Dominant subspace and low-rank approximations from block Krylov subspaces without a prescribed gap

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Abstract

We develop a novel convergence analysis of the classical deterministic block Krylov methods for the approximation of h-dimensional dominant subspaces and low-rank approximations of matrices $A \in \mathbb{K}^{m \times n}$ (where $\mathbb{K} = \mathbb{R}$ or \mathbb{C}) in the case that there is no singular gap at the index h i.e., if $\sigma_h = \sigma_{h+1}$ (where $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$ denote the singular values of A, and $p = \min\{m, n\}$). Indeed, starting with a (deterministic) matrix $X \in \mathbb{K}^{n \times r}$ with $r \geq h$ satisfying a compatibility assumption with some h-dimensional right dominant subspace of A, we show that block Krylov methods produce arbitrarily good approximations for both problems mentioned above. Our approach is based on recent work by Drineas, Ipsen, Kontopoulou and Magdon-Ismail on the approximation of structural left dominant subspaces. The main difference between our work and previous work on this topic is that instead of exploiting a singular gap at the prescribed index h (which is zero in this case) we exploit the nearest existing singular gaps.

Keywords. Dominant subspaces, low-rank approximation, singular value decomposition, principal angles.

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1 Introduction

Low-rank matrix approximation is a central problem in numerical linear algebra (see [21]). It is well known that truncated singular value decompositions (SVDs) of a matrix $A \in \mathbb{K}^{m \times n}$ (for $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$) produce optimal solutions to this problem ([2, 11, 15, 21]). Indeed, let $A = U\Sigma V^*$ be a SVD and let $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$ be the singular values of A, where $p = \min\{m, n\}$. Given $1 \leq h \leq \operatorname{rank}(A)$, recall that a truncated SVD of A is given by $A_h = U_h \Sigma_h V_h^*$, where the columns of U_h and V_h are the top h columns of U and V, respectively, and Σ_h is the diagonal matrix with main diagonal given by $\sigma_1, \ldots, \sigma_h$. In this case, we have that $||A - A_h||_{2,F} \leq ||A - B||_{2,F}$ for every $B \in \mathbb{K}^{m \times n}$ with $\operatorname{rank}(B) \leq h$, where $||\cdot||_{2,F}$ stand for spectral and Frobenius norms respectively. Nevertheless, it is well known that (in general) computation of a SVD of a matrix is expensive. This motivates the efficient numerical computation of approximations of truncated SVDs of matrices [6, 12, 13, 20, 21, 26, 27].

A closer look at the optimal approximations shows that they can be described as $A_h = P_h A$, where $P_h \in \mathbb{K}^{m \times m}$ is the orthogonal projection onto the range $R(U_h) = \mathcal{U}_h$, spanned by the top h columns of U. Hence, one of the main strategies for computing low-rank approximations is the computation of convenient h-dimensional subspaces $\mathcal{T} \subset \mathbb{K}^m$ and considering the corresponding low rank approximations. There are several methods for the efficient computation of low-rank approximations of the form PA for an orthogonal projection $P \in \mathbb{K}^{m \times m}$, based on the construction

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of convenient h-dimensional subspaces $R(P) = \mathcal{T}$ (equivalently, orthonormal sets of h vectors). Among others, implementations of the subspace iteration (or block power) and block Krylov methods have become very popular [6, 11, 12, 20, 21, 22, 26]. Yet, even if PA is a good low-rank approximation of A (that is, if $||PA - A||_2 \approx \sigma_{h+1}$), PA and A might not share some other features. For example, the singular values $\sigma_i(PA)$ and $\sigma_i(A)$ might be quite different for some $1 \leq i \leq h$. It could also be the case that the range $R(PA) \subset \mathbb{K}^m$ is not close to any h-dimensional left dominant subspace $\mathcal{U}_h \subset \mathbb{K}^m$ of A; here, the distance between subspaces is measured in terms of the principal angles between them (see [20]). Thus, to derive low-rank approximations that share some other features with A, it seems natural to consider first the construction of subspaces \mathcal{T} that are close to the subspaces \mathcal{U}_h . Once this is achieved, these subspaces can be used to construct approximated truncated SVDs of the form PA that do share some other features with A. Moreover, the subspaces \mathcal{T} themselves are also relevant in the study of principal component analysis [16] (since they are approximations of the principal components \mathcal{U}_h) and for the estimation of the leverage scores for the construction of CUR decompositions (see the recent survey [4] and the references therein).

As opposed to the low-rank approximation problem of the matrix A (see [5]), the singular gap $\sigma_h - \sigma_{h+1} \geq 0$ plays a role in the approximation of the h-dimensional left dominant subspace \mathcal{U}_h of A. Indeed, if the singular gap is positive then the condition number of computing the (uniquely determined) left dominant subspace \mathcal{U}_h of A depends (up to small factors) on the inverse of the singular gap $(\sigma_h - \sigma_{h+1})^{-1}$, irrespectively of the method being used to approximate \mathcal{U}_h (see [24, 25]). This fact is reflected in the convergence analysis of deterministic iterative methods used to compute approximations of \mathcal{U}_h , as those considered in [6, 22, 26]; indeed, in the deterministic setting, the upper bounds for the principal angles between \mathcal{U}_h and its approximations obtained in the previous works become arbitrarily large as the singular gap $\sigma_h - \sigma_{h+1} > 0$ tends to 0. Furthermore, in case the singular gap is zero then we get an infinite family of h-dimensional left dominant subspaces of A; this introduces a new problem, that is *choosing* a convenient h-dimensional left dominant subspace of A to approximate.

The previous facts could lead us to believe that the problem of approximating h-dimensional left dominant subspaces of A when the singular gap $\sigma_h - \sigma_{h+1} = 0$ is not well posed for its analysis in the deterministic setting. In this manuscript, we challenge this belief for the block Krylov iterative method. Indeed, in case $\sigma_h = \sigma_{h+1}$ we show that the existence of infinitely many h-dimensional left dominant subspaces of A can be used to our advantage, by developing a method for choosing a convenient such dominant subspace that is close to the subspace obtained by the block Krylov method. To do this we adapt some of the main ideas of [6], to deal with the approximation of left dominant subspaces. Indeed, we consider a starting guess matrix $X \in \mathbb{K}^{n \times r}$ that satisfies some compatibility assumptions with A, which can always be achieved even with r = h (i.e., for a minimal choice of r). Our approach is based on enclosing $\sigma_j > \sigma_{j+1} = \sigma_h = \sigma_k > \sigma_{k+1}$ in such a way that j < h and $k \ge h$ are the nearest indices for which there are singular gaps. These gaps appear explicitly in the upper bounds related to our convergence analysis of block Krylov methods. In this context, we show that block Krylov subspaces produce arbitrarily good hdimensional approximations of conveniently chosen left and right h-dominant subspaces. Moreover, we show that block Krylov spaces can also be used to compute arbitrarily good approximations of Aof rank at most h that share some other features with A, even when the singular gap $\sigma_h - \sigma_{h+1} = 0$ (see Section 2.4 for a detailed description of the problems mentioned above). Thus, our results complement the convergence analysis in [6]. Besides the fact that the no singular gap case is of interest (due to the common occurrence of repeated singular values in applications with some degree of symmetry), we believe that our approach to the convergence analysis of block Krylov iterative methods can be extended in different directions, not only to cover the convergence analysis of other methods but also to allow for a more general understanding of subspace approximation problems (e.g. for clustered singular values).

The paper is organized as follows. In Section 2 we recall the notions of principal angles between subspaces, dominant subspaces and their relation to SVDs and we describe the context and main

problems considered in this work. In Section 3 we state our main results on h-dimensional dominant subspace approximations (Section 3.1) and low-rank approximations by matrices of rank h (Section 3.2) when there is no singular gap at the index h. At the end of Section, we include some discussion on how is that our approach can be adapted to deal with more general situations (such as the clustered singular value case). In Section 4 we present the proofs of the results described in Section 3; some of these proofs require some technical facts that we consider in Section 5 (Appendix).

2 Preliminaries and description of the main context

We begin by recalling some geometric notions that play a central role in the convergence analysis of iterative algorithms. Then, we describe the context and problems that are the main motivation of our work.

2.1 Principal angles between subspaces

Let S, $T \subset \mathbb{K}^n$ be two subspaces of dimensions s and t respectively. Let $S \in \mathbb{K}^{n \times s}$ and $T \in \mathbb{K}^{n \times t}$ be isometries (i.e., matrices with orthonormal columns) such that R(S) = S and R(T) = T. Following [11], we define the principal angles between S and T, denoted

$$0 \le \theta_1(\mathcal{S}, \mathcal{T}) \le \ldots \le \theta_k(\mathcal{S}, \mathcal{T}) \le \frac{\pi}{2}$$
 where $k = \min\{s, t\}$,

determined by the identities $\cos(\theta_i(S, T)) = \sigma_i(S^*T) = \sigma_i(T^*S)$, for $1 \le i \le k$; in this case the roles of S and T are symmetric. If we assume that $s \le t$ (so k = s) the principal angles can be also determined in terms of the identities

$$\sin(\theta_{s-i+1}(\mathcal{S}, \mathcal{T})) = \sigma_i((I - TT^*)S) = \sigma_i((I - TT^*)SS^*) = \sigma_i((I - P_{\mathcal{T}})P_{\mathcal{S}}) \tag{1}$$

for $1 \leq i \leq s$, where $P_{\mathcal{H}} \in \mathbb{K}^{n \times n}$ denotes the orthogonal projection onto a subspace $\mathcal{H} \subset \mathbb{K}^n$; it is worth noticing that in this last case the roles of S and T (equivalently the roles of $P_{\mathcal{S}}$ and $P_{\mathcal{T}}$) are not symmetric (unless s = t). Principal angles can be considered as a vector valued measure of the distance between the subspaces S and T. Following [23] we let $\Theta(S, T) = \operatorname{diag}(\theta_1(S, T), \dots, \theta_s(S, T))$ denote the diagonal matrix with the principal angles in its main diagonal. As a consequence of the previous facts we get that

$$\|\sin\Theta(S,T)\|_{2,F} = \|(I-P_T)P_S\|_{2,F}$$

are (scalar measures of) the angular distances between S and T (see [11, 23]).

2.2 Dominant subspaces

We begin with a formal description of the class of dominant subspaces of a matrix, without assuming a singular gap. Let $A \in \mathbb{K}^{m \times n}$ and let $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$, where $p = \min\{m, n\}$, denote its singular values. Let $\mathcal{S}' \subset \mathbb{K}^m$ be a subspace of dimension $1 \leq h \leq \operatorname{rank}(A) \leq p$. We say that \mathcal{S}' is a left dominant subspace for A if \mathcal{S}' admits an orthonormal basis $\{w_1, \ldots, w_h\}$ such that $AA^*w_i = \sigma_i^2 w_i$, for $1 \leq i \leq h$. Equivalently, \mathcal{S}' is a left dominant subspace for A if the h largest singular values of $P_{\mathcal{S}'}A$ are $\sigma_1 \geq \ldots \geq \sigma_h$. In this case we have that

$$||P_{\mathcal{S}'}A - A|| \le ||QA - A||$$

for every orthogonal projection $Q \in \mathbb{K}^{m \times m}$ with $\operatorname{rank}(Q) = h$ and every unitarily invariant norm; that is, $P_{\mathcal{S}'}A$ is an optimal low-rank approximation of A (see [2, Section IV.3]).

On the other hand, we say that $S \subset \mathbb{K}^n$ is a right dominant subspace for A if S admits an orthonormal basis $\{z_1, \ldots, z_h\}$ such that $A^*Az_i = \sigma_i^2 z_i$, for $1 \leq i \leq h$. Similar remarks apply also to right dominant subspaces. It is interesting to notice that the class of h-dimensional left dominant subspaces of A coincides with the class of h-dimensional right dominant subspaces of A^* ; in what follows we will make use of this fact.

2.3Dominant subspaces and SVDs

Let $A = U\Sigma V^*$ be a full SVD for $A \in \mathbb{K}^{m \times n}$, where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$, $\Sigma \in \mathbb{R}^{m \times n}$ and $U \in \mathbb{K}^{m \times m}$ and $V \in \mathbb{K}^{n \times n}$ are unitary (orthogonal when $\mathbb{K} = \mathbb{R}$) matrices. In this case Σ is a (rectangular) diagonal matrix, with diagonal entries given by the singular values of A. In what follows we let u_i (respectively v_i) denote the columns of U (respectively of V).

Given $1 \leq h \leq m$, we define the subspace $\mathcal{U}_h = \operatorname{Span}\{u_1, \dots, u_h\} \subset \mathbb{K}^m$; similarly, if $1 \leq h \leq n$, we let $\mathcal{V}_h = \operatorname{Span}\{v_1,\ldots,v_h\} \subset \mathbb{K}^n$. Then, \mathcal{U}_h and \mathcal{V}_h are left and right dominant subspaces respectively. In case $\sigma_h > \sigma_{h+1}$ then it is well known that the left (respectively right) dominant subspace for A of dimension h is uniquely determined; hence, in this case \mathcal{U}_h and \mathcal{V}_h do not depend on our particular choice of SVD for A.

