

CONVERGENCE RATES OF INDIVIDUAL RITZ VALUES IN BLOCK PRECONDITIONED GRADIENT-TYPE EIGENSOLVERS

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ABSTRACT. Many popular eigensolvers for large and sparse Hermitian matrices or matrix pairs can be interpreted as accelerated block preconditioned gradient (BPG) iterations in order to analyze their convergence behavior by composing known estimates. An important feature of BPG is the cluster robustness, i.e., reasonable performance for computing clustered eigenvalues is ensured by a sufficiently large block size. This feature can easily be explained for exact-inverse (exact shift-inverse) preconditioning by adapting classical estimates on non-preconditioned eigensolvers, whereas the existing results for more general preconditioning are still improvable. We expect to extend certain sharp estimates for the corresponding vector iterations to BPG where proper bounds of convergence rates of individual Ritz values are to be derived. Such an extension has been achieved for BPG with fixed step sizes in [Math. Comp. 88 (2019), 2737–2765]. The present paper deals with the more practical case that the step sizes are implicitly optimized by the Rayleigh-Ritz method. Our new estimates improve some previous ones in view of concise and more flexible bounds.

1. Introduction

Solving eigenvalue problems of large and sparse Hermitian matrices or matrix pairs are of practical importance in various applications. Proper iterative methods with vectors or subspaces allow determining the desired eigenpairs with reasonable effort [1, 7]. The convergence behavior of such eigensolvers depends on the distribution of relevant eigenvalues as well as certain methodical characteristics including preconditioners and block sizes (dimensions of iterates).

As a simple example, we first consider the computation of the smallest eigenvalues of a symmetric positive definite matrix $A \in \mathbb{R}^{n \times n}$ by the preconditioned subspace iteration

$$(1.1) \quad X^{(\ell+1)} \xleftarrow{\text{RR}[s]} \text{span}\{X^{(\ell)} - TR^{(\ell)}\}.$$

Therein s denotes the block size. The current iterate $X^{(\ell)} \in \mathbb{R}^{n \times s}$ is assumed to have full rank and consists of orthonormal Ritz vectors of A in the subspace $\text{span}\{X^{(\ell)}\}$. The corresponding residuals form the block residual $R^{(\ell)} = AX^{(\ell)} - X^{(\ell)}\Theta^{(\ell)}$ with the diagonal matrix $\Theta^{(\ell)} \in \mathbb{R}^{s \times s}$ containing Ritz values. The term $TR^{(\ell)}$ can be determined by using an incomplete factorization of A or approximately solving a block linear system of the form $AE = R^{(\ell)}$. The underlying matrix T is called preconditioner and represents an approximate inverse of A for which the condition

$$(1.2) \quad \|I - TA\|_A \leq \gamma < 1$$

with the $n \times n$ identity matrix I ensures that the trial subspace $\mathcal{U}^{(\ell)} = \text{span}\{X^{(\ell)} - TR^{(\ell)}\}$ has dimension s according to [9, Lemma 3.1]. Finally, the Rayleigh-Ritz procedure $\text{RR}[s]$ extracts orthonormal Ritz vectors from $\mathcal{U}^{(\ell)}$ and builds with them the next iterate $X^{(\ell+1)}$. This elementary eigensolver is actually a block preconditioned gradient (BPG) iteration since the columns

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of $R^{(\ell)}$ are collinear with the gradient vectors of the Rayleigh quotient

$$\lambda : \mathbb{R}^n \setminus \{0\} \rightarrow \mathbb{R}, \quad \lambda(x) = \frac{x^T A x}{x^T x}$$

associated with the columns of $X^{(\ell)}$. For computing the first t eigenvalues of A concerning the eigenvalue arrangement $\lambda_1 \leq \dots \leq \lambda_n$, one can basically set a sufficiently large block size s for ensuring $\lambda_t \ll \lambda_{s+1}$ according to the well-known convergence theory [15] for the subspace iteration $X^{(\ell+1)} \xleftarrow{\text{RR}[s]} \text{span}\{A^{-1}X^{(\ell)}\}$ (i.e. the block power method for A^{-1}) which coincides with the special form of (1.1) for $T = A^{-1}$. Extending the trial subspace of (1.1) leads to more efficient eigensolvers such as

$$(1.3) \quad X^{(\ell+1)} \xleftarrow{\text{RR}[s]} \text{span}\{X^{(\ell)}, TR^{(\ell)}\}$$

which can be interpreted as a BPG iteration with optimized step sizes, and

$$(1.4) \quad X^{(\ell+1)} \xleftarrow{\text{RR}[s]} \text{span}\{X^{(\ell-1)}, X^{(\ell)}, TR^{(\ell)}\}$$

which corresponds to the locally optimal block preconditioned conjugate gradient (LOBPCG) method [5]. Moreover, it is advantageous to implement these eigensolvers in combination with deflation due to the different convergence rates of individual Ritz values. Deriving sharp bounds of these convergence rates is challenging for advanced eigensolvers. We review here some known results for the iterations (1.1) and (1.3).

1.1. Known results

The convergence behavior of (1.1) can be analyzed as in [3, Section 2] in terms of the eigenvalue arrangement $\lambda_1 \leq \dots \leq \lambda_n$ of A , the quality parameter γ from (1.2) for the preconditioner T , and the block size s . The resulting estimate for the i th Ritz value for an index $i \in \{1, \dots, s\}$ provides a bound which essentially depends on the convergence factor

$$(1.5) \quad \gamma + (1 - \gamma)\lambda_i/\lambda_{s+1}.$$

Its special form λ_i/λ_{s+1} for $\gamma = 0$, i.e., for $T = A^{-1}$, also appears in a classical angle estimate for the block power method for A^{-1} in [15]. However, the analysis in [3] requires a technical assumption on certain angles between the initial subspace $\text{span}\{X^{(0)}\}$ and the eigenvectors associated with the eigenvalues $\lambda_1, \dots, \lambda_s$. The gap $\lambda_{i+1} - \lambda_i$ for each $i \in \{1, \dots, s\}$ has to be sufficiently large for making the assumption practically reasonable. Although the convergence factor (1.5) is suitable for indicating the cluster robustness of (1.1), i.e., fast convergence for $i \ll s$ despite $\lambda_{i+1} - \lambda_i \approx 0$, the assumption limits the applicability.

A more flexible and concise estimate for (1.1) can be derived by [6, Section 5]. Therein an eigenvalue interval $(\lambda_j, \lambda_{j+1})$ with $j \geq i$ is used for locating the i th Ritz value in the current subspace iterate, and the distance ratio $(* - \lambda_j)/(\lambda_{j+1} - *)$ serves as a convergence measure. The corresponding convergence factor reads $\gamma + (1 - \gamma)\lambda_j/\lambda_{j+1}$. In particular, if the i th Ritz value reaches the interval $(\lambda_i, \lambda_{i+1})$, one gets the special form $\gamma + (1 - \gamma)\lambda_i/\lambda_{i+1}$ which is less accurate in comparison to (1.5) but still reasonable for sufficiently large $\lambda_{i+1} - \lambda_i$. Moreover, this result cannot be refined as (1.5) without further modifications since its theoretical sharpness can be verified by certain special iterates.

Our recent result in [21] uses a larger interval for the Ritz value location, namely, $(\lambda_{j-s+i}, \lambda_{j+1})$ with $j \geq s$. By defining an alternative quality parameter $\tilde{\gamma}$ for the preconditioner T concerning a geometric interpretation based on [9], we have achieved the convergence factor $\tilde{\gamma} + (1 - \tilde{\gamma})\lambda_{j-s+i}/\lambda_{j+1}$ with respect to $(* - \lambda_{j-s+i})/(\lambda_{j+1} - *)$. The final phase of (1.1) is characterized by $j = s$ where the distance ratio is simply $(* - \lambda_i)/(\lambda_{s+1} - *)$ and the convergence factor is

specialized as $\tilde{\gamma} + (1 - \tilde{\gamma})\lambda_i/\lambda_{s+1}$. This is comparable with (1.5), and can reasonably describe the cluster robustness since the technical assumption used in [3] is avoided.

The above estimates for (1.1) also provide preliminary bounds for the accelerated iterations (1.3) and (1.4). More direct bounds for (1.3) have been presented in [13] in terms of sums of Ritz value errors by generalizing some arguments from [16, 14] concerning vectorial gradient iterations, and in [12] by upgrading the analysis from [6] and adapting a sharp estimate from [10] for the single-vector version of (1.3). In comparison to the desirable convergence factor

$$(1.6) \quad \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \quad \text{with} \quad \kappa = \frac{\lambda_i(\lambda_n - \lambda_{s+1})}{\lambda_{s+1}(\lambda_n - \lambda_i)}$$

which can easily be shown to improve (1.5), the result from [13] contains some additional technical terms and only asymptotically indicates (1.6), whereas the result from [12] gives a suboptimal form of (1.6) with the index $i + 1$ instead of $s + 1$. These results for (1.3) need to be improved in order to build a proper basement for the convergence analysis of more complicated eigensolvers including LOBPCG.

1.2. Aim and overview

Our goal is to derive concise Ritz value estimates containing convergence factors like (1.6) for interpreting the cluster robustness of the BPG iteration (1.3). As the ratio λ_i/λ_{s+1} is a decisive term in (1.6), a fundamental idea is to skip the eigenvalues $\lambda_{i+1}, \dots, \lambda_s$ (or $\lambda_{j-s+i+1}, \dots, \lambda_j$ in a more general case with $j \geq s$) by utilizing certain auxiliary subspaces which are orthogonal (and A -orthogonal) to the associated eigenvectors x_{i+1}, \dots, x_s .

This idea arises from the analysis of an abstract block iteration by Knyazev [4], and has been adapted to the preconditioned subspace iteration (1.1) in [21]. By observing a partial iteration of (1.1) within the orthogonal complement of $\text{span}\{x_{i+1}, \dots, x_s\}$, some Ritz vectors in two successive subspace iterates are compared in a geometric way similarly to [9] for constructing a perturbed inverse vector iteration. The corresponding perturbation parameter $\tilde{\gamma}$ can be used as an alternative quality parameter of preconditioning in the further analysis. We note that this approach depends on the fact that the next subspace iterate in (1.1) is simply the current trial subspace, i.e., $\text{span}\{X^{(\ell+1)}\} = \text{span}\{X^{(\ell)} - TR^{(\ell)}\}$. Thus a direct comparison between Ritz vectors is enabled.

In contrast, the BPG iteration (1.3) cannot be described by an equality formula since the next subspace iterate is only a subset of the current trial subspace. The more complicated relation between Ritz vectors therein is analyzed in [12] using Sion's-minimax theorem via certain basis matrices instead of Ritz vectors. Consequently, for analyzing the cluster robustness of (1.3), we tend to update the above construction of an alternative quality parameter of preconditioning by means of basis matrices or subspaces.

For the sake of generality, we follow the introduction of the LOBPCG method in [5] and reformulate (1.3) for the generalized eigenvalue problem

$$(1.7) \quad Mv = \mu Av, \quad M, A \in \mathbb{C}^{n \times n} \text{ Hermitian, } \quad A \text{ positive definite}$$

where the target eigenvalues of the matrix pair (M, A) are the largest ones. Some conversions between (1.7) and practical eigenvalue problems are introduced in Section 2 together with a simple representation of the investigated iteration which does not limit the generality. Section 3 provides some auxiliary terms and intermediate arguments based on the analysis of an abstract block iteration from [4] and the analysis of the preconditioned subspace iteration (1.1) from [21]. A subspace-oriented interpretation of preconditioning in partial iterations of the BPG iteration (1.3) leads to multi-step estimates in Section 4 reflecting the cluster robustness. We additionally

discuss the possibility of deriving estimates under classical conditions like (1.2). Numerical experiments for illustrating the new results are given in Section 5.

2. Preliminaries

The generalized eigenvalue problem (1.7) can be used as a common form of several practical eigenvalue problems, e.g., computing a subset of the spectrum of a self-adjoint elliptic partial differential operator together with the associated eigenfunctions. Therein proper discretizations produce the standard eigenvalue problem $Lu = \lambda u$ of an Hermitian matrix $L \in \mathbb{C}^{n \times n}$ or the generalized eigenvalue problem

$$(2.1) \quad Lu = \lambda Su, \quad L, S \in \mathbb{C}^{n \times n} \text{ Hermitian, } S \text{ positive definite}$$

which formally includes $Lu = \lambda u$ by setting S as the $n \times n$ identity matrix I .

If the target eigenvalues of the matrix pair (L, S) are the smallest ones, we can transform (2.1) as $(L - \sigma S)u = (\lambda - \sigma)Su$ with a sufficiently small shift σ such that the matrix $\tilde{L} = L - \sigma S$ is positive definite. The shifted problem corresponds to (1.7) for $M = S$, $A = \tilde{L}$ and $\mu = (\lambda - \sigma)^{-1}$.

If some interior eigenvalues of (L, S) are first to be determined, a similar shifted problem with an indefinite and invertible \tilde{L} can be established. This cannot directly be covered by (1.7). Instead, we can consider the equivalent problem $(\tilde{L}S^{-1}\tilde{L})u = (\lambda - \sigma)\tilde{L}u$ as a special form of (1.7) with $M = \pm\tilde{L}$, $A = \tilde{L}S^{-1}\tilde{L}$ and $\mu = \pm(\lambda - \sigma)^{-1}$.

