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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 for the purpose of analyzing their convergence behavior by composing known estimates. An important feature of the BPG method is the cluster robustness, i.e., that reasonable performance for computing clustered eigenvalues is ensured by a sufficiently large block size. Concise estimates reflecting this feature can easily be derived for exact-inverse (exact shift-inverse) preconditioning. Therein, the BPG method is compatible with an abstract block iteration analyzed by Knyazev [Soviet J. Numer. Anal. Math. Modelling, 2 (1987), pp. 371–396]. An adaptation to more general preconditioning is difficult as some orthogonality properties cannot be preserved. Another analysis by Ovtchinnikov [Linear Algebra Appl., 415 (2006), pp. 140–166] provides sumwise estimates for Ritz values containing elegant convergence factors. However, additional technical terms lead to cumbersome bounds and could cause overestimations in the first steps. We expect to improve the existing results by deriving concise estimates for individual Ritz values. A mid-term goal has been achieved for the BPG iteration with fixed step sizes by the authors in [Math. Comp., 88 (2019), pp. 2737–2765]. The present paper deals with the more practical case that the step sizes are implicitly optimized by the Rayleigh–Ritz method.

Key words. preconditioned subspace eigensolvers, Ritz values, cluster robustness

AMS subject classifications. 65F15, 65N12, 65N25

1. Introduction.

Solving eigenvalue problems for large and sparse Hermitian matrices or matrix pairs are of practical importance in various applications. Appropriate iterative methods with vectors or subspaces allow to determine the desired eigenpairs with reasonable effort [1, 9]. The convergence behavior of such eigensolvers depends on the distribution of the 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

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

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 $\operatorname{span}\{X^{(\ell)}\}$. 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 the 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 a preconditioner and represents an approximate inverse of A for which the condition

$$\|I - TA\|_A \le \gamma < 1 \tag{1.2}$$

with the $n\times n$ identity matrix I ensures that the trial subspace $\mathcal{U}^{(\ell)} = \operatorname{span}\{X^{(\ell)} - TR^{(\ell)}\}$ has dimension s according to [11, Lemma 3.1]. It is not necessary to assume in (1.2) that T is symmetric positive definite. Nevertheless, for an arbitrary symmetric positive definite preconditioner $\widetilde{T}$, there exists a scalar $\omega \in \mathbb{R}$ so that $T = \omega\widetilde{T}$ fulfills (1.2); see the more general setup (2.2) for Hermitian matrices in our analysis following the pioneering work [5]

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on nonasymptotic convergence bounds for preconditioned subspace eigensolvers. Finally, the Rayleigh–Ritz procedure $\mathrm{RR}[s]$ 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 of $R^{(\ell)}$ are collinear with the gradient vectors of the Rayleigh quotient

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

associated with the columns of $X^{(\ell)}$. For computing the first t eigenvalues of A concerning the eigenvalue arrangement $\lambda_1 \leq \cdots \leq \lambda_n$, fast convergence can be ensured by $\lambda_t \ll \lambda_{s+1}$ according to the well-known convergence theory [17] for the subspace iteration $X^{(\ell+1)} \xleftarrow{\mathrm{RR}[s]} \mathrm{span}\{A^{-1}X^{(\ell)}\}$ (i.e., the block power method for A^{-1}), which coincides with the special form of (1.1) for $T = A^{-1}$. A practical stopping criterion utilizing the first t columns of the block residual $R^{(\ell)}$ can tell us whether the block size s is sufficiently large. In the negative case and if, in addition, s cannot be further enlarged due to storage limits, then one can combine (1.1) with deflation techniques; cf. the preconditioned steepest descent method with implicit deflation [4]. Then the target eigenvalues can be computed in several successive runs where $\lambda_{t_1+\cdots+t_{k-1}+t_k} \ll \lambda_{t_1+\cdots+t_{k-1}+s+1}$ is fulfilled in the kth run (t_j denotes the number of target eigenvalues obtained in the jth run).

Furthermore, extending the trial subspace of (1.1) leads to more efficient eigensolvers such as

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

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

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

which corresponds to the locally optimal block preconditioned conjugate gradient (LOBPCG) method [7]. Again, it is advantageous to implement these eigensolvers in combination with deflation due to the different convergence rates of the individual Ritz values. Deriving sharp bounds for 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 the preconditioned subspace iteration (1.1) can be analyzed as in [3, Section 2] in terms of the eigenvalue arrangement $\lambda_1 \leq \cdots \leq \lambda_n$ of A, the quality parameter γ from (1.2) for the preconditioner T, and the block size s. The resulting estimate for the ith Ritz value for an index $i \in \{1, \ldots, s\}$ provides a bound which essentially depends on the convergence factor

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

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 [17]. However, the analysis in [3] requires a technical assumption on certain angles between the initial subspace $\mathrm{span}\{X^{(0)}\}$ and the eigenvectors associated with the eigenvalues $\lambda_1, \ldots, \lambda_s$. The gap $\lambda_{i+1} - \lambda_i$, for each $i \in \{1, \ldots, s\}$, 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 [8, Section 5]. Therein, an eigenvalue interval $(\lambda_j, \lambda_{j+1})$ with $j \geq i$ is used for locating the ith Ritz value in the current

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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 ith Ritz value reaches the interval $(\lambda_i,\lambda_{i+1})$, then 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 [23] 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 $\widetilde{\gamma}$ for the preconditioner T concerning a geometric interpretation based on [11], we have achieved the convergence factor

$$\widetilde{\gamma}+(1-\widetilde{\gamma})\lambda_{j-s+i}/\lambda_{j+1} \tag{1.6}$$

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 to $\widetilde{\gamma}+(1-\widetilde{\gamma})\lambda_i/\lambda_{s+1}$. 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 accelerated iterations such as (1.3) and (1.4). More direct bounds for the BPG iteration (1.3) have been presented in [15] in terms of sums of Ritz value errors by generalizing some arguments from [18, 16] concerning vectorial gradient iterations. In [14], we have upgraded the analysis from [8] by adapting a sharp estimate from [12] for the single-vector version of (1.3), leading to bounds in terms of the convergence measure $(*-\lambda_j)/(\lambda_{j+1}-*)$ for individual Ritz values.

The result from [15] is somewhat cumbersome due to angle-dependent terms, and it indicates only asymptotically a concise convergence factor consisting of a few eigenvalues and a quality parameter as in (1.5) or (1.6). The limitation of [14] is similar to that of [8], i.e., the convergence factor

$$\frac{\tau+\gamma\,(2-\tau)}{(2-\tau)+\gamma\,\tau} \qquad \text{with} \quad \tau=\frac{\lambda_i(\lambda_n-\lambda_{i+1})}{\lambda_{i+1}(\lambda_n-\lambda_i)} \tag{1.7}$$

(using γ from (1.2) together with the letter τ instead of κ from [14] for the sake of avoiding confusion between κ and condition numbers) is close to 1 in the case $\lambda_i\approx\lambda_{i+1}$ and thus cannot indicate cluster robustness.

The recent analysis for the preconditioned subspace iteration (1.1) from [23] inspires an analogous approach for the BPG iteration (1.3) using $(*-\lambda_{j-s+i})/(\lambda_{j+1}-*)$ as the convergence measure. Therein the desired convergence factor

$$\frac{\tau+\widetilde{\gamma}\,(2-\tau)}{(2-\tau)+\widetilde{\gamma}\,\tau} \qquad \text{with} \quad \tau=\frac{\lambda_{j-s+i}(\lambda_n-\lambda_{j+1})}{\lambda_{j+1}(\lambda_n-\lambda_{j-s+i})} \tag{1.8}$$

is formally motivated by (1.7) and indicates the advantage of optimizing step sizes in the BPG method in addition to the cluster robustness. We note that the approach from [23] or the derivation of (1.6) can only be partially adapted to the BPG iteration for obtaining (1.8). In particular, the quality parameter $\widetilde{\gamma}$ needs to be constructed in another way concerning the Rayleigh–Ritz procedure.

1.2. Aim and overview. Our goal is to derive concise Ritz value estimates containing convergence factors like (1.8) for interpreting the cluster robustness of the BPG iteration (1.3). As the ratio $\lambda_{j-s+i}/\lambda_{j+1}$ is a decisive term in (1.8), a fundamental idea is to skip the eigenvalues $\lambda_{j-s+i+1},\dots,\lambda_j$ by utilizing certain auxiliary subspaces which are orthogonal (and A-orthogonal) to the associated eigenvectors $x_{j-s+i+1},\dots,x_j$.

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This idea arises from the analysis of an abstract block iteration by Knyazev [6] and has been adapted to the preconditioned subspace iteration (1.1) in [23]. By observing a partial iteration of (1.1) within the orthogonal complement of $\operatorname{span}\{x_{j-s+i+1},\dots,x_j\}$, some Ritz vectors in two successive subspace iterates are compared in a geometric way similarly to [11] for constructing a perturbed inverse vector iteration. The corresponding perturbation parameter $\widetilde{\gamma}$ 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., $\operatorname{span}\{X^{(\ell+1)}\} = \operatorname{span}\{X^{(\ell)} - TR^{(\ell)}\}$. Thus, a direct comparison between the Ritz vectors is allowed.