On the other hand, if $\sigma_h = \sigma_{h+1}$ then we have a continuum class of h-dimensional left dominant subspaces: indeed, let $0 \le j = j(h) < h < k = k(h)$ be given by $j(h) = \max\{0 \le \ell < h : \sigma_{\ell} > \sigma_{h}\}$, where we set $\sigma_0 = +\infty$ and $k = k(h) = \max\{1 \le \ell \le \operatorname{rank}(A) : \sigma_\ell = \sigma_h\}$. If we further let $\mathcal{U}_0 = \{0\}$ then, it is straightforward to check that an h-dimensional subspace \mathcal{S}' is a left dominant subspace for A if and only if there exists an (h-j)-dimensional subspace $\mathcal{U} \subset \mathcal{U}_k \ominus \mathcal{U}_j := \mathcal{U}_k \cap \mathcal{U}_i^{\perp} \subset \mathbb{K}^m$ such that $S' = U_j \oplus U$. Therefore, we have a natural parametrization of h-dimensional left dominant subspaces in terms of subspaces \mathcal{U} that vary over the Grassmann manifold of (h-j)-dimensional subspaces of $\mathcal{U}_k \ominus \mathcal{U}_j \subset \mathbb{K}^m$.

It is a basic fact in linear algebra that given S' a left dominant subspace of dimension $h \geq 1$, there exists a SVD, $A = U\Sigma V^*$ such that $S' = \mathcal{U}_h$ i.e., the subspace spanned by the top h columns of U; and a similar fact also holds for right dominant subspaces.

2.4 Main problems considered in this work

Throughout the rest of the paper we consider the following block Krylov algorithm for approximation of left dominant subspaces and computation of low-rank approximations (see [6]).

Algorithm 2.1 (Block Krylov algorithm for left dominant subspace and low-rank approximation)

Require: $A \in \mathbb{K}^{m \times n}$, starting guess $X \in \mathbb{K}^{n \times r}$; target rank $h \leq \operatorname{rank}(A)$; power $\ell \geq 0$.

$$K_{\ell} = K_{\ell}(A, X) := (AX \quad (AA^*)AX \quad \cdots \quad (AA^*)^{\ell}AX) \in \mathbb{K}^{m \times (\ell+1) \cdot r}$$

$$\mathcal{K}_{\ell} = \mathcal{K}_{\ell}(A, X) := R(K_{\ell}) \subset \mathbb{K}^m .$$

$$(2)$$

Test that $d := \dim \mathcal{K}_{\ell} \geq h$. In this case:

Ensure: $\hat{U}_h \in \mathbb{K}^{m \times h}$ with orthonormal columns

- 1: Compute an orthonormal basis $U_K \in \mathbb{K}^{m \times d}$ for \mathcal{K}_{ℓ} .
- 2: Set $W = U_K^* A \in \mathbb{K}^{d \times n}$ (notice that $\mathrm{rank}(W) \geq h$). 3: Compute $U_{W,h} \in \mathbb{K}^{d \times h}$ isometry, such that $R(U_{W,h})$ is a left dominant subspace of W. 4: Return: $U_K \in \mathbb{K}^{m \times d}$ and $\hat{U}_h = U_K U_{W,h} \in \mathbb{K}^{m \times h}$.

Once Algorithm 2.1 is performed, we consider the output matrices U_K and \hat{U}_h . We assume further that $\sigma_h = \sigma_{h+1}$; in this setting, our first main problem is to show the existence of some h-dimensional subspace $\mathcal{T} \subseteq \mathcal{K}_{\ell}$ that is close to some h-dimensional left dominant subspace \mathcal{U}_h of A. In this context, proximity between subspaces is measured by $\|\sin\Theta(\mathcal{U}_h,\mathcal{T})\|_{2,F}$ i.e., in terms of (the spectral or Frobenius norm of) the sines of the principal angles between the subspaces \mathcal{U}_h and \mathcal{T} (see Section 3.1). Once we establish the existence of $\mathcal{T} \subseteq \mathcal{K}_{\ell}$ as above, we get the low-rank approximation $P_{\mathcal{T}}A$ of A, where $P_{\mathcal{T}}$ denotes the orthogonal projection onto \mathcal{T} . We point out that the previous approach does not provide an effective way (algorithm) to compute \mathcal{T} .

Therefore our second main problem is to obtain upper bounds for the approximation error $||A - A_h||_{2,F}$, for the low-rank matrix $A_h = U_h U_h^* A$ computed in terms of the output of Algorithm

2.1. Further, we require that the upper bound for the approximation error of A by \hat{A}_h becomes arbitrarily close to $||A - A_h||_{2,F}$ (optimal approximation error as described at the beginning of Section 1) as the power ℓ increases. Hence, by solving this second problem, we obtain (in an effective way) the low-rank approximation \hat{A}_h of A (see Section 3.2) that behaves much like the optimal low-rank approximations A_h of A.

In the case that there is a singular gap i.e., $\sigma_h > \sigma_{h+1}$, these problems have been recently solved in [6]. In this work we adapt the approach considered in [6] to construct approximations of dominant spaces and low-rank approximation of A, based on the block Krylov subspaces \mathcal{K}_{ℓ} , in the case that there is no singular gap at the index h.

3 Main results

In this section, we state our main results related to dominant subspace approximations and low-rank matrix approximations in terms of block Krylov subspaces. The proofs of these results are considered in Section 4. At the end of this section, we include some comments and further research problems related to the present work.

Our results are motivated by the recent work of P. Drineas, I.C.F. Ipsen, E.M. Kontopoulou and M. Magdon-Ismail [6]. In that work, the authors merged a series of techniques, tools and arguments that lead to structural results related to the approximation of dominant subspaces from block Krylov spaces in the presence of a singular gap. The convergence analysis obtained in [6] has a deep influence in our present work; indeed, we shall follow some of the lines developed in that work, that we refer to as the *DIKM-I theory*. Of course, at some points, we have to depart from those arguments to deal with the no-singular-gap case.

3.1 Approximation of dominant subspaces by block Krylov spaces

In what follows we consider the convergence analysis of the block Krylov iterative method for approximating left dominant subspaces of a matrix A (Algorithm 2.1). Once the Algorithm 2.1 is performed, we describe the output matrix \hat{U}_h in terms of its columns $\hat{U}_h = (\hat{u}_1, \dots, \hat{u}_h)$. We also consider the matrices $\hat{U}_i = (\hat{u}_1, \dots, \hat{u}_i) \in \mathbb{K}^{m \times i}$, for $1 \leq i \leq h$.

As before, let $A \in \mathbb{K}^{m \times n}$ with singular values $\sigma_1 \geq \ldots \geq \sigma_p$, for $p = \min\{m, n\}$. Given $1 \leq h \leq \operatorname{rank}(A) \leq p$, we let $0 \leq j(h) < h$ be given by

$$j = j(h) = \max\{0 \le \ell < h : \sigma_{\ell} > \sigma_h\}$$
(3)

where we set $\sigma_0 = +\infty$ and

$$k = k(h) = \max\{1 \le \ell \le \operatorname{rank}(A) : \sigma_{\ell} = \sigma_h\}. \tag{4}$$

Since $h \leq \operatorname{rank}(A)$, we get that $\sigma_k = \sigma_h > 0$. As mentioned in the preceding sections, we will focus on the case when h < k (i.e., when $\sigma_h = \sigma_{h+1}$). Moreover, we will further assume that $h \leq r < k$ so that $\sigma_h = \sigma_r = \sigma_k$) where $X \in \mathbb{K}^{n \times r}$ is the starting guess in Algorithm 2.1; otherwise (if $k \leq r$) we could simply apply the DIKM-I theory, using the singular gap $\sigma_k > \sigma_{k+1}$ (since, in the generic case, X is full rank and satisfies the compatibility hypothesis of the DIKM-I theory). Let $A = U\Sigma V^*$ be a full SVD of A. In case $1 \leq k < p$ then we consider the following partitioning of U, Σ and V

$$\Sigma = \begin{pmatrix} \Sigma_k & \\ & \Sigma_{k,\perp} \end{pmatrix}$$
 , $U = \begin{pmatrix} U_k & U_{k,\perp} \end{pmatrix}$, $V = \begin{pmatrix} V_k & V_{k,\perp} \end{pmatrix}$.

Algorithm 2.1 will provide a reasonable output as long as the starting guess matrix satisfies certain compatibility conditions with A. Hence, we consider the following

Definition 3.1. Given $X \in \mathbb{K}^{n \times r}$ we say that (A, X) is h-compatible if there is an h-dimensional right dominant subspace $S \subset \mathbb{K}^n$ for A, with

$$\Theta(S, R(X)) < \frac{\pi}{2} I.$$

Given $X \in \mathbb{K}^{n \times r}$ notice that (A, X) is h-compatible if and only if $\dim(X^*\mathcal{S}) = h$, for some h-dimensional right dominant subspace \mathcal{S} of A.

Throughout the rest of the work, we fix $1 \leq h \leq \operatorname{rank}(A) \leq p = \min\{m,n\}$ and we let $0 \leq j = j(h) < h \leq k = k(h) \leq \operatorname{rank}(A)$ be defined as in Eqs. (3) and (4). The next result will allow us to show that block Krylov methods produce arbitrarily good approximations of right and left dominant subspaces under the previous hypothesis (see Remark 3.3 below). In what follows, given a matrix Z we let Z^{\dagger} denote its Moore-Penrose pseudo-inverse.

Theorem 3.2. Let $t \geq 0$ and let $\phi(x)$ be a polynomial of degree at most 2t + 1 with odd powers only, such that $\phi(\sigma_1), \ldots, \phi(\sigma_k) > 0$. Let (A, X) be h-compatible and let $\mathcal{K}_t = \mathcal{K}_t(A, X)$. Then, there exists an h-dimensional left dominant subspace \mathcal{S}' for A such that

$$\|\sin\Theta(\mathcal{K}_t,\mathcal{S}')\|_{2,F} \le 2\|\sin\Theta(R(V_k^*X),V_k^*\mathcal{V}_i)\|_{2,F} +$$

$$\|\phi(\Sigma_{k,\perp})\|_2 \|\phi(\Sigma_k)^{-1}\|_2 \|V_{k,\perp}^* X (V_k^* X)^{\dagger}\|_{2,F}$$
.

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In case j = 0 (respectively k = rank(A)) the first term (respectively the second term) should be omitted in the previous upper bound. Moreover, we have the inequality

$$\Theta(R(V_k^*X), V_k^*V_j) \le \Theta(R(X), V_j).$$

Proof. See Section 4.1.

We point out that Theorem 3.2 above is related to [6, Theorem 2.1] from the DIKM-I theory. In case $\sigma_h = \sigma_{h+1}$ (and hence k > h), the hypothesis in Theorem 3.2 involves the (continuum) class of h-dimensional left dominant subspaces of A; that is, we are allowed to consider any such dominant subspace to test our assumptions. In particular, the hypothesis is satisfied in a generic case.

As mentioned in Section 2.3, since $\sigma_j > \sigma_{j+1}$ and $\sigma_k > \sigma_{k+1}$ the subspaces $\mathcal{V}_j = R(V_j)$ and $\mathcal{V}_k = R(V_k)$ do not depend on the particular SVD of $A = U\Sigma V^*$ being considered. Hence, the principal angles $\Theta(R(V_k^*X), V_k^*\mathcal{V}_j)$ in Theorem 3.2 do not depend on the particular SVD of A, since they coincide with $\Theta(R(P_{\mathcal{V}_k}X), P_{\mathcal{V}_k}\mathcal{V}_j)$ (here $P_{\mathcal{V}_k} \in \mathbb{K}^{n \times n}$ denotes the orthogonal projection onto $\mathcal{V}_k \subset \mathbb{K}^n$).

To apply Theorem 3.2 we need to bound the principal angles $\Theta(R(V_k^*X), R(V_k^*V_j))$ (notice that [6, Theorem 2.1] does not require such bound). We remark that the second inequality in Theorem 3.2 provides an alternative method to have control of the previous principal angles.

Using the results from [28] we can interpret the second term in the upper bound in Theorem 3.2 as a measure of how close the subspaces R(X) and (the k-dimensional right dominant subspace) \mathcal{V}_k are; indeed, the smaller this second term is, the closer the subspaces are. The distance between these subspaces does not seem to have been considered before in the analysis of convergence of dominant subspaces obtained by block Krylov methods, under our present assumption that $h \leq r < k$ (where the dimension of the dominant subspace is strictly bigger than that of R(X)).

Remark 3.3 (Convergence analysis to dominant subspaces). Theorem 3.2 suggests a strategy to obtain a convergence analysis of subspaces obtained from the block Krylov method to h-dimensional left dominant subspaces. We now describe this strategy in detail for the benefit of the reader. With the notation of Theorem 3.2 we consider the following steps:

Step 1. Beginning with A, X and $q \ge 0$, we first consider the (auxiliary) block Krylov matrix

$$\tilde{K}_q := K_q(A^*, AX) = (A^*(AX) \quad (A^*A)A^*(AX) \quad \cdots \quad (A^*A)^q A^*(AX))$$

constructed in terms of $A^* \in \mathbb{K}^{n \times m}$ and (the auxiliary starting guess matrix) $AX \in \mathbb{K}^{m \times r}$. Assume that $1 \leq j < h$ so that $\sigma_j(A^*) = \sigma_j(A) > \sigma_{j+1}(A) = \sigma_{j+1}(A^*)$.