Some further specializations of (1.7) refer to Hermitian definite matrix pencils [8] and the linear response eigenvalue problem [2].

2.1. Considered iteration

We modify the iteration (1.3) in order to compute the largest eigenvalues of (M, A) from (1.7). With the block size s , the current iterate $V^{(\ell)} \in \mathbb{C}^{n \times s}$ has full rank and consists of A -orthonormal Ritz vectors of (M, A) in the subspace $\text{span}\{V^{(\ell)}\}$. The associated block residual reads $R_V^{(\ell)} = MV^{(\ell)} - AV^{(\ell)}\Theta_V^{(\ell)}$ with the diagonal Ritz value matrix $\Theta_V^{(\ell)} = V^{(\ell)*}MV^{(\ell)} \in \mathbb{R}^{s \times s}$. An approximate solution of the block linear system $AE = R_V^{(\ell)}$ is denoted by $\tilde{T}R_V^{(\ell)}$ with a Hermitian positive definite preconditioner \tilde{T} which is an approximate inverse of A . By using the smallest eigenvalue α and the largest eigenvalue β of the matrix product $\tilde{T}A$ (or $A^{1/2}\tilde{T}A^{1/2}$) which are both positive, it holds that

$$(2.2) \quad \|I - \omega\tilde{T}A\|_A \leq \gamma \quad \text{with} \quad \omega = \frac{2}{\beta + \alpha} \quad \text{and} \quad \gamma = \frac{\beta - \alpha}{\beta + \alpha} < 1.$$

This condition is a more natural form of (1.2) concerning an arbitrary Hermitian positive definite \tilde{T} and additional scaling. The trial subspace $\mathcal{U}_V^{(\ell)} = \text{span}\{V^{(\ell)}, \tilde{T}R_V^{(\ell)}\}$ evidently has at least dimension s . The next iterate $V^{(\ell+1)}$ is constructed by A -orthonormal Ritz vectors of (M, A) in $\mathcal{U}_V^{(\ell)}$ associated with the s largest Ritz values. We denote by $\text{RR}[M, A, s]$ the underlying Rayleigh-Ritz procedure. Then the modified version of (1.3) is represented by

$$(2.3) \quad V^{(\ell+1)} \xleftarrow{\text{RR}[M, A, s]} \text{span}\{V^{(\ell)}, \tilde{T}R_V^{(\ell)}\}.$$

The special form of (2.3) for $M = I$ is equivalent to (1.3). Therein all Ritz values are positive so that $\Theta_V^{(\ell)}$ is positive definite. By using its square root matrix $C = (\Theta_V^{(\ell)})^{1/2}$, one can construct the iterate $X^{(\ell)} = V^{(\ell)}C^{-1}$ for (1.3) due to the properties

$$\begin{aligned} X^{(\ell)*}X^{(\ell)} &= X^{(\ell)*}MX^{(\ell)} = C^{-1}V^{(\ell)*}MV^{(\ell)}C^{-1} = C^{-1}\Theta_V^{(\ell)}C^{-1} = I_s, \\ X^{(\ell)*}AX^{(\ell)} &= C^{-1}V^{(\ell)*}AV^{(\ell)}C^{-1} = C^{-2} = (\Theta_V^{(\ell)})^{-1}, \end{aligned}$$

i.e., the columns of $X^{(\ell)}$ are orthonormal Ritz vectors of A in $\text{span}\{X^{(\ell)}\}$, and the corresponding Ritz values are contained in $\Theta^{(\ell)} = (\Theta_V^{(\ell)})^{-1}$. In addition, the relation

$$\begin{aligned} R^{(\ell)} &= AX^{(\ell)} - X^{(\ell)}\Theta^{(\ell)} = AV^{(\ell)}C^{-1} - V^{(\ell)}C^{-1}(\Theta_V^{(\ell)})^{-1} \\ &= -(MV^{(\ell)} - AV^{(\ell)}\Theta_V^{(\ell)})C^{-3} = -R_V^{(\ell)}C^{-3} \end{aligned}$$

leads to the subspace equality $\text{span}\{X^{(\ell)}, TR^{(\ell)}\} = \text{span}\{V^{(\ell)}, \tilde{T}R_V^{(\ell)}\}$ for $T = \omega\tilde{T}$ concerning the conditions (1.2) and (2.2).

Furthermore, if (2.3) is applied to the practical problem (2.1), determining $\tilde{T}R_V^{(\ell)}$ refers to solving the block linear system $AE = R_V^{(\ell)}$ for $A = \tilde{L}$ or $A = \tilde{L}S^{-1}\tilde{L}$. The latter case can be implemented by solving two systems for \tilde{L} successively.

2.2. Convergence measure and simplified notation

We denote by μ_i the i th largest eigenvalue of (M, A) from (1.7), i.e., the eigenvalues are arranged as $\mu_1 \geq \dots \geq \mu_n$. With the Ritz values $\theta_1^{(\ell)} \geq \dots \geq \theta_s^{(\ell)}$ of (M, A) in the subspace $\text{span}\{V^{(\ell)}\}$, we set $\Theta_V^{(\ell)} = \text{diag}(\theta_1^{(\ell)}, \dots, \theta_s^{(\ell)})$. We measure the convergence of $\theta_i^{(\ell)}$ by the distance ratio $(\mu_{j-s+i} - *) / (* - \mu_{j+1})$ with a certain index $j \geq s$.

For an arbitrary shift $\sigma < \mu_n$, the iteration (2.3) and the above convergence measure are invariant for the substitution

$$(2.4) \quad M \leftrightarrow M - \sigma A, \quad \mu_i \leftrightarrow \mu_i - \sigma, \quad \theta_i^{(\ell)} \leftrightarrow \theta_i^{(\ell)} - \sigma.$$

Therefore assuming that M is positive definite does not limit the generality.

In addition, since the condition (2.2) is formulated with respect to the inner product induced by A , we can simplify the notation of matrices and vectors by using the representations

$$(2.5) \quad H = A^{-1/2}MA^{-1/2}, \quad y = A^{1/2}v, \quad Y = A^{1/2}V, \quad N = A^{1/2}(\omega\tilde{T})A^{1/2}$$

as in [21, Subsection 1.2]. Then (2.2) turns into

$$(2.6) \quad \|I - N\|_2 \leq \gamma < 1,$$

and (2.3) is equivalent to

$$(2.7) \quad Y^{(\ell+1)} \xleftarrow{\text{RR}[H,s]} \text{span}\{Y^{(\ell)}, N(HY^{(\ell)} - Y^{(\ell)}\Theta_V^{(\ell)})\}$$

where $\Theta_Y^{(\ell)} = \Theta_V^{(\ell)}$. The notation of eigenvalues and Ritz values remains unchanged.

Remark 2.1. For analyzing the convergence behavior of the BPG iteration (2.3), we only need to observe the accompanying iteration (2.7) for two Hermitian positive definite matrices: H with the arranged eigenvalues $\mu_1 \geq \dots \geq \mu_n$, and N satisfying (2.6). Therein the current iterate $Y^{(\ell)} \in \mathbb{C}^{n \times s}$ has full rank and its columns are orthonormal Ritz vectors of H in $\text{span}\{Y^{(\ell)}\}$ associated with the arranged Ritz values $\theta_1^{(\ell)} \geq \dots \geq \theta_s^{(\ell)}$, also contained in the diagonal matrix $\Theta_Y^{(\ell)}$. The Rayleigh-Ritz procedure $\text{RR}[H, s]$ extracts orthonormal Ritz vectors of H associated with the s largest Ritz values.

3. Approaches and auxiliary subspaces

In this section, we begin with exact-inverse preconditioning $\tilde{T} = A^{-1}$ in the BPG iteration (2.3) and introduce two approaches for the convergence analysis. The first approach is a comparative analysis where the trial subspace is simplified in order to apply estimates from [4] for an abstract block iteration. We particularly introduce some underlying auxiliary subspaces and

formulate with them the second approach. Therein proper vector iterations are constructed for preparing the analysis for general preconditioners based on our previous results from [12, 21].

3.1. Analysis via an abstract block iteration

In the case $\tilde{T} = A^{-1}$, we can set $N = I$ in the accompanying iteration (2.7). Then the trial subspace turns into

$$\text{span}\{Y^{(\ell)}, HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)}\} = \text{span}\{Y^{(\ell)}\Theta_Y^{(\ell)}, HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)}\} = \text{span}\{Y^{(\ell)}, HY^{(\ell)}\}$$

where the diagonal Ritz value matrix $\Theta_Y^{(\ell)}$ is invertible due to the positive definiteness of H . Therefore (2.7) is specialized as

$$(3.1) \quad Y^{(\ell+1)} \stackrel{\text{RR}[H,s]}{\leftarrow} \text{span}\{Y^{(\ell)}, HY^{(\ell)}\}.$$

For an arbitrary linear polynomial $p_1(\cdot)$, the iteration

$$(3.2) \quad Y^{(\ell+1)} = p_1(H)Y^{(\ell)}$$

does not converge faster than (3.1) since the Rayleigh-Ritz procedure thereof provides the best s approximate eigenvalues in the larger subspace $\text{span}\{Y^{(\ell)}, HY^{(\ell)}\}$ enclosing $\text{span}\{p_1(H)Y^{(\ell)}\}$.

Indeed, the iteration (3.1) can be regarded as a simply restarted version of the block Lanczos method and investigated based on the comparative analysis from [4, Section 2] by Knyazev. We reformulate the central estimate therein as follows.

Lemma 3.1 (reformulation of [4, (2.22)]). *With the settings from Remark 2.1, consider the iteration $Y^{(\ell+1)} = f(H)Y^{(\ell)}$ for $Y^{(\ell)} \in \mathbb{C}^{n \times s}$ and a function $f(\cdot)$ satisfying $|f(\mu_1)| \geq \dots \geq |f(\mu_s)| > 0$. If $Y^{(\ell)}$ has full rank and the s th largest Ritz value $\theta_s^{(\ell)}$ of H in $\text{span}\{Y^{(\ell)}\}$ is larger than μ_{s+1} , then $Y^{(\ell+1)}$ also has full rank. In addition, for the corresponding Ritz value $\theta_s^{(\ell+1)}$, it holds that*

$$(3.3) \quad \frac{\mu_s - \theta_s^{(\ell+1)}}{\theta_s^{(\ell+1)} - \mu_{s+1}} \leq \left(\frac{\max_{k=s+1, \dots, n} |f(\mu_k)|}{\min_{k=1, \dots, s} |f(\mu_k)|} \right)^2 \frac{\mu_s - \theta_s^{(\ell)}}{\theta_s^{(\ell)} - \mu_{s+1}}.$$

Applying Lemma 3.1 to (3.2) with

$$f(\mu) = p_1(\mu) = \mu - \frac{1}{2}(\mu_{s+1} + \mu_n)$$

yields the convergence factor

$$\frac{\max_{k=s+1, \dots, n} |f(\mu_k)|}{\min_{k=1, \dots, s} |f(\mu_k)|} = \frac{|f(\mu_{s+1})|}{|f(\mu_s)|} = \frac{\mu_{s+1} - \mu_n}{2\mu_s - \mu_{s+1} - \mu_n} = \frac{\kappa_s}{2 - \kappa_s} \quad \text{with} \quad \kappa_s = \frac{\mu_{s+1} - \mu_n}{\mu_s - \mu_n}$$

so that (3.3) provides a single-step estimate for (3.1) which can be applied recursively for multiple steps. A direct extension to the i th largest Ritz value for an arbitrary $i \leq s$ does not hold in general; cf. the numerical example in [20, Section 3 and Figure 1]. In contrast, the estimate [4, (2.20)] leads to the angle-dependent multi-step estimate

$$\frac{\mu_i - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_n} \leq \left(\frac{\kappa_i}{2 - \kappa_i} \right)^{2\ell} \tan^2 \varphi^{(0)} \quad \text{with} \quad \kappa_i = \frac{\mu_{s+1} - \mu_n}{\mu_i - \mu_n}$$

for (3.1) where $\varphi^{(0)}$ is the Euclidean angle between the initial subspace $\text{span}\{Y^{(0)}\}$ and the invariant subspace of H associated with the eigenvalues μ_1, \dots, μ_s . Furthermore, two angle-free multi-step estimates for (3.1) can be derived analogously to recent results from [21] for the block power method $Y^{(\ell+1)} = HY^{(\ell)}$ (and swapping the indices i and j in the notation therein).