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 [14] using Sion's-minimax theorem via certain basis matrices instead of Ritz vectors. Consequently, for analyzing the cluster robustness of (1.3) with the desired convergence factor (1.8), we need to update the construction of the quality parameter $\widetilde{\gamma}$ of preconditioning by means of basis matrices or subspaces.

For the sake of generality, we follow the introduction of the LOBPCG method in [7] and reformulate (1.3) for the generalized eigenvalue problem

$$Mv = \mu Av, \qquad M, A \in \mathbb{C}^{n\times n} \text{ Hermitian}, \quad A \text{ positive definite}, \tag{1.9}$$

where the target eigenvalues of the matrix pair (M, A) are the largest ones. Some conversions between (1.9) and practical eigenvalue problems are introduced in Section 2 together with a simple representation of the investigated iteration that does not limit the generality. Section 3 provides some auxiliary terms and intermediate arguments based on the analysis of an abstract block iteration from [6] and the analysis of the preconditioned subspace iteration (1.1) from [23]. A subspace-oriented interpretation of preconditioning is introduced in Lemma 3.3 with two invariant subspaces related to eigenvalues of indices $j-s+1,\dots,j-s+i$ and $j-s+i+1,\dots,j$ with which a stepwise mixture of two partial iterations of the BPG method is defined in (3.9). This enables an adaptation of relevant arguments from [14] to show decisive statements for preconditioning in Theorem 3.7 and leads to cluster-robust multi-step estimates in Section 4. 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 (1.9) 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, appropriate discretizations produce the standard eigenvalue problem $Lu = \lambda u$ of a Hermitian matrix $L \in \mathbb{C}^{n\times n}$ or the generalized eigenvalue problem

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

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, then we can transform (2.1) as $(L-\sigma S)u = (\lambda-\sigma)Su$ with a sufficiently small shift σ such that the matrix $\widetilde{L} = L - \sigma S$ is positive definite. The shifted problem corresponds to (1.9) for $M = S$, $A = \widetilde{L}$ and $\mu = (\lambda-\sigma)^{-1}$.

If some interior eigenvalues of (L, S) are first to be determined, then we can establish a similar shifted problem with an indefinite and invertible $\widetilde{L}$. This cannot directly be covered by (1.9). Instead, we can consider the equivalent problem $(\widetilde{L}S^{-1}\widetilde{L})u = (\lambda-\sigma)\widetilde{L}u$ as a special form of (1.9) with $M = \pm\widetilde{L}$, $A = \widetilde{L}S^{-1}\widetilde{L}$, and $\mu = \pm(\lambda-\sigma)^{-1}$.

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Some further specializations of (1.9) include Hermitian definite matrix pencils [10] and the linear response eigenvalue problem [2].

Our analysis focuses on a BPG iteration for solving (1.9); see Section 2.1. Therein, we consider the matrices M and A from (1.9) instead of L, S, and $\widetilde{L}$ mentioned above. Furthermore, we use a notation with respect to the inner product induced by A as in [23]; see Section 2.2.

2.1. Considered iteration. We modify the iteration (1.3) for computing the largest eigenvalues of (M, A) from (1.9). 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 $\operatorname{span}\{V^{(\ell)}\}$. 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 $\widetilde{T}R_V^{(\ell)}$ with a Hermitian positive definite preconditioner $\widetilde{T}$ that is an approximate inverse of A. By using the smallest eigenvalue α and the largest eigenvalue β of the matrix product $\widetilde{T}A$ (or $A^{1/2}\widetilde{T}A^{1/2}$), which are both positive, it holds that

$$\|I - \omega\widetilde{T}A\|_A \le \gamma \qquad \text{with} \quad \omega = \frac{2}{\beta+\alpha} \quad \text{and} \quad \gamma = \frac{\beta-\alpha}{\beta+\alpha} < 1. \tag{2.2}$$

This condition is a more natural form of (1.2) concerning an arbitrary Hermitian positive definite $\widetilde{T}$ and additional scaling. The trial subspace $\mathcal{U}_V^{(\ell)} = \operatorname{span}\{V^{(\ell)}, \widetilde{T}R_V^{(\ell)}\}$ 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 $\mathrm{RR}[M, A, s]$ the underlying Rayleigh–Ritz procedure. Then the modified version of (1.3) is represented by

$$V^{(\ell+1)} \xleftarrow{\mathrm{RR}[M,A,s]} \operatorname{span}\{V^{(\ell)}, \widetilde{T}R_V^{(\ell)}\}. \tag{2.3}$$

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

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

i.e., the columns of $X^{(\ell)}$ are orthonormal Ritz vectors of A in $\operatorname{span}\{X^{(\ell)}\}$, 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 $\operatorname{span}\{X^{(\ell)}, TR^{(\ell)}\} = \operatorname{span}\{V^{(\ell)}, \widetilde{T}R_V^{(\ell)}\}$ for $T = \omega\widetilde{T}$ concerning the conditions (1.2) and (2.2).

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

2.2. Convergence measure and A-notation. We denote by μ_i the ith largest eigenvalue of (M, A) from (1.9), i.e., the eigenvalues are arranged as $\mu_1 \ge \cdots \ge \mu_n$. With the Ritz values $\theta_1^{(\ell)} \ge \cdots \ge \theta_s^{(\ell)}$ of (M, A) in the subspace $\operatorname{span}\{V^{(\ell)}\}$, we set $\Theta_V^{(\ell)} = \operatorname{diag}(\theta_1^{(\ell)}, \ldots, \theta_s^{(\ell)})$.

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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 under the substitution

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

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 modify the notation of matrices and vectors by using the representations

$$H = A^{-1/2} M A^{-1/2}, \qquad y = A^{1/2} v, \qquad Y = A^{1/2} V, \qquad N = A^{1/2} (\omega \widetilde{T}) A^{1/2} \tag{2.5}$$

as in [23, Subsection 1.2]. Then, (2.2) turns into

$$\|I - N\|_2 \leq \gamma < 1, \tag{2.6}$$

and (2.3) is equivalent to

$$Y^{(\ell+1)} \;\xleftarrow{\mathrm{RR}[H,s]}\; \mathrm{span}\{Y^{(\ell)}, N(HY^{(\ell)} - Y^{(\ell)} \Theta_Y^{(\ell)})\}, \tag{2.7}$$

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 $\mu_1 \geq \cdots \geq \mu_n$ 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 $\mathrm{span}\{Y^{(\ell)}\}$ associated with the arranged Ritz values $\theta_1^{(\ell)} \geq \cdots \geq \theta_s^{(\ell)}$, also contained in the diagonal matrix $\Theta_Y^{(\ell)}$. The Rayleigh–Ritz procedure $\mathrm{RR}[H, s]$ 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 $\widetilde{T} = A^{-1}$ 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 so that one can apply estimates from [6] concerning an abstract block iteration. We particularly introduce some underlying auxiliary subspaces and formulate with them the second approach. Therein, certain vector iterations are constructed for preparing the analysis for general preconditioners based on our previous results from [14, 23].

3.1. Analysis via an abstract block iteration. In the case $\widetilde{T} = A^{-1}$, we can set $N = I$ in the accompanying iteration (2.7). Then the trial subspace turns into

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

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

$$Y^{(\ell+1)} \;\xleftarrow{\mathrm{RR}[H,s]}\; \mathrm{span}\{Y^{(\ell)}, HY^{(\ell)}\}. \tag{3.1}$$

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

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

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

Indeed, the iteration (3.1) can be regarded as a simply restarted version of the block Lanczos method and can be investigated based on the comparative analysis from [6, Section 2] by Knyazev. We reformulate the central estimate therein as follows:

LEMMA 3.1 (Reformulation of [6, (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 $|f(\mu_1)| \geq \cdots \geq |f(\mu_s)| > 0$. If $Y^{(\ell)}$ has full rank and the sth largest Ritz value $\theta_s^{(\ell)}$ of H in $\operatorname{span}\{Y^{(\ell)}\}$ 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*

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

Applying Lemma 3.1 to (3.2) with

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

yields the convergence factor

$$\frac{\max_{k=s+1,\ldots,n} |f(\mu_k)|}{\min_{k=1,\ldots,s} |f(\mu_k)|} = \frac{|f(\mu_{s+1})|}{|f(\mu_s)|} = \frac{\mu_{s+1} - \mu_n}{2\mu_s - \mu_{s+1} - \mu_n} = \frac{\tau_s}{2 - \tau_s},$$

with

$$\tau_s = \frac{\mu_{s+1} - \mu_n}{\mu_s - \mu_n},$$

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 ith largest Ritz value for an arbitrary $i \leq s$ does not hold in general; cf. the numerical example in [22, Section 3 and Figure 1]. In contrast, the estimate [6, (2.20)] leads to the angle-dependent multi-step estimate

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

for (3.1), where $\varphi^{(0)}$ is the Euclidean angle between the initial subspace $\operatorname{span}\{Y^{(0)}\}$ and the invariant subspace of H associated with the eigenvalues $\mu_1, \ldots, \mu_s$. Furthermore, two angle-free multi-step estimates for (3.1) can be derived analogously to recent results from [23] 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 [23, 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*

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

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

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

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For proving Lemma 3.2, we can first adapt the analysis from [23] to the iteration (3.2) and then extend the results to the accelerated iteration (3.1) by using again the subspace inclusion $\operatorname{span}\{p_1(H)Y^{(\ell)}\} \subseteq \operatorname{span}\{Y^{(\ell)}, HY^{(\ell)}\}$. An underlying proof technique is that one can select a subspace $\widetilde{\mathcal{Y}} \subseteq \operatorname{span}\{Y^{(\ell)}\}$ such that $\widetilde{\mathcal{Y}}$, $H\widetilde{\mathcal{Y}}$, and $p_1(H)\widetilde{\mathcal{Y}}$ are simultaneously orthogonal to the eigenvectors associated with the eigenvalues $\mu_{i+1}, \ldots, \mu_s$ or $\mu_{j-s+i+1}, \ldots, \mu_j$, 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 intermediate vector iterations within the subspace $\widetilde{\mathcal{Y}} + H\widetilde{\mathcal{Y}}$ and its counterpart for $N \approx I$ so that some arguments from [14, 23] can be utilized.

