j^T Y^T Z = e_j^T$ which turns into the linear system $(Z^T Y)\, g_j = e_j$ after transposing. Therein $Z^T Y$ is an invertible matrix, since the assumption $\angle_2\big(\mathcal{Y}, \mathcal{Z}\big) < \pi/2$ ensures, for each nonzero vector $g \in \mathbb{R}^s$, that

$$\angle_2\big(Yg, \mathcal{Z}\big) \;\le\; \max_{y\in\mathcal{Y}\backslash\{0\}} \angle_2\big(y, \mathcal{Z}\big) \;\overset{(1.31)}{=}\; \angle_2\big(\mathcal{Y}, \mathcal{Z}\big) < \pi/2$$

so that Yg is not orthogonal to $\mathcal{Z}$, and thus $(Z^T Y)g = Z^T(Yg) \neq 0$ (i.e., by contraposition, $(Z^T Y)g = 0$ implies that $g = 0$). Consequently, the linear system $(Z^T Y)\, g_j = e_j$ has exactly one solution so that y_j exists uniquely and can be represented by $y_j = Y g_j = Y(Z^T Y)^{-1} e_j$.

Subsequently, this representation applied to the vectors $y_1, \ldots, y_i$ for an arbitrary $i \in \{1, \ldots, s\}$ results in the block form

$$[y_1, \ldots, y_i] = Y(Z^T Y)^{-1}[e_1, \ldots, e_i]$$

which is a factorization of the matrix $\widetilde{Y} = [y_1, \ldots, y_i]$. Then $\widetilde{Y}$ has rank i since its three factors have full column rank. Correspondingly, the subspace $\widetilde{\mathcal{Y}} = \operatorname{span}\{y_1, \ldots, y_i\}$ has dimension i. Next, in order to determine the dimension of the subspace $\mathcal{U} = p(H)\widetilde{\mathcal{Y}} = \operatorname{span}\{p(H)y_1, \ldots, p(H)y_i\}$, we consider the associated matrix $U = p(H)\widetilde{Y} = [p(H)y_1, \ldots, p(H)y_i]$ together with the basis matrix $\widetilde{Z} = [z_1, \ldots, z_i] = Z\,[e_1, \ldots, e_i]$ of $\widetilde{\mathcal{Z}}$. Then we have

$$\begin{aligned} U^T \widetilde{Z} &= \widetilde{Y}^T \big(p(H)\big)^T \widetilde{Z} = \widetilde{Y}^T p(H)\widetilde{Z} = \widetilde{Y}^T [p(H)z_1, \ldots, p(H)z_i] \\ &= \widetilde{Y}^T [p(\mu_1)z_1, \ldots, p(\mu_i)z_i] = \widetilde{Y}^T \widetilde{Z} D \end{aligned}$$

with the diagonal matrix $D = \operatorname{diag}\big(p(\mu_1), \ldots, p(\mu_i)\big) \in \mathbb{R}^{i\times i}$. Therein $\widetilde{Y}^T \widetilde{Z}$ coincides with the $(i \times i)$-identity matrix I_i, namely,

$$\widetilde{Y}^T \widetilde{Z} = \big(Y(Z^T Y)^{-1}[e_1, \ldots, e_i]\big)^T \big(Z\,[e_1, \ldots, e_i]\big) = \big((Z^T Y)(Z^T Y)^{-1}[e_1, \ldots, e_i]\big)^T [e_1, \ldots, e_i] = I_i$$

(or by using the given orthogonality conditions), and the diagonal matrix D is invertible since its diagonal entries $p(\mu_j)$, $j = 1, \ldots, i$ with $i \in \{1, \ldots, s\}$, are all nonzero, namely,

$$\mu_j \ge \mu_i \ge \mu_s \ge \mu_{s+1} \quad\Rightarrow\quad 1 + 2\,\frac{\mu_j - \mu_{s+1}}{\mu_{s+1} - \mu_n} \ge 1 \quad\Rightarrow\quad p(\mu_j) = T_{k-1}\left(1 + 2\,\frac{\mu_j - \mu_{s+1}}{\mu_{s+1} - \mu_n}\right) \ge 1$$

according to the properties in (1.36). Consequently, $U^T\widetilde{Z} = \widetilde{Y}^T\widetilde{Z}D$ coincides with D, and is thus an invertible $(i\times i)$-matrix so that U has rank i and the subspace $\mathcal{U}$ has dimension i.

For deriving the estimate (2.34), we start with the property

$$\tan\angle_2\big(\mathcal{U},\widetilde{\mathcal{Z}}\big) \overset{(1.32)}{=} \max_{u\in\mathcal{U}\setminus\{0\}} \tan\angle_2\big(u,\widetilde{\mathcal{Z}}\big) = \max_{\widetilde{y}\in\widetilde{\mathcal{Y}}\setminus\{0\}} \tan\angle_2\big(p(H)\widetilde{y},\widetilde{\mathcal{Z}}\big)$$

based on $\mathcal{U}=p(H)\widetilde{\mathcal{Y}}$, and select a vector $w\in\widetilde{\mathcal{Y}}\setminus\{0\}$ which maximizes $\tan\angle_2\big(p(H)\widetilde{y},\widetilde{\mathcal{Z}}\big)$, i.e.,

$$\tan\angle_2\big(\mathcal{U},\widetilde{\mathcal{Z}}\big) = \tan\angle_2\big(p(H)w,\widetilde{\mathcal{Z}}\big).$$

Then the given orthogonality conditions ensure that $w\in\widetilde{\mathcal{Y}}\subset\operatorname{span}\{z_1,\dots,z_i,z_{s+1},\dots,z_n\}$ so that w can be expanded as $w=\sum_{j=1}^{i}\alpha_j z_j+\sum_{j=s+1}^{n}\alpha_j z_j$ with the coefficients $\alpha_j=z_j^Tw$. Moreover, in terms of the orthogonal projector $P=Q_1+\cdots+Q_s$ on $\mathcal{Z}$, we have $Pw=\sum_{j=1}^{i}\alpha_j z_j$ so that

$$\tan^2\angle_2\big(w,\mathcal{Z}\big) \overset{(1.33)}{=} \left(\frac{\|w-Pw\|_2}{\|Pw\|_2}\right)^2 = \frac{\big\|\sum_{j=s+1}^{n}\alpha_j z_j\big\|_2^2}{\big\|\sum_{j=1}^{i}\alpha_j z_j\big\|_2^2} = \frac{\sum_{j=s+1}^{n}\alpha_j^2}{\sum_{j=1}^{i}\alpha_j^2}. \tag{2.35}$$

Analogously, by using the expansion $p(H)w=\sum_{j=1}^{i}p(\mu_j)\,\alpha_j z_j+\sum_{j=s+1}^{n}p(\mu_j)\,\alpha_j z_j$ of the auxiliary vector $p(H)w$ and the orthogonal projector $Q=Q_1+\cdots+Q_i$ on $\widetilde{\mathcal{Z}}$, we have $Q\big(p(H)w\big)=\sum_{j=1}^{i}p(\mu_j)\,\alpha_j z_j$ so that

$$\tan^2\angle_2\big(p(H)w,\widetilde{\mathcal{Z}}\big) = \frac{\big\|\sum_{j=s+1}^{n}p(\mu_j)\,\alpha_j z_j\big\|_2^2}{\big\|\sum_{j=1}^{i}p(\mu_j)\,\alpha_j z_j\big\|_2^2} = \frac{\sum_{j=s+1}^{n}p^2(\mu_j)\,\alpha_j^2}{\sum_{j=1}^{i}p^2(\mu_j)\,\alpha_j^2}. \tag{2.36}$$

In addition, by applying again the properties in (1.36) to the shifted Chebyshev polynomial $p(\cdot)$, it holds that

$$p(\mu_j)\ge p(\mu_i)\ge 1 \quad\text{for}\quad j\in\{1,\dots,i\}, \qquad\text{and}\quad |p(\mu_j)|\le 1 \quad\text{for}\quad j\in\{s{+}1,\dots,n\}. \tag{2.37}$$

Summarizing the above yields

$$\begin{aligned}\tan^2\angle_2\big(\mathcal{U},\widetilde{\mathcal{Z}}\big) &= \tan^2\angle_2\big(p(H)w,\widetilde{\mathcal{Z}}\big) \overset{(2.36)}{=} \frac{\sum_{j=s+1}^{n}p^2(\mu_j)\,\alpha_j^2}{\sum_{j=1}^{i}p^2(\mu_j)\,\alpha_j^2} \overset{(2.37)}{\le} \frac{\sum_{j=s+1}^{n}\alpha_j^2}{\sum_{j=1}^{i}p^2(\mu_i)\,\alpha_j^2}\\ &= \big[T_{k-1}(1+2\gamma_i)\big]^{-2}\frac{\sum_{j=s+1}^{n}\alpha_j^2}{\sum_{j=1}^{i}\alpha_j^2} \overset{(2.35)}{=} \big[T_{k-1}(1+2\gamma_i)\big]^{-2}\tan^2\angle_2\big(w,\mathcal{Z}\big)\end{aligned}$$

and subsequently

$$\tan\angle_2\big(\mathcal{U},\widetilde{\mathcal{Z}}\big) \le \big[T_{k-1}(1+2\gamma_i)\big]^{-1}\tan\angle_2\big(w,\mathcal{Z}\big) \tag{2.38}$$

according to the positivity of the concerned values. Furthermore, since $w\in\widetilde{\mathcal{Y}}\setminus\{0\}$ and $\widetilde{\mathcal{Y}}\subseteq\mathcal{Y}$, it holds that

$$\tan\angle_2\big(w,\mathcal{Z}\big) \le \max_{y\in\mathcal{Y}\setminus\{0\}}\tan\angle_2\big(y,\mathcal{Z}\big) \overset{(1.32)}{=} \tan\angle_2\big(\mathcal{Y},\mathcal{Z}\big).$$

Combining this with (2.38) yields the estimate (2.34). □

Now the angle-dependent estimate (2.12) can be shown. The estimate is trivial in the case $\tan\angle_2(\mathcal{Y},\mathcal{Z})=\infty$. In the nontrivial case $\tan\angle_2(\mathcal{Y},\mathcal{Z})<\infty$, i.e., $\angle_2(\mathcal{Y},\mathcal{Z})<\pi/2$, Lemma 2.10 is applicable so that the estimate (2.34) holds. Moreover, the auxiliary subspace $\mathcal{U}=p(H)\widetilde{\mathcal{Y}}$ has dimension i and is a subset of the block-Krylov subspace $\mathcal{K}$. Then applying Lemma 2.9 to $\mathcal{V}=\mathcal{K}$ yields the estimate (2.30). Finally, (2.12) is achieved by combining (2.30) with (2.34).

Remark 2.11. *In Lemma 2.10, the auxiliary vectors* $y_1, \ldots, y_s$ *and the eigenvectors* $z_1, \ldots, z_s$ *form a biorthogonal system. Such auxiliary vectors have already been suggested by Rutishauser in [97] for investigating the block power method. Similar settings have been used in Saad's analysis [98]; cf. Theorem 2.3. However, it is somewhat artificial to assume the linear independence of the concerned orthogonal projections in a theorem. Instead, we suggest the more natural assumption* $\angle_2(\mathcal{Y}, \mathcal{Z}) < \pi/2$.

In comparison to Knyazev's analysis [44, 45] which did not provide formal estimates and derivations for Krylov subspace eigensolvers, we add some details for completeness, e.g., the verification of the dimension i *of the auxiliary subspace* $\mathcal{U} = p(H)\widetilde{\mathcal{Y}}$ *and the properties of the shifted Chebyshev polynomial* $p(\cdot)$ *in* (2.37).

2.3.2 Angle-free estimates on Ritz values

We consider the angle-free estimates (2.10) concerning the largest Ritz value in a Krylov subspace and (2.13) concerning the sth largest Ritz value in a block-Krylov subspace.

For deriving (2.10), we use again the auxiliary vector $p(H)y$ with $p(\alpha) = T_{k-1}\big(1 + 2\,\frac{\alpha-\mu_2}{\mu_2-\mu_m}\big)$ as in the derivation of the angle-dependent estimate (2.9). However, it is not meaningful to apply the eigenexpansion of $p(H)y$ to the derivation of (2.10) since the resulting estimate (2.29) is not angle-free. Instead, we can construct a further auxiliary vector $\widetilde{y} \in \mathbb{R}^n \backslash \{0\}$ which does not necessarily belong to the Krylov subspace but has the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \qquad \text{and} \qquad \frac{\mu_1 - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_2} \leq [\,T_{k-1}(1 + 2\gamma_1)\,]^{-2}\,\frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}\,. \tag{2.39}$$

The construction of $\widetilde{y}$ is based on a monotonicity argument of the Rayleigh quotient $\mu(\cdot)$ with respect to the expansion coefficients of the concerned vectors; cf. [44, Lemma 2.3.2] and [72, Lemma A.1]. We restate this argument in Lemma 2.12. Then a suitable $\widetilde{y}$ is introduced in Lemma 2.13 together with the verification of the properties in (2.39). By combining these properties with the evident relation $\theta_1 \geq \mu\big(p(H)y\big)$, the derivation of (2.10) is completed.

For deriving (2.13), we apply a similar approach. the monotonicity argument in Lemma 2.12 is slightly reformulated in favor of block-Krylov subspaces.

Arguments for Krylov subspaces

Lemma 2.12. *With Notation 1.4, let* u *be an arbitrary nonzero vector in* $\mathbb{R}^n$ *with* $\mu_i \geq \mu(u) \geq \mu_{i+1}$*, and define an orthonormal system* $\{z_1, \ldots, z_m\}$ *with respect to the eigenprojections* $Q_1 u, \ldots, Q_m u$ *of* u *analogously to* (2.16)*, i.e.,* $z_1, \ldots, z_m$ *are orthonormal eigenvectors associated with the eigenvalues* $\mu_1, \ldots, \mu_m$*, and* u *can be expanded as* $u = \sum_{l=1}^{m} \alpha_l\, z_l$ *with the coefficients* $\alpha_l = \|Q_l u\|_2$*. Then the vector* $v = \sum_{l=1}^{m} \beta_l\, z_l$ *with* $\beta_l \in \mathbb{R}$ *satisfies*

(a) $\mu(v) \geq \mu(u)$ *if* $|\beta_l| \geq |\alpha_l| \ \ \forall\, l \leq i$ *and* $|\beta_l| \leq |\alpha_l| \ \ \forall\, l > i$,

(b) $\mu(v) \leq \mu(u)$ *if* $|\beta_l| \leq |\alpha_l| \ \ \forall\, l \leq i$ *and* $|\beta_l| \geq |\alpha_l| \ \ \forall\, l > i$.

Proof. For proving the statement (a), we begin with the intermediate vector $u_i = u + (\beta_i - \alpha_i)\, z_i$, i.e., a slight modification of u where the coefficient α_i is replaced by β_i. We show the relation $\mu_i \geq \mu(u_i) \geq \mu(u)$ by regarding $\mu(u) = \big(\sum_{l=1}^{m} \mu_l\, \alpha_l^2\big)/\big(\sum_{l=1}^{m} \alpha_l^2\big)$ as the value $f(\alpha_i^2)$ of the function $f(\cdot)$ defined by

$$f(\xi) = \frac{\mu_i\, \xi + \sum_{l \in \{1,\ldots,m\} \backslash \{i\}} \mu_l\, \alpha_l^2}{\xi + \sum_{l \in \{1,\ldots,m\} \backslash \{i\}} \alpha_l^2} \quad \text{for} \quad \xi \in [\alpha_i^2, \infty).$$

The derivative of $f(\cdot)$ reads

$$\frac{\mu_i\big(\xi+\sum_{l\in\{1,\dots,m\}\setminus\{i\}}\alpha_l^2\big)-\big(\mu_i\,\xi+\sum_{l\in\{1,\dots,m\}\setminus\{i\}}\mu_l\,\alpha_l^2\big)}{\big(\xi+\sum_{l\in\{1,\dots,m\}\setminus\{i\}}\alpha_l^2\big)^2}=\frac{\sum_{l\in\{1,\dots,m\}\setminus\{i\}}(\mu_i-\mu_l)\,\alpha_l^2}{\big(\xi+\sum_{l\in\{1,\dots,m\}\setminus\{i\}}\alpha_l^2\big)^2}$$

so that its sign is constant and given by the sign of the constant term $\sum_{l\in\{1,\dots,m\}\setminus\{i\}}(\mu_i-\mu_l)\,\alpha_l^2$. Thus $f(\cdot)$ is either decreasing or nondecreasing on the interval $[\alpha_i^2,\,\infty)$. If $f(\cdot)$ is decreasing, it holds that

$$\mu(u)=f(\alpha_i^2)>\lim_{\xi\to\infty}f(\xi)=\mu_i$$

which contradicts the condition $\mu_i\geq\mu(u)$ in the lemma. Consequently, $f(\cdot)$ is nondecreasing so that the replacement $\alpha_i\to\beta_i$ with $|\beta_i|\geq|\alpha_i|$, i.e., with $\beta_i^2\geq\alpha_i^2$, results in

$$f(\alpha_i^2)\leq f(\beta_i^2)\leq\lim_{\xi\to\infty}f(\xi)\qquad\Rightarrow\qquad\mu_i\geq\mu(u_i)\geq\mu(u).$$

More generally, we define the intermediate vectors $u_{i+1},\,u_i,\,\dots,\,u_1$ by setting $u_{i+1}=u$ and $u_{j-1}=u_j+(\beta_{j-1}-\alpha_{j-1})\,z_{j-1}$ for $j=i{+}1,\,\dots,\,2$. Then the above approach inductively shows the relation $\mu_{j-1}\geq\mu(u_{j-1})\geq\mu(u_j)$ under the condition $\mu_{j-1}\geq\mu(u_j)$ which is ensured by $\mu_i\geq\mu(u)$ or by the result $\mu_j\geq\mu(u_j)$ of the previous step. In summary, we get

$$\mu(u_1)\geq\cdots\geq\mu(u_i)\geq\mu(u_{i+1})=\mu(u). \tag{2.40}$$

Additionally, we define the intermediate vectors $v_i,\,v_{i+1},\,\dots,\,v_m$ by setting $v_i=u_1$ and $v_{j+1}=v_j+(\beta_{j+1}-\alpha_{j+1})\,z_{j+1}$ for $j=i,\,\dots,\,m{-}1$. Then an analogous approach yields

$$\mu(v_m)\geq\cdots\geq\mu(v_{i+1})\geq\mu(v_i)=\mu(u_1).$$

Combining this with (2.40) and $v_m=v$ completes the proof of the statement (a). Furthermore, the statement (b) can be proved analogously or by reformulating the proof of (a) for $-H$. □

Based on Lemma 2.12, we can construct an auxiliary vector $\widetilde{y}$ satisfying (2.39) by scaling the eigenprojection Q_1y of the initial vector y.

Lemma 2.13. *With Notation 1.4, consider a Krylov subspace* $\mathcal{K}=\operatorname{span}\{y,Hy,\dots,H^{k-1}y\}$ *with the initial vector* $y\in\mathbb{R}^n\setminus\{0\}$*, and assume that* $\mu(y)>\mu_2$*. Then the eigenprojection* Q_1y *is nonzero, and an auxiliary vector* $\widetilde{y}$ *which possesses the properties in* (2.39) *is given by*

$$\widetilde{y}\;=\;p(\mu_1)\,Q_1y\;+\;\textstyle\sum_{l=2}^m Q_ly$$

with the polynomial $p(\alpha)=T_{k-1}\big(1+2\,\frac{\alpha-\mu_2}{\mu_2-\mu_m}\big)$ *depending on the Chebyshev polynomial* $T_{k-1}(\cdot)$.

Proof. The eigenprojection Q_1y is nonzero, since otherwise y belongs to the invariant subspace $\mathcal{Z}_2\oplus\cdots\oplus\mathcal{Z}_m$ so that $\mu_2\geq\mu(y)$ holds and contradicts the condition $\mu(y)>\mu_2$.

Next, we show that the auxiliary vector $\widetilde{y}$ possesses the properties in (2.39). According to (1.36), the shifted Chebyshev polynomial $p(\cdot)$ has the properties

$$p(\mu_1)>1\qquad\text{and}\qquad|p(\mu_l)|\leq1\quad\forall\,l\in\{2,\dots,m\}. \tag{2.41}$$

These can be combined with Lemma 2.12 in order to show the inequalities

$$\mu\big(p(H)y\big)\geq\mu(y),\qquad\mu\big(p(H)y\big)\geq\mu(\widetilde{y}),\qquad\mu(\widetilde{y})\geq\mu(y) \tag{2.42}$$

in a row where the first inequality serves to guarantee the condition $\mu\big(p(H)y\big) > \mu_2$ for proving the second inequality.

The first inequality in (2.42) is proved by regarding y and $p(H)y$ as u and v in Lemma 2.12. Since $\mu_1 \geq \mu(y) > \mu_2$, the condition $\mu_i \geq \mu(u) \geq \mu_{i+1}$ is fulfilled for $i=1$. Moreover, since $y = \sum_{l=1}^m Q_l y$ and $p(H)y = p(H)\big(\sum_{l=1}^m Q_l y\big) = \sum_{l=1}^m p(\mu_l)\, Q_l y$, the associated coefficients read $\alpha_l = \|Q_l y\|_2$ and $\beta_l = p(\mu_l)\, \|Q_l y\|_2$ for each $l \in \{1,\dots,m\}$. Then

$$|\beta_1| = \big|p(\mu_1)\big|\,|\alpha_1| \overset{(2.41)}{>} |\alpha_1|, \qquad \text{and} \quad |\beta_l| = \big|p(\mu_l)\big|\,|\alpha_l| \overset{(2.41)}{\leq} |\alpha_l| \quad \forall\, l>1.$$

Thus the statement (a) is applicable and shows that $\mu\big(p(H)y\big) \geq \mu(y)$.

For proving the second inequality in (2.42), we regard $p(H)y$ and $\widetilde{y}$ as u and v in Lemma 2.12. Therein $\mu_i \geq \mu(u) \geq \mu_{i+1}$ is also fulfilled for $i=1$ since $\mu_1 \geq \mu\big(p(H)y\big) \geq \mu(y) > \mu_2$ by using the first inequality in (2.42). In addition, the associated coefficients fulfill $|\alpha_l| = |p(\mu_l)|\, \|Q_l y\|_2$ for each $l \in \{1,\dots,m\}$, $|\beta_1| = |p(\mu_1)|\, \|Q_1 y\|_2$, and $|\beta_l| = \|Q_l y\|_2$ for each $l \in \{2,\dots,m\}$ according to the definition of $\widetilde{y}$. Then the statement (b) is applicable because

$$|\beta_1| = |\alpha_1|, \qquad \text{and} \quad |\beta_l| = \frac{|\alpha_l|}{|p(\mu_l)|} \overset{(2.41)}{\geq} |\alpha_l| \quad \forall\, l>1.$$

Therefore we get $\mu(v) \leq \mu(u)$, i.e., $\mu\big(p(H)y\big) \geq \mu(\widetilde{y})$.

In order to show the third inequality in (2.42), we regard y and $\widetilde{y}$ as u and v in Lemma 2.12. The condition $\mu_i \geq \mu(u) \geq \mu_{i+1}$ for $i=1$ is ensured by $\mu_1 \geq \mu(y) > \mu_2$ again. The associated coefficients read $\alpha_l = \|Q_l y\|_2$ for each $l \in \{1,\dots,m\}$, $\beta_1 = p(\mu_1)\, \|Q_1 y\|_2$, and $\beta_l = \|Q_l y\|_2$ for each $l \in \{2,\dots,m\}$ so that

$$|\beta_1| = \big|p(\mu_1)\big|\,|\alpha_1| \overset{(2.41)}{>} |\alpha_1|, \qquad \text{and} \quad |\beta_l| = |\alpha_l| \quad \forall\, l>1.$$

Thus the statement (a) is applicable and shows that $\mu(\widetilde{y}) \geq \mu(y)$.

Combining the second and third inequality in (2.42) results in the first property in (2.39).

The second property in (2.39) is trivial in the case $\sum_{l=2}^m Q_l y = 0$ since therein we have $y = Q_1 y$ and $\widetilde{y} = p(\mu_1)\, Q_1 y$ with $p(\mu_1) \neq 0$ due to (2.41) so that y and $\widetilde{y}$ are eigenvectors associated with μ_1. Thus $\mu(y) = \mu(\widetilde{y}) = \mu_1$, and both sides of the inequality in the property are zero. In the nontrivial case $\sum_{l=2}^m Q_l y \neq 0$, we represent y by $y = z + w$ with $z = Q_1 y$ and $w = \sum_{l=2}^m Q_l y$. Then w is nonzero so that the value $\mu(w)$ can be defined. Moreover, z and w are orthogonal projections of y to the eigenspace $\mathcal{Z}_1$ and the invariant subspace $\mathcal{Z}_2 \oplus \cdots \oplus \mathcal{Z}_m$, respectively. Thus $z^T w = 0$ and $z^T H w = 0$ hold so that

$$\mu(y) = \frac{z^T H z + w^T H w}{z^T z + w^T w} \qquad \Rightarrow \qquad \frac{\mu(z) - \mu(y)}{\mu(y) - \mu(w)} = \left(\frac{\|w\|_2}{\|z\|_2}\right)^2 > 0 \tag{2.43}$$

analogously to (2.31) and (2.32) in the proof of Lemma 2.9. Similarly, by using the expansion $\widetilde{y} = p(\mu_1)\, z + w$ corresponding to $y = z + w$ and the definition of $\widetilde{y}$, we get

$$\mu(\widetilde{y}) = \frac{\big(p(\mu_1)\, z\big)^T H \big(p(\mu_1)\, z\big) + w^T H w}{\big(p(\mu_1)\, z\big)^T \big(p(\mu_1)\, z\big) + w^T w} \qquad \Rightarrow \qquad \frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(w)} = \left(\frac{\|w\|_2}{\|p(\mu_1)\, z\|_2}\right)^2.$$

Combining this with (2.43) yields

$$\left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(w)}\right)\left(\frac{\mu(z) - \mu(y)}{\mu(y) - \mu(w)}\right)^{-1} = \left(\frac{1}{|p(\mu_1)|}\right)^2 = \big[\, T_{k-1}(1 + 2\gamma_1)\,\big]^{-2} \tag{2.44}$$

with the gap ratio $\gamma_1 = (\mu_1 - \mu_2)/(\mu_2 - \mu_m)$. In addition, the third inequality in (2.42) can be extended as $\mu(z) = \mu_1 \geq \mu(\widetilde{y}) \geq \mu(y) > \mu_2 \geq \mu(w)$. Consequently, we have

$$\left(\frac{\mu_1 - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_2}\right)\left(\frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}\right)^{-1} = \left(\frac{\mu_1 - \mu(\widetilde{y})}{\mu_1 - \mu(y)}\right)\left(\frac{\mu(y) - \mu_2}{\mu(\widetilde{y}) - \mu_2}\right)$$
$$\leq \left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(z) - \mu(y)}\right)\left(\frac{\mu(y) - \mu(w)}{\mu(\widetilde{y}) - \mu(w)}\right) = \left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(w)}\right)\left(\frac{\mu(z) - \mu(y)}{\mu(y) - \mu(w)}\right)^{-1}.$$

This extends (2.44) as $\left(\frac{\mu_1-\mu(\widetilde{y})}{\mu(\widetilde{y})-\mu_2}\right)\left(\frac{\mu_1-\mu(y)}{\mu(y)-\mu_2}\right)^{-1} \leq [\,T_{k-1}(1+2\gamma_1)\,]^{-2}$ which is equivalent to the second property in (2.39) in the nontrivial case. □

The verification in Lemma 2.13 allows us to apply the properties in (2.39) to the proof of the angle-free estimate (2.10). Since $p(H)y$ belongs to the Krylov subspace $\mathcal{K}$, we get $\theta_1 \geq \mu\big(p(H)y\big)$. Then $\theta_1 \geq \mu(\widetilde{y})$ holds according to the first property in (2.39). Subsequently, the monotonicity of the function $\big(\mu_1 - \cdot\,\big)/\big(\,\cdot - \mu_2\big)$ shows that $\big(\mu_1 - \theta_1\big)/\big(\theta_1 - \mu_2\big) \leq \big(\mu_1 - \mu(\widetilde{y})\big)/\big(\mu(\widetilde{y}) - \mu_2\big)$. Combining this with the second property in (2.39) implies (2.10).

For deriving the angle-free estimate (2.13) concerning block-Krylov subspaces, we generalize Lemmas 2.12 and 2.13 as Lemmas 2.14 and 2.15.

Arguments for block-Krylov subspaces

Lemma 2.14. *With Notation 1.5, let u be an arbitrary nonzero vector in $\mathbb{R}^n$ with $\mu_i \geq \mu(u) \geq \mu_{i+1}$, and expand u as $u = \sum_{l=1}^{n} \alpha_l\, z_l$ with the coefficients $\alpha_l = z_l^T u$. Then the vector $v = \sum_{l=1}^{n} \beta_l\, z_l$ with $\beta_l \in \mathbb{R}$ satisfies*

(a) $\mu(v) \geq \mu(u)$ *if* $|\beta_l| \geq |\alpha_l| \quad \forall\, l \leq i$ *and* $|\beta_l| \leq |\alpha_l| \quad \forall\, l > i$,

(b) $\mu(v) \leq \mu(u)$ *if* $|\beta_l| \leq |\alpha_l| \quad \forall\, l \leq i$ *and* $|\beta_l| \geq |\alpha_l| \quad \forall\, l > i$.

Proof. The proof of Lemma 2.12 with n instead of m shows the statements. □

We note that the assumption $\mu_i > \mu_{i+1}$ is not required in Lemma 2.14, but rather required in the angle-free estimate (2.13) for the index $i = s$ in order to avoid a less meaningful bound with $\gamma_s = 0$. In the following lemma, we construct an auxiliary vector $\widetilde{y}$ by adapting the properties (2.39) to a block-Krylov subspace.

Lemma 2.15. *With Notation 1.5, consider a block-Krylov subspace*

$$\mathcal{K} = \mathrm{span}\{Y, HY, \ldots, H^{k-1}Y\}$$

with a basis matrix $Y \in \mathbb{R}^{n\times s}$ of the initial subspace $\mathcal{Y}$, and let $\eta_1 \geq \cdots \geq \eta_s$ be the Ritz values of H in $\mathcal{Y}$. If $\eta_s > \mu_{s+1}$, then the subspace $p(H)\mathcal{Y}$ has dimension s where the polynomial $p(\cdot)$ is defined by $p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha-\mu_{s+1}}{\mu_{s+1}-\mu_n}\right)$ depending on the Chebyshev polynomial $T_{k-1}(\cdot)$. In addition, let $\widetilde{\eta}_1 \geq \cdots \geq \widetilde{\eta}_s$ be the Ritz values of H in $p(H)\mathcal{Y}$, and let y be a nonzero vector in $\mathcal{Y}$ for which $p(H)y$ is a Ritz vector in $p(H)\mathcal{Y}$ associated with $\widetilde{\eta}_s$. Then the auxiliary vector

$$\widetilde{y} \;=\; p(\mu_s)\, \textstyle\sum_{l=1}^{s} Q_l y \;+\; \sum_{l=s+1}^{n} Q_l y$$

possesses the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \qquad \text{and} \qquad \frac{\mu_s - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{s+1}} \leq [\,T_{k-1}(1+2\gamma_s)\,]^{-2}\, \frac{\mu_s - \mu(y)}{\mu(y) - \mu_{s+1}} \tag{2.45}$$

with the gap ratio $\gamma_s = (\mu_s - \mu_{s+1})/(\mu_{s+1} - \mu_n)$.

Proof. In order to determine the dimension of the subspace $p(H)\mathcal{Y}$, we use the invariant subspace $\mathcal{Z} = \text{span}\{z_1, \ldots, z_s\}$ together with its basis matrix $Z = [z_1, \ldots, z_s]$. The assumption $\eta_s > \mu_{s+1}$ ensures $\angle_2\big(\mathcal{Y}, \mathcal{Z}\big) < \pi/2$, since otherwise $\mathcal{Y}$ contains a nonzero vector $\widehat{y}$ with $\angle_2\big(\widehat{y}, \mathcal{Z}\big) = \pi/2$ according to (1.31), then $\widehat{y}$ belongs to $\text{span}\{z_{s+1}, \ldots, z_n\}$ so that $\mu_{s+1} \geq \mu(\widehat{y}) \geq \eta_s$ holds and contradicts $\eta_s > \mu_{s+1}$. Subsequently, $\angle_2\big(\mathcal{Y}, \mathcal{Z}\big) < \pi/2$ ensures that Z^TY is an invertible matrix; see the first paragraph in the proof of Lemma 2.10. In addition, similarly as in the second paragraph therein, we have

$$\big(p(H)Y\big)^T Z = Y^T\big(p(H)\big)^T Z = Y^T p(H) Z = Y^T Z D = (Z^TY)^T D$$

with the diagonal matrix $D = \text{diag}\big(p(\mu_1), \ldots, p(\mu_s)\big) \in \mathbb{R}^{s\times s}$, which is invertible since its diagonal entries are all nonzero according to (1.36). Thus $(p(H)Y)^T Z = (Z^TY)^T D$ is an invertible $(s \times s)$-matrix so that $p(H)Y$ has rank s and $p(H)\mathcal{Y}$ has dimension s.

For verifying that the auxiliary vector $\widetilde{y}$ possesses the properties in (2.45), we use the more detailed properties

$$p(\mu_1) \geq \cdots \geq p(\mu_s) > 1 \qquad \text{and} \qquad |p(\mu_l)| \leq 1 \quad \forall\, l \in \{s+1, \ldots, n\} \tag{2.46}$$

of the shifted Chebyshev polynomial $p(\cdot)$ based on (1.36). Therein $p(\mu_s) > 1$ holds since the relation $\mu_s \geq \eta_s > \mu_{s+1}$ results in $p(\mu_s) > p(\mu_{s+1}) = 1$.

The first property in (2.45) is denotationally identical with that in (2.39) and can thus be verified as in Lemma 2.13 by showing three inequalities in a row; cf. (2.42).

We first show the inequality $\mu\big(p(H)y\big) \geq \mu(y)$. Therein Lemma 2.14 cannot easily be applied with the index $i = s$ since the required condition $\mu_s \geq \mu(y) \geq \mu_{s+1}$ is not completely known in the above discussion, namely, $\mu_s \geq \mu(y)$ still needs to be verified. A suitable approach begins with the relation $\mu(y) \geq \eta_s > \mu_{s+1}$ so that the condition $\mu_i \geq \mu(y) \geq \mu_{i+1}$ is fulfilled for an index $i \in \{1, \ldots, s\}$ which is not necessarily s. Then we regard y and $p(H)y/p(\mu_i)$ as u and v in Lemma 2.14. The associated coefficients read $\alpha_l = z_l^T y$ and $\beta_l = p(\mu_l)\,(z_l^T y)/p(\mu_i)$ for each $l \in \{1, \ldots, n\}$. In addition, by using (2.46) and $i \leq s$, we get

$$\frac{p(\mu_1)}{p(\mu_i)} \geq \cdots \geq \frac{p(\mu_i)}{p(\mu_i)} = 1 \geq \cdots \geq \frac{p(\mu_s)}{p(\mu_i)} > 0, \qquad \left|\frac{p(\mu_l)}{p(\mu_i)}\right| \leq \left|\frac{1}{p(\mu_i)}\right| < 1 \quad \forall\, l > s$$

so that

$$|\beta_l| = \big|p(\mu_l)\,\alpha_l/p(\mu_i)\big| = \left|\frac{p(\mu_l)}{p(\mu_i)}\right| |\alpha_l| \begin{cases} \geq |\alpha_l| & \forall\, l \leq i, \\ \leq |\alpha_l| & \forall\, l > i. \end{cases}$$

Thus the statement (a) in Lemma 2.14 is applicable and shows that $\mu\big(p(H)y/p(\mu_i)\big) \geq \mu(y)$. This results in $\mu\big(p(H)y\big) \geq \mu(y)$ since $p(H)y/p(\mu_i)$ is collinear with $p(H)y$.

Moreover, since $p(H)y$ is a Ritz vector in $p(H)\mathcal{Y}$ associated with $\widetilde{\eta}_s$, it holds that $\mu\big(p(H)y\big) = \widetilde{\eta}_s \leq \mu_s$. Combining this with the already known relations $\mu\big(p(H)y\big) \geq \mu(y)$ and $\mu(y) \geq \eta_s > \mu_{s+1}$ yields $\mu_s \geq \mu\big(p(H)y\big) \geq \mu(y) > \mu_{s+1}$. Thus the condition $\mu_i \geq \mu(u) \geq \mu_{i+1}$ in Lemma 2.14 is fulfilled by $u = p(H)y$ or $u = y$ for the index $i = s$. Subsequently, we show the two inequalities

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \qquad \text{and} \qquad \mu(\widetilde{y}) \geq \mu(y)$$

in the first property in (2.45) by applying Lemma 2.14 as follows. By regarding $p(H)y$ and $\widetilde{y}$ as u and v, the associated coefficients read $\alpha_l = p(\mu_l)\,(z_l^T y)$ for each $l \in \{1, \ldots, n\}$, $\beta_l = p(\mu_s)\,(z_l^T y)$ for each $l \leq s$, and $\beta_l = z_l^T y$ for each $l > s$ according to the definition of $\widetilde{y}$. Then

$$|\beta_l| = \left|\frac{p(\mu_s)}{p(\mu_l)}\right| |\alpha_l| \overset{(2.46)}{\leq} |\alpha_l| \quad \forall\, l \leq s, \qquad \text{and} \quad |\beta_l| = \frac{|\alpha_l|}{|p(\mu_l)|} \overset{(2.46)}{\geq} |\alpha_l| \quad \forall\, l > s$$

so that we can apply the statement (b) and get $\mu\big(p(H)y\big) \geq \mu(\widetilde{y})$. Next, by regarding y and $\widetilde{y}$ as u and v, the α-coefficients are given by $\alpha_l = z_l^T y$ for each $l \in \{1, \dots, n\}$, and the β-coefficients remain as before. Then

$$|\beta_l| = \big|p(\mu_s)\big|\,|\alpha_l| \overset{(2.46)}{>} |\alpha_l| \quad \forall\, l \leq s, \qquad \text{and} \quad |\beta_l| = |\alpha_l| \quad \forall\, l > s$$

so that statement (a) is applicable and shows that $\mu(\widetilde{y}) \geq \mu(y)$.

In order to verify the second property in (2.45), we represent y by $y = z + w$ with $z = \sum_{l=1}^{s} Q_l y$ and $w = \sum_{l=s+1}^{n} Q_l y$. Correspondingly, $\widetilde{y}$ is represented by $\widetilde{y} = p(\mu_s)z + w$. It holds that $z \neq 0$ since otherwise $y = w \in \operatorname{span}\{z_{s+1}, \dots, z_n\}$ so that $\mu(y) \leq \mu_{s+1}$. This contradicts the already known relation $\mu_s \geq \mu(y) > \mu_{s+1}$. Furthermore, the property is trivial in the case $w = 0$ since therein $y = z \in \operatorname{span}\{z_1, \dots, z_s\}$ so that $\mu(y) \geq \mu_s$. Combing this with the relation $\mu_s \geq \mu(y) > \mu_{s+1}$ yields $\mu(y) = \mu_s$. In addition, it holds that $\widetilde{y} = p(\mu_s)z = p(\mu_s)y$ with $p(\mu_s) \neq 0$ due to (2.46) so that $\mu(\widetilde{y}) = \mu(y) = \mu_s$. Thus both sides of the inequality in the property are zero. In the nontrivial case $w \neq 0$, the value $\mu(w)$ can be defined. Then, analogously to the proof of Lemma 2.13, we get

$$\left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(w)}\right)\left(\frac{\mu(z) - \mu(y)}{\mu(y) - \mu(w)}\right)^{-1} = \left(\frac{1}{|p(\mu_s)|}\right)^2 = [\,T_{k-1}(1 + 2\gamma_s)\,]^{-2}$$

with the gap ratio $\gamma_s = (\mu_s - \mu_{s+1})/(\mu_{s+1} - \mu_n)$; cf. (2.44). In addition, based on the relation $\mu(z) \geq \mu_s \geq \mu(\widetilde{y}) \geq \mu(y) > \mu_{s+1} \geq \mu(w)$, it holds that

$$\begin{aligned}\left(\frac{\mu_s - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{s+1}}\right)\left(\frac{\mu_s - \mu(y)}{\mu(y) - \mu_{s+1}}\right)^{-1} &= \left(\frac{\mu_s - \mu(\widetilde{y})}{\mu_s - \mu(y)}\right)\left(\frac{\mu(y) - \mu_{s+1}}{\mu(\widetilde{y}) - \mu_{s+1}}\right) \\ &\leq \left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(z) - \mu(y)}\right)\left(\frac{\mu(y) - \mu(w)}{\mu(\widetilde{y}) - \mu(w)}\right) = \left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(w)}\right)\left(\frac{\mu(z) - \mu(y)}{\mu(y) - \mu(w)}\right)^{-1}.\end{aligned}$$

Summarizing the above yields $\left(\frac{\mu_s - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{s+1}}\right)\left(\frac{\mu_s - \mu(y)}{\mu(y) - \mu_{s+1}}\right)^{-1} \leq [\,T_{k-1}(1 + 2\gamma_s)\,]^{-2}$ which is an equivalent form of the second property in (2.45) in the nontrivial case. □

Now we apply Lemma 2.15 to the proof of the angle-free estimate (2.13). Since $p(H)\mathcal{Y}$ is an s-dimensional subspace within the block-Krylov subspace $\mathcal{K}$, it holds that $\widetilde{\eta}_s \leq \theta_s$ for the corresponding sth Ritz values based on the Courant-Fischer principles. Then we get $\theta_s \geq \widetilde{\eta}_s = \mu\big(p(H)y\big) \geq \mu(\widetilde{y})$ according to the first property in (2.45) so that the monotonicity of the function $\big(\mu_s - \cdot\,\big)/\big(\,\cdot - \mu_{s+1}\big)$ shows that $\big(\mu_s - \theta_s\big)/\big(\theta_s - \mu_{s+1}\big) \leq \big(\mu_s - \mu(\widetilde{y})\big)/\big(\mu(\widetilde{y}) - \mu_{s+1}\big)$. Moreover, the same monotonicity applied to $\mu(y) \geq \eta_s$ yields $\big(\mu_s - \mu(y)\big)/\big(\mu(y) - \mu_{s+1}\big) \leq \big(\mu_s - \eta_s\big)/\big(\eta_s - \mu_{s+1}\big)$. Combining these two inequalities with the second property in (2.45) implies (2.13).

2.3.3 Additional estimates on Ritz vectors

We consider the estimate (2.11) concerning the largest Ritz value in a Krylov subspace or a block-Krylov subspace and the estimate (2.14) concerning interior Ritz values in a block-Krylov subspace.

Indeed, these estimates hold in certain more general cases. In Lemma 2.16, we prove a reformulation of (2.11) in terms of $\mu(v)$ for an arbitrary nonzero vector v. In Lemma 2.17, we prove (2.14) for an arbitrary subspace.

Lemma 2.16. *With Notation 1.4, consider an arbitrary vector $v \in \mathbb{R}^n \backslash \{0\}$ satisfying $\mu(v) > \mu_2$. Then the eigenprojection $Q_1 v$ is nonzero, and*

$$\sin^2 \angle_2(v, z_1) \leq \frac{\mu_1 - \mu(v)}{\mu_1 - \mu_2} \tag{2.47}$$

holds for a normalized eigenvector z_1 which is collinear with $Q_1 v$. Furthermore, with Notation 1.5, consider an arbitrary vector $v \in \mathbb{R}^n \backslash \{0\}$ satisfying $\mu(v) \geq \mu_2$, and assume that $\mu_1 > \mu_2$. Then (2.47) holds for the eigenvector z_1 which is given in Notation 1.5.

Proof. With Notation 1.4, the condition $\mu(v) > \mu_2$ ensures $Q_1 v \neq 0$ since otherwise v belongs to $\mathcal{Z}_2 \oplus \cdots \oplus \mathcal{Z}_m$ so that $\mu_2 \geq \mu(v)$. By using $\widetilde{z}_1 = Q_1 v / \|Q_1 v\|_2$, the normalized eigenprojection z_1 is either $\widetilde{z}_1$ or $-\widetilde{z}_1$ so that $\sin^2 \angle_2(v, z_1) = \sin^2 \angle_2(v, \widetilde{z}_1) = \sin^2 \angle_2(\widetilde{z}_1, v)$. In addition, we extend $\widetilde{z}_1$ to an orthonormal system $\{\widetilde{z}_1, \ldots, \widetilde{z}_m\}$ analogously to (2.16), and use the expansion $v = \sum_{l=1}^m \alpha_l \, \widetilde{z}_l$ with the coefficients $\alpha_l = \|Q_l v\|_2$. Then $\mu(v) = \big(\sum_{l=1}^m \mu_l \, \alpha_l^2\big) / \big(\sum_{l=1}^m \alpha_l^2\big)$, and $\cos \angle_2(\widetilde{z}_1, v) = \alpha_1 / \|v\|_2$; cf. (2.18). Summarizing the above, we get

$$\frac{\mu_1 - \mu(v)}{\mu_1 - \mu_2} = \frac{\sum_{l=1}^m (\mu_1 - \mu_l) \, \alpha_l^2}{(\mu_1 - \mu_2) \sum_{l=1}^m \alpha_l^2} \geq \frac{\sum_{l=2}^m (\mu_1 - \mu_2) \, \alpha_l^2}{(\mu_1 - \mu_2) \sum_{l=1}^m \alpha_l^2} = \frac{\sum_{l=2}^m \alpha_l^2}{\sum_{l=1}^m \alpha_l^2} = 1 - \frac{\alpha_1^2}{\sum_{l=1}^m \alpha_l^2}$$

$$= 1 - \left(\frac{\alpha_1}{\|v\|_2} \right)^2 = 1 - \cos^2 \angle_2(\widetilde{z}_1, v) = \sin^2 \angle_2(\widetilde{z}_1, v) = \sin^2 \angle_2(v, z_1).$$

The estimate with Notation 1.5 can be proved analogously by setting $v = \sum_{l=1}^n \alpha_l \, z_l$ with the given eigenvectors $z_1, \ldots, z_n$. In the added case $\mu(v) = \mu_2$, the estimate reads $\sin^2 \angle_2(v, z_1) \leq 1$ and holds trivially. □

Applying Lemma 2.16 to certain Ritz vectors implies the estimate (2.11) in Theorem 2.4 and the formally same estimate in Theorem 2.5. Therein the assumption $\mu(y) > \mu_2$ in Theorem 2.4 for the initial vector y of a Krylov subspace leads to $\mu(u_1) = \theta_1 \geq \mu(y) > \mu_2$ for a Ritz vector u_1 associated with the largest Ritz value θ_1. Thus Lemma 2.16 with Notation 1.4 is applicable to u_1 and the eigenvector $z_1 = Q_1 y / \|Q_1 y\|_2$, and implies (2.11). Furthermore, the assumptions in Theorem 2.5 concerning a block-Krylov subspace ensure $\mu_1 > \mu_2$ and $\mu(u_1) = \theta_1 \geq \mu_2$ for a Ritz vector u_1 associated with the largest Ritz value θ_1. Thus Lemma 2.16 with Notation 1.5 is directly applicable. We remark that the estimate (2.47) also holds in the case $\mu(v) < \mu_2$ where the bound is larger than 1 so that the inequality is trivial.

The derivation of the estimate (2.14) concerning interior Ritz values is more complicated. We prove this estimate in Lemma 2.17 where an arbitrary subspace is considered. A basic idea of the proof is that the corresponding Ritz vectors can be investigated within a small subspace in order to determine a representation of $\sin^2 \angle_2(u_i, z_i)$ which is similar to the bound; see (2.51) below. Moreover, some relevant arguments from [44, 45, 47] are discussed in Remark 2.18 together with possible refinements.

Lemma 2.17. *With Notation 1.5, assume that the s largest eigenvalues $\mu_1, \ldots, \mu_s$ are distinct, and let $u_1, \ldots, u_s$ be orthonormal Ritz vectors of H in an arbitrary subspace $\mathcal{U} \subseteq \mathbb{R}^n$ associated with the s largest Ritz values $\theta_1 \geq \cdots \geq \theta_s$. If $\theta_{i-1} \geq \mu_i$, $\theta_i \geq \mu_{i+1}$, and $\theta_{i-1} > \theta_i$ for a certain $i \in \{2, \ldots, s\}$, then it holds that*

$$\sin^2 \angle_2(u_i, z_i) \leq 1 - \frac{(\mu_1 - \theta_i)(\theta_i - \mu_{i+1})(\theta_{i-1} - \mu_i)}{(\mu_1 - \mu_i)(\mu_i - \mu_{i+1})(\theta_{i-1} - \theta_i)}. \tag{2.48}$$

Proof. We begin with two simple cases. In the case $\mu_i = \theta_{i-1}$, the bound in (2.48) is equal to 1 so that (2.48) reads $\sin^2 \angle_2(u_i, z_i) \leq 1$ and holds trivially. In the case $\mu_i = \theta_i$, the bound in (2.48) is equal to 0 so that one needs to prove the equality $\sin^2 \angle_2(u_i, z_i) = 0$. Indeed, this equality is an extension of the Courant-Fischer principles under the given assumption that μ_i and μ_{i+1} are distinct, and $\theta_{i-1} > \theta_i$. Thereby each maximizer of $\mu(\cdot)$ in $\widehat{\mathcal{Z}} = \operatorname{span}\{z_i, \ldots, z_n\}$ is collinear with z_i, and each minimizer of $\mu(\cdot)$ in $\widehat{\mathcal{U}} = \operatorname{span}\{u_1, \ldots, u_i\}$ is collinear with u_i. Moreover, the dimension comparison $\dim\big(\widehat{\mathcal{Z}} \cap \widehat{\mathcal{U}}\big) = \dim \widehat{\mathcal{Z}} + \dim \widehat{\mathcal{U}} - \dim\big(\widehat{\mathcal{Z}} \cup \widehat{\mathcal{U}}\big) \geq (n - i + 1) + i - n = 1$

ensures that there exists a nonzero vector $v \in \widehat{\mathcal{Z}} \cap \widehat{\mathcal{U}}$ which satisfies $\mu_i \geq \mu(v) \geq \theta_i$. Then $\mu_i = \theta_i$ implies $\mu_i = \mu(v) = \theta_i$ so that v is collinear with z_i as a maximizer of $\mu(\cdot)$ in $\widehat{\mathcal{Z}}$ and collinear with u_i as a minimizer of $\mu(\cdot)$ in $\widehat{\mathcal{U}}$. Therefore z_i and u_i are collinear so that $\sin^2 \angle_2(u_i, z_i) = 0$.

Next, we consider the remaining case with the condition $\theta_{i-1} > \mu_i > \theta_i$ due to $\mu_i \neq \theta_{i-1}$, $\mu_i \neq \theta_i$, the assumption $\theta_{i-1} \geq \mu_i$, and the relation $\mu_i \geq \theta_i$. Therein we use the auxiliary subspaces

$$\mathcal{V} = \operatorname{span}\{v_1, v_2\} \qquad \text{and} \qquad \mathcal{W} = \operatorname{span}\{v_1, v_2, z_i\} = \mathcal{V} + \operatorname{span}\{z_i\}$$

where v_1 is an arbitrary normalized vector in the subspace $\widetilde{\mathcal{U}} = \operatorname{span}\{u_1, \ldots, u_{i-1}\}$, and v_2 is given by u_i. According to the properties

$$u_j^T u_i = 0 \qquad \text{and} \qquad u_j^T H u_i = 0 \qquad \forall\, j \in \{1, \ldots, i-1\},$$

we have $v_1^T v_2 = 0$ and $v_1^T H v_2 = 0$. Combining this with the symmetry of H yields

$$[v_1, v_2]^T [v_1, v_2] = \operatorname{diag}(1, 1) \qquad \text{and} \qquad [v_1, v_2]^T H [v_1, v_2] = \operatorname{diag}\big(\mu(v_1), \mu(v_2)\big),$$

i.e., v_1 and v_2 are orthonormal Ritz vectors in the subspace $\mathcal{V} = \operatorname{span}\{v_1, v_2\}$. Thus $\mathcal{V}$ has dimension 2, and $\mathcal{W}$ has dimension 2 or 3. If $\dim \mathcal{W} = 2$, we get $\mathcal{W} = \mathcal{V}$. Then the eigenvector z_i belongs to $\mathcal{V}$ and is thus a Ritz vector in $\mathcal{V}$ so that the corresponding Ritz value $\mu_i = \mu(z_i)$ coincides with either $\mu(v_1)$ or $\mu(v_2)$. Consequently, either $\mu_i \geq \theta_{i-1}$ or $\mu_i = \theta_i$ holds due to $\mu(v_1) \geq \min_{\widetilde{u} \in \widetilde{\mathcal{U}} \setminus \{0\}} \mu(\widetilde{u}) = \theta_{i-1}$ and $\mu(v_2) = \mu(u_i) = \theta_i$. This contradicts the condition $\theta_{i-1} > \mu_i > \theta_i$ of the current case. Thus $\mathcal{W}$ must have dimension 3. Then, since the eigenvector z_i belongs to $\mathcal{W}$, $\mu_i = \mu(z_i)$ is a Ritz value in $\mathcal{W}$. Moreover, the condition $\theta_{i-1} > \mu_i > \theta_i$ implies the relation

$$\max_{w \in \mathcal{W} \setminus \{0\}} \mu(w) \geq \mu(v_1) \geq \theta_{i-1} > \mu_i > \theta_i = \mu(v_2) \geq \min_{w \in \mathcal{W} \setminus \{0\}} \mu(w).$$

Therefore μ_i differs from the extreme Ritz values in $\mathcal{W}$ and can be denoted by φ_2 within the arrangement $\varphi_1 > \varphi_2 > \varphi_3$ of the Ritz values in $\mathcal{W}$. Correspondingly, z_i can be denoted by w_2 within the basis $\{w_1, w_2, w_3\}$ consisting of orthonormal Ritz vectors associated with $\varphi_1, \varphi_2, \varphi_3$. Then $\sin^2 \angle_2(u_i, z_i)$ coincides with $\sin^2 \angle_2(v_2, w_2) = \sin^2 \angle_2(w_2, v_2)$ and can be determined based on the expansions

$$v_1 = \psi_{1,1}\, w_1 + \psi_{2,1}\, w_2 + \psi_{3,1}\, w_3, \qquad v_2 = \psi_{1,2}\, w_1 + \psi_{2,2}\, w_2 + \psi_{3,2}\, w_3$$

with the coefficients $\psi_{j,l} = w_j^T v_l \in \mathbb{R}$. These expansions allow us to rewrite the properties

$$v_1^T v_2 = 0, \quad v_1^T H v_2 = 0, \quad v_1^T v_1 = 1, \quad v_2^T v_2 = 1, \quad v_1^T H v_1 = \mu(v_1), \quad v_2^T H v_2 = \mu(v_2)$$

in terms of $\psi_{j,l}$, φ_1, φ_2, φ_3, $\xi_1 = \mu(v_1)$, and $\xi_2 = \mu(v_2)$, namely,

$$\begin{aligned}
\psi_{1,1}\psi_{1,2} + \psi_{2,1}\psi_{2,2} + \psi_{3,1}\psi_{3,2} &= 0, & \varphi_1\psi_{1,1}\psi_{1,2} + \varphi_2\psi_{2,1}\psi_{2,2} + \varphi_3\psi_{3,1}\psi_{3,2} &= 0,\\
\psi_{1,1}^2 + \psi_{2,1}^2 + \psi_{3,1}^2 &= 1, & \psi_{1,2}^2 + \psi_{2,2}^2 + \psi_{3,2}^2 &= 1,\\
\varphi_1\psi_{1,1}^2 + \varphi_2\psi_{2,1}^2 + \varphi_3\psi_{3,1}^2 &= \xi_1, & \varphi_1\psi_{1,2}^2 + \varphi_2\psi_{2,2}^2 + \varphi_3\psi_{3,2}^2 &= \xi_2.
\end{aligned} \tag{2.49}$$

The first two equations in (2.49) can be transformed as

$$(\varphi_1 - \varphi_2)\psi_{2,1}\psi_{2,2} = (\varphi_3 - \varphi_1)\psi_{3,1}\psi_{3,2}, \qquad (\varphi_1 - \varphi_2)\psi_{1,1}\psi_{1,2} = (\varphi_2 - \varphi_3)\psi_{3,1}\psi_{3,2}.$$

Combining their squared forms with the other four equations in (2.49) yields a simple nonlinear system which has the solution

$$\begin{aligned} \psi_{1,1}^2 &= \frac{(\xi_1-\varphi_2)(\xi_1-\varphi_3)(\varphi_1-\xi_2)}{(\varphi_1-\varphi_2)(\varphi_1-\varphi_3)(\xi_1-\xi_2)}, & \psi_{1,2}^2 &= \frac{(\xi_2-\varphi_2)(\xi_2-\varphi_3)(\varphi_1-\xi_1)}{(\varphi_1-\varphi_2)(\varphi_1-\varphi_3)(\xi_2-\xi_1)}, \\ \psi_{2,1}^2 &= \frac{(\xi_1-\varphi_1)(\xi_1-\varphi_3)(\varphi_2-\xi_2)}{(\varphi_2-\varphi_1)(\varphi_2-\varphi_3)(\xi_1-\xi_2)}, & \psi_{2,2}^2 &= \frac{(\xi_2-\varphi_1)(\xi_2-\varphi_3)(\varphi_2-\xi_1)}{(\varphi_2-\varphi_1)(\varphi_2-\varphi_3)(\xi_2-\xi_1)}, \\ \psi_{3,1}^2 &= \frac{(\xi_1-\varphi_1)(\xi_1-\varphi_2)(\varphi_3-\xi_2)}{(\varphi_3-\varphi_1)(\varphi_3-\varphi_2)(\xi_1-\xi_2)}, & \psi_{3,2}^2 &= \frac{(\xi_2-\varphi_1)(\xi_2-\varphi_2)(\varphi_3-\xi_1)}{(\varphi_3-\varphi_1)(\varphi_3-\varphi_2)(\xi_2-\xi_1)}. \end{aligned} \tag{2.50}$$

Then $\sin^2\angle_2(u_i,z_i)$ is determined by

$$\begin{aligned} \sin^2\angle_2(u_i,z_i) = \sin^2\angle_2(w_2,v_2) = 1-\cos^2\angle_2(w_2,v_2) &\overset{(1.31)}{=} 1-\left(\frac{w_2^Tv_2}{\|w_2\|_2\,\|v_2\|_2}\right)^2 \\ = 1-\psi_{2,2}^2 = 1-&\frac{(\varphi_1-\xi_2)(\xi_2-\varphi_3)(\xi_1-\varphi_2)}{(\varphi_1-\varphi_2)(\varphi_2-\varphi_3)(\xi_1-\xi_2)} \end{aligned} \tag{2.51}$$

where we exchange the signs of some factors of $\psi_{2,2}^2$ so that the new factors are all nonnegative due to the relation $\varphi_1 \ge \mu(v_1) = \xi_1 > \varphi_2 > \mu(v_2) = \xi_2 \ge \varphi_3$. Subsequently, we can extend the representation (2.51) as the inequality (2.48) by using the relations

$$\varphi_1 \le \mu_1, \qquad \varphi_2 = \mu_i, \qquad \varphi_3 \le \mu_{i+1}, \qquad \xi_1 \ge \theta_{i-1}, \qquad \xi_2 = \theta_i. \tag{2.52}$$

Therein the relation $\varphi_3 \le \mu_{i+1}$ still needs to be verified, whereas the other relations evidently hold according to the above settings. We verify $\varphi_3 \le \mu_{i+1}$ in two subcases with respect to v_2 and the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1,\dots,z_{i-1}\}$.