Notice that if $\psi(x) \in \mathbb{K}[x]$ is any polynomial of degree at most 2q with even powers only and such that $\psi(\sigma_1) \geq \ldots \geq \psi(\sigma_j) > 0$ then $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2) V^* X$ is such that $R(\Psi_q) \subset \tilde{K}_q$; here we have used the convention $\Sigma^{2\ell} = (\Sigma^\ell)^* \cdot \Sigma^\ell \in \mathbb{K}^{n \times n}$ for the sake of simplicity. Moreover, it is well known that there are convenient choices of $\psi(x)$ which warrant that the angles between $R(\Psi_q)$ and (the j-dimensional left dominant subspace of A^*) \mathcal{V}_j become arbitrarily small as q increases.

Step 2. Assume that $k < \operatorname{rank}(A)$; an application of Theorem 3.2 to the matrix A, with starting guess matrix Ψ_q and t = 0 (so that $\phi(x) = x$), shows that there exists an h-dimensional left dominant subspace \mathcal{S}' of A such that

$$\|\sin\Theta(\mathcal{K}_{q+1}(A,X),\mathcal{S}')\|_{2,F} \le 2\|\sin\Theta(R(\Psi_q)),\mathcal{V}_j)\|_{2,F} + \frac{\sigma_{k+1}}{\sigma_k} \|V_{k,\perp}^* \Psi_q(V_k^* \Psi_q)^{\dagger}\|_{2,F}.$$
 (5)

where we have used the inclusion $\mathcal{K}_0(A^*, \Psi_q) \subset \mathcal{K}_{q+1}(A, X)$, the properties of principal angles described in Remark 4.2, and that $A^* = V \Sigma U^*$ is a SVD of A^* .

Step 3. As mentioned in Step 1., the first term in the upper bound in Eq. (5) is known to become arbitrarily small for convenient choices of $\psi(x)$; we will show that there are choices of $\psi(x)$ for which both the expressions $\|\sin\Theta(R(\Psi_q)), \mathcal{V}_j)\|_{2,F}$ and $\|V_{k,\perp}^*\Psi_q(V_k^*\Psi_q)^{\dagger}\|_{2,F}$ become arbitrarily small as q increases.

We point out that the cases in which j=0 or $k=\operatorname{rank}(A)$ can be tackled in a similar way. The reader will notice that Theorem 3.2 allows for other possible approaches to the convergence analysis of subspaces obtained from the block Krylov algorithm to h-dimensional left dominant subspaces.

In what follows we consider the different steps of the strategy for the convergence analysis of the block Krylov subspaces to the h-dimensional left dominant subspaces described in Remark 3.3. We begin by obtaining an upper bound related to the claim in Step 1. Thus, given A with singular values $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$ (with $p = \min\{m, n\}$), we introduce

$$\gamma_i = \frac{\sigma_i - \sigma_{i+1}}{\sigma_{i+1}} \ge 0$$
 for $1 \le i \le \operatorname{rank}(A) - 1$.

The following result is a straightforward consequence of the results from [6].

Theorem 3.4. Let (A, X) be h-compatible and assume that $1 \leq j < h$, so then $\gamma_j > 0$. Let $\psi(x) \in \mathbb{K}[x]$ be a polynomial of degree at most 2q with even powers only and such that $\psi(\sigma_1), \ldots, \psi(\sigma_j) > 0$. If we let $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$ then

$$\|\sin\Theta(R(\Psi_q), \mathcal{V}_j)\|_{2,F} \le \|\psi(\Sigma_{j,\perp})\|_2 \|\psi(\Sigma_j)^{-1}\|_2 \|V_{j,\perp}^* X (V_j^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_j)^2}$$

Proof. See Section 4.2. \Box

In the next result we obtain an upper bound required in Step 3 of Remark 3.3.

Theorem 3.5. Let (A, X) be h-compatible, let $q \ge 0$ and assume that $\sigma_{k+1} > 0$. Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. Then, $\psi(\sigma_1) \ge \ldots \ge \psi(\sigma_k) > 1$ and if we let $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$ then

$$\|\sin\Theta(R(\Psi_q), \mathcal{V}_j)\|_{2,F} \le \frac{\psi(\sigma_k)}{\psi(\sigma_j)} \|V_{j,\perp}^* X (V_j^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_j)^2}$$
 (6)

$$\|V_{k,\perp}^* \Psi_q(V_k^* \Psi_q)^{\dagger}\|_{2,F} \le \frac{1}{\psi(\sigma_k)} \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_k)^2}$$
(7)

Moreover, in this case we have

$$\frac{\psi(\sigma_k)}{\psi(\sigma_i)} \le \frac{1}{(1+\gamma_i)^{2q}} \quad and \quad \frac{1}{\psi(\sigma_k)} \le 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1+\gamma_k)}. \tag{8}$$

Proof. See Section 4.2.

Remark 3.6. Consider the notation in Theorem 3.5 above. We point out that the first inequality in Eq. (8) corresponds to a worst case scenario; moreover, numerical examples show that the upper bound can be (typically) tightened. Indeed, let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. For $x \ge 1$ we get the representation

$$T_{2q}(x) = \frac{(x + \sqrt{x^2 - 1})^{2q} + (x - \sqrt{x^2 - 1})^{2q}}{2}$$

For $1 \le \ell \le k+1$, set $\eta_{\ell} = \frac{\sigma_{\ell}}{\sigma_{\ell+1}} \ge 1$ so $\eta_{\ell} = 1 + \gamma_{\ell}$. Then $\frac{\sigma_{j}}{\sigma_{k+1}} = \eta_{j} \cdot \eta_{k} > 1$ and

$$\frac{\psi(\sigma_k)}{\psi(\sigma_j)} = \frac{T_{2q}(\eta_k)}{T_{2q}(\eta_j \cdot \eta_k)} = \frac{(\eta_k + \sqrt{\eta_k^2 - 1})^{2q} + (\eta_k - \sqrt{\eta_k^2 - 1})^{2q}}{\eta_j^{2q}(\eta_k + \sqrt{\eta_k^2 - \frac{1}{\eta_j^2}})^{2q} + (\eta_k - \sqrt{\eta_k^2 - \frac{1}{\eta_j^2}})^{2q}} \le \frac{1}{\eta_j^{2q}} = \frac{1}{(1 + \gamma_j)^{2q}}.$$

The upper bound above is sharp since

$$\lim_{\eta_k \to \infty} \frac{T_{2q}(\eta_k)}{T_{2q}(\eta_j \cdot \eta_k)} = \frac{1}{(1 + \gamma_j)^{2q}}.$$

Nevertheless, in the regime η_j , $\eta_k \in (1, 1+\varepsilon)$ for small $\varepsilon > 0$ (which is quiet relevant for applications) we can expect better upper bounds. Indeed, numerical examples show that if $1 < \eta_k \le \eta_j$ then we have that for $q \ge 1$,

$$\frac{\psi(\sigma_k)}{\psi(\sigma_j)} = \frac{T_{2q}(\eta_k)}{T_{2q}(\eta_j \cdot \eta_k)} \le 4 \frac{2^{-2q \min\{\sqrt{\gamma_j}, 1\}}}{(1 + \gamma_j)}, \tag{9}$$

which is a tighter upper bound than that in Eq. (8) for $\eta_j \in (1, 1 + \varepsilon)$ for small $\varepsilon > 0$. We conjecture that Eq. (9) is true (under the previous restrictions). In fact, notice that when $\eta_k \approx 1$ then $\frac{T_{2q}(\eta_k)}{T_{2q}(\eta_j \cdot \eta_k)} \approx \frac{1}{T_{2q}(\eta_j)}$, so Eq. (9) is true (see [6]). On the other hand, for $\gamma_j \geq 1$ then Eq. (8) shows that

$$\frac{\psi(\sigma_k)}{\psi(\sigma_j)} = \frac{T_{2q}(\eta_k)}{T_{2q}(\eta_j \cdot \eta_k)} \le \frac{1}{(1+\gamma_j)^{2q}} \le 2^{-2q}.$$

In the following result we apply the strategy described in Remark 3.3 and obtain upper bounds for the convergence of block Krylov subspaces to h-dimensional left dominant subspaces for the spectral norm (the Frobenius norm case can be handled similarly); to simplify the statement below, we consider the following constants: given a h-compatible pair (A, X) set $C(A, X, j, k)_{2,F} = C_{2,F}$ determined as follows. If $h \leq k < \text{rank}(A)$ and $1 \leq j$ then

$$C_{2,F}(V,X) = C_{2,F} = \max \left\{ 2 \|V_{j,\perp}^* X(V_j^* X)^{\dagger}\|_{2,F}, \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F} \right\}.$$
 (10)

If j = 0 we let $C_{2,F} = \|V_{k,\perp}^* X (V_k^* X)^{\dagger}\|_{2,F}$; if k = rank(A) then we set $C_{2,F} = 2 \|V_{j,\perp}^* X (V_j^* X)^{\dagger}\|_{2,F}$.

Theorem 3.7. Let (A, X) be h-compatible, assume that $0 \le j < h \le k < rank(A)$, and let $\mathcal{K}_{q+1} = \mathcal{K}_{q+1}(A, X) \subset \mathbb{K}^m$, for $q \ge 0$. Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. If we let $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$ then there exists an h-dimensional left dominant subspace S' of A such that:

$$\|\sin\Theta(R(A\Psi_q),\mathcal{S}')\|_{2,F} \le C_{2,F} \left(\frac{\psi(\sigma_k)}{\psi(\sigma_i)} \frac{1}{(1+\gamma_i)^2} + \frac{1}{\psi(\sigma_k)} \frac{1}{(1+\gamma_k)^3}\right),\tag{11}$$

where $C_{2,F} = C_{2,F}(V,X)$. In particular, since $R(A\Psi_q) \subset \mathcal{K}_{q+1}$ and $\dim R(A\Psi_q) \geq h$,

$$\|\sin\Theta(\mathcal{K}_{q+1},\mathcal{S}')\|_{2,F} \le C_{2,F} \left(\frac{1}{(1+\gamma_i)^{2(q+1)}} + 4 \frac{2^{-2q \min\{\sqrt{\gamma_k},1\}}}{(1+\gamma_k)^4} \right). \tag{12}$$

In case j = 0 then the first terms (in the expressions between parentheses) in Eqs. (11) and (12) should be omitted.

Proof. See Section 4.2.
$$\Box$$

As already mentioned, the upper bound in Eq. (11) can be obtained by following the three-step strategy in Remark 3.2. The reader can check that in case k = rank(A) (so that $\sigma_{k+1} = 0$) then we can set $\psi(x) = T_{2q}(x/\sigma_k) = T_{2q}(x/\sigma_{j+1})$ and get the bound in Eq. (11) omitting the second terms in the expressions between parentheses; in this case Eq. (12) becomes

$$\|\sin\Theta(\mathcal{K}_{q+1},\mathcal{S}')\|_{2,F} \le \frac{4C_{2,F}}{(1+\gamma_i)^3} 2^{-2q\min\{\sqrt{\gamma_j},1\}}.$$

We point out that Theorem 3.7 complements the convergence analysis described in [6, Corollary 2.5]. That is, this result can be applied in contexts in which [6, Corollary 2.5] can not be applied; moreover, Theorem 3.7 shows the existence of h-dimensional subspaces $\mathcal{T} \subseteq \mathcal{K}_{q+1} = \mathcal{K}_{q+1}(A, X)$ that are arbitrarily good approximations of some h-dimensional left dominant subspace \mathcal{S}' of A (for sufficiently large $q \geq 0$). As opposed to Theorem 3.2, Theorem 3.7 does not require a priori knowledge of $\Theta(R(V_k^*X), V_k^*V_j)$ (see the comments after Theorem 3.2). On the other hand, the speed at which the upper bound in Eq. (12) decreases depends on both gaps γ_j and γ_k ; in particular, this result warrants a better convergence speed when both singular gaps are significant.

3.2 Low-rank approximations from block Krylov methods

Notice that the upper bounds in Theorem 3.7 can be made arbitrarily small for large enough $q \ge 0$. Therefore the corresponding block Krylov subspace contains (arbitrarily good) approximate left dominant subspaces. Still, the previous results do not provide a practical method to compute such approximate dominant subspaces and the corresponding low-rank approximations. In this section we revisit Algorithm 2.1 without assuming a singular gap, as a practical way to construct low-rank approximations. Our approach to deal with this problem is based on the approximate left dominant subspaces of a matrix A; indeed, we follow arguments from [26].