3.2. Auxiliary subspaces. Following the sketch of the proof of Lemma 3.2, we introduce some auxiliary subspaces that are still useful for analyzing general preconditioning $N \approx I$. Constructing such subspaces does not support the implementation of BPG (2.7) and serves only as an analytic tool for the interpretation of preconditioning.

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

$$\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{j-s+i+1}, \ldots, z_j\}^{\perp} \qquad \textit{and} \qquad \widehat{\mathcal{Z}} = \operatorname{span}\{z_{j-s+1}, \ldots, z_{j-s+i}\}^{\perp}$$

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

$$\widetilde{\mathcal{Y}} = \mathcal{Y} \cap \widetilde{\mathcal{Z}}, \qquad \textit{and} \qquad \widehat{\mathcal{Y}} = \mathcal{Y} \cap \widehat{\mathcal{Z}}.$$

Then it holds that

$$\dim \widetilde{\mathcal{Y}} \geq i, \qquad \textit{and} \qquad \dim \widehat{\mathcal{Y}} \geq s - i. \tag{3.6}$$

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

$$\dim \widetilde{\mathcal{Y}} = i, \quad \dim \widehat{\mathcal{Y}} = s - i, \quad \dim(\widetilde{\mathcal{Y}} \cap \widehat{\mathcal{Y}}) = 0, \quad \textit{and} \quad \dim(\widetilde{\mathcal{Y}} + \widehat{\mathcal{Y}}) = s. \tag{3.7}$$

Proof. The statement (3.6) follows from

$$\begin{aligned} \dim \widetilde{\mathcal{Y}} &= \dim \mathcal{Y} + \dim \widetilde{\mathcal{Z}} - \dim(\mathcal{Y} + \widetilde{\mathcal{Z}}) \geq s + (n - s + i) - n = i, \\ \dim \widehat{\mathcal{Y}} &= \dim \mathcal{Y} + \dim \widehat{\mathcal{Z}} - \dim(\mathcal{Y} + \widehat{\mathcal{Z}}) \geq s + (n - i) - n = s - i. \end{aligned}$$

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

$$\begin{aligned} \dim \widetilde{\mathcal{Y}} > i \quad &\Rightarrow \quad \widetilde{\theta} \leq \text{the } (i+1)\text{st element in } \{\mu_1, \ldots, \mu_i, \mu_{s+1}, \ldots, \mu_n\} = \mu_{s+1}, \\ \dim \widehat{\mathcal{Y}} > s - i \quad &\Rightarrow \quad \widehat{\theta} \leq \text{the } (s-i+1)\text{st element in } \{\mu_{i+1}, \ldots, \mu_n\} = \mu_{s+1}. \end{aligned}$$

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

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

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

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

3.3. Analysis via vector iterations. The invariant subspaces $\widetilde{\mathcal{Z}}$ and $\widehat{\mathcal{Z}}$ introduced in Lemma 3.3 are further of importance for analyzing the BPG iteration (2.7) with general preconditioners. Therein, the direct generalization

$$\widetilde{Y}^{(\ell+1)} \xleftarrow{\mathrm{RR}[H,\widetilde{i}]} \operatorname{span}\{\widetilde{Y}^{(\ell)}, N(H\widetilde{Y}^{(\ell)} - \widetilde{Y}^{(\ell)}\Theta_{\widetilde{Y}}^{(\ell)})\}$$

of (3.8) is somewhat problematic since $\operatorname{span}\{N(H\widetilde{Y}^{(\ell)} - \widetilde{Y}^{(\ell)}\Theta_{\widetilde{Y}}^{(\ell)})\}$ for $N \approx I$ is not necessarily a subset of $\widetilde{\mathcal{Z}}$. Instead, following our previous results from [14, 23], we reformulate the trial subspace of (2.7) as

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

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

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

with $\widetilde{i} = \dim \widetilde{\mathcal{Y}}^{(\ell)}$, $\widehat{i} = \dim \widehat{\mathcal{Y}}^{(\ell)}$, and $\widetilde{s} = \dim \operatorname{span}\{\widetilde{Y}^{(\ell+\frac{1}{2})}, \widehat{Y}^{(\ell+\frac{1}{2})}\}$ for the current step index ℓ. The matrix $U^{(\ell)}$ coincides with $HY^{(\ell)}$ for $N = I$, and $\operatorname{span}\{U^{(\ell)}\}$ corresponds to the trial subspace of a BPG iteration with fixed step sizes for which some cluster robust estimates have been derived in [23]. The trial subspace of (2.7), i.e., $\operatorname{span}\{Y^{(\ell)}, U^{(\ell)}\}$, is split into $\widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^{(\ell)}$ and $\widehat{\mathcal{Y}}^{(\ell)} + \widehat{\mathcal{U}}^{(\ell)}$, which are subsets of $\widetilde{\mathcal{Z}}$ and $\widehat{\mathcal{Z}}$, 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 $\operatorname{span}\{Y^{(\ell)}, U^{(\ell)}\}$ in (2.7), the update by (3.9) leads to less improvement in the 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 some vector iterations within (3.9) as well as an alternative quality parameter for $N \approx I$.

We first discuss the dimensions of the 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 ℓth step of (3.9) with the invariant subspaces $\widetilde{\mathcal{Z}}$ and $\widehat{\mathcal{Z}}$ for $j = s$ from Lemma 3.3. If*

$$\dim \widetilde{\mathcal{Y}}^{(\ell)} = i, \qquad \dim \widehat{\mathcal{Y}}^{(\ell)} = s - i,$$

and the smallest Ritz values $\widetilde{\theta}$, $\widehat{\theta}$ of H in $\widetilde{\mathcal{Y}}^{(\ell)}$, $\widehat{\mathcal{Y}}^{(\ell)}$ are larger than μ_{s+1}, then it holds for the subspaces $\widetilde{\mathcal{Y}}' = \operatorname{span}\{\widetilde{Y}^{(\ell+\frac{1}{2})}\}$ and $\widehat{\mathcal{Y}}' = \operatorname{span}\{\widehat{Y}^{(\ell+\frac{1}{2})}\}$, that

$$\dim \widetilde{\mathcal{Y}}' = i, \qquad \dim \widehat{\mathcal{Y}}' = s - i,$$

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and the smallest Ritz values $\widetilde{\theta}'$, $\widehat{\theta}'$ of H in $\widetilde{\mathcal{Y}}'$, $\widehat{\mathcal{Y}}'$ are also larger than μ_{s+1}. Moreover,

$$\dim(\widetilde{\mathcal{Y}}' + \widehat{\mathcal{Y}}') = s, \quad \widetilde{\mathcal{Y}}^{(\ell+1)} = \widetilde{\mathcal{Y}}', \qquad \text{and} \qquad \widehat{\mathcal{Y}}^{(\ell+1)} = \widehat{\mathcal{Y}}'. \tag{3.10}$$

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

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

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

$$\widetilde{\mathcal{Y}}^{(\ell+1)} = \operatorname{span}\{Y^{(\ell+1)}\} \cap \widetilde{\mathcal{Z}} = (\widetilde{\mathcal{Y}}' \cap \widetilde{\mathcal{Z}}) + (\widehat{\mathcal{Y}}' \cap \widetilde{\mathcal{Z}}) = \widetilde{\mathcal{Y}}'$$

holds according to

$$\begin{aligned}
&\widetilde{\mathcal{Y}}' \subseteq (\widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^{(\ell)}) \subseteq \widetilde{\mathcal{Z}} \quad \Rightarrow \quad \widetilde{\mathcal{Y}}' \cap \widetilde{\mathcal{Z}} = \widetilde{\mathcal{Y}}', \\
&\widehat{\mathcal{Y}}' \subseteq (\widehat{\mathcal{Y}}^{(\ell)} + \widehat{\mathcal{U}}^{(\ell)}) \subseteq \widehat{\mathcal{Z}} \quad \Rightarrow \quad \widehat{\mathcal{Y}}' \cap \widehat{\mathcal{Z}} = \widehat{\mathcal{Y}}' \\
&\qquad \Rightarrow \quad \widehat{\mathcal{Y}}' \cap \widetilde{\mathcal{Z}} = \widehat{\mathcal{Y}}' \cap \widehat{\mathcal{Z}} \cap \widetilde{\mathcal{Z}} = \widehat{\mathcal{Y}}' \cap \operatorname{span}\{z_{s+1}, \ldots, z_n\} = \{0\},
\end{aligned}$$

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

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 $\widetilde{\mathcal{Z}}$ and $\widehat{\mathcal{Z}}$ for $j = s$ from Lemma 3.3 and $\dim \operatorname{span}\{Y^{(0)}\} = s$. If the smallest (sth largest) Ritz value $\theta_s^{(0)}$ of H in $\operatorname{span}\{Y^{(0)}\}$ is larger than μ_{s+1}, then it holds for each ℓ that*

$$\dim \widetilde{\mathcal{Y}}^{(\ell)} = i, \qquad \dim \widehat{\mathcal{Y}}^{(\ell)} = s - i, \qquad \text{and} \qquad \dim \operatorname{span}\{Y^{(\ell+1)}\} = s.$$

The partial Rayleigh–Ritz approximations in the ℓth step actually produce the subspaces $\widetilde{\mathcal{Y}}^{(\ell+1)}$ and $\widehat{\mathcal{Y}}^{(\ell+1)}$.