Lemma 3.2 (based on [21, Theorems 2.6 and 2.8]). *With the settings from Remark 2.1, consider the special form (3.1) of the iteration (2.7). If $\theta_s^{(0)} > \mu_{s+1}$, then it holds that*

$$(3.4) \quad \frac{\mu_i - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{s+1}} \leq \left(\frac{\kappa_i}{2 - \kappa_i} \right)^{2\ell} \frac{\mu_i - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{s+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{s+1} - \mu_n}{\mu_i - \mu_n}.$$

A more general estimate in the case $\mu_j \geq \theta_s^{(0)} > \mu_{j+1}$ with a certain index $j \geq s$ reads

$$(3.5) \quad \frac{\mu_{j-s+i} - \theta_i^{(\ell)}}{\theta_i^{(\ell)} - \mu_{j+1}} \leq \left(\frac{\kappa_i}{2 - \kappa_i} \right)^{2\ell} \frac{\mu_{j-s+i} - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{j+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}.$$

For proving Lemma 3.2, we can first adapt the analysis from [21] to the iteration (3.2) and then extend the results to the accelerated iteration (3.1) by using again the subspace inclusion $\text{span}\{p_1(H)Y^{(\ell)}\} \subseteq \text{span}\{Y^{(\ell)}, HY^{(\ell)}\}$. An underlying proof technique is that one can select a subspace $\tilde{\mathcal{Y}} \subseteq \text{span}\{Y^{(\ell)}\}$ such that $\tilde{\mathcal{Y}}$, $H\tilde{\mathcal{Y}}$ and $p_1(H)\tilde{\mathcal{Y}}$ are simultaneously orthogonal to the eigenvectors associated with the eigenvalues μ_{i+1}, \dots, μ_s or $\mu_{j-s+i+1}, \dots, \mu_j$ which can be skipped in the estimates. However, this approach cannot easily be adapted to the iteration (2.7) with an arbitrary $N \approx I$ except for some special cases such as that N has the same eigenvectors as H . A possible way out is to construct proper vector iterations within the subspace $\tilde{\mathcal{Y}} + H\tilde{\mathcal{Y}}$ and its counterpart for $N \approx I$ so that some arguments from [12, 21] can be utilized.

3.2. Auxiliary subspaces

Following the proof sketch of Lemma 3.2, we introduce some auxiliary subspaces which are still useful for analyzing general preconditioning $N \approx I$.

Lemma 3.3. *With the settings from Remark 2.1, let z_1, \dots, z_n be orthonormal eigenvectors of H associated with the eigenvalues $\mu_1 \geq \dots \geq \mu_n$. By using the invariant subspaces*

$$\tilde{\mathcal{Z}} = \text{span}\{z_{j-s+i+1}, \dots, z_j\}^\perp \quad \text{and} \quad \hat{\mathcal{Z}} = \text{span}\{z_{j-s+1}, \dots, z_{j-s+i}\}^\perp$$

for a certain index $j \geq s$ (therein the superscript $^\perp$ denotes orthogonal complement), define for an arbitrary subspace $\mathcal{Y} \subseteq \mathbb{C}^n$ of dimension s the auxiliary subspaces

$$\tilde{\mathcal{Y}} = \mathcal{Y} \cap \tilde{\mathcal{Z}}, \quad \text{and} \quad \hat{\mathcal{Y}} = \mathcal{Y} \cap \hat{\mathcal{Z}}.$$

Then it holds that

$$(3.6) \quad \dim \tilde{\mathcal{Y}} \geq i, \quad \text{and} \quad \dim \hat{\mathcal{Y}} \geq s - i.$$

If $j = s$, and the smallest Ritz values $\tilde{\theta}$, $\hat{\theta}$ of H in $\tilde{\mathcal{Y}}$, $\hat{\mathcal{Y}}$ are larger than μ_{s+1} , then

$$(3.7) \quad \dim \tilde{\mathcal{Y}} = i, \quad \dim \hat{\mathcal{Y}} = s - i, \quad \dim(\tilde{\mathcal{Y}} \cap \hat{\mathcal{Y}}) = 0, \quad \text{and} \quad \dim(\tilde{\mathcal{Y}} + \hat{\mathcal{Y}}) = s.$$

Proof. The statement (3.6) follows from

$$\dim \tilde{\mathcal{Y}} = \dim \mathcal{Y} + \dim \tilde{\mathcal{Z}} - \dim(\mathcal{Y} + \tilde{\mathcal{Z}}) \geq s + (n - s + i) - n = i,$$

$$\dim \hat{\mathcal{Y}} = \dim \mathcal{Y} + \dim \hat{\mathcal{Z}} - \dim(\mathcal{Y} + \hat{\mathcal{Z}}) \geq s + (n - i) - n = s - i.$$

If $j = s$, the additional assumption on Ritz values excludes the strict inequalities in (3.6) since

$$\dim \tilde{\mathcal{Y}} > i \quad \Rightarrow \quad \tilde{\theta} \leq \text{the } (i+1)\text{th element in } \{\mu_1, \dots, \mu_i, \mu_{s+1}, \dots, \mu_n\} = \mu_{s+1},$$

$$\dim \hat{\mathcal{Y}} > s - i \quad \Rightarrow \quad \hat{\theta} \leq \text{the } (s-i+1)\text{th element in } \{\mu_{i+1}, \dots, \mu_n\} = \mu_{s+1}.$$

Moreover, $\dim(\tilde{\mathcal{Y}} \cap \hat{\mathcal{Y}}) = 0$ holds since otherwise there would exist nonzero vectors in $\tilde{\mathcal{Y}} \cap \hat{\mathcal{Y}}$ and its superset $\tilde{\mathcal{Z}} \cap \hat{\mathcal{Z}} = \text{span}\{z_{s+1}, \dots, z_n\}$ so that the smallest Ritz values $\tilde{\theta}$, $\hat{\theta}$ would be not larger than μ_{s+1} . Consequently, $\dim(\tilde{\mathcal{Y}} + \hat{\mathcal{Y}}) = \dim \tilde{\mathcal{Y}} + \dim \hat{\mathcal{Y}} - \dim(\tilde{\mathcal{Y}} \cap \hat{\mathcal{Y}}) = s$. \square

Based on the statement (3.6) and the Courant-Fischer principles, the convergence of the i th Ritz value produced by (3.1) is not slower than that of the i th Ritz value by the iteration

$$(3.8) \quad \tilde{Y}^{(\ell+1)} \xleftarrow{\text{RR}[H, \tilde{i}]} \text{span}\{\tilde{Y}^{(\ell)}, H\tilde{Y}^{(\ell)}\} \quad \text{with} \quad \text{span}\{\tilde{Y}^{(0)}\} = \text{span}\{Y^{(0)}\} \cap \tilde{\mathcal{Z}}$$

and $\tilde{i} = \dim \text{span}\{\tilde{Y}^{(0)}\} \geq i$. Evidently, each iterate of (3.8) is contained columnwise in $\tilde{\mathcal{Z}}$ so that the estimate (3.5) can be derived by modifying Lemma 3.1 restricted to $\tilde{\mathcal{Z}}$. The statement (3.7) refers to the final phase of (3.1) and the estimate (3.4) under the assumption $\theta_s^{(0)} > \mu_{s+1}$ (then the corresponding $\tilde{\theta}$ and $\hat{\theta}$ are also larger than μ_{s+1}). Therein (3.1) can be split into two partial iterations with respect to $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$. Moreover, we can inductively adapt (3.7) to the respective subspace iterates; see Lemma 3.4.

3.3. Analysis via vector iterations

For analyzing the iteration (2.7) with general preconditioners, the direct generalization

$$\tilde{Y}^{(\ell+1)} \xleftarrow{\text{RR}[H, \tilde{i}]} \text{span}\{\tilde{Y}^{(\ell)}, N(H\tilde{Y}^{(\ell)} - \tilde{Y}^{(\ell)}\Theta_Y^{(\ell)})\}$$

of (3.8) is somewhat problematic since $\text{span}\{N(H\tilde{Y}^{(\ell)} - \tilde{Y}^{(\ell)}\Theta_Y^{(\ell)})\}$ for $N \approx I$ is not necessarily a subset of $\tilde{\mathcal{Z}}$. Instead, following our previous results from [12, 21], we reformulate the trial subspace of (2.7) as

$$\text{span}\{Y^{(\ell)}, N(HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)})\} = \text{span}\{Y^{(\ell)}, Y^{(\ell)}\Theta_Y^{(\ell)} + N(HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)})\}$$

and consider a stepwise mixture of two partial iterations concerning $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$, namely,

$$(3.9) \quad \begin{aligned} \tilde{\mathcal{Y}}^{(\ell)} &= \text{span}\{Y^{(\ell)}\} \cap \tilde{\mathcal{Z}}, & \hat{\mathcal{Y}}^{(\ell)} &= \text{span}\{Y^{(\ell)}\} \cap \hat{\mathcal{Z}}, \\ U^{(\ell)} &= Y^{(\ell)}\Theta_Y^{(\ell)} + N(HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)}), \\ \tilde{\mathcal{U}}^{(\ell)} &= \text{span}\{U^{(\ell)}\} \cap \tilde{\mathcal{Z}}, & \hat{\mathcal{U}}^{(\ell)} &= \text{span}\{U^{(\ell)}\} \cap \hat{\mathcal{Z}}, \\ \tilde{Y}^{(\ell+\frac{1}{2})} &\xleftarrow{\text{RR}[H, \tilde{i}]} \tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}, & \hat{Y}^{(\ell+\frac{1}{2})} &\xleftarrow{\text{RR}[H, \hat{i}]} \hat{\mathcal{Y}}^{(\ell)} + \hat{\mathcal{U}}^{(\ell)}, \\ Y^{(\ell+1)} &\xleftarrow{\text{RR}[H, \tilde{s}]} \text{span}\{\tilde{Y}^{(\ell+\frac{1}{2})}, \hat{Y}^{(\ell+\frac{1}{2})}\} \end{aligned}$$

with $\tilde{i} = \dim \tilde{\mathcal{Y}}^{(\ell)}$, $\hat{i} = \dim \hat{\mathcal{Y}}^{(\ell)}$ and $\tilde{s} = \dim \text{span}\{\tilde{Y}^{(\ell+\frac{1}{2})}, \hat{Y}^{(\ell+\frac{1}{2})}\}$ for the current step index ℓ . The matrix $U^{(\ell)}$ coincides with $HY^{(\ell)}$ for $N = I$, and $\text{span}\{U^{(\ell)}\}$ corresponds to the trial subspace of a BPG iteration with fixed step sizes for which some cluster robust estimates have been derived in [21]. The trial subspace of (2.7), i.e., $\text{span}\{Y^{(\ell)}, U^{(\ell)}\}$, is split into $\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}$ and $\hat{\mathcal{Y}}^{(\ell)} + \hat{\mathcal{U}}^{(\ell)}$ which are subsets of $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$, respectively. Therein two partial Rayleigh-Ritz approximations are determined and additionally refined together for extracting the next iterate. In comparison to the direct Rayleigh-Ritz approximation in the larger subspace $\text{span}\{Y^{(\ell)}, U^{(\ell)}\}$ in (2.7), the update by (3.9) leads to less improvement in Ritz values according to the Courant-Fischer principles. Thus investigating (3.9) can provide suitable Ritz value estimates for (2.7). The next task in this approach is to construct proper vector iterations within (3.9) as well as an alternative quality parameter for $N \approx I$.

We first discuss the dimensions of auxiliary subspaces in (3.9) for $j = s$ concerning the final phase of the iteration (2.7).

Lemma 3.4. *With the settings from Remark 2.1, consider the ℓ th step of (3.9) with the invariant subspaces $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$ for $j = s$ from Lemma 3.3. If $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$, $\dim \hat{\mathcal{Y}}^{(\ell)} = s - i$, and the smallest Ritz values $\tilde{\theta}$, $\hat{\theta}$ of H in $\tilde{\mathcal{Y}}^{(\ell)}$, $\hat{\mathcal{Y}}^{(\ell)}$ are larger than μ_{s+1} , then it holds for the subspaces*

$\tilde{\mathcal{Y}}' = \text{span}\{\tilde{Y}^{(\ell+\frac{1}{2})}\}$ and $\hat{\mathcal{Y}}' = \text{span}\{\hat{Y}^{(\ell+\frac{1}{2})}\}$, that $\dim \tilde{\mathcal{Y}}' = i$, $\dim \hat{\mathcal{Y}}' = s - i$, and the smallest Ritz values $\tilde{\theta}'$, $\hat{\theta}'$ of H in $\tilde{\mathcal{Y}}'$, $\hat{\mathcal{Y}}'$ are also larger than μ_{s+1} . Moreover,

$$(3.10) \quad \dim(\tilde{\mathcal{Y}}' + \hat{\mathcal{Y}}') = s, \quad \tilde{\mathcal{Y}}^{(\ell+1)} = \tilde{\mathcal{Y}}', \quad \text{and} \quad \hat{\mathcal{Y}}^{(\ell+1)} = \hat{\mathcal{Y}}'.$$

Proof. The given assumption leads to $\tilde{i} = i$ and $\hat{i} = s - i$ so that the partial Rayleigh-Ritz approximations produce $\tilde{\mathcal{Y}}'$ of dimension i and $\hat{\mathcal{Y}}'$ of dimension $s - i$. In addition, the smallest Ritz values $\tilde{\theta}'$, $\hat{\theta}'$ of H in $\tilde{\mathcal{Y}}'$, $\hat{\mathcal{Y}}'$ improve $\tilde{\theta}$, $\hat{\theta}$, namely,

$$\tilde{\theta}' = \theta_i(\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}) \geq \theta_i(\tilde{\mathcal{Y}}^{(\ell)}) = \tilde{\theta}, \quad \text{and} \quad \hat{\theta}' = \theta_{s-i}(\hat{\mathcal{Y}}^{(\ell)} + \hat{\mathcal{U}}^{(\ell)}) \geq \theta_{s-i}(\hat{\mathcal{Y}}^{(\ell)}) = \hat{\theta}.$$