If v_2 is orthogonal to $\mathcal{Z}$, then $v_2 \in \operatorname{span}\{z_i,\dots,z_n\}$ holds so that the vector $v = v_2 - Q_iv_2$ belongs to $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{i+1},\dots,z_n\}$. Moreover, v also belongs to $\mathcal{W} = \operatorname{span}\{v_1,v_2,z_i\}$ because of $v = v_2 - Q_iv_2 = v_2 - (z_i^Tv_2)\,z_i$, and v is nonzero since otherwise v_2 is collinear with z_i so that $\mathcal{W}$ has dimension 2 which contradicts the condition $\theta_{i-1} > \mu_i > \theta_i$ as mentioned above. Thus we get

$$\varphi_3 = \min_{w\in\mathcal{W}\setminus\{0\}} \mu(w) \le \mu(v) \le \max_{\widetilde{z}\in\widetilde{\mathcal{Z}}\setminus\{0\}} \mu(\widetilde{z}) = \mu_{i+1}.$$

If v_2 is not orthogonal to $\mathcal{Z}$, we verify $\varphi_3 \le \mu_{i+1}$ for a special normalized vector v_1 in $\widetilde{\mathcal{U}} = \operatorname{span}\{u_1,\dots,u_{i-1}\}$. Then the representation (2.51) remains valid since it is derived for arbitrary normalized $v_1 \in \widetilde{\mathcal{U}}$. For constructing a suitable v_1, we use the orthonormal basis matrices $\widetilde{U} = [u_1,\dots,u_{i-1}]$ and $Z = [z_1,\dots,z_{i-1}]$ and define v_1 by $v_1 = v/\|v\|_2$ with $v = \widetilde{U}g$ where $g \in \mathbb{R}^{i-1}$ satisfies the linear system $\big(Z^T\widetilde{U}\big)g = Z^Tv_2$. Therein Z^Tv_2 is nonzero since v_2 is not orthogonal to $\mathcal{Z}$, and $Z^T\widetilde{U}$ is an invertible matrix since otherwise there exists a nonzero $\widetilde{g} \in \mathbb{R}^{i-1}$ satisfying $Z^T\widetilde{U}\,\widetilde{g} = 0$ so that $\widetilde{U}\,\widetilde{g}$ is orthogonal to $\mathcal{Z}$ and belongs to $\widehat{\mathcal{Z}} = \operatorname{span}\{z_i,\dots,z_n\}$, then

$$\mu_i = \max_{\widehat{z}\in\widehat{\mathcal{Z}}\setminus\{0\}} \mu(\widehat{z}) \ge \mu\big(\widetilde{U}\,\widetilde{g}\big) \ge \min_{\widetilde{u}\in\widetilde{\mathcal{U}}\setminus\{0\}} \mu(\widetilde{u}) = \theta_{i-1}$$

contradicts the condition $\theta_{i-1} > \mu_i > \theta_i$. Thus v has the form $v = \widetilde{U}g = \widetilde{U}\big(Z^T\widetilde{U}\big)^{-1}\big(Z^Tv_2\big)$ and is nonzero. By using the orthogonal projector $Q = \sum_{l=1}^{i-1} Q_l = \sum_{l=1}^{i-1} z_lz_l^T = ZZ^T$ on $\mathcal{Z}$, we get

$$Qv = ZZ^Tv = ZZ^T\widetilde{U}\big(Z^T\widetilde{U}\big)^{-1}\big(Z^Tv_2\big) = ZZ^Tv_2 = Qv_2.$$

In addition, the eigenprojections $Q_i v$ and $Q_i v_2$ are collinear with z_i so that it holds, by considering the orthogonal projector $\widetilde{Q} = \sum_{l=i+1}^{n} Q_l$ on the invariant subspace $\widetilde{\mathcal{Z}} = \text{span}\{z_{i+1}, \ldots, z_n\}$, that

$$\begin{aligned} \mathcal{W} &= \text{span}\{v_1,\, v_2,\, z_i\} = \text{span}\{v,\, v_2,\, z_i\} = \text{span}\big\{Qv + Q_i v + \widetilde{Q}v,\ Qv_2 + Q_i v_2 + \widetilde{Q}v_2,\ z_i\big\} \\ &= \text{span}\big\{Qv + \widetilde{Q}v,\ Qv_2 + \widetilde{Q}v_2,\ z_i\big\} = \text{span}\big\{Qv + \widetilde{Q}v,\ Qv + \widetilde{Q}v_2,\ z_i\big\}. \end{aligned}$$

Therein $\widetilde{Q}v_2 \neq \widetilde{Q}v$ holds since otherwise $\mathcal{W}$ reads $\text{span}\{Qv + \widetilde{Q}v,\, z_i\}$ and thus has dimension 2. This contradicts the condition $\theta_{i-1} > \mu_i > \theta_i$ as mentioned above. Therefore the vector $(Qv + \widetilde{Q}v_2) - (Qv + \widetilde{Q}v) = \widetilde{Q}v_2 - \widetilde{Q}v$ is nonzero. Moreover, it belongs to both of $\mathcal{W}$ and $\widetilde{\mathcal{Z}}$ so that

$$\varphi_3 = \min_{w \in \mathcal{W}\setminus\{0\}} \mu(w) \leq \mu\big(\widetilde{Q}v_2 - \widetilde{Q}v\big) \leq \max_{\widetilde{z} \in \widetilde{\mathcal{Z}}\setminus\{0\}} \mu(\widetilde{z}) = \mu_{i+1}.$$

Finally, applying the relations in (2.52) yields

$$\frac{\varphi_1 - \xi_2}{\varphi_1 - \varphi_2} = \frac{\varphi_1 - \theta_i}{\varphi_1 - \mu_i} \geq \frac{\mu_1 - \theta_i}{\mu_1 - \mu_i}, \quad \frac{\xi_2 - \varphi_3}{\varphi_2 - \varphi_3} = \frac{\theta_i - \varphi_3}{\mu_i - \varphi_3} \geq \frac{\theta_i - \mu_{i+1}}{\mu_i - \mu_{i+1}}, \quad \frac{\xi_1 - \varphi_2}{\xi_1 - \xi_2} = \frac{\xi_1 - \mu_i}{\xi_1 - \theta_i} \geq \frac{\theta_{i-1} - \mu_i}{\theta_{i-1} - \theta_i}$$

so that (2.51) is extended as (2.48). Therein the assumption $\theta_i \geq \mu_{i+1}$ ensures that the bound in (2.48) does not exceed 1. □

Lemma 2.17 is directly applicable to the settings from Theorems 2.3 and 2.5 by regarding the concerned block-Krylov subspace as $\mathcal{U}$.

Remark 2.18. *The estimate* (2.48) *was presented in a similar form in [45, Theorem 2.2] without the assumption $\theta_{i-1} > \theta_i$. It was mentioned that a proof was given in [47]. However, the corresponding formulation in [47, Theorem 2] is slightly different, namely, $\theta_{i-1} > \mu_i$ and $\theta_i > \mu_{i+1}$ are assumed instead of $\theta_{i-1} \geq \mu_i$ and $\theta_i \geq \mu_{i+1}$ so that $\theta_{i-1} > \theta_i$ is ensured. Indeed, $\theta_{i-1} = \theta_i$ cannot be excluded by the assumption that the eigenvalues are distinct. As a simple example, we consider the matrix $H = \text{diag}(3,\, 2,\, 1)$ and the subspace $\mathcal{U} = \text{span}\{u_1, u_2\}$ with $u_1 = (-\frac{1}{2}, \frac{\sqrt{2}}{2}, -\frac{1}{2})^T$ and $u_2 = (\frac{1}{2}, \frac{\sqrt{2}}{2}, \frac{1}{2})^T$, then $\theta_{i-1} = \theta_i = 2 = \mu_i$ holds for $i = 2$, and the bound in* (2.48) *would contain $0/0$. Thus it is necessary to assume the relation $\theta_{i-1} > \theta_i$ or ensure it by another assumption. Moreover, the estimate* (2.48) *is of practical interest in the case that the concerned Ritz values are good approximations of the concerned eigenvalues. Therein $\theta_{i-1} = \theta_i$ is not meaningful since μ_{i-1} and μ_i are distinct.*

The proof in [47] is partially oversimplified. In particular, the determination of $\psi_{2,2}^2$ is described as "it is easily verified", and the verification of $\varphi_3 \leq \mu_{i+1}$ is explained by applying the Courant-Fischer principles to a subspace which corresponds to $(Q + Q_i)\mathcal{W}$ in our formulation. For the reader's convenience, we formulate a detailed determination of $\psi_{2,2}^2$ based on the proof of [44, Theorem 2.2.2], and verify $\varphi_3 \leq \mu_{i+1}$ by pointing out that $\mathcal{W}$ contains a nonzero vector which also belongs to $\text{span}\{z_{i+1}, \ldots, z_n\}$.

Furthermore, we note that the estimate (2.48) *does not make use of the information of the Ritz values $\theta_1, \ldots, \theta_{i-2}$. Thus we expect that these further Ritz values could contribute to some refinements of* (2.48)*. In [44, Lemma 2.2.2], a similar estimate is shown by using certain arguments suggested by Golub and Van Loan in an early edition of [34]; cf. [34, Subsection 12.6.2]. This estimate concerns orthogonal and nonnormalized Ritz vectors $\widetilde{v}_1, \ldots, \widetilde{v}_s$ in the subspace* $\text{span}\{\widetilde{v}_1, \ldots, \widetilde{v}_s\}$ *which is a subset of* $\text{span}\{w_1, \ldots, w_{s+1}\}$ *with orthonormal Ritz vectors $w_1, \ldots, w_{s+1}$. Explicit forms of $(\widetilde{v}_l^T w_j)^2$ are determined in terms of concerned Ritz values. In comparison to the explicit form of $\psi_{2,2}^2 = (w_2^T v_2)^2$ in* (2.50) *for orthonormal v_1 and v_2, [44,* *Lemma 2.2.2] applied to $s=2$ provides the representation*

$$(w_2^T \widetilde{v}_2)^2 = (\widetilde{v}_2^T w_2)^2 = \frac{\varphi_2 - \xi_1}{(\varphi_2 - \xi_2)(\varphi_2 - \varphi_1)(\varphi_2 - \varphi_3)}$$

under the stronger assumption $\varphi_1 > \xi_1 > \varphi_2 > \xi_2 > \varphi_3$, i.e., by excluding the cases $\varphi_1 = \xi_1$ and $\xi_2 = \varphi_3$. However, since $\widetilde{v}_2$ is nonnormalized, one requires a corresponding representation of its norm in order to determine the explicit form of $\sin^2 \angle_2(w_2, \widetilde{v}_2)$. Such an approach is already complicated for $s=2$ so that [44, Lemma 2.2.2] was not extended to any refinement of the estimate (2.48). Instead, we have achieved some refinements of (2.48) by considering two series of Lagrange polynomials based on the proof of Lemma 2.17; see Subsection 3.2.4 for the formulation with Notation 1.4 and Subsection 5.1.4 for the formulation with Notation 1.5. In addition, under the weaker assumption $\mu_{i-1} > \mu_i = \cdots = \mu_{i+t} > \mu_{i+t+1}$ for eigenvalues, an alternative estimate concerning $\sin^2 \angle_2\big(\mathrm{span}\{u_i, \ldots, u_{i+t}\}, \mathrm{span}\{z_i, \ldots, z_{i+t}\}\big)$ was suggested in [44, 45] without proof. We prove such an estimate in Subsection 5.1.4.

2.3.4 Improvements and further estimates

The classical estimates by Saad [98] and Knyazev [44, 45] are improved in this thesis concerning the four types of Krylov subspace eigensolvers introduced in Subsection 1.4.1 and their reciprocal representations in (1.29).

For the standard Krylov subspace iteration (1.29a), we denote the associated Krylov subspace $\widehat{\mathcal{K}}^k(y^{(0)})$ by $\mathcal{K} = \mathrm{span}\{y, Hy, \ldots, H^{k-1}y\}$, and present the following estimates in Chapter 3:

(i) Estimates on approximate eigenvectors which improve (2.1) and (2.4).

(ii) Angle-dependent estimates on Ritz values which improve (2.3) and (2.5).

(iii) Angle-free estimates on Ritz values which generalize (2.10).

(iv) Additional estimates on Ritz vectors which improve (2.11).

Subsequently, for the restarted Krylov subspace iteration (1.29b), we consider a series of Krylov subspaces $\widehat{\mathcal{K}}^k(y^{(\ell)})$, $\ell \in \mathbb{N}$. Therein we prefer those estimates of the form $f(y^{(\ell+1)}) \leq \varepsilon f(y^{(\ell)})$ with a convergence measure $f(\cdot)$ and a convergence factor $\varepsilon \in (0,1)$ since their recursive application results in the multistep estimate $f(y^{(\ell)}) \leq \varepsilon^\ell f(y^{(0)})$ for investigating $\widehat{\mathcal{K}}^k(y^{(\ell)})$ in terms of $\widehat{\mathcal{K}}^k(y^{(0)})$. However, the first two types of estimates from Chapter 3 are too different from the above form, whereas the type (iii) from Chapter 3 can match this form after modification. The modified estimates are presented in Chapter 4 and deal with the Ritz values in $\widehat{\mathcal{K}}^k(y^{(\ell)})$. These can easily be extended as estimates on Ritz vectors by using the type (iv) from Chapter 3. Moreover, some sharp estimates can be derived by using two further types of polynomials.

Next, for the block-Krylov subspace iteration (1.29c), the following estimates are presented in Chapter 5 concerning the block-Krylov subspace $\mathcal{K} = \mathrm{span}\{Y, HY, \ldots, H^{k-1}Y\}$ which corresponds to $\widehat{\mathcal{K}}^k(Y^{(0)})$.

(i) Estimates on approximate eigenvectors which improve (2.6).

(ii) Angle-dependent estimates on Ritz values which improve (2.8).

(iii) Angle-free estimates on Ritz values which generalize (2.13).

(iv) Additional estimates on Ritz vectors which improve (2.14).

Finally, for the restarted block-Krylov subspace iteration (1.29b) with the block-Krylov subspaces $\widehat{\mathcal{K}}^k(Y^{(\ell)})$, $\ell \in \mathbb{N}$, the angle-free estimates from Chapter 5 are modified in Chapter 6 in order to analyze the Ritz values in $\widehat{\mathcal{K}}^k(Y^{(\ell)})$. The associated Ritz vectors can be analyzed by combing the modified estimates with the type (iv) from Chapter 5.

3 Standard Krylov subspace iterations

In this chapter, we investigate standard Krylov subspace iterations of the type (1.22) with the reciprocal representation (1.29a). For this simple type of Krylov subspace eigensolvers, the convergence behavior concerning interior and clustered eigenvalues cannot always be predicted reasonably by using the classical estimates by Saad [98] which we have introduced in Theorems 2.1 and 2.2. In Saad's analysis, the initial vector of the considered Krylov subspace is somewhat overstressed for representing approximate eigenvectors so that some possibly large ratio-products occur in the bounds. Thus it would be better to distribute the burden of the initial vector to certain appropriate auxiliary vectors.

It is worthwhile to introduce some previous improvements of Saad's estimates and compare them with our results afterwards. In [112], van der Sluis and van der Vorst analyzed the convergence behavior of Ritz values in a Krylov subspace arising from the preconditioned conjugate gradient method. Therein Saad's estimates (2.3) and (2.5) for $i=1$ were reformulated concerning the approximation of the smallest eigenvalue of a symmetric matrix which corresponds to the preconditioned system matrix; see [112, Theorem 4.3]. In the accompanying numerical example with two clustered eigenvalues, these estimates did not give sufficiently accurate bounds due to small gap ratios and large ratio-products. Instead, a comparative approach by using other Ritz values stemming from certain modifications of the spectrum yields better bounds. Nevertheless, these bounds contain some auxiliary parameters so that an explicit improvement was not presented in [112], but rather in [105] by Sleijpen and van der Sluis. In particular, [105, Theorem 5.1] provided three alternative bounds which are better than the corresponding Chebyshev bound for low-dimensional Krylov subspaces or within that numerical example from [112] mentioned above. Another improvement of the estimate (2.3) for $i=1$ was presented in [61, Theorem 4.1] by Li. Although this improved estimate is equivalent to Knyazev's estimate (2.9), it was independently derived in terms of sine values. Additionally, the sharpness of the associated Chebyshev bound was discussed concerning the extreme points of the underlying shifted Chebyshev polynomial. Last but not least, we note that the estimates (2.3) and (2.5) for arbitrary i can be improved by partially modifying Saad's analysis similarly to [121, Theorem 1.8] by Yang and Yang. This is not a substantial improvement since the possibly large ratio-products are still contained.

We prefer Knyazev's analysis [44, 45] for improving Saad's estimates. As mentioned in Remark 2.6, some estimates for block-Krylov subspace iterations can be improved significantly by avoiding certain linear factors in the construction of auxiliary vectors. The corresponding arguments have been formulated in Section 2.3. However, the estimates for standard Krylov subspace iterations have only been improved for $i=1$. Thus this approach needs to be extended in order to achieve a complete improvement. In our convergence analysis for standard Krylov subspace iterations, we begin with the reciprocal representation (1.29a) concerning the eigenvalue problem of a symmetric matrix. For the sake of simplicity, the Krylov subspace $\widehat{\mathcal{K}}^k(y^{(0)})$ and the initial vector $y^{(0)}$ are denoted by $\mathcal{K}$ and y as in Chapter 2 for introducing classical estimates. Moreover, we add a natural assumption that $\mathcal{K}$ is not an invariant subspace. This usually holds true in practice due to pseudorandom initial vectors. In Section 3.1, we reformulate several available estimates in practical settings where clustered eigenvalues are under consideration. Section 3.2 is devoted to deriving new estimates which improve the estimates (2.1), (2.4) on approximate eigenvectors, the estimates (2.3), (2.5) on Ritz values, and the additional estimate (2.11) on Ritz vectors, respectively. Therein some new auxiliary vectors allow us to avoid the linear factors from Saad's analysis, and the auxiliary vectors can be eliminated within certain angles and moderate ratios.

Section 3.3 serves to compare the available estimates with the new estimates in several numerical tests. Finally, in Section 3.4, we reformulate our new estimates with respect to the description (1.22) concerning generalized matrix eigenvalue problems.

3.1 Available estimates

The settings in the works [112, 105, 61, 121] for improving Saad's estimates are not unified. In order to compare these previous improvements with our new estimates, we reformulate them with the settings from Theorems 2.1 and 2.2. From a practical perspective, we additionally assume that the considered Krylov subspace is not an invariant subspace. Indeed, this assumption excludes a trivial case of Saad's estimates and ensures that an auxiliary vector for the refined estimates is nonzero.

Lemma 3.1. *With Notation 1.4, consider a Krylov subspace* $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ *with the initial vector* $y \in \mathbb{R}^n \backslash \{0\}$*, and assume that* $\mathcal{K}$ *is not an invariant subspace. Then* $\mathcal{K}$ *contains no eigenvectors, and the following statements hold.*

(a) The values $\tan\angle_2(z_i, \mathcal{K})$*,* $\sin^2\angle_2(z_i, u_i)$ *and* $\mu_i - \theta_i$ *in Theorems 2.1 and 2.2 are nonzero.*

(b) The vector $\widetilde{y}$ *in Theorem 2.2 is nonzero.*

Proof. We first show that $\mathcal{K}$ contains no eigenvectors under the assumption that $\mathcal{K}$ is not an invariant subspace. By contraposition, if $\mathcal{K}$ contains an eigenvector, e.g., z with the corresponding eigenvalue μ, then, combining the eigenequation $Hz = \mu z$ with the representation $z = \sum_{j=1}^{k} \alpha_j H^{j-1} y$ implies $\sum_{j=1}^{k} \alpha_j H^j y = \sum_{j=1}^{k} \mu\, \alpha_j H^{j-1} y$. Subsequently, by using the largest index $l \in \{1, \ldots, k\}$ for which the coefficient α_l is nonzero, it holds that $\sum_{j=1}^{l} \alpha_j H^j y = \sum_{j=1}^{l} \mu\, \alpha_j H^{j-1} y$. Thus

$$H^l y \in \operatorname{span}\{y, Hy, \ldots, H^{l-1}y\} \qquad \Rightarrow \qquad H^k y \in \operatorname{span}\{H^{k-l}y, H^{k-l+1}y, \ldots, H^{k-1}y\}$$

so that

$$H\mathcal{K} = \operatorname{span}\{Hy, \ldots, H^{k-1}y\} + \operatorname{span}\{H^k y\} \subseteq \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\} = \mathcal{K}$$

holds, i.e., $\mathcal{K}$ would be an invariant subspace.

Based on this fact, we can verify the statements (a) and (b). Therein $\tan\angle_2(z_i, \mathcal{K})$ and $\sin^2\angle_2(z_i, u_i)$ are nonzero since otherwise $\mathcal{K}$ would contain the eigenvector z_i. For verifying $\mu_i - \theta_i \neq 0$, we use the property $\mathcal{K} \subseteq \operatorname{span}\{z_1, \ldots, z_m\}$ with the orthonormal system $\{z_1, \ldots, z_m\}$ defined in (2.16), then each maximizer of the Rayleigh quotient $\mu(\cdot)$ in $\widehat{\mathcal{Z}} = \operatorname{span}\{z_i, \ldots, z_m\}$ is collinear with z_i because of $\mu_i > \mu_{i+1}$. In addition, we use a subspace $\widehat{\mathcal{U}} = \operatorname{span}\{u_1, \ldots, u_i\}$ spanned by orthonormal Ritz vectors associated with the Ritz values $\theta_1 \geq \cdots \geq \theta_i$. If $i > 1$, the assumption $\theta_{i-1} > \mu_i$ in Theorems 2.1 and 2.2 implies $\theta_{i-1} > \theta_i$ so that each minimizer of $\mu(\cdot)$ in $\widehat{\mathcal{U}}$ is collinear with u_i. Moreover, this property holds trivially for $i = 1$. Then z_i and u_i would be collinear provided that $\mu_i = \theta_i$; cf. the first paragraph in the proof of Lemma 2.17. Consequently, $\mathcal{K}$ would contain the eigenvector z_i if $\mu_i - \theta_i = 0$ holds. Next, we verify (b) by contraposition. Beginning with $\widetilde{y} = 0$, i.e.,

$$\left(\prod_{j=i+1}^{i+t} (H - \mu_j I)\right) y = 0$$

with $i + t < k$, we get $Hy_{i+1} = \mu_{i+1}\, y_{i+1}$ for

$$y_{i+1} = \left(\prod_{j=i+2}^{i+t} (H - \mu_j I)\right) y.$$

Therein y_{i+1} belongs to $\mathcal{K}$ since the product in its definition corresponds to a polynomial of degree $t-1 < i+t < k$. If $y_{i+1} \neq 0$, then y_{i+1} is an eigenvector due to $Hy_{i+1} = \mu_{i+1}\, y_{i+1}$. If $y_{i+1} = 0$ and $t = 1$, it holds that $y = y_{i+1} = 0$ which contradicts $y \neq 0$. If $y_{i+1} = 0$ and $t > 1$, we get $Hy_{i+2} = \mu_{i+2}\, y_{i+2}$ for

$$y_{i+2} = \left(\prod_{j=i+3}^{i+t} (H - \mu_j I)\right) y.$$

Repeating this argumentation up to $y_{i+t} = y$ shows the existence of a certain eigenvector in $\mathcal{K}$. Thus $\mathcal{K}$ would contain an eigenvector if $\widetilde{y} = 0$ holds. □

According to the statement (a) in Lemma 3.1, we can restrict Theorems 2.1 and 2.2 to a nontrivial case by assuming that $\mathcal{K}$ is not an invariant subspace. Moreover, it would be better to emphasize the number of target eigenvalues and describe the clustered eigenvalues with a fixed index instead of the variable index $i+t$ in Theorem 2.2. Concerning the standard Krylov subspace iteration (1.29a), the s largest eigenvalues are target eigenvalues. Correspondingly, we consider an eigenvalue cluster which includes μ_s and denote by c the index of the smallest eigenvalue in this cluster, then μ_s and μ_{c+1} are well separated. For the reader's convenience, we adapt Theorems 2.1 and 2.2 to these practical settings.

Theorem 3.2. *With Notation 1.4, consider a Krylov subspace* $\mathcal{K} = \operatorname{span}\{y, Hy, \dots, H^{k-1}y\}$ *with the initial vector* $y \in \mathbb{R}^n \backslash \{0\}$*, and assume that* $\mathcal{K}$ *is not an invariant subspace. Let the eigenvalues* $\mu_1, \dots, \mu_s$ *be of practical interest, and the eigenvalues* μ_s*,* μ_{c+1} *be well separated for an index* $c \in [s, k)$*, then the following estimates hold.*

(I) Estimates on approximate eigenvectors: If the eigenprojection $Q_i y$ *of* y *is nonzero for an index* $i \in \{1, \dots, s\}$*, then it holds, in terms of the normalized eigenprojection* $z_i = Q_i y / \|Q_i y\|_2$*, the invariant subspace* $\mathcal{Z} = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_i$*, the gap ratio* $\gamma_i = (\mu_i - \mu_{i+1})/(\mu_{i+1} - \mu_m)$*, and the Chebyshev polynomial* $T_{k-i}(\cdot)$*, that*

$$\tan \angle_2\big(z_i, \mathcal{K}\big) \leq \frac{\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}}{T_{k-i}(1 + 2\gamma_i)} \, \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)}. \tag{3.1}$$

In addition, the vector

$$\widetilde{y} = \left(\prod_{j=i+1}^{c} (H - \mu_j I)\right) y$$

is nonzero, and

$$\tan \angle_2\big(z_i, \mathcal{K}\big) \leq \frac{\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}}{T_{k-c}(1 + 2\widetilde{\gamma}_i)} \, \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)}, \tag{3.2}$$

$$\tan \angle_2\big(z_i, \mathcal{K}\big) \leq \frac{\left(\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}\right) \left(\prod_{j=i+1}^{c} \frac{\mu_j - \mu_m}{\mu_i - \mu_j}\right)}{T_{k-c}(1 + 2\widetilde{\gamma}_i)} \, \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \tag{3.3}$$

hold with the gap ratio $\widetilde{\gamma}_i = (\mu_i - \mu_{c+1})/(\mu_{c+1} - \mu_m)$ *and the Chebyshev polynomial* $T_{k-c}(\cdot)$*.*

(II) Angle-dependent estimates on Ritz values: Denote by $\theta_1 \geq \cdots \geq \theta_s$ *the* s *largest Ritz values of* H *in* $\mathcal{K}$*, then*

$$\mu_i - \theta_i \leq (\mu_i - \mu_m) \left(\frac{\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}}{T_{k-i}(1 + 2\gamma_i)} \, \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \right)^2, \tag{3.4}$$

$$\mu_i - \theta_i \leq (\mu_i - \mu_m) \left(\frac{\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}}{T_{k-c}(1 + 2\widetilde{\gamma}_i)} \, \frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)} \right)^2 \tag{3.5}$$

and

$$\mu_i - \theta_i \leq (\mu_i - \mu_m) \left(\frac{\left(\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}\right) \left(\prod_{j=i+1}^{c} \frac{\mu_j - \mu_m}{\mu_i - \mu_j}\right)}{T_{k-c}(1 + 2\widetilde{\gamma}_i)} \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \right)^2 \tag{3.6}$$

hold for $i \in \{1, \ldots, s\}$ *with the terms from (I) by assuming* $\theta_{i-1} > \mu_i$ *in the case* $i > 1$.

In Theorem 3.2, we skip the additional estimate (2.2) on Ritz vectors since it cannot be improved significantly. The refined estimates (2.4) and (2.5) from Theorem 2.2 are simply reformulated by the substitution $i + t = c$.

With the settings from Theorem 3.2, the estimates in [105, Theorem 5.1] are reformulated as

$$\mu_1 - \theta_1 \leq (\mu_1 - \mu_m) \frac{\ln^2(4\tau + 2)}{(4k-2)^2}, \tag{3.7a}$$

$$\mu_1 - \theta_1 \leq (\mu_1 - \mu_m) \frac{\tau}{(2k-1)^2}, \tag{3.7b}$$

$$\mu_1 - \theta_1 \leq (\mu_1 - \mu_m)\, 5\, \tau\, \gamma\, e^{2 - (4k-2)\gamma^{1/2}} \tag{3.7c}$$

with $\tau = \tan^2 \angle_2(y, z_1)$ and $\gamma = (\mu_1 - \mu_2)/(\mu_1 - \mu_m)$ where the estimate (3.7c) requires the assumption $2k - 1 \geq \gamma^{-1/2}$. The original estimates concern the approximation of the smallest eigenvalue of a symmetric matrix. Thus applying them to $-H$ yields (3.7).

Subsequently, the estimate in [61, Theorem 4.1] is reformulated as

$$\mu_1 - \theta_1 \leq (\mu_1 - \mu_m) \frac{\varepsilon}{1 + \varepsilon} \qquad \text{with} \qquad \varepsilon = \left(\frac{\tan \angle_2(y, z_1)}{T_{k-1}(1 + 2\gamma_1)} \right)^2. \tag{3.8}$$

The estimate (3.8) can be derived by combining the inequalities

$$\frac{\mu_1 - \theta_1}{\mu_1 - \mu_m} \leq \sin^2 \angle_2(z_1, \mathcal{K}) \qquad \text{and} \qquad \sin^2 \angle_2(z_1, \mathcal{K}) \leq \frac{\varepsilon}{1 + \varepsilon}$$

which are equivalent to (2.28) and (3.1) for $i = 1$ in terms of tangent values. Correspondingly, (3.8) is equivalent to Knyazev's estimate (2.9).

Interestingly, we can generalize the estimate (3.8) to arbitrary $i \in \{1, \ldots, s\}$ by partially modifying Saad's analysis, inspired by [121, Theorem 1.8].

Theorem 3.3. *With the settings from Theorem 3.2, it holds that*

$$\mu_i - \theta_i \leq (\mu_i - \mu_m) \frac{\zeta}{1 + \zeta} \tag{3.9}$$

where ζ *is given by any of the squared terms in the estimates* (3.4)*,* (3.5) *and* (3.6)*.*

Proof. We first prove (3.9) for ζ from (3.4) based on Saad's analysis introduced in Subsections 2.2.1 and 2.2.2. Concerning the auxiliary vector $q(H)y$ with the polynomial $q(\cdot)$ defined by

$$q(\alpha) = \left(\prod_{j=1}^{i-1} (\alpha - \theta_j) \right) T_{k-i} \left(1 + 2 \frac{\alpha - \mu_{i+1}}{\mu_{i+1} - \mu_m} \right),$$

and the expansion $y = \sum_{l=1}^{m} \alpha_l z_l$ with the coefficients $\alpha_l = \|Q_l y\|_2$, Saad's analysis yields

$$\frac{\sum_{l=i+1}^{m} q^2(\mu_l)\, \alpha_l^2}{q^2(\mu_i)\, \alpha_i^2} \leq \left(\frac{\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}}{T_{k-i}(1 + 2\gamma_i)} \frac{\sin \angle_2(y, \mathcal{Z})}{\cos \angle_2(y, z_i)} \right)^2 = \zeta \tag{3.10}$$

analogously to (2.20). Subsequently, (2.21) is modified as

$$\begin{aligned}\mu\big(q(H)y\big) - \mu_m &= \frac{\sum_{l=1}^{m} (\mu_l - \mu_m)\, q^2(\mu_l)\, \alpha_l^2}{\sum_{l=1}^{m} q^2(\mu_l)\, \alpha_l^2} \;\geq\; \frac{\sum_{l=1}^{i} (\mu_l - \mu_m)\, q^2(\mu_l)\, \alpha_l^2}{\sum_{l=1}^{m} q^2(\mu_l)\, \alpha_l^2} \\ &\geq (\mu_i - \mu_m) \frac{\sum_{l=1}^{i} q^2(\mu_l)\, \alpha_l^2}{\sum_{l=1}^{m} q^2(\mu_l)\, \alpha_l^2} \;=\; (\mu_i - \mu_m) \left(1 + \frac{\sum_{l=i+1}^{m} q^2(\mu_l)\, \alpha_l^2}{\sum_{l=1}^{i} q^2(\mu_l)\, \alpha_l^2}\right)^{-1} \\ &\geq (\mu_i - \mu_m) \left(1 + \frac{\sum_{l=i+1}^{m} q^2(\mu_l)\, \alpha_l^2}{q^2(\mu_i)\, \alpha_i^2}\right)^{-1} \overset{(3.10)}{\geq} (\mu_i - \mu_m)\,(1+\zeta)^{-1}.\end{aligned}$$

Moreover, $\theta_i \geq \mu\big(q(H)y\big)$ holds since $q(H)y$ is orthogonal to the Ritz vectors associated with those Ritz values larger than θ_i. Then we get

$$\theta_i - \mu_m \;\geq\; \mu\big(q(H)y\big) - \mu_m \;\geq\; (\mu_i - \mu_m)\,(1+\zeta)^{-1} \qquad \Rightarrow \qquad \frac{\theta_i - \mu_m}{\mu_i - \mu_m} \;\geq\; (1+\zeta)^{-1}$$

so that

$$\frac{\mu_i - \theta_i}{\mu_i - \mu_m} \;=\; 1 - \frac{\theta_i - \mu_m}{\mu_i - \mu_m} \;\leq\; 1 - (1+\zeta)^{-1} \;=\; \frac{\zeta}{1+\zeta}.$$

Thus (3.9) holds for ζ from (3.4). Next, applying the above approach to the the auxiliary vector $\widetilde{q}(H)\widetilde{y}$ from Subsection 2.2.3 with the substitution $i + t = c$ yields (3.9) for ζ from the estimates (3.5) and (3.6). □

In comparison to (3.9), the estimates (3.4), (3.5) and (3.6) have the form $\mu_i - \theta_i \leq (\mu_i - \mu_m)\,\zeta$ so that (3.9) always provides better bounds, especially for large ζ. However, this improvement is not substantial since it does not avoid the possibly large ratio-products such as $\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}$. Furthermore, we note that the analysis in [121] results in some other estimates depending on the eigenvalues μ_{i-1} and μ_{i+1}. These estimates do not constantly provides better bounds than (3.4), (3.5) and (3.6) according to the numerical experiments in [121]. Thus (3.9) can be regarded as their robust variant.

3.2 New estimates

Our new estimates for standard Krylov subspace iterations are achieved by modifying the auxiliary vector $\widetilde{y}$ from Theorem 3.2 and by extending certain arguments for block-Krylov subspace iterations which are introduced in Section 2.3. A drawback of $\widetilde{y}$ is that it has to be multiplied with the linear factors $H - \mu_j I$ or $H - \theta_j I$ for $j = 1, \ldots, i-1$ in Saad's analysis so that the possibly large ratio-products $\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}$ and $\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}$ are contained in the bounds. Thus Saad's estimates can be improved by avoiding these linear factors.

In Subsection 3.2.1, we treat estimates on approximate eigenvectors. The construction of the auxiliary vectors $y_1, \ldots, y_s$ in Lemma 2.10 concerning the initial subspace of a block-Krylov subspace inspires us to modify the auxiliary vector $\widetilde{y}$ as

$$\widehat{y} = \Big(\prod\nolimits_{j \in \{1,\ldots,c\} \setminus \{i\}} (H - \mu_j I)\Big)\, y \tag{3.11}$$

with the settings from Theorem 3.2. Evidently, $\widehat{y}$ coincides with $\big(\prod_{j=1}^{i-1} (H - \mu_j I)\big)\widetilde{y}$ and already involves the linear factors $H - \mu_j I$ for $j = 1, \ldots, i-1$. Thus an estimate without $\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i}$ can be achieved in terms of $\widehat{y}$. Moreover, $\widehat{y}$ can be eliminated within an angle between two subspaces as in Lemma 2.10.

Subsection 3.2.2 deals with angle-dependent estimates on Ritz values. An estimate without $\prod_{j=1}^{i-1} \frac{\theta_j-\mu_m}{\theta_j-\mu_i}$ can be derived by using $\big(\prod_{j=1}^{i-1}(H-\theta_j I)\big)\widetilde{y}$ as an auxiliary vector. However, this vector cannot easily be eliminated within certain angles. Instead, we extend $\widehat{y}$ to a set of vectors

$$y_l = \Big(\prod_{j\in\{1,\ldots,c\}\setminus\{l\}} (H-\mu_j I)\Big)\, y, \qquad l = 1,\ldots,c \tag{3.12}$$

in order to adapt the proof techniques of Lemma 2.10 to standard Krylov subspace iterations. The bound in the resulting estimate is independent of auxiliary vectors.

In Subsection 3.2.3, we derive some angle-free estimates on Ritz values by using the vectors from (3.12) and extending certain arguments from Lemma 2.15. These estimates improve the angle-dependent estimates in the case of large angle terms. Moreover, the extended arguments are also applicable to the analysis for restarted and block variants in further chapters.

Subsection 3.2.4 is devoted to deriving additional estimates on Ritz vectors which can be combined with the above estimates on Ritz values. In comparison to the estimates (2.11) and (2.14), we present a better bound which makes use of further Ritz values and eigenvalues. The derivation is based on the proof of Lemma 2.17 and uses two series of Lagrange polynomials.

3.2.1 Estimates on approximate eigenvectors

We first improve the estimates (3.1), (3.2) and (3.3) on approximate eigenvectors with respect to the angle between an eigenvector z_i and the considered Krylov subspace $\mathcal{K}$. These estimates represent Saad's estimates (2.1) and (2.4) in the nontrivial case that $\mathcal{K}$ is not an invariant subspace. For improving them, we use a modified auxiliary vector (3.11) which can avoid the ratio-products in the bounds.

Theorem 3.4. *With the settings from Theorem 3.2, the auxiliary vector $\widehat{y}$ defined in* (3.11) *is nonzero, and*

$$\tan\angle_2(z_i,\mathcal{K}) \le \big[\,T_{k-c}(1+2\widetilde{\gamma}_i)\,\big]^{-1} \tan\angle_2(\widehat{y},\mathcal{Z}) \tag{3.13}$$

holds. Moreover,

$$\tan\angle_2(z_i,\mathcal{K}) \le \big[\,T_{k-c}(1+2\widetilde{\gamma}_i)\,\big]^{-1} \tan\angle_2(\mathcal{K}^c,\mathcal{Z}^c) \tag{3.14}$$

holds in terms of the Krylov subspace $\mathcal{K}^c = \operatorname{span}\{y, Hy, \ldots, H^{c-1}y\}$ and the invariant subspace $\mathcal{Z}^c = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_c$.

Proof. The property $\widehat{y} \neq 0$ can be shown analogously to the statement (b) in Lemma 3.1, namely, $\mathcal{K}$ contains no eigenvectors since it is not an invariant subspace, whereas $\widehat{y} = 0$ would imply the existence of an eigenvector in $\mathcal{K}$.

For deriving (3.13), we use the shifted Chebyshev polynomial $p(\cdot)$ defined by

$$p(\alpha) = T_{k-c}\left(1 + 2\,\frac{\alpha-\mu_{c+1}}{\mu_{c+1}-\mu_m}\right). \tag{3.15}$$

Then the vector $p(H)\widehat{y}$ can be represented by

$$p(H)\widehat{y} = p(H)\big(q(H)y\big) = q(H)\big(p(H)y\big) \qquad \text{with} \qquad q(\alpha) = \prod_{j\in\{1,\ldots,c\}\setminus\{i\}}(\alpha-\mu_j).$$

Therein the product of $q(\cdot)$ and $p(\cdot)$ is a polynomial of degree $(c-1)+(k-c) = k-1$ so that $p(H)\widehat{y}$ belongs to $\mathcal{K}$. Moreover, $p(\cdot)$ has the properties

$$p(\mu_i) > 1 \qquad \text{and} \qquad |p(\mu_l)| \le 1 \quad \forall\, l \in \{c+1,\ldots,m\} \tag{3.16}$$

according to (1.36). Next, we extend the eigenvector $z_i = Q_i y/\|Q_i y\|_2$ to an orthonormal system $\{z_1,\ldots,z_m\}$ as in (2.16), and expand y as $y = \sum_{l=1}^m \alpha_l\, z_l$ with $\alpha_l = \|Q_l y\|_2$. Then the vector

$p(H)y$ has the expansion $p(H)y = \sum_{l=1}^{m} p(\mu_l)\,\alpha_l\, z_l$, where the term $p(\mu_i)\,\alpha_i\, z_i$ is nonzero due to $p(\mu_i) > 1$ and $\alpha_i = \|Q_i y\|_2 > 0$. Thus $p(H)y \neq 0$. In addition, $p(H)\widehat{y} = q(H)\big(p(H)y\big) \neq 0$ can be shown by contraposition beginning with

$$\left(\prod_{j\in\{1,\ldots,c\}\setminus\{i\}} (H - \mu_j I)\right) \big(p(H)y\big) = 0$$

analogously to the statement (b) in Lemma 3.1. In summary, $p(H)\widehat{y}$ is a nonzero vector in $\mathcal{K}$ and the associated polynomial $p(\cdot)$ fulfills (3.16). Then

$$\tan^2 \angle_2(z_i, \mathcal{K}) \leq \tan^2 \angle_2\big(z_i, p(H)\widehat{y}\big) \qquad \text{and} \qquad \tan \angle_2(z_i, \mathcal{K}) \geq 0$$

hold according to (1.32) in Definition 1.6. Consequently, the derivation of (3.13) can be completed by showing the intermediate estimate

$$\tan^2 \angle_2\big(z_i, p(H)\widehat{y}\big) \leq \big[\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,\big]^{-2} \tan^2 \angle_2(\widehat{y}, \mathcal{Z}). \tag{3.17}$$

For showing (3.17), we begin with the expansion $\widehat{y} = q(H)y = \sum_{l=1}^{m} \beta_l\, z_l$ where $\beta_l = q(\mu_l)\,\alpha_l$. Since $q(\mu_l) = 0$ holds for each $l \in \{1,\ldots,c\}\setminus\{i\}$, a more precise expansion reads

$$\widehat{y} = \beta_i\, z_i + \sum_{l=c+1}^{m} \beta_l\, z_l$$

with $\beta_i = q(\mu_i)\,\alpha_i = \big(\prod_{j\in\{1,\ldots,c\}\setminus\{i\}} (\mu_i - \mu_j)\big)\, \|Q_i y\|_2 \neq 0$. Correspondingly, we expand the vector $p(H)\widehat{y}$ as

$$p(H)\widehat{y} = p(\mu_i)\,\beta_i\, z_i + \sum_{l=c+1}^{m} p(\mu_l)\,\beta_l\, z_l.$$

Then, according to (1.31), it holds that

$$\cos^2 \angle_2(z_i, \widehat{y}) = \left(\frac{z_i^T \widehat{y}}{\|z_i\|_2\, \|\widehat{y}\|_2}\right)^2 = \frac{(z_i^T \widehat{y})^2}{\|\widehat{y}\|_2^2} = \frac{\beta_i^2}{\beta_i^2 + \sum_{l=c+1}^{m} \beta_l^2}$$

so that $\tan^2 \angle_2(z_i, \widehat{y}) = \big(\cos^2 \angle_2(z_i, \widehat{y})\big)^{-1} - 1 = \big(\sum_{l=c+1}^{m} \beta_l^2\big)/\beta_i^2$. Analogously, we get

$$\tan^2 \angle_2\big(z_i, p(H)\widehat{y}\big) = \frac{\sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}{p^2(\mu_i)\,\beta_i^2}.$$

Combining these representations with (3.16) yields

$$\tan^2 \angle_2\big(z_i, p(H)\widehat{y}\big) \leq \frac{1}{p^2(\mu_i)} \left(\frac{\sum_{l=c+1}^{m} \beta_l^2}{\beta_i^2}\right) = \big[\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,\big]^{-2} \tan^2 \angle_2(z_i, \widehat{y}). \tag{3.18}$$

Moreover, according to (1.33) and $\widehat{y} = \beta_i\, z_i + \sum_{l=c+1}^{m} \beta_l\, z_l$, it holds that

$$\tan^2 \angle_2(\widehat{y}, \mathcal{Z}) = \left(\frac{\big\|\sum_{l=i+1}^{m} Q_l \widehat{y}\big\|_2}{\big\|\sum_{l=1}^{i} Q_l \widehat{y}\big\|_2}\right)^2 = \frac{\big\|\sum_{l=c+1}^{m} \beta_l\, z_l\big\|_2^2}{\big\|\beta_i\, z_i\big\|_2^2} = \frac{\sum_{l=c+1}^{m} \beta_l^2}{\beta_i^2} = \tan^2 \angle_2(z_i, \widehat{y}).$$

Thus (3.18) immediately implies (3.17).

For deriving (3.14), the relation

$$\tan^2 \angle_2(\widehat{y}, \mathcal{Z}^c) = \left(\frac{\big\|\sum_{l=c+1}^{m} Q_l \widehat{y}\big\|_2}{\big\|\sum_{l=1}^{c} Q_l \widehat{y}\big\|_2}\right)^2 = \frac{\big\|\sum_{l=c+1}^{m} \beta_l\, z_l\big\|_2^2}{\big\|\beta_i\, z_i\big\|_2^2} = \frac{\sum_{l=c+1}^{m} \beta_l^2}{\beta_i^2} = \tan^2 \angle_2(z_i, \widehat{y})$$

implies $\tan \angle_2(\widehat{y}, \mathcal{Z}^c) = \tan \angle_2(\widehat{y}, \mathcal{Z})$. In addition, the definition (3.11) of $\widehat{y}$ shows that $\widehat{y}$ belongs to $\mathcal{K}^c$ so that $\tan \angle_2(\widehat{y}, \mathcal{Z}^c) \leq \tan \angle_2(\mathcal{K}^c, \mathcal{Z}^c)$ holds according to (1.32) and $\dim \mathcal{K}^c = c \leq \dim \mathcal{Z}^c$. Then we get $\tan \angle_2(\widehat{y}, \mathcal{Z}) \leq \tan \angle_2(\mathcal{K}^c, \mathcal{Z}^c)$ which extends (3.13) as (3.14). □

In comparison to (3.2) and (3.3), the estimates (3.13) and (3.14) do not contain the ratio-products $\prod_{j=1}^{i-1} \frac{\mu_j-\mu_m}{\mu_j-\mu_i}$ and $\prod_{j=i+1}^{c} \frac{\mu_j-\mu_m}{\mu_i-\mu_j}$. Thus better bounds can be achieved in the case that μ_i is an interior element of an eigenvalue cluster. Furthermore, the special form of (3.13) with $c=i$, $\widetilde{\gamma}_i=\gamma_i$ and $\widehat{y} = \big(\prod_{j=1}^{i-1}(H-\mu_j I)\big)y$ directly improves (3.1) for $i>1$. In addition, (3.13) and (3.14) also hold in H-angles by assuming the positive definiteness of H. These variants can be transformed afterwards as estimates in M-angles concerning the generalized matrix eigenvalue problem (1.1).

Corollary 3.5. *With the settings from Theorem 3.2, assume that H is positive definite so that H-angles $\angle_H(\,\cdot\,,\,\cdot\,)$ can be defined as in Definition 1.6. Then the variants of the estimates* (3.13) *and* (3.14) *with $\angle_H(\,\cdot\,,\,\cdot\,)$ instead of $\angle_2(\,\cdot\,,\,\cdot\,)$ hold.*

Proof. Basically, we only need to show that the central inequality (3.18) in the proof of (3.13) and (3.14) holds with H-angles. By using the expansion $\widehat{y} = \beta_i z_i + \sum_{l=c+1}^{m} \beta_l z_l$ and the property

$$\|z_l\|_H^2 = z_l^T H z_l = \mu_l\,(z_l^T z_l) = \mu_l$$

of the orthonormal eigenvectors, we get

$$\cos^2 \angle_H(z_i,\widehat{y}) = \frac{(z_i^T H\widehat{y})^2}{\|z_i\|_H^2\,\|\widehat{y}\|_H^2} = \frac{(\mu_i\, z_i^T \widehat{y})^2}{\mu_i\,\|\widehat{y}\|_H^2} = \frac{\mu_i\,\beta_i^2}{\|\widehat{y}\|_H^2} = \frac{\mu_i\,\beta_i^2}{\mu_i\,\beta_i^2 + \sum_{l=c+1}^{m}\mu_l\,\beta_l^2}$$

so that $\tan^2 \angle_H(z_i,\widehat{y}) = \big(\cos^2 \angle_H(z_i,\widehat{y})\big)^{-1} - 1 = \big(\sum_{l=c+1}^{m}\mu_l\,\beta_l^2\big)/(\mu_i\,\beta_i^2)$. Analogously,

$$\tan^2 \angle_H\big(z_i, p(H)\widehat{y}\big) = \frac{\sum_{l=c+1}^{m}\mu_l\, p^2(\mu_l)\,\beta_l^2}{\mu_i\, p^2(\mu_i)\,\beta_i^2}$$

holds. Subsequently, (3.16) implies

$$\tan^2 \angle_H\big(z_i, p(H)\widehat{y}\big) \le \frac{1}{p^2(\mu_i)}\left(\frac{\sum_{l=c+1}^{m}\mu_l\,\beta_l^2}{\mu_i\,\beta_i^2}\right) = [\,T_{k-c}(1+2\widetilde{\gamma}_i)\,]^{-2}\,\tan^2 \angle_H(z_i,\widehat{y})$$

which is the H-variant of (3.18). □

3.2.2 Angle-dependent estimates on Ritz values

The angle-dependent estimates (3.4), (3.5) and (3.6) on Ritz values correspond to Saad's estimates (2.3) and (2.5). We can improve them by modifying the auxiliary vector $\widetilde{y}$ from Theorem 3.2 similarly as in (3.11) and Theorem 3.4. In addition, we partially modify Saad's analysis as in Theorem 3.3 in order to achieve a further refinement.

Theorem 3.6. *With the settings from Theorem 3.2, the auxiliary vector*

$$y^c = \left(\prod_{j=1}^{i-1}(H-\theta_j I)\right)\left(\prod_{j=i+1}^{c}(H-\mu_j I)\right) y$$

is nonzero, and

$$\mu_i - \theta_i \le (\mu_i - \mu_m)\,\frac{\psi}{1+\psi} \tag{3.19}$$

holds for

$$\psi = [\,T_{k-c}(1+2\widetilde{\gamma}_i)\,]^{-2}\left(\frac{\sin \angle_2(y^c,\mathcal{Z})}{\cos \angle_2(y^c, z_i)}\right)^2.$$

Proof. The property $y^c \neq 0$ can be shown by contraposition analogously to the statement (b) in Lemma 3.1. For deriving (3.19), we use the shifted Chebyshev polynomial $p(\cdot)$ defined in (3.15) as in the proof of Theorem 3.4. Then $p(H)y^c$ has the representation

$$p(H)y^c = p(H)\big(q(H)y\big) = q(H)\big(p(H)y\big) \quad \text{with} \quad q(\alpha) = \big(\textstyle\prod_{j=1}^{i-1}(\alpha-\theta_j)\big)\big(\prod_{j=i+1}^{c}(\alpha-\mu_j)\big).$$

Since the product of $q(\cdot)$ and $p(\cdot)$ is a polynomial of degree $(i-1)+(c-i)+(k-c) = k-1$, the vector $p(H)y^c$ belongs to $\mathcal{K}$. Moreover, by using the properties in (3.16) and the expansion $y = \sum_{l=1}^{m} \alpha_l z_l$ with respect to an orthonormal system $\{z_1, \ldots, z_m\}$ from (2.16), we can show that $p(H)y^c$ is a nonzero vector. Then the value $\mu\big(p(H)y^c\big)$ can be defined, and $\theta_i \geq \mu\big(p(H)y^c\big)$ holds since $p(H)y^c$ contains the linear factors $H - \theta_j I$ for $j = 1, \ldots, i-1$ so that $p(H)y^c$ is orthogonal to the Ritz vectors associated with those Ritz values larger than θ_i. Thus we can complete the derivation of (3.19) by showing the intermediate estimate

$$\mu_i - \mu\big(p(H)y^c\big) \leq (\mu_i - \mu_m)\,\frac{\psi}{1+\psi}. \tag{3.20}$$

Therein we use the expansion $y^c = q(H)y = \sum_{l=1}^{m} \beta_l z_l$ where $\beta_l = q(\mu_l)\,\alpha_l$. Since $q(\mu_l) = 0$ holds for each $l \in \{i+1, \ldots, c\}$, we get

$$y^c = \textstyle\sum_{l=1}^{i} \beta_l z_l + \sum_{l=c+1}^{m} \beta_l z_l$$

where $\beta_i = q(\mu_i)\,\alpha_i = \big(\prod_{j=1}^{i-1}(\mu_i-\theta_j)\big)\big(\prod_{j=i+1}^{c}(\mu_i-\mu_j)\big)\,\|Q_i y\|_2 \neq 0$ holds due to the assumption $\theta_{i-1} > \mu_i$ from Theorem 3.2. In addition, we use the corresponding expansion

$$p(H)y^c = \textstyle\sum_{l=1}^{i} p(\mu_l)\,\beta_l z_l + \sum_{l=c+1}^{m} p(\mu_l)\,\beta_l z_l$$

of $p(H)y^c$ in order to determine a lower bound of the difference $\mu\big(p(H)y^c\big) - \mu_m$, namely,

$$\begin{aligned}
\mu\big(p(H)y^c\big) - \mu_m \;&=\; \frac{\sum_{l=1}^{i}(\mu_l-\mu_m)\,p^2(\mu_l)\,\beta_l^2 + \sum_{l=c+1}^{m}(\mu_l-\mu_m)\,p^2(\mu_l)\,\beta_l^2}{\sum_{l=1}^{i} p^2(\mu_l)\,\beta_l^2 + \sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}\\
&\geq\; (\mu_i-\mu_m)\,\frac{\sum_{l=1}^{i} p^2(\mu_l)\,\beta_l^2}{\sum_{l=1}^{i} p^2(\mu_l)\,\beta_l^2 + \sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}\\
&=\; (\mu_i-\mu_m)\left(1+\frac{\sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}{\sum_{l=1}^{i} p^2(\mu_l)\,\beta_l^2}\right)^{-1} \;\geq\; (\mu_i-\mu_m)\left(1+\frac{\sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}{p^2(\mu_i)\,\beta_i^2}\right)^{-1}.
\end{aligned} \tag{3.21}$$

Subsequently, by using (3.16) again, we get

$$\frac{\sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}{p^2(\mu_i)\,\beta_i^2} \leq \frac{1}{p^2(\mu_i)}\left(\frac{\sum_{l=c+1}^{m}\beta_l^2}{\beta_i^2}\right) = [\,T_{k-c}(1+2\widetilde{\gamma}_i)\,]^{-2}\left(\frac{\sum_{l=c+1}^{m}\beta_l^2}{\beta_i^2}\right). \tag{3.22}$$

Moreover, according to (1.31), (1.33), and the expansion $y^c = \sum_{l=1}^{i}\beta_l z_l + \sum_{l=c+1}^{m}\beta_l z_l$, it holds that

$$\cos^2\angle_2(y^c, z_i) = \cos^2\angle_2(z_i, y^c) = \left(\frac{z_i^T y^c}{\|z_i\|_2\,\|y^c\|_2}\right)^2 = \frac{(z_i^T y^c)^2}{\|y^c\|_2^2} = \frac{\beta_i^2}{\|y^c\|_2^2},$$

$$\sin^2\angle_2(y^c, \mathcal{Z}) = \left(\frac{\|\sum_{l=i+1}^{m} Q_l y^c\|_2}{\|y^c\|_2}\right)^2 = \frac{\|\sum_{l=c+1}^{m}\beta_l z_l\|_2^2}{\|y^c\|_2^2} = \frac{\sum_{l=c+1}^{m}\beta_l^2}{\|y^c\|_2^2}.$$

Consequently, (3.22) can be rewritten as

$$\frac{\sum_{l=c+1}^{m} p^2(\mu_l)\,\beta_l^2}{p^2(\mu_i)\,\beta_i^2} \leq [\,T_{k-c}(1+2\widetilde{\gamma}_i)\,]^{-2}\left(\frac{\sin\angle_2(y^c, \mathcal{Z})}{\cos\angle_2(y^c, z_i)}\right)^2 = \psi.$$

Combining this with (3.21) yields

$$\mu\big(p(H)y^c\big) - \mu_m \;\geq\; (\mu_i - \mu_m)\,(1+\psi)^{-1} \quad\Rightarrow\quad \frac{\mu\big(p(H)y^c\big) - \mu_m}{\mu_i - \mu_m} \;\geq\; (1+\psi)^{-1}$$

so that

$$\frac{\mu_i - \mu\big(p(H)y^c\big)}{\mu_i - \mu_m} \;=\; 1 - \frac{\mu\big(p(H)y^c\big) - \mu_m}{\mu_i - \mu_m} \;\leq\; 1 - (1+\psi)^{-1} \;=\; \frac{\psi}{1+\psi}$$

holds and implies (3.20). □

The estimate (3.19) does not depend on $\prod_{j=1}^{i-1} \frac{\theta_j - \mu_m}{\theta_j - \mu_i}$ and $\prod_{j=i+1}^{c} \frac{\mu_j - \mu_m}{\mu_i - \mu_j}$ which are contained in (3.5) and (3.6). Thus (3.19) provides better bounds in the case that μ_i is an interior element of an eigenvalue cluster. In addition, a direct improvement of (3.4) for $i > 1$ is given by the special form of (3.19) with $c = i$, $\widetilde{\gamma}_i = \gamma_i$ and $y^c = y^i = \big(\prod_{j=1}^{i-1}(H - \theta_j I)\big)y$.

However, the auxiliary vector y^c is not necessarily orthogonal to the eigenspaces associated with $\mu_1, \ldots, \mu_{i-1}$ so that it cannot easily be eliminated within an angle between two subspaces as in (3.14). In order to overcome this drawback, we extend $\widehat{y}$ to a set of vectors defined in (3.12). These vectors enable an adaptation of the proof techniques from Lemma 2.10 to standard Krylov subspace iterations and can be eliminated within the resulting estimate afterwards.

Theorem 3.7. *With the settings from Theorem 3.2, the auxiliary vectors defined in* (3.12) *are nonzero, and*

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_m} \leq [\,T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2}\, \tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) \tag{3.23}$$

holds in terms of the Krylov subspace $\mathcal{K}^c = \operatorname{span}\{y, Hy, \ldots, H^{c-1}y\}$ *and the invariant subspace* $\mathcal{Z}^c = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_c$. *Moreover,*

$$\mu_i - \theta_i \leq (\mu_i - \mu_m)\,\frac{\psi}{1+\psi} \tag{3.24}$$

holds for $\psi = [\,T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2}\, \tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c)$.

Proof. The auxiliary vectors $y_1, \ldots, y_c$ defined in (3.12) are nonzero since otherwise $\mathcal{K}$ would be an invariant subspace; cf. the proof of the statement (b) in Lemma 3.1.

The estimate (3.23) holds trivially in the case $\tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) = \infty$. Thus we only need to show (3.23) in the case $\tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) < \infty$. Therein we represent $\tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c)$ by $\tan^2 \angle_2(\mathcal{K}^c, \mathcal{V})$ with $\mathcal{V} = \operatorname{span}\{z_1, \ldots, z_c\}$ concerning the orthonormal system $\{z_1, \ldots, z_m\}$ defined in (2.16) with respect to the eigenprojections of y. This representation can be verified by using the orthogonal projector $Q = \sum_{j=1}^{c} Q_j$ on $\mathcal{Z}^c$ and the orthogonal projector $P = \sum_{l=1}^{c} z_l z_l^T$ on $\mathcal{V}$ as follows. Beginning with the expansion $w = \sum_{l=1}^{m} (z_l^T w)\, z_l$ of an arbitrary nonzero vector $w \in \mathcal{K}^c$, we get

$$Qw = \textstyle\sum_{l=1}^{m} (z_l^T w)\, Q z_l = \sum_{l=1}^{m} (z_l^T w)\,\big(\sum_{j=1}^{c} Q_j z_l\big) = \sum_{l=1}^{c} (z_l^T w)\, z_l = \sum_{l=1}^{c} z_l z_l^T w = Pw$$

so that

$$\tan^2 \angle_2(w, \mathcal{Z}^c) = \frac{\|w - Qw\|_2^2}{\|Qw\|_2^2} = \frac{\|w - Pw\|_2^2}{\|Pw\|_2^2} = \tan^2 \angle_2(w, \mathcal{V})$$

holds according to (1.33). Then, by considering the relation $\dim \mathcal{K}^c = c = \dim \mathcal{V} \leq \dim \mathcal{Z}^c$ and applying the angle properties in (1.32), we get

$$\tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) = \max_{w \in \mathcal{K}^c \setminus \{0\}} \tan^2 \angle_2(w, \mathcal{Z}^c) = \max_{w \in \mathcal{K}^c \setminus \{0\}} \tan^2 \angle_2(w, \mathcal{V}) = \tan^2 \angle_2(\mathcal{K}^c, \mathcal{V}). \tag{3.25}$$

Subsequently, we use the auxiliary vectors defined in (3.12) which belong to $\mathcal{K}^c$ by definition and have already been shown to be nonzero. A further property of these vectors is that $z_t^T y_l = 0$ holds for each $t \in \{1, \dots, c\} \backslash \{l\}$, namely,

$$z_t^T y_l = z_t^T \left(\prod_{j \in \{1,\dots,c\} \backslash \{l\}} (H - \mu_j I) \right) y = (H z_t - \mu_t z_t)^T \left(\prod_{j \in \{1,\dots,c\} \backslash \{l,t\}} (H - \mu_j I) \right) y = 0.$$

In addition, $z_l^T y_l$ is nonzero for each $l \in \{1, \dots, c\}$, since otherwise y_l is orthogonal to all of $z_1, \dots, z_c$ and thus orthogonal to $\mathcal{V}$ so that

$$\angle_2(y_l, \mathcal{V}) = \pi/2 \qquad \Rightarrow \qquad \tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) \overset{(3.25)}{=} \tan^2 \angle_2(\mathcal{K}^c, \mathcal{V}) \geq \tan^2 \angle_2(y_l, \mathcal{V}) = \infty.$$

This contradicts the condition $\tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) < \infty$ of the current case. In summary, we get

$$[z_1, \dots, z_c]^T [y_1, \dots, y_c] = \operatorname{diag}(z_1^T y_1, \dots, z_c^T y_c) \quad \text{with} \quad z_l^T y_l \neq 0 \quad \forall\, l \in \{1, \dots, c\}. \tag{3.26}$$

Thus $[z_1, \dots, z_c]^T [y_1, \dots, y_c]$ is an invertible matrix so that $y_1, \dots, y_c$ are linearly independent.