Proof. Applying Lemma 3.3 to $\mathcal{Y} = \operatorname{span}\{Y^{(0)}\}$ implies $\dim \widetilde{\mathcal{Y}}^{(0)} = i$, $\dim \widehat{\mathcal{Y}}^{(0)} = s - i$ by the first two equalities in (3.7), whose assumption is verified by the fact that the smallest Ritz values $\widetilde{\theta}$ and $\widehat{\theta}$ of H in the subsets $\widetilde{\mathcal{Y}}^{(0)}$ and $\widehat{\mathcal{Y}}^{(0)}$ of $\operatorname{span}\{Y^{(0)}\}$ 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. ∎

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

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

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

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

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

Now we can focus on the first partial iteration in (3.9) and define certain vector iterations for characterizing the ith 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 $\widetilde{\theta}'$ the ith largest Ritz value of H in $\widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^{(\ell)}$. Then the following statements hold:*

(a) For each ℓ, the matrix $U^{(\ell)}$ has full rank, and $\dim \widetilde{\mathcal{U}}^{(\ell)} \geq i$.

(b) In the special case $N = I$, the subspace $\widetilde{\mathcal{U}}^{(\ell)}$ coincides with $H\widetilde{\mathcal{Y}}^{(\ell)}$, and there exists a nonzero vector $\widetilde{y} \in \widetilde{\mathcal{Y}}^{(\ell)}$ for which the largest Ritz value $\widetilde{\theta}^{\diamond}$ of H in $\operatorname{span}\{\widetilde{y}, H\widetilde{y}\}$ *does not exceed $\widetilde{\theta}'$.*

(c) In the general case $N \approx I$, consider an orthonormal matrix $\widetilde{U} \in \mathbb{C}^{n\times i}$ with $\operatorname{span}\{\widetilde{U}\} \subseteq \widetilde{\mathcal{U}}^{(\ell)}$, *and an orthonormal basis matrix $\widetilde{Y}$ of $\widetilde{\mathcal{Y}}^{(\ell)}$. Let $\mu(\cdot)$ be the Rayleigh quotient with respect to H. If the matrix $\widetilde{R} = H\widetilde{Y} - \widetilde{Y}\widetilde{Y}^*H\widetilde{Y}$ has full rank and*

$$\|(H\widetilde{Y} - \widetilde{U}\widetilde{U}^*H\widetilde{Y})(\widetilde{R}^*\widetilde{R})^{-1/2}\|_2 \leq \widetilde{\gamma} \qquad \text{for a certain } \widetilde{\gamma} < 1, \tag{3.11}$$

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

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

and the largest Ritz value $\widetilde{\theta}^{\diamond}$ of H in $\operatorname{span}\{\widetilde{y}, \widetilde{u}\}$ *does not exceed $\widetilde{\theta}'$.*

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

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

for matching the notation in [23, 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, $\dim \widetilde{\mathcal{U}}^{(\ell)} \geq i$ can be shown analogously to (3.6) in Lemma 3.3.

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

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

(where $\widetilde{\mathcal{Z}} = H\widetilde{\mathcal{Z}}$ is ensured by the positive definiteness of H). Following the property $\dim \widetilde{\mathcal{Y}}^{(\ell)} = i$ from Lemma 3.5 or Lemma 3.6, we use an arbitrary basis matrix $\widetilde{Y} \in \mathbb{C}^{n\times i}$ of $\widetilde{\mathcal{Y}}^{(\ell)}$ so that the subspace $\widetilde{\mathcal{U}}' = \widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^{(\ell)}$ can be represented by $\operatorname{span}\{\widetilde{Y}, H\widetilde{Y}\}$. We denote by t the dimension of $\widetilde{\mathcal{U}}'$ and by $V \in \mathbb{C}^{n\times t}$ a basis matrix of $\widetilde{\mathcal{U}}'$ whose columns $v_1, \ldots, v_t$

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are orthonormal Ritz vectors associated with the Ritz values $\varphi_1 \geq \cdots \geq \varphi_t$ of H in $\widetilde{\mathcal{U}}'$. Then we get the orthogonal projector $P = VV^*$ on $\widetilde{\mathcal{U}}'$ and the diagonal Ritz value matrix $V^*HV = \operatorname{diag}(\varphi_1, \ldots, \varphi_t)$. Moreover, the ith largest Ritz value $\widetilde{\theta}'$ of H in $\widetilde{\mathcal{U}}'$ is the largest Ritz value of H in $\widetilde{\mathcal{U}}^\diamond = \operatorname{span}\{v_i, \ldots, v_t\}$. Based on the dimension comparison

$$\dim(\widetilde{\mathcal{Y}}^{(\ell)} \cap \widetilde{\mathcal{U}}^\diamond) = \dim \widetilde{\mathcal{Y}}^{(\ell)} + \dim \widetilde{\mathcal{U}}^\diamond - \dim(\widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^\diamond) \geq i + (t - i + 1) - t = 1,$$

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

$$H\widetilde{y} = P(H\widetilde{y}) = PH(P\widetilde{y}) = VV^*HVV^*\widetilde{y} = V \operatorname{diag}(\varphi_1, \ldots, \varphi_t)\, V^*\widetilde{y}.$$

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

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

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

so that

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

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

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

where the second inequality uses the fact that $\widetilde{Y}\widetilde{Y}^*H\widetilde{Y}e$ is the orthogonal projection of $H\widetilde{Y}e$ on $\operatorname{span}\{\widetilde{Y}\}$. Thus (3.12) is fulfilled by $\widetilde{y} = \widetilde{Y}e$ and $\widetilde{u} = \widetilde{U}(\widetilde{U}^*H\widetilde{Y}e)$. Specific $\widetilde{y}$ and $\widetilde{u}$ possessing the additional property can be constructed analogously to the proof of [14, Theorem 3.2] (using Sion's-minimax theorem). Therein, the largest Ritz value $\widetilde{\theta}^\diamond$ of H in $\operatorname{span}\{\widetilde{y}, \widetilde{u}\}$ does not exceed the ith largest Ritz value $\widetilde{\theta}^\bullet$ of H in $\operatorname{span}\{\widetilde{Y}, \widetilde{U}\}$. Consequently, we get $\widetilde{\theta}^\diamond \leq \widetilde{\theta}^\bullet \leq \widetilde{\theta}'$ according to $\operatorname{span}\{\widetilde{Y}, \widetilde{U}\} \subseteq (\widetilde{\mathcal{Y}}^{(\ell)} + \widetilde{\mathcal{U}}^{(\ell)})$ and the Courant–Fischer principles. ∎

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

$$\widetilde{y}^\diamond \xleftarrow{\mathrm{RR}[H,1]} \operatorname{span}\{\widetilde{y}, H\widetilde{y}\} \tag{3.13}$$

for deriving an intermediate estimate. Since $\widetilde{y}$ and $H\widetilde{y}$ are contained in the invariant subspace $\widetilde{\mathcal{Z}}$, we adapt an estimate from [13, 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 $\widetilde{y}$ belongs to the invariant subspace $\widetilde{\mathcal{Z}}$ defined in Lemma 3.3 and $\mu(\widetilde{y})$ is located in the eigenvalue interval $(\mu_{j+1}, \mu_{j-s+i}]$, then it holds that*

$$\frac{\mu_{j-s+i} - \mu(\widetilde{y}^\diamond)}{\mu(\widetilde{y}^\diamond) - \mu_{j+1}} \leq \left(\frac{\tau_i}{2 - \tau_i}\right)^2 \frac{\mu_{j-s+i} - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \qquad \text{with} \quad \tau_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}. \tag{3.14}$$

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Proof. The iteration (3.13) is equivalent to

$$\widetilde{Z}^*\widetilde{y}^\diamond \xleftarrow{\mathrm{RR}[\widetilde{Z}^*H\widetilde{Z},1]} \operatorname{span}\{\widetilde{Z}^*\widetilde{y},\,(\widetilde{Z}^*H\widetilde{Z})\widetilde{Z}^*\widetilde{y}\}$$

with the orthonormal basis matrix $\widetilde{Z} = [z_1, \ldots, z_{j-s+i}, z_{j+1}, \ldots, z_n]$ of $\widetilde{\mathcal{Z}}$. Then, (3.14) is achieved by adapting [13, Theorem 4.1] to the matrix $\widetilde{Z}^*H\widetilde{Z}$ and the corresponding Rayleigh quotient $\widetilde{\mu}(\cdot)$ together with simple reformulations based on

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

for arbitrary nonzero vectors w from $\widetilde{\mathcal{Z}}$. ∎

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

$$\widetilde{y}^\diamond \xleftarrow{\mathrm{RR}[H,1]} \operatorname{span}\{\widetilde{y},\widetilde{u}\} \tag{3.15}$$

suggested by the statement (c) in Theorem 3.7. The derivation is essentially based on [12].