Thus $\tilde{\theta}'$ and $\hat{\theta}'$ are also larger than μ_{s+1} . Subsequently, the property $\dim(\tilde{\mathcal{Y}}' + \hat{\mathcal{Y}}') = s$ can be shown analogously to the last equality in (3.7). Then $\tilde{s} = s$, and

$$\tilde{\mathcal{Y}}^{(\ell+1)} = \text{span}\{Y^{(\ell+1)}\} \cap \tilde{\mathcal{Z}} = (\tilde{\mathcal{Y}}' \cap \tilde{\mathcal{Z}}) + (\hat{\mathcal{Y}}' \cap \tilde{\mathcal{Z}}) = \tilde{\mathcal{Y}}'$$

holds according to

$$\begin{aligned} \tilde{\mathcal{Y}}' &\subseteq (\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}) \subseteq \tilde{\mathcal{Z}} &\Rightarrow &\tilde{\mathcal{Y}}' \cap \tilde{\mathcal{Z}} = \tilde{\mathcal{Y}}', \\ \hat{\mathcal{Y}}' &\subseteq (\hat{\mathcal{Y}}^{(\ell)} + \hat{\mathcal{U}}^{(\ell)}) \subseteq \hat{\mathcal{Z}} &\Rightarrow &\hat{\mathcal{Y}}' \cap \hat{\mathcal{Z}} = \hat{\mathcal{Y}}' \\ &&&\Rightarrow \hat{\mathcal{Y}}' \cap \tilde{\mathcal{Z}} = \hat{\mathcal{Y}}' \cap \hat{\mathcal{Z}} \cap \tilde{\mathcal{Z}} = \hat{\mathcal{Y}}' \cap \text{span}\{z_{s+1}, \dots, z_n\} = \{0\} \end{aligned}$$

where the last equality is ensured by $\hat{\theta}' > \mu_{s+1}$. The verification of $\hat{\mathcal{Y}}^{(\ell+1)} = \hat{\mathcal{Y}}'$ is analogous. \square

Lemma 3.4 enables an inductive proof of the following properties of (3.9) under a natural assumption on the initial subspace.

Lemma 3.5. *With the settings from Remark 2.1, consider the iteration (3.9) with the invariant subspaces $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$ for $j = s$ from Lemma 3.3 and $\dim \text{span}\{Y^{(0)}\} = s$. If the smallest (sth largest) Ritz value $\theta_s^{(0)}$ of H in $\text{span}\{Y^{(0)}\}$ is larger than μ_{s+1} , then it holds for each ℓ , that $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$, $\dim \hat{\mathcal{Y}}^{(\ell)} = s - i$, and $\dim \text{span}\{Y^{(\ell+1)}\} = s$. The partial Rayleigh-Ritz approximations in the ℓ th step actually produce the subspaces $\tilde{\mathcal{Y}}^{(\ell+1)}$ and $\hat{\mathcal{Y}}^{(\ell+1)}$.*

Proof. Applying Lemma 3.3 to $\mathcal{Y} = \text{span}\{Y^{(0)}\}$ implies $\dim \tilde{\mathcal{Y}}^{(0)} = i$ and $\dim \hat{\mathcal{Y}}^{(0)} = s - i$ by the first two equalities in (3.7) whose assumption is verified by the fact that the smallest Ritz values $\tilde{\theta}$ and $\hat{\theta}$ of H in the subsets $\tilde{\mathcal{Y}}^{(0)}$ and $\hat{\mathcal{Y}}^{(0)}$ of $\text{span}\{Y^{(0)}\}$ are at least $\theta_s^{(0)}$ and thus larger than μ_{s+1} . Therefore Lemma 3.4 is already applicable to $\ell = 0$. Moreover, the statements for ℓ in Lemma 3.4 immediately verify the assumption for $\ell + 1$. Recursively applying Lemma 3.4 completes the proof. \square

Lemma 3.5 motivates an approach for estimating the convergence rate of the i th Ritz value in the final phase of the iteration (2.7) by observing the partial subspace iterate $\tilde{\mathcal{Y}}^{(\ell)}$ in (3.9). The other partial subspace iterate $\hat{\mathcal{Y}}^{(\ell)}$ plays an important role in the background for ensuring $\dim \text{span}\{Y^{(\ell+1)}\} = s$. Extending Lemma 3.5 to the more general case $j \geq s$ requires certain assumptions on the initial subspace $\text{span}\{Y^{(0)}\}$ which are much more technical than the natural assumption $\theta_s^{(0)} > \mu_{s+1}$. It is remarkable that opposite properties such as $\dim \tilde{\mathcal{Y}}^{(\ell)} > i$ rarely occur in numerical tests with randomly generated initial guesses. Therefore we simply use an empirical assumption for analyzing (3.9) in the case $j \geq s$.

Lemma 3.6. *With the settings from Remark 2.1, consider the iteration (3.9) with the invariant subspaces $\tilde{\mathcal{Z}}$ and $\hat{\mathcal{Z}}$ for $j \geq s$ from Lemma 3.3. Assume for each ℓ that $\dim \text{span}\{Y^{(\ell)}\} = s$, $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$, and $\dim \hat{\mathcal{Y}}^{(\ell)} = s - i$. Then the partial Rayleigh-Ritz approximations in the ℓ th step actually produce the subspaces $\tilde{\mathcal{Y}}^{(\ell+1)}$ and $\hat{\mathcal{Y}}^{(\ell+1)}$.*

Proof. The statement cannot be proved by directly applying Lemma 3.4 due to the dependence on Ritz values. Instead,

$$\tilde{\mathcal{Y}}^{(\ell+1)} = (\text{span}\{Y^{(\ell+1)}\} \cap \tilde{\mathcal{Z}}) \supseteq (\tilde{\mathcal{Y}}' \cap \tilde{\mathcal{Z}}) = \tilde{\mathcal{Y}}' \quad \Rightarrow \quad \tilde{\mathcal{Y}}^{(\ell+1)} = \tilde{\mathcal{Y}}'$$

holds since $\dim \tilde{\mathcal{Y}}' = i$ and $\dim \tilde{\mathcal{Y}}^{(\ell+1)} = i$ (by adapting the assumption to $\ell + 1$). The equality $\hat{\mathcal{Y}}^{(\ell+1)} = \hat{\mathcal{Y}}'$ holds analogously. \square

Now we can focus on the first partial iteration in (3.9) and define certain vector iterations for characterizing the i th Ritz value.

Theorem 3.7. *With the settings from Remark 2.1, consider the iteration (3.9) under the assumption from Lemma 3.5 or Lemma 3.6, and denote by $\tilde{\theta}'$ the i th largest Ritz value of H in $\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}$. Then the following statements hold:*

- (a) *For each ℓ , the matrix $U^{(\ell)}$ has full rank, and $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$.*
- (b) *In the special case $N = I$, the subspace $\tilde{\mathcal{U}}^{(\ell)}$ coincides with $H\tilde{\mathcal{Y}}^{(\ell)}$, and there exists a nonzero vector $\tilde{y} \in \tilde{\mathcal{Y}}^{(\ell)}$ for which the largest Ritz value $\tilde{\theta}^\circ$ of H in $\text{span}\{\tilde{y}, H\tilde{y}\}$ does not exceed $\tilde{\theta}'$.*
- (c) *In the general case $N \approx I$, consider an orthonormal matrix $\tilde{U} \in \mathbb{C}^{n \times i}$ with $\text{span}\{\tilde{U}\} \subseteq \tilde{\mathcal{U}}^{(\ell)}$, and an orthonormal basis matrix \tilde{Y} of $\tilde{\mathcal{Y}}^{(\ell)}$. Let $\mu(\cdot)$ be the Rayleigh quotient with respect to H . If the matrix $\tilde{R} = H\tilde{Y} - \tilde{Y}\tilde{Y}^*H\tilde{Y}$ has full rank, and*

$$(3.11) \quad \|(H\tilde{Y} - \tilde{U}\tilde{U}^*H\tilde{Y})(\tilde{R}^*\tilde{R})^{-1/2}\|_2 \leq \tilde{\gamma} < 1,$$

then there exist nonzero vectors $\tilde{y} \in \text{span}\{\tilde{Y}\}$ and $\tilde{u} \in \text{span}\{\tilde{U}\}$ such that

$$(3.12) \quad \|H\tilde{y} - \tilde{u}\|_2 \leq \tilde{\gamma}\|H\tilde{y} - \mu(\tilde{y})\tilde{y}\|_2,$$

and the largest Ritz value $\tilde{\theta}^\circ$ of H in $\text{span}\{\tilde{y}, \tilde{u}\}$ does not exceed $\tilde{\theta}'$.

Proof. (a) According to Lemma 3.5 or Lemma 3.6, we get $\dim \text{span}\{Y^{(\ell)}\} = s$ for each ℓ . The corresponding $U^{(\ell)}$ can be represented by

$$U^{(\ell)} = Y^{(\ell)}\Theta_Y^{(\ell)} + N(HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)}) = Y'\Theta$$

$$\text{with } Y = Y^{(\ell)}, \quad \Theta = \Theta_Y^{(\ell)} \quad \text{and} \quad Y' = Y - N(Y - HY\Theta^{-1})$$

for matching the notation in [21, Lemma 3.1] where a BPG iteration with fixed step sizes is analyzed, and Y' can be shown to have full rank. Then $U^{(\ell)} = Y'\Theta$ also has full rank since the diagonal Ritz value matrix $\Theta = \Theta_Y^{(\ell)}$ is invertible due to the positive definiteness of H . Subsequently, $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$ can be shown analogously to (3.6) in Lemma 3.3.

- (b) For $N = I$, the matrix $U^{(\ell)}$ becomes $HY^{(\ell)}$ so that

$$\tilde{\mathcal{U}}^{(\ell)} = \text{span}\{U^{(\ell)}\} \cap \tilde{\mathcal{Z}} = \text{span}\{HY^{(\ell)}\} \cap (H\tilde{\mathcal{Z}}) = H(\text{span}\{Y^{(\ell)}\} \cap \tilde{\mathcal{Z}}) = H\tilde{\mathcal{Y}}^{(\ell)}$$

(where $\tilde{\mathcal{Z}} = H\tilde{\mathcal{Z}}$ is ensured by the positive definiteness of H). Following the property $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$ from Lemma 3.5 or Lemma 3.6, we use an arbitrary basis matrix $\tilde{Y} \in \mathbb{C}^{n \times i}$ of $\tilde{\mathcal{Y}}^{(\ell)}$ so that the subspace $\tilde{\mathcal{U}}' = \tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)}$ can be represented by $\text{span}\{\tilde{Y}, H\tilde{Y}\}$. We denote by \bar{i} the dimension of $\tilde{\mathcal{U}}'$, and by $V \in \mathbb{C}^{n \times \bar{i}}$ a basis matrix of $\tilde{\mathcal{U}}'$ whose columns $v_1, \dots, v_{\bar{i}}$ are orthonormal Ritz vectors associated with the Ritz values $\varphi_1 \geq \dots \geq \varphi_{\bar{i}}$ of H in $\tilde{\mathcal{U}}'$. Then we get the orthogonal projector $P = VV^*$ on $\tilde{\mathcal{U}}'$ and the diagonal Ritz value matrix $V^*HV = \text{diag}(\varphi_1, \dots, \varphi_{\bar{i}})$. Moreover, the i th largest Ritz value $\tilde{\theta}'$ of H in $\tilde{\mathcal{U}}'$ is the largest Ritz value of H in $\tilde{\mathcal{U}}^\circ = \text{span}\{v_i, \dots, v_{\bar{i}}\}$. Based on the dimension comparison

$$\dim(\tilde{\mathcal{Y}}^{(\ell)} \cap \tilde{\mathcal{U}}^\circ) = \dim \tilde{\mathcal{Y}}^{(\ell)} + \dim \tilde{\mathcal{U}}^\circ - \dim(\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^\circ) \geq i + (\bar{i} - i + 1) - \bar{i} = 1,$$

we can select a nonzero vector \tilde{y} from $\tilde{\mathcal{Y}}^{(\ell)} \cap \tilde{\mathcal{U}}^\circ$. According to $\tilde{y} \in \tilde{\mathcal{Y}}^{(\ell)}$ and $H\tilde{y} \in H\tilde{\mathcal{Y}}^{(\ell)} = \tilde{\mathcal{U}}^{(\ell)}$, the vectors \tilde{y} and $H\tilde{y}$ are contained in $\tilde{\mathcal{U}}'$ so that

$$H\tilde{y} = P(H\tilde{y}) = PH(P\tilde{y}) = VV^*HV V^*\tilde{y} = V \operatorname{diag}(\varphi_1, \dots, \varphi_i) V^*\tilde{y}.$$

In addition, $\tilde{y} \in \tilde{\mathcal{U}}^\circ$ and the orthogonality between the columns of V ensure that the first $i-1$ entries of $V^*\tilde{y}$ are equal to zero. This property is preserved in the vector $\operatorname{diag}(\varphi_1, \dots, \varphi_i) V^*\tilde{y}$ so that $H\tilde{y}$ belongs to $\tilde{\mathcal{U}}^\circ$. Therefore $\operatorname{span}\{\tilde{y}, H\tilde{y}\}$ is a subset of $\tilde{\mathcal{U}}^\circ$, and the largest Ritz value $\tilde{\theta}^\circ$ of H in $\operatorname{span}\{\tilde{y}, H\tilde{y}\}$ is bounded from above by $\tilde{\theta}'$ which is the largest Ritz value of H in $\tilde{\mathcal{U}}^\circ$.