This property allows us to construct proper subspaces for proving the estimate (3.23), namely, the subspaces

$$\widetilde{\mathcal{Y}} = \operatorname{span}\{y_1, \dots, y_i\} \subseteq \mathcal{K}^c, \qquad \widetilde{\mathcal{Z}} = \operatorname{span}\{z_1, \dots, z_i\} \subseteq \mathcal{V}$$

can be used for deriving the intermediate estimate

$$\tan^2 \angle_2\big(p(H)\widetilde{\mathcal{Y}}, \widetilde{\mathcal{Z}}\big) \leq [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \tan^2 \angle_2(\mathcal{K}^c, \mathcal{Z}^c) \tag{3.27}$$

where $p(\cdot)$ is the shifted Chebyshev polynomial defined in (3.15).

The derivation of (3.27) begins with the relation

$$\tan \angle_2\big(p(H)\widetilde{\mathcal{Y}}, \widetilde{\mathcal{Z}}\big) = \max_{u \in p(H)\widetilde{\mathcal{Y}} \backslash \{0\}} \tan \angle_2\big(u, \widetilde{\mathcal{Z}}\big) = \max_{\widetilde{y} \in \widetilde{\mathcal{Y}} \backslash \{0\}} \tan \angle_2\big(p(H)\widetilde{y}, \widetilde{\mathcal{Z}}\big)$$

which enables the representation of $\tan \angle_2\big(p(H)\widetilde{\mathcal{Y}}, \widetilde{\mathcal{Z}}\big)$ by $\tan \angle_2\big(p(H)w, \widetilde{\mathcal{Z}}\big)$ with a vector $w \in \widetilde{\mathcal{Y}} \backslash \{0\}$ maximizing $\tan \angle_2\big(p(H)\widetilde{y}, \widetilde{\mathcal{Z}}\big)$. Moreover, the property $z_t^T y_l = 0 \ \forall\, t \in \{1, \dots, c\} \backslash \{l\}$ ensures that $\widetilde{\mathcal{Y}}$ is a subset of the invariant subspace $\operatorname{span}\{z_1, \dots, z_i, z_{c+1}, \dots, z_m\}$. Thus w can be expanded as $w = \sum_{j=1}^{i} \alpha_j z_j + \sum_{j=c+1}^{m} \alpha_j z_j$ with the coefficients $\alpha_j = z_j^T w$, and it holds that $Pw = \sum_{j=1}^{i} \alpha_j z_j$ in terms of the orthogonal projector $P = \sum_{l=1}^{c} z_l z_l^T$ on $\mathcal{V}$. Then we get

$$\tan^2 \angle_2\big(w, \mathcal{V}\big) = \frac{\|w - Pw\|_2^2}{\|Pw\|_2^2} = \frac{\big\| \sum_{j=c+1}^{m} \alpha_j z_j \big\|_2^2}{\big\| \sum_{j=1}^{i} \alpha_j z_j \big\|_2^2} = \frac{\sum_{j=c+1}^{m} \alpha_j^2}{\sum_{j=1}^{i} \alpha_j^2}. \tag{3.28}$$

Next, a similar representation of $\tan \angle_2\big(p(H)w, \widetilde{\mathcal{Z}}\big)$ can be achieved by using the expansion $p(H)w = \sum_{j=1}^{i} p(\mu_j)\, \alpha_j z_j + \sum_{j=c+1}^{m} p(\mu_j)\, \alpha_j z_j$ and the orthogonal projector $\widetilde{P} = \sum_{l=1}^{i} z_l z_l^T$ on $\widetilde{\mathcal{Z}}$. Therein $\widetilde{P}\big(p(H)w\big) = \sum_{j=1}^{i} p(\mu_j)\, \alpha_j z_j$ holds so that

$$\tan^2 \angle_2\big(p(H)w, \widetilde{\mathcal{Z}}\big) = \frac{\big\| \sum_{j=c+1}^{m} p(\mu_j)\, \alpha_j z_j \big\|_2^2}{\big\| \sum_{j=1}^{i} p(\mu_j)\, \alpha_j z_j \big\|_2^2} = \frac{\sum_{j=c+1}^{m} p^2(\mu_j)\, \alpha_j^2}{\sum_{j=1}^{i} p^2(\mu_j)\, \alpha_j^2}. \tag{3.29}$$

Moreover, the shifted Chebyshev polynomial $p(\cdot)$ has the properties

$$p(\mu_j) \geq p(\mu_i) > 1 \quad \forall\ j \in \{1, \dots, i\}, \qquad |p(\mu_j)| \leq 1 \quad \forall\ j \in \{c+1, \dots, m\} \tag{3.30}$$

based on (1.36). Summarizing the above yields

$$\begin{aligned}\tan^2\angle_2\big(p(H)\widetilde{\mathcal{Y}},\widetilde{\mathcal{Z}}\big) &= \tan^2\angle_2\big(p(H)w,\widetilde{\mathcal{Z}}\big) \overset{(3.29)}{=} \frac{\sum_{j=c+1}^m p^2(\mu_j)\,\alpha_j^2}{\sum_{j=1}^i p^2(\mu_j)\,\alpha_j^2} \overset{(3.30)}{\leq} \frac{\sum_{j=c+1}^m \alpha_j^2}{\sum_{j=1}^i p^2(\mu_i)\,\alpha_j^2}\\ &= \big[T_{k-c}(1+2\widetilde{\gamma}_i)\big]^{-2}\frac{\sum_{j=c+1}^m \alpha_j^2}{\sum_{j=1}^i \alpha_j^2} \overset{(3.28)}{=} \big[T_{k-c}(1+2\widetilde{\gamma}_i)\big]^{-2}\tan^2\angle_2\big(w,\mathcal{V}\big).\end{aligned}$$

Combining this with

$$\tan^2\angle_2\big(w,\mathcal{V}\big) \leq \max_{w\in\mathcal{K}^c\setminus\{0\}}\tan^2\angle_2(w,\mathcal{V}) = \tan^2\angle_2\big(\mathcal{K}^c,\mathcal{V}\big) \overset{(3.25)}{=} \tan^2\angle_2(\mathcal{K}^c,\mathcal{Z}^c)$$

(where the inequality holds because of $w\in\widetilde{\mathcal{Y}}\setminus\{0\}$ and $\widetilde{\mathcal{Y}}\subseteq\mathcal{K}^c$) yields (3.27).

Finally, we extend (3.27) as the estimate (3.23). Therein we need to verify that the subspace $p(H)\widetilde{\mathcal{Y}}$ has dimension i in order to apply the Courant-Fischer principles. We use the generating vectors $p(H)y_1,\dots,p(H)y_i$ of $p(H)\widetilde{\mathcal{Y}}$ and the property

$$z_t^T\big(p(H)y_l\big) = \big(p(H)z_t\big)^T y_l = \big(p(\mu_t)z_t\big)^T y_l = p(\mu_t)\,\big(z_t^T y_l\big)$$

for the indices $t,l\in\{1,\dots,i\}$. Then

$$[z_1,\dots,z_i]^T[p(H)y_1,\dots,p(H)y_i] = \operatorname{diag}\big(p(\mu_1)\,z_1^T y_1,\dots,p(\mu_i)\,z_i^T y_i\big) \tag{3.31}$$

holds analogously to (3.26). Moreover, $p(\mu_l)>1>0$ and $z_l^T y_l\neq 0$ hold for each $l\in\{1,\dots,i\}$ according to (3.30) and (3.26). Thus the matrix product in (3.31) is an invertible matrix so that $p(H)y_1,\dots,p(H)y_i$ are linearly independent, and $\dim\big(p(H)\widetilde{\mathcal{Y}}\big)=i$. Consequently, there are i Ritz values of H in $p(H)\widetilde{\mathcal{Y}}$. We denote them by $\beta_1\geq\cdots\geq\beta_i$. In addition, $p(H)\widetilde{\mathcal{Y}}$ is a subset of $\mathcal{K}$ since the generating vectors $p(H)y_1,\dots,p(H)y_i$ belong to $\mathcal{K}$ by considering the degree of the associated polynomial. Then the relation $p(H)\widetilde{\mathcal{Y}}\subseteq\mathcal{K}\subseteq\operatorname{span}\{z_1,\dots,z_m\}$ holds so that $\beta_i\leq\theta_i\leq\mu_i$ holds according to the Courant-Fischer principles. Furthermore, we use a Ritz vector u in $p(H)\widetilde{\mathcal{Y}}$ associated with β_i, and expand u as $u=\widetilde{z}+\widetilde{w}$ with its orthogonal projections $\widetilde{z}\in\widetilde{\mathcal{Z}}=\operatorname{span}\{z_1,\dots,z_i\}$ and $\widetilde{w}\in\operatorname{span}\{z_{i+1},\dots,z_m\}$. Then the intermediate estimate

$$\frac{\mu_i-\theta_i}{\theta_i-\mu_m}\leq\frac{\mu_i-\beta_i}{\beta_i-\mu_m}\leq\tan^2\angle_2\big(p(H)\widetilde{\mathcal{Y}},\widetilde{\mathcal{Z}}\big)$$

can be shown analogously as in Lemma 2.9. Combining this with (3.27) yields (3.23).

Moreover, (3.23) implies (3.24) by using the relation

$$\frac{\mu_i-\theta_i}{\mu_i-\mu_m}=\frac{\mu_i-\theta_i}{\theta_i-\mu_m}\left(1+\frac{\mu_i-\theta_i}{\theta_i-\mu_m}\right)^{-1}$$

and the monotonicity of the function $(\,\cdot\,)/(1+\,\cdot\,)$. □

The estimate (3.23) does not require the assumption $\theta_{i-1}>\mu_i$ from Theorem 3.2 and generalizes Knyazev's estimate (2.9). The bound in (3.23) is actually the squared value of the bound in the estimate (3.14) on approximate eigenvectors. Nevertheless, the auxiliary vector $\widehat{y}$ for deriving (3.14) needs to be strengthened by further auxiliary vectors from (3.12) in order to derive (3.23).

The estimate (3.24) is equivalent to (3.23). An important feature of (3.24) is, in comparison to (3.4), (3.5), (3.6) and (3.19), that it does not depend on the Ritz values in the current Krylov subspace and thus provides an a priori bound.

3.2.3 Angle-free estimates on Ritz values

The estimates in the previous subsections require certain angle terms such as $\tan\angle_2(\mathcal{K}^c, \mathcal{Z}^c)$. These terms avoid the possibly large ratio-products, but can still be suboptimal for providing appropriate bounds for low-dimensional Krylov subspaces where the Chebyshev factors are only moderate. For such a case, we derive some angle-free estimates based on Knyazev's estimate (2.10). Therein we use again the auxiliary vectors from (3.12), and extend certain arguments from Lemma 2.15.

Theorem 3.8. *With the settings from Theorem 3.2, the auxiliary vectors defined in* (3.12) *are nonzero. Moreover,*

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_{c+1}} \leq [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \, \frac{\mu_i - \eta}{\eta - \mu_{c+1}} \tag{3.32}$$

holds for the smallest Ritz value η of H in the Krylov subspace $\mathcal{K}^c = \mathrm{span}\{y, Hy, \ldots, H^{c-1}y\}$ by assuming $\eta > \mu_{c+1}$, and

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_{i+1}} \leq [\, T_{k-i}(1 + 2\gamma_i)\,]^{-2} \, \frac{\mu_i - \varphi}{\varphi - \mu_{i+1}} \tag{3.33}$$

holds for the smallest Ritz value φ of H in $\mathcal{K}^i = \mathrm{span}\{y, Hy, \ldots, H^{i-1}y\}$ by assuming $\varphi > \mu_{i+1}$.

Proof. As mentioned at the beginning of the proof of Theorem 3.7, the statement that the auxiliary vectors $y_1, \ldots, y_c$ defined in (3.12) are nonzero can be shown by contraposition analogously to the statement (b) in Lemma 3.1.

For deriving the estimate (3.32), we use $y_1, \ldots, y_c$ together with the orthonormal system $\{z_1, \ldots, z_m\}$ defined in (2.16) with respect to the eigenprojections of the initial vector y of $\mathcal{K}$. According to their definition in (3.12), $y_1, \ldots, y_c$ belong to $\mathcal{K}^c$, and $z_t^T y_l = 0$ holds for distinct $t,\, l \in \{1, \ldots, c\}$. In addition, the assumption $\eta > \mu_{c+1}$ for (3.32) ensures that $z_l^T y_l \neq 0$ holds for each $l \in \{1, \ldots, c\}$, since otherwise there exists a y_l with the property $z_t^T y_l = 0 \;\; \forall\, t \in \{1, \ldots, c\}$, i.e., y_l is orthogonal to $\mathrm{span}\{z_1, \ldots, z_c\}$ and thus belongs to the invariant subspace $\mathrm{span}\{z_{c+1}, \ldots, z_m\}$ so that

$$\mu_{c+1} \;=\; \max_{\widetilde{z} \,\in\, \mathrm{span}\{z_{c+1}, \ldots, z_m\} \setminus \{0\}} \mu(\widetilde{z}) \;\geq\; \mu(y_l) \;\geq\; \min_{\widetilde{y} \,\in\, \mathcal{K}^c \setminus \{0\}} \mu(\widetilde{y}) \;=\; \eta$$

holds and contradicts $\eta > \mu_{c+1}$. Consequently, $[z_1, \ldots, z_c]^T [y_1, \ldots, y_c]$ is an invertible matrix so that $y_1, \ldots, y_c$ are linearly independent; cf. (3.26). Then $\widetilde{\mathcal{Y}} = \mathrm{span}\{y_1, \ldots, y_i\}$ is an i-dimensional subspace within $\mathcal{K}^c$. Moreover, by using the shifted Chebyshev polynomial $p(\cdot)$ defined in (3.15), the subspace $p(H)\widetilde{\mathcal{Y}}$ is an i-dimensional subspace within $\mathcal{K}$ as shown by the relation (3.31) in the proof of Theorem 3.7. Thus we denote by $\widetilde{\eta}_1 \geq \cdots \geq \widetilde{\eta}_i$ the Ritz values of H in $p(H)\widetilde{\mathcal{Y}}$.

Similarly as in Lemma 2.15, we represent $\widetilde{\eta}_i$ by $\mu\big(p(H)w\big)$ where $p(H)w$ is an associated Ritz vector in $p(H)\widetilde{\mathcal{Y}}$ with a corresponding $w \in \widetilde{\mathcal{Y}} \setminus \{0\}$. Then we verify that the vector

$$\widetilde{w} \;=\; p(\mu_i) \textstyle\sum_{l=1}^{i} z_l z_l^T w \;+\; \sum_{l=c+1}^{m} z_l z_l^T w$$

possesses the properties

$$\mu\big(p(H)w\big) \geq \mu(\widetilde{w}) \geq \mu(w) \tag{3.34}$$

and

$$\frac{\mu_i - \mu(\widetilde{w})}{\mu(\widetilde{w}) - \mu_{c+1}} \leq [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \, \frac{\mu_i - \mu(w)}{\mu(w) - \mu_{c+1}}. \tag{3.35}$$

The property (3.34) is verified by showing the inequalities

$$\mu\big(p(H)w\big) \geq \mu(w), \qquad \mu\big(p(H)w\big) \geq \mu(\widetilde{w}), \qquad \mu(\widetilde{w}) \geq \mu(w) \tag{3.36}$$

in a row. The concerned vectors belong to the invariant subspace $\operatorname{span}\{z_1, \ldots, z_i, z_{c+1}, \ldots, z_m\}$, for which the following statements hold analogously to Lemma 2.12.

Let u be an arbitrary nonzero vector in $\operatorname{span}\{z_1, \ldots, z_i, z_{c+1}, \ldots, z_m\}$ with $\mu_{\tau_j} \geq \mu(u) \geq \mu_{\tau_{j+1}}$ for two neighboring indices τ_j and τ_{j+1} from the arranged index set $\tau = \{1, \ldots, i,\, c+1, \ldots, m\}$, and expand u as $u = \sum_{l=1}^{\#\tau} \alpha_{\tau_l} z_{\tau_l}$ with the cardinality $\#\tau$ and the coefficients $\alpha_{\tau_l} = z_{\tau_l}^T u$. Then the vector $v = \sum_{l=1}^{\#\tau} \beta_{\tau_l} z_{\tau_l}$ with $\beta_{\tau_l} \in \mathbb{R}$ satisfies

(a) $\mu(v) \geq \mu(u)$ if $|\beta_{\tau_l}| \geq |\alpha_{\tau_l}| \;\; \forall\, l \leq j$ and $|\beta_{\tau_l}| \leq |\alpha_{\tau_l}| \;\; \forall\, l > j$,

(b) $\mu(v) \leq \mu(u)$ if $|\beta_{\tau_l}| \leq |\alpha_{\tau_l}| \;\; \forall\, l \leq j$ and $|\beta_{\tau_l}| \geq |\alpha_{\tau_l}| \;\; \forall\, l > j$.

In addition, it holds that

$$p(\mu_{\tau_1}) \geq \cdots \geq p(\mu_{\tau_i}) = p(\mu_i) \geq p(\mu_c) > 1, \qquad \text{and} \quad |p(\mu_{\tau_l})| \leq 1 \quad \forall\, l > i \tag{3.37}$$

according to (1.36).

For showing the first inequality in (3.36), the relation

$$\mu(w) \;\geq\; \min_{\widetilde{y} \in \widetilde{\mathcal{Y}} \setminus \{0\}} \mu(\widetilde{y}) \;\geq\; \min_{\widetilde{y} \in \mathcal{K}^c \setminus \{0\}} \mu(\widetilde{y}) \;=\; \eta \;>\; \mu_{c+1} \tag{3.38}$$

ensures that the condition $\mu_{\tau_j} \geq \mu(w) \geq \mu_{\tau_{j+1}}$ is fulfilled for a $j \in \{1, \ldots, i\}$. Then w and $p(H)w/p(\mu_{\tau_j})$ can be regarded as u and v in the above variant of Lemma 2.12. The associated coefficients read $\alpha_{\tau_l} = z_{\tau_l}^T w$ and $\beta_{\tau_l} = p(\mu_{\tau_l})\,(z_{\tau_l}^T w)/p(\mu_{\tau_j})$. Since $\tau_j \leq \tau_i$, (3.37) implies

$$\frac{p(\mu_{\tau_1})}{p(\mu_{\tau_j})} \geq \cdots \geq \frac{p(\mu_{\tau_j})}{p(\mu_{\tau_j})} = 1 \geq \cdots \geq \frac{p(\mu_{\tau_i})}{p(\mu_{\tau_j})} > 0, \qquad \left|\frac{p(\mu_{\tau_l})}{p(\mu_{\tau_j})}\right| \leq \left|\frac{1}{p(\mu_{\tau_j})}\right| < 1 \quad \forall\, l > i$$

so that

$$|\beta_{\tau_l}| = \big|p(\mu_{\tau_l})\,\alpha_{\tau_l}/p(\mu_{\tau_j})\big| = \left|\frac{p(\mu_{\tau_l})}{p(\mu_{\tau_j})}\right| |\alpha_{\tau_l}| \begin{cases} \geq |\alpha_{\tau_l}| & \forall\, l \leq j, \\ \leq |\alpha_{\tau_l}| & \forall\, l > j. \end{cases}$$

Then applying the statement (a) shows that $\mu\big(p(H)w/p(\mu_{\tau_j})\big) \geq \mu(w)$ which leads to the inequality $\mu\big(p(H)w\big) \geq \mu(w)$ by using the collinearity of $p(H)w/p(\mu_{\tau_j})$ and $p(H)w$.

Subsequently, we extend the first inequality in (3.36) as

$$\mu_i \geq \widetilde{\eta}_i = \mu\big(p(H)w\big) \geq \mu(w) > \mu_{c+1} \tag{3.39}$$

according to the Courant-Fischer principles and (3.38). Then the condition $\mu_{\tau_j} \geq \mu(u) \geq \mu_{\tau_{j+1}}$ in the above variant of Lemma 2.12 is fulfilled by $u = p(H)w$ or $u = w$ for $j = i$, and the remaining two inequalities in (3.36) can be shown as follows.

By regarding $p(H)w$ and $\widetilde{w}$ as u and v, the associated coefficients read $\alpha_{\tau_l} = p(\mu_{\tau_l})\,(z_{\tau_l}^T w)$ for each $l \in \{1, \ldots, \#\tau\}$, $\beta_{\tau_l} = p(\mu_{\tau_i})\,(z_{\tau_l}^T w)$ for each $l \leq i$, and $\beta_{\tau_l} = z_{\tau_l}^T w$ for each $l > i$ according to $\tau_i = i$ and the definition of $\widetilde{w}$. Then (3.37) implies

$$|\beta_{\tau_l}| = \left|\frac{p(\mu_{\tau_i})}{p(\mu_{\tau_l})}\right| |\alpha_{\tau_l}| \leq |\alpha_{\tau_l}| \quad \forall\, l \leq i, \qquad |\beta_{\tau_l}| = \frac{|\alpha_{\tau_l}|}{|p(\mu_{\tau_l})|} \geq |\alpha_{\tau_l}| \quad \forall\, l > i$$

so that the statement (b) is applicable and results in $\mu\big(p(H)w\big) \geq \mu(\widetilde{w})$. Similarly, by regarding w and $\widetilde{w}$ as u and v, the α-coefficients read $\alpha_{\tau_l} = z_{\tau_l}^T w$ for each $l \in \{1, \ldots, \#\tau\}$ so that

$$|\beta_{\tau_l}| = \big|p(\mu_{\tau_i})\big|\,|\alpha_{\tau_l}| > |\alpha_{\tau_l}| \quad \forall\, l \leq i, \qquad |\beta_{\tau_l}| = |\alpha_{\tau_l}| \quad \forall\, l > i.$$

Thus the statement (a) is applicable and yields $\mu(\widetilde{w}) \geq \mu(w)$. This completes the verification of the property (3.34).

For verifying the property (3.35), we represent w and $\widetilde{w}$ by

$$w = z + \widetilde{z} \qquad \text{and} \qquad \widetilde{w} = p(\mu_i)z + \widetilde{z}$$

with $z = \sum_{l=1}^{i} z_l z_l^T w$ and $\widetilde{z} = \sum_{l=c+1}^{m} z_l z_l^T w$. Therein z is nonzero since otherwise $w = \widetilde{z} \in \operatorname{span}\{z_{c+1}, \ldots, z_m\}$ holds and leads to $\mu(w) \leq \mu_{c+1}$ which contradicts (3.38).

Furthermore, in the case $\widetilde{z} = 0$, it holds that $w = z \in \operatorname{span}\{z_1, \ldots, z_i\}$ which implies $\mu(w) \geq \mu_i$. Combining this with (3.39) yields $\mu(w) = \mu_i$. In addition, $\widetilde{w} = p(\mu_i)z = p(\mu_i)w$ holds where $p(\mu_i)$ is nonzero due to (3.37). Then we get $\mu(\widetilde{w}) = \mu(w) = \mu_i$ so that both sides of the inequality in (3.35) are zero. Thus (3.35) holds trivially.

In the case $\widetilde{z} \neq 0$, the value $\mu(\widetilde{z})$ can be defined. Then

$$\left(\frac{\mu(z) - \mu(\widetilde{w})}{\mu(\widetilde{w}) - \mu(\widetilde{z})}\right)\left(\frac{\mu(z) - \mu(w)}{\mu(w) - \mu(\widetilde{z})}\right)^{-1} = \left(\frac{1}{|p(\mu_i)|}\right)^2 = [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \tag{3.40}$$

holds analogously to (2.44) in the proof of Lemma 2.13 despite different settings. In addition, according to (3.34), (3.39) and the definitions of z, $\widetilde{z}$, the relation $\mu(z) \geq \mu_i \geq \mu(\widetilde{w}) \geq \mu(w) > \mu_{c+1} \geq \mu(\widetilde{z})$ holds and implies

$$\left(\frac{\mu_i - \mu(\widetilde{w})}{\mu(\widetilde{w}) - \mu_{c+1}}\right)\left(\frac{\mu_i - \mu(w)}{\mu(w) - \mu_{c+1}}\right)^{-1} = \left(\frac{\mu_i - \mu(\widetilde{w})}{\mu_i - \mu(w)}\right)\left(\frac{\mu(w) - \mu_{c+1}}{\mu(\widetilde{w}) - \mu_{c+1}}\right)$$

$$\leq \left(\frac{\mu(z) - \mu(\widetilde{w})}{\mu(z) - \mu(w)}\right)\left(\frac{\mu(w) - \mu(\widetilde{z})}{\mu(\widetilde{w}) - \mu(\widetilde{z})}\right) = \left(\frac{\mu(z) - \mu(\widetilde{w})}{\mu(\widetilde{w}) - \mu(\widetilde{z})}\right)\left(\frac{\mu(z) - \mu(w)}{\mu(w) - \mu(\widetilde{z})}\right)^{-1}.$$

Combining this with (3.40) completes the verification of the property (3.35).

Finally, we apply (3.34) and (3.35) to the proof of the estimate (3.32). Since $p(H)\widetilde{\mathcal{Y}}$ is an i-dimensional subspace within $\mathcal{K}$, the corresponding ith Ritz values $\widetilde{\eta}_i$, θ_i in descending order fulfill $\theta_i \geq \widetilde{\eta}_i$ according to the Courant-Fischer principles. Then (3.34) extends this relation as $\theta_i \geq \widetilde{\eta}_i = \mu\big(p(H)w\big) \geq \mu(\widetilde{w})$ so that the monotonicity of the function $\big(\mu_i - \cdot\,\big)/\big(\,\cdot - \mu_{c+1}\big)$ implies $\big(\mu_i - \theta_i\big)/\big(\theta_i - \mu_{c+1}\big) \leq \big(\mu_i - \mu(\widetilde{w})\big)/\big(\mu(\widetilde{w}) - \mu_{c+1}\big)$. In addition, $\mu(w) \geq \eta$ holds due to (3.38) so that $\big(\mu_i - \mu(w)\big)/\big(\mu(w) - \mu_{c+1}\big) \leq \big(\mu_i - \eta\big)/\big(\eta - \mu_{c+1}\big)$. Combining these two inequalities with (3.35) yields (3.32).

The estimate (3.33) can be shown by the same approach with the special setting $c = i$. □

The estimates (3.32) and (3.33) supplement the angle-dependent estimates (3.19) and (3.23) in the case of low-dimensional Krylov subspaces. We can generalize them in Chapter 4 to arbitrarily located Ritz values η and φ in order to investigate restarted Krylov subspace iterations where the angle-dependent estimates cannot be applied to multiple steps. Moreover, in Chapter 5, we can adapt some arguments in the proof of Theorem 3.8 to block-Krylov subspace iterations in order to generalize the angle-free estimate (2.13) to further Ritz values.

3.2.4 Additional estimates on Ritz vectors

For analyzing the Ritz vectors in the considered Krylov subspace, we can combine some additional estimates such as (2.11) and (2.14) with the estimates on Ritz values derived in the previous subsections. Therein (2.14) can easily be adapted to standard Krylov subspace iterations. The bound in (2.14) only makes use of two Ritz values θ_{i-1} and θ_i for analyzing a Ritz vector associated with θ_i. Thus we expect that the bound could be refined by adding further Ritz values. We aim to extend the term

$$\frac{(\mu_1 - \theta_i)(\theta_i - \mu_{i+1})(\theta_{i-1} - \mu_i)}{(\mu_1 - \mu_i)(\mu_i - \mu_{i+1})(\theta_{i-1} - \theta_i)}$$

in (2.14) as

$$\Bigg(\prod_{j=1,\ j\neq i}^{s+1} \frac{\theta_i - \mu_j}{\mu_i - \mu_j}\Bigg)\Bigg(\prod_{j=1,\ j\neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j}\Bigg)$$

based on the proof of Lemma 2.17. The first product in the extended term is actually the value of the ith Lagrange polynomial at θ_i concerning an interpolation problem for $\mu_1, \dots, \mu_{s+1}$, whereas the second product concerns an interpolation problem for $\theta_1, \dots, \theta_s$.

The central part of the derivation of this extension is solving a generalized form of the system (2.49). Since the result of this part can be reused in Chapter 5 concerning block-Krylov subspace iterations, we explicitly formulate it in the following lemma where the subspaces $\mathcal{V}$ and $\mathcal{W}$ correspond to span$\{u_1, \dots, u_s\}$ and span$\{u_1, \dots, u_s, z_i\}$ for orthonormal Ritz vectors $u_1, \dots, u_s$ and a normalized eigenvector z_i.

Lemma 3.9. *Consider a symmetric matrix $H \in \mathbb{R}^{n\times n}$ and arbitrary subspaces $\mathcal{V} \subseteq \mathcal{W} \subseteq \mathbb{R}^n$ with $\dim \mathcal{V} = s \geq 2$ and $\dim \mathcal{W} = s + 1$. Let $\xi_1 \geq \cdots \geq \xi_s$ and $\varphi_1 \geq \cdots \geq \varphi_{s+1}$ be the Ritz values of H in $\mathcal{V}$ and in $\mathcal{W}$, respectively. If these Ritz values are distinct, then the associated orthonormal Ritz vectors $v_1, \dots, v_s$ and $w_1, \dots, w_{s+1}$ are unique up to sign, and*

$$(w_t^T v_l)^2 = \left(\prod_{j=1,\ j\neq t}^{s+1} \frac{\xi_l - \varphi_j}{\varphi_t - \varphi_j}\right)\left(\prod_{j=1,\ j\neq l}^{s} \frac{\varphi_t - \xi_j}{\xi_l - \xi_j}\right) \tag{3.41}$$

holds for each $t \in \{1, \dots, s+1\}$ and each $l \in \{1, \dots, s\}$.

Proof. For each distinct Ritz value, all associated Ritz vectors are collinear. Thus only two normalized Ritz vectors exist, and have different signs. Consequently, the squared values $\big(w_t^T v_l\big)^2$ are unique.

In order to determine $\big(w_t^T v_l\big)^2$ in terms of Ritz values, we denote $w_t^T v_l$ by $\psi_{t,l}$ concerning the expansions $v_l = \sum_{t=1}^{s+1} \psi_{t,l}\, w_t$, $l = 1, \dots, s$. Then, by using the properties $w_d^T w_t = \delta_{d,t}$ and $w_d^T H w_t = \varphi_t \delta_{d,t}$ with Kronecker delta, the properties

$$\begin{aligned} &v_c^T v_l = 0, \quad v_c^T H v_l = 0 \qquad \text{for} \quad c, l \in \{1, \dots, s\} \ \text{ with } \ c < l, \\ &v_l^T v_l = 1, \quad v_l^T H v_l = \xi_l \qquad \text{for} \quad l \in \{1, \dots, s\} \end{aligned}$$

can be rewritten as

$$\begin{aligned} &\textstyle\sum_{t=1}^{s+1} \psi_{t,c}\, \psi_{t,l} = 0, \qquad \sum_{t=1}^{s+1} \varphi_t\, \psi_{t,c}\, \psi_{t,l} = 0 \qquad \text{for} \quad c, l \in \{1, \dots, s\} \ \text{ with } \ c < l, \\ &\textstyle\sum_{t=1}^{s+1} \psi_{t,l}^2 = 1, \qquad \sum_{t=1}^{s+1} \varphi_t\, \psi_{t,l}^2 = \xi_l \qquad \text{for} \quad l \in \{1, \dots, s\}. \end{aligned} \tag{3.42}$$

This is a nonlinear system of $s(s-1) + 2s = s(s+1)$ equations for $s(s+1)$ ψ-terms. The solution is unique up to sign since the squared values $\psi_{t,l}^2 = \big(w_t^T v_l\big)^2$ are unique. Thus we only need to show that this nonlinear system is fulfilled by certain ψ-terms stemming from (3.41). For instance, we set

$$\psi_{t,l} = \sigma_{t,l} \left(\prod_{j=1,\ j\neq t}^{s+1} \frac{\xi_l - \varphi_j}{\varphi_t - \varphi_j}\right)^{1/2} \left(\prod_{j=1,\ j\neq l}^{s} \frac{\varphi_t - \xi_j}{\xi_l - \xi_j}\right)^{1/2} \tag{3.43}$$

with $\sigma_{t,l} = -1$ for $2 \leq t \leq l$ and otherwise $\sigma_{t,l} = 1$. Then (3.43) can be shown to fulfill (3.42) as follows.

We begin with the first two types of equations in (3.42) and reformulate them as

$$\textstyle\sum_{t=2}^{s+1} (\varphi_1 - \varphi_t)\, \psi_{t,c}\, \psi_{t,l} = 0, \qquad \sum_{t=1}^{s} (\varphi_t - \varphi_{s+1})\, \psi_{t,c}\, \psi_{t,l} = 0$$

by using row reduction. This results in

$$\begin{aligned} &\textstyle\sum_{t=2}^{s+1} \operatorname{sign}(\psi_{t,c}\,\psi_{t,l})\sqrt{(\varphi_1-\varphi_t)^2\,\psi_{t,c}^2\,\psi_{t,l}^2} = 0,\\ &\textstyle\sum_{t=1}^{s} \operatorname{sign}(\psi_{t,c}\,\psi_{t,l})\sqrt{(\varphi_t-\varphi_{s+1})^2\,\psi_{t,c}^2\,\psi_{t,l}^2} = 0 \end{aligned} \tag{3.44}$$

by using the fact that the terms $\varphi_1 - \varphi_t$ and $\varphi_t - \varphi_{s+1}$ are positive. Then we verify that (3.44) is fulfilled by (3.43). Beginning with

$$\begin{aligned} \psi_{t,c}^2\,\psi_{t,l}^2 &= \left(\prod_{j=1,\ j\neq t}^{s+1}\frac{\xi_c-\varphi_j}{\varphi_t-\varphi_j}\right)\left(\prod_{j=1,\ j\neq c}^{s}\frac{\varphi_t-\xi_j}{\xi_c-\xi_j}\right)\left(\prod_{j=1,\ j\neq t}^{s+1}\frac{\xi_l-\varphi_j}{\varphi_t-\varphi_j}\right)\left(\prod_{j=1,\ j\neq l}^{s}\frac{\varphi_t-\xi_j}{\xi_l-\xi_j}\right)\\ &= \frac{\left(\prod_{j=1,\ j\neq t}^{s+1}(\xi_c-\varphi_j)(\xi_l-\varphi_j)\right)(\varphi_t-\xi_l)(\varphi_t-\xi_c)\left(\prod_{j=1,\ j\neq c,\ j\neq l}^{s}(\varphi_t-\xi_j)^2\right)}{\left(\prod_{j=1,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)^2\right)\left(\prod_{j=1,\ j\neq c}^{s}(\xi_c-\xi_j)\right)\left(\prod_{j=1,\ j\neq l}^{s}(\xi_l-\xi_j)\right)}\\ &= \frac{\left(\prod_{j=1}^{s+1}(\xi_c-\varphi_j)(\xi_l-\varphi_j)\right)\left(\prod_{j=1,\ j\neq c,\ j\neq l}^{s}(\varphi_t-\xi_j)^2\right)}{\left(\prod_{j=1,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)^2\right)\left(\prod_{j=1,\ j\neq c}^{s}(\xi_c-\xi_j)\right)\left(\prod_{j=1,\ j\neq l}^{s}(\xi_l-\xi_j)\right)}, \end{aligned}$$

we get

$$\begin{aligned} (\varphi_1-\varphi_t)^2\,\psi_{t,c}^2\,\psi_{t,l}^2 &= \eta_{c,l}\left(\frac{p_{c,l}(\varphi_t)}{\prod_{j=2,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)}\right)^2,\\ (\varphi_t-\varphi_{s+1})^2\,\psi_{t,c}^2\,\psi_{t,l}^2 &= \eta_{c,l}\left(\frac{p_{c,l}(\varphi_t)}{\prod_{j=1,\ j\neq t}^{s}(\varphi_t-\varphi_j)}\right)^2 \end{aligned} \tag{3.45}$$

with a parameter $\eta_{c,l}$ and a polynomial $p_{c,l}(\cdot)$ defined by

$$\eta_{c,l} = \frac{\left(\prod_{j=1}^{s+1}(\xi_c-\varphi_j)(\xi_l-\varphi_j)\right)}{\left(\prod_{j=1,\ j\neq c}^{s}(\xi_c-\xi_j)\right)\left(\prod_{j=1,\ j\neq l}^{s}(\xi_l-\xi_j)\right)}, \qquad p_{c,l}(\alpha) = \textstyle\prod_{j=1,\ j\neq c,\ j\neq l}^{s}(\alpha-\xi_j).$$

Therein $\eta_{c,l}$ is independent of the index t. Moreover, if $\eta_{c,l}$ is nonzero, then the above representation of $\eta_{c,l}$ contains exactly $c+l+(c-1)+(l-1) = 2(c+l-1)$ negative factors according to the Courant-Fischer principles and the relation $\xi_1 > \cdots > \xi_s$. Thus $\eta_{c,l}$ is either zero or positive. In contrast, the signs of the other factors in (3.45) depend on t, namely, if $p_{c,l}(\varphi_t) \neq 0$, then

$$\frac{p_{c,l}(\varphi_t)}{\prod_{j=2,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)} = \frac{\prod_{j=1,\ j\neq c,\ j\neq l}^{s}(\varphi_t-\xi_j)}{\prod_{j=2,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)} \begin{cases} <0 & \text{for } t\leq c,\\ >0 & \text{for } t\in(c,l],\\ <0 & \text{for } t>l, \end{cases}$$

$$\frac{p_{c,l}(\varphi_t)}{\prod_{j=1,\ j\neq t}^{s}(\varphi_t-\varphi_j)} = \frac{\prod_{j=1,\ j\neq c,\ j\neq l}^{s}(\varphi_t-\xi_j)}{\prod_{j=1,\ j\neq t}^{s}(\varphi_t-\varphi_j)} \begin{cases} >0 & \text{for } t\leq c,\\ <0 & \text{for } t\in(c,l],\\ >0 & \text{for } t>l. \end{cases}$$

In addition, the definition of the σ-terms shows that

$$\operatorname{sign}(\psi_{t,c}\,\psi_{t,l}) = \sigma_{t,c}\sigma_{t,l} \begin{cases} >0 & \text{for } t\leq c,\\ <0 & \text{for } t\in(c,l],\\ >0 & \text{for } t>l. \end{cases}$$

Summarizing the above, we get

$$\begin{aligned} \textstyle\sum_{t=2}^{s+1} \operatorname{sign}(\psi_{t,c}\,\psi_{t,l})\sqrt{(\varphi_1-\varphi_t)^2\,\psi_{t,c}^2\,\psi_{t,l}^2} &= -\sqrt{\eta_{c,l}}\;\textstyle\sum_{t=2}^{s+1} \dfrac{p_{c,l}(\varphi_t)}{\prod_{j=2,\ j\neq t}^{s+1}(\varphi_t-\varphi_j)}, \\ \textstyle\sum_{t=1}^{s} \operatorname{sign}(\psi_{t,c}\,\psi_{t,l})\sqrt{(\varphi_t-\varphi_{s+1})^2\,\psi_{t,c}^2\,\psi_{t,l}^2} &= \sqrt{\eta_{c,l}}\;\textstyle\sum_{t=1}^{s} \dfrac{p_{c,l}(\varphi_t)}{\prod_{j=1,\ j\neq t}^{s}(\varphi_t-\varphi_j)}. \end{aligned} \tag{3.46}$$

In (3.46), the sums on the right-hand sides can be shown to be zero. For a better readability, we show this property afterwards by Lemma 3.10. Then (3.46) results in (3.44) so that the first two types of equations in (3.42) are verified.

Next, we verify the remaining types of equations in (3.42) by using two series of Lagrange polynomials $q_t(\cdot)$ and $\widetilde{q}_l(\cdot)$ defined by

$$q_t(\xi) = \prod_{j=1,\ j\neq t}^{s+1} \frac{\xi-\varphi_j}{\varphi_t-\varphi_j} \qquad \text{and} \qquad \widetilde{q}_l(\varphi) = \prod_{j=1,\ j\neq l}^{s} \frac{\varphi-\xi_j}{\xi_l-\xi_j}.$$

Since the polynomial $\widetilde{q}_l(\cdot)$ has degree $s-1$ and trivially interpolates the $s+1$ pairs $\big(\varphi_t,\,\widetilde{q}_l(\varphi_t)\big)$, $t=1,\dots,s+1$, it coincides with the interpolating polynomial $\sum_{t=1}^{s+1}\widetilde{q}_l(\varphi_t)\,q_t(\cdot)$. Thus

$$\begin{aligned} \sum_{t=1}^{s+1}\psi_{t,l}^2 &= \sum_{t=1}^{s+1}\left(\prod_{j=1,\ j\neq t}^{s+1}\frac{\xi_l-\varphi_j}{\varphi_t-\varphi_j}\right)\left(\prod_{j=1,\ j\neq l}^{s}\frac{\varphi_t-\xi_j}{\xi_l-\xi_j}\right) \\ &= \sum_{t=1}^{s+1} q_t(\xi_l)\,\widetilde{q}_l(\varphi_t) = \sum_{t=1}^{s+1}\widetilde{q}_l(\varphi_t)\,q_t(\xi)\Big|_{\xi=\xi_l} = \widetilde{q}_l(\xi_l) = 1. \end{aligned}$$

Furthermore, the polynomial $\widehat{q}_l(\cdot)$ defined by $\widehat{q}_l(\varphi) = \varphi\,\widetilde{q}_l(\varphi)$ has degree s and trivially interpolates the $s+1$ pairs $\big(\varphi_t,\,\varphi_t\,\widetilde{q}_l(\varphi_t)\big)$, $t=1,\dots,s+1$. Thus it coincides with the interpolating polynomial $\sum_{t=1}^{s+1}\varphi_t\,\widetilde{q}_l(\varphi_t)\,q_t(\cdot)$ so that

$$\begin{aligned} \sum_{t=1}^{s+1}\varphi_t\,\psi_{t,l}^2 &= \sum_{t=1}^{s+1}\varphi_t\left(\prod_{j=1,\ j\neq t}^{s+1}\frac{\xi_l-\varphi_j}{\varphi_t-\varphi_j}\right)\left(\prod_{j=1,\ j\neq l}^{s}\frac{\varphi_t-\xi_j}{\xi_l-\xi_j}\right) \\ &= \sum_{t=1}^{s+1}\varphi_t\,q_t(\xi_l)\,\widetilde{q}_l(\varphi_t) = \sum_{t=1}^{s+1}\varphi_t\,\widetilde{q}_l(\varphi_t)\,q_t(\xi)\Big|_{\xi=\xi_l} = \widehat{q}_l(\xi_l) = \xi_l\,\widetilde{q}_l(\xi_l) = \xi_l. \end{aligned}$$

In summary, (3.43) fulfills (3.42) so that the corresponding squared values result in (3.41). □

Additionally, we formulate the omitted part of the above proof concerning the representation (3.46). The property that the sums on the right-hand sides in (3.46) are zero can be shown in the following more general form.

Lemma 3.10. *Let $\alpha_1,\dots,\alpha_k\in\mathbb{R}$ be pairwise different, and let $p(\cdot)$ be an arbitrary real polynomial of degree $k-2$. Then it holds that*

$$\sum_{i=1}^{k}\frac{p(\alpha_i)}{\prod_{j=1,\ j\neq i}^{k}(\alpha_i-\alpha_j)} = 0. \tag{3.47}$$

Proof. We first consider the case $k=2$. Therein $p(\cdot)$ is a constant function so that $p(\alpha_1)=p(\alpha_2)$, and $p(\alpha_1)/(\alpha_1-\alpha_2) + p(\alpha_2)/(\alpha_2-\alpha_1) = 0$ holds trivially.

In the nontrivial case $k \geq 3$, we represent $p(\cdot)$ by $p(\alpha) = \sum_{s=0}^{k-2} \eta_s \alpha^s$ and prove (3.47) by verifying the property

$$\sum_{i=1}^{k} \frac{\alpha_i^s}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} = 0 \qquad \forall\ s \in \{0, \ldots, k-2\}. \tag{3.48}$$

We apply the Lagrange polynomials $l_1(\cdot), \ldots, l_k(\cdot)$ concerning an interpolation problem for $\alpha_1, \ldots, \alpha_k$, namely,

$$l_i(\alpha) = \prod_{j=1,\ j\neq i}^{k} \frac{\alpha - \alpha_j}{\alpha_i - \alpha_j} = \frac{\alpha^{k-1} - \left(\sum_{j=1,\ j\neq i}^{k} \alpha_j\right) \alpha^{k-2} + q_i(\alpha)}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)}, \qquad i = 1, \ldots, k$$

where $q_i(\cdot)$ is a corresponding real polynomial whose degree is not larger than $k-3$.

We verify the property (3.48) for $s = 0$ by using the $(k-1)$ th derivative of $l_i(\cdot)$, i.e.,

$$l_i^{(k-1)}(\alpha) = \frac{(k-1)!}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)}.$$

In addition, since $\sum_{i=1}^{k} l_i(\cdot)$ is a constant function with the value 1, it holds that

$$\sum_{i=1}^{k} l_i^{(k-1)}(\alpha) = \left(\sum_{i=1}^{k} l_i\right)^{(k-1)}(\alpha) = \frac{d^{\,k-1}}{d\,\alpha^{k-1}}\, 1 = 0.$$

Then (3.48) for $s = 0$ is verified as follows.

$$\sum_{i=1}^{k} \frac{\alpha_i^0}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} = \frac{1}{(k-1)!} \sum_{i=1}^{k} \frac{(k-1)!}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} = \frac{1}{(k-1)!} \sum_{i=1}^{k} l_i^{(k-1)}(\alpha) = 0.$$

In order to verify (3.48) for $s \in \{1, \ldots, k-2\}$, we use the $(k-2)$ th derivative of $l_i(\cdot)$, i.e.,

$$l_i^{(k-2)}(\alpha) = \frac{(k-1)!\,\alpha - (k-2)!\left(\sum_{j=1,\ j\neq i}^{k} \alpha_j\right)}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)}. \tag{3.49}$$

Moreover, the polynomial $\sum_{i=1}^{k} \alpha_i^{s-1} l_i(\cdot)$ interpolates the pairs $\left(\alpha_i,\, \alpha_i^{s-1}\right)$. The uniqueness of interpolating polynomial implies $\sum_{i=1}^{k} \alpha_i^{s-1} l_i(\alpha) = \alpha^{s-1}$ since the monomial α^{s-1} interpolates the same pairs and has degree $s-1 \leq k-3 < k-1$. Thus

$$\sum_{i=1}^{k} \alpha_i^{s-1} l_i^{(k-2)}(\alpha) = \left(\sum_{i=1}^{k} \alpha_i^{s-1} l_i\right)^{(k-2)}(\alpha) = \frac{d^{\,k-2}}{d\,\alpha^{k-2}}\, \alpha^{s-1} = 0. \tag{3.50}$$

Next, applying the representation (3.49) to $\widetilde{\alpha} = \left(\sum_{j=1}^{k} \alpha_j\right)/(k-1)$ yields

$$l_i^{(k-2)}(\widetilde{\alpha}) \overset{(3.49)}{=} \frac{(k-2)!\left(\sum_{j=1}^{k} \alpha_j\right) - (k-2)!\left(\sum_{j=1,\ j\neq i}^{k} \alpha_j\right)}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} = \frac{(k-2)!\,\alpha_i}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)}$$

so that

$$\begin{aligned} \sum_{i=1}^{k} \frac{\alpha_i^s}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} &= \frac{1}{(k-2)!} \sum_{i=1}^{k} \frac{\alpha_i^{s-1} (k-2)!\,\alpha_i}{\prod_{j=1,\ j\neq i}^{k} (\alpha_i - \alpha_j)} \\ &= \frac{1}{(k-2)!} \sum_{i=1}^{k} \alpha_i^{s-1} l_i^{(k-2)}(\widetilde{\alpha}) \overset{(3.50)}{=} 0. \end{aligned}$$

This completes the verification of the property (3.48). □

Applying Lemma 3.10 to $\varphi_2, \ldots, \varphi_{s+1}$ or $\varphi_1, \ldots, \varphi_s$ together with the polynomial $p_{c,l}(\cdot)$ of degree $s-2$ shows that the sums on the right-hand sides in (3.46) are zero.

Now we return to the analysis of the Ritz vectors in a Krylov subspace, and refine the estimates (2.11), (2.14) by applying Lemma 3.9.

Theorem 3.11. *With Notation 1.4, consider a Krylov subspace* $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ *with the initial vector* $y \in \mathbb{R}^n \backslash \{0\}$*, and let* $u_1, \ldots, u_s$ *be orthonormal Ritz vectors of* H *in* $\mathcal{K}$ *associated with the s largest Ritz values* $\theta_1 \geq \cdots \geq \theta_s$*. If* $\theta_j > \mu_{j+1}$ *for each* $j \in \{1, \ldots, s\}$*, then the eigenprojection* $Q_i y$ *is nonzero for each* $i \in \{1, \ldots, s\}$*, and* $\theta_1, \ldots, \theta_s$ *are distinct. Moreover, it holds, in terms of the normalized eigenprojection* $z_i = Q_i y / \|Q_i y\|_2$*, that*

$$\sin^2 \angle_2(u_i, z_i) \leq 1 - \left(\prod_{j=1,\ j \neq i}^{s+1} \frac{\theta_i - \mu_j}{\mu_i - \mu_j} \right) \left(\prod_{j=1,\ j \neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j} \right). \tag{3.51}$$

Proof. We show the property $Q_i y \neq 0$ for $i \in \{1, \ldots, s\}$ inductively by using the Courant-Fischer principles. If $Q_1 y = 0$, then $\mathcal{K}$ is a subset of $\mathcal{Z}_2 \oplus \cdots \oplus \mathcal{Z}_m$ so that $\theta_1 \leq \mu_2$. This contradicts the assumption $\theta_j > \mu_{j+1}$ for $j=1$. Therefore $Q_1 y \neq 0$ holds. In the further induction steps, the condition $Q_l y \neq 0 \ \ \forall\, l < i$ implies $Q_i y \neq 0$ since otherwise $\mathcal{K}$ is a subset of $\operatorname{span}\{Q_1 y, \ldots, Q_{i-1} y\} \oplus \mathcal{Z}_{i+1} \oplus \cdots \oplus \mathcal{Z}_m$ so that $\theta_i \leq \mu_{i+1}$ which contradicts the assumption $\theta_j > \mu_{j+1}$ for $j=i$. Based on the property $Q_i y \neq 0$, we can define $z_i = Q_i y / \|Q_i y\|_2$ for each $i \in \{1, \ldots, s\}$. Then $\mathcal{K}$ is a subset of $\mathcal{Y} \oplus \widetilde{\mathcal{Y}}$ with

$$\mathcal{Y} = \operatorname{span}\{z_1, \ldots, z_s\} \qquad \text{and} \qquad \widetilde{\mathcal{Y}} = \operatorname{span}\{Q_{s+1} y, \ldots, Q_m y\},$$

and the relation $\mu_j \geq \theta_j$ holds for each $j \in \{1, \ldots, s\}$ according to the Courant-Fischer principles. Combining this with the assumption $\theta_j > \mu_{j+1}$ yields

$$\mu_1 \geq \theta_1 > \mu_2 \geq \theta_2 > \cdots > \mu_s \geq \theta_s > \mu_{s+1} \tag{3.52}$$

so that $\theta_1, \ldots, \theta_s$ are distinct.

For deriving the estimate (3.51), we use the auxiliary subspaces

$$\mathcal{U} = \operatorname{span}\{u_1, \ldots, u_s\} \qquad \text{and} \qquad \mathcal{W} = \operatorname{span}\{u_1, \ldots, u_s, z_i\} = \mathcal{U} + \operatorname{span}\{z_i\}.$$

Evidently, the orthonormal Ritz vectors $u_1, \ldots, u_s$ in $\mathcal{K}$ are also Ritz vectors in $\mathcal{U}$, and $\theta_1, \ldots, \theta_s$ are the corresponding Ritz values. Thus $\mathcal{U}$ has dimension s, and $\mathcal{W}$ has dimension s or $s+1$.

If $\dim \mathcal{W} = s$, the eigenvector z_i belongs to $\mathcal{U}$ and is a Ritz vector in $\mathcal{U}$. Since the Ritz values $\theta_1, \ldots, \theta_s$ are distinct, the associated Ritz vectors belong to $\operatorname{span}\{u_1\}, \ldots, \operatorname{span}\{u_s\}$, respectively. Thus z_i belongs to $\operatorname{span}\{u_j\}$ for a certain $j \in \{1, \ldots, s\}$ so that $\mu_i = \mu(z_i) = \mu(u_j) = \theta_j \in \{\theta_1, \ldots, \theta_s\}$. Moreover, according to (3.52), μ_i is located in $[\theta_1, \infty)$ for $i=1$ and in $[\theta_i, \theta_{i-1})$ for $i \in \{2, \ldots, s\}$. Therefore $\mu_i = \theta_i$ holds, and z_i belongs to $\operatorname{span}\{u_i\}$. Then u_i and z_i are collinear nonzero vectors so that $\sin^2 \angle_2(u_i, z_i) = 0$. In addition, the bound in (3.51) is equal to 0 for $\mu_i = \theta_i$. Thus (3.51) holds trivially.

If $\dim \mathcal{W} = s+1$, we can denote the Ritz values in $\mathcal{W}$ by $\varphi_1 \geq \cdots \geq \varphi_{s+1}$. Then, according to

$$\mathcal{U} \ \subseteq \ \mathcal{W} \ = \ \mathcal{U} + \operatorname{span}\{z_i\} \ \subseteq \ \mathcal{K} + \operatorname{span}\{z_i\} \ \subseteq \ \mathcal{Y} \oplus \widetilde{\mathcal{Y}} + \operatorname{span}\{z_i\} \ = \ \mathcal{Y} \oplus \widetilde{\mathcal{Y}}$$

and the Courant-Fischer principles, it holds that

$$\mu_j \geq \varphi_j \geq \theta_j \quad \forall\, j \in \{1, \ldots, s\}, \qquad \text{and} \qquad \mu_{s+1} \geq \max_{\widetilde{y} \in \widetilde{\mathcal{Y}} \backslash \{0\}} \mu(\widetilde{y}) \geq \varphi_{s+1}.$$

Combining this with the assumption $\theta_j > \mu_{j+1}$ yields

$$\mu_j \geq \varphi_j \geq \theta_j > \mu_{j+1} \geq \varphi_{j+1} \qquad \forall\, j \in \{1, \ldots, s\} \tag{3.53}$$

so that $\varphi_1, \ldots, \varphi_{s+1}$ are distinct. Subsequently, the eigenvector z_i belongs to $\mathcal{W}$ and is a Ritz vector in $\mathcal{W}$. Thus the corresponding Ritz value $\mu_i = \mu(z_i)$ is contained in $\{\varphi_1, \ldots, \varphi_{s+1}\}$. In addition, the relation (3.53) shows that μ_i is located in $[\varphi_1, \infty)$ for $i=1$ and in $[\varphi_i, \varphi_{i-1})$ for $i \in \{2, \ldots, s+1\}$. Therefore $\mu_i = \varphi_i$ holds. Correspondingly, z_i can be denoted by w_i within the basis $\{w_1, \ldots, w_{s+1}\}$ consisting of orthonormal Ritz vectors associated with $\varphi_1, \ldots, \varphi_{s+1}$. Then $\sin^2 \angle_2(u_i, z_i)$ is equal to $\sin^2 \angle_2(u_i, w_i)$ and $\sin^2 \angle_2(w_i, u_i)$. By using the expansions

$$u_l = \textstyle\sum_{t=1}^{s+1} \psi_{t,l}\, w_t, \qquad l = 1, \ldots, s$$

with the coefficients $\psi_{t,l} = w_t^T u_l \in \mathbb{R}$, it holds that

$$\sin^2 \angle_2(u_i, z_i) = 1 - \cos^2 \angle_2(w_i, u_i) \overset{(1.31)}{=} 1 - \left(\frac{w_i^T u_i}{\|w_i\|_2\, \|u_i\|_2} \right)^2 = 1 - \psi_{i,i}^2. \tag{3.54}$$

Moreover, since the concerned Ritz values are distinct, Lemma 3.9 is applicable to $\mathcal{V} = \mathcal{U}$ and $\mathcal{W}$ so that (3.41) for $\xi = \theta$ and $t = l = i$ implies

$$\psi_{i,i}^2 = (w_i^T u_i)^2 = \left(\prod_{j=1,\ j \neq i}^{s+1} \frac{\theta_i - \varphi_j}{\varphi_i - \varphi_j} \right) \left(\prod_{j=1,\ j \neq i}^{s} \frac{\varphi_i - \theta_j}{\theta_i - \theta_j} \right).$$

Then, by using (3.53) and $\mu_i = \varphi_i$, we get

$$\begin{aligned} \psi_{i,i}^2 &= \left(\prod_{j=1}^{i-1} \frac{\varphi_j - \theta_i}{\varphi_j - \mu_i} \right) \left(\prod_{j=i+1}^{s+1} \frac{\theta_i - \varphi_j}{\mu_i - \varphi_j} \right) \left(\prod_{j=1,\ j \neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j} \right) \\ &\geq \left(\prod_{j=1}^{i-1} \frac{\mu_j - \theta_i}{\mu_j - \mu_i} \right) \left(\prod_{j=i+1}^{s+1} \frac{\theta_i - \mu_j}{\mu_i - \mu_j} \right) \left(\prod_{j=1,\ j \neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j} \right) \\ &= \left(\prod_{j=1,\ j \neq i}^{s+1} \frac{\theta_i - \mu_j}{\mu_i - \mu_j} \right) \left(\prod_{j=1,\ j \neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j} \right) \end{aligned}$$

which extends (3.54) as the estimate (3.51). □

The proof of Theorem 3.11 does not use the assumption that $\mathcal{K}$ is not an invariant subspace. Instead, the assumption $\theta_j > \mu_{j+1}$ ensures that the concerned Ritz values are distinct so that Lemma 3.9 is applicable. Alternatively, one can use the slightly weaker assumption $\theta_j \geq \mu_{j+1}$ in order to include the trivial case $\mu_i = \theta_{i-1}$ as in Lemma 2.17 which is a rare case in practice. Moreover, as mentioned in Remark 2.18, the arguments from [34, Subsection 12.6.2] are not suitable for proving Theorem 3.11 since a stronger assumption $\varphi_j > \xi_j = \theta_j$ is required and the considered Ritz vectors are nonnormalized.

3.3 Numerical comparisons

We demonstrate the benefit of our new estimates by several numerical examples. Similarly as in the works [98, 112, 105, 61, 121], we use diagonal matrices as test-matrices. There is no loss of generality since the estimates are invariant under a transformation with proper orthonormal eigenvectors. Nevertheless, more practical examples are presented afterwards in Chapter 7 concerning generalized matrix eigenvalue problems arising from the finite element discretization of an elliptic operator.

3.3.1 Improvements

We first compare our estimates from Subsections 3.2.1 and 3.2.2 with the corresponding available estimates from Section 3.1, and discuss the observed improvements. Therein the following two test-matrices are used.

Test-matrix 1

We consider the eigenvalue problem of the negative Laplacian operator $-\Delta$ on the domain $[0, 6\pi]^3$ with homogeneous Dirichlet boundary conditions, and set the reciprocals of its eigenvalues

$$\lambda_{i_1} + \lambda_{i_2} + \lambda_{i_3} \qquad \text{with} \qquad \lambda_{i_1}, \lambda_{i_2}, \lambda_{i_3} \in \left\{ \left(\tfrac{1}{6}\right)^2, \left(\tfrac{2}{6}\right)^2, \ldots, \left(\tfrac{20}{6}\right)^2 \right\}$$

in descending order as diagonal entries of a diagonal matrix $H \in \mathbb{R}^{n \times n}$ with $n = 8000$, i.e., the inverse of H corresponds to a restriction of $-\Delta$ with respect to the eigenfunctions associated with the above eigenvalues. The 5 largest distinct eigenvalues of H are well separated, namely,

$$\mu_1 = 12, \qquad \mu_2 = 6, \qquad \mu_3 = 4, \qquad \mu_4 = 3.\overline{27}, \qquad \mu_5 = 3,$$

and the smallest distinct eigenvalue reads $\mu_{694} = 0.03$. Concerning the settings of Theorem 3.2, we set $c = 4$ for those estimates with the Chebyshev polynomial $T_{k-c}(\cdot)$.