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 $\widetilde{y}$ and $\widetilde{u}$ belong to the invariant subspace $\widetilde{\mathcal{Z}}$ defined in Lemma 3.3 and satisfy the condition (3.12) with a certain $\widetilde{\gamma} \in [0,1)$ and $\mu(\widetilde{y})$ is located in the eigenvalue interval $(\mu_{j+1}, \mu_{j-s+i}]$, then it holds that*

$$\frac{\mu_{j-s+i} - \mu(\widetilde{y}^\diamond)}{\mu(\widetilde{y}^\diamond) - \mu_{j+1}} \le \left(\frac{\tau_i + \widetilde{\gamma}\,(2-\tau_i)}{(2-\tau_i) + \widetilde{\gamma}\,\tau_i}\right)^2 \frac{\mu_{j-s+i} - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{j+1}} \quad \text{with} \quad \tau_i = \frac{\mu_{j+1} - \mu_n}{\mu_{j-s+i} - \mu_n}. \tag{3.16}$$

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

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

The condition (3.12) can be reformulated as

$$\|\widetilde{H}\check{y} - \check{u}\|_2 \le \widetilde{\gamma}\,\|\widetilde{H}\check{y} - \widetilde{\mu}(\check{y})\check{y}\|_2$$

since $\|w\|_2 = \|\widetilde{Z}\widetilde{Z}^*w\|_2 = \|\widetilde{Z}^*w\|_2$ holds for arbitrary $w \in \widetilde{\mathcal{Z}}$. Thus, $\check{u}$ belongs to a ball $\mathcal{B}_{\widetilde{\gamma},\check{y}}$ centered at $\widetilde{H}\check{y}$ with the radius $\widetilde{\gamma}\,\|\widetilde{H}\check{y} - \widetilde{\mu}(\check{y})\check{y}\|_2$. Then the trial subspace $\operatorname{span}\{\check{y},\check{u}\}$ is characterized by a cone as in [12, Section 2] so that the geometric analysis therefrom is applicable. Adapting [12, Theorem 2.2] yields (3.16). ∎

4. Main results. The analysis of the auxiliary iteration (3.9) via vector iterations from Section 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.

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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 $\mu_1 \geq \cdots \geq \mu_n$. 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 $\operatorname{span}\{Y^{(\ell)}\}$, 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 $\operatorname{span}\{Y^{(0)}\}$ together with the invariant subspaces $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{i+1}, \dots, z_s\}^\perp$ and $\widehat{\mathcal{Z}} = \operatorname{span}\{z_1, \dots, z_i\}^\perp$. Then,

$$\dim \widetilde{\mathcal{Y}}^{(\ell)} = i \qquad \text{and} \qquad \dim \widetilde{\mathcal{U}}^{(\ell)} \geq i \qquad \text{hold for each } \ell.$$

Moreover, consider an orthonormal matrix $\widetilde{U} \in \mathbb{C}^{n \times i}$ with $\operatorname{span}\{\widetilde{U}\} \subseteq \widetilde{\mathcal{U}}^{(\ell)}$ and an orthonormal basis matrix $\widetilde{Y}$ of $\widetilde{\mathcal{Y}}^{(\ell)}$, and let $\mu(\cdot)$ be the Rayleigh quotient with respect to H. If the matrix $\widetilde{R} = H\widetilde{Y} - \widetilde{Y}\widetilde{Y}^* H\widetilde{Y}$ has full rank and

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

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

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

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 $\operatorname{span}\{Y^{(0)}\}$ together with the invariant subspaces $\widetilde{\mathcal{Z}} = \operatorname{span}\{z_{j-s+i+1}, \dots, z_j\}^\perp$ and $\widehat{\mathcal{Z}} = \operatorname{span}\{z_{j-s+1}, \dots, z_{j-s+i}\}^\perp$. Assume for each ℓ that $\dim \operatorname{span}\{Y^{(\ell)}\} = s$, $\dim \widetilde{\mathcal{Y}}^{(\ell)} = i$, and $\dim \widehat{\mathcal{Y}}^{(\ell)} = s - i$. Then,

$$\dim \widetilde{\mathcal{U}}^{(\ell)} \geq i,$$

and a similar estimate for (2.7) reads

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

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

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

If $\operatorname{span}\{Y^{(\ell)}\}$ contains no eigenvectors, then we use [23, Lemma 3.1], where $U^{(\ell)}$ is analyzed within a BPG iteration with fixed step sizes. This implies

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

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

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

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

$$\frac{\mu_i - \widetilde{\theta}^{\diamond}}{\widetilde{\theta}^{\diamond} - \mu_{s+1}} \leq \left(\frac{\tau_i + \widetilde{\gamma}\,(2-\tau_i)}{(2-\tau_i) + \widetilde{\gamma}\,\tau_i}\right)^2 \frac{\mu_i - \mu(\widetilde{y})}{\mu(\widetilde{y}) - \mu_{s+1}} \qquad \text{with} \quad \tau_i = \frac{\mu_{s+1} - \mu_n}{\mu_i - \mu_n},$$

which can be extended as

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

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

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

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

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. □

REMARK 4.2. Theorem 4.1 extends the estimates for a BPG iteration with fixed step sizes from [23, Theorem 3.2 and Theorem 3.3] to the iteration (2.7) with implicitly optimized step sizes. The statement (a) indicates that the ith Ritz value strictly increases until some eigenvectors are enclosed by the subspace iterate. In addition, a reformulation of [14, (3.7)] leads to the sharp estimate

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

for the sth 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, then we can reset the index ℓ to 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 ith Ritz value in the first steps of (2.7). The assumption on the subspace dimensions is usually fulfilled in numerical tests with randomly generated initial guesses.

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

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

which is similar to (4.1) with $i = s$. These two estimates for the sth Ritz value in the final phase of (2.7) only differ in the quality parameters γ and $\widetilde{\gamma}$. We also note that $\theta_s^{(0)}$ cannot be replaced by $\theta_i^{(0)}$ in (4.1) and (4.2); cf. a counterexample in [22, Section 3] corresponding to the BPG iteration with exact-inverse preconditioning.

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REMARK 4.4. In comparison to the results from [15], our multi-step estimate (4.1) indicates that the single-step convergence rate is asymptotically bounded by the factor $\widetilde{q}_i^2$ with $\widetilde{q}_i = \big(\tau_i + \widetilde{\gamma}\,(2-\tau_i)\big)/\big((2-\tau_i) + \widetilde{\gamma}\,\tau_i\big)$ similarly to the asymptotic convergence factor $q_{k,m}$ presented in [15, Corollary 1] (despite a typo with a redundant exponent 2). If adapted to Theorem 4.1 (with $k \to i$ and $m \to s$), then $q_{k,m}$ becomes

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

which is slightly larger than $\widetilde{q}_i$ for $\widetilde{\gamma} = \gamma$. However, the nonasymptotic estimate in [15, 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 [15, 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 $\tau = \mu_{s+1}/\mu_i$ (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 $\widetilde{\gamma}$. The convergence rates of the 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). As an analytic tool, the auxiliary iteration (3.9) is transformed into (4.4) to define a suitable quality parameter of preconditioning.

THEOREM 4.5. *Consider the generalized eigenvalue problem (1.9) 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 $\operatorname{span}\{V^{(\ell)}\}$ of (2.3). Therein, $\Theta_V^{(\ell)} = \operatorname{diag}(\theta_1^{(\ell)}, \dots, \theta_s^{(\ell)})$, $R_V^{(\ell)} = MV^{(\ell)} - AV^{(\ell)}\Theta_V^{(\ell)}$, and the preconditioner $\widetilde{T}$ 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 $\operatorname{span}\{V^{(\ell)}\}$, then $\theta_i^{(\ell+1)} > \theta_i^{(\ell)}$.

(b) If $\theta_s^{(0)} > \mu_{s+1}$, consider the auxiliary iteration

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

using the same initial subspace $\operatorname{span}\{V^{(0)}\}$ together with the invariant subspaces $\widetilde{\mathcal{W}} = \operatorname{span}\{w_{i+1}, \dots, w_s\}^{\perp_A}$ and $\widehat{\mathcal{W}} = \operatorname{span}\{w_1, \dots, w_i\}^{\perp_A}$. Then,

$$\widetilde{i} = \dim \widetilde{\mathcal{V}}^{(\ell)} = i \quad \text{and} \quad \dim \widetilde{\mathcal{U}}^{(\ell)} \geq i \qquad \text{hold for each } \ell.$$

Moreover, consider an A-orthonormal matrix $\widetilde{U} \in \mathbb{C}^{n\times i}$ with $\operatorname{span}\{\widetilde{U}\} \subseteq \widetilde{\mathcal{U}}^{(\ell)}$ 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 the matrix $\widetilde{R} = A^{-1}M\widetilde{V} - \widetilde{V}\widetilde{V}^*M\widetilde{V}$ 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).