(c) The existence of \tilde{U} follows from (a). Vectors \tilde{y} and \tilde{u} satisfying (3.12) can be constructed by using an arbitrary nonzero vector $c \in \mathbb{C}^i$, namely, (3.11) ensures

$$\|(H\tilde{Y} - \tilde{U}\tilde{U}^*H\tilde{Y})(\tilde{R}^*\tilde{R})^{-1/2}c\|_2 \leq \tilde{\gamma}\|c\|_2$$

so that

$$\|(H\tilde{Y} - \tilde{U}\tilde{U}^*H\tilde{Y})e\|_2 \leq \tilde{\gamma}\|(\tilde{R}^*\tilde{R})^{1/2}e\|_2 \quad \text{for } e = (\tilde{R}^*\tilde{R})^{-1/2}c.$$

Subsequently, by using $\|(\tilde{R}^*\tilde{R})^{1/2}e\|_2 = \sqrt{e^*\tilde{R}^*\tilde{R}e} = \|\tilde{R}e\|_2$ and the definition of \tilde{R} , we get

$$\|H\tilde{Y}e - \tilde{U}\tilde{U}^*H\tilde{Y}e\|_2 \leq \tilde{\gamma}\|H\tilde{Y}e - \tilde{Y}\tilde{Y}^*H\tilde{Y}e\|_2 \leq \tilde{\gamma}\|H\tilde{Y}e - \tilde{Y}e\mu(\tilde{Y}e)\|_2$$

where the second inequality uses the fact that $\tilde{Y}\tilde{Y}^*H\tilde{Y}e$ is the orthogonal projection of $H\tilde{Y}e$ on $\operatorname{span}\{\tilde{Y}\}$. Thus (3.12) is fulfilled by $\tilde{y} = \tilde{Y}e$ and $\tilde{u} = \tilde{U}(\tilde{U}^*H\tilde{Y}e)$. Specific \tilde{y} and \tilde{u} possessing the additional property can be constructed analogously to the proof of [12, Theorem 3.2] (using Sion's-minimax theorem). Therein the largest Ritz value $\tilde{\theta}^\circ$ of H in $\operatorname{span}\{\tilde{y}, \tilde{u}\}$ does not exceed the i th largest Ritz value $\tilde{\theta}^\circ$ of H in $\operatorname{span}\{\tilde{Y}, \tilde{U}\}$. Consequently, we get $\tilde{\theta}^\circ \leq \tilde{\theta}^\circ \leq \tilde{\theta}'$ according to $\operatorname{span}\{\tilde{Y}, \tilde{U}\} \subseteq (\tilde{\mathcal{Y}}^{(\ell)} + \tilde{\mathcal{U}}^{(\ell)})$ and the Courant-Fischer principles. \square

The statement (b) in Theorem 3.7 suggests the vector iteration

$$(3.13) \quad \tilde{y}^\circ \xleftarrow{\operatorname{RR}[H,1]} \operatorname{span}\{\tilde{y}, H\tilde{y}\}$$

for deriving an intermediate estimate. Since \tilde{y} and $H\tilde{y}$ are contained in the invariant subspace $\tilde{\mathcal{Z}}$, we adapt an estimate from [11, Theorem 4.1] for vectorial gradient iterations as follows.

Lemma 3.8. *With the settings from Remark 2.1, consider the iteration (3.13), and let $\mu(\cdot)$ be the Rayleigh quotient with respect to H . If \tilde{y} belongs to the invariant subspace $\tilde{\mathcal{Z}}$ defined in Lemma 3.3, and $\mu(\tilde{y})$ is located in the eigenvalue interval $(\mu_{j+1}, \mu_{j-s+i}]$, then it holds that*

$$(3.14) \quad \frac{\mu_{j-s+i} - \mu(\tilde{y}^\circ)}{\mu(\tilde{y}^\circ) - \mu_{j+1}} \leq \left(\frac{\kappa_i}{2 - \kappa_i} \right)^2 \frac{\mu_{j-s+i} - \mu(\tilde{y})}{\mu(\tilde{y}) - \mu_{j+1}} \quad \text{with } \kappa_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}.$$

Proof. The iteration (3.13) is equivalent to

$$\tilde{Z}^*\tilde{y}^\circ \xleftarrow{\operatorname{RR}[\tilde{Z}^*H\tilde{Z},1]} \operatorname{span}\{\tilde{Z}^*\tilde{y}, (\tilde{Z}^*H\tilde{Z})\tilde{Z}^*\tilde{y}\}$$

with the orthonormal basis matrix $\tilde{Z} = [z_1, \dots, z_{j-s+i}, z_{j+1}, \dots, z_n]$ of $\tilde{\mathcal{Z}}$. Then (3.14) is achieved by adapting [11, Theorem 4.1] to the matrix $\tilde{Z}^*H\tilde{Z}$ and the corresponding Rayleigh quotient $\tilde{\mu}(\cdot)$ together with simple reformulations based on

$$\tilde{\mu}(\tilde{Z}^*w) = \frac{(\tilde{Z}^*w)^*(\tilde{Z}^*H\tilde{Z})(\tilde{Z}^*w)}{(\tilde{Z}^*w)^*(\tilde{Z}^*w)} = \frac{(\tilde{Z}\tilde{Z}^*w)^*H(\tilde{Z}\tilde{Z}^*w)}{w^*(\tilde{Z}\tilde{Z}^*w)} = \frac{w^*Hw}{w^*w} = \mu(w)$$

for arbitrary nonzero vectors w from $\tilde{\mathcal{Z}}$. \square

A similar intermediate estimate for $N \approx I$ can be derived within the iteration

$$(3.15) \quad \tilde{y}^\circ \xleftarrow{\operatorname{RR}[H,1]} \operatorname{span}\{\tilde{y}, \tilde{u}\}$$

suggested by the statement (c) in Theorem 3.7. The derivation is essentially based on [10].

Lemma 3.9. *With the settings from Remark 2.1, consider the iteration (3.15), and let $\mu(\cdot)$ be the Rayleigh quotient with respect to H . If \tilde{y} and \tilde{u} belong to the invariant subspace $\tilde{\mathcal{Z}}$ defined in Lemma 3.3 and satisfy the condition (3.12) with a certain $\tilde{\gamma} \in [0, 1)$, and $\mu(\tilde{y})$ is located in the eigenvalue interval $(\mu_{j+1}, \mu_{j-s+i}]$, then it holds that*

$$(3.16) \quad \frac{\mu_{j-s+i} - \mu(\tilde{y}^\diamond)}{\mu(\tilde{y}^\diamond) - \mu_{j+1}} \leq \left(\frac{\kappa_i + \tilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \tilde{\gamma}\kappa_i} \right)^2 \frac{\mu_{j-s+i} - \mu(\tilde{y})}{\mu(\tilde{y}) - \mu_{j+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}.$$

Proof. As in the proof of Lemma 3.8, we define the matrix $\tilde{H} = \tilde{Z}^* H \tilde{Z}$ and the corresponding Rayleigh quotient $\tilde{\mu}(\cdot)$ so that (3.15) is equivalent to

$$\tilde{y}^\diamond \xleftarrow{\text{RR}[\tilde{H}, 1]} \text{span}\{\tilde{y}, \tilde{u}\} \quad \text{with} \quad \tilde{y}^\diamond = \tilde{Z}^* \tilde{y}^\diamond, \quad \tilde{y} = \tilde{Z}^* \tilde{y} \quad \text{and} \quad \tilde{u} = \tilde{Z}^* \tilde{u}.$$

The condition (3.12) can be reformulated as

$$\|\tilde{H}\tilde{y} - \tilde{u}\|_2 \leq \tilde{\gamma} \|\tilde{H}\tilde{y} - \tilde{\mu}(\tilde{y})\tilde{y}\|_2$$

since $\|w\|_2 = \|\tilde{Z}\tilde{Z}^*w\|_2 = \|\tilde{Z}^*w\|_2$ holds for arbitrary $w \in \tilde{\mathcal{Z}}$. Thus \tilde{u} belongs to a ball $\mathcal{B}_{\tilde{\gamma}, \tilde{y}}$ centred at $\tilde{H}\tilde{y}$ with the radius $\tilde{\gamma} \|\tilde{H}\tilde{y} - \tilde{\mu}(\tilde{y})\tilde{y}\|_2$. Then the trial subspace $\text{span}\{\tilde{y}, \tilde{u}\}$ is characterized by a cone as in [10, Section 2] so that the geometric analysis therefrom is applicable. Adapting [10, Theorem 2.2] yields (3.16). \square

4. Main results

The analysis of the auxiliary iteration (3.9) via vector iterations from Subsection 3.3 results in multi-step estimates for (2.7) in Theorem 4.1 and corresponding estimates for the BPG iteration (2.3) in Theorem 4.5. The results are formulated for general preconditioning and contain estimates for $N = I$ as special forms.

Theorem 4.1. *With the settings from Remark 2.1 concerning the iteration (2.7), let z_1, \dots, z_n be orthonormal eigenvectors of H associated with the eigenvalues $\mu_1 \geq \dots \geq \mu_n$. Then the following statements hold:*

- (a) *The Ritz values produced by (2.7) fulfill $\theta_i^{(\ell+1)} \geq \theta_i^{(\ell)}$ for each ℓ and $i \in \{1, \dots, s\}$. If there are no eigenvectors in $\text{span}\{Y^{(\ell)}\}$, then $\theta_i^{(\ell+1)} > \theta_i^{(\ell)}$.*
- (b) *If $\theta_s^{(0)} > \mu_{s+1}$, consider the auxiliary iteration (3.9) using the same initial subspace $\text{span}\{Y^{(0)}\}$ together with the invariant subspaces $\tilde{\mathcal{Z}} = \text{span}\{z_{i+1}, \dots, z_s\}^\perp$ and $\tilde{\mathcal{Z}} = \text{span}\{z_1, \dots, z_i\}^\perp$. Then $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$ and $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$ hold for each ℓ . Moreover, consider an orthonormal matrix $\tilde{U} \in \mathbb{C}^{n \times i}$ with $\text{span}\{\tilde{U}\} \subseteq \tilde{\mathcal{U}}^{(\ell)}$, and an orthonormal basis matrix \tilde{Y} of $\tilde{\mathcal{Y}}^{(\ell)}$, and let $\mu(\cdot)$ be the Rayleigh quotient with respect to H . If the matrix $\tilde{R} = H\tilde{Y} - \tilde{Y}\tilde{Y}^*H\tilde{Y}$ has full rank, and*

$$\|(H\tilde{Y} - \tilde{U}\tilde{U}^*H\tilde{Y})(\tilde{R}^*\tilde{R})^{-1/2}\|_2 \leq \tilde{\gamma} < 1$$

is fulfilled for each $\ell < L$ as in (3.11), then

$$(4.1) \quad \frac{\mu_i - \theta_i^{(L)}}{\theta_i^{(L)} - \mu_{s+1}} \leq \left(\frac{\kappa_i + \tilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \tilde{\gamma}\kappa_i} \right)^{2L} \frac{\mu_i - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{s+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{s+1} - \mu_n}{\mu_i - \mu_n}$$

holds for the Ritz values produced by (2.7).