Test-matrix 2

The multiplicity of the eigenvalues of an elliptic operator can be perturbed by a nonuniform discretization. Based on this fact, we modify the multiple eigenvalues of the underlying negative Laplacian operator for generating Test-matrix 1 by successively adding the perturbation 0.001. For instance, the triple eigenvalue $\lambda = \left(\frac{1}{6}\right)^2 + \left(\frac{1}{6}\right)^2 + \left(\frac{2}{6}\right)^2 = \frac{1}{6}$ is modified as an eigenvalue cluster $\{\frac{1}{6}, \frac{1}{6} + 0.001, \frac{1}{6} + 0.002\}$. Subsequently, the reciprocals of the modified eigenvalues are set in descending order as diagonal entries of a diagonal matrix $H \in \mathbb{R}^{n \times n}$ with $n = 8000$. All eigenvalues of this H are simple. The 5 largest eigenvalues and the smallest eigenvalue read

$$\mu_1 = 12, \qquad \mu_2 = 6, \qquad \mu_3 \approx 5.9642, \qquad \mu_4 \approx 5.9289, \qquad \mu_5 = 4, \qquad \mu_{8000} = 0.03.$$

Since μ_4 is the smallest eigenvalue in the cluster $\{\mu_2, \mu_3, \mu_4\}$ and well separated from μ_5, we set $c = 4$ for those estimates with the Chebyshev polynomial $T_{k-c}(\cdot)$ concerning the settings of Theorem 3.2.

Our numerical tests are divided according to the types of estimates.

Estimates on approximate eigenvectors

The estimates (3.13) and (3.14) from Subsection 3.2.1 are directly comparable with Saad's refined estimates (3.2) and (3.3). In particular, the bound in (3.13) cannot exceed the bound in (3.2) since the relation $\widehat{y} = \left(\prod_{j=1}^{i-1}(H - \mu_j I)\right)\widetilde{y}$ results in

$$\tan^2 \angle_2(\widehat{y}, \mathcal{Z}) \leq \left(\prod_{j=1}^{i-1} \frac{\mu_j - \mu_m}{\mu_j - \mu_i} \right)^2 \left(\frac{\sin \angle_2(\widetilde{y}, \mathcal{Z})}{\cos \angle_2(\widetilde{y}, z_i)} \right)^2$$

which can be shown based on the proof of (3.13). Moreover, it can be observed that (3.14) significantly improves (3.3) for certain initial vectors y with $\mu(y) \in (\mu_{c+1}, \mu_c)$. Therein we select 1000 pseudorandom vectors as y, and build the corresponding Krylov subspaces $\mathcal{K}$. The numerical maxima of $\tan \angle_2(z_i, \mathcal{K})$ and the computed bounds are documented in tables and figures.

For Test-matrix 1, we increase the dimension of $\mathcal{K}$ up to $k = 15$, and document the associated data for the indices $i \in \{1, 2, 3\}$. In addition, we consider the basic estimate (3.1). The numerical maxima of $\tan\angle_2(z_i, \mathcal{K})$ are documented for each $k \in \{1, \ldots, 15\}$, whereas the computed bounds are documented for $k \geq i$ or $k \geq c = 4$ including the trivial case $k - i = 0$ or $k - c = 0$ (i.e., the associated Chebyshev polynomial is a constant function with the value 1). The data for $k = 15$ are listed in Table 3.1, and drawn together with the data for $k < 15$ in Figure 3.1 (semi-log plot). The following features can be observed in this example.

- The new estimate (3.13) coincides with the refined estimate (3.2) for $i = 1$, and improves it for $i \in \{2, 3\}$. Moreover, both of them improve the basic estimate (3.1). The rate of improvement increases with k due to the relation $\widetilde{\gamma}_i > \gamma_i$ of the corresponding gap ratios.
- The new estimate (3.14) improves the refined estimate (3.3). The improvement is significant for $i = 3$ where (3.14) is slightly less accurate than (3.13) and more accurate than (3.2). The curves for (3.14) and (3.3) are parallel to those for (3.13) and (3.2) so that they provide better bounds than the basic estimate (3.1) for sufficiently large k.

Table 3.1: Comparison between several estimates on approximate eigenvectors for Test-matrix 1 with respect to the numerical maxima NM of $\tan\angle_2(z_i, \mathcal{K})$ and the computed bounds. The associated parameters are set as $c = 4$ and $k = 15$.

i	NM	(3.1)	(3.2)	(3.3)	(3.13)	(3.14)
1	1.24×10^{-13}	2.92×10^{-7}	1.33×10^{-11}	6.98×10^{-10}	1.33×10^{-11}	2.87×10^{-10}
2	5.32×10^{-9}	1.81×10^{-4}	1.00×10^{-6}	4.31×10^{-5}	9.04×10^{-7}	4.24×10^{-6}
3	1.45×10^{-5}	1.58×10^{-1}	1.37×10^{-2}	2.21×10^{-1}	6.33×10^{-3}	6.46×10^{-3}

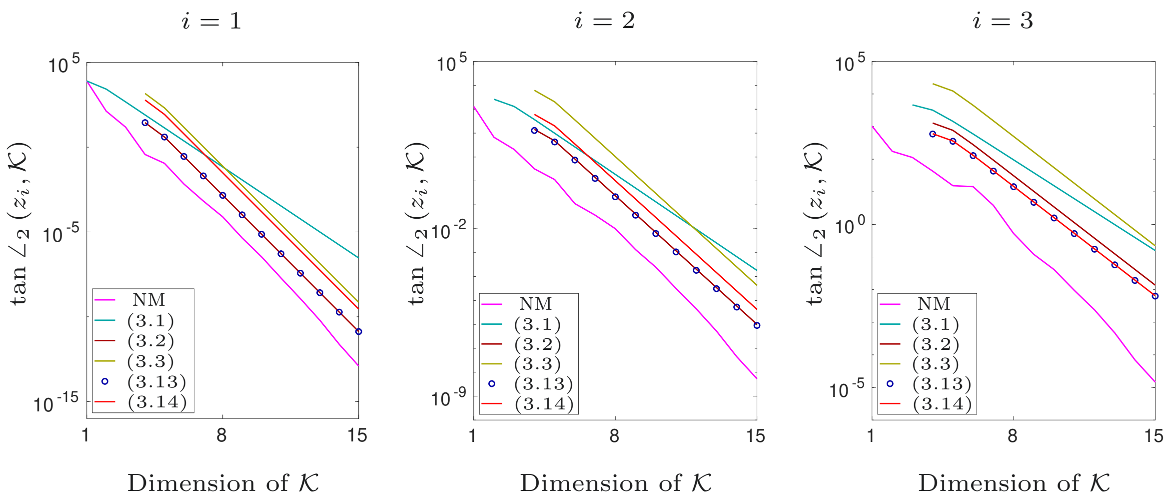

Figure 3.1: More data for the comparison in Table 3.1 with $k \leq 15$.

For Test-matrix 2, we build Krylov subspaces $\mathcal{K}$ up to a higher dimension $k = 18$ since the value $\tan\angle_2(z_i, \mathcal{K})$ decreases slowly for $i \in \{2, 3\}$ corresponding to clustered eigenvalues. The data documentation is similar to that for Test-matrix 1. The results are presented in Table 3.2 and Figure 3.2 together with the following features.

- The basic estimate (3.1) provides better bounds for small k, but cannot reasonably predict the convergence rate of $\tan\angle_2(z_i, \mathcal{K})$ for $i \in \{2, 3\}$ as the gap ratio γ_i is close to 0 due to clustered eigenvalues. In contrast, the curves for the other estimates are nearly parallel to the last part of the curve for $\tan\angle_2(z_i,\mathcal{K})$ so that the convergence rate can be revealed.

- For $i=1$, the new estimate (3.13) coincides with the refined estimate (3.2), whereas (3.14) is much less accurate than the other estimates because of the large differences between the term $\tan\angle_2(\mathcal{K}^c,\mathcal{Z}^c)$ from (3.14) and the trigonometric terms from the other estimates. Nevertheless, these differences are dramatically reduced for $i\in\{2,3\}$ concerning clustered eigenvalues so that (3.14) significantly improves (3.3) and can also overtake (3.2).

Table 3.2: Comparison between several estimates on approximate eigenvectors for Test-matrix 2 with respect to the numerical maxima NM of $\tan\angle_2(z_i,\mathcal{K})$ and the computed bounds. The associated parameters are set as $c=4$ and $k=18$.

i	NM	(3.1)	(3.2)	(3.3)	(3.13)	(3.14)
1	1.21×10^{-14}	2.65×10^{-10}	1.90×10^{-12}	2.93×10^{-11}	1.90×10^{-12}	6.56×10^{-8}
2	8.27×10^{-5}	2.35×10^{2}	3.51×10^{-2}	3.61×10^{-1}	2.84×10^{-2}	5.74×10^{-2}
3	1.65×10^{-4}	3.96×10^{4}	1.73×10^{-1}	7.26×10^{-1}	5.75×10^{-2}	6.64×10^{-2}

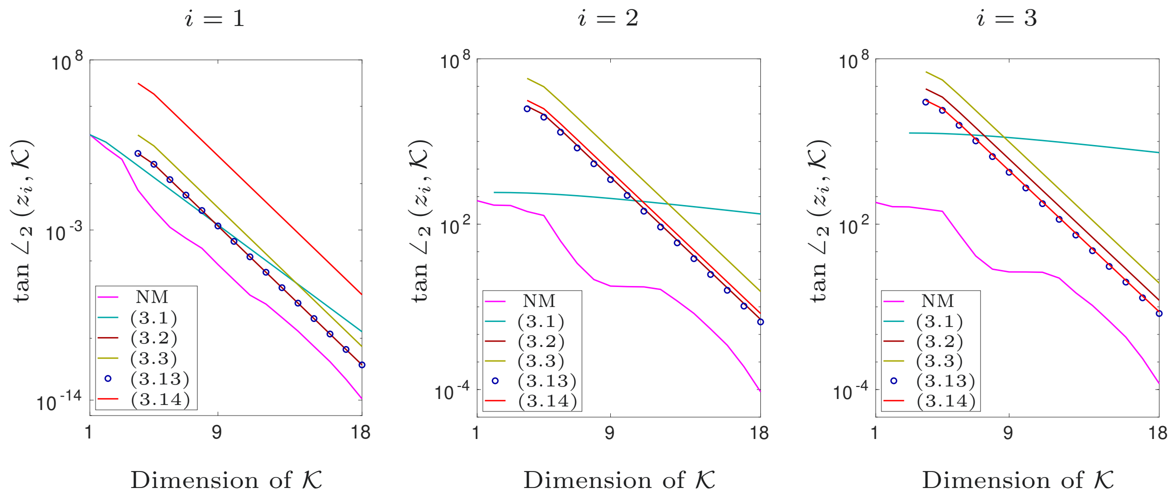

Figure 3.2: More data for the comparison in Table 3.2 with $k\le 18$.

Angle-dependent estimates on Ritz values

We compare the estimates (3.19) and (3.24) from Subsection 3.2.2 with Saad's refined estimates (3.5) and (3.6). Indeed, (3.19) already improves the further refinement of (3.5) in Theorem 3.3 in the sense of

$$\left(\frac{\sin\angle_2(y^c,\mathcal{Z})}{\cos\angle_2(y^c,z_i)}\right)^2\le\left(\prod_{j=1}^{i-1}\frac{\theta_j-\mu_m}{\theta_j-\mu_i}\right)^2\left(\frac{\sin\angle_2(\widetilde{y},\mathcal{Z})}{\cos\angle_2(\widetilde{y},z_i)}\right)^2$$

which can be proved by using the relation $y^c=\left(\prod_{j=1}^{i-1}(H-\theta_jI)\right)\widetilde{y}$; cf. the proof of (3.19). For the reader's convenience, we additionally consider the basic estimate (3.4), and denote by (3.4)*, (3.5)*, (3.6)* the refinements of (3.4), (3.5), (3.6) in Theorem 3.3. As mentioned at the end of Subsection 3.2.2, the estimate (3.24) has the advantage that it provides an a priori bound which is independent of the Ritz values $\theta_1,\ldots,\theta_{i-1}$ in the current Krylov subspace. Moreover, it can significantly improve (3.6)* for certain initial vectors y with $\mu(y) \in (\mu_{c+1}, \mu_c)$. The numerical test uses 1000 pseudorandom initial vectors and the corresponding Krylov subspaces $\mathcal{K}$. We document the numerical maxima of the difference $\mu_i - \theta_i$ and the computed bounds.

For Test-matrix 1, we build $\mathcal{K}$ up to the dimension $k = 14$. The associated data are documented for the indices $i \in \{1, 2, 3\}$. In particular, the numerical maxima of $\mu_1 - \theta_1$ are documented up to $k = 11$ since the value is smaller than 10^{-16} for $k > 11$. For $i \in \{2, 3\}$, the estimate (3.24) is applicable to more dimension numbers than the other estimates which require the assumption $\theta_{i-1} > \mu_i$. The obtained data are given in Table 3.3 and Figure 3.3. In addition, we remark the following features.

- The bounds in the compared estimates have the common form $\zeta/(1+\zeta)$ where ζ denotes certain squared terms containing Chebyshev factors; cf. Theorem 3.3. For small k, these bounds are close to the constant $\mu_i - \mu_m$ which means that ζ is much larger than 1. Thus the estimates with the symbol * improve their basic variants especially for low-dimensional Krylov subspaces.
- The new estimate (3.19) is the most accurate one among the compared estimates, whereas the refinement (3.4)* of the basic estimate (3.4) is much less accurate. Furthermore, the new estimate (3.24) improves the refined estimate (3.6)*. The improvement is significant for $i \in \{2, 3\}$ where (3.24) is only slightly less accurate than (3.19).
- Additionally, the estimates in (3.7) stemming from [105, Theorem 5.1] are indeed less accurate than (3.4)* within the current example as shown in the left subfigure in Figure 3.4. Therein the estimates can only be compared for $i = 1$ since the estimates in (3.7) have not been generalized to arbitrary indices. We note that two estimates in (3.7) are even less accurate than the basic estimate (3.4). Nevertheless, (3.7) can provide better bounds within a model problem from [105] which can be constructed equivalently by setting

$$
\begin{aligned}
&H = \operatorname{diag}(\mu_1, \ldots, \mu_{900}) \quad \text{with} \quad \mu_1 = -0.034, \quad \mu_2 = -0.082, \quad \mu_3 = -0.127, \\
&\quad \mu_4 = -0.155, \quad \mu_5 = -0.190, \quad \mu_i = -0.2 - \frac{i-6}{894} \quad \text{for} \quad i = 6, \ldots, 900, \\
&\quad \text{and} \quad y = (1, \ldots, 1)^T \in \mathbb{R}^{900}.
\end{aligned}
\tag{3.55}
$$

Therein the best bound is provided by (3.7a) for $k < 14$ and by (3.7c) for $k \in [14, 28]$; see the right subfigure in Figure 3.4. The new estimate (3.19) overtakes them for $k > 28$.

Table 3.3: Comparison between several angle-dependent estimates on Ritz values for Test-matrix 1 with respect to the numerical maxima NM of $\mu_i - \theta_i$ and the computed bounds. The associated parameters are set as $c = 4$, $k = 11$ for $i = 1$, and $k = 14$ for $i > 1$. The symbol * denotes the refinement of the concerned estimate in Theorem 3.3.

i	NM	(3.4)*	(3.5)*	(3.6)*	(3.19)	(3.24)
1	4.69×10^{-15}	1.30×10^{-6}	2.92×10^{-12}	8.20×10^{-9}	2.92×10^{-12}	2.53×10^{-9}
2	1.92×10^{-13}	4.76×10^{-5}	3.54×10^{-9}	6.65×10^{-6}	2.86×10^{-9}	6.25×10^{-9}
3	1.66×10^{-8}	5.41×10^{-1}	6.85×10^{-3}	1.23×10^{0}	1.45×10^{-3}	2.54×10^{-3}

For Test-matrix 2, the dimension of $\mathcal{K}$ is increased up to $k = 20$ in order to observe sufficiently small $\mu_i - \theta_i$ for $i \in \{2, 3\}$ where μ_i is located in an eigenvalue cluster. We document the data similarly as for Test-matrix 1. The numerical maxima of $\mu_1 - \theta_1$ subceed 10^{-16} for $k > 12$ and are thus documented up to $k = 12$. We present the results in Table 3.4 and Figure 3.5 together with the following features.

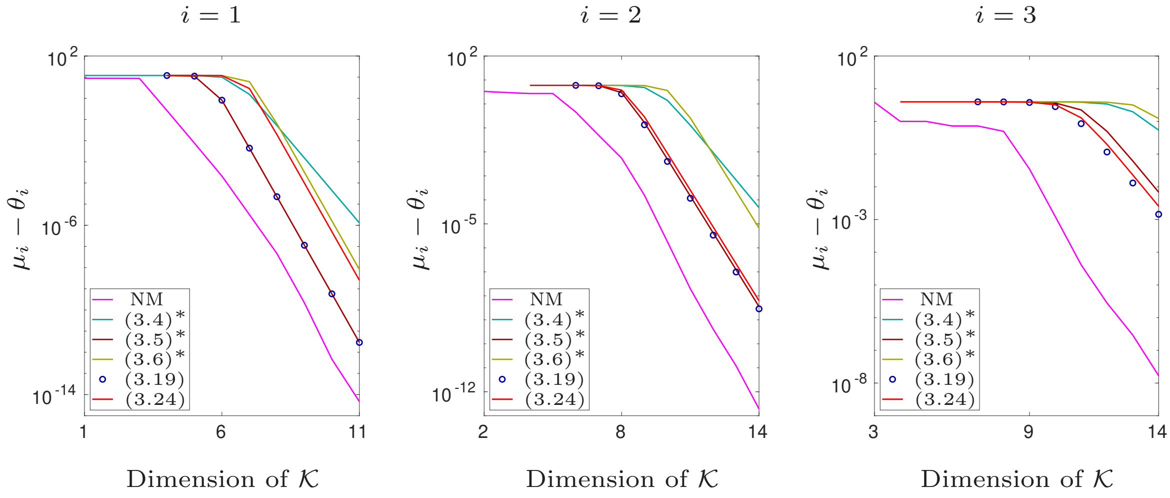

Figure 3.3: More data for the comparison in Table 3.3 with $k \leq 11$ for $i = 1$ and $k \leq 14$ for $i > 1$.

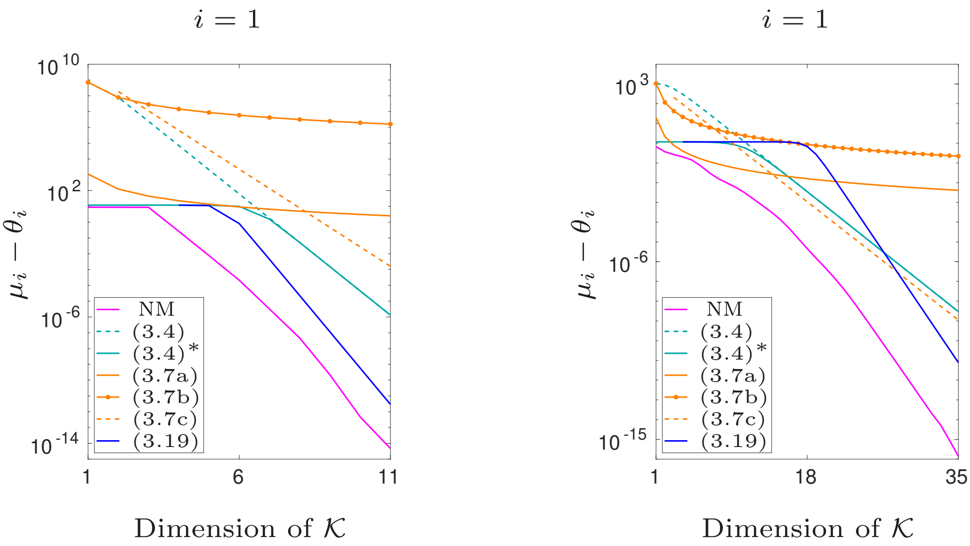

Figure 3.4: Additional comparison between several angle-dependent estimates on Ritz values including the (orange) estimates in (3.7). Left: Comparison for Test-matrix 1. Right: Comparison for the example (3.55).

- The refinement (3.4)* of the basic estimate (3.4) provides the best bound for $i=1$ and $k<9$, but cannot meaningfully describe the reduction of the difference $\mu_i-\theta_i$ for $i\in\{2,\,3\}$. The underlying fact is that the gap ratio γ_i is bounded away from 0 for $i=1$ because of $\mu_1\gg\mu_2$, but close to 0 for $i\in\{2,\,3\}$ as μ_2,μ_3,μ_4 are clustered. The other four estimates in the comparison are suitable for clustered eigenvalues.
- For $i=1$, the new estimate (3.19) and the refined estimate (3.5)* provide the same bound, whereas (3.24) gives a considerable overestimation since the term $\tan\angle_2(\mathcal{K}^c,\mathcal{Z}^c)$ from (3.24) is much larger than the trigonometric terms from the other estimates. However, their differences are moderate for $i\in\{2,\,3\}$ so that (3.24) provides significantly better bounds than (3.6)*. Moreover, (3.19) is more accurate than (3.5)* for $i\in\{2,\,3\}$, and (3.24) overtakes (3.5)* for $i=3$.
- Additionally, the estimates in (3.7) are less accurate than (3.4)* and partially less accurate than (3.4) within the current example; see the left subfigure in Figure 3.6. However, since μ_1 is well separated from μ_2 in the current example, it would be better to consider a further example with $\mu_1\approx\mu_2$. Indeed, a variant of the model problem from [105] corresponding to (3.55) was used in [112], and can be equivalently constructed by setting

$$\begin{aligned} &H=\operatorname{diag}(\mu_1,\dots,\mu_{900}) \quad \text{with} \quad \mu_1=-0.034, \quad \mu_2=-0.0341, \quad \mu_3=-0.082,\\ &\quad \mu_4=-0.127, \quad \mu_5=-0.155, \quad \mu_6=-0.190,\\ &\quad \mu_i=-0.2-\frac{i-7}{893} \quad \text{for} \quad i=7,\dots,900, \quad \text{and} \quad y=(1,\dots,1)^T\in\mathbb{R}^{900}. \end{aligned} \tag{3.56}$$

Within (3.56), the best bound is provided by (3.4)* for $k<3$, by (3.7a) for $k\in[3,35]$, and by (3.19) for $k>35$; see the right subfigure in Figure 3.6. The estimate (3.7c) is not applicable for $k\le 45$ due to the assumption $2k-1\ge\gamma^{-1/2}$.

Table 3.4: Comparison between several angle-dependent estimates on Ritz values for Test-matrix 2 with respect to the numerical maxima NM of $\mu_i-\theta_i$ and the computed bounds. The associated parameters are set as $c=4$, $k=12$ for $i=1$, and $k=20$ for $i>1$. The symbol * denotes the refinement of the concerned estimate in Theorem 3.3.

i	NM	(3.4)*	(3.5)*	(3.6)*	(3.19)	(3.24)
1	2.49×10^{-16}	1.47×10^{-9}	4.59×10^{-11}	1.07×10^{-8}	4.59×10^{-11}	1.78×10^{-1}
2	1.01×10^{-7}	5.97×10^{0}	1.08×10^{-4}	1.12×10^{-2}	7.09×10^{-5}	3.67×10^{-4}
3	5.37×10^{-7}	5.93×10^{0}	3.63×10^{-3}	6.30×10^{-2}	4.07×10^{-4}	5.09×10^{-4}

3.3.2 Supplements

The estimates from Subsections 3.2.3 and 3.2.4 serve to supplement the angle-dependent estimates. More precisely, the angle-free estimates (3.32) and (3.33) can provide better bounds for low-dimensional Krylov subspaces and can be extended concerning restarted Krylov subspace iterations. The additional estimate (3.51) can be combined with those estimates on Ritz values in order to analyze the associated Ritz vectors.

Sharpness of angle-free estimates

The benefit of the angle-free estimates (3.32) and (3.33) can be demonstrated by extending the comparison from [83, Section 2.1]. We use the Test-matrix 1 from Subsection 3.3.1 which has

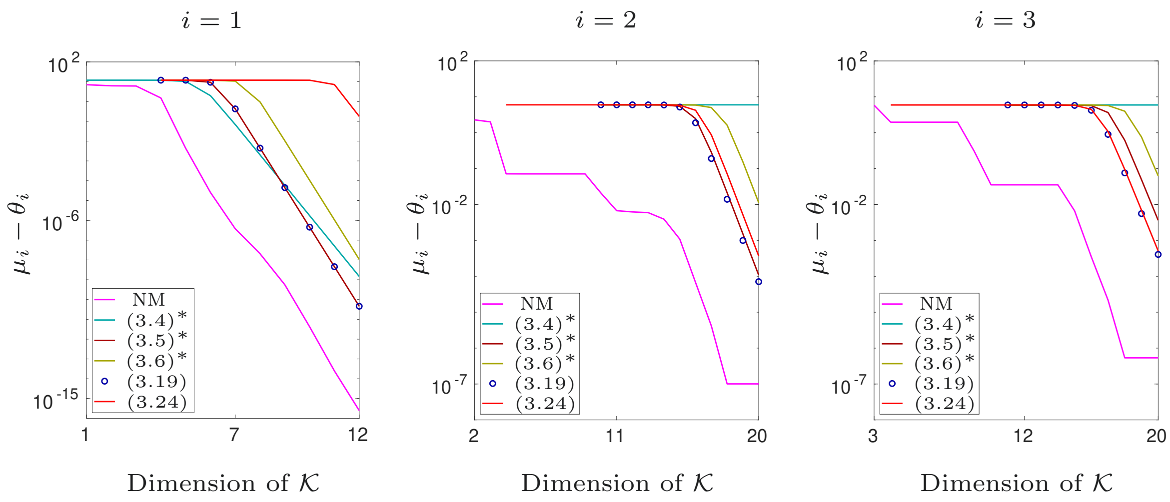

Figure 3.5: More data for the comparison in Table 3.4 with $k \leq 12$ for $i = 1$ and $k \leq 20$ for $i > 1$.

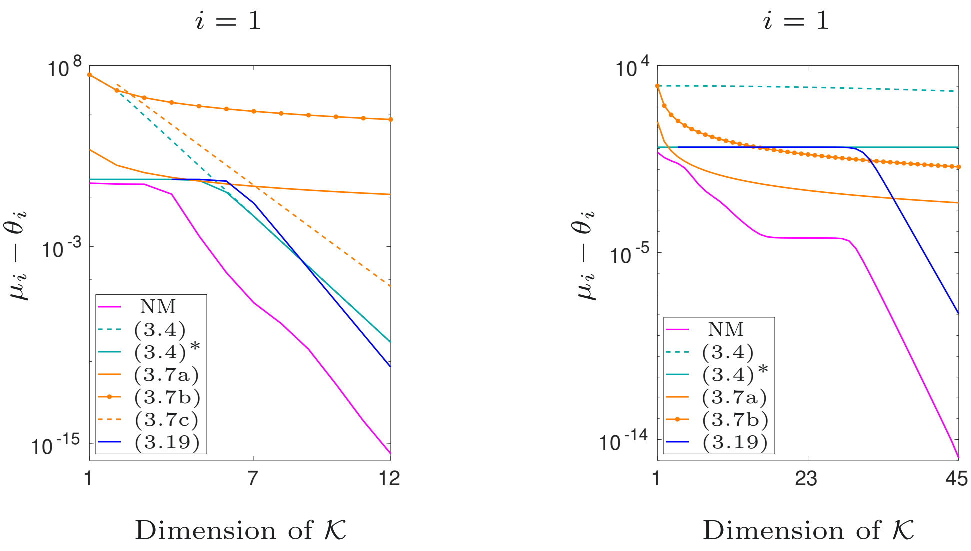

Figure 3.6: Additional comparison between several angle-dependent estimates on Ritz values including the (orange) estimates in (3.7). Left: Comparison for Test-matrix 2. Right: Comparison for the example (3.56).

a similar eigenvalue distribution as the test-matrix from [83]. For a systematic formulation, we regard (3.33) as a special form of (3.32) for $c = i$, and compare (3.32) with the generally most accurate angle-dependent estimate (3.19). We reformulate (3.32) as

$$\left(\frac{\mu_i - \theta_i}{\theta_i - \mu_{c+1}}\right)\left(\frac{\mu_i - \eta}{\eta - \mu_{c+1}}\right)^{-1} \leq [\,T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2}$$

where the bound is independent of the initial vector of the considered Krylov subspace. Thus we can observe the numerical maxima of

$$\left(\frac{\mu_i - \theta_i}{\theta_i - \mu_{c+1}}\right)\left(\frac{\mu_i - \eta}{\eta - \mu_{c+1}}\right)^{-1} \tag{3.57}$$

for sufficiently many sample initial vectors in order to check the sharpness of (3.32). Correspondingly, we determine for each sample initial vector a lower bound $\widetilde{\theta}_i$ of θ_i by the estimate (3.19), and observe the numerical maxima of

$$\left(\frac{\mu_i - \widetilde{\theta}_i}{\widetilde{\theta}_i - \mu_{c+1}}\right)\left(\frac{\mu_i - \eta}{\eta - \mu_{c+1}}\right)^{-1} \tag{3.58}$$

for discussing the sharpness of (3.19) in comparison to (3.32). Therein (3.58) is a variable bound for (3.57), whereas $[\,T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2}$ is a constant bound and denoted by CB.

We first set $i = 1$, $c = 1$, $k = 3$. Similarly as in [83, Section 2.1], we select 100 equidistant points α from the interval $(\mu_2, \mu_1) = (6, 12)$. For each α, we construct 3600 pseudorandom vectors y satisfying $\mu(y) = \alpha$, and build the corresponding Krylov subspaces $\mathcal{K}$. After computing the required terms, the numerical maxima of (3.57) and (3.58) are plotted versus $\mu(y)$ together with $\text{CB} = [\,T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2}$ in the left subfigure in Figure 3.7. We note that the constant bound CB is more accurate than variable bound (3.58), and nearly sharp for $\mu(y) \approx \mu_1$. In addition, we plot a variant $(3.58)^\circ$ of (3.58) where the lower bound $\widetilde{\theta}_i$ of θ_i is determined by the basic estimate (3.4) as in [83]. This variant is slightly less accurate than (3.58) so that CB is the best bound in the current test.

In the second test, we set $i = 1$, $c = 2$, $k = 3$. Then $c + 1$ reads 3 so that μ_3 is a relevant eigenvalue for the estimates. Therefore we consider the interval $(\mu_3, \mu_2) = (4, 6)$ together with the interval $(\mu_2, \mu_1) = (6, 12)$, and select from each of them 100 equidistant points α. The further computation is similar to that in the first test. Subsequently, the numerical maxima of (3.57) and (3.58) are presented together with CB in the right subfigure in Figure 3.7. Since certain values are considerably large, we use the semi-log plot. On the interval (μ_3, μ_2), CB is more accurate than (3.58), and nearly sharp for $\mu(y) \approx \mu_2$. Interestingly, (3.58) overtakes CB on (μ_2, μ_1).

In the next three tests, we set $i = 2$ together with $[c = 2,\ k = 3]$, $[c = 2,\ k = 4]$ or $[c = 3,\ k = 4]$ where the interval $(\mu_4, \mu_3) = (3.\overline{27}, 4)$ is added for $c = 3$. We present the corresponding numerical maxima of (3.57) and (3.58) together with CB in the subfigures in Figure 3.8. In the test with $[c = 2,\ k = 3]$, CB is always more accurate than (3.58), and sharp on the interval (μ_2, μ_1). Moreover, the numerical maxima of (3.58) are nonpositive for certain points in (μ_3, μ_2), i.e., the lower bound $\widetilde{\theta}_i$ cannot exceed μ_{c+1}. These nonpositive values are omitted in the plot. In the test with $[c = 2,\ k = 4]$, CB is also always more accurate than (3.58), but not sharp on (μ_2, μ_1). The curve of (3.57) is similar to that in the first test. In the test with $[c = 3,\ k = 4]$, CB is less accurate than (3.58) on (μ_3, μ_2), but overtakes (3.58) on the other two intervals. The graphic for $\mu(y)$ between μ_4 and μ_2 is similar to the graphic in the second test.

In summary, CB is more accurate than (3.58) for $c = i$. Although it can possibly be overtaken by (3.58) for $c > i$, its value is always much smaller than 1 so that the overestimation is controllable. Correspondingly, we prefer the angle-free estimate (3.32) and its special form (3.33) in the case of low-dimensional Krylov subspaces.

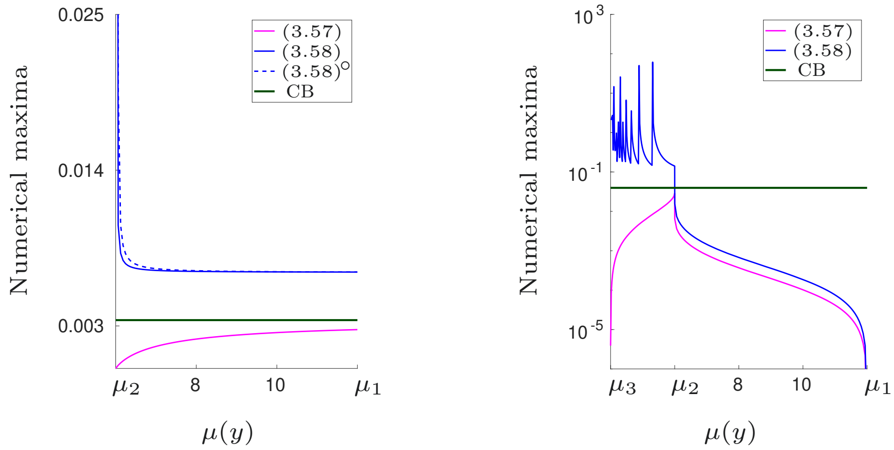

Figure 3.7: Comparison between the angle-dependent estimate (3.19) and the angle-free estimate (3.32). Therein the variable bound (3.58) corresponds to (3.19), and the constant bound CB $= [T_{k-c}(1+2\widetilde{\gamma}_i)]^{-2}$ corresponds to (3.32). The numerical maxima of these two bounds and the ratio (3.57) are compared for various sample initial vectors y and then plotted versus $\mu(y)$. Left: Comparison for $i=1$, $c=1$, $k=3$. Right: Comparison for $i=1$, $c=2$, $k=3$.

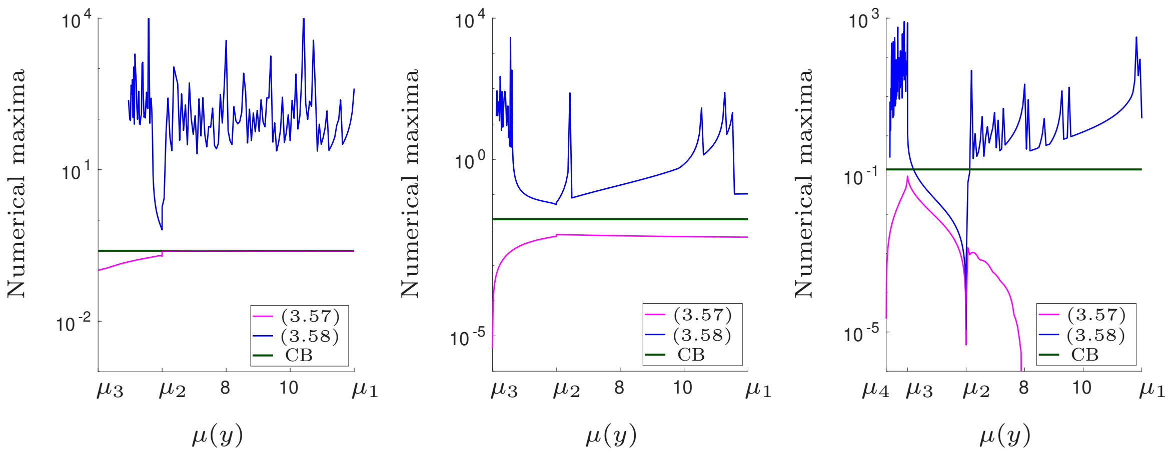

Figure 3.8: Comparison between the angle-dependent estimate (3.19) and the angle-free estimate (3.32). Therein the variable bound (3.58) corresponds to (3.19), and the constant bound CB $= [T_{k-c}(1+2\widetilde{\gamma}_i)]^{-2}$ corresponds to (3.32). The numerical maxima of these two bounds and the ratio (3.57) are compared for various sample initial vectors y and then plotted versus $\mu(y)$. Left: Comparison for $i=2$, $c=2$, $k=3$. Center: Comparison for $i=2$, $c=2$, $k=4$. Right: Comparison for $i=2$, $c=3$, $k=4$.

Improvement of estimates on Ritz vectors

The central estimate (3.51) in Subsection 3.2.4 improves the estimate (2.11) and the adapted form of (2.14) to standard Krylov subspace iterations. We discuss the improvement within the test presented in Table 3.3 and Figure 3.3. The tested Krylov subspaces $\mathcal{K}$ have dimension 14, and the assumption $\theta_j > \mu_{j+1}\ \forall\ j \in \{1, \ldots, s\}$ of (3.51) is fulfilled for $s = 7$. Concerning the sine squared $\text{SQ}_i = \sin^2 \angle_2(u_i, z_i)$, we compare (3.51) with (2.11) for $i = 1$, and with (2.14) for $i \in \{2, \ldots, 7\}$. However, we omit the result for $i = 1$ since the values subceed 10^{-16}. The results for $i \in \{2, \ldots, 7\}$ are presented in Table 3.5. We note that (3.51) significantly improves (2.14) in the sense of relative error. For completeness, we compare (3.51) with (2.11) by using $\mathcal{K}$ of dimension 10. Therein SQ_1 reads 4.48×10^{-14}, and (3.51) gives the bound 5.45×10^{-14} which is better than the bound 7.82×10^{-14} by (2.11).

Table 3.5: Comparison between the estimates (3.51) and (2.14) on Ritz vectors concerning the sine squared $\text{SQ}_i = \sin^2 \angle_2(u_i, z_i)$ for Test-matrix 1 from Subsection 3.3.1.

i	2	3	4	5	6	7
SQ_i	4.42×10^{-14}	7.03×10^{-9}	6.61×10^{-11}	1.04×10^{-9}	1.19×10^{-1}	7.84×10^{-2}
(3.51)	5.01×10^{-14}	9.19×10^{-9}	8.88×10^{-11}	1.37×10^{-9}	1.91×10^{-1}	1.74×10^{-1}
(2.14)	9.59×10^{-14}	2.91×10^{-8}	4.45×10^{-10}	5.45×10^{-9}	3.71×10^{-1}	2.06×10^{-1}

Furthermore, the estimates on Ritz values can be extended by (3.51), (2.11) and (2.14) since their bounds are monotonically increasing with respect to the errors of the concerned Ritz values. For instance, we extend (3.24) by (3.51) and (2.14) and apply the combinations to SQ_3 in Table 3.5. Therein (3.24)+(3.51) gives the bound 3.49×10^{-3}, whereas (3.24)+(2.14) gives the bound 4.44×10^{-3}. These bounds are independent of the exact Ritz values in the current Krylov subspace and are thus a priori bounds. In contrast, the bound in the estimate (2.2) does not possess the above monotonicity so that (2.2) has to use the exact Ritz values for analyzing the associated Ritz vectors.

3.4 Reformulation for generalized matrix eigenvalue problems

We reformulate the new estimates from Section 3.2 for generalized matrix eigenvalue problems with Notation 1.1. The reformulation is elementary and based on reversing the substitutions (1.26) and (1.30). The results are directly applicable to standard Krylov subspace iterations of the type (1.22).

Theorem 3.12. *With Notation 1.1, consider a Krylov subspace*

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

with the initial vector $x \in \mathbb{R}^n \backslash \{0\}$, and assume that $\mathcal{K}$ is not an invariant subspace. Let the eigenvalues $\lambda_1, \ldots, \lambda_s$ be of practical interest, and the reciprocals of λ_s λ_{c+1} be well separated for an index $c \in [s, k)$, then the following estimates hold.

(I) Estimates on approximate eigenvectors: The auxiliary vector

$$\widehat{x} = \Big(\prod\nolimits_{j\in\{1,\ldots,c\}\backslash\{i\}} \big(A^{-1}M - \lambda_j^{-1}I\big)\Big)\, x$$

is nonzero. If the eigenprojection $P_i x$ of x is nonzero for an index $i \in \{1, \ldots, s\}$, then it holds, in terms of the A-normalized eigenprojection $w_i = P_i x / \|P_i x\|_A$, the invariant *subspace* $\mathcal{W} = \mathcal{W}_1 \oplus \cdots \oplus \mathcal{W}_i$, *the gap ratio* $\widetilde{\gamma}_i = (\lambda_i^{-1} - \lambda_{c+1}^{-1})/(\lambda_{c+1}^{-1} - \lambda_m^{-1})$, *and the Chebyshev polynomial* $T_{k-c}(\cdot)$, *that*

$$\tan \angle_A(w_i, \mathcal{K}) \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-1} \tan \angle_A(\widehat{x}, \mathcal{W}). \tag{3.59}$$

In addition,

$$\tan \angle_A(w_i, \mathcal{K}) \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-1} \tan \angle_A(\mathcal{K}^c, \mathcal{W}^c) \tag{3.60}$$

holds in terms of the Krylov subspace $\mathcal{K}^c = \operatorname{span}\{x,\ A^{-1}Mx,\ \ldots,\ (A^{-1}M)^{c-1}x\}$ *and the invariant subspace* $\mathcal{W}^c = \mathcal{W}_1 \oplus \cdots \oplus \mathcal{W}_c$.

(II) *Angle-dependent estimates on Ritz values: Denote by* $\vartheta_1, \ldots, \vartheta_s$ *the* s *reciprocally largest Ritz values of* (A, M) *in* $\mathcal{K}$. *Then the auxiliary vector*

$$x^c = \Big(\prod_{j=1}^{i-1} (A^{-1}M - \vartheta_j^{-1} I)\Big) \Big(\prod_{j=i+1}^{c} (A^{-1}M - \lambda_j^{-1} I)\Big)\, x$$

is nonzero, and

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_m^{-1}} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \left(\frac{\sin \angle_A(x^c, \mathcal{W})}{\cos \angle_A(x^c, w_i)} \right)^2 \tag{3.61}$$

holds with the terms from (I) by assuming $\vartheta_{i-1}^{-1} > \lambda_i^{-1}$ *in the case* $i > 1$. *Moreover,*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_m^{-1}} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \tan^2 \angle_A(\mathcal{K}^c, \mathcal{W}^c) \tag{3.62}$$

holds without assuming $\vartheta_{i-1}^{-1} > \lambda_i^{-1}$.

(III) *Angle-free estimates on Ritz values: In addition to (II), assume that the reciprocally smallest Ritz value* α *of* (A, M) *in* $\mathcal{K}^c$ *fulfills* $\alpha^{-1} > \lambda_{c+1}^{-1}$. *Then*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_{c+1}^{-1}} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \, \frac{\lambda_i^{-1} - \alpha^{-1}}{\alpha^{-1} - \lambda_{c+1}^{-1}} \tag{3.63}$$

holds. Similarly, by assuming $\beta^{-1} > \lambda_{i+1}^{-1}$ *for the reciprocally smallest Ritz value* β *of* (A, M) *in* $\mathcal{K}^i = \operatorname{span}\{x,\ A^{-1}Mx,\ \ldots,\ (A^{-1}M)^{i-1}x\}$,

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_{i+1}^{-1}} \le [\, T_{k-i}(1 + 2\gamma_i)\,]^{-2} \, \frac{\lambda_i^{-1} - \beta^{-1}}{\beta^{-1} - \lambda_{i+1}^{-1}} \tag{3.64}$$

holds in terms of the (smaller) gap ratio $\gamma_i = (\lambda_i^{-1} - \lambda_{i+1}^{-1})/(\lambda_{i+1}^{-1} - \lambda_m^{-1})$ *and the Chebyshev polynomial* $T_{k-i}(\cdot)$.

(IV) *Additional estimates on Ritz vectors: Let* $v_1, \ldots, v_s$ *be* A*-orthonormal Ritz vectors associated with* $\vartheta_1, \ldots, \vartheta_s$. *If* $\vartheta_j^{-1} > \lambda_{j+1}^{-1}$ *for each* $j \in \{1, \ldots, s\}$, *then the eigenprojection* $P_i x$ *is nonzero for each* $i \in \{1, \ldots, s\}$, *and* $\vartheta_1, \ldots, \vartheta_s$ *are distinct. Moreover, it holds, in terms of the* A*-normalized eigenprojection* $w_i = P_i x / \|P_i x\|_A$, *that*

$$\sin^2 \angle_A(v_i, w_i) \le 1 - \left(\prod_{j=1,\ j\ne i}^{s+1} \frac{\vartheta_i^{-1} - \lambda_j^{-1}}{\lambda_i^{-1} - \lambda_j^{-1}} \right) \left(\prod_{j=1,\ j\ne i}^{s} \frac{\lambda_i^{-1} - \vartheta_j^{-1}}{\vartheta_i^{-1} - \vartheta_j^{-1}} \right). \tag{3.65}$$

If M is positive definite, then the estimates (3.59) and (3.60) also hold in M-angles, and the estimates (3.63) and (3.64) can be simplified as

$$\frac{\vartheta_i - \lambda_i}{\lambda_{c+1} - \vartheta_i} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_i)\,]^{-2} \, \frac{\alpha - \lambda_i}{\lambda_{c+1} - \alpha} \quad \text{and} \quad \frac{\vartheta_i - \lambda_i}{\lambda_{i+1} - \vartheta_i} \le [\, T_{k-i}(1 + 2\gamma_i)\,]^{-2} \, \frac{\beta - \lambda_i}{\lambda_{i+1} - \beta}$$

since the concerned eigenvalues and Ritz values are positive.

4 Restarted Krylov subspace iterations

For solving large-scale matrix eigenvalue problems, standard Krylov subspace iterations usually need to be restarted because of their high storage requirement. The resulting low-dimensional Krylov subspaces are subsets of an underlying Krylov subspace with increasing dimension. The approximations of eigenvalues and eigenvectors produced in these low-dimensional Krylov subspaces are generally less accurate than the approximations from the corresponding standard Krylov subspace iteration with respect to the number of outer steps. Nevertheless, the total computation time for reaching an expected accuracy can be reduced due to the smaller extent of the involved Rayleigh-Ritz procedure.

In comparison to the popularity of restarted Krylov subspace iterations, their convergence behavior has rarely been analyzed in a sound way as for standard Krylov subspace iterations. A reason might be that some of the classical estimates are locally applicable to single steps and can asymptotically show the global convergence in the case that the dimensions of the involved Krylov subspaces are sufficiently large. The restarting prevents applying these estimates in a nonasymptotical and practical way. For instance, Saad's estimates formulated in Theorem 3.2 require the initial vector of the current Krylov subspace for building the bounds, whereas the convergence measures on the left-hand sides are not related to the initial vector of the next Krylov subspace. Thus they cannot be applied to multiple steps for deriving a priori bounds. Combining Theorem 3.2 with the additional estimate (2.2) is also problematic due to the dependence of (2.2) on exact Ritz values. Therefore we aim to enrich the convergence analysis for restarted Krylov subspace iterations by flexible and more accurate estimates, especially for small Krylov subspaces.

In this chapter, we investigate restarted Krylov subspace iterations of the type (1.23) by observing the reciprocal representation (1.29b) concerning standard matrix eigenvalue problems with Notation 1.4. In Section 4.1, we review several of our previous results from [83, 125] on a simply restarted version of (1.29b). In particular, we introduce an extension of Knyazev's estimate (2.10) to the case that the initial approximate eigenvalue is located in an arbitrary interval between consecutive eigenvalues. In addition, a geometry-flavored analysis yields sharp estimates on Ritz vectors and Ritz values. Therein the bounds are supported by a variable number of eigenvalues, whereas the Chebyshev bounds only use three eigenvalues. Section 4.2 is devoted to investigating the general version of (1.29b). The angle-free estimates on Ritz values from Subsection 3.2.3 are extended to arbitrarily located initial Ritz values by using the same basic idea as for extending (2.10). The resulting estimates can be combined with the additional estimates from Subsection 3.2.4 for providing estimates on Ritz vectors. In Section 4.3, the main results are reformulated for their application to the description (1.23) of restarted Krylov subspace iterations concerning generalized matrix eigenvalue problems with Notation 1.1.

4.1 Estimates for simple restarting

The simply restarted version of (1.29b) with $c = s = 1$, i.e.,

$$y^{(\ell+1)} \quad \leftarrow \quad \widehat{\mathrm{RR}}\left(\widehat{\mathcal{K}}^k(y^{(\ell)}), 1\right) \quad \text{with fixed } k > 1, \tag{4.1}$$

has been investigated in [83, 125] as an extension of the gradient iteration

$$y^{(\ell+1)} = y^{(\ell)} + \omega^{(\ell)} \left(H y^{(\ell)} - \mu(y^{(\ell)}) y^{(\ell)} \right). \tag{4.2}$$

A particular motivation was that the convergence analysis for (4.2) from [80] has successfully been generalized in [79] to the preconditioned gradient iteration (1.4). Since (1.4) corresponds to the PINVIT method $\mathscr{P}_2$ as described in Subsection 1.3.1, it is expected that the investigation of related Krylov subspace iterations such as (4.1) could contribute to the completion of the convergence theory of the PINVIT hierarchy.

The simply restarted Krylov subspace iteration (4.1) generates a series of Krylov subspaces

$$\widehat{\mathcal{K}}^k(y^{(\ell)}) = \operatorname{span}\{y^{(\ell)}, Hy^{(\ell)}, \ldots, H^{k-1}y^{(\ell)}\}, \quad \ell = 0, 1, 2, \ldots$$

for a symmetric matrix $H \in \mathbb{R}^{n\times n}$ with Notation 1.4 and approximates the largest eigenvalue of H by the largest Ritz values in the involved Krylov subspaces. The initial vector of the next Krylov subspace is simply a Ritz vector in the current Krylov subspace associated with the largest Ritz value.

We first discuss the applicability of Saad's estimates formulated in Theorem 3.2. Since the iteration (4.1) focuses on the largest eigenvalue, we only need to consider a special form of Theorem 3.2 with $i=1$. Therein the invariant subspace $\mathcal{Z} = \mathcal{Z}_1 \oplus \cdots \oplus \mathcal{Z}_i$ is actually the eigenspace $\mathcal{Z}_1$ associated with the largest eigenvalue μ_1. The angle $\angle_2(y,\mathcal{Z})$ is thus simplified as

$$\angle_2(y,\mathcal{Z}) = \angle_2(y,\mathcal{Z}_1) = \angle_2(y,Q_1y) = \angle_2(y,z_1)$$

with the normalized eigenprojection $z_1 = Q_1y/\|Q_1y\|_2$, and the trigonometric term $\sin\angle_2(y,\mathcal{Z})/\cos\angle_2(y,z_i)$ for $i=1$ coincides with $\tan\angle_2(y,z_1)$. Moreover, the ratio-products in Theorem 3.2 are reduced to 1 for $i=1$. Consequently, the basic estimates (3.1) and (3.4) are simplified as

$$\begin{aligned}\tan\angle_2\big(z_1,\mathcal{K}\big) &\le [\,T_{k-1}(1+2\gamma_1)\,]^{-1}\,\tan\angle_2(y,z_1),\\ \mu_1-\theta_1 &\le (\mu_1-\mu_m)\Big([\,T_{k-1}(1+2\gamma_1)\,]^{-1}\,\tan\angle_2(y,z_1)\Big)^2,\end{aligned}$$

and the refined estimates can be simplified in a similar way. Evidently, these simplified estimates can be applied to single steps of (4.1) by setting $y = y^{(\ell)}$ and $\mathcal{K} = \widehat{\mathcal{K}}^k(y^{(\ell)})$. However, one cannot combine the resulting inequalities regarding consecutive Krylov subspaces in order to derive a priori bounds. An indirect combination with further inequalities such as

$$\tan\angle_2(y^{(\ell+1)},z_1) \le C^{(\ell)}\tan\angle_2\big(z_1,\widehat{\mathcal{K}}^k(y^{(\ell)})\big)$$

based on the additional estimate (2.2) is possible but impractical, namely, the distance paramter δ_i in (2.2) has to use exact Ritz values instead of estimated Ritz values; cf. the last paragraph of Subsection 3.3.2.

Several suitable estimates for the iteration (4.1) have been achieved in our previous works [83, 125]. Therein we note that Knyazev's estimate (2.10) introduced in Theorem 2.4 can be applied recursively for deriving a priori bounds. The single-step estimate

$$\frac{\mu_1-\mu(y^{(\ell+1)})}{\mu(y^{(\ell+1)})-\mu_2} \le [\,T_{k-1}(1+2\gamma_1)\,]^{-2}\,\frac{\mu_1-\mu(y^{(\ell)})}{\mu(y^{(\ell)})-\mu_2} \tag{4.3}$$

based on (2.10) trivially leads to the multi-step estimate

$$\frac{\mu_1-\mu(y^{(\ell)})}{\mu(y^{(\ell)})-\mu_2} \le [\,T_{k-1}(1+2\gamma_1)\,]^{-2\ell}\,\frac{\mu_1-\mu(y^{(0)})}{\mu(y^{(0)})-\mu_2}.$$

Moreover, (4.3) gives a tighter bound in comparison to Saad's estimate (3.4); cf. the numerical example in [83, Section 2.1]. Nevertheless, since (4.3) requires the somewhat strong assumption $\mu(y^{(\ell)}) > \mu_2$, it is desirable to extend (4.3) to the more general case $\mu_j > \mu(y^{(\ell)}) > \mu_{j+1}$ concerning two consecutive eigenvalues. An extension by [83, Theorem 3.1] reads

$$\frac{\mu_j-\mu(y^{(\ell+1)})}{\mu(y^{(\ell+1)})-\mu_{j+1}} \le [\,T_{k-1}(1+2\gamma_j)\,]^{-2}\,\frac{\mu_j-\mu(y^{(\ell)})}{\mu(y^{(\ell)})-\mu_{j+1}} \tag{4.4}$$

with the gap ratio $\gamma_j = (\mu_j - \mu_{j+1})/(\mu_{j+1} - \mu_m)$. In addition, the sharpness of (4.4) has been discussed in [125]. We note that (4.4) is not sharp for Krylov subspaces of dimension $k > 2$. From an analytical point of view, the cause is that the contained Chebyshev factor $[\,T_{k-1}(1+2\gamma_j)\,]^{-2}$ is derived from the solution of an optimization problem on the interval $[\mu_m, \mu_{j+1}]$ whereas the desired sharp convergence factor should solve a similar optimization problem concerning a finite number of points in $[\mu_m, \mu_{j+1}]$, namely, the eigenvalues $\mu_{j+1}, \ldots, \mu_m$. From an comparative point of view, we note that $[\,T_{k-1}(1+2\gamma_j)\,]^{-2}$ only uses three eigenvalues whereas a sharp estimate on Ritz vectors from [83, Theorem 3.1] requires $k+1$ eigenvalues. By extending the proof of this sharp estimate, a sharp variant of (4.4) has been derived in [125]. The bound depends on certain interpolating polynomials which have similar properties like shifted Chebyshev polynomials.

The further part of this section is devoted to reviewing the main estimates from [83, 125]. Some proof techniques are also useful for investigating the general version of restarted Krylov subspace iterations in Section 4.2.

4.1.1 Basic estimates

We begin with the above-mentioned extended estimate (4.4) from [83]. For completeness, we embed this estimate in the following theorem.

Theorem 4.1. *With Notation 1.4, consider the restarted Krylov subspace iteration* (1.29b) *with* $c = s = 1$ *where* $y^{(\ell+1)}$ *is a Ritz vector of* H *in* $\widehat{\mathcal{K}}^k(y^{(\ell)})$ *associated with the largest Ritz value. Assume that the involved Krylov subspaces are not invariant subspaces, and let* $\mu(\cdot)$ *be the Rayleigh quotient with respect to* H *as defined in* (1.34)*. Then* $\mu(y^{(\ell+1)}) > \mu(y^{(\ell)})$ *holds for each* ℓ *so that the sequence* $\big(\mu(y^{(\ell)})\big)_{\ell\in\mathbb{N}}$ *is strictly increasing. In addition, the estimate* (4.4) *holds in the case* $\mu_j > \mu(y^{(\ell)}) > \mu_{j+1}$ *for a certain index* $j \in \{1, \ldots, m-1\}$.

The simple inequality $\mu(y^{(\ell+1)}) > \mu(y^{(\ell)})$ serves to supplement the estimate (4.4) in the special case $\mu(y^{(\ell)}) = \mu_j$ where (4.4) would lead to the trivial inequality $\mu(y^{(\ell+1)}) \geq \mu(y^{(\ell)})$. Indeed, $\mu(y^{(\ell+1)}) > \mu(y^{(\ell)})$ is ensured by the assumption that the involved Krylov subspaces are not invariant subspaces. If $\mu(y^{(\ell+1)}) = \mu(y^{(\ell)})$ holds, i.e., $\mu(y^{(\ell)})$ is equal to the largest Ritz value $\theta_1^{(\ell)}$ in $\widehat{\mathcal{K}}^k(y^{(\ell)})$, then $y^{(\ell)}$ is a maximizer of $\mu(\cdot)$ and thus a Ritz vector associated with $\theta_1^{(\ell)}$. Consequently, the residual $Hy^{(\ell)} - \theta_1^{(\ell)} y^{(\ell)}$ which evidently belongs to $\widehat{\mathcal{K}}^k(y^{(\ell)})$ must be orthogonal to $\widehat{\mathcal{K}}^k(y^{(\ell)})$. This means that the residual is zero so that $y^{(\ell)}$ is an eigenvector. Therefore $\widehat{\mathcal{K}}^k(y^{(\ell)}) = \operatorname{span}\{y^{(\ell)}\}$ holds and contradicts that $\widehat{\mathcal{K}}^k(y^{(\ell)})$ is not an invariant subspace.

The estimate (4.4) can be derived in the form

$$\frac{\mu_j - \theta_1}{\theta_1 - \mu_{j+1}} \leq [\,T_{k-1}(1+2\gamma_j)\,]^{-2}\,\frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}} \tag{4.5}$$

with $\theta_1 = \mu(y^{(\ell+1)})$ and $y = y^{(\ell)}$. Therein θ_1 is the largest Ritz value in the Krylov subspace $\mathcal{K} = \widehat{\mathcal{K}}^k(y^{(\ell)}) = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$, and the initial vector y fulfills $\mu_j > \mu(y) > \mu_{j+1}$. In the nontrivial case $\mu_j > \theta_1$ (otherwise the left-hand side of (4.5) is nonpositive), we can show that the auxiliary vector

$$\widetilde{y} \,=\, p(\mu_j)\,\textstyle\sum_{l=1}^{j} Q_l y \,+\, \sum_{l=j+1}^{m} Q_l y$$

with the shifted Chebyshev polynomial $p(\alpha) = T_{k-1}\big(1 + 2\,\frac{\alpha - \mu_{j+1}}{\mu_{j+1} - \mu_m}\big)$ possesses the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \qquad \text{and} \qquad \frac{\mu_j - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \leq [\,T_{k-1}(1+2\gamma_j)\,]^{-2}\,\frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}}\,.$$

Their verification is analogous to the proof of Lemma 2.13. Subsequently, the first property implies $\theta_1 \geq \mu\big(p(H)y\big) \geq \mu(\widetilde{y})$ by considering $p(H)y \in \mathcal{K}$ so that the second property can be extended as (4.5) by using the monotonicity of the function $\big(\mu_j - \,\cdot\,\big)/\big(\,\cdot\, - \mu_{j+1}\big)$.

Combining (4.4) with $\mu(y^{(\ell+1)}) > \mu(y^{(\ell)})$ shows that the sequence $\big(\mu(y^{(\ell)})\big)_{\ell\in\mathbb{N}}$ converges to the largest eigenvalue μ_1 provided that the corresponding Krylov subspaces $\widehat{\mathcal{K}}^k(y^{(\ell)})$ are not invariant subspaces. In the practically rare case that any $\widehat{\mathcal{K}}^k(y^{(\ell)})$ is an invariant subspace, then the residuals of the Ritz vectors in $\widehat{\mathcal{K}}^k(y^{(\ell)})$ are zero so that the Ritz vectors become eigenvectors. Consequently, an eigenvalue is given by $\mu(y^{(\ell+1)})$ which is the largest Ritz value in $\widehat{\mathcal{K}}^k(y^{(\ell)})$.

Furthermore, if $\mu(y^{(\ell)})$ reaches the final interval (μ_2, μ_1), the additional estimate (2.11) is applicable and gives

$$\sin^2 \angle_2(y^{(\ell+1)}, z_1) \leq \frac{\mu_1 - \mu(y^{(\ell+1)})}{\mu_1 - \mu_2}$$

where z_1 is the normalized eigenprojection of $y^{(\ell)}$ on the eigenspace $\mathcal{Z}_1$. Combining this with (4.4) for $j=1$ yields a Ritz vector estimate depending on $\mu(y^{(\ell)})$.