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(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* $\operatorname{span}\{V^{(0)}\}$ *together with the invariant subspaces* $\widetilde{\mathcal{W}} = \operatorname{span}\{w_{j-s+i+1}, \dots, w_j\}^{\perp_A}$ *and* $\widehat{\mathcal{W}} = \operatorname{span}\{w_{j-s+1}, \dots, w_{j-s+i}\}^{\perp_A}$. *Assume for each* ℓ *that* $\dim \operatorname{span}\{V^{(\ell)}\} = s$, $\widetilde{i} = \dim \widetilde{\mathcal{V}}^{(\ell)} = i$, *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 explicitly extends our analysis of the block preconditioned steepest descent iteration from [14]. Therein, we consider the computation of the smallest eigenvalues of the matrix pair (A, M) for Hermitian positive definite matrices $A, M \in \mathbb{C}^{n\times n}$. The estimate (4.2) turns into

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

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:

$$\begin{aligned}
&\operatorname{span}\{\widetilde{V}^{(\ell)}\} = \operatorname{span}\{V^{(\ell)}\} \cap \widetilde{\mathcal{W}}, && \widetilde{V}^{(\ell+\frac{1}{2})} \xleftarrow{\mathrm{RR}[M,A,\widetilde{i}]} \operatorname{span}\{\widetilde{V}^{(\ell)}, TR_{\widetilde{V}}^{(\ell)}\},\\
&\operatorname{span}\{\widehat{V}^{(\ell)}\} = \operatorname{span}\{V^{(\ell)}\} \cap \widehat{\mathcal{W}}, && \widehat{V}^{(\ell+\frac{1}{2})} \xleftarrow{\mathrm{RR}[M,A,\widehat{i}]} \operatorname{span}\{\widehat{V}^{(\ell)}, TR_{\widehat{V}}^{(\ell)}\},\\
&V^{(\ell+1)} \xleftarrow{\mathrm{RR}[M,A,\widetilde{s}]} \operatorname{span}\{\widetilde{V}^{(\ell+\frac{1}{2})}, \widehat{V}^{(\ell+\frac{1}{2})}\},
\end{aligned} \tag{4.5}$$

where R denotes block residuals. In the case $\widetilde{i} = \dim \operatorname{span}\{\widetilde{V}^{(\ell)}\} = 1$, the first partial iteration in (4.5) is a vectorial gradient iteration. A geometric relation between two successive iterates $\widetilde{v}$ and $\widetilde{v}'$ can be derived based on [12, Theorem 3.1], namely, there is a rational function $f(\cdot)$ satisfying $\widetilde{v}^{\diamond} = f(A^{-1}M)\widetilde{v}$ and $\mu(\widetilde{v}') \geq \mu(\widetilde{v}^{\diamond})$. Moreover, $\widetilde{v}^{\diamond}$ can be regarded as the next iterate generated by a special preconditioner $T^{\diamond}$. Therefore, the convergence of the largest Ritz value in (4.5) is decelerated by using such $T^{\diamond}$. The corresponding first partial iteration can be simplified since $\operatorname{span}\{\widetilde{V}^{(\ell+\frac{1}{2})}\} \subseteq \widetilde{\mathcal{W}}$ is ensured by $\widetilde{v}^{\diamond} = f(A^{-1}M)\widetilde{v}$. 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 essentially due to differences between the eigenspaces of (M, A) and those of the preconditioner (except for polynomial preconditioning). Occasionally, we can apply the estimate with γ for $i = 1$ similarly to a deflation, i.e., analyzing the convergence rate of the $(i+1)$st Ritz value provided that the first i Ritz values are sufficiently close to the target eigenvalues.

5. Numerical experiments. We demonstrate the main results and discuss their accuracy by several numerical examples. In the first example, we implement the accompanying iteration (2.7) (using the symbol N for preconditioners) for a test matrix from [23] and illustrate Theorem 4.1. The further examples, using discretized Laplacian eigenvalue problems, are concerned with the BPG iteration (2.3) (with the symbol $\widetilde{T}$ for preconditioners) and Theorem 4.5.

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Example I. We reuse the diagonal matrix $H = \operatorname{diag}(\mu_1, \ldots, \mu_n)$ from [23, Exp. I] with $n = 6000$ and $\mu_i = 10.07 - 0.01\,i$, for $i \le 6$. 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 $\mu_1, \ldots, \mu_s$ 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=eta*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 $\mu_i - \theta_i^{(\ell)}$, $i \in \{1, \ldots, 6\}$, by solid curves in Figure 5.1. This immediately reflects the monotone convergence stated in Theorem 4.1(a).

For verifying Theorem 4.1(b), we determine the quality parameter $\widetilde{\gamma}$ 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 $\widetilde{\gamma}$ in the estimate (4.1) with an index adaptation. Therein,

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

The resulting bounds for $\mu_i - \theta_i^{(\ell)}$ are displayed by dashed curves in Figure 5.1. In addition, their counterparts based on the single-step estimates from [14], i.e.,

$$\frac{\mu_i - \theta_i^{(L)}}{\theta_i^{(L)} - \mu_{i+1}} \le \left(\frac{\widehat{\tau}_i + \widetilde{\gamma}\,(2 - \widehat{\tau}_i)}{(2 - \widehat{\tau}_i) + \widetilde{\gamma}\,\widehat{\tau}_i} \right)^{2L} \frac{\mu_i - \theta_i^{(0)}}{\theta_i^{(0)} - \mu_{i+1}} \qquad \text{with} \quad \widehat{\tau}_i = \frac{\mu_{i+1} - \mu_n}{\mu_i - \mu_n}, \tag{5.1}$$

are displayed by dotted curves. Therein, the numerical values of $\widetilde{\gamma}$ are slightly smaller than those of γ from (2.2). Thus, the bounds by (5.1) with γ instead of $\widetilde{\gamma}$ are at most as good as the bounds in dotted curves.

These two types of curves coincide for $i = s = 6$. The difference between them is substantial for $i \in \{1, \ldots, 5\}$ due to $\mu_i \approx \mu_{i+1}$. The dashed curves clearly reflect the cluster robustness, whereas the dotted curves wrongly predict a stagnation. Furthermore, the accuracy of bounds in the 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.

Theorem 4.1(c) can be verified 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 square domain $[0, 1]^2$ with homogeneous Dirichlet boundary conditions. The discretization matrix A using a five-point star is a well-know block tridiagonal matrix. We use A of size $n = 10000$ and $M = I$ for setting up (1.9). The six largest eigenvalues of (M, A) approximate the reciprocals of $\alpha\pi^2$ for $\alpha \in \{2, 5, 5, 8, 10, 10\}$.

The BPG iteration (2.3) with the block size $s = 6$ is implemented for three preconditioners $\widetilde{T} \in \{T_1, T_2, T_3\}$ by `ichol(A,struct('type','ict','droptol',eta))`, for $\eta \in \{10^{-5}, 10^{-4}, 10^{-3}\}$. Similarly to Example I, the Ritz value errors in the slowest run concerning 1000 random initial subspaces are illustrated by solid curves in Figure 5.2.

We particularly demonstrate Theorem 4.5(b). Therein, the quality parameter $\widetilde{\gamma}$ in (4.1) is determined for each iteration step after $\theta_s^{(\ell)} > \mu_{s+1}$ by using the auxiliary iteration (4.4). The respective maxima are

$$\widetilde{\gamma} \approx 0.0931 \ \text{ for } T_1, \qquad \widetilde{\gamma} \approx 0.4325 \ \text{ for } T_2, \qquad \widetilde{\gamma} \approx 0.5595 \ \text{ for } T_3.$$

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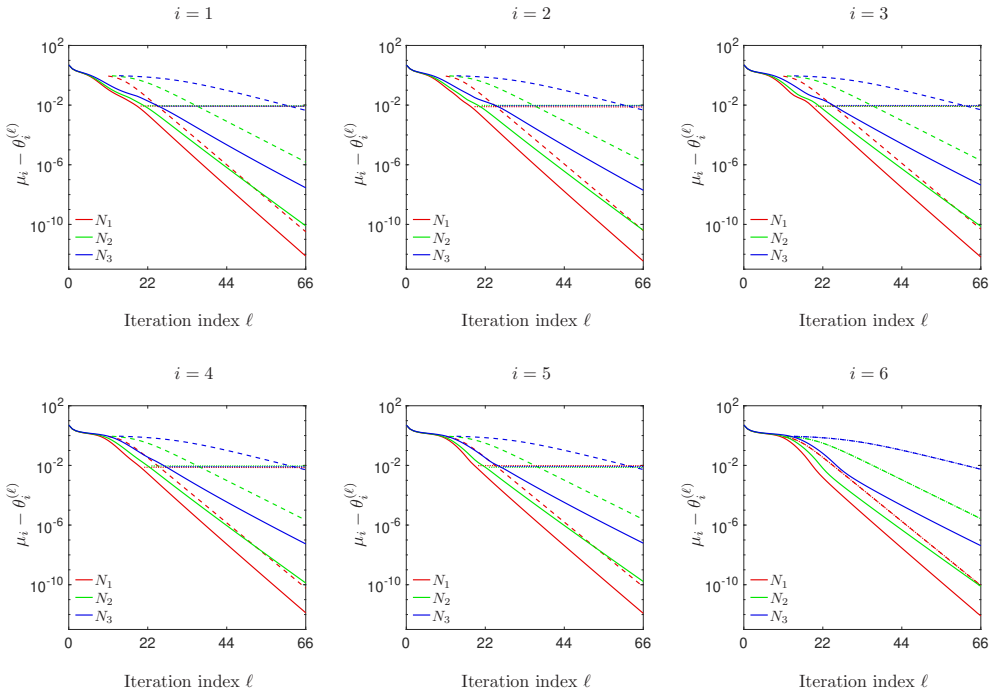

FIG. 5.1. *Cluster robustness of the accompanying iteration (2.7) applied to Example I. Solid curves: Ritz value errors in the slowest run among 1000 runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.1. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.*

The resulting bounds in dashed curves are appropriate for each Ritz value. Their counterparts by (5.1) in dotted curves are mostly reasonable for $i \in \{1,\, 3,\, 4,\, 6\}$, where μ_i and μ_{i+1} are not clustered and the bounds are more accurate in the first steps. Moreover, the dotted curves cannot be drawn for $i \in \{2,\, 5\}$ since the distance ratio in (5.1) is degenerate due to $\mu_i = \mu_{i+1}$.