For the next results, we consider Algorithm 2.1 with input: $A \in \mathbb{K}^{m \times n}$, starting guess $X \in \mathbb{K}^{n \times r}$ and power $\ell = q+1$ for some $q \geq 0$; we set our target rank to $1 \leq h \leq \text{rank }(A)$. Once the algorithm stops, we consider the output matrices U_K and \hat{U}_h ; we further describe \hat{U}_h in terms of its columns, $\hat{U}_h = (\hat{u}_1, \dots, \hat{u}_h) \in \mathbb{K}^{m \times h}$. In this case we set

$$\hat{U}_i = (\hat{u}_1, \dots, \hat{u}_i) \in \mathbb{K}^{m \times i} , \quad \text{for} \quad 1 \le i \le h.$$
 (13)

As before, we let $j = j(h) < h \le k = k(h)$ be defined as in Eqs. (3) and (4), and we consider the notation used so far. Further, given $1 \le i \le h$ we let $A_i = U_i \Sigma_i V_i^* \in \mathbb{K}^{m \times n}$ denote a best rank-i approximation of A (so that $||A - A_i||_2 = \sigma_{i+1}$).

Let (A, X) be h-compatible and let $q \ge 0$. In what follows we make use of the constants $\delta(A, X, q, j, k)_{2,F} = \delta_{2,F}$ given by: for $k < \operatorname{rank}(A)$ then let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q, $\psi(x) = T_{2q}(x/\sigma_{k+1})$ and set

$$\delta_{2,F} := \sqrt{2} \, C_{2,F} \, \left(\frac{\psi(\sigma_k)}{\psi(\sigma_i)} \, \frac{1}{(1+\gamma_i)} + \frac{1}{\psi(\sigma_k)} \, \frac{1}{(1+\gamma_k)^2} \right) \,, \tag{14}$$

where $C_{2,F}$ is defined as in Eq. (10). In case j=0 the first term should be omitted. In case $k=\operatorname{rank}(A)$ then let $\psi(x)=T_{2q}(x/\sigma_k)=T_{2q}(x/\sigma_{j+1})$ and set

$$\delta_{2,F} := \frac{\sqrt{2}}{\psi(\sigma_j)} \frac{C_{2,F}}{(1+\gamma_j)}. \tag{15}$$

Theorem 3.8. Let (A, X) be h-compatible and let $q \ge 0$ be such that $\delta_2 \le 1$. Let U_K be the output of Algorithm 2.1 with the power parameter set to $q + 1 \ge 1$. Then there exists an h-dimensional right dominant subspace $\tilde{\mathcal{S}}$ of A such that

$$||AP_{\tilde{S}} - U_K U_K^* A P_{\tilde{S}}||_{2,F} \le \sigma_{h+1} \cdot \delta_{2,F}.$$
 (16)

Proof. See Section 4.3.

Although rather technical, the previous result allows us to get the following estimates for the first h singular values of A.

Theorem 3.9. Let (A, X) be h-compatible and let $q \ge 0$ be such that $\delta_2 \le 1$. Let $\hat{A}_h = \hat{U}_h \hat{U}_h^* A$, where \hat{U}_h is the output of Algorithm 2.1 with the power parameter set to $q + 1 \ge 1$. Then,

$$\sigma_i - \sigma_{h+1} \cdot \delta_2 \le \sigma_i(\hat{A}_h) \le \sigma_i \quad \text{for} \quad 1 \le i \le h.$$
 (17)

Proof. See Section 4.3. \Box

Theorem 3.10. Let (A, X) be h-compatible and let $q \ge 0$ be such that $\delta_2 \le 1$. Let \hat{U}_h be the output of Algorithm 2.1 with the power parameter set to $q + 1 \ge 1$. Then, for every $1 \le i \le h$ we have that

$$||A - \hat{U}_i \hat{U}_i^* A||_{2,F} \le ||A - A_i||_{2,F} + \sigma_{i+1} \cdot \delta_F,$$
(18)

where $\delta_{2,F}$ are defined in Eq. (14) or (15).

Proof. See Section 4.3.
$$\Box$$

Using the previous results together with estimates for $\delta_{2,F}$ as defined in Eqs. (14) and (15) we can obtain the following upper bounds for the approximation of singular values and approximation errors using the block Krylov Algorithm 2.1.

Theorem 3.11. Let (A, X) be h-compatible, let $0 \le j < h \le k < rank(A)$, and let $C_{2,F}$ be defined as in Eq. (10). Assume that

$$\sqrt{2} C_2 \left(\frac{1}{(1+\gamma_j)^{2q+1}} + 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1+\gamma_k)^3} \right) \le 1,$$
(19)

where we follow the convention: $\gamma_0 = +\infty$ in case j = 0. Let \hat{U}_h be the output of Algorithm (2.1) with the power parameter set to $q + 1 \ge 1$; Let

$$\hat{A}_i = \hat{U}_i \hat{U}_i^* A$$
 for $1 \le i \le h$,

be the rank-i approximation of A obtained from Algorithm 2.1. Then, for $1 \le i \le h$:

$$\sigma_i - \sigma_{h+1} \cdot \sqrt{2} C_2 \left(\frac{1}{(1+\gamma_j)^{2q+1}} + 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1+\gamma_k)^3} \right) \le \sigma_i(\hat{A}_h) \le \sigma_i$$

and

$$||A - \hat{U}_i \hat{U}_i^* A||_{2,F} \le ||A - A_i||_{2,F} + \sigma_{i+1} \cdot \sqrt{2} C_F \left(\frac{1}{(1 + \gamma_j)^{2q+1}} + 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1 + \gamma_k)^3} \right).$$

Proof. See Section 4.3.

Theorem 3.11 complements the analysis in the deterministic setting obtained in [6, Corollary 2.6]. That is, this result can be applied in contexts in which [6, Corollary 2.6] can not be applied (i.e., when there is no singular gap). Theorem 3.11 shows that the distance $||A - \hat{A}_h(q)||_{2,F}$, between the low-rank approximations $\hat{A}_h(q)$ of A obtained from the block Krylov method and A, converges to the minimial distance $||A - A_h||_{2,F}$ as the power parameter (number of iterations) $q \ge 0$ increases. Moreover, it also shows the convergence of the first h singular values of \hat{A}_h to the corresponding singular values of A. Thus, our approach follows the paradigm introduced in [20] for the assessment of the quality of low-rank approximations. On the other hand, the speed at which the upper bounds in Theorem 3.11 decrease depends on both gaps γ_j and γ_k ; that is, this result warrants better convergence speeds when both singular gaps are significant.

Remark 3.12. There is a vast literature related to low-rank approximation, both from a deterministic and randomized point of view, taking into account singular gaps, or disregarding these gaps (see the survey [17]).

Randomized methods [7, 8, 12, 13, 20] typically draw a random $n \times r$ matrix X (a starting guess matrix) and consider the random subspace $R(X) \subset \mathbb{K}^n$ given by the range of X. One of the advantages of this approach is that it is possible to prove that, with high probability, X satisfies some compatibility properties with the structure of A, regardless of the particular choice of A (see [5]); on the other hand, the conclusions of the randomized approach then typically hold with high probability. Thus, these conclusions do not apply to particular choices of matrices X. In this setting, the work [20] contains a deep analysis of the block Krylov method for low-rank approximations, when the starting guess matrix is drawn from a standard Gaussian random matrix. The gap-independent bounds obtained in [20, Theorems 10 and 12] (see also [20, Theorems 11 and 12]) imply that a number $O(1/\sqrt{\varepsilon})$ of iterations in Algorithm 2.1 are required to warrant (with high probability) that $||A - \hat{A}_h(q)||_2 \le (1+\varepsilon)||A - A_h||_2$ and $|\sigma_i(A)^2 - \sigma_i(\hat{A}_h)^2| \le \varepsilon \sigma_h(A)^2$, for $1 \le i \le h$.

Notice that we follow a deterministic approach where we consider a fixed (deterministic) $n \times r$ matrix X satisfying a set of specific (explicit) compatibility hypotheses with the structure of A (that hold in generic cases) and obtain conclusions that hold for the particular matrices X and A. In our deterministic setting, Theorem 3.11 implies (for a fixed h-compatible pair (A, X) and $1 \le j < h \le k < \operatorname{rank}(A)$) that

$$||A - \hat{U}_i \hat{U}_i^* A||_{2,F} \le ||A - A_i||_{2,F} + \sigma_{i+1} \cdot 2\sqrt{2} C_F \max \left\{ \frac{1}{(1 + \gamma_j)^{2q+1}}, 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1 + \gamma_k)^3} \right\},$$

where $C_F = \max\{2 \|V_{j,\perp}^* X(V_j^* X)^{\dagger}\|_F$, $\|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_F\}$. Hence, if q is the smallest integer satisfying

$$\log(\frac{2\sqrt{2}C_F}{\varepsilon}) \le \min\{(2q+1)\,\log(1+\gamma_j)\,,\,2\,\log(2)\,q\,\min\{\sqrt{\gamma_k},1\}\}\$$

then Algorithm 2.1 provides a low-rank approximation of A such that $||A - \hat{A}_h(q)||_2 \le (1 + \varepsilon) ||A - A_h||_2$, $|\sigma_i(A)^2 - \sigma_i(\hat{A}_h)^2| \le \varepsilon \sigma_h(A)^2$, for $1 \le i \le h$. Thus Theorem 3.11 implies that, (for fixed

A and X), a number $O((\min\{2\log(1+\gamma_j), 2\sqrt{2}\min\{\sqrt{\gamma_k}, 1\}\})^{-1}\log(\frac{2\sqrt{2}C_F}{\varepsilon}))$ of iterations in Algorithm 2.1 are required to achieve the previously mentioned approximation errors. On the other hand, we remark that it is well known that an analysis of convergence such as that derived in Theorem 3.7 (for dominant subspaces) or Theorem 3.11 can be used to obtain upper bounds for the approximation errors in the randomized setting (for example, see Saibaba's work in the context of the Subspace Iteration Method [22]). We will consider these issues elsewhere.

Remark 3.13. As a final comment, we point out that the present results together with the results from [6] do not cover the complete picture of the convergence analysis of deterministic block Krylov methods. For example, assume that we are interested in computing an approximation of an h-dimensional dominant subspace of the matrix A in the case that there is a small singular gap $\sigma_h > \sigma_{h+1}$, for which $\gamma_h \approx 0$ (so $\frac{\sigma_h}{\sigma_{h+1}} \approx 1$). This situation corresponds, for example, to the case where σ_h lies in a cluster of singular values $\sigma_{j+1} > \ldots > \sigma_h > \ldots > \sigma_k$, for $1 \leq j < h < k < \operatorname{rank}(A)$ and $\sigma_{j+1} - \sigma_k \approx 0$. In this case [6, Theorem 2.1] exhibits a rather slow speed of convergence with respect to the power parameter (number of iterations) $q \geq 0$. Although our approach does not apply directly to the case where σ_h lies in a cluster of singular values, it seems that our results and techniques could shed some light on the convergence analysis in this case. Indeed, let us consider the following heuristic argument: let $A = U\Sigma V^*$ and assume that $\sigma_{j+1} \geq \ldots \geq \sigma_h \geq \ldots \geq \sigma_k > 0$, for $1 \leq j < h < k$ and set $\varepsilon = \sigma_{j+1} - \sigma_k \approx 0$. Let us construct an auxiliary matrix

$$A_{\text{aux}} = U \Sigma_{\text{aux}} V^*$$
, $\Sigma_{\text{aux}} = \text{diag}(\sigma_1, \dots, \sigma_j, c, \dots, c, \sigma_{k+1}, \dots, \sigma_p)$

where $p = \min\{m, n\}$ and $c = 1/2(\sigma_{j+1} + \sigma_k)$. We will use the key fact that the dominant subspaces \mathcal{U}_j and \mathcal{U}_k of A and A_{aux} of dimensions j and k, respectively, coincide (although h-dimensional dominant subspaces of A and A_{aux} do not necessarily coincide). Similarly, the gaps γ_j , $\tilde{\gamma}_j > 0$ and γ_k , $\tilde{\gamma}_k > 0$ of A and A_{aux} are *comparable*.

Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$ and let $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$. Then, by Theorem 3.5 we get that $\|\sin\Theta(R(\Psi_q)), \mathcal{V}_j)\|_{2,F}$ and $\|V_{k,\perp}^*\Psi_q(V_k^*\Psi_q)^{\dagger}\|_{2,F}$ decay (as a function of the number of iterations) in terms of the enveloping gaps γ_j and γ_k . Hence, if we now apply Theorem 3.2 to the auxiliary matrix A_{aux} with starting guess Ψ_q and with t=0, we see that there exists an h-dimensional left dominant subspace $\mathcal{S}'_{\text{aux}}$ of A_{aux} such that

$$\|\sin\Theta(R(A_{\mathrm{aux}}\Psi_q),\mathcal{S}'_{\mathrm{aux}})\|_{2,F} \leq 2\|\sin\Theta(R(\Psi_q)),\mathcal{V}_j)\|_{2,F} + \frac{1}{1+\tilde{\gamma}_k}\|V_{k,\perp}^*\Psi_q(V_k^*\Psi_q)^{\dagger}\|_{2,F}.$$

It seems reasonable to expect that the difference between $\Theta(R(A\Psi_q), \mathcal{S}'_{aux})$ and $\Theta(R(A_{aux}\Psi_q), \mathcal{S}'_{aux})$ can be bounded in terms of some measure of the *spread* of the cluster $\sigma_j \geq \ldots \geq \sigma_k$. Assuming this last fact and putting together the previous estimates, we now conclude that

$$\|\sin\Theta(\mathcal{K}_{q+1},\mathcal{S}'_{\text{aux}})\|_{2,F} \le \|\sin\Theta(R(A\Psi_q),\mathcal{S}'_{\text{aux}})\|_{2,F}$$

where the upper bound would decay in terms of the gaps γ_j and γ_k and the power parameter; here we have used that $R(A\Psi_q) \subset \mathcal{K}_{q+1} = R(K_{q+1}(A,X))$.