4.1.2 Sharp estimates

The basic Ritz value estimate (4.5) is only sharp in the case $k=2$ where (4.5) is reduced to an estimate for a steepest ascent iteration from [80] :

$$\frac{\mu_j - \theta_1}{\theta_1 - \mu_{j+1}} \leq \left(\frac{\kappa}{2-\kappa}\right)^2 \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}} \qquad \text{with} \qquad \kappa = \frac{\mu_{j+1} - \mu_m}{\mu_j - \mu_m}. \tag{4.6}$$

The estimate (4.6) is sharp in the sense that the inequality in (4.6) becomes an equality in the limit case $\mu(y) \to \mu_j$ within an invariant subspace of H associated with the eigenvalues μ_j, μ_{j+1} and μ_m. An accompanying estimate from [80] on a Ritz vector u_1 associated with θ_1 reads

$$\tan \angle_2(u_1, \mathcal{Z}_1) \leq \kappa \tan \angle_2(y, \mathcal{Z}_1) \qquad \text{with} \qquad \kappa = \frac{\mu_2 - \mu_m}{\mu_1 - \mu_m}. \tag{4.7}$$

The sharpness of (4.7) is related to the limit case $\mu(y) \to \mu_2$ (instead of $\mu(y) \to \mu_1$) within an invariant subspace of H associated with the eigenvalues μ_1, μ_2 and μ_m. In addition, if H is positive definite, (4.7) also holds in H-angles. In [83], the H-variant of (4.7) is extended to larger Krylov subspaces of degree $k > 2$. The resulting estimate can easily be modified with respect to Euclidean angles, namely,

$$\tan \angle_2(u_1, \mathcal{Z}_1) \leq \prod_{l=1}^{k-1} \frac{\mu_2 - \mu_{m+1-l}}{\mu_1 - \mu_{m+1-l}} \tan \angle_2(y, \mathcal{Z}_1). \tag{4.8}$$

The convergence factor in (4.8) is a ratio-product which evidently generalizes the convergence factor κ in (4.7). Moreover, (4.8) is sharp by considering the limit case $\mu(y) \to \mu_2$ within a $(k+1)$-dimensional invariant subspace of H associated with the eigenvalues $\mu_1, \mu_2, \mu_{m-k+2}, \ldots, \mu_m$.

Therefore we attempted in [125] to derive a more accurate bound with $k+1$ eigenvalues in order to improve the estimate (4.5) where the gap ratio γ_j only depends on three eigenvalues. The analysis in [125] begins with the case $\mu(y) > \mu_2$. Therein the auxiliary subspace

$$\mathcal{U} \;=\; \operatorname{span}\{w_1\} + \mathcal{K} \;=\; \operatorname{span}\{w_1, y, Hy, \ldots, H^{k-1}y\} \tag{4.9}$$

is constructed with the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ and the eigenprojection $w_1 = Q_1 y$ (which is nonzero since otherwise $\mu(y) \leq \mu_2$). Certain properties of $\mathcal{U}$ allow us to formulate a mini-dimensional analysis.

Lemma 4.2. *With Notation 1.4, consider the subspace $\mathcal{U}$ defined by (4.9). Assume that $\mathcal{K}$ is not an invariant subspace and that $\mu(y) > \mu_2$. Let U be an orthonormal basis matrix of $\mathcal{U}$. Then $\mathcal{U}$ possesses the following properties concerning the representations*

$$\widehat{H} = U^T H U \qquad \textit{and} \qquad \widehat{y} = U^T y.$$

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

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

The Ritz pairs (θ, v) of H in $\mathcal{K}$ correspond to the Ritz pairs $(\theta, U^T v)$ of $\widehat{H}$ in $\widehat{\mathcal{K}}$.

(ii) The subspace $\mathcal{U}$ has dimension $k+1$. The Ritz values $\alpha_1 \geq \cdots \geq \alpha_{k+1}$ of H in $\mathcal{U}$ are strictly interlaced by the Ritz values $\theta_1 \geq \cdots \geq \theta_k$ of H in $\mathcal{K}$, namely,

$$\alpha_1 > \theta_1 > \alpha_2 > \cdots > \alpha_k > \theta_k > \alpha_{k+1}. \tag{4.10}$$

In addition, $\alpha_1, \ldots, \alpha_{k+1}$ are distinct eigenvalues of $\widehat{H}$. The eigenvalue α_1 coincides with μ_1, and the associated eigenspace is $\operatorname{span}\{U^T w_1\}$.

(iii) Let $\widehat{u}_1, \ldots, \widehat{u}_{k+1}$ be orthonormal eigenvectors of $\widehat{H}$ associated with $\alpha_1, \ldots, \alpha_{k+1}$, and let $\widehat{\mu}(\cdot)$ be the Rayleigh quotient with respect to $\widehat{H}$. Then the affine space

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

contains a vector

$$\widetilde{y} = \widehat{u}_1 + \textstyle\sum_{l=2}^{k+1} \beta_l \widehat{u}_l$$

for which $U\widetilde{y}$ is collinear with y and all coefficients β_l are nonzero. Moreover, the level set

$$\mathcal{S} = \{\widehat{u} \in \widehat{\mathcal{U}} \ ; \ \widehat{\mu}(\widehat{u}) = \theta_1\}$$

corresponds to an ellipsoid, i.e., the coefficients $\widehat{\beta}_l$ in the representation $\widehat{u} = \widehat{u}_1 + \sum_{l=2}^{k+1} \widehat{\beta}_l \widehat{u}_l$ fulfill the ellipsoid equation

$$\sum_{l=2}^{k+1} \widehat{\beta}_l^2 \left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_l} \right)^{-1} = 1. \tag{4.11}$$

Lemma 4.2 summarizes several arguments from [83, Lemmas 3.3 and 3.4] which have been used for deriving the sharp Ritz vector estimate (4.8). In particular, the ellipsoid equation (4.11) is derived by

$$\theta_1 = \widehat{\mu}(\widehat{u}) = \frac{\widehat{u}^T \widehat{H} \widehat{u}}{\widehat{u}^T \widehat{u}} = \frac{\alpha_1 + \sum_{l=2}^{k+1} \alpha_l \widehat{\beta}_l^2}{1 + \sum_{l=2}^{k+1} \widehat{\beta}_l^2} \qquad \Rightarrow \qquad \sum_{l=2}^{k+1} (\theta_1 - \alpha_l) \widehat{\beta}_l^2 = \alpha_1 - \theta_1.$$

The ratios $(\alpha_1 - \theta_1)/(\theta_1 - \alpha_l)$, $l = 2, \ldots, k+1$ are positive due to (4.10) and correspond to the squares of the semi-axes of the ellipsoid. Subsequently, another sharp estimate is derived depending on the Ritz values $\alpha_1, \ldots, \alpha_{k+1}$ of H in $\mathcal{U}$.

Theorem 4.3. *With the settings from Lemma 4.2, it holds that*

$$\left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_2} \right) \left(\frac{\alpha_1 - \mu(y)}{\mu(y) - \alpha_2} \right)^{-1} \leq [\, p(\alpha_1) \,]^{-2}. \tag{4.12}$$

Therein $p(\cdot)$ is a polynomial of degree $k-1$ which interpolates the pairs $\big(\alpha_l, (-1)^l\big)$, $l = 2, \ldots, k+1$. The equality in (4.12) is attained in the limit case $\mu(y) \to \alpha_1$.

Theorem 4.3 can be proved based on a geometric argument concerning the accompanying Krylov subspace $\widehat{\mathcal{K}}$, the affine space $\widehat{\mathcal{U}}$ and the level set $\mathcal{S}$ introduced in Lemma 4.2; cf. the proof of [125, Theorem 3.1] for details. For the reader's convenience, we formulate a proof sketch.

We first note that the $\widehat{\mathcal{U}}$-representation of $\mathcal{S}$ with respect to the basis vectors $\widehat{u}_2, \ldots, \widehat{u}_{k+1}$ is an ellipsoid defined by (4.11), whereas the $\widehat{\mathcal{U}}$-representation of the intersection $\widehat{\mathcal{U}} \cap \widehat{\mathcal{K}}$ is a tangential hyperplane of this ellipsoid. The point of tangency corresponds to a Ritz vector of $\widehat{H}$ in $\widehat{\mathcal{K}}$ associated with θ_1. Next, by using the coefficients β_l of the vector $\widetilde{y}$ from Lemma 4.2, the $\widehat{\mathcal{U}}$-representations of $\widehat{\mathcal{K}} \cap \big(\widehat{u}_1 + \mathrm{span}\{\widehat{u}_l\}\big)$ can be shown to have the coordinates

$$\beta_l \kappa_l \qquad \text{with} \qquad \kappa_l = \prod_{i=2,\ i\neq l}^{k+1} \frac{\alpha_l - \alpha_i}{\alpha_1 - \alpha_i}, \qquad l = 2, \ldots, k+1.$$

In addition, the coordinates of the above-mentioned point of tangency are given by

$$(\delta_l \beta_l \kappa_l)^{-1} \qquad \text{with} \qquad \delta_l = \left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_l}\right)^{-1}, \qquad l = 2, \ldots, k+1.$$

Combining this with certain trigonometric transformations yields

$$\left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_2}\right)\left(\frac{\alpha_1 - \mu(y)}{\mu(y) - \alpha_2}\right)^{-1} \leq \frac{\left(\sum_{l=2}^{k+1} \kappa_l^{-1}\right)^2}{\left(\sum_{l=2}^{k+1} \delta_l \beta_l^2\right)\left(\sum_{l=2}^{k+1} \delta_l^{-1} \beta_l^{-2} \kappa_l^{-2}\right)}. \tag{4.13}$$

By using the Cauchy-Schwarz inequality, we get

$$\left(\sum_{l=2}^{k+1} \delta_l \beta_l^2\right)^{1/2} \left(\sum_{l=2}^{k+1} \delta_l^{-1} \beta_l^{-2} \kappa_l^{-2}\right)^{1/2} \geq \sum_{l=2}^{k+1} \big(\delta_l^{1/2} \beta_l\big)\big(\delta_l^{-1/2} \beta_l^{-1} |\kappa_l|^{-1}\big) = \sum_{l=2}^{k+1} |\kappa_l|^{-1}$$

which extends (4.13) as

$$\left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_2}\right)\left(\frac{\alpha_1 - \mu(y)}{\mu(y) - \alpha_2}\right)^{-1} \leq \frac{\left(\sum_{l=2}^{k+1} \kappa_l^{-1}\right)^2}{\left(\sum_{l=2}^{k+1} |\kappa_l|^{-1}\right)^2}.$$

The right-hand side can be reformulated as the term $[\,p(\alpha_1)\,]^{-2}$ with the interpolating polynomial $p(\cdot)$ from Theorem 4.3 by considering that the values of the associated Lagrange basis polynomials at α_1 are just κ_l^{-1}. This completes the derivation of the estimate (4.12). In the limit case $\mu(y) \to \alpha_1$, we can verify that each inequality utilized in the derivation turns into an equality so that the equality in (4.12) is attained.

Furthermore, the estimate (4.12) can easily be extended as

$$\left(\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2}\right)\left(\frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}\right)^{-1} \leq \left(\frac{\alpha_1 - \theta_1}{\theta_1 - \alpha_2}\right)\left(\frac{\alpha_1 - \mu(y)}{\mu(y) - \alpha_2}\right)^{-1} \leq [\,p(\alpha_1)\,]^{-2} = [\,p(\mu_1)\,]^{-2}.$$

However, the term $[\,p(\mu_1)\,]^{-2}$ still depends on the Ritz values $\alpha_2, \ldots, \alpha_{k+1}$. By discussing the monotonicity of $[\,p(\alpha_1)\,]^{-2}$ with respect to these Ritz values, we can describe an upper bound of $[\,p(\alpha_1)\,]^{-2}$ in terms of certain eigenvalues in order to formulate a more practical estimate.

Lemma 4.4. *With the settings from Lemma 4.2, it holds that*

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2} \leq \left(\min_{\tau} p_\tau(\mu_1)\right)^{-2} \frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}.$$

Therein τ denotes an arbitrary $(k-2)$-element subset of the index set $\{3, \ldots, m-1\}$, and $p_\tau(\cdot)$ is a polynomial of degree $k-1$ which interpolates the pairs $\big(\mu_2, 1\big)$, $\big(\mu_m, (-1)^{k+1}\big)$ and $\big(\mu_{\tau_l}, (-1)^l\big)$, $l = 3, \ldots, k$ with the indices $\tau_l \in \tau$ in ascending order.

Lemma 4.4 can be proved by using the Newton form of the interpolating polynomial $p(\cdot)$; cf. the proof of [125, Lemma 3.2].

In the more general case $\mu_j > \mu(y) > \mu_{j+1}$, a slight modification of Lemma 4.2, Theorem 4.3 and Lemma 4.4 yields the following result.

Lemma 4.5. *With Notation 1.4, consider the subspace*

$$\mathcal{U} = \operatorname{span}\{w_j\} + \mathcal{K} = \operatorname{span}\{w_j, y, Hy, \ldots, H^{k-1}y\}$$

which is constructed with the Krylov subspace $\mathcal{K} = \operatorname{span}\{y, Hy, \ldots, H^{k-1}y\}$ *and the eigenprojection* $w_j = Q_j y$. *Assume that* $\mathcal{K}$ *is not an invariant subspace and that* $\mu_j > \mu(y) > \mu_{j+1}$ *for a certain index* $j \in \{1, \ldots, m-1\}$. *If* w_j *is nonzero, then* $\mathcal{U}$ *has dimension* $k+1$ *so that one can denote by* $\alpha_1 \geq \cdots \geq \alpha_{k+1}$ *the Ritz values of* H *in* $\mathcal{U}$. *In addition, if* $\mu_{j+1} \geq \alpha_2$, *then the estimate* (4.12) *holds for the largest Ritz value* θ_1 *of* H *in* $\mathcal{K}$. *Furthermore,* $\theta_1 \geq \mu_j$ *holds trivially for* $j > m-k$. *In the case* $j \leq m-k$, *it holds that*

$$\frac{\mu_j - \theta_1}{\theta_1 - \mu_{j+1}} \leq \Big(\min_{\tau} p_\tau(\mu_j)\Big)^{-2} \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}}.$$

Therein τ *denotes an arbitrary* $(k-2)$*-element subset of the index set* $\{j+2, \ldots, m-1\}$, *and* $p_\tau(\cdot)$ *is a polynomial of degree* $k-1$ *which interpolates the pairs* $\big(\mu_{j+1}, 1\big)$, $\big(\mu_m, (-1)^{k+1}\big)$ *and* $\big(\mu_{\tau_l}, (-1)^l\big)$, $l = 3, \ldots, k$ *with the indices* $\tau_l \in \tau$ *in ascending order.*

Nevertheless, the estimates in Lemmas 4.4 and 4.5 are not explicit since the bounds depend on a minimization problem. Explicit estimates have been achieved only in the case $k=3$.

Theorem 4.6. *With Notation 1.4, consider the Krylov subspace* $\mathcal{K} = \operatorname{span}\{y, Hy, H^2y\}$ *which is not an invariant subspace. Let* $\mu(\cdot)$ *be the Rayleigh quotient with respect to* H *as defined in* (1.34). *If* $\mu(y) > \mu_2$, *then*

$$\frac{\mu_1 - \theta_1}{\theta_1 - \mu_2} \leq [\,q(\mu_1)\,]^{-2} \frac{\mu_1 - \mu(y)}{\mu(y) - \mu_2}$$

holds for the largest Ritz value θ_1 *of* H *in* $\mathcal{K}$. *Therein* $q(\cdot)$ *is a quadratic polynomial which interpolates the pairs* $\big(\mu_2, 1\big)$, $\big(\mu_\xi, -1\big)$ *and* $\big(\mu_m, 1\big)$, *and* μ_ξ *is an eigenvalue which has the smallest distance to* $(\mu_2 + \mu_m)/2$ *among the eigenvalues* $\mu_3, \ldots, \mu_{m-1}$. *Moreover, if* $\mu_j > \mu(y) > \mu_{j+1}$ *for a certain index* $j \in \{1, \ldots, m-1\}$, *then* $\theta_1 \geq \mu_j$ *holds trivially for* $j > m-3$. *In the case* $j \leq m-3$, *it holds that*

$$\frac{\mu_j - \theta_1}{\theta_1 - \mu_{j+1}} \leq [\,q(\mu_j)\,]^{-2} \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}} \tag{4.14}$$

Therein $q(\cdot)$ *is a quadratic polynomial interpolating the pairs* $\big(\mu_{j+1}, 1\big)$, $\big(\mu_\xi, -1\big)$ *and* $\big(\mu_m, 1\big)$, *and* μ_ξ *is an eigenvalue which has the smallest distance to* $(\mu_{j+1} + \mu_m)/2$ *among the eigenvalues* $\mu_{j+2}, \ldots, \mu_{m-1}$.

Theorem 4.6 can be proved by characteristically solving the minimization problem from Lemma 4.4; cf. the proof of [125, Lemma 3.4]. It is remarkable that the estimate (4.14) is not based on Lemma 4.5 and does not require the technical assumptions $w_j \neq 0$ and $\mu_{j+1} \geq \alpha_2$. The proof of (4.14) is analogous to that of (4.5) by using the fact that $q(\cdot)$ has similar properties in comparison to the shifted Chebyshev polynomial $p(\cdot)$ defined by $p(\alpha) = T_{k-1}\big(1 + 2\,\frac{\alpha - \mu_{j+1}}{\mu_{j+1} - \mu_m}\big)$. Moreover, the sharpness of (4.14) can be interpreted similarly to Theorem 4.3, namely, the equality is attained in the limit case $\mu(y) \to \mu_j$ within an invariant subspace associated with the eigenvalues μ_j, μ_{j+1}, μ_ξ, μ_m.

4.2 Estimates for general restarting

We consider further the general version of the restarted Krylov subspace iteration (1.29b) with $c \geq s \geq 1$. Therein the construction of the next Krylov subspace $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$ usually does not begin with an explicit initial vector $y^{(\ell+1)}$, but rather begins with the subset $\widehat{\mathcal{K}}^c(y^{(\ell+1)})$

which can be spanned by c orthonormal Ritz vectors associated with the c largest Ritz values in $\widehat{\mathcal{K}}^k(y^{(\ell)})$; cf. the thick-restart Lanczos method [118]. Alternatively, one can determine $\widehat{\mathcal{K}}^c(y^{(\ell+1)})$ by a shifted QR algorithm where the shifts are given by the remaining Ritz values in $\widehat{\mathcal{K}}^k(y^{(\ell)})$; cf. the implicitly restarted Lanczos method [19]. Concerning the convergence analysis for (1.29b), the angle-free estimates (3.32) and (3.33) on Ritz values from Subsection 3.2.3 are applicable, however, with strong assumptions on some initial Ritz values. Extending these estimates to arbitrarily located initial Ritz values can considerably improve their applicability. Based on the proof techniques of (3.32) and (3.33), we derive new estimates in two types: single-step estimates and multi-step estimates. The single-step estimates can also generalize the estimate (4.4) for simple restarting.

4.2.1 Single-step estimates

For investigating the general version of (1.29b) with $c \geq s \geq 1$, it does not make sense to consider the value $\mu(y^{(\ell)})$ as in (4.4) since the initial vector $y^{(\ell)}$ is usually not explicitly determined for $\ell > 0$. In the special case $c = s = 1$, the value $\mu(y^{(\ell)})$ coincides with the largest Ritz value $\theta_1^{(\ell-1)}$ of H in $\widehat{\mathcal{K}}^k(y^{(\ell-1)})$ for $\ell > 0$. Thus (4.4) can be rewritten as

$$\frac{\mu_j - \theta_1^{(\ell)}}{\theta_1^{(\ell)} - \mu_{j+1}} \leq [\,T_{k-1}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \theta_1^{(\ell-1)}}{\theta_1^{(\ell-1)} - \mu_{j+1}}.$$

By regarding this form, we aim to generalize (4.4) to the s largest Ritz values in the involved Krylov subspaces. The generalization is comparable with the estimate (3.33) for the standard Krylov subspace iteration (1.29a). Moreover, we shift the step index ℓ by 1 in order to formulate the resulting estimate in a conventional way. For completeness, we provide an additional estimate for the first step.

Theorem 4.7. *With Notation 1.4, consider the restarted Krylov subspace iteration* (1.29b) *where the subset $\widehat{\mathcal{K}}^c(y^{(\ell+1)})$ of $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$ is spanned by orthonormal Ritz vectors of H in $\widehat{\mathcal{K}}^k(y^{(\ell)})$ associated with the c largest Ritz values. Assume that the involved Krylov subspaces are not invariant subspaces, and denote by $\theta_1^{(\ell)} \geq \cdots \geq \theta_s^{(\ell)}$ the s largest Ritz values of H in $\widehat{\mathcal{K}}^k(y^{(\ell)})$ for $s \leq c$ and the step index ℓ. Then*

$$\theta_i^{(\ell+1)} > \theta_i^{(\ell)} \tag{4.15}$$

holds for each ℓ and each $i \in \{1,\dots,s\}$ so that the sequences $\big(\theta_i^{(\ell)}\big)_{\ell\in\mathbb{N}}$ are strictly increasing.

Furthermore, if $\mu_j > \theta_i^{(\ell)} > \mu_{j+1}$ is fulfilled for certain indices $i \in \{1,\dots,s\}$ and $j \in \{i,\dots,m-c+i-1\}$, then it holds, in terms of the gap ratio $\gamma_j = (\mu_j - \mu_{j+1})/(\mu_{j+1} - \mu_m)$ and the Chebyshev polynomial $T_{k-c}(\cdot)$, that

$$\frac{\mu_j - \theta_i^{(\ell+1)}}{\theta_i^{(\ell+1)} - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}. \tag{4.16}$$

In addition,

$$\frac{\mu_j - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \varphi_i}{\varphi_i - \mu_{j+1}} \tag{4.17}$$

holds for the ith largest Ritz value φ_i of H in the Krylov subspace $\widehat{\mathcal{K}}^c(y^{(0)})$ by assuming $\mu_j > \varphi_i > \mu_{j+1}$.

Proof. We first construct an auxiliary subspace $\mathcal{U}$ concerning the generating orthonormal Ritz vectors $u_1,\dots,u_c$ of $\widehat{\mathcal{K}}^c(y^{(\ell+1)})$. These Ritz vectors are selected from $\widehat{\mathcal{K}}^k(y^{(\ell)})$ by the iteration

(1.29b) and correspond to the c largest Ritz values $\theta_1^{(\ell)} \geq \cdots \geq \theta_c^{(\ell)}$. Since the statements of Theorem 4.7 are formulated for the ith largest Ritz value, we consider the subspace $\mathcal{U} = \operatorname{span}\{u_1, \ldots, u_i\}$. Evidently, $\mathcal{U}$ is a subset of $\widehat{\mathcal{K}}^c(y^{(\ell+1)})$. Moreover, $u_1, \ldots, u_i$ are automatically Ritz vectors of H in $\mathcal{U}$ associated with the Ritz values $\theta_1^{(\ell)} \geq \cdots \geq \theta_i^{(\ell)}$, and it holds that

$$\begin{aligned} H^t\,\mathcal{U} \;\subseteq\; H^t\,\widehat{\mathcal{K}}^c(y^{(\ell+1)}) \;&=\; H^t \operatorname{span}\{y^{(\ell+1)}, Hy^{(\ell+1)}, \ldots, H^{c-1}y^{(\ell+1)}\} \\ &=\; \operatorname{span}\{H^t y^{(\ell+1)}, H^{1+t}y^{(\ell+1)}, \ldots, H^{c-1+t}y^{(\ell+1)}\} \;\subseteq\; \widehat{\mathcal{K}}^k(y^{(\ell+1)}) \end{aligned}$$

for each $t \in \{0, \ldots, k-c\}$. This ensures that the block-Krylov subspace

$$\mathcal{K} = \operatorname{span}\{U, HU, \ldots, H^{k-c}U\}$$

with the basis matrix $U = [u_1, \ldots, u_i]$ of $\mathcal{U}$ is a subset of the Krylov subspace $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$. Thus the relation

$$\mathcal{U} \;\subseteq\; \mathcal{K} \;\subseteq\; \widehat{\mathcal{K}}^k(y^{(\ell+1)})$$

holds. According to the Courant-Fischer principles, we get

$$\theta_i^{(\ell)} \leq \theta_i \leq \theta_i^{(\ell+1)} \tag{4.18}$$

for the ith largest Ritz value θ_i of H in $\mathcal{K}$.

Next, we construct an auxiliary y concerning $\mathcal{U}$ and $\mathcal{K}$. We use orthonormal Ritz vectors $w_1, \ldots, w_d$ of H in $\mathcal{K}$ associated with the Ritz values $\theta_1 \geq \cdots \geq \theta_d$ where d denotes $\dim \mathcal{K}$. Then the intersection of the subspaces $\mathcal{U}$ and $\mathcal{W}_{i,d} = \operatorname{span}\{w_i, \ldots, w_d\}$ contains nonzero vectors according to

$$\dim\big(\mathcal{U} \cap \mathcal{W}_{i,d}\big) = \dim \mathcal{U} + \dim \mathcal{W}_{i,d} - \dim\big(\mathcal{U} + \mathcal{W}_{i,d}\big) \geq i + (d-i+1) - d = 1.$$

We select an arbitrary nonzero vector y from $\mathcal{U} \cap \mathcal{W}_{i,d}$. Then the vector $H^t y$ belongs to $\mathcal{K}$ for each $t \in \{0, \ldots, k-c\}$ because of

$$y \in \mathcal{U} \qquad \Rightarrow \qquad H^t y \;\in\; H^t\,\mathcal{U} \;=\; \operatorname{span}\{H^t U\} \;\subseteq\; \mathcal{K}.$$

In addition, $W^T H^t y = (W^T H W)^t (W^T y)$ holds for the Ritz basis matrix $W = [w_1, \ldots, w_d]$. We show this property inductively by considering that WW^T is the orthogonal projector on $\mathcal{K}$:

$$\begin{aligned} W^T H^t y &= W^T H H^{t-1} y = (W^T H)(W W^T)(H^{t-1} y) \\ &= (W^T H W)(W^T H^{t-1} y) = \cdots = (W^T H W)^t (W^T y). \end{aligned}$$

Consequently, the vector $H^t y$ can be represented by

$$H^t y = (WW^T)(H^t y) = W (W^T H W)^t (W^T y).$$

Therein $W^T H W$ is actually a diagonal matrix $\operatorname{diag}(\theta_1, \ldots, \theta_d)$ containing Ritz values. Moreover, since y belongs to $\mathcal{W}_{i,d} = \operatorname{span}\{w_i, \ldots, w_d\}$, the Ritz vectors $w_1, \ldots, w_{i-1}$ are orthogonal to y. In summary, we get

$$H^t y = W \begin{pmatrix} \theta_1 & & & & & \\ & \ddots & & & & \\ & & \theta_{i-1} & & & \\ & & & \theta_i & & \\ & & & & \ddots & \\ & & & & & \theta_d \end{pmatrix}^t \begin{pmatrix} 0 \\ \vdots \\ 0 \\ w_i^T y \\ \vdots \\ w_d^T y \end{pmatrix} = W \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \theta_i^t w_i^T y \\ \vdots \\ \theta_d^t w_d^T y \end{pmatrix} \in \mathcal{W}_{i,d}$$

for each $t \in \{0, \dots, k-c\}$ so that y has the property that

$$p(H)y \text{ belongs to } \mathcal{W}_{i,d} \text{ for an arbitrary real polynomial } p(\cdot) \text{ of degree } k-c. \tag{4.19}$$

Now the estimate (4.15) can be shown by contraposition. Since (4.18) implies $\theta_i^{(\ell+1)} \geq \theta_i^{(\ell)}$, we only need to exclude the equality $\theta_i^{(\ell+1)} = \theta_i^{(\ell)}$. If this equality holds, then (4.18) implies $\theta_i = \theta_i^{(\ell)}$. In addition, the property (4.19) shows that the Krylov subspace

$$\widetilde{\mathcal{K}} = \operatorname{span}\{y, Hy, \dots, H^{k-c}y\}$$

is a subset of $\mathcal{W}_{i,d}$. Then the relation

$$\theta_i^{(\ell)} = \min_{u \in \mathcal{U}\setminus\{0\}} \mu(u) \leq \mu(y) \leq \max_{w \in \widetilde{\mathcal{K}}\setminus\{0\}} \mu(w) \leq \max_{w \in \mathcal{W}_{i,d}\setminus\{0\}} \mu(w) = \theta_i.$$

holds due to $y \in \mathcal{U}\setminus\{0\}$, $y \in \widetilde{\mathcal{K}}\setminus\{0\}$ and $\widetilde{\mathcal{K}} \subseteq \mathcal{W}_{i,d}$. Combining this with $\theta_i = \theta_i^{(\ell)}$ yields

$$\mu(y) = \max_{w \in \widetilde{\mathcal{K}}\setminus\{0\}} \mu(w)$$

so that the initial vector y of the Krylov subspace $\widetilde{\mathcal{K}}$ is a maximizer of the Rayleigh quotient $\mu(\cdot)$ in $\widetilde{\mathcal{K}}$ and thus a Ritz vector. Then the residual $r = Hy - \mu(y)y$ belongs to $\widetilde{\mathcal{K}}$ because of $k > c$ and is orthogonal to $\widetilde{\mathcal{K}}$. Consequently, r is zero, and y is an eigenvector so that there exists an eigenvector in $\mathcal{U}$ and thus also in $\widehat{\mathcal{K}}^k(y^{(\ell)})$. This contradicts the assumption that $\widehat{\mathcal{K}}^k(y^{(\ell)})$ is not an invariant subspace; cf. Lemma 3.1.

The estimate (4.16) holds trivially in the case $\mu_j \leq \theta_i^{(\ell+1)}$ as the left-hand side is nonpositive. In the nontrivial case $\mu_j > \theta_i^{(\ell+1)}$, the relation (4.18) is extended as

$$\mu_j > \theta_i^{(\ell+1)} \geq \theta_i \geq \theta_i^{(\ell)} > \mu_{j+1}$$

due to the assumption $\theta_i^{(\ell)} > \mu_{j+1}$. Then the monotonicity of the function $\big(\mu_j - \cdot\,\big)/\big(\,\cdot - \mu_{j+1}\big)$ allows us to derive (4.16) from the intermediate estimate

$$\frac{\mu_j - \theta_i}{\theta_i - \mu_{j+1}} \leq \big[\,T_{k-c}(1 + 2\gamma_j)\,\big]^{-2} \, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}. \tag{4.20}$$

For proving (4.20), we use the auxiliary vector y together with a shifted Chebyshev polynomial $p(\cdot)$ defined by

$$p(\alpha) = T_{k-c}\left(1 + 2\,\frac{\alpha - \mu_{j+1}}{\mu_{j+1} - \mu_m}\right). \tag{4.21}$$

Therein $|p(\mu_l)| > 1$ holds for each $l \in \{1, \dots, j\}$ due to (1.36). This ensures that $p(H)y$ is nonzero since otherwise the eigenprojection $Q_l y$ would be zero for each $l \in \{1, \dots, j\}$, namely,

$$0 = Q_l\, p(H)y = p(\mu_l)\, Q_l y \quad \wedge \quad |p(\mu_l)| > 1 \qquad \Rightarrow \qquad Q_l y = 0,$$

and y would belong to the invariant subspace $\mathcal{Z}_{j+1} \oplus \cdots \oplus \mathcal{Z}_m$ so that

$$\mu_{j+1} \geq \mu(y) \geq \min_{u \in \mathcal{U}\setminus\{0\}} \mu(u) = \theta_i^{(\ell)}$$

holds and contradicts the assumption $\theta_i^{(\ell)} > \mu_{j+1}$. In addition, the property (4.19) shows that $p(H)y$ belongs to $\mathcal{W}_{i,d}$. Thus

$$p(H)y \in \mathcal{W}_{i,d}\setminus\{0\} \quad \Rightarrow \quad \mu\big(p(H)y\big) \leq \max_{w \in \mathcal{W}_{i,d}\setminus\{0\}} \mu(w) = \theta_i. \tag{4.22}$$

Subsequently, based on the proof of Theorem 3.8, we can verify that the vector

$$\widetilde{y} = p(\mu_j) \sum_{l=1}^{j} Q_l y + \sum_{l=j+1}^{m} Q_l y$$

possesses the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \qquad \text{and} \qquad \frac{\mu_j - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}}. \quad (4.23)$$

Combining (4.22) and the first property in (4.23) yields the relation $\theta_i \geq \mu\big(p(H)y\big) \geq \mu(\widetilde{y})$. Then the monotonicity of the function $\big(\mu_j - \,\cdot\,\big)/\big(\,\cdot\, - \mu_{j+1}\big)$ extends the second property in (4.23) as

$$\frac{\mu_j - \theta_i}{\theta_i - \mu_{j+1}} \leq \frac{\mu_j - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2}\, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}$$

which implies the intermediate estimate (4.20) and further the estimate (4.16).

The estimate (4.17) can be shown in a similar way by constructing the auxiliary subspace $\mathcal{U}$ with orthonormal Ritz vectors in $\widehat{\mathcal{K}}^c(y^{(0)})$. □

The main estimate (4.16) in Theorem 4.7 is a direct generalization of the estimate (4.4) for simple restarting, but not a direct extension of the estimate (3.33) for the standard Krylov subspace iteration (1.29a). The Chebyshev polynomial $T_{k-c}(\cdot)$ in (4.16) cannot be replaced by $T_{k-i}(\cdot)$ as in (3.33) for the sake of a more accurate bound, since $T_{k-i}(\cdot)$ demands the block-Krylov subspace $\operatorname{span}\{U, HU, \ldots, H^{k-i}U\}$ which is not necessarily a subset of the Krylov subspace $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$. Thus the proof of (4.16) cannot be adapted to $T_{k-i}(\cdot)$.

Furthermore, in the case $k - c = 2$, the Chebyshev term $[\,T_{k-c}(1+2\gamma_j)\,]^{-2}$ in (4.16) can be refined by the term $[\,q(\mu_j)\,]^{-2}$ from the estimate (4.14). The refinement in a more general case will be a topic in future work.

4.2.2 Multi-step estimates

The single-step estimate (4.16) for the restarted Krylov subspace iteration (1.29b) can be applied recursively and extended by the additional estimate (4.17). This results in the multi-step estimate

$$\frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}} \leq [\,T_{k-c}(1+2\gamma_j)\,]^{-2(\ell+1)}\, \frac{\mu_j - \varphi_i}{\varphi_i - \mu_{j+1}}. \quad (4.24)$$

However, the gap ratio γ_j can possibly lead to an overestimation in the case of clustered eigenvalues. Thus we prefer to derive a better multi-step estimate analogously to the estimate (3.32) from Theorem 3.8.

Theorem 4.8. *With the settings from Theorem 4.7, if the smallest Ritz value η of H in the Krylov subspace $\widehat{\mathcal{K}}^c(y^{(0)})$ fulfills $\mu_j > \eta > \mu_{j+1}$ for a certain $j \in \{c, \ldots, m-1\}$, then it holds, in terms of the gap ratio $\widetilde{\gamma}_{i,j} = (\mu_{j-c+i} - \mu_{j+1})/(\mu_{j+1} - \mu_m)$ and the Chebyshev polynomial $T_{k-c}(\cdot)$, that*

$$\frac{\mu_{j-c+i} - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}} \leq [\,T_{k-c}(1+2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\, \frac{\mu_{j-c+i} - \eta}{\eta - \mu_{j+1}}. \quad (4.25)$$

Proof. In the case $\mu_{j-c+i} \leq \theta_i^{(\ell)}$, (4.25) holds trivially since the left-hand side is nonpositive.

In the nontrivial case $\mu_{j-c+i} > \theta_i^{(\ell)}$, we consider the subspace iteration

$$\mathcal{Y}^{(t+1)} = p(H)\, \mathcal{Y}^{(t)} \quad (4.26)$$

with $\mathcal{Y}^{(-1)} = \widehat{\mathcal{K}}^c(y^{(0)})$ and the shifted Chebyshev polynomial $p(\cdot)$ defined by (4.21). The restarted Krylov subspace iteration (1.29b) is actually an acceleration of (4.26) since (1.29b) applies the Rayleigh-Ritz procedure to an extended subspace. Based on the Courant-Fischer principles, the relation $\theta_i^{(\ell)} \geq \eta_i^{(\ell)}$ holds for the ith largest Ritz value $\eta_i^{(\ell)}$ of H in $\mathcal{Y}^{(\ell)}$. In addition, the monotonicity of the function $\big(\mu_{j-c+i} - \cdot\big)/\big(\cdot - \mu_{j+1}\big)$ allows us to derive (4.25) from the intermediate estimate

$$\frac{\mu_{j-c+i} - \eta_i^{(\ell)}}{\eta_i^{(\ell)} - \mu_{j+1}} \leq \big[\,T_{k-c}(1 + 2\widetilde{\gamma}_{i,j})\,\big]^{-2(\ell+1)} \, \frac{\mu_{j-c+i} - \eta}{\eta - \mu_{j+1}}. \tag{4.27}$$

In order to show (4.27), we first verify that the subspace $\mathcal{Y}^{(\ell)}$ has at least dimension i so that the ith largest Ritz value $\eta_i^{(\ell)}$ exists. For this purpose, we define an orthonormal system $\{z_1, \ldots, z_m\}$ with respect to the eigenprojections $Q_l y^{(0)}$ of the initial vector $y^{(0)}$ as in (2.16). Then the dimension of the intersection of $\mathcal{Y}^{(-1)} = \widehat{\mathcal{K}}^c(y^{(0)})$ and the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1, \ldots, z_{j-c+i}, z_{j+1}, \ldots, z_m\}$ is at least i, namely,

$$\dim\big(\mathcal{Y}^{(-1)} \cap \mathcal{Z}\big) = \dim \mathcal{Y}^{(-1)} + \dim \mathcal{Z} - \dim\big(\mathcal{Y}^{(-1)} + \mathcal{Z}\big) \geq c + (m - c + i) - m = i.$$

Consequently, there exists an i-dimensional subspace $\widetilde{\mathcal{Y}} \subseteq \big(\mathcal{Y}^{(-1)} \cap \mathcal{Z}\big)$, and it holds that

$$\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}} \subseteq \Big(\big(p(H)\big)^{\ell+1}\mathcal{Y}^{(-1)} \cap \big(p(H)\big)^{\ell+1}\mathcal{Z}\Big) \subseteq \big(\mathcal{Y}^{(\ell)} \cap \mathcal{Z}\big).$$

Thus $\dim \mathcal{Y}^{(\ell)} \geq i$ can be verified by showing that $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}}$ has dimension i.

Therein we use an arbitrary basis matrix $\widetilde{Y} \in \mathbb{R}^{n\times i}$ of $\widetilde{\mathcal{Y}}$. Then the matrix product

$$\widetilde{Z}^T\widetilde{Y} \in \mathbb{R}^{j\times i} \qquad \text{with} \qquad \widetilde{Z} = [z_1, \ldots, z_j]$$

(note that $i \leq s \leq c \leq j$) has full rank, since otherwise there exists a nonzero vector $g \in \mathbb{R}^i$ with $\widetilde{Z}^T\widetilde{Y}g = 0$, i.e., the subspace $\widetilde{\mathcal{Y}}$ contains a nonzero vector $\widetilde{y} = \widetilde{Y}g$ which is orthogonal to $\operatorname{span}\{\widetilde{Z}\}$ and belongs to $\operatorname{span}\{z_{j+1}, \ldots, z_m\}$. Thus

$$\mu_{j+1} \;\geq\; \mu(\widetilde{y}) \;\geq\; \min_{w \in \widetilde{\mathcal{Y}}\setminus\{0\}} \mu(w) \;\geq\; \min_{w \in \mathcal{Y}^{(-1)}\setminus\{0\}} \mu(w) \;=\; \eta$$

holds and contradicts the assumption $\eta > \mu_{j+1}$. Based on that $\widetilde{Z}^T\widetilde{Y} \in \mathbb{R}^{j\times i}$ has full rank, the matrix product $\widetilde{Z}^T\Big(\big(p(H)\big)^{\ell+1}\widetilde{Y}\Big) \in \mathbb{R}^{j\times i}$ also has full rank by considering the transformation

$$\begin{aligned}
\widetilde{Z}^T\Big(\big(p(H)\big)^{\ell+1}\widetilde{Y}\Big) &= \widetilde{Z}^T\Big(\big(p(H)\big)^{\ell+1}\Big)^T\widetilde{Y} = \Big(\big(p(H)\big)^{\ell+1}\widetilde{Z}\Big)^T\widetilde{Y} \\
&= \Big(\big(p(H)\big)^{\ell+1}[z_1, \ldots, z_j]\Big)^T\widetilde{Y} = \Big(\Big[\big(p(\mu_1)\big)^{\ell+1}z_1, \ldots, \big(p(\mu_j)\big)^{\ell+1}z_j\Big]\Big)^T\widetilde{Y} \\
&= \Big([z_1, \ldots, z_j] \operatorname{diag}\Big(\big(p(\mu_1)\big)^{\ell+1}, \ldots, \big(p(\mu_j)\big)^{\ell+1}\Big)\Big)^T\widetilde{Y} \\
&= \operatorname{diag}\Big(\big(p(\mu_1)\big)^{\ell+1}, \ldots, \big(p(\mu_j)\big)^{\ell+1}\Big)\,\big(\widetilde{Z}^T\widetilde{Y}\big)
\end{aligned}$$

and the property $|p(\mu_l)| > 1$ for each $l \in \{1, \ldots, j\}$ due to (1.36) applied to (4.21). This ensures that $\big(p(H)\big)^{\ell+1}\widetilde{Y}$ has full rank so that $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}}$ has dimension i.

Next, we denote by α the smallest Ritz value in $\widetilde{\mathcal{Y}}$ and by β the smallest Ritz value (which is also the ith largest Ritz value) in $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}}$, then we get

$$\begin{aligned}
\widetilde{\mathcal{Y}} \subseteq \mathcal{Y}^{(-1)} \qquad &\Rightarrow \qquad \alpha \geq \eta > \mu_{j+1}, \\
\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}} \subseteq \mathcal{Y}^{(\ell)} \qquad &\Rightarrow \qquad \beta \leq \eta_i^{(\ell)} \leq \theta_i^{(\ell)} < \mu_{j-c+i}
\end{aligned}$$

by applying the Courant-Fischer principles to the smallest Ritz values α and η or to the ith largest Ritz values β and $\eta_i^{(\ell)}$. Therefore the intermediate estimate (4.27) can be shown by verifying the inequality

$$\frac{\mu_{j-c+i}-\beta}{\beta-\mu_{j+1}} \leq \big[\,T_{k-c}(1+2\widetilde{\gamma}_{i,j})\,\big]^{-2(\ell+1)}\,\frac{\mu_{j-c+i}-\alpha}{\alpha-\mu_{j+1}}. \tag{4.28}$$

Therein we use a Ritz vector $\widehat{w}$ in $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}}$ associated with β which can be represented by $\widehat{w}=\big(p(H)\big)^{\ell+1}w$ with a nonzero vector $w=\widetilde{Y}g\in\widetilde{\mathcal{Y}}$. Since $\widetilde{\mathcal{Y}}$ and $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{Y}}$ are subsets of the invariant subspace $\mathcal{Z}=\operatorname{span}\{z_1,\ldots,z_{j-c+i},z_{j+1},\ldots,z_m\}$, the vectors w and $\widehat{w}$ belong to $\mathcal{Z}$. Correspondingly, we define the auxiliary vector

$$\widetilde{w} \;=\; \big(p(\mu_{j-c+i})\big)^{\ell+1}\,\textstyle\sum_{l=1}^{j-c+i} z_l z_l^T w \;+\; \sum_{l=j+1}^{m} z_l z_l^T w.$$

Then the properties $\mu(\widehat{w})\geq\mu(\widetilde{w})\geq\mu(w)$ and

$$\frac{\mu_{j-c+i}-\mu(\widetilde{w})}{\mu(\widetilde{w})-\mu_{j+1}} \leq \big[\,T_{k-c}(1+2\widetilde{\gamma}_{i,j})\,\big]^{-2(\ell+1)}\,\frac{\mu_{j-c+i}-\mu(w)}{\mu(w)-\mu_{j+1}} \tag{4.29}$$

can be verified analogously to the properties (3.34) and (3.35) in the proof of Theorem 3.8. It is remarkable that the powered polynomial $\big(p(\cdot)\big)^{\ell+1}$ possesses similar properties as introduced in (3.37) related to (1.36). The verification of (4.28) is subsequently completed by extending (4.29) with the relation $\mu_{j-c+i}>\beta=\mu(\widehat{w})\geq\mu(\widetilde{w})\geq\mu(w)\geq\alpha>\mu_{j+1}$. □

The gap ratio $\widetilde{\gamma}_{i,j}$ in the estimate (4.25) can be bounded away from zero for sufficiently large c. Thus (4.25) can reasonably describe the cluster robustness of restarted Krylov subspace iterations. Based on (4.25), we aim to optimize the choice of the parameter c for implementing restarted Krylov subspace iterations in future work.

4.3 Reformulation for generalized matrix eigenvalue problems

In order to apply the main results in this chapter to restarted Krylov subspace iterations of the type (1.23), we reformulate them for generalized matrix eigenvalue problems with Notation 1.1.

Theorem 4.9. *With Notation 1.1, consider restarted Krylov subspace iterations of the type* (1.23) *where the subset $\mathcal{K}^c(x^{(\ell+1)})$ of $\mathcal{K}^k(x^{(\ell+1)})$ is spanned by A-orthonormal Ritz vectors of (A,M) in $\mathcal{K}^k(x^{(\ell)})$ associated with the c reciprocally largest Ritz values. Assume that the involved Krylov subspaces are not invariant subspaces, and denote by $\vartheta_1^{(\ell)},\ldots,\vartheta_s^{(\ell)}$ the s reciprocally largest Ritz values of (A,M) in $\mathcal{K}^k(x^{(\ell)})$ for $s\leq c$ and the step index ℓ. Then*

$$(\vartheta_i^{(\ell+1)})^{-1} \;>\; (\vartheta_i^{(\ell)})^{-1} \tag{4.30}$$

holds for each ℓ and each $i\in\{1,\ldots,s\}$ so that the Ritz value sequences $\big(\vartheta_i^{(\ell)}\big)_{\ell\in\mathbb{N}}$ are reciprocally strictly increasing.

Furthermore, if $\lambda_j^{-1}>\big(\vartheta_i^{(\ell)}\big)^{-1}>\lambda_{j+1}^{-1}$ is fulfilled for certain indices $i\in\{1,\ldots,s\}$ and $j\in\{i,\ldots,m-c+i-1\}$, then it holds, in terms of the gap ratio $\gamma_j=(\lambda_j^{-1}-\lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1}-\lambda_m^{-1})$ and the Chebyshev polynomial $T_{k-c}(\cdot)$, that

$$\frac{\lambda_j^{-1}-(\vartheta_i^{(\ell+1)})^{-1}}{(\vartheta_i^{(\ell+1)})^{-1}-\lambda_{j+1}^{-1}} \leq \big[\,T_{k-c}(1+2\gamma_j)\,\big]^{-2}\,\frac{\lambda_j^{-1}-(\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1}-\lambda_{j+1}^{-1}}. \tag{4.31}$$

In addition,

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(0)})^{-1}}{(\vartheta_i^{(0)})^{-1} - \lambda_{j+1}^{-1}} \le [\, T_{k-c}(1 + 2\gamma_j)\,]^{-2} \, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}} \tag{4.32}$$

holds for the ith reciprocally largest Ritz value α_i of (A, M) in the Krylov subspace $\mathcal{K}^c(x^{(0)})$ by assuming $\lambda_j^{-1} > \alpha_i^{-1} > \lambda_{j+1}^{-1}$. The corresponding multi-step estimate

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \le [\, T_{k-c}(1 + 2\gamma_j)\,]^{-2(\ell+1)} \, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}} \tag{4.33}$$

can be improved by

$$\frac{\lambda_{j-c+i}^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)} \, \frac{\lambda_{j-c+i}^{-1} - \beta^{-1}}{\beta^{-1} - \lambda_{j+1}^{-1}} \tag{4.34}$$

concerning clustered eigenvalues. Therein β is the reciprocally smallest Ritz value of (A, M) in $\mathcal{K}^c(x^{(0)})$ and assumed to fulfill $\lambda_j^{-1} > \beta^{-1} > \lambda_{j+1}^{-1}$ for a certain $j \in \{c, \ldots, m-1\}$, and the gap ratio $\widetilde{\gamma}_{i,j}$ is defined by $\widetilde{\gamma}_{i,j} = (\lambda_{j-c+i}^{-1} - \lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1} - \lambda_m^{-1})$.

If M is positive definite, then the concerned eigenvalues and Ritz values are positive so that the estimates in Theorem 4.9 can be formulated in a simpler way. For instance, (4.31) and (4.34) can be simplified as

$$\frac{\vartheta_i^{(\ell+1)} - \lambda_j}{\lambda_{j+1} - \vartheta_i^{(\ell+1)}} \le [\, T_{k-c}(1 + 2\gamma_j)\,]^{-2} \, \frac{\vartheta_i^{(\ell)} - \lambda_j}{\lambda_{j+1} - \vartheta_i^{(\ell)}}$$

and

$$\frac{\vartheta_i^{(\ell)} - \lambda_{j-c+i}}{\lambda_{j+1} - \vartheta_i^{(\ell)}} \le [\, T_{k-c}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)} \, \frac{\beta - \lambda_{j-c+i}}{\lambda_{j+1} - \beta}.$$

5 Block-Krylov subspace iterations

The block implementation of standard Krylov subspace iterations enables the determination of entire eigenspaces associated with multiple eigenvalues. Therein the block size, i.e., the dimension of the initial subspace, can be set equal to a presumed upper bound of the multiplicities of the target eigenvalues. Moreover, the cluster robustness is expected to be improved based on the analysis of the block power method by Rutishauser [97]. Indeed, a basic idea from [97] on constructing auxiliary vectors orthogonal to certain eigenvectors has also been utilized by Saad [98] and Knyazev [44, 45] for investigating block-Krylov subspace iterations; see the corresponding estimates introduced in Theorems 2.3 and 2.5. In Saad's analysis, an auxiliary vector $\widetilde{y}$ is set orthogonal to the eigenvectors associated with the eigenvalues $\mu_{i+1}, \ldots, \mu_{i+s-1}$ in order to obtain a sufficiently large gap ratio $(\mu_i - \mu_{i+s})/(\mu_{i+s} - \mu_n)$. However, this overlooks the case that the eigenvalues $\mu_1, \ldots, \mu_i$ are clustered. Consequently, some ratio-products in the resulting bounds could be very large. In Knyazev's analysis, several auxiliary vectors y_j for $j \in \{1, \ldots, s\}$ are set orthogonal to the eigenvectors associated with the eigenvalues μ_l for $l \in \{1, \ldots, s\} \backslash \{j\}$. Then another gap ratio $(\mu_i - \mu_{s+1})/(\mu_{s+1} - \mu_n)$ can be obtained by using the auxiliary subspace $\operatorname{span}\{y_1, \ldots, y_i\}$ which is orthogonal to the eigenvectors associated with the eigenvalues $\mu_{i+1}, \ldots, \mu_s$. This results in better bounds without problematic ratio-products. A further benefit is that these auxiliary vectors can be eliminated in the final form of the estimates. It is remarkable that Saad's estimates have been improved by Yang and Yang in [121, Theorem 2.5] as well as by Li and Zhang in [62, Theorems 4.1 and 5.1]. The analysis from [121] can be modified in order to derive a better estimate as in Theorem 3.3. The analysis from [62] aims to estimate invariant subspaces instead of single eigenvectors, and Ritz value sums instead of single Ritz values. Nevertheless, as mentioned in [62, Section 6], the resulting estimates cannot directly be compared with Saad's estimates.

In this chapter, we investigate block-Krylov subspace iterations of the type (1.24) in terms of the reciprocal representation (1.29c). We denote by $\mathcal{K}$ and Y the block-Krylov subspace $\widehat{\mathcal{K}}^k(Y^{(0)})$ and an associated basis matrix $Y^{(0)}$ of the initial subspace. In particular, we extend Knyazev's analysis in order to achieve directly comparable improvements of Saad's estimates. In Section 5.1, we consider (1.29c) with sufficiently large block sizes. Therein the dimension t of the initial subspace is not less than an index $c \geq s$ for which the eigenvalue μ_{c+1} is well separated from the smallest target eigenvalue μ_s. The new results include estimates on approximate eigenvectors, Ritz values and Ritz vectors. Section 5.2 deals with small block sizes, i.e., the case $t < c$ regarding the above-mentioned setting in Section 5.1. This case is of greater practical interest for reducing the storage requirement. The estimates from Section 5.1 can easily be modified by using a new interpretation of the considered Block-Krylov subspace. In Section 5.3, the achieved results are reformulated for the description (1.24) of block-Krylov subspace iterations.

5.1 Estimates for large block sizes

We begin with a summary of Saad's estimates for block-Krylov subspace iterations. Analogously to Lemma 3.1, we can adapt Theorem 2.3 to a nontrivial case by assuming that the considered block-Krylov subspace is not an invariant subspace. Moreover, we prefer to denote by t the dimension of the initial subspace and by s the number of target eigenvalues since these two sizes are not necessarily equal in practice. Concerning clustered eigenvalues, the size of a possible eigenvalue cluster containing the target eigenvalues is denoted by c. The main estimates from

Theorem 2.3 can be reformulated with respect to these practical settings as follows.

Theorem 5.1. *With Notation 1.5, consider a block-Krylov subspace*

$$\mathcal{K} = \operatorname{span}\{Y, HY, \dots, H^{k-1}Y\}$$

with a basis matrix $Y \in \mathbb{R}^{n\times t}$ of the initial subspace $\mathcal{Y}$, and assume that $\mathcal{K}$ is not an invariant subspace. Let $\mu_1, \dots, \mu_s$ be the target eigenvalues, and let the eigenvalues μ_s and μ_{c+1} be well separated for an index $c \geq s$. Then the following estimates hold for each $i \in \{1, \dots, s\}$.

(I) An estimate on approximate eigenvectors: The intersection of the subspaces $\mathcal{Y}$ and $\widehat{\mathcal{Z}} = \operatorname{span}\{z_1, \dots, z_i, z_{i+t} \dots, z_n\}$ contains a nonzero vector $\widehat{y}$. By using $\widehat{y}$ as an auxiliary vector, it holds, in terms of the set σ_i of all distinct eigenvalues larger than μ_i, the cardinality $\#\sigma_i$ of σ_i, the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1, \dots, z_i\}$, the gap ratio $\widehat{\gamma}_i = (\mu_i - \mu_{i+t})/(\mu_{i+t} - \mu_n)$, and the Chebyshev polynomial $T_{k-1-\#\sigma_i}(\cdot)$, that

$$\tan \angle_2\big(z_i, \mathcal{K}\big) \leq \frac{\prod_{\mu\in\sigma_i} \frac{\mu-\mu_n}{\mu-\mu_i}}{T_{k-1-\#\sigma_i}(1+2\widehat{\gamma}_i)} \, \frac{\sin \angle_2(\widehat{y}, \mathcal{Z})}{|\cos \angle_2(\widehat{y}, z_i)|}. \tag{5.1}$$

(II) An angle-dependent estimate on Ritz values: In addition to (I), denote by $\theta_1 \geq \cdots \geq \theta_s$ the s largest Ritz values of H in $\mathcal{K}$, then it holds, in terms of the set $\widetilde{\sigma}_i$ of all distinct Ritz values larger than θ_i, and the cardinality $\#\widetilde{\sigma}_i$ of $\widetilde{\sigma}_i$, that

$$\mu_i - \theta_i \leq (\mu_i - \mu_n) \left(\frac{\prod_{\theta\in\widetilde{\sigma}_i} \frac{\theta-\mu_n}{\theta-\mu_i}}{T_{k-1-\#\widetilde{\sigma}_i}(1+2\widehat{\gamma}_i)} \, \frac{\sin \angle_2(\widehat{y}, \mathcal{Z})}{\cos \angle_2(\widehat{y}, z_i)} \right)^2 \tag{5.2}$$

where $\theta_{i-1} > \mu_i$ is assumed in the case $i > 1$.

The auxiliary vector $\widehat{y}$ in Theorem 5.1 is constructed in a natural way. The existence of $\widehat{y}$ is ensured by the dimension inequality

$$\dim\big(\mathcal{Y} \cap \widehat{\mathcal{Z}}\big) = \dim \mathcal{Y} + \dim \widehat{\mathcal{Z}} - \dim\big(\mathcal{Y} + \widehat{\mathcal{Z}}\big) \geq t + (n-t+1) - n = 1.$$

In comparison to the auxiliary vector $\widetilde{y}$ in Theorem 2.3, $\widehat{y}$ is not unique and can be orthogonal to z_i. Therefore $\cos \angle_2(\widehat{y}, z_i)$ is not necessarily positive, and the estimates (5.1) and (5.2) include the practically rare case that the bounds are infinite. In addition, by modifying the proof of [121, Theorem 2.5], the estimate (5.2) can be slightly improved; cf. Theorem 3.3. The improved estimate reads

$$\mu_i - \theta_i \leq (\mu_i - \mu_n)\frac{\zeta}{1+\zeta} \qquad \text{with} \qquad \zeta = \left(\frac{\prod_{\theta\in\widetilde{\sigma}_i} \frac{\theta-\mu_n}{\theta-\mu_i}}{T_{k-1-\#\widetilde{\sigma}_i}(1+2\widehat{\gamma}_i)} \, \frac{\sin \angle_2(\widehat{y}, \mathcal{Z})}{\cos \angle_2(\widehat{y}, z_i)} \right)^2. \tag{5.3}$$

Furthermore, if the dimension t of the initial subspace $\mathcal{Y}$ is not less than c, then the gap ratio $\widehat{\gamma}_i$ can be bounded away from zero due to the obvious relation

$$\mu_i \geq \mu_s \gg \mu_{c+1} \geq \mu_{t+1} \geq \mu_{i+t}\,.$$

Consequently, the Chebyshev factors in the estimates (5.1), (5.2) and (5.3) are reasonable for $t \geq c$. However, the ratio-products $\prod_{\mu\in\sigma_i} \frac{\mu-\mu_n}{\mu-\mu_i}$ and $\prod_{\theta\in\widetilde{\sigma}_i} \frac{\theta-\mu_n}{\theta-\mu_i}$ could be very large if the eigenvalues $\mu_1, \dots, \mu_i$ are clustered. The following analysis aims to overcome this drawback.

5.1.1 Estimates on approximate eigenvectors

We first improve the estimate (5.1) on approximate eigenvectors which corresponds to Saad's estimate (2.6). The problematic ratio-product $\prod_{\mu\in\sigma_i}\frac{\mu-\mu_n}{\mu-\mu_i}$ arises from the multiplication of the auxiliary vector $\widehat{y}$ or $\widetilde{y}$ with linear factors $H-\mu I$ for $\mu>\mu_i$; cf. Remark 2.6. In order to eliminate this ratio-product in the bound, we construct another auxiliary vector which belongs to the invariant subspace associated with $\mu_i, \mu_{t+1}, \ldots, \mu_n$. Then μ_i is the first relevant eigenvalue in the corresponding analysis so that linear factors $H-\mu I$ for $\mu>\mu_i$ are not required. Moreover, the auxiliary vector can be eliminated at the end of the derivation.