Furthermore, the estimate (4.1) implies a less accurate alternative

$$\mu_t - \theta_t^{(L)} \le \left(\frac{\tau_i + \widetilde{\gamma}\,(2 - \tau_i)}{(2 - \tau_i) + \widetilde{\gamma}\,\tau_i} \right)^{2L} \frac{\mu_t - \theta_s^{(0)}}{\theta_s^{(0)} - \mu_{s+1}}\,(\mu_t - \mu_{s+1}), \qquad \text{for } t \in \{1, \ldots, i\}, \tag{5.2}$$

and further a multi-step estimate for $\sum_{t=1}^{i}(\mu_t - \theta_t^{(L)})$, which can asymptotically be compared with [15, Theorem 3]. Figure 5.3 presents a comparison between the corresponding single-step convergence factors by using the same data as in Figure 5.2. The convergence factor from (5.2) does not depend on the iterates and is thus constant; see the dashed lines. In contrast, the convergence factor from [15, Theorem 3] contains some variable terms which cause overestimations in the first steps; see the dotted curves.

Subsequently, we repeat the numerical experiments from Figure 5.2 for some clustered eigenvalues. 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 (1.9) for $n = 9534$ and $M = I$. The six largest eigenvalues build two tight clusters $\{\mu_1, \mu_2\}$ and $\{\mu_3, \ldots, \mu_6\}$. We construct preconditioners T_1, T_2, T_3 by `ichol` as mentioned above. The quality parameter reads

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

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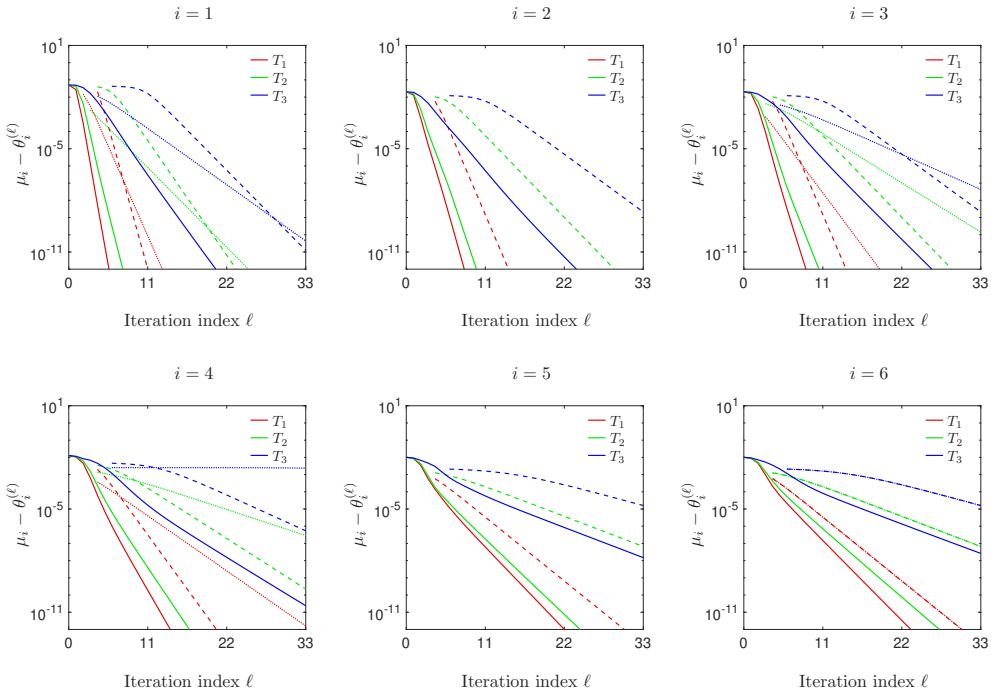

FIG. 5.2. *Cluster robustness of the BPG iteration (2.3) applied to the Laplacian eigenvalue problem on a square domain in Example II. Solid curves: Ritz value errors in the slowest run among* 1000 *runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.5. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.*

The comparison in Figure 5.4 indicates again the advantage of the bounds by Theorem 4.5, displayed in dashed curves. Their counterparts (5.1) in dotted curves are only reasonable for $i \in \{2,\ 6\}$, where μ_i and μ_{i+1} are not clustered. Moreover, the dotted curves vanish for $i = 5$ since μ_5 and μ_6 coincide.

Example III. We consider the Laplacian eigenvalue problem on a 2D tulip-like domain with homogeneous Dirichlet boundary conditions; see Figure 5.5. The boundary consists of three parts:

$$\Gamma_1 = \big\{\big(1.2\sin(t) + 0.3\sin(4t),\ -\cos(t) - 0.5\cos(2t)\big)^T;\ t \in [-\pi,\ \pi)\big\},$$
$$\Gamma_2 = \big\{\big(0,\ 0.5\,t\big)^T;\ t \in (0,\ 1)\big\}, \qquad \Gamma_3 = \big\{\big(0,\ 0.5(1-t)\big)^T;\ t \in (0,\ 1]\big\}.$$

We generate matrix eigenvalue problems successively by an adaptive finite element discretization depending on the residuals of approximate eigenfunctions associated with the three smallest operator eigenvalues; cf. [23, Appendix] and some relevant graphics in Figure 5.5. We repeat the numerical experiments from Figure 5.2 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 block size $s = 6$. The target eigenvalues are partially clustered ($\mu_2 \approx \mu_3$). Concerning the comparison between the new result (4.1) and a previous result reformulated in (5.1), we first compare their decisive terms τ_i and $\widehat{\tau}_i$. For

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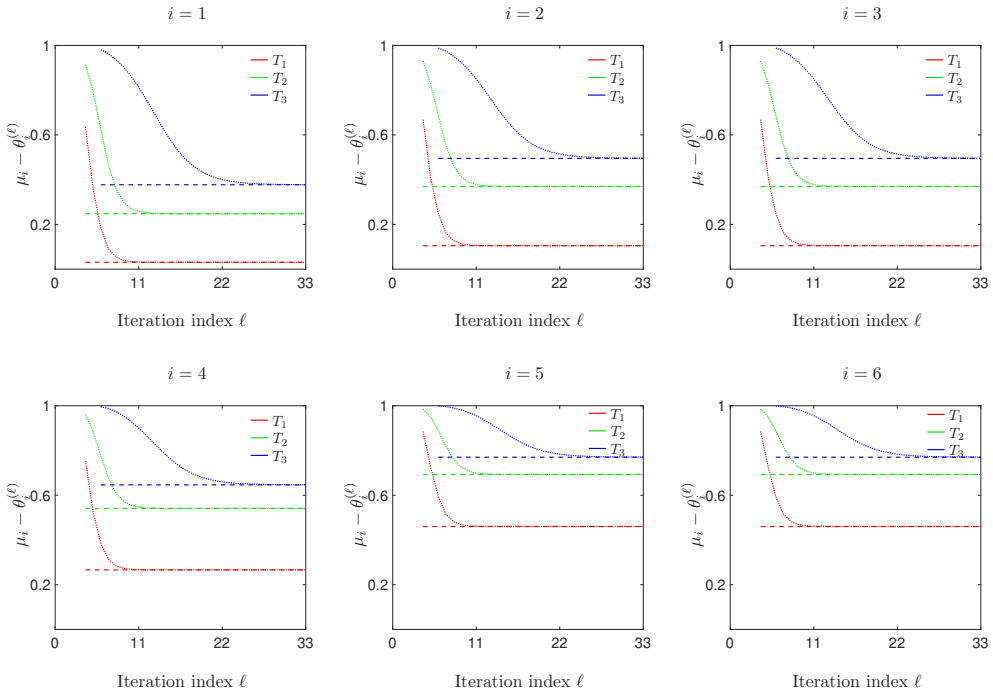

FIG. 5.3. *Comparison between convergence factors in two sumwise estimates using data from Figure 5.2. Dashed lines: Convergence factors based on Theorem 4.5. Dotted curves: Convergence factors based on [15, Theorem 3].*

$i \in \{1, \ldots, 6\}$, we have

$$\begin{aligned} \tau_i &\in \{0.1993,\ 0.4628,\ 0.4687,\ 0.6279,\ 0.7307,\ 0.9459\}, \\ \widehat{\tau}_i &\in \{0.4306,\ 0.9875,\ 0.7464,\ 0.8593,\ 0.7725,\ 0.9459\}. \end{aligned} \tag{5.3}$$

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 $\widetilde{\gamma}$ with respect to the auxiliary iteration (4.4) reads

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

Figure 5.6 presents a bound comparison for the Ritz value errors in the slowest run concerning 1000 random initial subspaces. The dashed curves display the new bounds by (4.1). They generally have steeper slopes than the dotted curves containing bounds by (5.1). The slope difference mainly depends on the terms τ_i and $\widehat{\tau}_i$; cf. their values given in (5.3). The maximal difference appears for $i = 2$, where the dotted curves are almost constant. As an explanation, we note that the corresponding τ-value $\widehat{\tau}_2 \approx 0.9875$ is close to 1, and the convergence factor is at least $\widehat{\tau}_2/(2 - \widehat{\tau}_2)$ for each test preconditioner. Such an overestimation can also be caused by a slightly smaller τ-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 $\widehat{\tau}_4$ (dotted), τ_6, and $\widehat{\tau}_6$ (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 $\widetilde{\gamma} < 0.5$, is costly with respect to inner steps and the total time.