At this point, we remark that the subspaces $S'_{\text{aux}} = S'_{\text{aux}}(q)$ are not necessarily dominant subspaces of A. Yet, the subspaces S'_{aux} satisfy that there exist (h-j)-dimensional subspaces $\mathcal{U} \subset \mathcal{U}_k \ominus \mathcal{U}_j$ such that $S'_{\text{aux}} = \mathcal{U}_j \oplus \mathcal{U}$. Using this last fact we could show that $\|A - P_{S'_{\text{aux}}}A\|_{2,F}$ can be bounded by $\|A - A_j\|_{2,F} + \|(\sigma_{\ell+j} - c)_{\ell=1}^{k-j}\|_{2,F}$, where $\|A - A_j\|_{2,F} \approx \|A - A_h\|_{2,F}$ and $\|(\sigma_{\ell+j} - c)_{\ell=1}^{k-j}\|_{2,F} \approx 0$, because we are assuming that $\sigma_{j+1} \geq \ldots \geq \sigma_k$ forms a cluster of singular values. That is, even when S'_{aux} is not an h-dimensional left dominant subspace of A, it would behave much like one. Thus, in case $\gamma_h > 0$ and $\gamma_h \approx 0$ but with significant gaps γ_j and γ_k , we would conclude the existence of the subspaces $S'_{\text{aux}}(q)$ that become close to \mathcal{K}_{q+1} rather fast, as $q \geq 0$ increases. In this case S'_{aux} could be used to study the low-rank approximations obtained

from Algorithm 2.1 (similarly to the way that we have used the existence of a dominant subspace of A lying close to \mathcal{K}_{q+1} to study low-rank approximations obtained from Algorithm 2.1). We will consider this type of analysis elsewhere.

4 Proofs of the main results

In this section we present detailed proofs of our main results. Some of our arguments make use of some basic facts from matrix analysis, that we develop in Section 5 (Appendix). We begin by recalling the notation introduced so far; then we consider some general facts about block Krylov spaces, principal angles and principal vectors between subspaces that are needed for developing the proofs below.

Notation 4.1. We keep the notation and assumptions introduced so far; hence, we consider:

- 1. $A \in \mathbb{K}^{m \times n}$ with singular values $\sigma_1 \ge \dots \sigma_p \ge 0$, with $p = \min\{m, n\}$.
- 2. $1 \le h \le \operatorname{rank}(A) \le p$; moreover, we let $0 \le j(h) < h$ be given by

$$j = j(h) = \max\{0 \le \ell < h : \sigma_{\ell} > \sigma_h\} < h$$

where we set $\sigma_0 = +\infty$ and

$$k = k(h) = \max\{1 \le \ell \le \operatorname{rank}(A) : \sigma_{\ell} = \sigma_h\} \ge h$$
.

- 3. A starting guess $X \in \mathbb{K}^{n \times r}$ such that (A, X) is h-compatible; that is, we assume that there exists an h-dimensional right dominant subspace S of A such that $\Theta(R(X), S) < \frac{\pi}{2}I$. In this case, $\dim X^*S = h$; in particular $r \geq \operatorname{rank}(X) \geq h$.
- 4. For any $\ell \geq 0$ we consider $K_{\ell} = K_{\ell}(A, X)$ constructed in terms of A and X as in Eq. (2), that is

$$K_{\ell} = K_{\ell}(A, X) = (AX \quad (AA^*)AX \quad \dots \quad (AA^*)^{\ell}AX) \in \mathbb{K}^{m \times (\ell+1)r}$$

and consider the block Krylov space $\mathcal{K}_{\ell} = \mathcal{K}_{\ell}(A, X) = R(K_{\ell})$.

5. $A = U\Sigma V^*$ a SVD of A. Given $1 \le \ell \le \operatorname{rank}(A)$ we consider the partitions

$$\Sigma = \begin{pmatrix} \Sigma_{\ell} & \\ & \Sigma_{\ell,\perp} \end{pmatrix} , \quad U = \begin{pmatrix} U_{\ell} & U_{\ell,\perp} \end{pmatrix} , \quad V = \begin{pmatrix} V_{\ell} & V_{\ell,\perp} \end{pmatrix} . \tag{20}$$

Since the pair (A, X) is h-compatible then we further assume that $R(V_h^*X) = R(V_h)$; this can always be done by choosing a convenient SVD of A.

Notice that for every polynomial $\varphi(x) \in \mathbb{K}[x]$ of degree at most ℓ we get that the range of $\varphi(AA^*)AX \in \mathbb{K}^{m \times r}$ is contained in \mathcal{K}_{ℓ} . In terms of a SVD of A, we get that

$$\varphi(AA^*)AX = U\varphi(\Sigma^2)\Sigma V^*X = U\varphi(\Sigma)V^*X$$

where $\phi(x) = x \varphi(x^2) \in \mathbb{K}[x]$ is a polynomial of degree at most $2\ell + 1$ with odd powers only, and represents a generalized matrix function (see [1, 14]). Here $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_p) \in \mathbb{R}^{m \times n}$, where $p = \min\{m, n\}$; hence,

$$\phi(\Sigma) = \operatorname{diag}(\phi(\sigma_1), \dots, \phi(\sigma_p)) \in \mathbb{K}^{m \times n}$$

In this case we write

$$\Phi := U\phi(\Sigma)V^*X \in \mathbb{K}^{m \times r}, \tag{21}$$

so by the previous facts, $R(\Phi) \subset \mathcal{K}_{\ell}$. Let \mathcal{S} be an h-dimensional right dominant subspace \mathcal{S} of A such that $\Theta(R(X),\mathcal{S}) < \frac{\pi}{2}I$ as above. As already mentioned, we can consider a SVD of $A = U\Sigma V^*$ in such a way that $\mathcal{S} = \mathcal{V}_h$. In this case, $R(V_h^*X) = R(V_h^*)$: if we assume further that $\phi(\sigma_i) \neq 0$ for $1 \leq i \leq h$ (so $\phi(\Sigma_h) \in \mathbb{K}^{h \times h}$ is an invertible matrix) then $\dim R(\Phi) \geq h$, where Φ is defined as in Eq. (21). We will further consider similar facts related to convenient block decompositions of a SVD of A.

Remark 4.2. We mention some further properties of the principal angles between subspaces (see Section 2.1 for definitions) that we will need in what follows. Let $\mathcal{S}, \mathcal{T} \subset \mathbb{K}^n$ be two subspaces such that $s = \dim \mathcal{S} \leq \dim \mathcal{T} = t$. If $\mathcal{S}' \subset \mathcal{S}$ and $\mathcal{T} \subset \mathcal{T}'$ are subspaces with dimensions s' and t' respectively, then

$$\|\Theta(S, T')\|_{2,F} \le \|\Theta(S, T)\|_{2,F}$$
, $\|\sin\Theta(S, T')\|_{2,F} \le \|\sin\Theta(S, T)\|_{2,F}$

and similarly

$$\|\Theta(\mathcal{S}',\mathcal{T})\|_{2,F} \leq \|\Theta(\mathcal{S},\mathcal{T})\|_{2,F} \quad , \quad \|\sin\Theta(\mathcal{S}',\mathcal{T})\|_{2,F} \leq \|\sin\Theta(\mathcal{S},\mathcal{T})\|_{2,F} \, ,$$

which follow from the definition of principal angles (see Eq. (1)). On the other hand, dim $S^{\perp} = n - s \ge n - t = \dim \mathcal{T}^{\perp}$ and therefore, for $1 \le j \le \min\{s, n - t\}$,

$$\sin(\theta_{(n-t)-j+1}(\mathcal{S}^{\perp}, \mathcal{T}^{\perp})) = \sigma_i((I - P_{\mathcal{S}^{\perp}})P_{\mathcal{T}^{\perp}}) = \sigma_i(P_{\mathcal{S}}(I - P_{\mathcal{T}})) = \sin(\theta_{s-j+1}(\mathcal{S}, \mathcal{T})).$$

By the previous identity, we see that the positive angles between S and T coincide with the positive angles between S^{\perp} and T^{\perp} Notice that as a consequence of this last fact we get that

$$\|\Theta(S, T)\|_{2,F} = \|\Theta(S^{\perp}, T^{\perp})\|_{2,F}.$$
 (22)

Remark 4.3 (Principal vectors between subspaces). In what follows we shall also make use of the principal vectors associated with the subspaces \mathcal{S} , $\mathcal{T} \subset \mathbb{K}^n$ such that $s = \dim \mathcal{S} \leq \dim \mathcal{T} = t$: indeed, by the construction of the principal angles, we get that there exist orthonormal systems $\{u_1, \ldots, u_s\} \subset \mathcal{S}$ and $\{v_1, \ldots, v_s\} \subset \mathcal{T}$ such that

$$\langle u_i, v_j \rangle = \delta_{ij} \cos(\theta_j(\mathcal{S}, \mathcal{T})) \quad \text{for} \quad 1 \le i, j \le s,$$

where δ_{ij} is Kronecker's delta function. We say that $\{u_1, \ldots, u_s\}$ and $\{v_1, \ldots, v_s\}$ are the principal vectors (directions) associated with the subspaces \mathcal{S} and \mathcal{T} . Notice that the previous facts imply, in particular, that the subspaces $\mathcal{S}_j = \operatorname{Span}\{u_1, \ldots, u_j\} \subset \mathcal{S}$ and $\mathcal{T}_j = \operatorname{Span}\{v_1, \ldots, v_j\} \subset \mathcal{T}$ are such that

$$\Theta(S_j, \mathcal{T}_j) = \operatorname{diag}(\theta_1(S, \mathcal{T}), \dots, \theta_j(S, \mathcal{T})) \in \mathbb{R}^{j \times j} \quad \text{ for } \quad 1 \leq j \leq s.$$

In this case we say that $\{u_1, \ldots, u_j\} \subset \mathcal{S}$ are principal vectors corresponding to $(\mathcal{S}, \mathcal{T}, j)$ (here it is implicit that $1 \leq j \leq s = \min\{\dim \mathcal{S}, \dim \mathcal{T}\}$). If $\tilde{\mathcal{S}} \subset \mathcal{S}$ and $\tilde{\mathcal{T}} \subset \mathcal{T}$ are two j-dimensional subspaces then, it follows that $\Theta(\mathcal{S}_j, \mathcal{T}_j) \leq \Theta(\tilde{\mathcal{S}}, \tilde{\mathcal{T}})$; that is, \mathcal{S}_j and \mathcal{T}_j are j-dimensional subspaces of \mathcal{S} and \mathcal{T} respectively, that are at minimal angular (vector-valued) distance.

4.1 Proof of Theorem 3.2

We now present a proof of Theorem 3.2. We divide our arguments into steps.

Proof. Step 1: adapting the DIKM-I theory to the present context. Consider Notation 4.1. By construction $\sigma_j > \sigma_{j+1} = \sigma_h = \sigma_k$. We first assume that $1 \leq j$ and $k < \operatorname{rank}(A) \leq p = \min\{m, n\}$. Since $k < \operatorname{rank}(A)$ then $\sigma_h = \sigma_k > \sigma_{k+1} > 0$.

We consider $X \in \mathbb{K}^{n \times r}$ such $\dim(\mathcal{X}) = s \geq h$ and such that there exists a right dominant subspace $\mathcal{S} \subset \mathbb{K}^n$ of dimension h with $\Theta(\mathcal{S}, \mathcal{X}) < \pi/2I$, where $\mathcal{X} = R(X) \subset \mathbb{K}^n$ denotes the

range of X. Consider $A = U\Sigma V^*$ a full SVD. We now consider the partitioning as in Eq. (20) corresponding to the index $1 \le k \le \operatorname{rank}(A)$. It is worth noticing that Σ_k , $R(U_k) = \mathcal{U}_k$ and $R(V_k) = \mathcal{V}_k$ do not depend on the particular choice of a SVD of A; also notice that the partition is well defined since $k < \operatorname{rank}(A)$. Let $\phi(x)$ be a polynomial of degree 2t + 1 with odd powers only, such that $\phi(\sigma_1), \ldots, \phi(\sigma_k) > 0$; hence $\phi(\Sigma_k)$ is invertible.