- (c) *If $\theta_s^{(0)}$ is located in $(\mu_{j+1}, \mu_j]$ for a certain $j \geq s$, consider the auxiliary iteration (3.9) using the same initial subspace $\text{span}\{Y^{(0)}\}$ together with the invariant subspaces $\tilde{\mathcal{Z}} = \text{span}\{z_{j-s+i+1}, \dots, z_j\}^\perp$ and $\tilde{\mathcal{Z}} = \text{span}\{z_{j-s+1}, \dots, z_{j-s+i}\}^\perp$. Assume for each ℓ that*

$\dim \text{span}\{Y^{(\ell)}\} = s$, $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$, and $\dim \hat{\mathcal{Y}}^{(\ell)} = s - i$. Then $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$, and a similar estimate for (2.7) reads

$$(4.2) \quad \frac{\mu_{j-s+i} - \theta_i^{(L)}}{\theta_i^{(L)} - \mu_{j+1}} \leq \left(\frac{\kappa_i + \tilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \tilde{\gamma}\kappa_i} \right)^{2L} \frac{\mu_{j-s+i} - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{j+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}.$$

Proof. (a) The trivial relation $\theta_i^{(\ell+1)} \geq \theta_i^{(\ell)}$ follows from the optimality of the Rayleigh-Ritz procedure. For showing its strict version, we represent the trial subspace of (2.7) by

$$\text{span}\{Y^{(\ell)}, U^{(\ell)}\} \quad \text{with} \quad U^{(\ell)} = Y^{(\ell)}\Theta_Y^{(\ell)} + N(HY^{(\ell)} - Y^{(\ell)}\Theta_Y^{(\ell)}).$$

If $\text{span}\{Y^{(\ell)}\}$ contains no eigenvectors, we use [21, Lemma 3.1] where $U^{(\ell)}$ is analyzed within a BPG iteration with fixed step sizes. This implies

$$\theta_i^{(\ell+1)} = \theta_i(\text{span}\{Y^{(\ell)}, U^{(\ell)}\}) \geq \theta_i(\text{span}\{U^{(\ell)}\}) > \theta_i(\text{span}\{Y^{(\ell)}\}) = \theta_i^{(\ell)}.$$

(b) Combining Lemma 3.5 and Theorem 3.7 yields $\dim \tilde{\mathcal{Y}}^{(\ell)} = i$, $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$ and suggests a vector iteration concerning $\text{span}\{\tilde{y}, \tilde{u}\}$. Moreover, for the respective smallest (i th largest) Ritz values $\tilde{\theta}_i^{(\ell)}$ and $\tilde{\theta}_i^{(\ell+1)}$ of H in $\tilde{\mathcal{Y}}^{(\ell)}$ and $\tilde{\mathcal{Y}}^{(\ell+1)}$, the Courant-Fischer principles ensure

$$\mu_i \geq \tilde{\theta}_i^{(\ell+1)} = \tilde{\theta}' \geq \tilde{\theta}^\circ \geq \mu(\tilde{y}) \geq \tilde{\theta}_i^{(\ell)}$$

(where $\tilde{\theta}^{(\ell+1)} = \tilde{\theta}'$ follows from Lemma 3.5), i.e., the sequence $(\tilde{\theta}_i^{(\ell)})_{\ell \in \mathbb{N}}$ is nondecreasing. Thus $\tilde{\theta}_i^{(\ell)} \geq \tilde{\theta}_i^{(0)} \geq \theta_s^{(0)} > \mu_{s+1}$ holds so that the above Ritz values and $\mu(\tilde{y})$ are all located in $(\mu_{s+1}, \mu_i]$. Then Lemma 3.9 with $j = s$ leads to

$$\frac{\mu_i - \tilde{\theta}^\circ}{\tilde{\theta}^\circ - \mu_{s+1}} \leq \left(\frac{\kappa_i + \tilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \tilde{\gamma}\kappa_i} \right)^2 \frac{\mu_i - \mu(\tilde{y})}{\mu(\tilde{y}) - \mu_{s+1}} \quad \text{with} \quad \kappa_i = \frac{\mu_{s+1} - \mu_n}{\mu_i - \mu_n}$$

which can be extended as

$$\frac{\mu_i - \tilde{\theta}_i^{(\ell+1)}}{\tilde{\theta}_i^{(\ell+1)} - \mu_{s+1}} \leq \left(\frac{\kappa_i + \tilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \tilde{\gamma}\kappa_i} \right)^2 \frac{\mu_i - \tilde{\theta}_i^{(\ell)}}{\tilde{\theta}_i^{(\ell)} - \mu_{s+1}}$$

by using the monotonicity of $(\mu_i - *) / (* - \mu_{s+1})$. Recursively applying this intermediate estimate results in (4.1) due to $\theta_i^{(L)} \geq \tilde{\theta}_i^{(L)}$ and $\tilde{\theta}_i^{(0)} \geq \theta_s^{(0)}$.

(c) Combining Lemma 3.6 and Theorem 3.7 leads to $\dim \tilde{\mathcal{U}}^{(\ell)} \geq i$ and a vector iteration. The estimate (4.2) is trivial for $\theta_i^{(L)} \geq \mu_{j-s+i}$. If $\theta_i^{(L)} < \mu_{j-s+i}$, we get

$$\mu_{j-s+i} > \theta_i^{(L)} \geq \tilde{\theta}_i^{(L)} \geq \tilde{\theta}_i^{(\ell+1)} = \tilde{\theta}' \geq \tilde{\theta}^\circ \geq \mu(\tilde{y}) \geq \tilde{\theta}_i^{(\ell)} \geq \tilde{\theta}_i^{(0)} \geq \theta_s^{(0)} > \mu_{j+1}$$

for $\ell < L$ similarly to (b). Then (4.2) is derived by Lemma 3.9 with $j \geq s$ and a recursive reformulation as well as monotonicity arguments. \square

Remark 4.2. Theorem 4.1 extends the estimates for a BPG iteration with fixed step sizes from [21, Theorem 3.2 and Theorem 3.3] to the iteration (2.7) with implicitly optimized step sizes. The statement (a) indicates that the i th Ritz value strictly increases until some eigenvectors are enclosed by the subspace iterate. In addition, a reformulation of [12, (3.7)] leads to the sharp estimate

$$(4.3) \quad \frac{\mu_j - \theta_s^{(\ell+1)}}{\theta_s^{(\ell+1)} - \mu_{j+1}} \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^2 \frac{\mu_j - \theta_s^{(\ell)}}{\theta_s^{(\ell)} - \mu_{j+1}} \quad \text{with} \quad \kappa = \frac{\mu_{j+1} - \mu_n}{\mu_j - \mu_n}$$

for the s th Ritz value in the case $\theta_s^{(\ell)} \in (\mu_{j+1}, \mu_j)$ with $j \geq s$ using the quality parameter γ from (2.6). Combining this with (a) shows that $\theta_s^{(\ell)}$ can converge to an eigenvalue μ_j with $j > s$ and otherwise can exceed μ_{s+1} . If $\theta_s^{(\ell)} > \mu_{s+1}$ occurs, we can reset the index ℓ as 0 and apply the statement (b) to the further steps. The statement (c) formally generalizes (b) to arbitrarily located $\theta_s^{(0)}$ and provides a supplement to (4.3) for discussing the convergence of the i th Ritz

value in the first steps of (2.7). The assumption on subspace dimensions is usually fulfilled in numerical tests with randomly generated initial guesses.

Remark 4.3. For evaluating the quality parameter $\tilde{\gamma}$ in the estimates (4.1) and (4.2), we can follow the introduction of (3.11) and determine the auxiliary subspaces $\tilde{\mathcal{Y}}^{(\ell)} = \text{span}\{Y^{(\ell)}\} \cap \tilde{\mathcal{Z}}$ and $\tilde{\mathcal{U}}^{(\ell)} = \text{span}\{U^{(\ell)}\} \cap \tilde{\mathcal{Z}}$ via the invariant subspace $\text{span}\{z_{j-s+1}, \dots, z_j\}$. Furthermore, it is remarkable that (4.3) with $j = s$ implies

$$\frac{\mu_s - \theta_s^{(L)}}{\theta_s^{(L)} - \mu_{s+1}} \leq \left(\frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \right)^{2L} \frac{\mu_s - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{s+1}} \quad \text{with} \quad \kappa = \frac{\mu_{s+1} - \mu_n}{\mu_s - \mu_n}$$

which is similar to (4.1) with $i = s$. These two estimates for the s th Ritz value in the final phase of (2.7) only differ in the quality parameters γ and $\tilde{\gamma}$.

Remark 4.4. In comparison to the results from [13], our multi-step estimate (4.1) indicates that the single-step convergence rate is asymptotically bounded by \tilde{q}_i^2 with $\tilde{q}_i = (\kappa_i + \tilde{\gamma}(2 - \kappa_i)) / ((2 - \kappa_i) + \tilde{\gamma}\kappa_i)$ similarly to the asymptotic convergence factor $q_{k,m}$ presented in [13, Corollary 1] (despite typo with a redundant exponent 2). If adapted to Theorem 4.1 (with $k \rightarrow i$ and $m \rightarrow s$), $q_{k,m}$ becomes

$$q_i = \frac{\kappa + \gamma(2 - \kappa)}{(2 - \kappa) + \gamma\kappa} \quad \text{with} \quad \kappa = \frac{\mu_{s+1}}{\mu_i}$$

which is slightly larger than \tilde{q}_i for $\tilde{\gamma} = \gamma$. However, the nonasymptotic estimate in [13, Corollary 1] is formulated for a sum of Ritz value errors corresponding to $\sum_{t=1}^i (\mu_t - \theta_t^{(\ell)})$. Therein the convergence bound contains q_i^2 and $\sum_{t=1}^s (\mu_t - \theta_t^{(\ell)})$ together with a technical term which is not explicitly given. The main estimate in [13, Theorem 3] uses a convergence factor depending on certain angles and a ratio corresponding to $\mu_{s+1}/\theta_i^{(\ell)}$ as a counterpart of the above $\kappa = \mu_{s+1}/\mu_i$ (in the original formulation, μ_k^i/μ_{m+1} should be corrected as μ_{m+1}/μ_k^i). In Theorem 4.1, we have achieved a concise convergence factor by using the alternative quality parameter $\tilde{\gamma}$. The convergence rates of individual Ritz values do not need to be analyzed in a mixed form.

Finally, we reformulate Theorem 4.1 as explicit statements for the BPG iteration (2.3) by using the substitutions (2.4) and (2.5).

Theorem 4.5. *Consider the generalized eigenvalue problem (1.7) with A -orthonormal eigenvectors w_1, \dots, w_n of (M, A) associated with the eigenvalues $\mu_1 \geq \dots \geq \mu_n$, and let $\theta_1^{(\ell)} \geq \dots \geq \theta_s^{(\ell)}$ be the Ritz values of (M, A) in the subspace iterate $\text{span}\{V^{(\ell)}\}$ of (2.3). Therein $\Theta_V^{(\ell)} = \text{diag}(\theta_1^{(\ell)}, \dots, \theta_s^{(\ell)})$, $R_V^{(\ell)} = MV^{(\ell)} - AV^{(\ell)}\Theta_V^{(\ell)}$, and the preconditioner \tilde{T} satisfies (2.2). Then the following statements hold:*

- (a) *The Ritz values produced by (2.3) fulfill $\theta_i^{(\ell+1)} \geq \theta_i^{(\ell)}$ for each ℓ and $i \in \{1, \dots, s\}$. If there are no eigenvectors in $\text{span}\{V^{(\ell)}\}$, then $\theta_i^{(\ell+1)} > \theta_i^{(\ell)}$.*
- (b) *If $\theta_s^{(0)} > \mu_{s+1}$, consider the auxiliary iteration*

$$\begin{aligned} \tilde{V}^{(\ell)} &= \text{span}\{V^{(\ell)}\} \cap \tilde{\mathcal{W}}, & \hat{V}^{(\ell)} &= \text{span}\{V^{(\ell)}\} \cap \hat{\mathcal{W}}, \\ U^{(\ell)} &= V^{(\ell)}\Theta_V^{(\ell)} + T(MV^{(\ell)} - AV^{(\ell)}\Theta_V^{(\ell)}) \quad \text{with} \quad T = \omega\tilde{T} \quad \text{from (2.2)}, \\ (4.4) \quad \tilde{U}^{(\ell)} &= \text{span}\{U^{(\ell)}\} \cap \tilde{\mathcal{W}}, & \hat{U}^{(\ell)} &= \text{span}\{U^{(\ell)}\} \cap \hat{\mathcal{W}}, \\ \tilde{V}^{(\ell+\frac{1}{2})} &\xleftarrow{\text{RR}[M, A, \tilde{a}]} \tilde{V}^{(\ell)} + \tilde{U}^{(\ell)}, & \hat{V}^{(\ell+\frac{1}{2})} &\xleftarrow{\text{RR}[M, A, \hat{a}]} \hat{V}^{(\ell)} + \hat{U}^{(\ell)}, \\ V^{(\ell+1)} &\xleftarrow{\text{RR}[M, A, \tilde{s}]} \text{span}\{\tilde{V}^{(\ell+\frac{1}{2})}, \hat{V}^{(\ell+\frac{1}{2})}\} \end{aligned}$$

using the same initial subspace $\text{span}\{V^{(0)}\}$ together with the invariant subspaces $\widetilde{\mathcal{W}} = \text{span}\{w_{i+1}, \dots, w_s\}^{\perp A}$ and $\widehat{\mathcal{W}} = \text{span}\{w_1, \dots, w_i\}^{\perp A}$. Then $\widetilde{i} = \dim \widetilde{\mathcal{V}}^{(\ell)} = i$ and $\dim \widetilde{\mathcal{U}}^{(\ell)} \geq i$ hold for each ℓ . Moreover, consider an A -orthonormal matrix $\widetilde{U} \in \mathbb{C}^{n \times i}$ with $\text{span}\{\widetilde{U}\} \subseteq \widetilde{\mathcal{U}}^{(\ell)}$, and an A -orthonormal basis matrix \widetilde{V} of $\widetilde{\mathcal{V}}^{(\ell)}$, and let $\mu(\cdot)$ be the Rayleigh quotient with respect to (M, A) . If $\widetilde{R} = A^{-1}M\widetilde{V} - \widetilde{V}\widetilde{V}^*M\widetilde{V}$ has full rank, and $\widehat{R} = (A^{-1}M\widetilde{V} - \widetilde{U}\widetilde{U}^*M\widetilde{V})(\widetilde{R}^*A\widetilde{R})^{-1/2}$ fulfills $\|\widehat{R}^*A\widehat{R}\|_2^{1/2} \leq \widetilde{\gamma} < 1$ for each $\ell < L$, then the multi-step estimate (4.1) holds for the Ritz values produced by (2.3).