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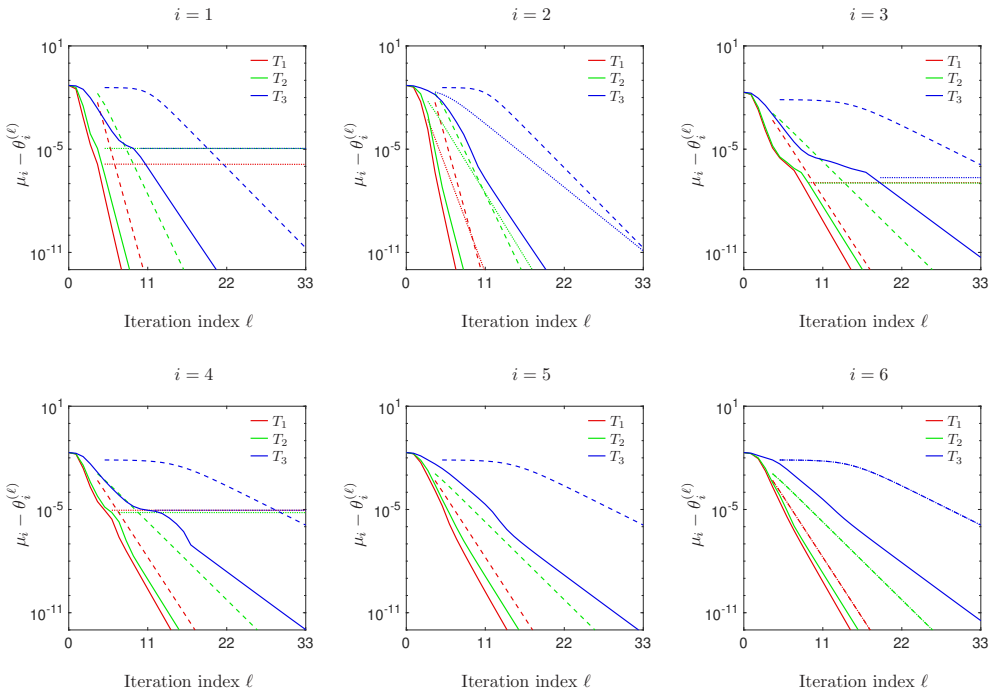

FIG. 5.4. *Cluster robustness of the BPG iteration (2.3) applied to the Laplacian eigenvalue problem on a rectangle domain in Example II. Solid curves: Ritz value errors in the slowest run among* 1000 *runs with random initial subspaces. Dashed curves: Bounds determined by Theorem 4.5. Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.*

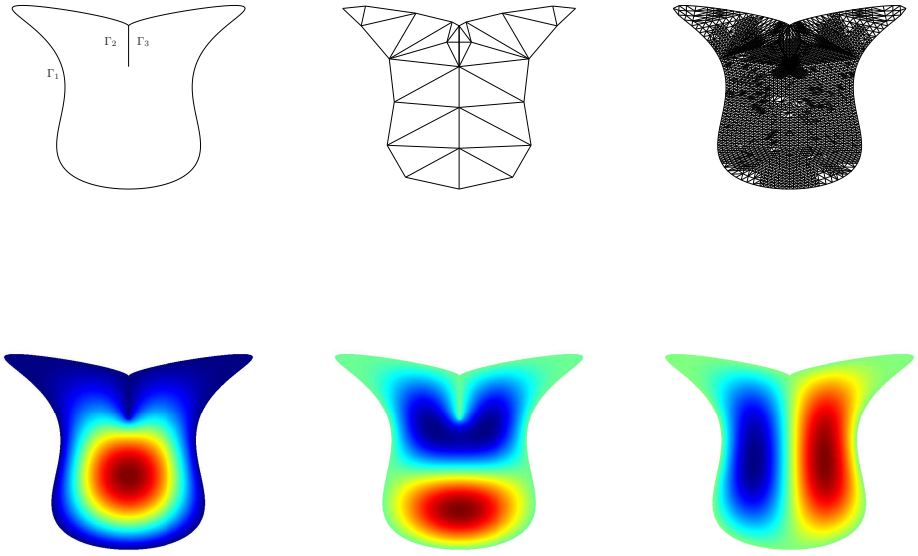

FIG. 5.5. *Laplacian eigenvalue problem for Example III. First row: domain, initial grid, and an adaptively refined grid. Second row: approximate eigenfunctions (top view) associated with the three smallest operator eigenvalues whose residuals are used for the grid refinement.*

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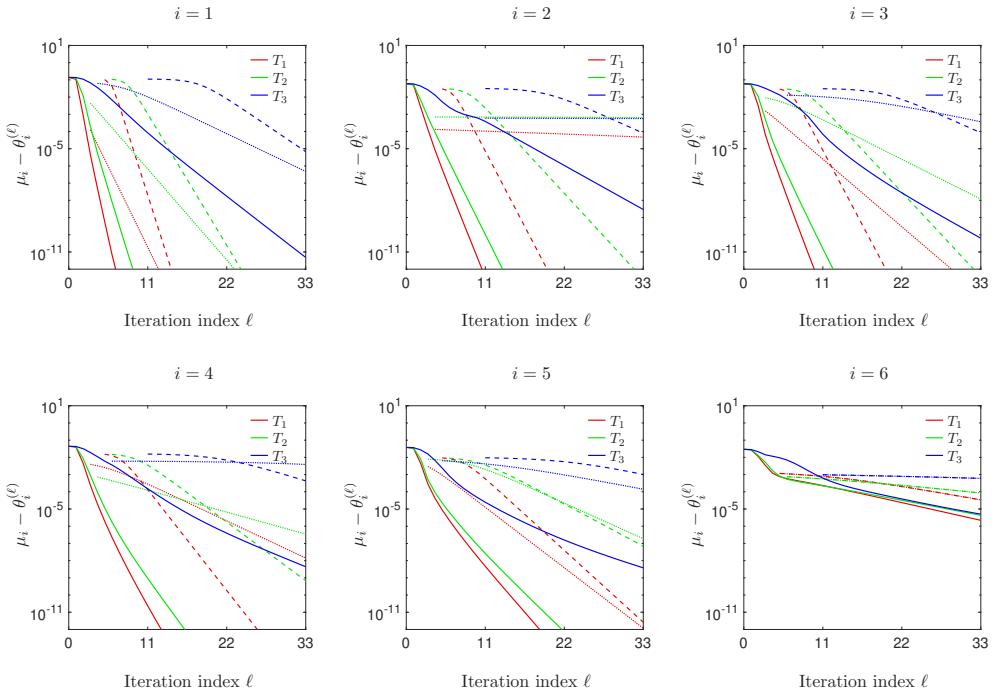

FIG. 5.6. *Cluster robustness of the BPG iteration* (2.3) *applied to Example III. Solid curves: Ritz value errors in the slowest run among* 1000 *runs with random initial subspaces. Dashed curves: Bounds determined by Theorem* 4.5. *Dotted curves: Bounds based on single-step estimates with neighboring eigenvalues.*

6. Conclusion. The cluster robustness of block preconditioned gradient (BPG) eigensolvers with sufficiently large block sizes is studied by deriving concise convergence bounds of the individual Ritz values. A basic argument in our analysis is that the Rayleigh–Ritz (RR) approximation in the trial 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 [6]. The previous analysis [23] 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, 15]. This approach is upgraded in the present paper by adapting some geometric arguments from our analysis of the (block) preconditioned steepest descent iteration [12, 14]. The achieved multi-step estimates improve the sumwise estimates from [15] 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 [19, 20, 21]. Extending our analysis of BPG to more powerful eigensolvers is desirable in our future research. The first step would be a thorough analysis of the single-vector version of LOBPCG by comparing it to a nonrestarted Davidson iteration. The advantage of the CG-like extension of the trial subspace

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by previous iterates would be more deeply investigated based on the first observations in [7] and also the similar topic "global quasi optimality" [21] for restarted Davidson methods.

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