Step 2: applying the DIKM-I theory to the adapted model. We let $\mathcal{K}_t = \mathcal{K}_t(A, X)$ denote the block Krylov subspace and let $P_t \in \mathbb{K}^{m \times m}$ denote the orthogonal projection onto \mathcal{K}_t . Notice that if we let $\Phi \in \mathbb{K}^{m \times r}$ be as in Eq. (21) then $R(\Phi) \subset \mathcal{K}_t$. Consider for now an arbitrary h-dimensional subspace $\mathcal{S}' \subset \mathbb{K}^m$. Then

$$\|\sin\Theta(\mathcal{K}_t, \mathcal{S}')\|_{2,F} = \|(I - P_t)P_{\mathcal{S}'}\|_{2,F} \le \|(I - \Phi\Phi^{\dagger})P_{\mathcal{S}'}\|_{2,F},$$
(23)

where we have used that $\dim \mathcal{K}_t \geq \dim R(\Phi) \geq \dim \mathcal{S}' = h$. We now consider the decomposition $\Phi = \Phi_k + \Phi_{k,\perp}$, where

$$\Phi_k \equiv U_k \phi(\Sigma_k) V_k^* X$$
 and $\Phi_{k,\perp} \equiv U_{k,\perp} \phi(\Sigma_{k,\perp}) V_{k,\perp}^* X$.

By [6, Lemma 4.2] (see also [18]) we get that

$$||(I - \Phi \Phi^{\dagger}) P_{S'}||_{2,F} \le ||P_{S'} - \Phi B||_{2,F} \quad \text{for} \quad B \in \mathbb{K}^{r \times m}.$$

By the previous inequality we get that

$$\|(I - \Phi\Phi^{\dagger})P_{S'}\|_{2,F} \le \|(I - \Phi\Phi_k^{\dagger})P_{S'}\|_{2,F}. \tag{24}$$

We can further estimate

$$\|(I - \Phi \Phi_k^{\dagger}) P_{\mathcal{S}'}\|_{2,F} \le \|(I - \Phi_k \Phi_k^{\dagger}) P_{\mathcal{S}'}\|_{2,F} + \|\Phi_{k,\perp} \Phi_k^{\dagger} P_{\mathcal{S}'}\|_{2,F}. \tag{25}$$

Step 3: dealing with the fact that $R(V_k^*X) \neq R(V_k^*)$. We now consider the two terms to the right of Eq. (25). In our present case, we have to deal with the fact that $R(V_k^*X) \neq R(V_k^*)$ when h < k. Indeed, since $\Theta(S, \mathcal{X}) < \pi/2I$ and $S \subset R(V_k)$ we see that if we let

$$\mathcal{W} \equiv R(V_k^* X) = V_k^* \mathcal{X} \subset \mathbb{K}^k$$

then $k \geq \dim(\mathcal{W}) := d \geq h$. Let

$$\mathcal{T} = \phi(\Sigma_k)\mathcal{W} \subset \mathbb{K}^k$$
.

Since, by hypothesis, $\phi(\Sigma_k) \in \mathbb{R}^{k \times k}$ is an invertible matrix then dim $\mathcal{T} = d$ and

$$\Phi_k \Phi_k^{\dagger} = U_k P_{\mathcal{T}} U_k^* \,. \tag{26}$$

We now consider $\mathcal{H}' = \operatorname{Span}\{e_1, \dots, e_j\} \subset \mathbb{K}^k$, where $j = j(h) \geq 1$ and $\{e_1, \dots, e_k\}$ denotes the canonical basis of \mathbb{K}^k ; notice that $\mathcal{H}' = R(V_k^*V_j)$. We also consider the principal angles

$$\Theta(\mathcal{W}, \mathcal{H}') = \operatorname{diag}(\theta_1(\mathcal{W}, \mathcal{H}'), \dots, \theta_j(\mathcal{W}, \mathcal{H}')) \in \mathbb{R}^{j \times j}.$$

By Proposition 5.1 we get that

$$\Theta(\mathcal{W}, \mathcal{H}') \le \Theta(\mathcal{X}, \mathcal{V}_j) < \frac{\pi}{2} I,$$

since $V_j \subset R(V_k)$ and $V_k^* V_j = \mathcal{H}'$, and the second inequality above follows from the fact that $\theta_i(\mathcal{X}, \mathcal{V}_j) \leq \theta_i(\mathcal{X}, \mathcal{S}) < \frac{\pi}{2}$, for $1 \leq i \leq j$, since $V_j \subset \mathcal{S}$ (see Section 2.1).

Step 4: computing the left dominant subspace S'. Let $\{w_1, \ldots, w_j\} \subset W$ and $\{f_1, \ldots, f_j\} \subset \mathcal{H}'$ be the principal vectors associated with W and \mathcal{H}' (as described in Section 2.1). Let W'

Span $\{w_1, \ldots, w_j\} \subset \mathcal{W}$; in this case, $\Theta(\mathcal{W}, \mathcal{H}') = \Theta(\mathcal{W}', \mathcal{H}')$, by construction. Consider the subspace $\mathcal{T}' = \phi(\Sigma_k) \mathcal{W}' \subset \mathcal{T}$ so $\dim(\mathcal{T}') = \dim(\mathcal{W}') = j = \dim(\mathcal{H}')$; since \mathcal{H}' is an invariant subspace of $\phi(\Sigma_k)$ then Proposition 5.2 implies that

$$\|\sin\Theta(\mathcal{T}',\mathcal{H}')\|_{2,F} \le \|\sin\Theta(\mathcal{W}',\mathcal{H}')\|_{2,F} = \|\sin\Theta(\mathcal{W},\mathcal{H}')\|_{2,F}$$

since $\|\phi(\Sigma_k)(I - P_{\mathcal{H}'})\|_2 \|\phi(\Sigma_k)^{-1}\|_2 = 1$, where we used that $\phi(\sigma_i) \ge \phi(\sigma_k) > 0$, for $1 \le i \le k$ and that $\phi(\sigma_{j+1}) = \phi(\sigma_k)$.

Let $\mathcal{T}'' = \mathcal{T} \ominus \mathcal{T}'$ so dim $\mathcal{T}'' = d - j$ and $\mathcal{T}'' \subset (\mathcal{T}')^{\perp}$. Since dim $((\mathcal{T}')^{\perp}) = \dim((\mathcal{H}')^{\perp})$, by Eq. (22) we see that

$$\|\Theta(\mathcal{T}'',(\mathcal{H}')^{\perp})\|_{2,F} \leq \|\Theta((\mathcal{T}')^{\perp},(\mathcal{H}')^{\perp})\|_{2,F} = \|\Theta(\mathcal{T}',\mathcal{H}')\|_{2,F} \leq \|\Theta(\mathcal{W},\mathcal{H}')\|_{2,F}.$$

Let $\{y_1, \ldots, y_{d-j}\} \subset \mathcal{T}''$ and $\{z_1, \ldots, z_{d-j}\} \subset (\mathcal{H}')^{\perp}$ be the principal vectors associated with \mathcal{T}'' and $(\mathcal{H}')^{\perp}$. Then, if we let $\mathcal{H}'' = \operatorname{Span}\{z_1, \ldots, z_{h-j}\}$ we have that $\dim \mathcal{H}'' = h - j$,

$$\|\sin\Theta(\mathcal{T}'',\mathcal{H}'')\|_{2,F} \le \|\sin\Theta(\mathcal{T}'',(\mathcal{H}')^{\perp})\|_{2,F} \le \|\sin\Theta(\mathcal{W},\mathcal{H}')\|_{2,F}$$
.

On the one hand, we have that $\mathcal{T} = \mathcal{T}' \oplus \mathcal{T}''$; on the other hand, we have that

$$\mathcal{S}' := U_k(\mathcal{H}' \oplus \mathcal{H}'') = \mathcal{U}_i \oplus U_k \mathcal{H}'' \subseteq \mathcal{U}_k \subseteq \mathbb{K}^m$$

is an h-dimensional left dominant subspace of A (see Section 2.3).

Step 5: obtaining some more upper bounds. Since

$$\|\sin\Theta(\mathcal{T}',\mathcal{H}')\|_{2,F}$$
, $\|\sin\Theta(\mathcal{T}'',\mathcal{H}'')\|_{2,F} \le \|\sin\Theta(\mathcal{W},\mathcal{H}')\|_{2,F}$

then Proposition 5.3 implies that $\|\sin\Theta(\mathcal{T},\mathcal{H}'\oplus\mathcal{H}'')\|_{2,F} \leq 2\|\sin\Theta(\mathcal{W},\mathcal{H}')\|_{2,F}$. Hence

$$\|(I - \Phi_k \Phi_k^{\dagger}) P_{\mathcal{S}'}\|_{2,F} = \|\sin\Theta(U_k \mathcal{T}, \mathcal{S}')\|_{2,F} \le 2 \|\sin\Theta(\mathcal{W}, \mathcal{H}')\|_{2,F},$$
(27)

since U_k is an isometry and $R(\Phi_k) = U_k \mathcal{T}$ (see Eq. (26)).

By Proposition 5.4, since $W = R(V_k^*X)$,

$$\Phi_k^{\dagger} = (V_k^* X)^{\dagger} (U_k \phi(\Sigma_k) P_{\mathcal{W}})^{\dagger}.$$

Since $U_k \in \mathbb{K}^{m \times k}$ has a trivial kernel, we get that

$$(U_k \phi(\Sigma_k) P_{\mathcal{W}})^{\dagger} = (\phi(\Sigma_k) P_{\mathcal{W}})^{\dagger} (U_k P_{\mathcal{T}})^{\dagger} = (\phi(\Sigma_k) P_{\mathcal{W}})^{\dagger} P_{\mathcal{T}} U_k^* = (\phi(\Sigma_k) P_{\mathcal{W}})^{\dagger} U_k^*$$

where we have used Proposition 5.4, that $(U_k P_T)^{\dagger} = (U_k P_T)^* = P_T U_k^*$ since $U_k P_T$ is a partial isometry and that $\ker((\phi(\Sigma_k)P_{\mathcal{W}})^{\dagger})^{\perp} = \mathcal{T}$. The previous facts show that

$$\Phi_{k,\perp}\Phi_k^{\dagger}P_{\mathcal{S}'} = U_{k,\perp}\phi(\Sigma_{k,\perp})V_{k,\perp}^*X(V_k^*X)^{\dagger}(\phi(\Sigma_k)P_{\mathcal{W}})^{\dagger}U_k^*P_{\mathcal{S}'}$$

so then,

$$\|\Phi_{k,\perp}\Phi_k^{\dagger} P_{\mathcal{S}'}\|_{2,F} \le \|\phi(\Sigma_{k,\perp})\|_2 \|\phi(\Sigma_k)^{-1}\|_2 \|V_{k,\perp}^* X (V_k^* X)^{\dagger}\|_{2,F}.$$
(28)

The result now follows from the estimates in Eqs. (23), (24) and (25) together with the bounds in Eqs. (27) and (28).

The cases in which j=0 or $k=\operatorname{rank}(A)$ can be dealt with similar arguments. Indeed, notice that if j=0 then we can take $\tilde{\mathcal{T}}\subset\mathcal{T}$ such that $\dim\tilde{\mathcal{T}}=h$, and set $\mathcal{S}'=U_k\tilde{\mathcal{T}}$. By construction, $\mathcal{S}'\subset R(\Phi_k)$ is a left dominant subspace of A (in this case any subspace of \mathcal{U}_k is a dominant subspace of A). Finally, in case $k=\operatorname{rank}(A)$ then $\Sigma_{k,\perp}=0$ and then $\phi(\Sigma_{k,\perp})=0$, so that we also get $\Phi_{k,\perp}=0$.

Some comments related to the previous proof are in order. We have followed the general lines of the proof of [6, Theorem 2.1]. Nevertheless, the assumption in [6] (i.e., that $R(V_k^*X) = R(V_k^*)$) automatically implies that $\|(I - \Phi_k \Phi_k^{\dagger}) P_{S'}\|_{2,F} = 0$ in Eq. (24). Since we are only assuming that the pair (A, X) is h-compatible, our arguments need to include Steps 3, 4 and the first part of Step 5.

With the notation of the proof, a careful inspection of the arguments above shows that the subspace S' can be computed explicitly (in terms of several objects that we describe below). We include the following pseudo-code of the construction of S', for the convenience of the reader. In the code, we invoke the construction (in terms of convenient singular value decompositions) of principal vectors corresponding to triplets (S, \mathcal{T}, j) as considered in Remark 4.3. We keep using Notation 4.1.

Algorithm 4.1 (Construction of S' as in Theorem 3.2)

Require: $A = U\Sigma V^* \in \mathbb{K}^{m\times n}$ a SVD of A, (a compatible) starting guess $X \in \mathbb{K}^{n\times r}$; rank parameters $0 \le j < h < k \le \text{rank}(A)$; power parameter $t \ge 0$; a polynomial $\phi(x) \in \mathbb{K}[x]$ of degree at most 2t + 1 with odd powers only, such that $\phi(\sigma_1), \ldots, \phi(\sigma_k) > 0$. Set

$$\mathcal{W} = R(V_k^* X)$$
, $\mathcal{T} = \phi(\Sigma_k) \mathcal{W}$, $\mathcal{H}' = R(V_k^* V_i)$.

Ensure: An h-dimensional left dominant subspace S' of A.