Theorem 5.2. *With the settings from Theorem 5.1, if the dimension t of $\mathcal{Y}$ is not less than c, then it holds for each $i\in\{1,\ldots,s\}$, in terms of the invariant subspace $\mathcal{Z}^t=\operatorname{span}\{z_1,\ldots,z_t\}$, the gap ratio $\gamma_{i,t}=(\mu_i-\mu_{t+1})/(\mu_{t+1}-\mu_n)$ and the Chebyshev polynomial $T_{k-1}(\cdot)$, that*

$$\tan\angle_2(z_i,\mathcal{K})\le\left[T_{k-1}(1+2\gamma_{i,t})\right]^{-1}\tan\angle_2(\mathcal{Y},\mathcal{Z}^t). \tag{5.4}$$

Proof. The estimate (5.4) holds trivially in the case $\tan\angle_2(\mathcal{Y},\mathcal{Z}^t)=\infty$. In the nontrivial case $\tan\angle_2(\mathcal{Y},\mathcal{Z}^t)<\infty$, we use an arbitrary nonzero vector y from the intersection of $\mathcal{Y}$ and the invariant subspace $\mathcal{Z}=\operatorname{span}\{z_i,z_{t+1},\ldots,z_n\}$ associated with the eigenvalues $\mu_i,\mu_{t+1},\ldots,\mu_n$. The existence of y is based on the fact that $\mathcal{Y}\cap\mathcal{Z}$ has at least dimension 1, namely,

$$\dim\big(\mathcal{Y}\cap\mathcal{Z}\big)=\dim\mathcal{Y}+\dim\mathcal{Z}-\dim\big(\mathcal{Y}+\mathcal{Z}\big)\ge t+(n-t+1)-n=1.$$

For deriving (5.4), we define a shifted Chebyshev polynomial $p(\cdot)$ by

$$p(\alpha)=T_{k-1}\left(1+2\,\frac{\alpha-\mu_{t+1}}{\mu_{t+1}-\mu_n}\right), \tag{5.5}$$

and consider y together with the vector $w=p(H)y$. Since y belongs to $\mathcal{Z}$, the eigenexpansion $y=\sum_{l=1}^n\alpha_l\,z_l$ with $\alpha_l=z_l^Ty$ is reduced to

$$y=\alpha_i\,z_i+\textstyle\sum_{l=t+1}^n\alpha_l\,z_l.$$

Thus w has the expansion

$$w=p(H)y=p(\mu_i)\,\alpha_i\,z_i+\textstyle\sum_{l=t+1}^n p(\mu_l)\,\alpha_l\,z_l.$$

Moreover, the coefficient α_i is nonzero since otherwise y belongs to the orthogonal complement $\operatorname{span}\{z_{t+1},\ldots,z_n\}$ of $\mathcal{Z}^t$ so that $\frac{1}{2}\pi=\angle_2(y,\mathcal{Z}^t)\le\angle_2(\mathcal{Y},\mathcal{Z}^t)$ holds and contradicts the condition $\tan\angle_2(\mathcal{Y},\mathcal{Z}^t)<\infty$ of the current case. Then we show the intermediate estimate

$$\tan^2\angle_2\big(z_i,w\big)\le\left[T_{k-1}(1+2\gamma_{i,t})\right]^{-2}\tan^2\angle_2(z_i,y) \tag{5.6}$$

as follows: The representation

$$\cos^2\angle_2(z_i,y)=\left(\frac{z_i^Ty}{\|z_i\|_2\,\|y\|_2}\right)^2=\frac{(z_i^Ty)^2}{\|y\|_2^2}=\frac{\alpha_i^2}{\alpha_i^2+\sum_{l=t+1}^n\alpha_l^2}$$

based on (1.31) is equivalent to $\tan^2\angle_2(z_i,y)=\big(\sum_{l=t+1}^n\alpha_l^2\big)/\alpha_i^2$. Analogously, we get

$$\tan^2\angle_2\big(z_i,w\big)=\frac{\sum_{l=t+1}^n p^2(\mu_l)\,\alpha_l^2}{p^2(\mu_i)\,\alpha_i^2}.$$

Combining these representations with the properties

$$p(\mu_i)>1\qquad\text{and}\qquad|p(\mu_l)|\le1\quad\forall\,l\in\{t+1,\ldots,n\}$$

based on (1.36) yields

$$\tan^2 \angle_2\big(z_i, w\big) \le \frac{\sum_{l=t+1}^{n} \alpha_l^2}{p^2(\mu_i)\,\alpha_i^2} \overset{(5.5)}{=} \big[\,T_{k-1}(1+2\gamma_{i,t})\,\big]^{-2} \tan^2 \angle_2(z_i, y)$$

so that (5.6) holds.

Finally, we obtain (5.4) by extending (5.6) with the relations

$$\tan^2 \angle_2(z_i, \mathcal{K}) \le \tan^2 \angle_2\big(z_i, w\big) \quad \text{and} \quad \tan^2 \angle_2(z_i, y) = \tan^2 \angle_2(y, \mathcal{Z}^t) \le \tan^2 \angle_2(\mathcal{Y}, \mathcal{Z}^t).$$

Therein the first relation is ensured by

$$y \in \mathcal{Y} = \operatorname{span}\{Y\} \quad \Rightarrow \quad w = p(H)y \in \operatorname{span}\{Y, HY, \dots, H^{k-1}Y\} = \mathcal{K}$$

and (1.32). The equality in the second relation is shown by

$$\tan^2 \angle_2(y, \mathcal{Z}^t) = \left(\frac{\big\| \sum_{l=t+1}^{n} Q_l y \big\|_2}{\big\| \sum_{l=1}^{t} Q_l y \big\|_2} \right)^2 = \frac{\big\| \sum_{l=t+1}^{n} \alpha_l\, z_l \big\|_2^2}{\big\| \alpha_i\, z_i \big\|_2^2} = \frac{\sum_{l=t+1}^{n} \alpha_l^2}{\alpha_i^2} = \tan^2 \angle_2(z_i, y)$$

based on (1.33), whereas the inequality follows from (1.32). The resulting quadratic representation of (5.4) is equivalent to (5.4) since the concerned tangent values $\tan \angle_2(z_i, \mathcal{K})$ and $\tan \angle_2(\mathcal{Y}, \mathcal{Z}^t)$ are nonnegative due to (1.32). □

The proof of Theorem 5.2 is partially analogous to that of Theorem 3.4. An essential difference is that the auxiliary vector y for Theorem 5.2 is built by the intersection of two subspaces. The choice of y is inspired by Rutishauser's analysis of the block power method [97].

The estimate (5.4) has a simple and concise form in comparison to (5.1). The bound does not depend on auxiliary vectors and ratio-products. This improves the applicability and the accuracy of the estimate, especially in the case of clustered eigenvalues. An earlier improvement has been presented in [122, Theorem 1] where the construction of auxiliary vectors is similar to that in Theorem 2.3, i.e., concerning the linear independence of the orthogonal projections of certain eigenvectors to the initial subspace $\mathcal{Y}$.

Moreover, the estimate (5.4) also holds in H-angles provided that H is positive definite. The proof is analogous to that of Corollary 3.5.

Corollary 5.3. *With the settings from Theorems 5.1 and 5.2, assume that H is positive definite so that H-angles $\angle_H(\,\cdot\,,\,\cdot\,)$ can be defined as in Definition 1.6. Then the variant of the estimate (5.4) with $\angle_H(\,\cdot\,,\,\cdot\,)$ instead of $\angle_2(\,\cdot\,,\,\cdot\,)$ holds.*

5.1.2 Angle-dependent estimates on Ritz values

The angle-dependent estimate (5.2) on Ritz values also contains an auxiliary vector and a ratio-product as in (5.1). For improving (5.2), we note that Knyazev's analysis from [45, Section 2] concerning an abstract subspace iteration results in a suitable angle-dependent estimate. This estimate has been formulated as (2.12) in Theorem 2.5 for a comparison with Saad's estimate (2.8), and can be reformulated with respect to the practical settings mentioned at the beginning of Section 5.1 as follows.

Theorem 5.4. *With the settings from Theorem 5.1, if the dimension t of $\mathcal{Y}$ is not less than c, then it holds for each $i \in \{1, \dots, s\}$, in terms of the invariant subspace $\mathcal{Z}^t = \operatorname{span}\{z_1, \dots, z_t\}$, the gap ratio $\gamma_{i,t} = (\mu_i - \mu_{t+1})/(\mu_{t+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-1}(\cdot)$, that*

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_n} \le \big[\,T_{k-1}(1+2\gamma_{i,t})\,\big]^{-2} \tan^2 \angle_2(\mathcal{Y}, \mathcal{Z}^t). \tag{5.7}$$

Proof. The proof is based on the arguments for block-Krylov subspaces introduced in Lemmas 2.9 and 2.10; cf. the paragraph before Remark 2.11.

Since (5.7) is trivial for $\tan \angle_2(\mathcal{Y}, \mathcal{Z}^t) = \infty$, we only need to consider the nontrivial case $\tan \angle_2(\mathcal{Y}, \mathcal{Z}^t) < \infty$. Therein Lemma 2.10 is applicable by setting $s = t$, $\mathcal{Z} = \mathcal{Z}^t$ and $\gamma_i = \gamma_{i,t}$. Consequently, one can construct an auxiliary subspace $\mathcal{Y}^i = \operatorname{span}\{y_1, \dots, y_i\}$ with unique vectors $y_j \in \mathcal{Y}$, $j = 1, \dots, t$, satisfying $y_j^T z_j = 1$ and $y_j^T z_l = 0$ for each $l \in \{1, \dots, t\} \setminus \{j\}$. A further auxiliary subspace $\mathcal{U} = p(H)\mathcal{Y}^i$ is constructed with the shifted Chebyshev polynomial $p(\cdot)$ defined by (5.5). Then the estimate (2.34) results in

$$\tan \angle_2\big(\mathcal{U}, \mathcal{Z}^i\big) \le [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-1} \tan \angle_2\big(\mathcal{Y}, \mathcal{Z}^t\big)$$

with the invariant subspace $\mathcal{Z}^i = \operatorname{span}\{z_1, \dots, z_i\}$. In addition, the subspace $\mathcal{U}$ has dimension i and is a subset of the block-Krylov subspace $\mathcal{K}$. Then Lemma 2.9 is applicable by setting $\mathcal{V} = \mathcal{K}$ and $\widetilde{\mathcal{Z}} = \mathcal{Z}^i$. The estimate (2.30) leads to

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_n} \le \tan^2 \angle_2\big(\mathcal{U}, \mathcal{Z}^i\big) \le \Big([\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-1} \tan \angle_2\big(\mathcal{Y}, \mathcal{Z}^t\big)\Big)^2$$

so that (5.7) holds. □

Furthermore, the estimate (5.7) can easily be compared with the estimates (5.2) and (5.3) by using the equivalent form

$$\mu_i - \theta_i \le (\mu_i - \mu_n)\,\frac{\zeta}{1 + \zeta} \qquad \text{with} \qquad \zeta = [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-2} \tan^2 \angle_2(\mathcal{Y}, \mathcal{Z}^t).$$

The comparison shows certain advantages of (5.7), namely, the assumption $\theta_{i-1} > \mu_i$ is not required and the bound does not depend on the auxiliary vector $\widehat{y}$ or the Ritz values in the current block-Krylov subspace.

5.1.3 Angle-free estimates on Ritz values

The angle terms in the bounds of angle-dependent estimates are still improvable. The improvement is especially desirable for low-dimensional block-Krylov subspaces where the Chebyshev factors are not sufficiently small. An angle-free estimate based on Knyazev's analysis from [45, Section 2] has already been introduced as (2.13) in Theorem 2.5. Its reformulation with respect to the practical settings mentioned at the beginning of Section 5.1 reads

$$\frac{\mu_t - \theta_t}{\theta_t - \mu_{t+1}} \le [\,T_{k-1}(1 + 2\gamma_t)\,]^{-2}\,\frac{\mu_t - \eta}{\eta - \mu_{t+1}}. \tag{5.8}$$

Therein η denotes the smallest Ritz value of H in $\mathcal{Y}$ and the gap ratio γ_t is defined by $\gamma_t = (\mu_t - \mu_{t+1})/(\mu_{t+1} - \mu_n)$. However, (5.8) concerns only one Ritz value θ_t, and the corresponding eigenvalue μ_t is not necessarily a target eigenvalue due to $t \ge c \ge s$. Therefore it is meaningful to extend (5.8) to the s largest Ritz values which approximate the target eigenvalues.

Theorem 5.5. *With the settings from Theorem 5.1, if the dimension t of $\mathcal{Y}$ is not less than c, and the smallest Ritz value η of H in $\mathcal{Y}$ fulfills $\eta > \mu_{t+1}$, then it holds for each $i \in \{1, \dots, s\}$, in terms of the gap ratio $\gamma_{i,t} = (\mu_i - \mu_{t+1})/(\mu_{t+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-1}(\cdot)$, that*

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_{t+1}} \le [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-2}\,\frac{\mu_i - \eta}{\eta - \mu_{t+1}}. \tag{5.9}$$

Proof. We first construct two auxiliary subspaces similarly to the proof of Theorem 5.4. By using the invariant subspace $\mathcal{Z}^t = \operatorname{span}\{z_1, \ldots, z_t\}$, the assumption $\eta > \mu_{t+1}$ ensures that $\angle_2(\mathcal{Y}, \mathcal{Z}^t)$ is smaller than $\pi/2$, since otherwise there exists a nonzero vector $y \in \mathcal{Y}$ with $\angle_2(y, \mathcal{Z}^t) = \pi/2$ according to (1.31), then y belongs to $\operatorname{span}\{z_{t+1}, \ldots, z_n\}$ so that $\mu_{t+1} \geq \mu(y) \geq \eta$ holds and contradicts $\eta > \mu_{t+1}$. Then Lemma 2.10 is applicable by setting $s = t$ and $\mathcal{Z} = \mathcal{Z}^t$. Consequently, there exist unique vectors $y_j \in \mathcal{Y}$, $j = 1, \ldots, t$, satisfying $y_j^T z_j = 1$ and $y_j^T z_l = 0$ for each $l \in \{1, \ldots, t\} \backslash \{j\}$. In addition, we get two i-dimensional auxiliary subspaces

$$\mathcal{Y}^i = \operatorname{span}\{y_1, \ldots, y_i\} \qquad \text{and} \qquad \mathcal{U} = p(H)\mathcal{Y}^i$$

with the shifted Chebyshev polynomial $p(\cdot)$ defined by (5.5). The orthogonality $y_j^T z_l = 0$ ensures that $\mathcal{Y}^i$ is a subset of the invariant subspace $\operatorname{span}\{z_1, \ldots, z_i, z_{t+1}, \ldots, z_n\}$, i.e., for each $y \in \mathcal{Y}^i$, the eigenexpansion $y = \sum_{l=1}^n z_l z_l^T y$ is reduced to

$$y = \textstyle\sum_{l=1}^i z_l z_l^T y + \sum_{l=t+1}^n z_l z_l^T y. \tag{5.10}$$

The next part of the proof is analogous to the proof of Theorem 3.8. Thus we skip some lengthy details. We denote by $\widetilde{\eta}_1 \geq \cdots \geq \widetilde{\eta}_i$ the Ritz values of H in $\mathcal{U}$, and consider a Ritz vector u associated with $\widetilde{\eta}_i$. According to $\mathcal{U} = p(H)\mathcal{Y}^i$, we represent u by $u = p(H)y$ with a corresponding nonzero vector $y \in \mathcal{Y}^i$. Subsequently, we construct the vector

$$\widetilde{y} \;=\; p(\mu_i) \textstyle\sum_{l=1}^i z_l z_l^T y \;+\; \sum_{l=t+1}^n z_l z_l^T y$$

based on the expansion (5.10), and verify that $\widetilde{y}$ possesses the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \tag{5.11}$$

and

$$\frac{\mu_i - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{t+1}} \leq \big[\,T_{k-1}(1 + 2\gamma_{i,t})\,\big]^{-2} \, \frac{\mu_i - \mu(y)}{\mu(y) - \mu_{t+1}}. \tag{5.12}$$

The property (5.11) is verified by showing the inequalities

$$\mu\big(p(H)y\big) \geq \mu(y), \qquad \mu\big(p(H)y\big) \geq \mu(\widetilde{y}), \qquad \mu(\widetilde{y}) \geq \mu(y)$$

in a row by using Lemma 2.14 restricted to the invariant subspace $\operatorname{span}\{z_1, \ldots, z_i, z_{t+1}, \ldots, z_n\}$; cf. the verification of (3.34) in the proof of Theorem 3.8.

The property (5.12) is verified analogously to (3.35). Therein we use the representations

$$y = z + \widetilde{z} \qquad \text{and} \qquad \widetilde{y} = p(\mu_i)z + \widetilde{z}$$

with the parts $z = \sum_{l=1}^i z_l z_l^T y$ and $\widetilde{z} = \sum_{l=t+1}^n z_l z_l^T y$. Then the case $z = 0$ can be excluded by the relation $\mu(y) \geq \eta > \mu_{t+1}$. In addition, if $\widetilde{z} = 0$, we can show that $\mu(\widetilde{y}) = \mu(y) = \mu_i$ so that (5.12) holds trivially. If $\widetilde{z} \neq 0$, then the value $\mu(\widetilde{z})$ can be defined, and the intermediate estimate

$$\left(\frac{\mu(z) - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu(\widetilde{z})}\right)\left(\frac{\mu(z) - \mu(y)}{\mu(y) - \mu(\widetilde{z})}\right)^{-1} = \left(\frac{1}{|p(\mu_i)|}\right)^2 = \big[\,T_{k-1}(1 + 2\gamma_{i,t})\,\big]^{-2} \tag{5.13}$$

holds; cf. (2.44) in the proof of Lemma 2.13. Subsequently, the relation $\mu(z) \geq \mu_i \geq \mu(\widetilde{y}) \geq \mu(y) > \mu_{t+1} \geq \mu(\widetilde{z})$ based on (5.11) implies

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

Combining this with (5.13) yields (5.12).

Finally, the relation $\theta_i \geq \widetilde{\eta}_i = \mu(u) = \mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \geq \eta$ based on the Courant-Fischer principles and (5.11) extends (5.12) as the estimate (5.9) by using the monotonicity of the function $\big(\mu_i - \cdot\big)/\big(\cdot - \mu_{t+1}\big)$. □

A remarkable advantage of the angle-free estimate (5.9) against the angle-dependent estimate (5.7) is that the convergence measure $\big(\mu_i - \cdot\big)/\big(\cdot - \mu_{t+1}\big)$ enables a direct generalization for investigating a series of block-Krylov subspaces arising from restarted block-Krylov subspace iterations. Moreover, by slightly modifying the proof of (5.9), a similar estimate

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_{i+1}} \leq [\,T_{k-1}(1 + 2\gamma_i)\,]^{-2}\, \frac{\mu_i - \eta_i}{\eta_i - \mu_{i+1}} \tag{5.14}$$

can be shown for the ith largest Ritz value η_i of H in the initial subspace $\mathcal{Y}$. In Chapter 6, we improve the applicability of (5.9) and (5.14) by generalizing them to arbitrarily located Ritz values η and η_i.

5.1.4 Additional estimates on Ritz vectors

The Ritz value estimates from Subsections 5.1.2 and 5.1.3 can be combined with the additional estimates on Ritz vectors introduced in Theorem 2.5. A similar but more accurate Ritz vector estimate has been derived in Theorem 3.11 concerning a Krylov subspace and Notation 1.4. A slight modification of its proof results in the following counterpart concerning an arbitrary subspace and Notation 1.5.

Theorem 5.6. *With Notation 1.5, let $u_1, \ldots, u_s$ be orthonormal Ritz vectors of H in a subspace $\mathcal{U} \subseteq \mathbb{R}^n$ associated with the s largest Ritz values $\theta_1 \geq \cdots \geq \theta_s$. If $\theta_j > \mu_{j+1}$ for each $j \in \{1, \ldots, s\}$, then it holds that*

$$\sin^2 \angle_2(u_i, z_i) \leq 1 - \left(\prod_{j=1,\ j\neq i}^{s+1} \frac{\theta_i - \mu_j}{\mu_i - \mu_j} \right) \left(\prod_{j=1,\ j\neq i}^{s} \frac{\mu_i - \theta_j}{\theta_i - \theta_j} \right). \tag{5.15}$$

In Theorem 5.6, the eigenvectors z_i are directly given by Notation 1.5 and do not depend on the subspace $\mathcal{U}$. In contrast to this, the eigenvectors z_i in Theorem 3.11 are related to eigenprojections of the initial vector of the concerned Krylov subspace.

A limitation of Theorem 5.6 is that the assumption $\theta_j > \mu_{j+1}$ is only reasonable in the case that the s largest eigenvalues are distinct; cf. Theorem 2.5. The following variant regarding a multiple eigenvalue has been suggested in [44, 45], however, without proof. Thus we add a proof which is based on some arguments from [47] concerning the simpler estimate (2.14).

Theorem 5.7. *With Notation 1.5, let $u_1, \ldots, u_s$ be orthonormal Ritz vectors of H in a subspace $\mathcal{U} \subseteq \mathbb{R}^n$ associated with the s largest Ritz values $\theta_1 \geq \cdots \geq \theta_s$. Consider the subspaces $\mathcal{U}_i = \operatorname{span}\{u_i, \ldots, u_{i+a}\}$ and $\mathcal{Z}_i = \operatorname{span}\{z_i, \ldots, z_{i+a}\}$ for certain i and a with $2 \leq i \leq i + a \leq s$. If $\mu_{i-1} > \mu_i = \cdots = \mu_{i+a} > \mu_{i+a+1}$, i.e., $\mu_i, \ldots, \mu_{i+a}$ correspond to a multiple eigenvalue, and the Ritz values fulfill $\theta_{i-1} \geq \mu_i$, $\theta_{i+a} \geq \mu_{i+a+1}$, $\theta_{i-1} > \theta_i$, then it holds that*

$$\sin^2 \angle_2\big(\mathcal{U}_i, \mathcal{Z}_i\big) \leq 1 - \frac{(\mu_1 - \theta_{i+a})(\theta_{i+a} - \mu_{i+a+1})(\theta_{i-1} - \mu_i)}{(\mu_1 - \mu_i)(\mu_i - \mu_{i+a+1})(\theta_{i-1} - \theta_{i+a})} \tag{5.16}$$

Proof. If $\mu_i = \theta_{i-1}$, the bound in (5.16) is equal to 1 so that the inequality holds trivially. Otherwise, it holds that $\theta_{i-1} > \mu_i$ due to $\mu_i \neq \theta_{i-1}$ and the assumption $\theta_{i-1} \geq \mu_i$.

For deriving (5.16) in the case $\theta_{i-1} > \mu_i$, we represent $\sin^2 \angle_2(\mathcal{U}_i, \mathcal{Z}_i)$ by $\sin^2 \angle_2(u, z)$ with certain auxiliary vectors u and z. We first select a normalized vector $u \in \mathcal{U}_i$ satisfying

$$\sin^2 \angle_2(u, \mathcal{Z}_i) = \max_{\widehat{u} \in \mathcal{U}_i \setminus \{0\}} \sin^2 \angle_2(\widehat{u}, \mathcal{Z}_i) = \sin^2 \angle_2(\mathcal{U}_i, \mathcal{Z}_i).$$

Subsequently, we construct a normalized vector $z \in \mathcal{Z}_i$ by using u and the orthogonal projector $P_i = \sum_{l=i}^{i+a} Q_l$ on $\mathcal{Z}_i$. If $P_i u \neq 0$, we set $z = P_i u / \|P_i u\|_2$, then $\|z\|_2 = \|u\|_2 = 1$ so that

$$\cos \angle_2(u, z) \overset{(1.31)}{=} u^T z = \frac{u^T P_i u}{\|P_i u\|_2} = \frac{u^T P_i^2 u}{\|P_i u\|_2} = \frac{u^T P_i^T P_i u}{\|P_i u\|_2} = \frac{\|P_i u\|_2^2}{\|P_i u\|_2} = \|P_i u\|_2, \tag{5.17}$$

and consequently

$$\sin^2 \angle_2(u, z) = 1 - \|P_i u\|_2^2 = \|u\|_2^2 - \|P_i u\|_2^2 = \|u - P_i u\|_2^2 \overset{(1.33)}{=} \sin^2 \angle_2(u, \mathcal{Z}_i).$$

If $P_i u = 0$, i.e., $u \perp \mathcal{Z}_i$, we select an arbitrary normalized vector from $\mathcal{Z}_i$ as z, then $u \perp z$ holds so that $\angle_2(u, z) = \pi/2 = \angle_2(u, \mathcal{Z}_i)$. Thus we get

$$\sin^2 \angle_2(u, z) = \sin^2 \angle_2(u, \mathcal{Z}_i) = \sin^2 \angle_2(\mathcal{U}_i, \mathcal{Z}_i)$$

in both cases for constructing z.

Next, we derive an estimate on $\sin^2 \angle_2(u, z)$ by using two auxiliary subspaces analogously to the proof of Lemma 2.17. We set $\mathcal{V} = \operatorname{span}\{v_1, v_2\}$ and $\mathcal{W} = \operatorname{span}\{v_1, v_2, z\} = \mathcal{V} + \operatorname{span}\{z\}$ where v_2 is simply

$$v_2 = u$$

and the definition of v_1 depends on P_i and the orthogonal projectors

$$Q = \sum_{l=1}^{i-1} Q_l, \qquad \widetilde{Q} = \sum_{l=i+a+1}^{n} Q_l, \qquad P = zz^T$$

on the subspaces $\mathcal{Z} = \operatorname{span}\{z_1, \ldots, z_{i-1}\}$, $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{i+a+1}, \ldots, z_n\}$, $\operatorname{span}\{z\}$.

For defining v_1, we construct two auxiliary vectors $\widetilde{u}$ and $\widetilde{v}$.

The vector $\widetilde{u}$ is constructed in $\widetilde{\mathcal{U}} = \operatorname{span}\{u_1, \ldots, u_{i-1}\}$ with respect to v_2 and $\mathcal{Z}$. If v_2 is orthogonal to $\mathcal{Z}$, we select an arbitrary nonzero vector from $\widetilde{\mathcal{U}}$ as $\widetilde{u}$. Otherwise, we use the orthonormal basis matrices $\widetilde{U} = [u_1, \ldots, u_{i-1}]$ and $Z = [z_1, \ldots, z_{i-1}]$, and define $\widetilde{u} = \widetilde{U} g$ with the unique solution g of the linear system $(Z^T \widetilde{U}) g = Z^T v_2$. Then $\widetilde{u}$ is nonzero and fulfills $Q\widetilde{u} = Q v_2$; cf. the construction of $v = \widetilde{U} g$ in the proof of Lemma 2.17.

In order to construct $\widetilde{v}$, we use the fact that $\mathcal{Z}_i = \operatorname{span}\{z_i, \ldots, z_{i+a}\}$ is an eigenspace due to the assumption $\mu_i = \cdots = \mu_{i+a}$. Then the above-constructed vector z belonging to $\mathcal{Z}_i$ is a normalized eigenvector, and it holds for the orthogonal projectors P and P_i that

$$\begin{aligned} PH &= zz^T H = z\,(Hz)^T = z\,(\mu_i z)^T = \mu_i zz^T = \mu_i P, \\ P_i H &= \textstyle\sum_{l=i}^{i+a} Q_l H = \sum_{l=i}^{i+a} z_l z_l^T H = \sum_{l=i}^{i+a} \mu_i z_l z_l^T = \mu_i P_i. \end{aligned} \tag{5.18}$$

Moreover, the relation $P_i u = P u$ holds in both cases for constructing z. If $P_i u \neq 0$, we have

$$z = P_i u / \|P_i u\|_2 \qquad \Rightarrow \qquad P_i u = \|P_i u\|_2\, z \overset{(5.17)}{=} (u^T z) z = zz^T u = P u.$$

If $P_i u = 0$, it holds that $u \perp \mathcal{Z}_i$ so that $u \perp z$, $z^T u = 0$, and thus $P u = zz^T u = 0 = P_i u$. In addition, we get

$$P_i H u \overset{(5.18)}{=} \mu_i P_i u = \mu_i P u \overset{(5.18)}{=} P H u.$$

Based on $P_i u = Pu$ and $P_i Hu = PHu$, we define $\widetilde{v}$ by

$$\widetilde{v} = \big(Q + P + \widetilde{Q}\big)\widetilde{u}$$

so that $\widetilde{v}$ has the properties

$$\widetilde{v}^T v_2 = \widetilde{u}^T\big(Q + P + \widetilde{Q}\big)u = \widetilde{u}^T\big(Q + P_i + \widetilde{Q}\big)u = \widetilde{u}^T u = 0,$$
$$\widetilde{v}^T H v_2 = \widetilde{u}^T\big(Q + P + \widetilde{Q}\big)Hu = \widetilde{u}^T\big(Q + P_i + \widetilde{Q}\big)Hu = \widetilde{u}^T Hu = 0.$$

Therein $\widetilde{u}^T u = 0$ and $\widetilde{u}^T Hu = 0$ hold because of $\widetilde{u} \in \widetilde{\mathcal{U}}$, $u \in \mathcal{U}_i$, $\widetilde{\mathcal{U}} \perp \mathcal{U}_i$ and $\widetilde{\mathcal{U}} \perp H\mathcal{U}_i$.

A further property $\mu(\widetilde{v}) \geq \mu(\widetilde{u})$ can be verified by Lemma 2.14 as follows. Since P_i can be represented by $P_i = \sum_{l=i}^{i+a} \widetilde{z}_l \widetilde{z}_l^T$ with an arbitrary orthonormal basis $\{\widetilde{z}_i, \dots, \widetilde{z}_{i+a}\}$ of $\mathcal{Z}_i$, we select such an orthonormal basis with $\widetilde{z}_i = z$. Then $\widetilde{u}$ can be expanded as

$$\widetilde{u} \;=\; \big(Q + P_i + \widetilde{Q}\big)\widetilde{u} \;=\; Q\widetilde{u} + (\widetilde{z}_i^T\widetilde{u})\widetilde{z}_i + \textstyle\sum_{l=i+1}^{i+a}(\widetilde{z}_l^T\widetilde{u})\widetilde{z}_l + \widetilde{Q}\widetilde{u}. \tag{5.19}$$

Combining this with the definition of $\widetilde{v}$ and the orthogonality between projectors yields

$$\widetilde{v} \;=\; \big(Q + P + \widetilde{Q}\big)\widetilde{u} \;\overset{(5.19)}{=}\; Q\widetilde{u} + (\widetilde{z}_i^T\widetilde{u})\widetilde{z}_i + \widetilde{Q}\widetilde{u} \;=\; Q\widetilde{u} + (\widetilde{z}_i^T\widetilde{u})\widetilde{z}_i + \textstyle\sum_{l=i+1}^{i+a} 0\,\widetilde{z}_l + \widetilde{Q}\widetilde{u}. \tag{5.20}$$

This allows us to regard $\widetilde{u}$ and $\widetilde{v}$ as u and v in Lemma 2.14, namely, we apply Lemma 2.14 to the final expansions in (5.19) and (5.20) by symbolizing the associated coefficients with α_l and β_l. Then α_l and β_l coincide for each $l \leq i$ and each $l \geq i+a+1$, and $\beta_l = 0$ for the other indices. In addition, since $\widetilde{u}$ belongs to $\widetilde{\mathcal{U}}$ spanned by the Ritz vectors $u_1, \dots, u_{i-1}$, the relation $\mu(\widetilde{u}) \geq \theta_{i-1} > \mu_i$ holds and ensures $\mu_j \geq \mu(\widetilde{u}) \geq \mu_{j+1}$ for an index $j \in \{1, \dots, i-1\}$. Thus the description of α_l and β_l is updated concerning the index j as

$$|\beta_l| = |\alpha_l| \quad \forall\, l \leq j \qquad \text{and} \qquad |\beta_l| \leq |\alpha_l| \quad \forall\, l > j$$

so that the statement (a) in Lemma 2.14 implies $\mu(\widetilde{v}) \geq \mu(\widetilde{u})$.

In summary, the auxiliary vector $\widetilde{v}$ fulfills

$$\widetilde{v}^T v_2 = \widetilde{v}^T H v_2 = 0, \qquad \mu(\widetilde{v}) \geq \mu(\widetilde{u}) \geq \theta_{i-1} > \mu_i. \tag{5.21}$$

Then we define v_1 by $v_1 = \widetilde{v}/\|\widetilde{v}\|_2$ so that (5.21) leads to

$$[v_1, v_2]^T[v_1, v_2] = \operatorname{diag}(1, 1) \qquad \text{and} \qquad [v_1, v_2]^T H[v_1, v_2] = \operatorname{diag}\big(\mu(v_1), \mu(v_2)\big).$$

Thus v_1 and v_2 are orthonormal Ritz vectors in the subspace $\mathcal{V} = \operatorname{span}\{v_1, v_2\}$. According to (5.21) and the Courant-Fischer principles, the Ritz values $\xi_1 = \mu(v_1)$ and $\xi_2 = \mu(v_2)$ fulfill

$$\xi_1 = \mu(v_1) = \mu(\widetilde{v}) \geq \theta_{i-1} > \mu_i \geq \theta_i = \max_{\widehat{u} \in \mathcal{U}_i \setminus \{0\}} \mu(\widehat{u}) \geq \mu(u) = \mu(v_2) = \xi_2. \tag{5.22}$$

Next, we observe $\mathcal{V}$ within the subspace $\mathcal{W}$. The vectors v_1 and v_2 are linear independent due to (5.21). This ensures $\dim \mathcal{V} = 2$, and $\dim \mathcal{W} \in \{2, 3\}$ holds because of $\mathcal{W} = \mathcal{V} + \operatorname{span}\{z\}$.

In the case $\dim \mathcal{W} = 2$, the eigenvector z belongs to $\mathcal{V}$ and is thus a Ritz vector in $\mathcal{V}$. More precisely, z belongs to either $\operatorname{span}\{v_1\}$ or $\operatorname{span}\{v_2\}$ since the Ritz values ξ_1 and ξ_2 are distinct due to (5.22). However, if $z \in \operatorname{span}\{v_1\}$, then it holds that $\mu_i = \mu(z) = \mu(v_1) = \xi_1$ which contradicts the relation $\xi_1 > \mu_i$ from (5.22). Thus $z \in \operatorname{span}\{v_2\}$, and z is collinear with u because of $v_2 = u$, then $\sin^2 \angle_2\big(\mathcal{U}_i, \mathcal{Z}_i\big) = \sin^2 \angle_2(u, z) = 0$ so that the estimate (5.16) holds trivially.

In the case $\dim \mathcal{W} = 3$, we denoted by $\varphi_1 \geq \varphi_2 \geq \varphi_3$ the Ritz values in $\mathcal{W}$. Then the relation $\varphi_3 \leq \mu_{i+a+1}$ can be verified by using a nonzero vector from the intersection of $\mathcal{W} = \operatorname{span}\{v_1, v_2, z\}$ and $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{i+a+1}, \dots, z_n\}$.

We first show the existence of such a vector concerning the construction of v_1, namely, $v_1 = \widetilde{v}/\|\widetilde{v}\|_2$ with $\widetilde{v} = \big(Q + P + \widetilde{Q}\big)\widetilde{u}$ and $\widetilde{u} \in \operatorname{span}\{u_1, \dots, u_{i-1}\}\backslash\{0\}$ where $Q\widetilde{u} = Qv_2$ holds in the subcase that v_2 is not orthogonal to $\mathcal{Z} = \operatorname{span}\{z_1, \dots, z_{i-1}\}$. A useful property is

$$P_i v_2 = P_i u = \|P_i u\|_2\, z$$

based on the definition $v_2 = u$ and the construction of z (including the trivial case $P_i u = 0$).

If v_2 is orthogonal to $\mathcal{Z}$, i.e., the projection Qv_2 is zero, then the vector $v = v_2 - \|P_i u\|_2\, z$ belonging to $\mathcal{W}$ also belongs to $\widetilde{\mathcal{Z}}$, namely,

$$v = v_2 - \|P_i u\|_2\, z = v_2 - P_i v_2 = \big(Qv_2 + P_i v_2 + \widetilde{Q}v_2\big) - P_i v_2 = \widetilde{Q}v_2 \in \widetilde{\mathcal{Z}}.$$

Moreover, v is nonzero since otherwise v_2 is either zero or collinear with z so that $\dim \mathcal{W} = 2$.

If v_2 is not orthogonal to $\mathcal{Z}$, then $Q\widetilde{u} = Qv_2$ holds so that

$$\begin{aligned}
\mathcal{W} = \operatorname{span}\{v_1,\ v_2,\ z\} &= \operatorname{span}\{\widetilde{v},\ v_2,\ z\} = \operatorname{span}\big\{\big(Q + P + \widetilde{Q}\big)\widetilde{u},\ Qv_2 + P_i v_2 + \widetilde{Q}v_2,\ z\big\}\\
&= \operatorname{span}\big\{Q\widetilde{u} + (z^T\widetilde{u})z + \widetilde{Q}\widetilde{u},\ Qv_2 + \|P_i u\|_2\, z + \widetilde{Q}v_2,\ z\big\}\\
&= \operatorname{span}\big\{Q\widetilde{u} + \widetilde{Q}\widetilde{u},\ Qv_2 + \widetilde{Q}v_2,\ z\big\} = \operatorname{span}\big\{Q\widetilde{u} + \widetilde{Q}\widetilde{u},\ Q\widetilde{u} + \widetilde{Q}v_2,\ z\big\}.
\end{aligned}$$

Subsequently, the vector $v = \big(Q\widetilde{u} + \widetilde{Q}v_2\big) - \big(Q\widetilde{u} + \widetilde{Q}\widetilde{u}\big)$ from $\mathcal{W}$ fulfills $v = \widetilde{Q}v_2 - \widetilde{Q}\widetilde{u}$ and thus belongs to $\widetilde{\mathcal{Z}}$. Moreover, v is nonzero since otherwise $\mathcal{W}$ coincides with $\operatorname{span}\{Q\widetilde{u} + \widetilde{Q}\widetilde{u},\ z\}$ and thus has dimension 2.

Therefore there exists a nonzero vector v in $\mathcal{W} \cap \widetilde{\mathcal{Z}}$ in both subcases. Consequently, we get

$$\varphi_3 = \min_{w \in \mathcal{W}\backslash\{0\}} \mu(w) \leq \mu(v) \leq \max_{\widetilde{z} \in \widetilde{\mathcal{Z}}\backslash\{0\}} \mu(\widetilde{z}) = \mu_{i+a+1}.$$

Combining this with the assumption $\mu_i = \mu_{i+a} > \mu_{i+a+1}$ and the relation $\xi_1 > \mu_i$ from (5.22) yields

$$\varphi_1 \geq \xi_1 > \mu_i > \mu_{i+a+1} \geq \varphi_3. \tag{5.23}$$

In addition, since the eigenvector z is a Ritz vector in $\mathcal{W}$, the eigenvalue $\mu_i = \mu(z)$ is a Ritz value belonging to the set $\{\varphi_1, \varphi_2, \varphi_3\}$. Then $\mu_i = \varphi_2$ holds according to (5.23). Correspondingly, z can be denoted by w_2 within a basis $\{w_1, w_2, w_3\}$ consisting of orthonormal Ritz vectors in $\mathcal{W}$ associated with $\varphi_1, \varphi_2, \varphi_3$.

Finally, $\sin^2 \angle_2(u, z)$ is determined analogously to the proof of Lemma 2.17, namely,

$$\sin^2 \angle_2(u, z) = \sin^2 \angle_2(v_2, w_2) = \sin^2 \angle_2(w_2, v_2) = 1 - \frac{(\varphi_1 - \xi_2)(\xi_2 - \varphi_3)(\xi_1 - \varphi_2)}{(\varphi_1 - \varphi_2)(\varphi_2 - \varphi_3)(\xi_1 - \xi_2)},$$

cf. (2.51). Then, by using the relations

$$\varphi_1 \leq \mu_1, \qquad \varphi_2 = \mu_i, \qquad \varphi_3 \leq \mu_{i+a+1}, \qquad \xi_1 \geq \theta_{i-1}$$

based on (5.22), we get

$$\frac{\varphi_1 - \xi_2}{\varphi_1 - \varphi_2} = \frac{\varphi_1 - \xi_2}{\varphi_1 - \mu_i} \geq \frac{\mu_1 - \xi_2}{\mu_1 - \mu_i}, \quad \frac{\xi_2 - \varphi_3}{\varphi_2 - \varphi_3} = \frac{\xi_2 - \varphi_3}{\mu_i - \varphi_3} \geq \frac{\xi_2 - \mu_{i+a+1}}{\mu_i - \mu_{i+a+1}}, \quad \frac{\xi_1 - \varphi_2}{\xi_1 - \xi_2} = \frac{\xi_1 - \mu_i}{\xi_1 - \xi_2} \geq \frac{\theta_{i-1} - \mu_i}{\theta_{i-1} - \xi_2}$$

so that

$$\sin^2 \angle_2(u,z) \le 1 - \frac{(\mu_1-\xi_2)(\xi_2-\mu_{i+a+1})(\theta_{i-1}-\mu_i)}{(\mu_1-\mu_i)(\mu_i-\mu_{i+a+1})(\theta_{i-1}-\xi_2)}. \tag{5.24}$$

Moreover, by using $\xi_2 = \mu(u) \ge \theta_{i+a} \ge \mu_{i+a+1}$, it holds that

$$\frac{\mu_1-\xi_2}{\theta_{i-1}-\xi_2} \ge \frac{\mu_1-\theta_{i+a}}{\theta_{i-1}-\theta_{i+a}}, \qquad \xi_2-\mu_{i+a+1} \ge \theta_{i+a}-\mu_{i+a+1}.$$

Combining this with (5.24) and $\sin^2 \angle_2(u,z) = \sin^2 \angle_2\big(\mathcal{U}_i, \mathcal{Z}_i\big)$ yields the estimate (5.16). □

In future work, we aim to improve the estimate (5.16) by using more Ritz values in order to achieve a more accurate bound. The main challenge is the generalization of the central part of the proof, i.e., the definition of v_1.

5.2 Estimates for small block sizes

In this section, we investigate block-Krylov subspace iterations with small block sizes. Concerning the reciprocal representation (1.29c) and the practical settings mentioned at the beginning of Section 5.1, we consider the case that the dimension t of the initial subspace is less than the cluster parameter c.

In this case, the eigenvalues μ_i and μ_{i+t} are not necessarily well separated so that the gap ratio $\widehat{\gamma}_i$ in the estimates (5.1), (5.2) and (5.3) could be close to zero. The corresponding Chebyshev factors are thus not suitable. Fortunately, the main estimates for large block sizes presented in Section 5.1 can easily be modified by interpreting the block-Krylov subspace $\mathcal{K}$ as a superset of an auxiliary block-Krylov subspace.

Lemma 5.8. *With the settings from Theorem 5.1, assume that the dimension t of $\mathcal{Y}$ is less than c, and select a low-dimensional block-Krylov subspace $\mathcal{K}^b = \operatorname{span}\{Y, HY, \ldots, H^{b-1}Y\}$ satisfying*

$$\dim \operatorname{span}\{Y, HY, \ldots, H^{b-2}Y\} < c \le d = \dim \mathcal{K}^b.$$

Then $\mathcal{K} = \operatorname{span}\{Y, HY, \ldots, H^{k-1}Y\}$ is a superset of the auxiliary block-Krylov subspace

$$\widetilde{\mathcal{K}} = \operatorname{span}\big\{\widetilde{Y}, H\widetilde{Y}, \ldots, H^{k-b}\widetilde{Y}\big\}$$

with a basis matrix $\widetilde{Y} \in \mathbb{R}^{n\times d}$ of the initial subspace $\widetilde{\mathcal{Y}} = \mathcal{K}^b$.

Proof. For each $t \in \{0, \ldots, k-b\}$, it holds that

$$\begin{aligned} \operatorname{span}\big\{H^t\widetilde{Y}\big\} &= H^t\widetilde{\mathcal{Y}} = H^t\mathcal{K}^b = H^t\operatorname{span}\{Y, HY, \ldots, H^{b-1}Y\} \\ &= \operatorname{span}\{H^tY, H^{1+t}Y, \ldots, H^{b-1+t}Y\} \subseteq \mathcal{K}. \end{aligned}$$

Thus the relation $\widetilde{\mathcal{K}} \subseteq \mathcal{K}$ holds. □

This interpretation of $\mathcal{K}$ is indeed inspired by the construction of the auxiliary block-Krylov subspace $\operatorname{span}\{U, HU, \ldots, H^{k-c}U\}$ in the proof of Theorem 4.7. Applying the results from Section 5.1 to the auxiliary block-Krylov subspace $\widetilde{\mathcal{K}}$ leads to suitable estimates for block-Krylov subspace iterations with small block sizes. The bounds depend on the initial subspace $\widetilde{\mathcal{Y}} = \mathcal{K}^b$.

Theorem 5.9. *With the settings from Theorem 5.1, if the dimension t of $\mathcal{Y}$ is less than c, then the following estimates hold for each $i \in \{1, \ldots, s\}$, in terms of the low-dimensional block-Krylov subspace $\mathcal{K}^b$ from Lemma 5.8, the invariant subspace $\mathcal{Z}^d = \operatorname{span}\{z_1, \ldots, z_d\}$, the gap ratio $\gamma_{i,d} = (\mu_i - \mu_{d+1})/(\mu_{d+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-b}(\cdot)$.*

(I) An estimate on approximate eigenvectors:

$$\tan \angle_2(z_i, \mathcal{K}) \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-1} \tan \angle_2(\mathcal{K}^b, \mathcal{Z}^d). \tag{5.25}$$

(II) An angle-dependent estimate on Ritz values:

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_n} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \tan^2 \angle_2(\mathcal{K}^b, \mathcal{Z}^d). \tag{5.26}$$

(III) An angle-free estimates on Ritz values:

$$\frac{\mu_i - \theta_i}{\theta_i - \mu_{d+1}} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \frac{\mu_i - \widetilde{\eta}}{\widetilde{\eta} - \mu_{d+1}} \tag{5.27}$$

where the smallest Ritz value $\widetilde{\eta}$ of H in $\mathcal{K}^b$ is assumed to be larger than μ_{d+1}.

Proof. For proving the estimate (5.25), we apply Theorem 5.2 to the auxiliary block-Krylov subspace $\widetilde{\mathcal{K}}$ with the initial subspace $\widetilde{\mathcal{Y}} = \mathcal{K}^b$ based on Lemma 5.8. By considering $\dim \widetilde{\mathcal{Y}} = d$ and that $\widetilde{\mathcal{K}}$ has degree $k - b + 1$, we get

$$\tan \angle_2(z_i, \widetilde{\mathcal{K}}) \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-1} \tan \angle_2(\mathcal{K}^b, \mathcal{Z}^d) \tag{5.28}$$

from the estimate (5.4). In addition, the relation $\widetilde{\mathcal{K}} \subseteq \mathcal{K}$ from Lemma 5.8 implies the inequality $\tan \angle_2(z_i, \mathcal{K}) \leq \tan \angle_2(z_i, \widetilde{\mathcal{K}})$ according to (1.32). Thus (5.25) follows from (5.28).

The proof of (5.26) is analogous. Applying Theorem 5.4 to $\widetilde{\mathcal{K}}$ yields

$$\frac{\mu_i - \widetilde{\theta}_i}{\widetilde{\theta}_i - \mu_n} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \tan^2 \angle_2(\mathcal{K}^b, \mathcal{Z}^d) \tag{5.29}$$

based on (5.7). Therein $\widetilde{\theta}_i$ is the ith largest Ritz value of H in $\widetilde{\mathcal{K}}$. Then $\widetilde{\theta}_i \leq \theta_i$ holds according to $\widetilde{\mathcal{K}} \subseteq \mathcal{K}$ and the Courant-Fischer principles. Subsequently, an extension of (5.29) due to the monotonicity of the function $(\mu_i - \cdot)/(\cdot - \mu_n)$ results in (5.26).

Finally, the estimate (5.27) is proved by applying Theorem 5.5 to $\widetilde{\mathcal{K}}$. Therein the estimate (5.9) turns into

$$\frac{\mu_i - \widetilde{\theta}_i}{\widetilde{\theta}_i - \mu_{d+1}} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \frac{\mu_i - \widetilde{\eta}}{\widetilde{\eta} - \mu_{d+1}}$$

which implies (5.27) by using $\widetilde{\theta}_i \leq \theta_i$ and the monotonicity of the function $(\mu_i - \cdot)/(\cdot - \mu_{d+1})$. □

In Theorem 5.9, the gap ratio $\gamma_{i,d}$ can be bounded away from zero because of $\mu_i \geq \mu_s \gg \mu_{c+1} \geq \mu_{d+1}$. This enables a reasonable description of the cluster robustness of block-Krylov subspace iterations with small block sizes. Furthermore, the Ritz value estimates (5.26) and (5.27) can be extended as Ritz vector estimates by using the additional estimates from Theorems 5.6 and 5.7.

5.3 Reformulation for generalized matrix eigenvalue problems

We reformulate the new estimates achieved in this chapter in terms of generalized matrix eigenvalue problems with Notation 1.2. The results are directly applicable to block-Krylov subspace iterations of the type (1.24), and generalize the corresponding estimates for standard Krylov subspace iterations listed in Theorem 3.12.

Theorem 5.10. *With Notation 1.2, consider a block-Krylov subspace*

$$\mathcal{K} = \operatorname{span}\{X,\, A^{-1}MX,\, \ldots,\, (A^{-1}M)^{k-1}X\}$$

with a basis matrix $X \in \mathbb{R}^{n\times t}$ *of the initial subspace* $\mathcal{X}$*, and assume that* $\mathcal{K}$ *is not an invariant subspace. Let* $\lambda_1, \ldots, \lambda_s$ *be the target eigenvalues, and let the eigenvalues* λ_s *and* λ_{c+1} *be well separated for an index* $c \geq s$*. Then the following estimates hold for each* $i \in \{1, \ldots, s\}$*.*

(I) Estimates on approximate eigenvectors: If the dimension t *of* $\mathcal{X}$ *is not less than* c*, then it holds, in terms of the invariant subspace* $\mathcal{W}^t = \operatorname{span}\{w_1, \ldots, w_t\}$*, the gap ratio* $\gamma_{i,t} = (\lambda_i^{-1} - \lambda_{t+1}^{-1})/(\lambda_{t+1}^{-1} - \lambda_n^{-1})$ *and the Chebyshev polynomial* $T_{k-1}(\cdot)$*, that*

$$\tan \angle_A(w_i, \mathcal{K}) \leq [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-1} \tan \angle_A(\mathcal{X}, \mathcal{W}^t). \tag{5.30}$$

If t *is less than* c*, one can select a low-dimensional block-Krylov subspace* $\mathcal{K}^b = \operatorname{span}\{X,$ $A^{-1}MX,\, \ldots,\, (A^{-1}M)^{b-1}X\}$ *satisfying*

$$\dim \operatorname{span}\{X,\, A^{-1}MX,\, \ldots,\, (A^{-1}M)^{b-2}X\} < c \leq d = \dim \mathcal{K}^b.$$

Then it holds, in terms of the invariant subspace $\mathcal{W}^d = \operatorname{span}\{w_1, \ldots, w_d\}$*, the gap ratio* $\gamma_{i,d} = (\lambda_i^{-1} - \lambda_{d+1}^{-1})/(\lambda_{d+1}^{-1} - \lambda_n^{-1})$ *and the Chebyshev polynomial* $T_{k-b}(\cdot)$*, that*

$$\tan \angle_A(w_i, \mathcal{K}) \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-1} \tan \angle_A(\mathcal{K}^b, \mathcal{W}^d). \tag{5.31}$$

(II) Angle-dependent estimates on Ritz values: In addition to (I), denote by $\vartheta_1, \ldots, \vartheta_s$ *the* s *reciprocally largest Ritz values of* (A, M) *in* $\mathcal{K}$*. If the dimension* t *of* $\mathcal{X}$ *is not less than* c*, then it holds that*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_n^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-2} \tan^2 \angle_A(\mathcal{X}, \mathcal{W}^t). \tag{5.32}$$

If t *is less than* c*, then*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_n^{-1}} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \tan^2 \angle_A(\mathcal{K}^b, \mathcal{W}^d). \tag{5.33}$$

(III) Angle-free estimates on Ritz values: In addition to (II), if the dimension t *of* $\mathcal{X}$ *is not less than* c*, and the reciprocally smallest Ritz value* α *of* (A, M) *in* $\mathcal{X}$ *fulfills* $\alpha^{-1} > \lambda_{t+1}^{-1}$*, then it holds that*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_{t+1}^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-2} \frac{\lambda_i^{-1} - \alpha^{-1}}{\alpha^{-1} - \lambda_{t+1}^{-1}}. \tag{5.34}$$

If t *is less than* c*, and the reciprocally smallest Ritz value* $\widetilde{\alpha}$ *of* (A, M) *in* $\mathcal{K}^b$ *fulfills* $\widetilde{\alpha}^{-1} > \lambda_{d+1}^{-1}$*, then*

$$\frac{\lambda_i^{-1} - \vartheta_i^{-1}}{\vartheta_i^{-1} - \lambda_{d+1}^{-1}} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2} \frac{\lambda_i^{-1} - \widetilde{\alpha}^{-1}}{\widetilde{\alpha}^{-1} - \lambda_{d+1}^{-1}}. \tag{5.35}$$

(IV) Additional estimates on Ritz vectors: Let $v_1, \ldots, v_s$ *be* A*-orthonormal Ritz vectors associated with* $\vartheta_1, \ldots, \vartheta_s$*. If* $\vartheta_j^{-1} > \lambda_{j+1}^{-1}$ *for each* $j \in \{1, \ldots, s\}$*, then it holds that*

$$\sin^2 \angle_A(v_i, w_i) \leq 1 - \left(\prod_{j=1,\ j\neq i}^{s+1} \frac{\vartheta_i^{-1} - \lambda_j^{-1}}{\lambda_i^{-1} - \lambda_j^{-1}}\right)\left(\prod_{j=1,\ j\neq i}^{s} \frac{\lambda_i^{-1} - \vartheta_j^{-1}}{\vartheta_i^{-1} - \vartheta_j^{-1}}\right). \tag{5.36}$$

If $\lambda_{i-1}^{-1} > \lambda_i^{-1} = \cdots = \lambda_{i+a}^{-1} > \lambda_{i+a+1}^{-1}$ *holds for certain* i *and* a *with* $2 \leq i \leq i+a \leq s$*, i.e.,* $\lambda_i, \ldots, \lambda_{i+a}$ *correspond to a multiple eigenvalue, and the Ritz values fulfill*

$$\vartheta_{i-1}^{-1} \geq \lambda_i^{-1}, \quad \vartheta_{i+a}^{-1} \geq \lambda_{i+a+1}^{-1}, \quad \vartheta_{i-1}^{-1} > \vartheta_i^{-1},$$

then the estimate

$$\sin^2 \angle_A\big(\mathcal{V}_i, \mathcal{W}_i\big) \leq 1 - \frac{(\lambda_1^{-1} - \vartheta_{i+a}^{-1})(\vartheta_{i+a}^{-1} - \lambda_{i+a+1}^{-1})(\vartheta_{i-1}^{-1} - \lambda_i^{-1})}{(\lambda_1^{-1} - \lambda_i^{-1})(\lambda_i^{-1} - \lambda_{i+a+1}^{-1})(\vartheta_{i-1}^{-1} - \vartheta_{i+a}^{-1})} \tag{5.37}$$

holds for the subspaces $\mathcal{V}_i = \operatorname{span}\{v_i, \ldots, v_{i+a}\}$ *and* $\mathcal{W}_i = \operatorname{span}\{w_i, \ldots, w_{i+a}\}$.

If M is positive definite, then the estimates (5.30) and (5.31) also hold in M-angles, and the estimates (5.34) and (5.35) can be simplified as

$$\frac{\vartheta_i - \lambda_i}{\lambda_{t+1} - \vartheta_i} \leq [\,T_{k-1}(1 + 2\gamma_{i,t})\,]^{-2}\, \frac{\alpha - \lambda_i}{\lambda_{t+1} - \alpha} \quad \text{and} \quad \frac{\vartheta_i - \lambda_i}{\lambda_{d+1} - \vartheta_i} \leq [\,T_{k-b}(1 + 2\gamma_{i,d})\,]^{-2}\, \frac{\widetilde{\alpha} - \lambda_i}{\lambda_{d+1} - \widetilde{\alpha}}$$

since the concerned eigenvalues and Ritz values are positive.

6 Restarted block-Krylov subspace iterations

The storage requirement of block-Krylov subspace iterations is generally higher than that of standard Krylov subspace iterations. Therefore it is more necessary to restart block-Krylov subspace iterations for solving large-scale matrix eigenvalue problems. In addition, restarted block-Krylov subspace iterations are generally more cluster robust than restarted Krylov subspace iterations. Their performance depends on the degree of the associated low-dimensional block-Krylov subspaces. A proper degree can provide a considerable compromise between the storage requirement and the convergence rate with respect to the number of outer steps so that the total computation time can significantly be reduced.

The convergence theory of restarted block-Krylov subspace iterations is in a similar situation in comparison to that of restarted Krylov subspace iterations mentioned at the beginning of Chapter 4. There is hardly any direct analysis, and restarting is an obstacle for applying those known estimates which only concern nonrestarted iterations. In our previous work [122], we note that a suitable and concise estimate can be derived based on Knyazev's estimate [45, Equation (2.22)] for an abstract subspace iteration; see the corresponding estimate (2.13) introduced in Theorem 2.5. However, since this estimate only concerns one Ritz value, namely, the smallest Ritz value in an s-dimensional subspace iterate, a generalization to all Ritz values was attempted and has been achieved in [122, Theorem 2]. Nevertheless, the description of the cluster robustness is still improvable.

In this chapter, we investigate restarted block-Krylov subspace iterations of the type (1.25) by observing the reciprocal representation (1.29d) concerning standard matrix eigenvalue problems with Notation 1.5. In Section 6.1, we consider (1.29d) with constant block sizes, i.e., the dimension of the first subspace iterate $\mathcal{Y}^{(0)} = \operatorname{span}\{Y^{(0)}\}$ is set equal to the number c of extracted Ritz vectors so that all subspace iterates $\mathcal{Y}^{(\ell)}$ have dimension c. The generalized estimate from [122, Theorem 2] can be applied to this version of (1.29d) after slight reformulation. Furthermore, we extend the angle-free estimate (5.9) on Ritz values from Subsection 5.1.3 to arbitrarily located initial Ritz values in order to formulate a cluster robust estimate. Further estimates on Ritz vectors can be obtained by using the additional estimates from Subsection 5.1.4. Section 6.2 is devoted to investigating (1.29d) with enlarged block sizes, i.e., the dimension t of $\mathcal{Y}^{(0)}$ is less than c, whereas further subspace iterates $\mathcal{Y}^{(\ell)}$ have dimension c due to the settings in (1.29d). Indeed, restarted Krylov subspace iterations are included in this case by setting $t=1$. For the convergence analysis, we can simply extend the estimates from Section 6.1 by an additional estimate for the first step. In Section 6.3, we reformulate the new results with respect to the description (1.25) of restarted block-Krylov subspace iterations.

6.1 Estimates for constant block sizes

The restarted block-Krylov subspace iteration (1.29d) constructs block-Krylov subspaces

$$\widehat{\mathcal{K}}^k(Y^{(\ell)}) = \operatorname{span}\{Y^{(\ell)}, HY^{(\ell)}, \dots, H^{k-1}Y^{(\ell)}\}, \quad \ell = 0,\, 1,\, 2,\, \dots$$

for a symmetric matrix $H \in \mathbb{R}^{n\times n}$ with Notation 1.5. This iteration aims at the s largest eigenvalues of H and extracts c Ritz vectors in each step in order to generate the next subspace iterate, i.e., the initial subspace of the next block-Krylov subspace. Properly enlarging c can improve the cluster robustness. The improvement in single steps can be interpreted by using the

Chebyshev type estimates from Section 5.1 for $t = c$, namely, the gap ratio

$$(\mu_i - \mu_{c+1})/(\mu_{c+1} - \mu_n)$$

is increasing with c so that the corresponding Chebyshev factor is decreasing. Moreover, one can naturally select c as the dimension t of the first subspace iterate $\mathcal{Y}^{(0)} = \mathrm{span}\{Y^{(0)}\}$. The choice $t \neq c$ seems uninteresting in the sense that further subspace iterates $\mathcal{Y}^{(\ell)} = \mathrm{span}\{Y^{(\ell)}\}$ have dimension c anyway. Indeed, the dimension of the generated block-Krylov subspaces can be reduced for $t < c$. For instance, in the case $t = 1$, one can show that (1.29d) coincides with the restarted Krylov subspace iteration(1.29b) due to the equivalence between implicit restart and thick-restart [19, 118]. Then the generated block-Krylov subspaces are actually Krylov subspaces. Thus we prefer to investigate (1.29d) in two versions: (1.29d) with $t = c$ in the current section, and (1.29d) with $t < c$ in Section 6.2.

For investigating (1.29d) with $t = c$, some Chebyshev type estimates for block-Krylov subspace iterations from Chapter 5 can only be applied in a limited way. As an example, we discuss the applicability of the estimate (5.4) on approximate eigenvectors. By setting $t = c$, $\mathcal{Y} = \mathcal{Y}^{(\ell)}$ and $\mathcal{K} = \widehat{\mathcal{K}}^k(Y^{(\ell)})$, we get

$$\tan\angle_2\big(z_i,\, \widehat{\mathcal{K}}^k(Y^{(\ell)})\big) \le [\,T_{k-1}(1 + 2\gamma_{i,c})\,]^{-1} \tan\angle_2\big(\mathcal{Y}^{(\ell)}, \mathcal{Z}^c\big)$$

which is applicable to each single step as an a posteriori estimate. However, it cannot directly be extended for estimating $\tan\angle_2\big(z_i,\, \widehat{\mathcal{K}}^k(Y^{(\ell)})\big)$ in terms of $\tan\angle_2\big(\mathcal{Y}^{(0)}, \mathcal{Z}^c\big)$. Although the additional estimate (2.7) can formally contribute to an indirect extension, the associated distance parameters and projectors prevent a reasonable application.