- (c) If $\theta_s^{(0)}$ is located in $(\mu_{j+1}, \mu_j]$ for a certain $j \geq s$, consider the auxiliary iteration (4.4) using the same initial subspace $\text{span}\{V^{(0)}\}$ together with the invariant subspaces $\widetilde{\mathcal{W}} = \text{span}\{w_{j-s+i+1}, \dots, w_j\}^{\perp A}$ and $\widehat{\mathcal{W}} = \text{span}\{w_{j-s+1}, \dots, w_{j-s+i}\}^{\perp A}$. Assume for each ℓ that $\dim \text{span}\{V^{(\ell)}\} = s$, $\widetilde{i} = \dim \widetilde{\mathcal{V}}^{(\ell)} = i$, and $\widehat{i} = \dim \widehat{\mathcal{V}}^{(\ell)} = s - i$. Then $\dim \widetilde{\mathcal{U}}^{(\ell)} \geq i$, and a similar estimate for (2.3) is given by (4.2).

A further reformulation of Theorem 4.5 for extending the convergence analysis of the block preconditioned steepest descent iteration from [12] refers to the computation of the smallest eigenvalues of the matrix pair (A, M) for Hermitian positive definite $A, M \in \mathbb{C}^{n \times n}$. Therein the estimate (4.2) turns into

$$(4.5) \quad \frac{\vartheta_i^{(L)} - \lambda_{j-s+i}}{\lambda_{j+1} - \vartheta_i^{(L)}} \leq \left(\frac{\kappa_i + \widetilde{\gamma}(2 - \kappa_i)}{(2 - \kappa_i) + \widetilde{\gamma}\kappa_i} \right)^{2L} \frac{\vartheta_s^{(0)} - \lambda_{j-s+i}}{\lambda_{j+1} - \vartheta_s^{(0)}} \quad \text{with} \quad \kappa_i = \frac{\lambda_{j-s+i}(\lambda_n - \lambda_{j+1})}{\lambda_{j+1}(\lambda_n - \lambda_{j-s+i})}$$

where λ and ϑ denote eigenvalues and Ritz values of (A, M) in ascending order.

Remark 4.6. Although the parameter $\widetilde{\gamma}$ cannot easily be replaced by γ from (2.2) in our analysis, mainly due to additional modifications of the preconditioned term $U^{(\ell)}$ by intersections in (4.4), the corresponding estimates with γ still provide reasonable bounds in numerical experiments. An analysis directly using γ should avoid additional modifications as in the following auxiliary iteration:

$$(4.6) \quad \begin{aligned} \text{span}\{\widetilde{\mathcal{V}}^{(\ell)}\} &= \text{span}\{V^{(\ell)}\} \cap \widetilde{\mathcal{W}}, & \widetilde{V}^{(\ell+\frac{1}{2})} &\stackrel{\text{RR}[M, A, \widetilde{i}]}{\leftarrow} \text{span}\{\widetilde{\mathcal{V}}^{(\ell)}, TR_{\widetilde{V}}^{(\ell)}\}, \\ \text{span}\{\widehat{\mathcal{V}}^{(\ell)}\} &= \text{span}\{V^{(\ell)}\} \cap \widehat{\mathcal{W}}, & \widehat{V}^{(\ell+\frac{1}{2})} &\stackrel{\text{RR}[M, A, \widehat{i}]}{\leftarrow} \text{span}\{\widehat{\mathcal{V}}^{(\ell)}, TR_{\widehat{V}}^{(\ell)}\}, \\ V^{(\ell+1)} &\stackrel{\text{RR}[M, A, \widehat{s}]}{\leftarrow} \text{span}\{\widetilde{V}^{(\ell+\frac{1}{2})}, \widehat{V}^{(\ell+\frac{1}{2})}\} \end{aligned}$$

where R denotes block residuals. In the case $\widetilde{i} = \dim \text{span}\{\widetilde{\mathcal{V}}^{(\ell)}\} = 1$, the first partial iteration in (4.6) is a vectorial gradient iteration. A geometric relation between two successive iterates \widetilde{v} and \widetilde{v}' can be derived based on [10, Theorem 3.1], namely, there is a rational function $f(\cdot)$ satisfying $\widetilde{v}^\circ = f(A^{-1}M)\widetilde{v}$ and $\mu(\widetilde{v}') \geq \mu(\widetilde{v}^\circ)$. Moreover, \widetilde{v}° can be regarded as the next iterate generated by a special preconditioner T° . Therefore the convergence of the largest Ritz value in (4.6) is decelerated by using such T° . The corresponding first partial iteration can be simplified since $\text{span}\{\widetilde{\mathcal{V}}^{(\ell+\frac{1}{2})}\} \subseteq \widetilde{\mathcal{W}}$ is ensured by $\widetilde{v}^\circ = f(A^{-1}M)\widetilde{v}$. This results in (4.2) with $\widetilde{\gamma} = \gamma$ for $i = 1$. Nevertheless, a generalization to arbitrary $i \in \{1, \dots, s\}$ requires further assumptions on partial iterations. Occasionally, we can apply the estimate with γ for $i = 1$ similarly to a deflation, i.e., analyzing the convergence rate of the $(i+1)$ th Ritz value provided that the first i Ritz values are sufficiently close to the target eigenvalues.

5. Numerical experiments

We consider several numerical examples in order to demonstrate the main results and discuss their accuracy. In the first example, we implement the accompanying iteration (2.7) for a test

matrix from [21], and illustrate Theorem 4.1. The further examples using discretized Laplacian eigenvalue problems are concerned with the BPG iteration (2.3) and Theorem 4.5.

Example I. We reuse the diagonal matrix $H = \text{diag}(\mu_1, \dots, \mu_n)$ from [21, Experiment I] with $n = 6000$ and $\mu_i = 10.07 - 0.01i$ for $i \leq 6$. The further eigenvalues (diagonal entries) of H are given by equidistant points between 9 and 1.

We implement the iteration (2.7) with the block size $s = 6$ where the target eigenvalues μ_1, \dots, μ_s are tightly clustered. We test three preconditioners, denoted by N_1, N_2, N_3 . The first one is simply $N_1 = I$, whereas N_2 and N_3 are generated by random sparse perturbations of I , namely, $N = \text{eta} * \text{sprand}(n, n, 5/n)$; $N = N' + I + N$ with $\eta \in \{0.09, 0.16\}$. For each preconditioner, we compare 1000 runs with random initial subspaces, and illustrate the slowest run with respect to the Ritz value errors $\mu_i - \theta_i^{(\ell)}$, $i \in \{1, \dots, 6\}$ by solid curves in Figure 1. This immediately reflects the monotone convergence in the statement (a) of Theorem 4.1.

For checking the statement (b), we determine the quality parameter $\tilde{\gamma}$ by evaluating (3.11) within the auxiliary iteration (3.9) for each iteration step after the Ritz value $\theta_s^{(\ell)}$ exceeds μ_{s+1} . The corresponding maximum is used as $\tilde{\gamma}$ in the estimate (4.1) with an index adaptation. Therein

$$\tilde{\gamma} = 0 \text{ for } N_1, \quad \tilde{\gamma} \approx 0.2429 \text{ for } N_2, \quad \tilde{\gamma} \approx 0.5285 \text{ for } N_3.$$

The resulting bounds for $\mu_i - \theta_i^{(\ell)}$ are plotted by dashed curves in Figure 1. In addition, their counterparts based on the single-step estimates from [12], i.e., those using $(\mu_{i+1} - \mu_n)/(\mu_i - \mu_n)$ instead of $(\mu_{s+1} - \mu_n)/(\mu_i - \mu_n)$ in (4.1), are displayed by dotted curves.

These two types of bounds coincide for $i = s = 6$. The difference between them is substantial for $i \in \{1, \dots, 5\}$ due to $\mu_i \approx \mu_{i+1}$. The bounds in dashed curves clearly reflect the cluster robustness, whereas the bounds in dotted curves wrongly predict a stagnation. Furthermore, the accuracy of bounds in dashed curves apparently depends on the accuracy of preconditioning, and could be improved for less accurate preconditioners. This motivates a future task for defining a more effective quality parameter.

The statement (c) can be checked in a similar way. We omit the illustration since it only concerns a few iteration steps for random initial subspaces. A reasonable illustration requires certain special initial subspaces.

Example II. We consider the Laplacian eigenvalue problem on the rectangle domain $[0, 2] \times [0, 1]$ with a slit $\{1\} \times [0.1, 0.9]$ and homogeneous Dirichlet boundary conditions. The five-point star discretization with the mesh size $1/70$ results in a standard eigenvalue problem which can be reformulated as (1.7) for $n = 9534$ and $M = I$. The six largest eigenvalues build two tight clusters $\{\mu_1, \mu_2\}$ and $\{\mu_3, \dots, \mu_6\}$.

The BPG iteration (2.3) with the block size $s = 6$ is implemented for three preconditioners T_1, T_2, T_3 constructed by

$$\text{ichol}(A, \text{struct}('type', 'ict', 'droptol', \text{eta})) \text{ for } \eta \in \{10^{-5}, 10^{-4}, 10^{-3}\}.$$

Similarly to Example I, Ritz value errors in the slowest run concerning 1000 random initial subspaces are illustrated by solid curves in Figure 2.

We particularly demonstrate the statement (b) of Theorem 4.5. Therein the quality parameter $\tilde{\gamma}$ is determined for each iteration step after $\theta_s^{(\ell)} > \mu_{s+1}$ by using the auxiliary iteration (4.4). The respective maxima are

$$\tilde{\gamma} \approx 0.0295 \text{ for } T_1, \quad \tilde{\gamma} \approx 0.2344 \text{ for } T_2, \quad \tilde{\gamma} \approx 0.5168 \text{ for } T_3.$$

The resulting bounds in dashed curves are appropriate for each Ritz value. Their counterparts based on [12] in dotted curves are only reasonable for $i \in \{2, 6\}$ where μ_i and μ_{i+1} are not

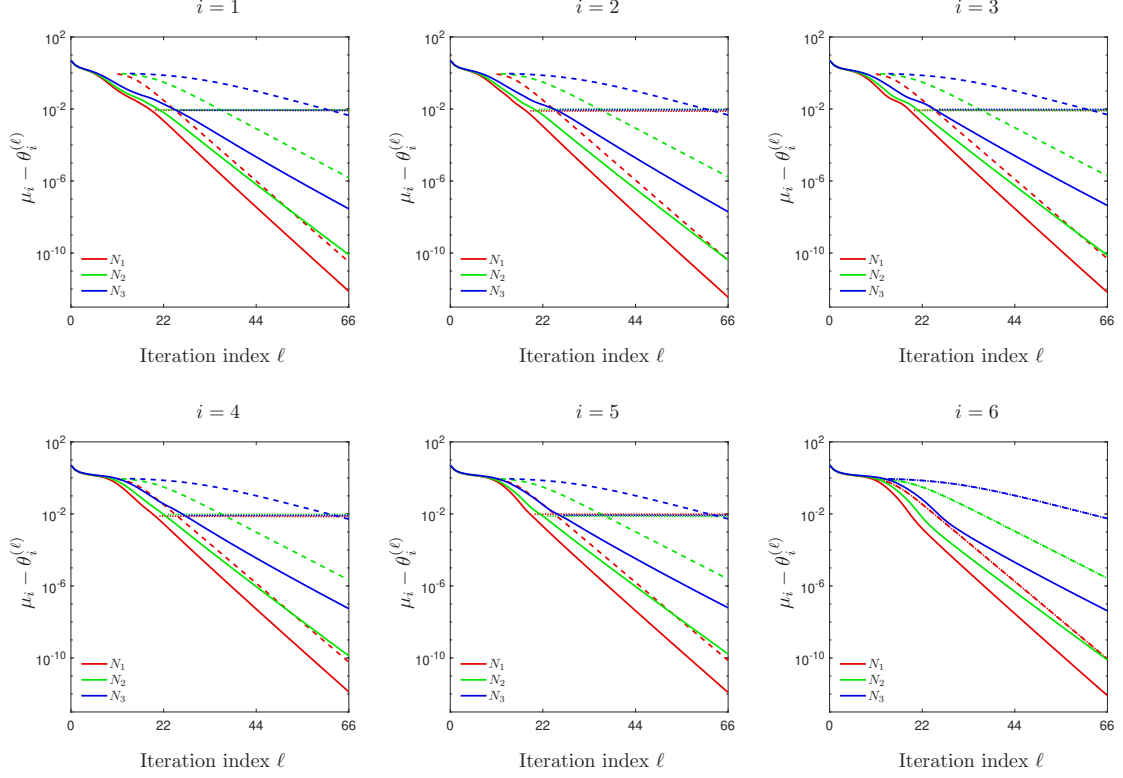


FIGURE 1. Cluster robustness of the accompanying iteration (2.7) applied to Example I. Solid curves: Ritz value errors in the slowest run among 1000 runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.1. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.

clustered and the bounds are more accurate in the first steps. Moreover, the dotted curves cannot be drawn for $i = 5$ since μ_5 and μ_6 coincide. The new bounds are thus advantageous for clustered and multiple eigenvalues.