- 1: Compute principal vectors $\{w_1, \ldots, w_j\} \subset \mathcal{W}$ corresponding to $(\mathcal{W}, \mathcal{H}', j)$.
- 2: Set $\mathcal{W}' = \operatorname{Span}\{w_1, \dots, w_j\} \subset \mathcal{W}$ and compute $\mathcal{T}'' = \mathcal{T} \ominus \phi(\Sigma_k)\mathcal{W}'$.
- 3: Compute principal vectors $\{z_1,\ldots,z_{h-j}\}\subset (\mathcal{H}')^{\perp}$ corresponding to $(\mathcal{T}'',\,(\mathcal{H}')^{\perp},h-j)$.
- 4: Set $\mathcal{H}'' = \operatorname{Span}\{z_1, \dots, z_{h-j}\}$ and $\mathcal{S}' := U_k(\mathcal{H}' \oplus \mathcal{H}'') = U_j \oplus U_k(\mathcal{H}'')$.
- 5: Return: the left dominant subspace $\mathcal{S}' \subset \mathbb{K}^m$.

4.2 Proofs of Theorems 3.4, 3.5 and 3.7

Proof of Theorem 3.4. Under our present assumptions we have that $\Theta(R(X), \mathcal{V}_j) < \pi/2 I_j$ i.e. $R(V_j^*X) = \mathcal{V}_j$. In this case we can argue as in the proof of [6, Proof of Theorem 2.1] and conclude that

$$\|\sin\Theta(R(\Psi_q), \mathcal{V}_j)\|_{2,F} \leq \|\psi(\Sigma_{j,\perp}) \cdot \Sigma_{j,\perp}^2\|_2 \|(\psi(\Sigma_j) \cdot \Sigma_j^2)^{-1}\|_2 \|V_{j,\perp}^* X(V_j^* X)^{\dagger}\|_{2,F}.$$

where we used that $\psi(\sigma_1), \ldots, \psi(\sigma_j) > 0$ so that in this case $\psi(\Sigma_j) \cdot \Sigma_j^2$ is an invertible matrix. Moreover,

$$\|\psi(\Sigma_{j,\perp})\cdot\Sigma_{j,\perp}^2\|_2 \|(\psi(\Sigma_j)\cdot\Sigma_j^2)^{-1}\|_2 \leq \|\psi(\Sigma_{j,\perp})\|_2 \|\psi(\Sigma_j)^{-1}\|_2 \left(\frac{\sigma_{j+1}}{\sigma_i}\right)^2.$$

The result now follows from the previous inequalities and the identity $\sigma_{j+1}/\sigma_j = (1+\gamma_j)^{-1}$.

In what follows we make use of the next result from [6].

Lemma 4.4 ([6]). Assume that k < rank(A), so that $\sigma_k > \sigma_{k+1} > 0$, and let

$$\gamma_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_{k+1}} > 0.$$

Let $T_{2q}(x) \in \mathbb{R}[x]$ be the Chebyshev polynomial of the first kind of degree 2q. Then $T_{2q}(x)$ has even powers only. Furthermore, if we set $\psi(x) = T_{2q}(x/\sigma_{k+1})$ then

$$\psi(\sigma_1) > \dots > \psi(\sigma_{k+1}) = 1$$
 , $\psi(\sigma_i) \ge \frac{1}{4} (1 + \gamma_k) 2^{2q \min\{\sqrt{\gamma_k}, 1\}}$, for $1 \le i \le k$,

and $|\psi(\sigma_i)| \leq 1$, for $i \geq k+1$. Hence,

$$\|\psi(\Sigma_k)^{-1}\|_2 \|\psi(\Sigma_{k,\perp})\|_2 \le 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{1 + \gamma_k}.$$

We point out that the inequalities $\psi(\sigma_1) \geq \ldots \geq \psi(\sigma_{k+1})$ in the lemma above are a consequence of the super-linear growth for large input values (i.e., in this case for $x \geq \sigma_{k+1}$) of the gap amplifying Chebyshev polynomials (see [6]).

Proof of Theorem 3.5. Let $T_{2q}(x) \in \mathbb{R}[x]$ be the Chebyshev polynomial of the first kind of degree 2q. Since $\sigma_{k+1} > 0$ we can set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. By Lemma 4.4 we get that $\psi(\sigma_1) > \ldots > \psi(\sigma_{k+1}) = 1$ and hence

$$\|\psi(\Sigma_j)^{-1}\|_2 = \frac{1}{\psi(\sigma_j)}$$
 and $\|\psi(\Sigma_{j+1})\|_2 = \psi(\sigma_{j+1}) = \psi(\sigma_k)$.

Thus, Eq. (6) follows from Theorem 3.4 and the identities above.

Consider $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$; then

$$V_{k,\perp}^* \Psi_q (V_k^* \Psi_q)^\dagger = (\psi(\Sigma_{k,\perp}) \cdot \Sigma_{k,\perp}^2) V_{k,\perp}^* X ((\psi(\Sigma_k) \cdot \Sigma_k^2) V_k^* X)^\dagger \,.$$

Since $\psi(\Sigma_k) \cdot \Sigma_k^2 \in \mathbb{K}^{k \times k}$ is invertible, then Proposition 5.4 implies that

$$((\psi(\Sigma_k)\cdot\Sigma_k^2)V_k^*X)^\dagger = (V_k^*X)^\dagger ((\psi(\Sigma_k)\cdot\Sigma_k^2)P_{R(V_k^*X)})^\dagger.$$

Hence, the previous identities imply that

$$\|V_{k,\perp}^* \Psi_q(V_k^* \Psi_q)^{\dagger}\|_{2,F} \leq \|\psi(\Sigma_{k,\perp}) \cdot \Sigma_{k,\perp}^2\|_2 \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F} \|(\psi(\Sigma_k) \cdot \Sigma_k^2)^{-1}\|_2.$$

Again, by Lemma 4.4, we get that $\|\psi(\Sigma_{k,\perp})\cdot\Sigma_{k,\perp}^2\|_2 \leq \sigma_{k+1}^2$ while $\|(\psi(\Sigma_k)\cdot\Sigma_k^2)^{-1}\|_2 \leq (\psi(\sigma_k)\sigma_k^2)^{-1}$. Putting everything together, we get that

$$||V_{k,\perp}^* \Psi_q(V_k^* \Psi_q)^{\dagger}||_{2,F} \le \frac{1}{\psi(\sigma_k)} ||V_{k,\perp}^* X(V_k^* X)^{\dagger}||_{2,F} \left(\frac{\sigma_{k+1}}{\sigma_k}\right)^2.$$

Thus, Eq. (7) now follows from the previous inequalities and the identity $\sigma_{k+1}/\sigma_k = (1+\gamma_k)^{-1}$. Finally, notice that the first inequality in Eq. (8) was shown in Remark 3.6, while the second inequality is a consequence of Lemma 4.4.

Recall that given an h-compatible pair (A, X) we defined $C(A, X, j, k)_{2,F} = C_{2,F}$ as follows: if $h \le k < \text{rank}(A)$ and $1 \le j$ then

$$C_{2,F}(V,X) = C_{2,F} = \max \left\{ 2 \|V_{j,\perp}^* X(V_j^* X)^{\dagger}\|_{2,F}, \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F} \right\}. \tag{29}$$

If j = 0 we let $C_{2,F} = \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F}$; if k = rank(A) then we set $C_{2,F} = 2 \|V_{j,\perp}^* X(V_j^* X)^{\dagger}\|_{2,F}$.

Proof of Theorem 3.7. Assume first that $1 \leq j < h \leq k < \operatorname{rank}(A)$; notice that $\sigma_h = \sigma_k > \sigma_{k+1} > 0$, since $k < \operatorname{rank}(A)$. To obtain the claimed convergence analysis we follow the strategy described in Remark 3.3. Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. By Theorem 3.5, if we let $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2)V^*X$ then

$$\|\sin\Theta(R(\Psi_q), \mathcal{V}_j)\|_{2,F} \le \frac{\psi(\sigma_k)}{\psi(\sigma_j)} \|V_{j,\perp}^* X (V_j^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_j)^2}$$
(30)

$$\|V_{k,\perp}^* \Psi_q(V_k^* \Psi_q)^{\dagger}\|_{2,F} \le \frac{1}{\psi(\sigma_k)} \|V_{k,\perp}^* X(V_k^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_k)^2}. \tag{31}$$

Since $V_h^*\Psi_q = \psi(\Sigma_h) \Sigma_h^2 V_h^* X$ then $R(V_h^*\Psi_q) = R(V_h^*)$ so that the pair (A, Ψ_q) is h-compatible and $\dim \Psi_q \geq h$. If we apply Theorem 3.2 to this last pair with t=0 and $\phi(x)=x$ and consider Eqs. (30) and (31) above, we conclude that there exists an h-dimensional left dominant subspace $\mathcal{S}' \subset \mathbb{K}^m$ for A such that

$$\|\sin\Theta(\mathcal{K}_{0}(A,\Psi_{q}),\mathcal{S}')\|_{2,F} \leq 2\frac{\psi(\sigma_{k})}{\psi(\sigma_{j})} \|V_{j,\perp}^{*}X(V_{j}^{*}X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_{j})^{2}} + \frac{1}{1+\gamma_{k}} \frac{1}{\psi(\sigma_{k})} \|V_{k,\perp}^{*}X(V_{k}^{*}X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_{k})^{2}}.$$

where we have used the identity $\sigma_{k+1}/\sigma_k = (1+\gamma_k)^{-1}$. Since $x^2 \psi(x) \in \mathbb{R}[x]$ is a degree 2(q+1) polynomial with even powers only, then we get that $R(\Psi_q) \subset \mathbb{R}(\tilde{K}_q)$ where

$$\tilde{K}_q := K_q(A^*, AX) = (A^*(AX) \quad (A^*A)A^*(AX) \quad \cdots \quad (A^*A)^q A^*(AX)) \in \mathbb{K}^{n \times (q+1)r}$$
.

Thus, $\mathcal{K}_0(A, \Psi_q) \subset \mathcal{K}_0(A, \tilde{K}_q) \subset \mathcal{K}_{q+1}(A, X)$; using the properties of principal angles and the estimates above, we now see that

$$\|\sin\Theta(\mathcal{K}_{q+1}(A,X),\mathcal{S}')\|_{2,F} \leq \|\sin\Theta(\mathcal{K}_{0}(A,\Psi_{q}),\mathcal{S}')\|_{2,F}$$

$$\leq C_{2,F} \left(\frac{\psi(\sigma_{k})}{\psi(\sigma_{j})} \frac{1}{(1+\gamma_{j})^{2}} + \frac{1}{\psi(\sigma_{k})} \frac{1}{(1+\gamma_{k})^{3}}\right),$$

where $C_{2,F} = C_{2,F}(A, X)$ is defined as in Eq. (29).

The case j = 0 can be treated with similar arguments (the details are left to the reader). \square

Remark 4.5 (Construction of \mathcal{S}' as in Theorem 3.7). A simple inspection of the proof above shows that the h-dimensional left dominant subspace $\mathcal{S}' \subset \mathbb{K}^m$ as in Theorem 3.7 can be constructed using Algorithm 4.1 with starting guess $\Psi_q = V(\psi(\Sigma) \cdot \Sigma^2) V^* X \in \mathbb{K}^{n \times r}$ and setting t = 0 (the rest of the parameters remain the same). Notice that this is in accordance with the general strategy described in Remark 3.3.

4.3 Proof of Theorems 3.8, 3.9, 3.10 and 3.11.

Throughout this section we consider Notation 4.1 and the notation from Theorem 3.10. In particular, we consider Algorithm 2.1 with input: $A \in \mathbb{K}^{m \times n}$, starting guess $X \in \mathbb{K}^{n \times r}$; moreover, we set our target rank to: $1 \leq h \leq \text{rank }(A)$. We let $U_K \in \mathbb{K}^{m \times d}$ denote the matrix whose columns form an orthonormal basis of the Krylov space \mathcal{K}_{q+1} constructed in terms of A and X, for some fixed $q \geq 0$; further, we let $\hat{U}_i \in \mathbb{K}^{m \times i}$ denote the matrix whose columns are the top i columns of the output \hat{U}_h of Algorithm 2.1, for $1 \leq i \leq h$. We mostly focus on the case in which $1 \leq j < h \leq k < \text{rank}(A)$; notice that in this case we have that $\sigma_h = \sigma_k > 0$, since $h \leq \text{rank}(A)$. The cases j = 0 or k = rank(A) can be treated with similar arguments (the details are left to the reader).