In contrast to this, the angle-free estimates (5.9) and (5.14) on Ritz values can be extended into practical a priori estimates. In particular, (5.14) can be reformulated as

$$\frac{\mu_i - \theta_i^{(\ell+1)}}{\theta_i^{(\ell+1)} - \mu_{i+1}} \le [\,T_{k-1}(1 + 2\gamma_i)\,]^{-2}\, \frac{\mu_i - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{i+1}} \tag{6.1}$$

concerning the ith largest Ritz value $\theta_i^{(\ell)}$ in the block-Krylov subspace $\widehat{\mathcal{K}}^k(Y^{(\ell)})$. Its recursive application results in

$$\frac{\mu_i - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{i+1}} \;\le\; [\,T_{k-1}(1 + 2\gamma_i)\,]^{-2\ell}\, \frac{\mu_i - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{i+1}} \;\le\; [\,T_{k-1}(1 + 2\gamma_i)\,]^{-2(\ell+1)}\, \frac{\mu_i - \eta_i}{\eta_i - \mu_{i+1}} \tag{6.2}$$

concerning the ith largest Ritz value η_i in the first subspace iterate $\mathcal{Y}^{(0)}$. However, the estimate (6.1) requires the assumption that the Ritz value $\theta_i^{(\ell)}$ already exceeds μ_{i+1} so that its application is restricted to the final phase of the considered iteration. In our previous work [122], an extension of (6.1) has been achieved under the weaker assumption that $\theta_i^{(\ell)}$ is located in the interval (μ_{j+1}, μ_j) for an arbitrary index $j \in \{i, \ldots, n - c + i - 1\}$. The corresponding Chebyshev factor reads $[\,T_{k-1}(1 + 2\gamma_j)\,]^{-2}$ with the gap ratio $\gamma_j = (\mu_j - \mu_{j+1})/(\mu_{j+1} - \mu_n)$. Moreover, in the case $k = 3$, this Chebyshev factor can be improved as the factor $[\,q(\mu_j)\,]^{-2}$ with an interpolating polynomial $q(\cdot)$ similarly to Theorem 4.6. Nevertheless, both factors are related to the distance $\mu_j - \mu_{j+1}$ and cannot reasonably describe the cluster robustness.

In the further part of this section, we review the main results from [122] for restarted block-Krylov subspace iterations, and improve them by new cluster robust estimates based on the estimate (5.9) from Subsection 5.1.3 concerning block-Krylov subspace iterations.

6.1.1 Single-step estimates

We first review [122, Theorem 2 and Corollary 2] in the following modified formulation with respect to certain practical settings for the restarted block-Krylov subspace iteration (1.29d).

Theorem 6.1. *With Notation 1.5, consider the restarted block-Krylov subspace iteration* (1.29d) *where the initial subspace* $\mathcal{Y}^{(\ell+1)} = \operatorname{span}\{Y^{(\ell+1)}\}$ *of* $\widehat{\mathcal{K}}^k(Y^{(\ell+1)})$ *is spanned by orthonormal Ritz vectors of* H *in* $\widehat{\mathcal{K}}^k(Y^{(\ell)})$ *associated with the* c *largest Ritz values. Assume that none of the subspace iterates* $\mathcal{Y}^{(\ell)} = \operatorname{span}\{Y^{(\ell)}\}$ *contains eigenvectors, and that the dimension* t *of* $\mathcal{Y}^{(0)} = \operatorname{span}\{Y^{(0)}\}$ *is equal to* c*. Denote by* $\theta_1^{(\ell)} \geq \cdots \geq \theta_s^{(\ell)}$ *the* s *largest Ritz values of* H *in* $\widehat{\mathcal{K}}^k(Y^{(\ell)})$ *for* $s \leq c$ *and the step index* ℓ*. Then*

$$\theta_i^{(\ell+1)} > \theta_i^{(\ell)} \tag{6.3}$$

holds for each ℓ *and each* $i \in \{1, \ldots, s\}$ *so that the sequences* $\big(\theta_i^{(\ell)}\big)_{\ell \in \mathbb{N}}$ *are strictly increasing.*

Furthermore, if $\mu_j > \theta_i^{(\ell)} > \mu_{j+1}$ *is fulfilled for certain indices* $i \in \{1, \ldots, s\}$ *and* $j \in \{i, \ldots, n-c+i-1\}$*, then it holds, in terms of the gap ratio* $\gamma_j = (\mu_j - \mu_{j+1})/(\mu_{j+1} - \mu_n)$ *and the Chebyshev polynomial* $T_{k-1}(\cdot)$*, that*

$$\frac{\mu_j - \theta_i^{(\ell+1)}}{\theta_i^{(\ell+1)} - \mu_{j+1}} \leq \big[\, T_{k-1}(1 + 2\gamma_j)\big]^{-2} \, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}. \tag{6.4}$$

In addition,

$$\frac{\mu_j - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{j+1}} \leq \big[\, T_{k-1}(1 + 2\gamma_j)\big]^{-2} \, \frac{\mu_j - \varphi_i}{\varphi_i - \mu_{j+1}} \tag{6.5}$$

holds for the i*th largest Ritz value* φ_i *of* H *in* $\mathcal{Y}^{(0)}$ *by assuming* $\mu_j \geq \varphi_i > \mu_{j+1}$*.*

The settings from Theorem 6.1 are, despite the differences between the considered iterations, similar to those from Theorem 4.7 concerning the restarted Krylov subspace iteration (1.29b). Correspondingly, the proof of [122, Theorem 2 and Corollary 2] can be improved structurally based on the proof of Theorem 4.7. For the reader's convenience, we formulate a proof sketch.

The first step serves to generate an i-dimensional auxiliary subspace $\mathcal{U}$ within the subspace iterate $\mathcal{Y}^{(\ell+1)}$. By using the generating vectors $u_1, \ldots, u_c$ of $\mathcal{Y}^{(\ell+1)}$, i.e., orthonormal Ritz vectors in $\widehat{\mathcal{K}}^k(Y^{(\ell)})$ associated with the c largest Ritz values $\theta_1^{(\ell)} \geq \cdots \geq \theta_c^{(\ell)}$, we set $\mathcal{U} = \operatorname{span}\{u_1, \ldots, u_i\} = \operatorname{span}\{U\}$ with the basis matrix $U = [u_1, \ldots, u_i]$. Then $\mathcal{U}$ is subset of $\mathcal{Y}^{(\ell+1)}$ so that the block-Krylov subspace

$$\mathcal{K} = \operatorname{span}\{U, HU, \ldots, H^{k-1}U\}$$

is a subset of $\widehat{\mathcal{K}}^k(Y^{(\ell+1)})$. In comparison to this, the proof of Theorem 4.7 constructs a block-Krylov subspace of degree $k - c$ which is a subset of the Krylov subspace $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$.

Next, an auxiliary nonzero vector y is selected from the intersection of the subspaces $\mathcal{U}$ and $\mathcal{W}_{i,d} = \operatorname{span}\{w_i, \ldots, w_d\}$ by considering orthonormal Ritz vectors $w_1, \ldots, w_d$ of H in $\mathcal{K}$ associated with the Ritz values $\theta_1 \geq \cdots \geq \theta_d$ with $d = \dim \mathcal{K}$. The existence of y follows from a dimension inequality. Moreover, it can be shown that $p(H)y$ belongs to $\mathcal{W}_{i,d}$ for an arbitrary real polynomial $p(\cdot)$ of degree $k-1$. The auxiliary vector for Theorem 4.7 is constructed in the same way, but with a polynomial of degree $k - c$.

For proving (6.3), we use the relation $\mathcal{U} \subseteq \mathcal{K} \subseteq \widehat{\mathcal{K}}^k(Y^{(\ell+1)})$ which implies $\theta_i^{(\ell)} \leq \theta_i \leq \theta_i^{(\ell+1)}$ according to the Courant-Fischer principles. In addition, the equality $\theta_i^{(\ell)} = \theta_i^{(\ell+1)}$ would cause that there exist eigenvectors in $\mathcal{U}$ and thus in $\mathcal{Y}^{(\ell+1)}$, i.e., a contradiction to the assumption that none of the subspace iterates contains eigenvectors. In the proof of Theorem 4.7, such an equality contradicts the assumption that the Krylov subspace $\widehat{\mathcal{K}}^k(y^{(\ell+1)})$ is not an invariant subspace.

The remaining part of the proof only slightly differs from the corresponding part of the proof of Theorem 4.7. The main estimate (6.4) is based on the intermediate estimate

$$\frac{\mu_j - \theta_i}{\theta_i - \mu_{j+1}} \leq \big[\, T_{k-1}(1 + 2\gamma_j)\big]^{-2} \, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}. \tag{6.6}$$

Therein a shifted Chebyshev polynomial $p(\cdot)$ defined by $p(\alpha) = T_{k-1}\Big(1 + 2\,\frac{\alpha-\mu_{j+1}}{\mu_{j+1}-\mu_n}\Big)$ is used to construct the vector

$$\widetilde{y} \,=\, p(\mu_j)\, \textstyle\sum_{l=1}^{j} Q_l y \,+\, \sum_{l=j+1}^{n} Q_l y$$

with eigenprojections $Q_l y$ of y. Then the properties

$$\mu\big(p(H)y\big) \geq \mu(\widetilde{y}) \geq \mu(y) \qquad \text{and} \qquad \frac{\mu_j - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \leq \big[\, T_{k-1}(1+2\gamma_j)\,\big]^{-2}\, \frac{\mu_j - \mu(y)}{\mu(y) - \mu_{j+1}}$$

can be verified and result in (6.6) according to the monotonicity of $(\mu_j - \cdot\,)/(\,\cdot - \mu_{j+1})$. This completes the derivation of (6.4). The estimate (6.5) can be derived analogously with a subset $\mathcal{U}$ of the first subspace iterate $\mathcal{Y}^{(0)}$.

Additionally, [122, Theorem 3] gives an improvement of (6.4) in the case $k\!=\!3$.

Theorem 6.2. *With the settings from Theorem 6.1, the estimate*

$$\frac{\mu_j - \theta_i^{(\ell+1)}}{\theta_i^{(\ell+1)} - \mu_{j+1}} \leq \big[\, q(\mu_j)\,\big]^{-2}\, \frac{\mu_j - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}}. \tag{6.7}$$

holds for $\theta_i^{(\ell)} \in (\mu_{j+1}, \mu_j)$ and $k = 3$. Therein $q(\cdot)$ is a quadratic polynomial which interpolates the pairs $\big(\mu_{j+1}, 1\big)$, $\big(\mu_\xi, -1\big)$ and $\big(\mu_n, 1\big)$, and μ_ξ is an eigenvalue which has the smallest distance to $(\mu_{j+1} + \mu_n)/2$ among the eigenvalues $\mu_{j+2}, \ldots, \mu_{n-1}$.

The estimate (6.7) can be derived analogously to (6.4) since the polynomial $q(\cdot)$ has similar properties as the shifted Chebyshev polynomial $p(\cdot)$ used in the derivation of (6.4). The sharpness of (6.7) can be interpreted by the limit case $\theta_i^{(\ell)} \to \mu_j$ concerning an invariant subspace associated with the eigenvalues μ_j, μ_{j+1}, μ_ξ, μ_n. However, if the distance $\mu_j - \mu_{j+1}$ is nearly zero, then both of the convergence factors $[\,q(\mu_j)\,]^{-2}$ and $[\,T_{k-1}(1 + 2\gamma_j)\,]^{-2}$ are close to 1. This seems to contradict the cluster robustness of restarted block-Krylov subspace iterations. Indeed, the sharpness of (6.7) concerns single steps, and the actual convergence rate can possibly be close to 1 in several early steps; cf. the numerical example shown in [122, Figure 2]. Thus the cluster robustness should be discussed with respect to multiple steps.

6.1.2 Multi-step estimates

The single-step estimates (6.4) and (6.7) can be applied recursively to multiple steps of the restarted block-Krylov subspace iteration (1.29d). The resulting estimates extend the similar estimate (6.2) to arbitrary eigenvalue intervals, and can be combined in order to analyze the entire convergence history. Nevertheless, the associated convergence factors need to be improved for describing the cluster robustness. For this purpose, we extend the angle-free estimate (5.9) on Ritz values from Subsection 5.1.3 in the following theorem. The proof is analogous to that of Theorem 4.8 concerning the restarted Krylov subspace iteration (1.29b).

Theorem 6.3. *With the settings from Theorem 6.1, if the smallest Ritz value η of H in the first subspace iterate $\mathcal{Y}^{(0)}$ fulfills $\mu_j > \eta > \mu_{j+1}$ for a certain $j \in \{c, \ldots, n-1\}$, then it holds for each $i \in \{1, \ldots, s\}$, in terms of the gap ratio $\widetilde{\gamma}_{i,j} = (\mu_{j-c+i} - \mu_{j+1})/(\mu_{j+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-1}(\cdot)$, that*

$$\frac{\mu_{j-c+i} - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}} \leq \big[\, T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,\big]^{-2(\ell+1)}\, \frac{\mu_{j-c+i} - \eta}{\eta - \mu_{j+1}}. \tag{6.8}$$

Proof. The case $\mu_{j-c+i} \leq \theta_i^{(\ell)}$ is trivial where the left-hand side of (6.8) is nonpositive.

In the nontrivial case $\mu_{j-c+i} > \theta_i^{(\ell)}$, we derive (6.8) by observing the subspace iteration $\mathcal{W}^{(t+1)} = p(H)\,\mathcal{W}^{(t)}$ with $\mathcal{W}^{(-1)} = \mathcal{Y}^{(0)}$ and the shifted Chebyshev polynomial $p(\cdot)$ defined by $p(\alpha) = T_{k-1}\left(1 + 2\,\frac{\alpha-\mu_{j+1}}{\mu_{j+1}-\mu_n}\right)$. This iteration is accelerated by the restarted block-Krylov subspace iteration (1.29d) in the sense that the Rayleigh-Ritz procedure is applied to an extended subspace. The Courant-Fischer principles imply the relation $\theta_i^{(\ell)} \geq \eta_i^{(\ell)}$ for the ith largest Ritz value $\eta_i^{(\ell)}$ of H in $\mathcal{W}^{(\ell)}$. Therefore (6.8) can be derived from the intermediate estimate

$$\frac{\mu_{j-c+i} - \eta_i^{(\ell)}}{\eta_i^{(\ell)} - \mu_{j+1}} \leq [\,T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\,\frac{\mu_{j-c+i} - \eta}{\eta - \mu_{j+1}} \tag{6.9}$$

due to the monotonicity of the function $(\mu_{j-c+i} - \cdot\,)/(\,\cdot - \mu_{j+1})$.

In order to show (6.9), we adapt the derivation of the intermediate estimate (4.27) from the proof of Theorem 4.8.

First, the subspace $\mathcal{W}^{(\ell)}$ has at least dimension i so that the ith largest Ritz value $\eta_i^{(\ell)}$ exists. This property is verified by using the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1, \ldots, z_{j-c+i}, z_{j+1}, \ldots, z_n\}$ given by Notation 1.5. The intersection of the subspaces $\mathcal{W}^{(-1)} = \mathcal{Y}^{(0)}$ and $\mathcal{Z}$ has at least dimension i because of

$$\dim\left(\mathcal{W}^{(-1)} \cap \mathcal{Z}\right) = \dim \mathcal{W}^{(-1)} + \dim \mathcal{Z} - \dim\left(\mathcal{W}^{(-1)} + \mathcal{Z}\right) \geq c + (n - c + i) - n = i.$$

Thus we can select an i-dimensional subspace $\widetilde{\mathcal{W}} \subseteq \left(\mathcal{W}^{(-1)} \cap \mathcal{Z}\right)$. Then the relation

$$\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}} \subseteq \left(\big(p(H)\big)^{\ell+1}\mathcal{W}^{(-1)} \cap \big(p(H)\big)^{\ell+1}\mathcal{Z}\right) \subseteq \left(\mathcal{W}^{(\ell)} \cap \mathcal{Z}\right)$$

holds so that the property $\dim \mathcal{W}^{(\ell)} \geq i$ can be verified by showing $\dim \big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}} = i$; cf. the proof of Theorem 4.8 for details.

Next, we denote by α the smallest Ritz value in $\widetilde{\mathcal{W}}$ and by β the ith largest Ritz value in $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}}$. Then it holds that

$$\begin{aligned} \widetilde{\mathcal{W}} \subseteq \mathcal{W}^{(-1)} \qquad &\Rightarrow \qquad \alpha \geq \eta > \mu_{j+1}, \\ \big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}} \subseteq \mathcal{W}^{(\ell)} \qquad &\Rightarrow \qquad \beta \leq \eta_i^{(\ell)} \leq \theta_i^{(\ell)} < \mu_{j-c+i} \end{aligned}$$

according to the Courant-Fischer principles. Consequently, we can show (6.9) by verifying

$$\frac{\mu_{j-c+i} - \beta}{\beta - \mu_{j+1}} \leq [\,T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\,\frac{\mu_{j-c+i} - \alpha}{\alpha - \mu_{j+1}}. \tag{6.10}$$

The verification of (6.10) makes use of a Ritz vector $\widehat{w}$ in $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}}$ associated with β. There exists evidently a nonzero vector $w \in \widetilde{\mathcal{W}}$ satisfying $\widehat{w} = \big(p(H)\big)^{\ell+1}w$. Moreover, both of w and $\widehat{w}$ belong to the invariant subspace $\mathcal{Z} = \operatorname{span}\{z_1, \ldots, z_{j-c+i}, z_{j+1}, \ldots, z_n\}$ because $\widetilde{\mathcal{W}}$ and $\big(p(H)\big)^{\ell+1}\widetilde{\mathcal{W}}$ are subsets of $\mathcal{Z}$. Thus we select an auxiliary vector

$$\widetilde{w} = \big(p(\mu_{j-c+i})\big)^{\ell+1} \textstyle\sum_{l=1}^{j-c+i} z_l z_l^T w + \sum_{l=j+1}^{n} z_l z_l^T w$$

in order to analyze the relation between $\mu(w)$ and $\mu(\widehat{w})$. More precisely, we can show the properties $\mu(\widehat{w}) \geq \mu(\widetilde{w}) \geq \mu(w)$ and

$$\frac{\mu_{j-c+i} - \mu(\widetilde{w})}{\mu(\widetilde{w}) - \mu_{j+1}} \leq [\,T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\,\frac{\mu_{j-c+i} - \mu(w)}{\mu(w) - \mu_{j+1}} \tag{6.11}$$

analogously to (3.34) and (3.35) in the proof of Theorem 3.8. Therein the properties from (3.37) can easily be adapted to the powered polynomial $\big(p(\cdot)\big)^{\ell+1}$. Finally, the relation $\mu_{j-c+i} > \beta = \mu(\widehat{w}) \geq \mu(\widetilde{w}) \geq \mu(w) \geq \alpha > \mu_{j+1}$ enables an extension of (6.11) which yields (6.10).

This completes the proof of the intermediate estimate (6.9) so that the estimate (6.8) holds. □

In comparison to the multi-step estimates derived from (6.4) and (6.7), the estimate (6.8) can make a better prediction of the number of required outer steps for reaching acceptable approximations. The Chebyshev factor with the gap ratio $\widetilde{\gamma}_{i,j}$ describes an average convergence rate, whereas the ratio $(\mu_{j-c+i}-\eta)/(\eta-\mu_{j+1})$ serves to avoid an underestimation of the possible slowdown in early steps.

Furthermore, the estimates (5.15) and (5.16) from Subsection 5.1.4 can be combined with (6.8) in order to analyze the associated Ritz vectors in the case that the bound for $\theta_i^{(\ell)}$ exceeds μ_{i+1} or μ_{i+a+1} (i.e., the largest eigenvalue smaller than μ_i). In future work, we are interested in deriving direct Ritz vector estimates similarly to (4.8).

6.2 Estimates for enlarged block sizes

This section deals with restarted block-Krylov subspace iterations with enlarged block sizes. Concerning the reciprocal representation (1.29d) and the discussion at the beginning of Section 6.1, we consider the case that the dimension t of the first subspace iterate $\mathcal{Y}^{(0)} = \operatorname{span}\{Y^{(0)}\}$ is less than the cluster parameter c. Since the further subspace iterates $\mathcal{Y}^{(\ell)}$ with $\ell \geq 1$ still have dimension c, the estimates from Section 6.1 are partially applicable. We only need to additionally analyze the relation between $\mathcal{Y}^{(0)}$ and $\mathcal{Y}^{(1)}$. Based on Lemma 5.8 and the subsequent analysis for block-Krylov subspace iterations with small block sizes from Section 5.2, several additional estimates are achieved.

Theorem 6.4. *With the settings from Theorem 6.1, assume that the dimension t of $\mathcal{Y}^{(0)}$ is less than c, and select a low-dimensional block-Krylov subspace $\widehat{\mathcal{K}}^b(Y^{(0)})$ satisfying*

$$\dim \widehat{\mathcal{K}}^{b-1}(Y^{(0)}) < c \leq d = \dim \widehat{\mathcal{K}}^{b}(Y^{(0)}),$$

i.e., the smallest block-Krylov subspace which is initialized by $\mathcal{Y}^{(0)}$ and has at least dimension c. Then $\widehat{\mathcal{K}}^k(Y^{(0)})$ is a superset of the auxiliary block-Krylov subspace

$$\widetilde{\mathcal{K}} = \operatorname{span}\big\{\widetilde{Y}, H\widetilde{Y}, \dots, H^{k-b}\widetilde{Y}\big\}$$

with a basis matrix $\widetilde{Y} \in \mathbb{R}^{n\times d}$ of the initial subspace $\widetilde{\mathcal{Y}} = \widehat{\mathcal{K}}^b(Y^{(0)})$. In addition, the following estimates hold for the ith largest Ritz value $\theta_i^{(0)}$ of H in $\widehat{\mathcal{K}}^k(Y^{(0)})$ where $i \in \{1,\dots,d\}$.

(I) If the ith largest Ritz value φ_i of H in $\widehat{\mathcal{K}}^b(Y^{(0)})$ fulfills $\mu_j > \varphi_i > \mu_{j+1}$ for a certain $j \in \{i,\dots,n-d+i-1\}$, then it holds, in terms of the gap ratio $\gamma_j = (\mu_j - \mu_{j+1})/(\mu_{j+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-b}(\cdot)$, that

$$\frac{\mu_j - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{j+1}} \leq [\,T_{k-b}(1+2\gamma_j)\,]^{-2}\,\frac{\mu_j - \varphi_i}{\varphi_i - \mu_{j+1}}. \tag{6.12}$$

(II) If the smallest Ritz value η of H in $\widehat{\mathcal{K}}^b(Y^{(0)})$ fulfills $\mu_j > \eta > \mu_{j+1}$ for a certain $j \in \{d,\dots,n-1\}$, then it holds, in terms of the gap ratio $\widehat{\gamma}_{i,j} = (\mu_{j-d+i} - \mu_{j+1})/(\mu_{j+1} - \mu_n)$ and the Chebyshev polynomial $T_{k-b}(\cdot)$, that

$$\frac{\mu_{j-d+i} - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{j+1}} \leq [\,T_{k-b}(1+2\widehat{\gamma}_{i,j})\,]^{-2}\,\frac{\mu_{j-d+i} - \eta}{\eta - \mu_{j+1}}. \tag{6.13}$$

Proof. The relation $\widetilde{\mathcal{K}} \subseteq \widehat{\mathcal{K}}^k(Y^{(0)})$ is obtained directly from Lemma 5.8.

The proof of (6.12) is based on a counterpart of the estimate (6.5) concerning the auxiliary block-Krylov subspace $\widetilde{\mathcal{K}}$ and its initial subspace $\widetilde{\mathcal{Y}} = \widehat{\mathcal{K}}^b(Y^{(0)})$, namely,

$$\frac{\mu_j - \widetilde{\theta}_i}{\widetilde{\theta}_i - \mu_{j+1}} \leq [\, T_{k-b}(1 + 2\gamma_j)\,]^{-2} \, \frac{\mu_j - \varphi_i}{\varphi_i - \mu_{j+1}} \tag{6.14}$$

for the ith largest Ritz value $\widetilde{\theta}_i$ of H in $\widetilde{\mathcal{K}}$. Moreover, the relation $\widetilde{\mathcal{K}} \subseteq \widehat{\mathcal{K}}^k(Y^{(0)})$ implies $\widetilde{\theta}_i \leq \theta_i^{(0)}$ according to the Courant-Fischer principles. Combining this with the monotonicity of the function $(\mu_j - \cdot\,)/(\,\cdot - \mu_{j+1})$ enables an extension of (6.14) which results in (6.12).

Analogously, we prove (6.13) by using a counterpart of the estimate (6.8) for $\ell = 0$ which reads

$$\frac{\mu_{j-d+i} - \widetilde{\theta}_i}{\widetilde{\theta}_i - \mu_{j+1}} \leq [\, T_{k-b}(1 + 2\widehat{\gamma}_{i,j})\,]^{-2} \, \frac{\mu_{j-d+i} - \eta}{\eta - \mu_{j+1}}.$$

Extending this by $\widetilde{\theta}_i \leq \theta_i^{(0)}$ and the monotonicity of $(\mu_{j-d+i} - \cdot\,)/(\,\cdot - \mu_{j+1})$ yields (6.13). □

The estimate (6.12) can easily be combined with (6.4) in order to formulate a multi-step estimate. However, it is slightly complicated to combine the estimates (6.13) and (6.8) due to the difference between μ_{j-d+i} and μ_{j-c+i}. For convenience, we can apply (6.13) to $i = c$ in order to determine a lower bound $\widetilde{\eta}$ of $\theta_c^{(0)}$, i.e. the cth largest Ritz value in $\widehat{\mathcal{K}}^k(Y^{(0)})$ as well as the smallest Ritz value in $\mathcal{Y}^{(1)}$. Subsequently, adapting (6.8) to $\mathcal{Y}^{(1)}$ and $\widetilde{\eta}$ yields

$$\frac{\mu_{j-c+i} - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}} \leq [\, T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2\ell} \, \frac{\mu_{j-c+i} - \widetilde{\eta}}{\widetilde{\eta} - \mu_{j+1}}.$$

Indeed, these multi-step estimates for the restarted block-Krylov subspace iteration (1.29d) formally generalize the multi-step estimates for the restarted Krylov subspace iteration (1.29b) introduced in Section 4.2. This corresponds to the fact that (1.29b) coincides with a special version of (1.29d) where the first subspace iterate $\mathcal{Y}^{(0)}$ has dimension 1.

6.3 Reformulation for generalized matrix eigenvalue problems

Concerning the application to restarted block-Krylov subspace iterations of the type (1.25), we reformulate the main results in this chapter for generalized matrix eigenvalue problems with Notation 1.2.

Theorem 6.5. *With Notation 1.2, consider restarted block-Krylov subspace iterations of the type* (1.25) *where the initial subspace* $\mathcal{X}^{(\ell+1)} = \operatorname{span}\{X^{(\ell+1)}\}$ *of* $\mathcal{K}^k(X^{(\ell+1)})$ *is spanned by A-orthonormal Ritz vectors of* (A, M) *in* $\mathcal{K}^k(X^{(\ell)})$ *associated with the c reciprocally largest Ritz values. Assume that none of the subspace iterates* $\mathcal{X}^{(\ell)} = \operatorname{span}\{X^{(\ell)}\}$ *contains eigenvectors, and that the dimension t of* $\mathcal{X}^{(0)} = \operatorname{span}\{X^{(0)}\}$ *is equal to c. Denote by* $\vartheta_1^{(\ell)}, \ldots, \vartheta_s^{(\ell)}$ *the s reciprocally largest Ritz values of* (A, M) *in* $\mathcal{K}^k(X^{(\ell)})$ *for* $s \leq c$ *and the step index* ℓ. *Then*

$$(\vartheta_i^{(\ell+1)})^{-1} > (\vartheta_i^{(\ell)})^{-1} \tag{6.15}$$

holds for each ℓ *and each* $i \in \{1, \ldots, s\}$ *so that the Ritz value sequences* $\big(\vartheta_i^{(\ell)}\big)_{\ell \in \mathbb{N}}$ *are reciprocally strictly increasing.*

Furthermore, if $\lambda_j^{-1} > (\vartheta_i^{(\ell)})^{-1} > \lambda_{j+1}^{-1}$ *is fulfilled for certain indices* $i \in \{1, \ldots, s\}$ *and* $j \in \{i, \ldots, n-c+i-1\}$, *then it holds, in terms of the gap ratio* $\gamma_j = (\lambda_j^{-1} - \lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1} - \lambda_n^{-1})$ *and the Chebyshev polynomial* $T_{k-1}(\cdot)$, *that*

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(\ell+1)})^{-1}}{(\vartheta_i^{(\ell+1)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_j)\,]^{-2}\, \frac{\lambda_j^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}}. \tag{6.16}$$

In addition,

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(0)})^{-1}}{(\vartheta_i^{(0)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_j)\,]^{-2}\, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}} \tag{6.17}$$

holds for the i*th reciprocally largest Ritz value* α_i *of* (A, M) *in* $\mathcal{X}^{(0)}$ *by assuming* $\lambda_j^{-1} \geq \alpha_i^{-1} > \lambda_{j+1}^{-1}$. *Combining* (6.16) *and* (6.17) *results in the multi-step estimate*

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_j)\,]^{-2(\ell+1)}\, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}}. \tag{6.18}$$

Another multi-step estimate concerning clustered eigenvalues reads

$$\frac{\lambda_{j-c+i}^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\, \frac{\lambda_{j-c+i}^{-1} - \beta^{-1}}{\beta^{-1} - \lambda_{j+1}^{-1}} \tag{6.19}$$

with the gap ratio $\widetilde{\gamma}_{i,j} = (\lambda_{j-c+i}^{-1} - \lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1} - \lambda_n^{-1})$. *Therein the relation* $\lambda_j^{-1} > \beta^{-1} > \lambda_{j+1}^{-1}$ *is assumed for a certain* $j \in \{c, \ldots, n-1\}$ *and the reciprocally smallest Ritz value* β *of* (A, M) *in* $\mathcal{X}^{(0)}$.

Next, if the dimension t *of* $\mathcal{X}^{(0)}$ *is less than* c, *one can select a low-dimensional block-Krylov subspace* $\mathcal{K}^b(X^{(0)})$ *satisfying*

$$\dim \mathcal{K}^{b-1}(X^{(0)}) < c \leq d = \dim \mathcal{K}^b(X^{(0)}).$$

Then the estimate (6.18) *can be modified as*

$$\frac{\lambda_j^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\gamma_j)\,]^{-2\ell}\, [\,T_{k-b}(1 + 2\gamma_j)\,]^{-2}\, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}} \tag{6.20}$$

where α_i *denotes the* i*th reciprocally largest Ritz value of* (A, M) *in* $\mathcal{K}^b(X^{(0)})$. *Moreover, the estimate* (6.19) *can be modified as*

$$\frac{\lambda_{j-c+i}^{-1} - (\vartheta_i^{(\ell)})^{-1}}{(\vartheta_i^{(\ell)})^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-1}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2\ell}\, \frac{\lambda_{j-c+i}^{-1} - \vartheta^{-1}}{\vartheta^{-1} - \lambda_{j+1}^{-1}} \tag{6.21}$$

where ϑ *denotes the reciprocally smallest Ritz value of* (A, M) *in* $\mathcal{X}^{(1)}$. *Subsequently,* (6.21) *can be extended by a lower bound of* ϑ^{-1} *obtained from the additional estimate*

$$\frac{\lambda_{j-d+c}^{-1} - \vartheta^{-1}}{\vartheta^{-1} - \lambda_{j+1}^{-1}} \leq [\,T_{k-b}(1 + 2\widehat{\gamma}_{c,j})\,]^{-2}\, \frac{\lambda_{j-d+c}^{-1} - \beta^{-1}}{\beta^{-1} - \lambda_{j+1}^{-1}}$$

with the gap ratio $\widehat{\gamma}_{c,j} = (\mu_{j-d+c} - \mu_{j+1})/(\mu_{j+1} - \mu_n)$ *and the reciprocally smallest Ritz value* β *of* (A, M) *in* $\mathcal{K}^b(X^{(0)})$.

If M is positive definite, then the concerned eigenvalues and Ritz values are positive so that the formulation of Theorem 6.5 can be simplified as in Theorem 4.9.

7 Numerical experiments

By now we have investigated four types of Krylov subspace eigensolvers which are introduced in Subsection 1.4.1. These eigensolvers aim at the reciprocally largest eigenvalues of a matrix pair (A, M) described in the abstract problem (1.1), and are especially applicable to discretized eigenvalue problems of second-order self-adjoint elliptic partial differential operators. In this context, we have combined several Krylov subspace eigensolvers with adaptive finite element discretizations for the numerical experiments in [83, 125, 122] by using our software "Adaptive-Multigrid-Preconditioned (AMP) Eigensolver" [124].

The AMP Eigensolver deals mainly with the negative Laplace operator on user-defined 2D domains. Its central part is written in FORTRAN based on the libraries BLAS and LAPACK. Additionally, a graphical user interface in Matlab serves to simplify the initialization and to illustrate the results. By applying the residual-based error estimator from [77], this software enables a fast adaptive grid refinement and multigrid preconditioning; see the manual in [124] for more details. Therein the AMP Eigensolver is tested on a standard PC with Intel Xeon 3.2GHz CPU and 31.4GiB RAM plus disk swapping. Concerning a classical operator eigenvalue problem from [77] where the domain is given by the unit circle with a slit along the horizontal axis, we constructed a mesh hierarchy up to 85,611,460 nodes and obtained six significant figures of the main target eigenvalue within 582.86 seconds.

This chapter is devoted to demonstrating the accuracy of the new convergence estimates achieved in Chapters 3 to 6. The performance of the investigated Krylov subspace eigensolvers is illustrated together with the corresponding bounds within three model problems generated by the AMP Eigensolver. In Section 7.1, we introduce the model problems and indicate the target eigenvalues of the involved matrix pairs. The first two model problems are extracted from adaptively refined grids. The resulting matrices A and M are stiffness matrix and mass matrix so that both of them are positive definite. The third model problem is related to the first one and concerns an invertible shifted matrix $A_\sigma = A - \sigma M$. Therein the matrix pair $(A_\sigma M^{-1} A_\sigma,\ A_\sigma)$ is of interest and subsequently denoted by (A, M). In Section 7.2, our convergence estimates are graphically compared with computational data by means of numerical maxima over 1000 tests. We discuss the accuracy with respect to the eigenvalue distribution and the cluster parameter concerning possible tasks for future research.

7.1 Model problems

Various model problems have been generated by the AMP Eigensolver [124] in our previous works for investigating Krylov subspace eigensolvers [83, 125, 122] and their preconditioned variants [82, 126]. In particular, the model problems from [126] serve to demonstrate the benefit of some cluster robust estimates for the PINVIT method $\mathscr{P}_{1,s}$ introduced in Subsection 1.3.1. Since the cluster robustness is an essential feature of our new estimates for Krylov subspace eigensolvers, we reuse the model problems from [126] as the first two model problems in this chapter. For the reader's convenience, we introduce some details for their derivation from the AMP Eigensolver.

Model problem I (MP1)

We begin with the Laplacian eigenvalue problem $-\Delta u = \lambda u$ on a 2D mushroom-shaped domain;

see Figure 7.1. The boundary of the domain is given by $\Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ with the parts

$$\Gamma_1 = \big\{\big(\cos(t)+\tfrac{1}{3}\cos(3t),\, \sin(t)+\tfrac{1}{4}\sin(4t)\big)^T;\ t \in [0,\, 2\pi)\big\},$$
$$\Gamma_2 = \big\{\big(\tfrac{4}{3}(1-t),\, 0\big)^T;\ t \in (0,\, 1)\big\}, \qquad \Gamma_3 = \big\{\big(\tfrac{4}{3}t,\, 0\big)^T;\ t \in [0,\, 1)\big\}$$

where Γ_2 and Γ_3 correspond to the two sides of a slit along the horizontal axis. After setting homogeneous Dirichlet boundary conditions on $\Gamma_1 \cup \Gamma_2$ and homogeneous Neumann boundary conditions on Γ_3, we construct a mesh hierarchy by combining the LOBPCG method [48] with an adaptive finite element discretization within the AMP Eigensolver.

The initial grid has only 5 degrees of freedom and results in a matrix eigenvalue problem of dimension 5. This small problem can easily be solved by a shifted QR algorithm. For each matrix pair (A, M) from further grids with growing dimension, we compute the three smallest eigenvalues by the LOBPCG method with the block size 3. In addition, we apply the residual-based error estimator from [77] to the approximate eigenfunctions associated with the smallest eigenvalue in order to adaptively refine the current grid.

Since the corresponding eigenfunction has an unbounded derivative at the origin, the refinement depths increase rapidly near the origin; see the initial grid and three further grids in Figure 7.1. Moreover, the mesh hierarchy provides multigrid preconditioners for solving the involved matrix eigenvalue problems. The computational performance is displayed in the third row in Figure 7.1. In the left subfigure, the solid curve stands for the cumulative time for the whole computation, and the marked curve denotes the time for the computation within the current grid. The centred subfigure presents the convergence history of the three smallest matrix eigenvalues $\lambda_1^{(A,M)} < \lambda_2^{(A,M)} < \lambda_3^{(A,M)}$ toward the corresponding operator eigenvalues $\lambda_1^{(-\Delta)} < \lambda_2^{(-\Delta)} < \lambda_3^{(-\Delta)}$ which are taken approximately from the 82nd grid with 22,219,374 nodes. The approximate distances $\lambda_i^{(A,M)} - \lambda_i^{(-\Delta)}$ are displayed in the marked/dashed/solid curves for $i = 1, 2, 3$, respectively. The right subfigure shows information of the residual-based error estimator. The norms of estimated residual vectors with respect to quadratic elements are denoted by the solid curve. The tolerances for solving matrix eigenvalue problems form the dashed curve. The residual norms of the computed approximate eigenfunctions with respect to linear elements are contained in the marked curve. In addition, the values of $\lambda_1^{(A,M)}$ from six selected grids are listed in Table 7.1.

Table 7.1: The smallest matrix eigenvalues $\lambda_1^{(A,M)}$ computed by using LOBPCG within AMP Eigensolver. These converge to the smallest operator eigenvalue $\lambda_1^{(-\Delta)} \approx 8.895049$.

level	1	23	36	51	62	78
nodes	27	3810	31504	390322	1572517	17712651
d.o.f.	5	3582	30838	387963	1567785	17696832
$\lambda_1^{(A,M)}$	12.33746	8.913402	8.897231	8.895217	8.895089	8.895050

For demonstrating the accuracy of our new convergence estimates, we use the generalized matrix eigenvalue problem $Ax = \lambda Mx$ from the 62nd grid with 1,567,785 degrees of freedom. The five smallest matrix eigenvalues read

$$\lambda_1 \approx 8.895089, \quad \lambda_2 \approx 13.77993, \quad \lambda_3 \approx 21.63029, \quad \lambda_4 \approx 25.08266, \quad \lambda_5 \approx 29.64299.$$

Their reciprocals are well separated so that the selection of the cluster parameter c in the estimates is less strict; see Section 7.2 for details.

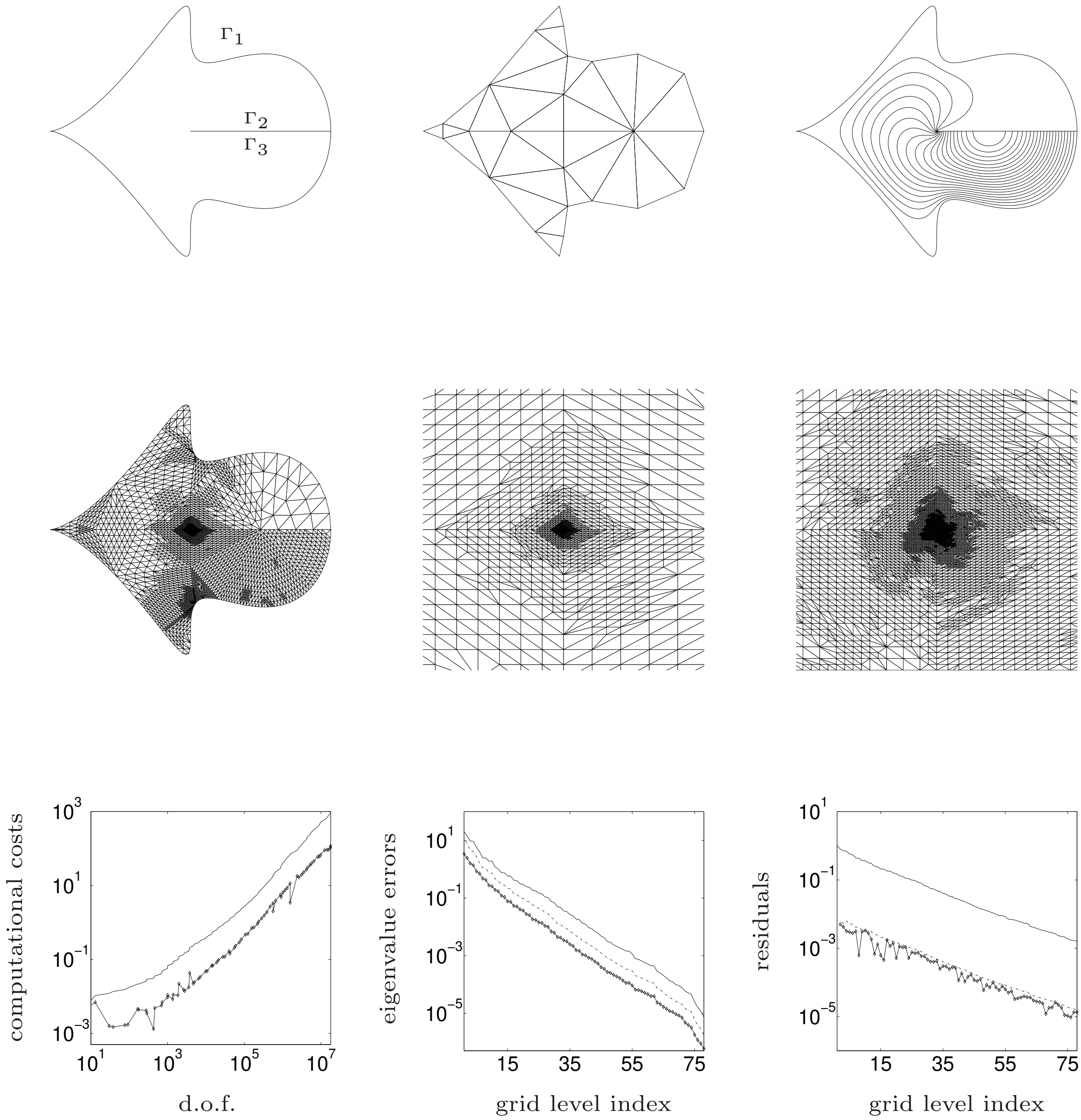

Figure 7.1: Solving MP1 with the AMP Eigensolver. *First row*: (left) the domain for the Laplacian eigenvalue problem $-\Delta u = \lambda u$ and its boundary in three parts, (center) the initial grid, (right) the contour lines of an eigenfunction associated with the smallest eigenvalue $\lambda_1^{(-\Delta)}$. *Second row*: three grids from the adaptive grid refinement with the grid levels 23, 36 and 51; see Table 7.1 for the corresponding numbers of nodes and degrees of freedom. The 36th and 51st grids are displayed by square-shaped sectional enlargements around the origin with side lengths 10^{-4} and 10^{-6}. *Third row*: computational information including (left) cumulative time for the whole computation and computation time in current grids, (center) approximate distances $\lambda_i^{(A,M)} - \lambda_i^{(-\Delta)}$ between the matrix eigenvalues $\lambda_i^{(A,M)}$ and the operator eigenvalues $\lambda_i^{(-\Delta)}$ for $i = 1, 2, 3$, (right) information of the residual-based error estimator for the adaptive grid refinement.

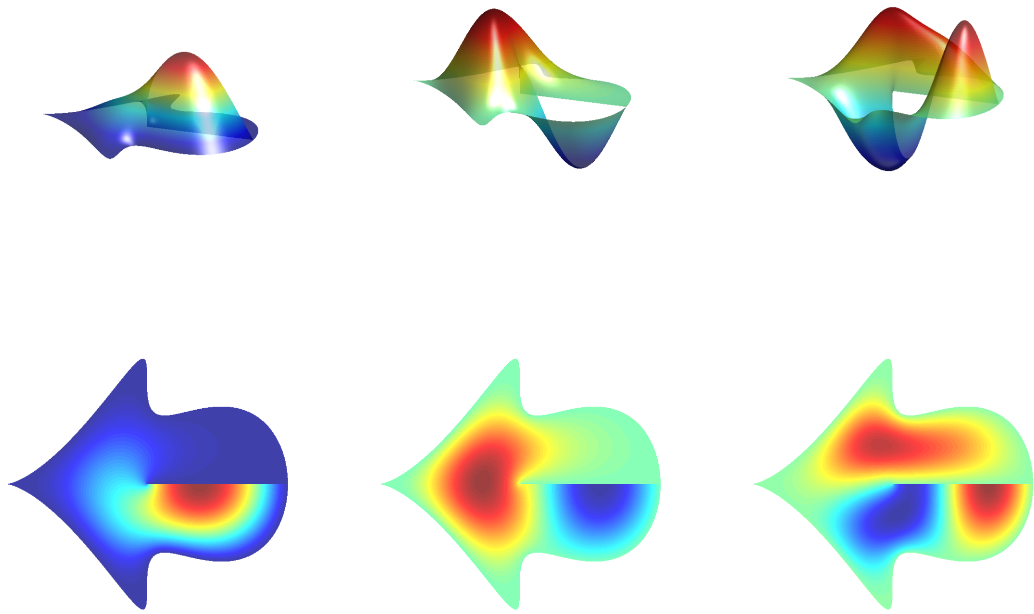

Figure 7.2: Approximate eigenfunctions associated with the three smallest eigenvalues for MP1. *First row*: side view. *Second row*: top view.

Model problem II (MP2)

In order to construct a model problem with clustered eigenvalues, we connect three circle subdomains by a thin annulus; see Figure 7.3. The circle subdomains have the same radius $r = 1.5$ and are centred at $(-\sqrt{3}, -1)^T$, $(\sqrt{3}, -1)^T$, $(0, 2)^T$, respectively. The annulus is centred at the origin with the radii $r_1 = 1.2$ and $r_2 = 1.5$. The Laplacian eigenvalue problem $-\Delta u = \lambda u$ is considered again, but with only homogeneous Dirichlet boundary conditions. Applying the AMP Eigensolver results in a sequence of matrix eigenvalue problems on 63 adaptively refined grids. The refinement is based on the residuals of the approximate eigenfunctions associated with the three smallest eigenvalues. The parts of approximate eigenfunctions on the circle subdomains are similar to the well-known peak eigenfunction on the unit circle.

For the numerical experiments in Section 7.2, we use the generalized eigenvalue problem $Ax = \lambda Mx$ from the 36th grid with 1,509,276 degrees of freedom. The nine smallest eigenvalues build two clusters, namely,

$$\lambda_1, \lambda_2, \lambda_3 \in (2.559876,\ 2.559941), \qquad \lambda_4, \ldots, \lambda_9 \in (6.495853,\ 6.500676).$$

Therefore it is meaningful to select an index $c \geq 3$ as the cluster parameter concerning the computation of the three smallest eigenvalues.

Model problem III (MP3)

We modify the model problem MP1 by setting the three smallest eigenvalues which are larger than the shift $\sigma = 60$ as target eigenvalues. The modified model problem is essentially the computation of the three smallest positive eigenvalues of the matrix pair $(A_\sigma M^{-1} A_\sigma,\ A_\sigma)$ with $A_\sigma = A - \sigma M$. We denote this matrix pair by (A, M) for the numerical experiments in Section

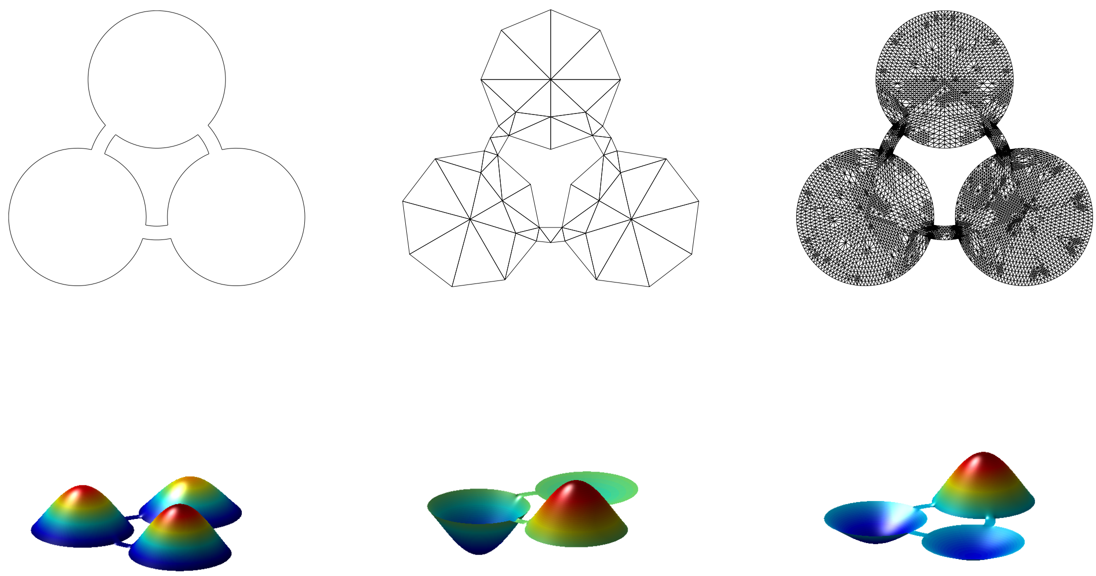

Figure 7.3: Solving MP2 with the AMP Eigensolver. *First row*: (left) the domain for the Laplacian eigenvalue problem $-\Delta u = \lambda u$, (center) the initial grid, (right) the 12th grid from the adaptive grid refinement. *Second row*: approximate eigenfunctions associated with the three smallest eigenvalues.

7.2. The five smallest positive eigenvalues read

$$\lambda_1 \approx 0.7823530, \quad \lambda_2 \approx 5.460023, \quad \lambda_3 \approx 11.69693, \quad \lambda_4 \approx 13.76184, \quad \lambda_5 \approx 21.69704.$$

The relatively large distance between λ_1^{-1} and λ_2^{-1} in comparison to that in MP1 leads to a slightly different convergence behavior of the Krylov subspace eigensolvers.

7.2 Illustration of bounds

In order to demonstrate the accuracy of our new convergence estimates, we implement the investigated Krylov subspace eigensolvers for the three model problems from Section 7.1, and compare the bounds with the corresponding computational data by means of numerical maxima.

7.2.1 Standard Krylov subspace iterations

We test standard Krylov subspace iterations of the type (1.22) with 1000 pseudorandom initial vectors $x^{(0)}$. Numerical maxima with respect to various convergence measures are documented for illustrating the bounds in the main estimates from Theorem 3.12. We skip the angle-free estimates on Ritz values since their extensions to restarted Krylov subspace iterations will be illustrated in Subsection 7.2.2.

Estimate (3.60) on approximate eigenvectors

The estimate (3.60) deals with the tangent value $\tan \angle_A(w_i, \mathcal{K})$ of the A-angle between an eigenvector w_i and the current Krylov subspace $\mathcal{K} = \mathcal{K}^k(x^{(0)})$. Therein w_i is collinear with the eigenprojection of the initial vector $x = x^{(0)}$ associated with the eigenvalue λ_i. Moreover, this angle is actually the A-angle between w_i and its A-orthogonal projection to $\mathcal{K}$ which can be interpreted as an approximate eigenvector in $\mathcal{K}$. The bound in (3.60) consists of the Chebyshev factor $[T_{k-c}(1+2\widetilde{\gamma}_i)]^{-1}$ and the tangent value $\tan\angle_A(\mathcal{K}^c,\mathcal{W}^c)$. The cluster parameter c is required for defining the gap ratio $\widetilde{\gamma}_i = (\lambda_i^{-1}-\lambda_{c+1}^{-1})/(\lambda_{c+1}^{-1}-\lambda_m^{-1})$, the low-dimensional Krylov subspace $\mathcal{K}^c = \mathcal{K}^c(x^{(0)})$ and the invariant subspace $\mathcal{W}^c$ associated with the first c eigenvalues.

For illustrating the bound in (3.60), we document the numerical maxima NM of $\tan\angle_A(w_i,\mathcal{K})$ over 1000 tests for $i\in\{1,2,3\}$ within each model problem from Section 7.1. The convergence behavior of the investigated standard Krylov subspace iterations is shown in Figure 7.4 by plotting NM versus the degree k of the current Krylov subspace $\mathcal{K}$. Therein k is also the dimension of $\mathcal{K}$ since the considered Krylov subspaces are not invariant subspaces. The convergence behavior clearly depends on the eigenvalue distribution. In MP1, the reciprocals of the target eigenvalues are well separated. Correspondingly, a strictly monotone convergence is observed, and the average convergence rate for $i\in\{2,3\}$ deteriorates in comparison to that for $i=1$. It is remarkable that the stepwise convergence rate can be predicted by the bound in (3.60) with various c. The bound with $c=i$ is suitable for a middle phase, whereas the bound with a larger c can match the final phase. In MP2, the clustered reciprocals of the target eigenvalues cause a staircase-shaped convergence. The convergence rate is close to 1 in many steps before the final phase. This can be reflected by the bound in (3.60) with $c=i$ for $i\in\{1,2\}$. For predicting the convergence rate in the final phase, we can set $c=3$ in the bound. The choice $c=9$ concerning the next cluster leads to overestimation before the final phase, but can slightly refine the prediction of the number of required steps for reaching an acceptable approximation. In MP3, we see a similar convergence history in comparison to that in MP1 as the reciprocals of the target eigenvalues are also well separated. The main difference is the faster convergence for $i=1$ due to the relatively large distance between λ_1^{-1} and λ_2^{-1}. Summarizing the above, we can apply the estimate (3.60) with various c and merge the corresponding bounds into a reasonable global bound, namely, by using smaller c for earlier phases and a sufficiently large c for the final phase.

Angle-dependent estimate (3.62) on Ritz values

The estimate (3.62) formally uses the square of the bound in (3.60) for analyzing the relative position $(\lambda_i^{-1}-\vartheta_i^{-1})/(\vartheta_i^{-1}-\lambda_m^{-1})$ where ϑ_i is the ith reciprocally largest Ritz value of (A,M) in $\mathcal{K}=\mathcal{K}^k(x^{(0)})$. It would be more convenient to observe the distance $\lambda_i^{-1}-\vartheta_i^{-1}$ in the numerical tests. Thus we reformulate (3.62) as

$$\lambda_i^{-1}-\vartheta_i^{-1} \le (\lambda_i^{-1}-\lambda_m^{-1})\,\frac{\psi}{1+\psi} \qquad \text{with} \qquad \psi = [T_{k-c}(1+2\widetilde{\gamma}_i)]^{-2}\,\tan^2\angle_A(\mathcal{K}^c,\mathcal{W}^c). \tag{7.1}$$

In Figure 7.5, we plot the numerical maxima NM of $\lambda_i^{-1}-\vartheta_i^{-1}$ over 1000 tests for $i\in\{1,2,3\}$ concerning the model problems from Section 7.1. The observation indicates that the convergence behavior with respect to $\lambda_i^{-1}-\vartheta_i^{-1}$ also depends on the eigenvalue distribution, but differs from that with respect to $\tan\angle_A(w_i,\mathcal{K})$ in the first phase. In particular, the ith Ritz value only exists for $k\ge i$ so that the NM of $\lambda_i^{-1}-\vartheta_i^{-1}$ are documented as of $k=i$. Moreover, a minor reduction in the first step is observed for all examples except for $i=1$ in MP2. The ratio $\psi/(1+\psi)$ in the reformulated estimate (7.1) is close to 1 for very large ψ appearing in the first phase. Therefore the corresponding bound curves have a nearly constant initial part, and provide a proper prediction of the convergence rate in a second part where appropriate. The number of required steps for reaching an acceptable approximation cannot be predicted accurately, especially for $i=3$ in MP3.

Additional estimate (3.65) on Ritz vectors

The estimate (3.65) deals with the sine squared $\sin^2\angle_A(v_i,w_i)$ of the A-angle between a Ritz vector v_i in the current Krylov subspace $\mathcal{K}=\mathcal{K}^k(x^{(0)})$ and an eigenvector w_i as considered in (3.60). The bound in (3.65) depends on the Ritz values in $\mathcal{K}$ so that (3.65) is actually an a posteriori estimate. Nevertheless, combining (3.65) with (3.62) enables an a priori estimate.