Example III. We consider the Laplacian eigenvalue problem on a 2D tulip-like domain with homogeneous Dirichlet boundary conditions; see Figure 3. The boundary consists of three parts:

$$\begin{aligned} \Gamma_1 &= \{(1.2 \sin(t) + 0.3 \sin(4t), -\cos(t) - 0.5 \cos(2t))^T; t \in [-\pi, \pi)\}, \\ \Gamma_2 &= \{(0, 0.5t)^T; t \in (0, 1)\}, \quad \Gamma_3 = \{(0, 0.5(1-t))^T; t \in (0, 1)\}. \end{aligned}$$

We generate matrix eigenvalue problems successively by an adaptive finite element discretization depending on residuals of approximate eigenfunctions associated with the three smallest operator eigenvalues; cf. [21, Appendix] and some relevant graphics in Figure 3. We repeat the numerical experiments in Example II for the matrix pair (M, A) from the 41st grid of the discretization with $n = 1,522,640$ degrees of freedom. The largest eigenvalues of (M, A) approximate the reciprocals of the smallest operator eigenvalues.

We observe again the BPG iteration (2.3) with the block size $s = 6$. The target eigenvalues are partially clustered ($\mu_2 \approx \mu_3$). Concerning the comparison between new results in Theorem 4.5 and previous results based on [12], we first compare their decisive terms $\kappa_i = (\mu_{s+1} - \mu_n) / (\mu_i - \mu_n)$ and $\hat{\kappa}_i = (\mu_{i+1} - \mu_n) / (\mu_i - \mu_n)$. For $i \in \{1, \dots, 6\}$, we have

$$(5.1) \quad \begin{aligned} \kappa_i &\in \{0.1993, 0.4628, 0.4687, 0.6279, 0.7307, 0.9459\}, \\ \hat{\kappa}_i &\in \{0.4306, 0.9875, 0.7464, 0.8593, 0.7725, 0.9459\}. \end{aligned}$$

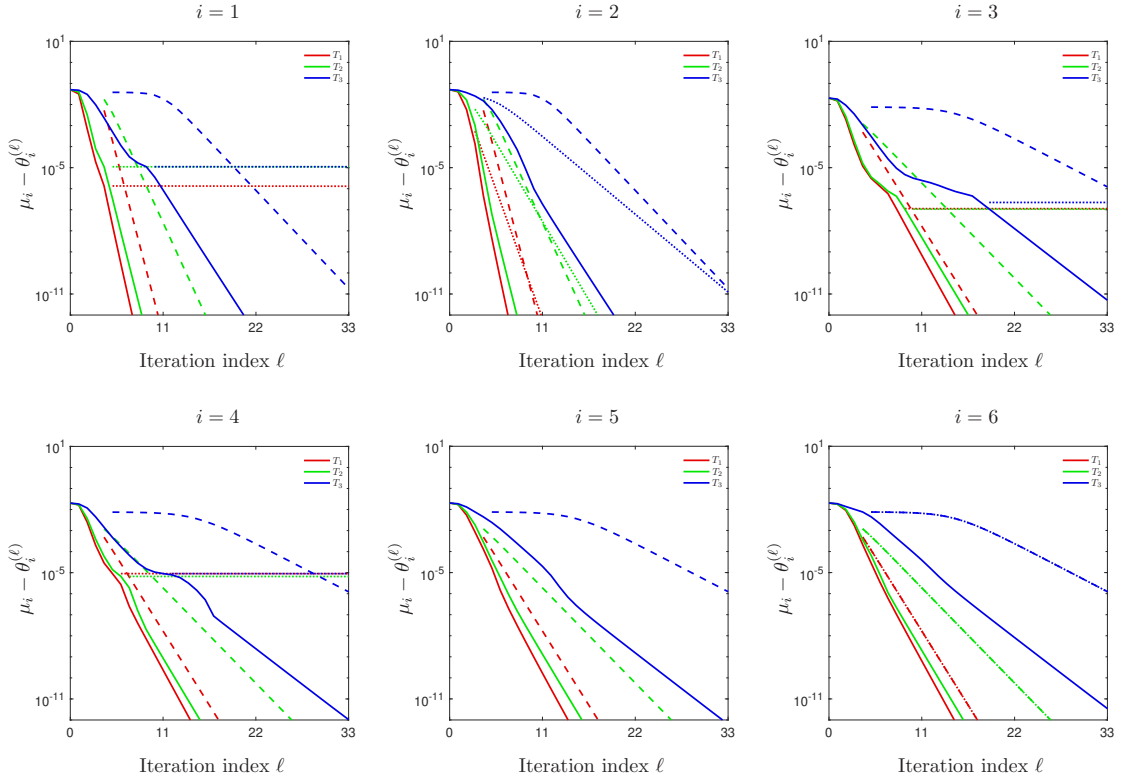


FIGURE 2. Cluster robustness of the BPG iteration (2.3) applied to Example II. Solid curves: Ritz value errors in the slowest run among 1000 runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.5. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.

The test preconditioners T_1, T_2, T_3 are constructed by `ichol` with $\eta \in \{10^{-7}, 10^{-6}, 10^{-5}\}$ as `droptol`. The quality parameter $\tilde{\gamma}$ with respect to the auxiliary iteration (4.4) reads

$$\tilde{\gamma} \approx 0.1116 \text{ for } T_1, \quad \tilde{\gamma} \approx 0.3563 \text{ for } T_2, \quad \tilde{\gamma} \approx 0.6652 \text{ for } T_3.$$

Figure 4 presents a bound comparison for Ritz value errors in the slowest run concerning 1000 random initial subspaces. The dashed curves display new bounds from Theorem 4.5. They generally have steeper slopes than the dotted curves containing bounds based on [12]. The slope difference mainly depends on the terms κ_i and $\hat{\kappa}_i$; cf. their values given in (5.1). The maximal difference appears for $i = 2$ where the dotted curves are almost constant. As an explanation, we note that the corresponding κ value $\hat{\kappa}_2 \approx 0.9875$ is close to 1, and the convergence factor is at least $\hat{\kappa}_2/(2 - \hat{\kappa}_2)$ for each test preconditioner. Such an overestimation can also be caused by a slightly smaller κ value between 0.85 and 0.95 for a moderate preconditioner; cf. the blue curves for $i \in \{4, 6\}$ corresponding to T_3 combined with $\hat{\kappa}_4$ (dotted), κ_6 and $\hat{\kappa}_6$ (dashed and dotted). Deriving sharper bounds in the case of moderate preconditioners is potentially important for large-scale discretized eigenvalue problems where generating more accurate preconditioners, e.g. with $\tilde{\gamma} < 0.5$, is costly with respect to inner steps and the total time.

Conclusion

The cluster robustness of block preconditioned gradient (BPG) eigensolvers with sufficiently large block sizes is studied by deriving proper convergence bounds of individual Ritz values. A basic argument in our analysis is that the Rayleigh-Ritz (RR) approximation in the trial

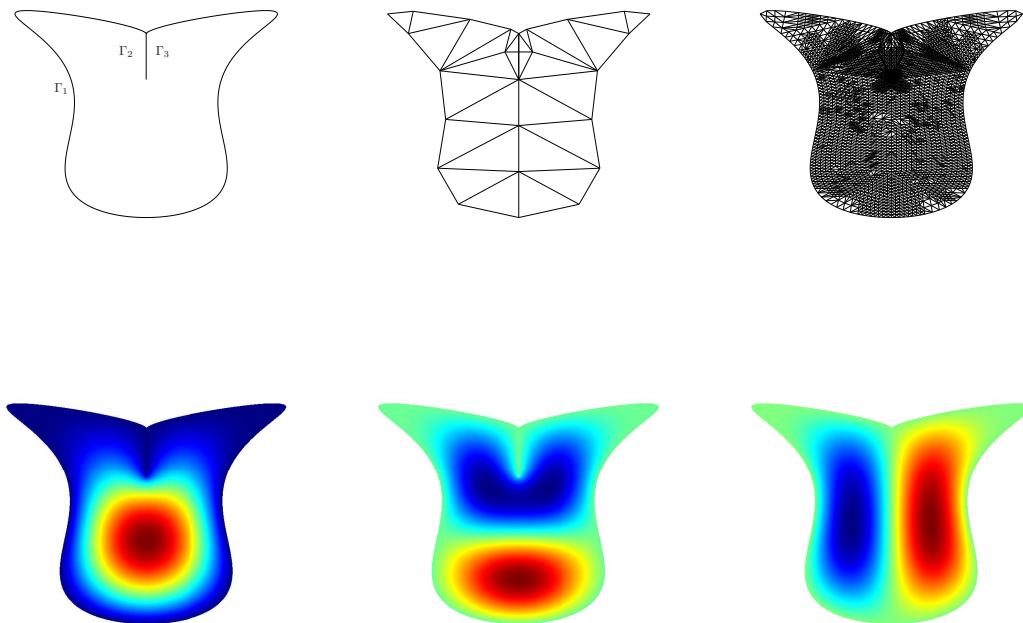


FIGURE 3. Laplacian eigenvalue problem for Example III. First row: domain, initial grid and an adaptively refined grid. Second row: approximate eigenfunctions (top view) associated with the three smallest operator eigenvalues whose residuals are used for the grid refinement.

subspace of BPG can be decelerated by applying RR to certain lower-dimensional subspaces. This motivates auxiliary iterations whose iterates are orthogonal to eigenvectors associated with some possibly clustered eigenvalues. The relevant eigenvalues in the resulting bound are thus not close to each other and reflect a cluster-independent convergence rate. The construction of such auxiliary iterations is relatively easy for exact-inverse preconditioning by using the classical analysis of an abstract block iteration [4]. The previous analysis [21] deals with an arbitrary Hermitian positive definite preconditioner, but focuses on fixed step sizes which correspond to the block power method rather than a block gradient iteration. Therein an alternative quality parameter for the preconditioner leads to concise bounds under weaker assumptions in comparison to [3, 13]. This approach is upgraded in the present paper by adapting some geometric arguments from our analysis of the (block) preconditioned steepest descent iteration [10, 12]. The achieved multi-step estimates improve the sumwise estimates from [13] in the sense of more intuitive convergence factors and the applicability to individual Ritz values. It is remarkable that BPG as two-block iterations are not necessarily cluster robust for small block sizes. This drawback can be overcome by three(or more)-block iterations such as LOBPCG and restarted Davidson methods [17, 18, 19]. Extending our analysis of BPG to more powerful eigensolvers is desirable in our future research.

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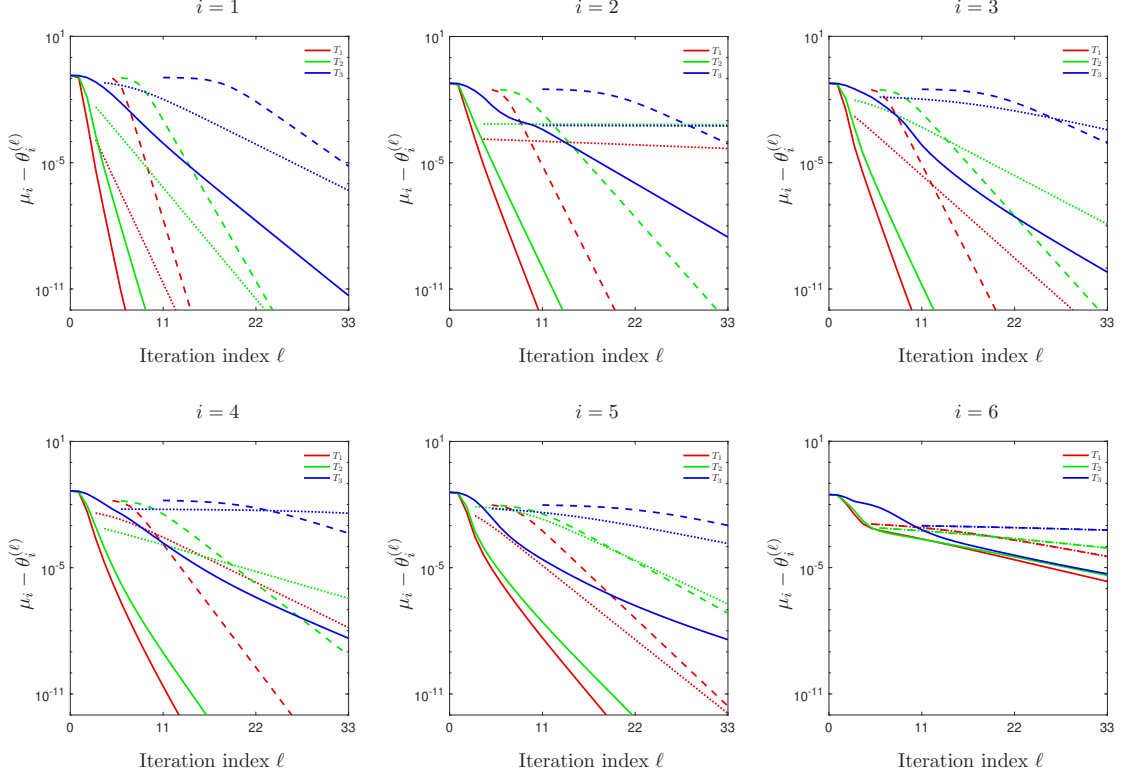


FIGURE 4. Cluster robustness of the BPG iteration (2.3) applied to Example III. Solid curves: Ritz value errors in the slowest run among 1000 runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.5. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.

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