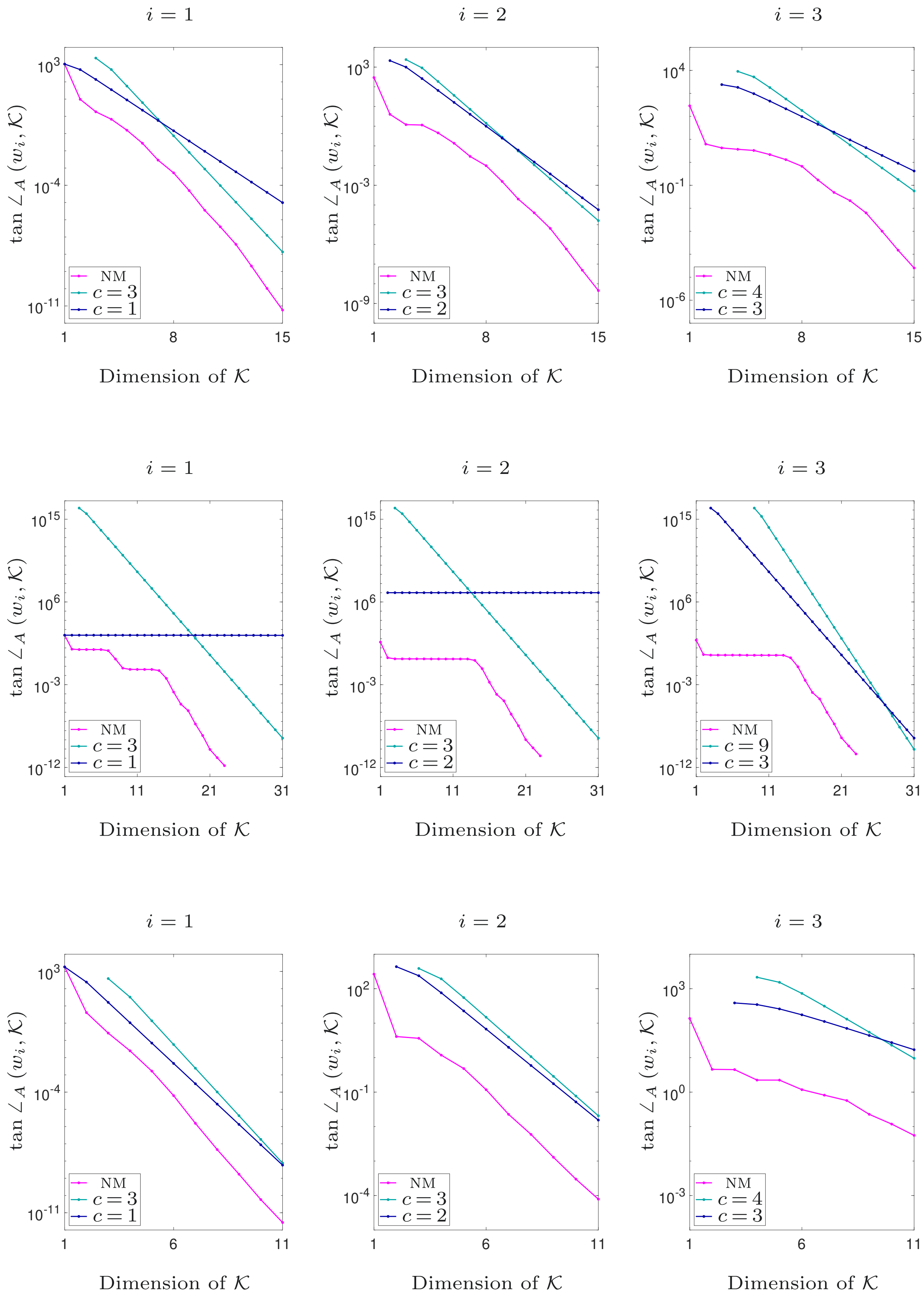

Figure 7.4: Illustration of the bound in the estimate (3.60) with various c in comparison to the numerical maxima NM of $\tan\angle_A(w_i,\mathcal{K})$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

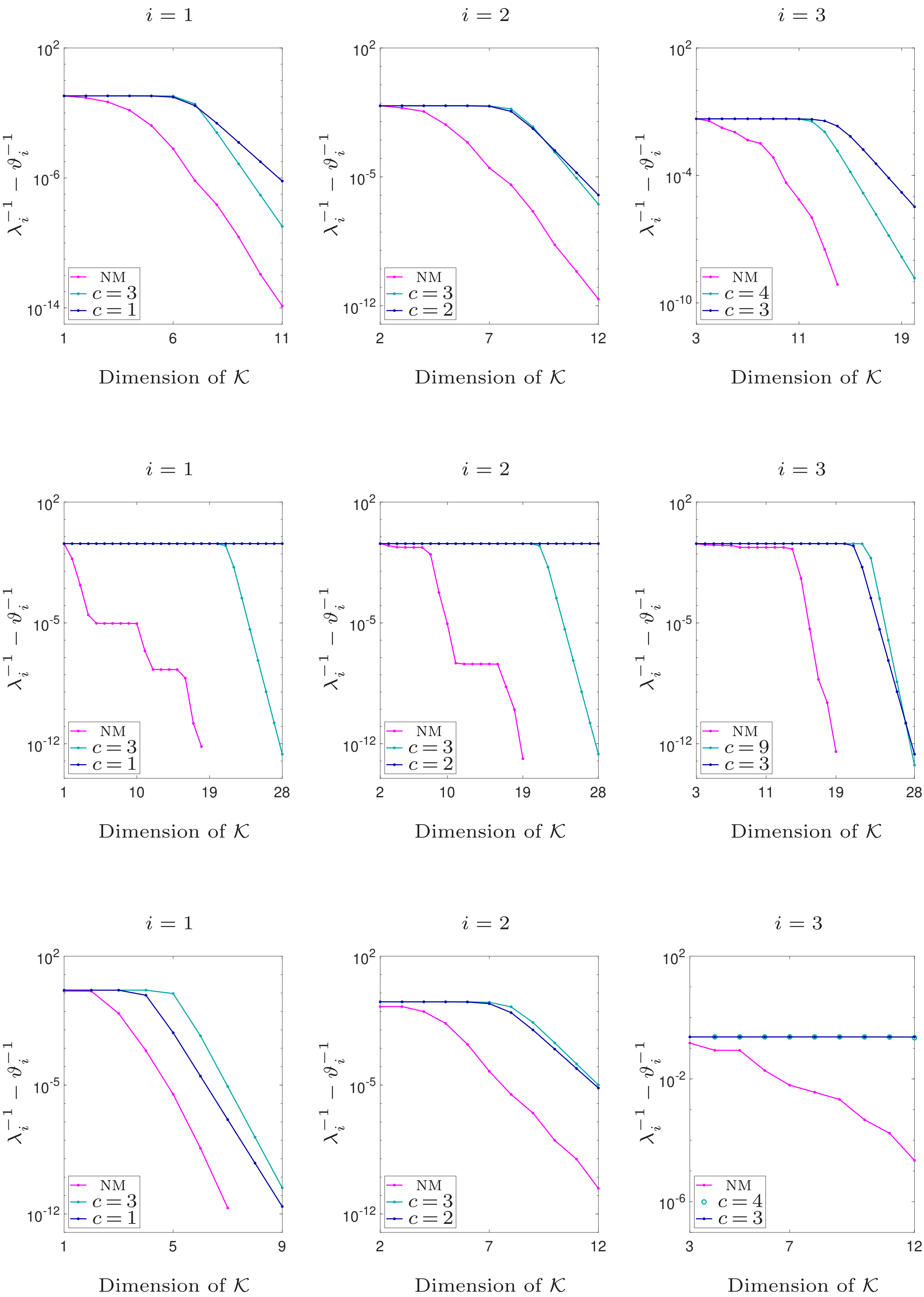

Figure 7.5: Illustration of the bound in the equivalent form (7.1) of the estimate (3.62) with various c in comparison to the numerical maxima NM of $\lambda_i^{-1} - \vartheta_i^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

For illustrating the bounds in these two estimates, we document the numerical maxima NM of $\sin^2 \angle_A(v_i, w_i)$ over 1000 tests for $i \in \{1, 2, 3\}$ concerning the model problems from Section 7.1. As observed in Figure 7.6, the convergence behavior with respect to $\sin^2 \angle_A(v_i, w_i)$ is similar to that with respect to the measure $\lambda_i^{-1} - \vartheta_i^{-1}$. This reflects a strong link between Ritz vectors and Ritz values. Next, we extend the estimates by the trivial bound 1 in the case that the assumption $\vartheta_j^{-1} > \lambda_{j+1}^{-1}\ \ \forall\, j \in \{1, \ldots, 3\}$, or its variant with estimated ϑ_j^{-1} from (3.62), does not hold. The graphical comparison between NM and the bound in (3.65) shows a high accuracy of (3.65) with exact Ritz values, especially in MP2 where the target eigenvalues are clustered. In addition, we consider the estimate combination "(3.65)+(3.62)" where the cluster parameter c is selected as in the cyan curves in Figure 7.5. For simplicity, we denote this combination by "(3.62)" in the legends in Figure 7.6. The observation reflects a lower accuracy which is caused by the limited quality of the estimate (3.62).

7.2.2 Restarted Krylov subspace iterations

In this subsection, restarted Krylov subspace iterations of the type (1.23) are tested with 1000 pseudorandom initial vectors $x^{(0)}$ for each model problem from Section 7.1. Therein we set $k = 6$, $c = s = 3$, and denote by $\vartheta_i^{(\ell)}$ the ith reciprocally largest Ritz value of (A, M) in the Krylov subspace $\mathcal{K}^k(x^{(\ell)})$. The numerical maxima NM of the distance $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ over 1000 tests are documented for $i \in \{1, 2, 3\}$, and plotted versus the iteration index ℓ in Figure 7.7. Moreover, we denote by $\vartheta_i^{(-1)}$ the ith reciprocally largest Ritz value of (A, M) in the low-dimensional Krylov subspace $\mathcal{K}^c(x^{(0)})$ concerning the multi-step estimates (4.33) and (4.34) from Theorem 4.9. Thus the iterations formally begin with the index -1. The dependence of their convergence behavior on the eigenvalue distribution can be interpreted as follows. In MP1 and MP3, the well-separated reciprocals of the target eigenvalues ensure a strictly monotone convergence with respect to inner steps within each outer step as observed in Figure 7.5. Correspondingly, the distance $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ is strictly decreasing. In MP2, a staircase-shaped convergence would be observed for a sufficiently large Krylov subspace; cf. the second row in Figure 7.5. However, the Krylov subspaces $\mathcal{K}^k(x^{(\ell)})$ in the tested restarted Krylov subspace iterations only have dimension 6 so that a slow local convergence can occur within $\mathcal{K}^k(x^{(\ell)})$. This leads to a minor reduction of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ in a few outer steps, but does not cause a slow global convergence.

Furthermore, suitable bounds for $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ are obtained by reformulating the estimates (4.33) and (4.34) as

$$\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1} \le \lambda_i^{-1} - \frac{\lambda_j^{-1} + \psi\, \lambda_{j+1}^{-1}}{1 + \psi} \quad \text{with} \quad \psi = [\, T_{k-c}(1 + 2\gamma_j)\,]^{-2(\ell+1)}\, \frac{\lambda_j^{-1} - \alpha_i^{-1}}{\alpha_i^{-1} - \lambda_{j+1}^{-1}} \tag{7.2}$$

and

$$\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1} \le \lambda_i^{-1} - \frac{\lambda_{j-c+i}^{-1} + \psi\, \lambda_{j+1}^{-1}}{1 + \psi} \quad \text{with} \quad \psi = [\, T_{k-c}(1 + 2\widetilde{\gamma}_{i,j})\,]^{-2(\ell+1)}\, \frac{\lambda_{j-c+i}^{-1} - \beta^{-1}}{\beta^{-1} - \lambda_{j+1}^{-1}}. \tag{7.3}$$

Therein α_i and β are Ritz values in $\mathcal{K}^c(x^{(0)})$. Their reciprocals belong to the interval $(\lambda_{j+1}^{-1}, \lambda_j^{-1})$. If the reciprocals of the corresponding Ritz values in the current $\mathcal{K}^c(x^{(\ell)})$ leave this interval, we update α_i and β by these Ritz values and determine a new interval. The observation in Figure 7.7 shows that (4.33) coincides with (4.34) for $i = 3 = c$. In addition, (4.33) is more accurate than (4.34) for $i \in \{1, 2\}$ in MP1 and MP3 where the reciprocals of the target eigenvalues are well separated. However, (4.33) cannot reflect the cluster robustness in MP2 since the gap ratio γ_j is close to zero in the final phase for $i \in \{1, 2\}$ so that the Chebyshev factor $[\, T_{k-c}(1 + 2\gamma_j)\,]^{-2(\ell+1)}$ cannot be bounded away from 1. In contrast, (4.34) can reasonably predict the convergence rate in the final phase, in spite of overestimation for earlier phases.

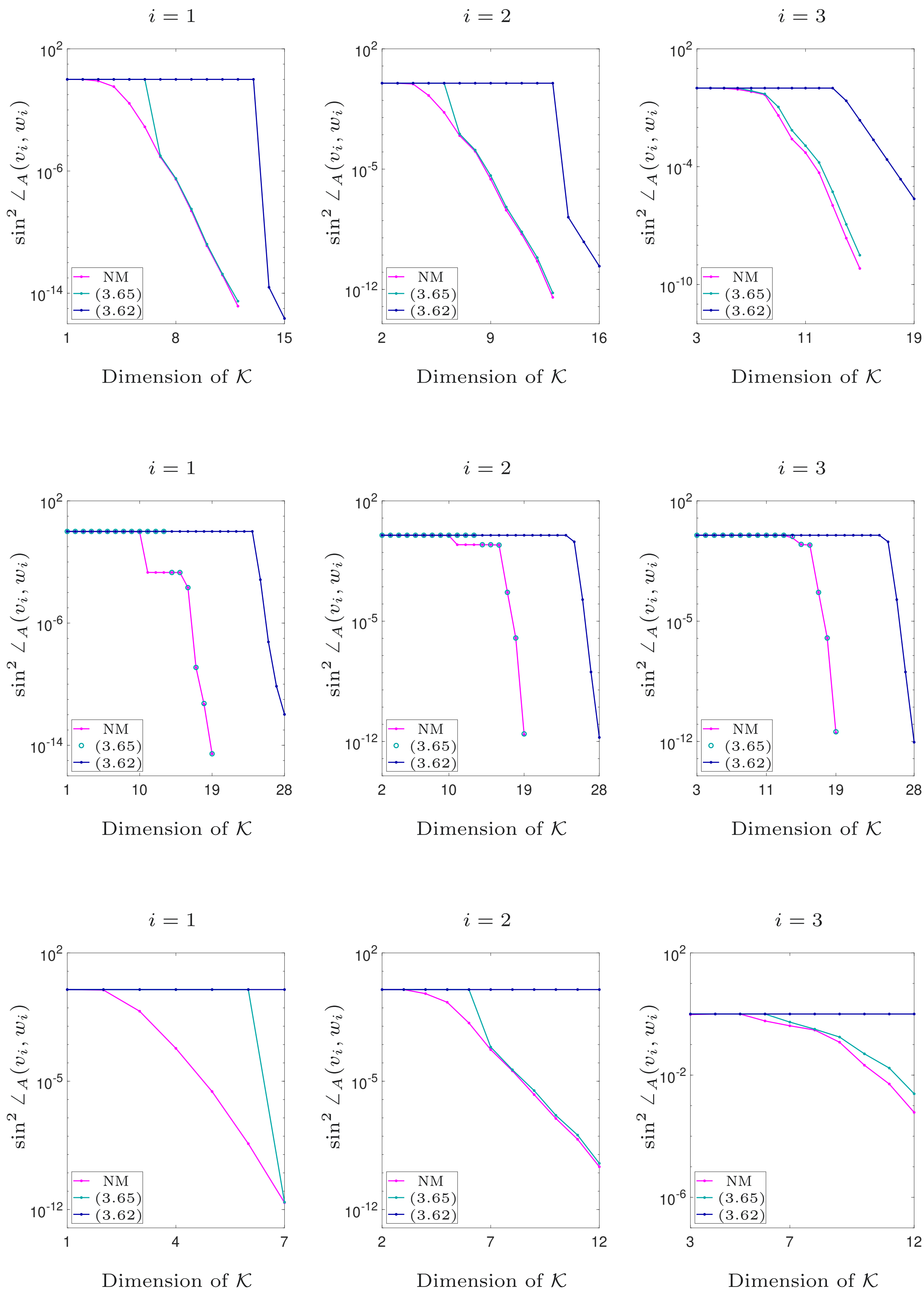

Figure 7.6: Illustration of the bound in the estimate (3.65) and the bound in the estimate combination "(3.65)+(3.62)" (denoted by "(3.62)" in the legends) in comparison to the numerical maxima NM of $\sin^2 \angle_A(v_i, w_i)$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

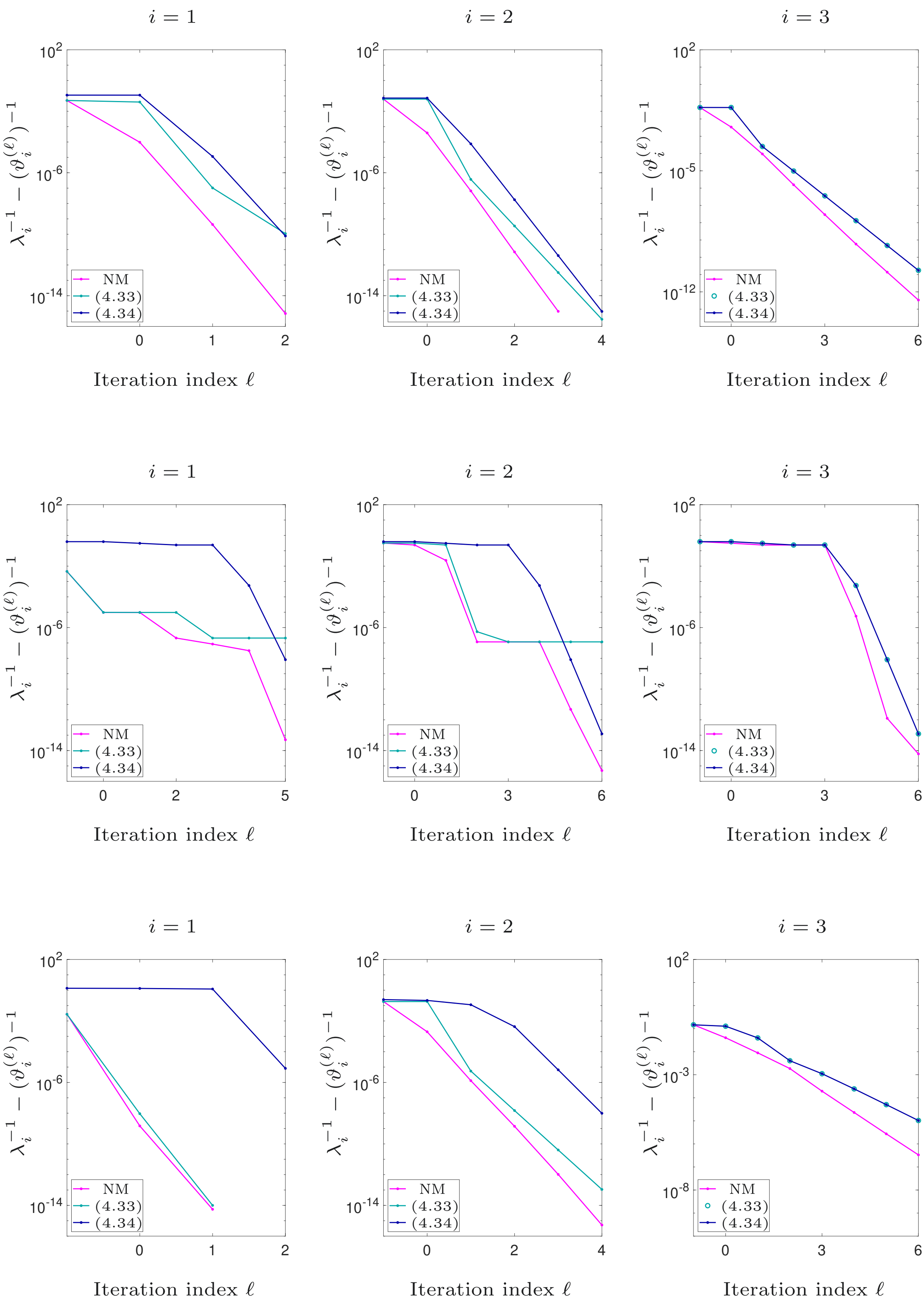

Figure 7.7: Illustration of the bounds in the equivalent forms (7.2) and (7.3) of the estimates (4.33) and (4.34) in comparison to the numerical maxima NM of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

7.2.3 Block-Krylov subspace iterations

We consider further block-Krylov subspace iterations of the type (1.24). By using 1000 pseudo-random initial subspaces $\mathrm{span}\{X^{(0)}\}$, we document numerical maxima with respect to various convergence measures corresponding to the main estimates from Theorem 5.10. The angle-free estimates on Ritz values are treated within their extensions to restarted block-Krylov subspace iterations in Subsection 7.2.4.

Estimates (5.30) and (5.31) on approximate eigenvectors

The estimates (5.30) and (5.31) serve to analyze the tangent value $\tan\angle_A(w_i,\mathcal{K})$ of the A-angle between an eigenvector w_i associated with the eigenvalue λ_i and the current block-Krylov subspace $\mathcal{K}=\mathcal{K}^k(X^{(0)})$. This angle is also the A-angle between w_i and its A-orthogonal projection to $\mathcal{K}$ which is an approximate eigenvector in $\mathcal{K}$, but usually not a Ritz vector. The application of these estimates depends on the dimension t of the initial subspace $\mathcal{X}=\mathrm{span}\{X^{(0)}\}$ and the cluster parameter c. In the case $t\geq c$, the estimate (5.30) is applicable and provides the bound $[\,T_{k-1}(1+2\gamma_{i,t})\,]^{-1}\tan\angle_A(\mathcal{X},\mathcal{W}^t)$ with the gap ratio $\gamma_{i,t}=(\lambda_i^{-1}-\lambda_{t+1}^{-1})/(\lambda_{t+1}^{-1}-\lambda_n^{-1})$ and the invariant subspace $\mathcal{W}^t=\mathrm{span}\{w_1,\dots,w_t\}$. In the case $t<c$, we use a low-dimensional block-Krylov subspace $\mathcal{K}^b=\mathcal{K}^b(X^{(0)})$ of degree b and dimension $d\geq c$. Then the estimate (5.31) provides the bound $[\,T_{k-b}(1+2\gamma_{i,d})\,]^{-1}\tan\angle_A(\mathcal{K}^b,\mathcal{W}^d)$ with the gap ratio $\gamma_{i,d}=(\lambda_i^{-1}-\lambda_{d+1}^{-1})/(\lambda_{d+1}^{-1}-\lambda_n^{-1})$ and the invariant subspace $\mathcal{W}^d=\mathrm{span}\{w_1,\dots,w_d\}$.

For illustrating the bounds in (5.30) and (5.31), we set $c=3$ according to the eigenvalue distribution in the model problems from Section 7.1. Subsequently, we document the numerical maxima NM of $\tan\angle_A(w_i,\mathcal{K})$ over 1000 tests for $i\in\{1,2,3\}$ where the dimension t of the initial subspace $\mathcal{X}=\mathrm{span}\{X^{(0)}\}$ is set equal to 3 for (5.30) and equal to 2 for (5.31). The documented NM are plotted versus the degree k of the current block-Krylov subspace $\mathcal{K}$ in Figure 7.8 for (5.30) and in Figure 7.9 for (5.31). It is remarkable that the convergence behavior with respect to NM depends weakly on the dimension t in MP1 and MP3. The main influence of t is that more steps are required for reaching an acceptable approximation by using smaller t. A significant dependence of the convergence behavior on t is observed in MP2 where the reciprocals of the target eigenvalues are clustered. If t is smaller than the cluster size, a staircase-shaped convergence occurs, namely, the reduction of $\tan\angle_A(w_i,\mathcal{K})$ nearly stagnates in a middle phase. Furthermore, as observed in Figure 7.8, the bound in (5.30) is reasonable for $i\in\{1,2\}$ in MP1 and MP3 as well as for $i\in\{1,2,3\}$ in MP2. A more accurate bound for $i=3$ in MP1 and MP3 can be constructed by applying (5.31) with a larger c. In Figure 7.9, the bound in (5.31) is determined with $b=2$ and $d=4$, and can provide a proper prediction of the convergence rate in the final phase.

Angle-dependent estimates (5.32) and (5.33) on Ritz values

The estimates (5.32) and (5.33) deal with the relative position $(\lambda_i^{-1}-\vartheta_i^{-1})/(\vartheta_i^{-1}-\lambda_n^{-1})$ of the ith reciprocally largest Ritz value ϑ_i of (A,M) in the current block-Krylov subspace $\mathcal{K}=\mathcal{K}^k(X^{(0)})$. The bounds coincide with the squares of the bounds in (5.30) and (5.31), respectively. Concerning the observation of the distance $\lambda_i^{-1}-\vartheta_i^{-1}$, we reformulate (5.32) and (5.33) as

$$\lambda_i^{-1}-\vartheta_i^{-1}\leq(\lambda_i^{-1}-\lambda_n^{-1})\,\frac{\psi}{1+\psi}\qquad\text{with}\qquad\psi=[\,T_{k-1}(1+2\gamma_{i,t})\,]^{-2}\,\tan^2\angle_A(\mathcal{X},\mathcal{W}^t)\tag{7.4}$$

and

$$\lambda_i^{-1}-\vartheta_i^{-1}\leq(\lambda_i^{-1}-\lambda_n^{-1})\,\frac{\psi}{1+\psi}\qquad\text{with}\qquad\psi=[\,T_{k-b}(1+2\gamma_{i,d})\,]^{-2}\,\tan^2\angle_A(\mathcal{K}^b,\mathcal{W}^d).\tag{7.5}$$

The corresponding bounds are illustrated in comparison to the numerical maxima NM of $\lambda_i^{-1}-\vartheta_i^{-1}$ over 1000 tests for $i\in\{1,2,3\}$. Therein we use $c=3$ as the cluster parameter. The dimension

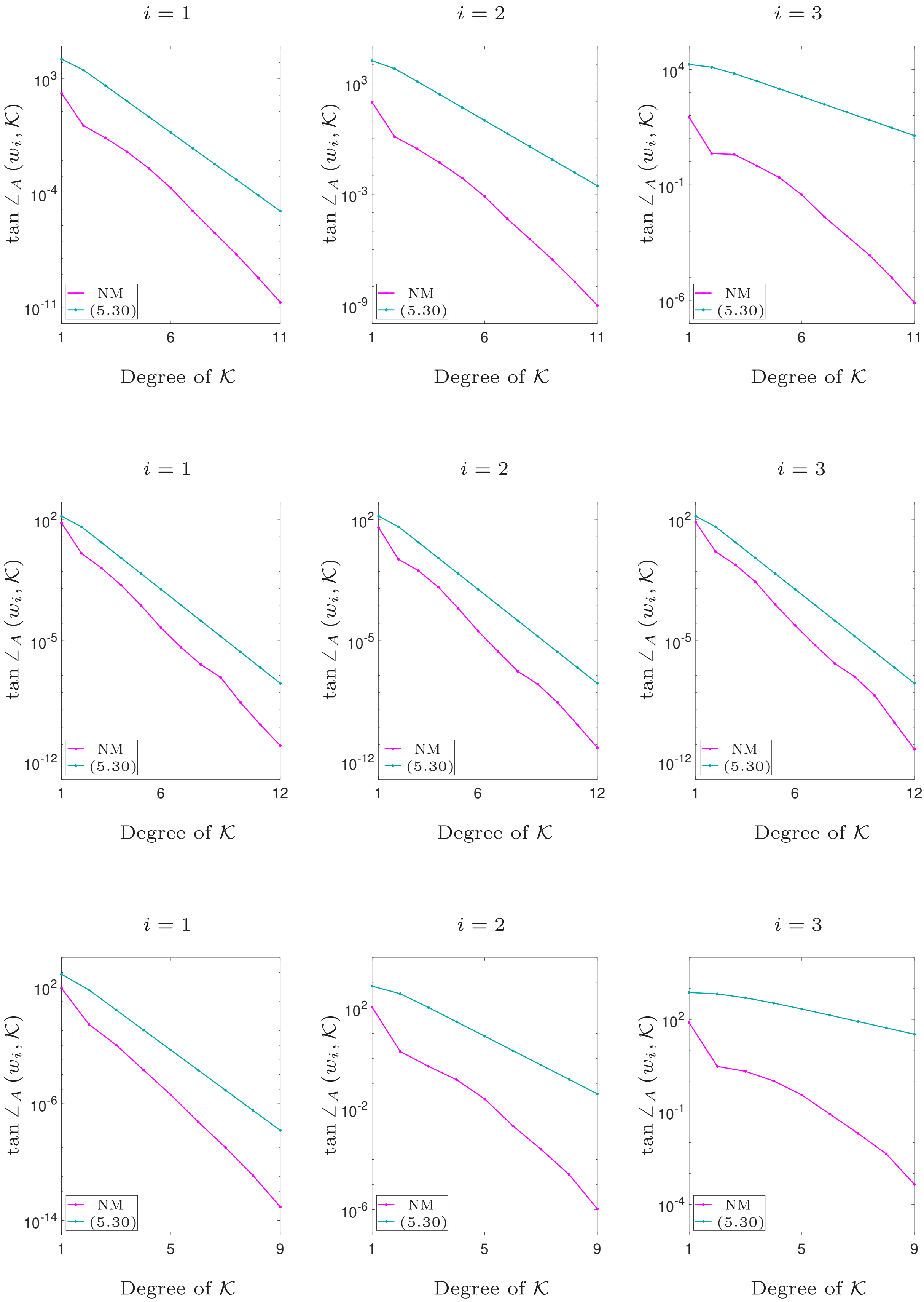

Figure 7.8: Illustration of the bound in the estimate (5.30) in comparison to the numerical maxima NM of $\tan \angle_A(w_i, \mathcal{K})$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

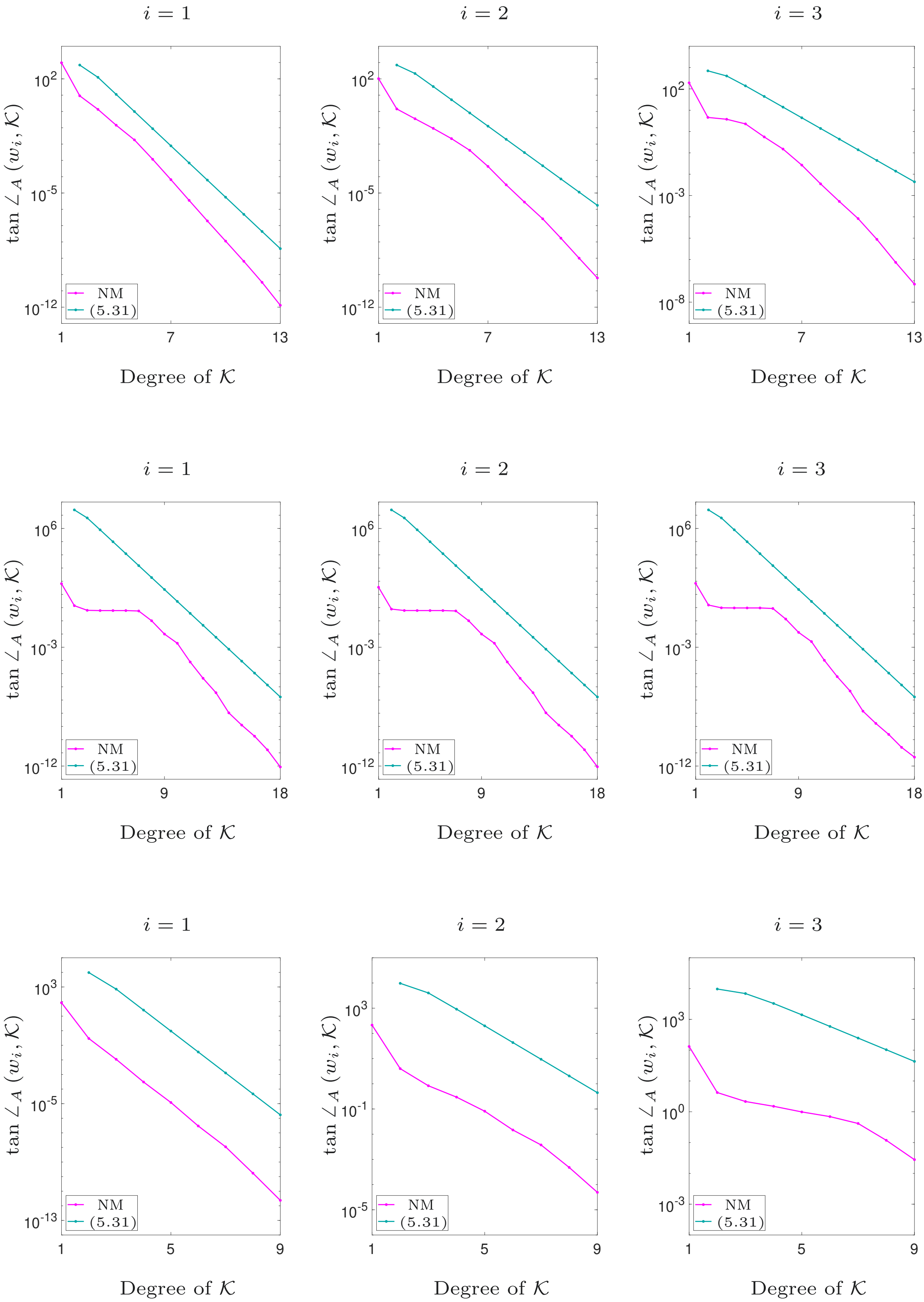

Figure 7.9: Illustration of the bound in the estimate (5.31) in comparison to the numerical maxima NM of $\tan \angle_A(w_i, \mathcal{K})$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

t of the initial subspace $\mathcal{X} = \operatorname{span}\{X^{(0)}\}$ is set equal to 3 for presenting (5.32) in Figure 7.10 and equal to 2 for presenting (5.33) in Figure 7.11. The convergence behavior is similar to that with respect to $\tan \angle_A(w_i, \mathcal{K})$. A strictly monotone convergence is observed in the most examples, whereas a staircase-shaped convergence occurs in the case $t = 2 < c$ in MP2 due to clustered eigenvalues. The observation of the bounds indicates that the convergence rate in the final phase can generally be predicted by the Chebyshev factor, but the prediction of the number of required steps for reaching an acceptable approximation is not always accurate; cf. the example $i = 3$ in MP1 and MP3.

Additional estimate (5.36) on Ritz vectors

The estimate (5.36) serves to analyze the sine squared $\sin^2 \angle_A(v_i, w_i)$ of the A-angle between a Ritz vector v_i in the current block-Krylov subspace $\mathcal{K} = \mathcal{K}^k(X^{(0)})$ and an eigenvector w_i. Moreover, we can combine (5.36) with (5.32) or (5.33) in order to construct an a priori estimate.

In Figure 7.12, we illustrate the bound in the estimate (5.36) and the bound in the estimate combination "(5.36)+(5.32)". Therein the numerical maxima NM of $\sin^2 \angle_A(v_i, w_i)$ over 1000 tests are documented for $i \in \{1, 2, 3\}$ and compared with the corresponding bounds. Similarly to the numerical experiment for (3.65) in Figure 7.6, the estimate (5.36) provides an accurate bound by using exact Ritz values, whereas the bound in "(5.36)+(5.32)" is less accurate due to the limited quality of (5.32) observed in Figure 7.10.

7.2.4 Restarted block-Krylov subspace iterations

In this subsection, we test restarted block-Krylov subspace iterations of the type (1.25) with 1000 pseudorandom initial subspaces $\mathcal{X}^{(0)} = \operatorname{span}\{X^{(0)}\}$ for each model problem from Section 7.1. Therein we denote by $\vartheta_i^{(\ell)}$ the ith reciprocally largest Ritz value of (A, M) in the block-Krylov subspace $\mathcal{K}^k(X^{(\ell)})$, and document the numerical maxima NM of the distance $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ over 1000 tests for $i \in \{1, 2, 3\}$. The cluster parameter c is set equal to 3 which is also the number s of target eigenvalues. Concerning the multi-step estimates from Theorem 6.5, we consider two cases with respect to the dimension t of $\mathcal{X}^{(0)}$. For $t = 3 = c$, we set $k = 4$ and illustrate the bounds in the estimates (6.18) and (6.19); see Figure 7.13. For $t = 2 < c$, we set $k = 5$ and illustrate the bounds in the estimates (6.20) and (6.21); see Figure 7.14. The corresponding NM of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ are plotted versus the iteration index ℓ where $\vartheta_i^{(-1)}$ is the ith reciprocally largest Ritz value of (A, M) in $\mathcal{X}^{(0)}$ or the low-dimensional block-Krylov subspace $\mathcal{K}^b(X^{(0)})$. The observation in these two figures reflects the dependence of the convergence behavior on the choice of t and k. Setting t equal to a proper cluster parameter c can avoid a staircase-shaped convergence caused by clustered eigenvalues as in MP2. Moreover, the dimension of $\mathcal{K}^k(X^{(\ell)})$ is not constantly equal to kc. For instance, with $t = 3 = c$ and $k = 4$ in Figure 7.13, the dimension of $\mathcal{K}^k(X^{(\ell)})$ is reduced to 6 after the distance $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ for $i \in \{1, 2\}$ has reached 10^{-12}. This can lead to a slow convergence of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ for $i = 3$ in MP1 and MP3. If t is smaller than c, the dimension of $\mathcal{K}^k(X^{(\ell)})$ is between kt and kc at the beginning, and can be smaller than kt in the final phase, e.g., equal to 7 in the case with $t = 2 < c$ and $k = 5$ in Figure 7.14.

Subsequently, we build suitable bounds for $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$ by reformulating the above-mentioned multi-step estimates from Theorem 6.5 analogously to (7.2) and (7.3) in Subsection 7.2.2. As observed in Figure 7.13 and Figure 7.14, the estimates (6.19) and (6.21) with the cluster-dependent gap ratio $\widetilde{\gamma}_{i,j} = (\lambda_{j-c+i}^{-1} - \lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1} - \lambda_n^{-1})$ can reflect the cluster robustness and reasonably predict the convergence rate in the final phase, whereas the estimates (6.18) and (6.20) with the simple gap ratio $\gamma_j = (\lambda_j^{-1} - \lambda_{j+1}^{-1})/(\lambda_{j+1}^{-1} - \lambda_n^{-1})$ are more accurate for the first steps.

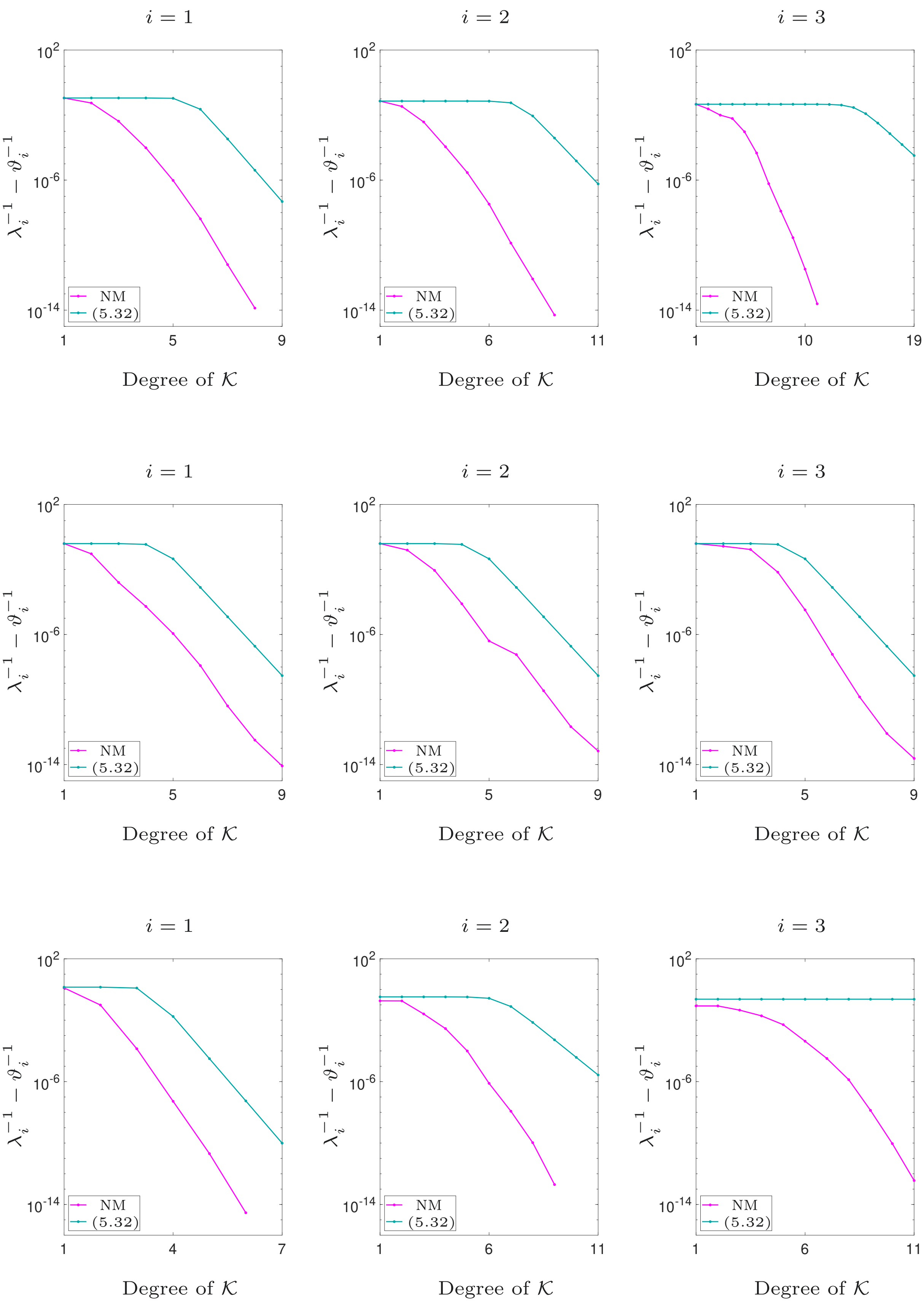

Figure 7.10: Illustration of the bound in the equivalent form (7.4) of the estimate (5.32) in comparison to the numerical maxima NM of $\lambda_i^{-1} - \vartheta_i^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

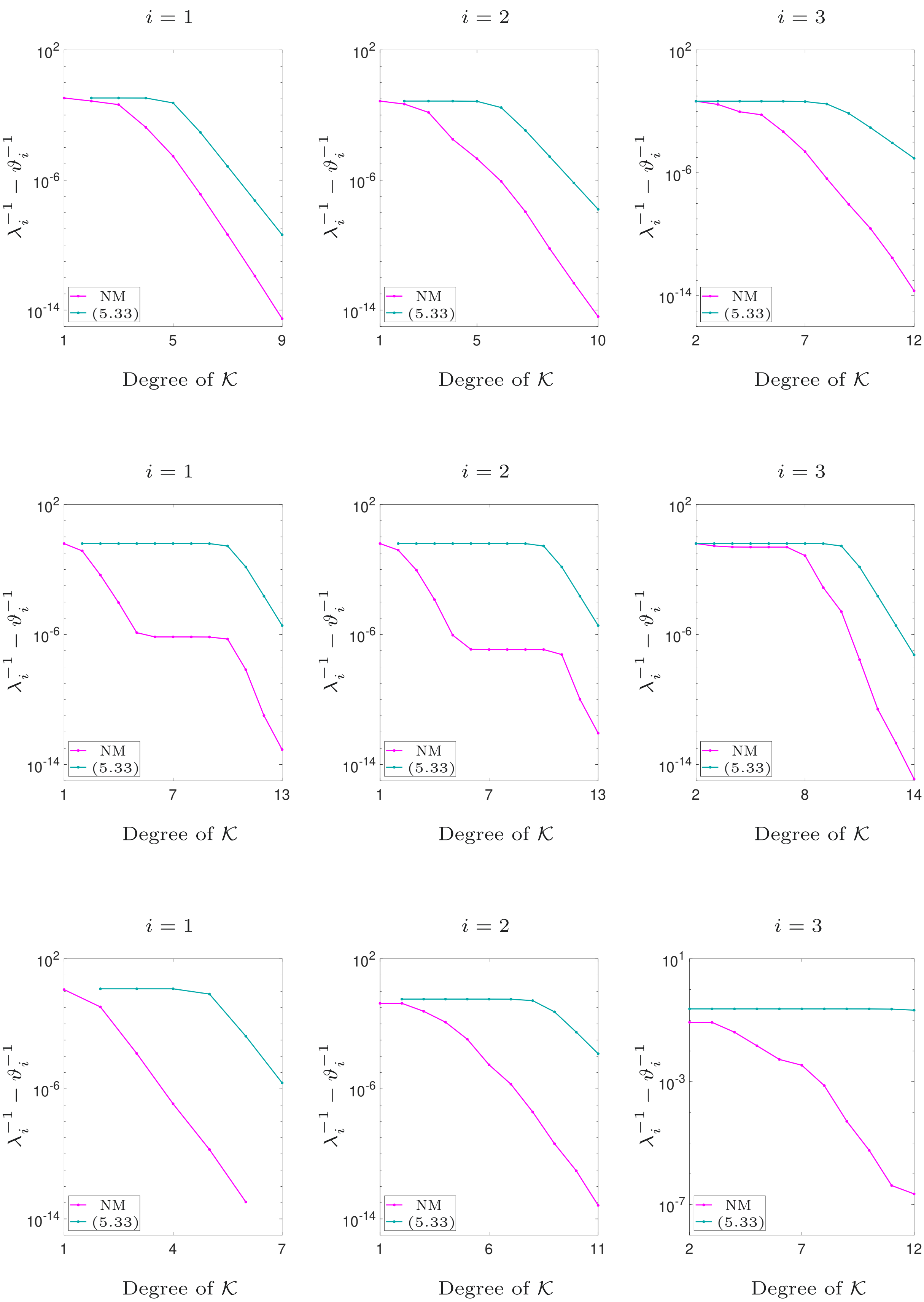

Figure 7.11: Illustration of the bound in the equivalent form (7.5) of the estimate (5.33) in comparison to the numerical maxima NM of $\lambda_i^{-1} - \vartheta_i^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

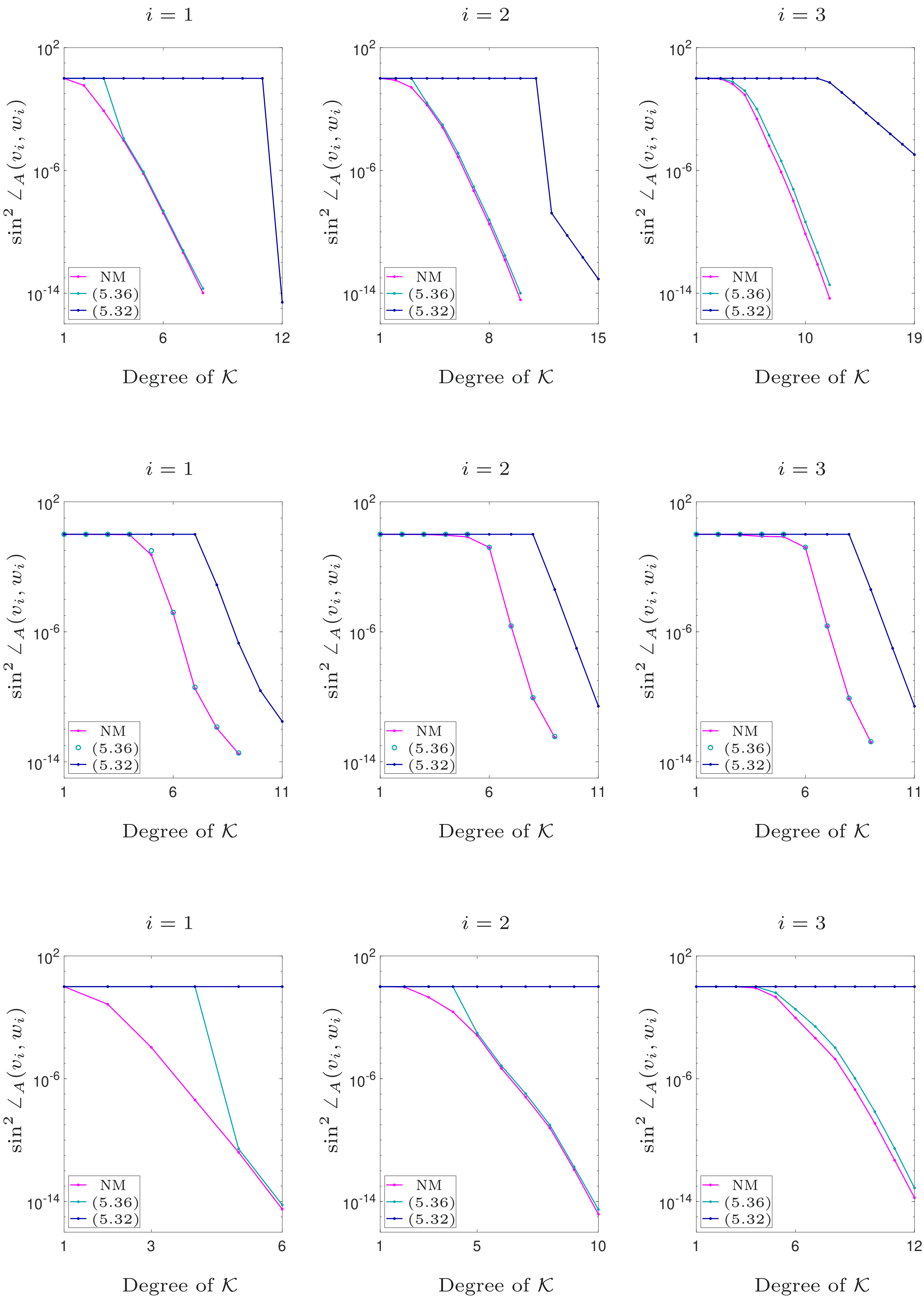

Figure 7.12: Illustration of the bound in the estimate (5.36) and the bound in the estimate combination "(5.36)+(5.32)" (denoted by "(5.32)" in the legends) in comparison to the numerical maxima NM of $\sin^2 \angle_A(v_i, w_i)$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

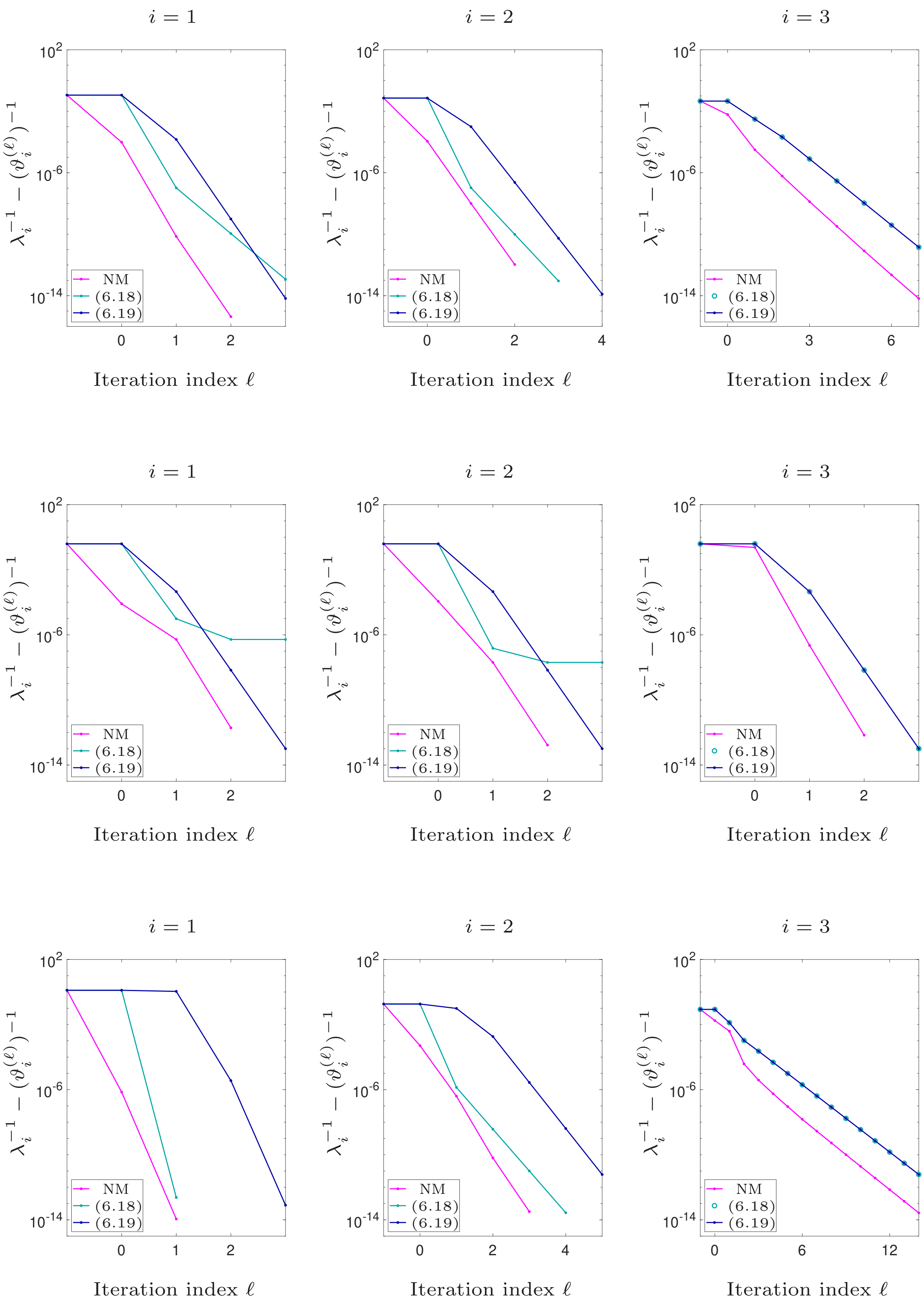

Figure 7.13: Illustration of the bounds in equivalent forms of the estimates (6.18) and (6.19) in comparison to the numerical maxima NM of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

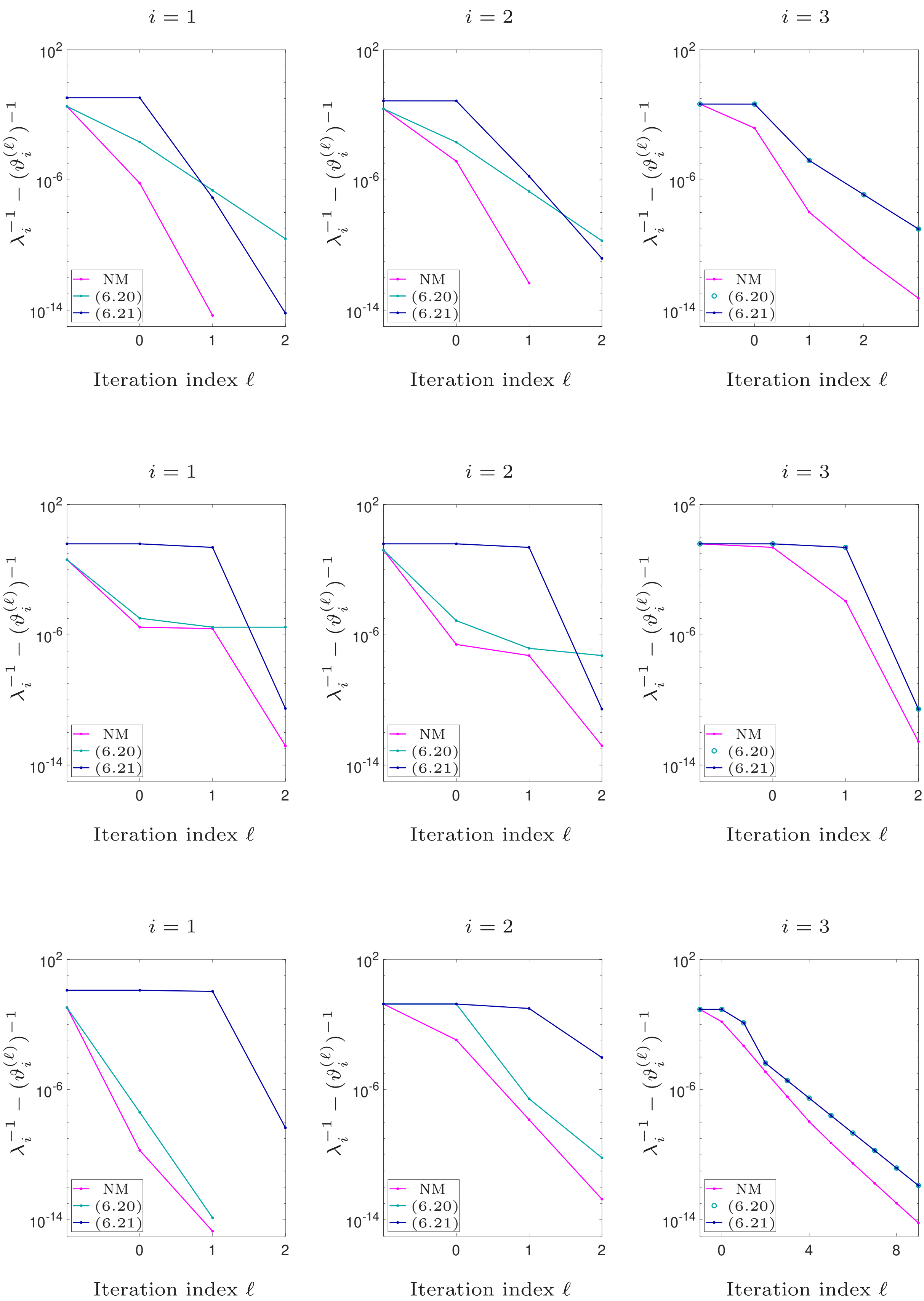

Figure 7.14: Illustration of the bounds in equivalent forms of the estimates (6.20) and (6.21) in comparison to the numerical maxima NM of $\lambda_i^{-1} - (\vartheta_i^{(\ell)})^{-1}$. *First row*: MP1. *Second row*: MP2. *Third row*: MP3.

8 Conclusion and outlook

Efficient and memory-saving numerical algorithms are of considerable importance for solving modern eigenvalue problems arsing from various scientific and technological activities. Such algorithms break through the limitations of classical matrix-based eigensolvers. Indeed, most of modern eigenvalue problems cannot be solved in a fully analytical way as the famous Abel-Ruffini theorem predicts that there is no closed-form expression for the roots of general polynomials whose degrees exceed four. Analytical solutions are only known for simple problems, e.g., tiny matrix eigenvalue problems and model operator eigenvalue problems on very regular domains. Moreover, matrix transformations are limited to small matrix eigenvalue problems due to their usually cubic time complexity. Therefore vector iterations and subspace iterations are preferred for developing modern eigensolvers, and significant advances have been made in recent decades. Nevertheless, the convergence behavior of many popular eigensolvers have only been partially or indirectly analyzed. More reasonable convergence estimates are desired for the further development of these eigensolvers.

In this context, the present thesis contributes to the convergence theory of Krylov subspace eigensolvers by providing new a priori estimates which significantly improve the comparable classical estimates. The investigated eigensolvers deal with discretized eigenvalue problems of second-order self-adjoint elliptic partial differential operators and serve to compute a moderate number of eigenvalues and the associated eigenfunctions. The classical estimates from [42, 90, 98, 94] concerning standard matrix eigenvalue problems can be applied to these eigensolvers after proper reformulations. However, the application is limited due to several drawbacks. In particular, the dependence of the bounds on the current (block-)Krylov subspace is an obstacle to deriving practical a priori estimates for restarted iterations.

In order to overcome these drawbacks, we modify the underlying proof techniques by extending the analysis of the block power method [97] and the analysis of certain abstract iterations for matrix functions [44, 45]. The resulting estimates provide considerably better bounds in the case of clustered eigenvalues. Moreover, their concise forms and natural assumptions enable further progress in the convergence analysis of restarted iterations. A remarkable fact is that Krylov subspace iterations can be interpreted as block-Krylov subspace iterations whose initial subspaces are Krylov subspaces. This allows us to extend our previous results on simple restarting [83, 125] to implicit or thick restarting.

In summary, we have investigated four types of Krylov subspace eigensolvers: standard Krylov subspace iterations (SK), restarted Krylov subspace iterations (RK), block-Krylov subspace iterations (BK) and restarted block-Krylov subspace iterations (RBK). For each of SK and BK, we have achieved four types of new estimates: (i) estimates on approximate eigenvectors, (ii) angle-dependent estimates on Ritz values, (iii) angle-free estimates on Ritz values, (iv) additional estimates on Ritz vectors. The types (i) and (ii) are direct improvements of the classical Chebyshev type estimates from [98] by Saad. Therein certain overestimations are avoided by using low-dimensional auxiliary subspaces which are subsets of small (block-)Krylov subspaces. The type (iii) provides a refinement of (ii) concerning restarted iterations, whereas the type (iv) can be combined with (ii) or (iii) for analyzing Ritz vectors in the final phase of the considered iteration. Furthermore, we have extended the type (iii) to arbitrarily located initial Ritz values. The extended estimates serve to investigate RK and RBK. Therein the Chebyshev factors can be improved additionally in terms of interpolation polynomials on the basis of an ellipsoidal interpretation of the relevant approximate eigenvectors.

Many of our estimates are derived inter alia with the following steps: (1) constructing auxiliary vectors which are orthogonal to an invariant subspace associated with several interior eigenvalues, (2) analyzing intermediate terms concerning shifted Chebyshev polynomials, (3) combining intermediate estimates by using angle relations or the monotonicity of relative positions in eigenvalue intervals. The step (1) enables a restriction of the analysis where the selected interior eigenvalues are skipped. This results in sufficiently large gap ratios for the step (2) so that suitable Chebyshev factors can be obtained. An important proof technique in (2) is splitting intermediate terms with respect to two invariant subspaces corresponding to the desired gap ratios. The step (3) serves to eliminate intermediate terms in the final bounds so that a priori estimates can be achieved.

In the numerical experiments for demonstrating our estimates, we observe that the Chebyshev factors can reasonably predict the convergence rate in the final phase of the considered iteration. It is challenging to accurately analyze every phase without further assumptions. In particular, the cluster robustness of Krylov subspace eigensolvers essentially depends on their initial vectors or initial subspaces. If the size of an eigenvalue cluster exceeds the dimension of an initial subspace, then slow convergence can occur in the first steps of the considered iteration. Nevertheless, our estimates can still reflect the cluster robustness in the sense of the entire convergence history.

Our outlook on future research includes the following topics: (I) improving the Chebyshev factors concerning (block-)Krylov subspaces of arbitrary degree, (II) deriving analogous estimates on sums of Ritz values which approximate clustered eigenvalues as well as on subspaces spanned by the associated Ritz vectors, (III) extending the current convergence analysis to related preconditioned eigensolvers.

The topic (I) is a continuation of our geometric investigation of Krylov subspace eigensolvers. The Chebyshev factors are sharp only in the case that the associated Chebyshev polynomial is linear. A considerable improvement has already been achieved for the quadratic case, whereas improvements for further cases are limited to intermediate estimates which depend on Ritz values in certain auxiliary subspaces. The desired general improvements are expected to be helpful for investigating preconditioned eigensolvers within the topic (III).

The topic (II) is inspired by indirect improvements of Saad's estimates for block-Krylov subspace iterations suggested by Li and Zhang [62]. These improvements are essentially generalizations with respect to alternative convergence measures. We aim to avoid some problematic terms such as possibly large ratio-products on the basis of the new proof techniques from the present thesis. Furthermore, this topic is related to the majorization error bounds from [49] by Knyazev and Argentati. Therein Ritz values are analyzed within arranged sets, and principal angles between subspaces are utilized for constructing suitable bounds.

The topic (III) is devoted to deepening the convergence theory of the hierarchy of preconditioned eigensolvers introduced in [75]. As mentioned in Subsection 1.3.2, we plan to investigate the single-vector method $\mathscr{P}_k$ with $k \geq 3$ by combining our analysis of restarted Krylov subspace iterations with proper interpretation of preconditioning. A next task is to derive cluster robust estimates for the block method $\mathscr{P}_{k,s}$ with $k \geq 2$ based on our analysis of $\mathscr{P}_{1,s}$ from [126]. Moreover, we are also interested in deriving similar estimates for further preconditioned eigensolvers such as the generalized Davidson method [68] and the more recent methods [56, 114, 115, 110, 111, 18, 54].

Last but not least, we expect that these topics can contribute to the convergence analysis for Krylov subspace methods in the area "linear response eigenvalue problems" [7] where the known estimates have similar drawbacks as the above-mentioned classical estimates.

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