In what follows we make use of the constants $\delta_{2,F}$ given by: for k < rank(A) then let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q, $\psi(x) = T_{2q}(x/\sigma_{k+1})$ and set

$$\delta_{2,F} := \sqrt{2} C_{2,F} \left(\frac{\psi(\sigma_k)}{\psi(\sigma_j)} \frac{1}{(1+\gamma_j)} + \frac{1}{\psi(\sigma_k)} \frac{1}{(1+\gamma_k)^2} \right), \tag{32}$$

where $C_{2,F}$ is defined as in Eq. (29). In case j=0 the first term should be omitted. In case $k=\operatorname{rank}(A)$ and $1\leq j$, then let $\psi(x)=T_{2q}(x/\sigma_k)$ and set

$$\delta_{2,F} := \frac{\sqrt{2}}{\psi(\sigma_j)} \frac{C_{2,F}}{(1+\gamma_j)}. \tag{33}$$

Proof of Theorem 3.8. We first assume that $1 \leq j < h \leq k < \text{rank}(A)$ so $\gamma_k > 0$. Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$. Consider $\tilde{\Psi}_q := U\left(\psi(\Sigma) \cdot \Sigma\right) V^*X \in \mathbb{K}^{m \times r}$ and notice that $A^*\tilde{\Psi}_q = V\left(\left(\psi(\Sigma) \cdot \Sigma^2\right) V^*X = \Psi_q$. Arguing as in the proof of Theorem 3.5 we get that

$$\|\sin\Theta(R(\tilde{\Psi}_q),\mathcal{U}_j)\|_{2,F} \le \frac{\psi(\sigma_k)}{\psi(\sigma_j)} \|V_{j,\perp}^* X (V_j^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_j)},$$

$$\|U_{k,\perp}^* \tilde{\Psi}_q(U_k^* \tilde{\Psi}_q)^{\dagger}\|_{2,F} \leq \frac{1}{\psi(\sigma_k)} \|V_{k,\perp}^* X (V_k^* X)^{\dagger}\|_{2,F} \frac{1}{(1+\gamma_k)}.$$

Notice that $U_h^*\tilde{\Psi}_q = \psi(\Sigma_h) \, \Sigma_h^2 \, V_h^* X$ so that $R(U_h^*\tilde{\Psi}_q) = R(U_h^*)$ and the pair $(A^*, \tilde{\Psi}_q)$ is h-compatible. Using the previous estimates together with Theorem 3.2 applied to the matrix A^* , the starting guess matrix $\tilde{\Psi}_q$ and t=0 (with $\phi(x)=x$) we get that there exists an h-dimensional right dominant subspace $\tilde{\mathcal{S}} \subset \mathbb{K}^n$ of A such that

$$\|\sin\Theta(R(\Psi_q),\tilde{\mathcal{S}})\|_{2,F} \le C_{2,F} \left(\frac{\psi(\sigma_k)}{\psi(\sigma_i)} \frac{1}{(1+\gamma_i)} + \frac{1}{\psi(\sigma_k)} \frac{1}{(1+\gamma_k)^2}\right) = \frac{\delta_{2,F}}{\sqrt{2}},\tag{34}$$

where we have used that $R(A^*\tilde{\Psi}_q) = R(\Psi_q)$ and $C_{2,F}$ is defined as in Eq. (29). Hence, by Eq. (34) and our hypotheses we now see that

$$\Theta(R(\Psi_q), \tilde{\mathcal{S}}) \le \frac{\pi}{4} I. \tag{35}$$

On the other hand, arguing as in the proof of Theorem 3.7 we see that $R(A\Psi_q) \subset \mathcal{K}_{q+1}(A,X)$. We now set $A_{\tilde{S}} = A P_{\tilde{S}}$, where $P_{\tilde{S}}$ denotes the orthogonal projection onto $\tilde{S} \subset \mathbb{K}^n$. In this case we get that $A = A_{\tilde{S}} + (A - A_{\tilde{S}})$ so that $A_{\tilde{S}}(A - A_{\tilde{S}})^* = A P_{\tilde{S}}(I - P_{\tilde{S}})A^* = 0$. If we let $V_{\tilde{S}} \in \mathbb{K}^{n \times h}$ denote the top right singular vectors of $A_{\tilde{S}}$ then $R(V_{\tilde{S}}) = \tilde{S}$. Notice that Eq. (35) implies that $R(V_{\tilde{S}}^*\Psi_q) = R(V_{\tilde{S}}^*)$ so we can apply Lemma 5.6 in this context. Hence, we consider the principal vectors $\{w_1, \ldots, w_h\} \subset \Psi_q$, corresponding to the pair of subspaces $(R(\Psi_q), \tilde{S})$; we also let $Q \in \mathbb{K}^{n \times h}$ be an isometry with columns w_1, \ldots, w_h so that $R(AQ) \subset R(A\Psi_q) \subset \mathcal{K}_{q+1}$. Recall that U_K (being the output of Algorithm 2.1 with power parameter set to q+1) denotes the matrix whose columns form an orthonormal basis of the Krylov space \mathcal{K}_{q+1} . Then, the previous facts together with Lemma 5.6 show that

$$||A_{\tilde{S}} - U_K U_K^* A_{\tilde{S}}||_{2,F} \leq ||(I - AQ(AQ)^{\dagger}) A_{\tilde{S}}||_{2,F} = ||A_{\tilde{S}} - AQ(AQ)^{\dagger} A_{\tilde{S}}||_{2,F} \leq ||A - A_{\tilde{S}}||_{2} ||\tan \Theta(R(\Psi_q), \tilde{S})||_{2,F}.$$

On the one hand, $||A - A_{\tilde{S}}||_2 = \sigma_{h+1}$, since \tilde{S} is an h-dimensional right dominant subspace of A. On the other hand, Eq. (35) also implies that

$$\|A-A_{\tilde{\mathcal{S}}}\|_2 \|\tan\Theta(R(\Psi_q),\tilde{\mathcal{S}})\|_{2,F} \leq \sigma_{h+1} \sqrt{2} \|\sin\Theta(R(\Psi_q),\tilde{\mathcal{S}})\|_{2,F} \leq \sigma_{h+1} \, \delta_{2,F} \,,$$

where we have also used Eq. (34).

Proof of Theorem 3.9. We keep using the notation from the proof of Theorem 3.8 above. As a consequence of Theorem 3.8 and Lidskii's inequality for singular values, we get that

$$|\sigma_i(A P_{\tilde{\mathcal{S}}}) - \sigma_i(U_K U_K^* A P_{\tilde{\mathcal{S}}})| \le ||A P_{\tilde{\mathcal{S}}} - U_K U_K^* A P_{\tilde{\mathcal{S}}}||_2 \le \sigma_{h+1} \delta_2, \ 1 \le i \le h.$$

Therefore, for $1 \leq i \leq h$, we have that

$$\sigma_i(A) \ge \sigma_i(U_K U_K^* A) = \sigma_i(\hat{A}_h) \ge \sigma_i(U_K U_K^* A P_{\tilde{S}}) \ge \sigma_i(A P_{\tilde{S}}) - \sigma_{h+1} \delta_2.$$

The result now follows from the previous facts and the identities $\sigma_i(AP_{\tilde{S}}) = \sigma_i(A)$, for $1 \leq i \leq h$. \square

Proof of Theorem 3.10. We keep using the notation from the proof of Theorem 3.8 above. In particular, we consider the existence of an h-dimensional right dominant subspace $\tilde{\mathcal{S}}$ for A that satisfies Eq. (34). We now argue as in the proof of [6, Theorem 2.3.] and consider the estimate for the Frobenius norm first. Indeed, by [3, Lemma 8] we have that

$$A - \hat{U}_i \hat{U}_i^* A = A - U_K (U_K^* A)_i \quad \text{for} \quad 1 \le i \le h,$$

where $(U_K^*A)_i$ denotes a best rank-*i* approximation of U_K^*A . By the same result, we also get that $U_K(U_K^*A)_i$ is a best rank-*i* approximation of A from $R(U_K)$ in the Frobenius norm i.e.,

$$||A - U_K(U_K^*A)_i||_F = \min_{\text{rank}(Y) < i} ||A - U_KY||_F.$$
(36)

We now consider a SVD, $A = U\Sigma V^*$ such that the top h columns of V span the h-dimensional right dominant subspace $R(V_h) = \mathcal{V}_h = \tilde{\mathcal{S}}$ (recall that this can always be done). For $1 \leq i \leq h$ we set

$$A = A_i + A_{i,\perp}$$
 where $A_i = U_i \Sigma_i V_i^*$ and $A_{i,\perp} = A - A_i$

Then, by [6, Lemma 7.2] we get that

$$||A - \hat{U}_i \hat{U}_i^* A||_F^2 \le ||A - A_i||_F^2 + ||A_i - U_K U_K^* A_i||_F^2.$$
(37)

Now we bound the second term in Eq. (37). Under the present notation, we get that $\Theta(R(V_h), R(\Psi_q)) \leq \frac{\pi}{4} I_h$, by Eq. (35). Hence, $\Theta(R(V_i), R(\Psi_q)) \leq \frac{\pi}{4} I_i$ (see Section 2.1) and we see that $R(V_i^* \Psi_q) = R(V_i^*)$, for $1 \leq i \leq h$. Thus, we can apply Lemma 5.6 in this context. Hence, we consider the principal vectors $\{w_1, \ldots, w_i\} \subset R(\Psi_q)$ corresponding to the pair $(R(\Psi_q), R(V_i))$. Moreover, we let $Q \in \mathbb{K}^{n \times i}$ be an isometry with $R(Q) = \operatorname{Span}\{w_1, \ldots, w_i\}$ so that $R(AQ) \subset R(A\Psi_q) \subset \mathcal{K}_{q+1}$. The previous facts together with Lemma 5.6 show that

$$||A_{i} - U_{K}U_{K}^{*}A_{i}||_{F} \leq ||(I - AQ(AQ)^{\dagger})A_{i}||_{F} = ||A_{i} - AQ(AQ)^{\dagger}A_{i}||_{F}$$

$$\leq ||A - A_{i}||_{2} ||\tan \Theta(R(\Psi_{q}), R(V_{i}))||_{F}$$

$$\leq ||A - A_{i}||_{2} ||\tan \Theta(R(\Psi_{q}), R(V_{h}))||_{F}.$$

By Eq. (35) we get that $\Theta(R(V_h), R(\Psi_q)) = \Theta(\tilde{S}, R(\Psi_q)) \leq \frac{\pi}{4} I$; then,

$$\| \tan \Theta(R(\Psi_q), R(V_h)) \|_F \le \sqrt{2} \| \sin \Theta(R(\Psi_q), R(V_h)) \|_F \le \delta_F$$

where we have used Eq. (34). Therefore, the previous inequalities imply that

$$||A - \hat{U}_i \hat{U}_i^* A||_F^2 \le ||A - A_i||_F^2 + (\sigma_{i+1} \cdot \delta_F)^2.$$
(38)

This proves the upper bound in Eq. (18) for the Frobenius norm. To prove the bound for the spectral norm, recall that by [12, Theorem 3.4.] we get that Eq. (38) implies that

$$||A - \hat{U}_i \hat{U}_i^* A||_2^2 \le ||A - A_i||_2^2 + (\sigma_{i+1} \cdot \delta_F)^2$$
,

since $\operatorname{rank}(\hat{U}_i\hat{U}_i^*A) \leq i$. The upper bound in (18) for the spectral norm follows from this last fact.

Proof of Theorem 3.11. Let us fix an h-compatible pair (A, X) and assume that $0 \le j < h \le k < \operatorname{rank}(A)$. We follow the conventions: $\gamma_0 = +\infty$ in case j = 0. Let $T_{2q}(x)$ be the Chebyshev polynomial of the first kind of degree 2q and set $\psi(x) = T_{2q}(x/\sigma_{k+1})$; in this case, by Theorem 3.5 we get that

$$\frac{\psi(\sigma_k)}{\psi(\sigma_j)} \le \frac{1}{(1+\gamma_j)^{2q}} \quad \text{and} \quad \frac{1}{\psi(\sigma_k)} \le 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1+\gamma_k)}.$$

Hence, if we let $\delta_{2,F}$ be defined as in Eq. (32) then we get that

$$\delta_{2,F} \le \sqrt{2} C_{2,F} \left(\frac{1}{(1+\gamma_j)^{2q+1}} + 4 \frac{2^{-2q \min\{\sqrt{\gamma_k}, 1\}}}{(1+\gamma_k)^3} \right). \tag{39}$$

Thus, if Eq. (19) is satisfied then $\delta_2 \leq 1$. In this case, we can apply Theorems 3.9 and 3.10 and get, for $1 \leq i \leq h$:

$$\sigma_i - \sigma_{h+1} \cdot \delta_2 \le \sigma_i(\hat{A}_h) \le \sigma_i$$
 and $||A - \hat{U}_i\hat{U}_i^*A||_{2,F} \le ||A - A_i||_{2,F} + \sigma_{i+1} \cdot \delta_F$.

Therefore, the result is a consequence of the previous two bounds together with the estimate in Eq. (39).

5 Appendix

In this section we include several technical results that were used in the proofs of the main results. Most of these technical results are elementary and can be found in the literature; we include the versions that are best suited for our exposition together with their proofs, for the convenience of the reader.

Proposition 5.1. Let $V \in \mathbb{K}^{n \times k}$ be an isometry and let \mathcal{V}' , $\mathcal{X} \subset \mathbb{K}^n$ be subspaces such that $\dim \mathcal{X} \geq \dim \mathcal{V}' = j$, $\mathcal{V}' \subset (\ker V^*)^{\perp} = R(V)$ and $\Theta(\mathcal{X}, \mathcal{V}') < \pi/2 I_j$. Then $\mathcal{W} = V^* \mathcal{X} \subset \mathbb{K}^k$ is such that $\dim \mathcal{W} \geq j$ and if we let $\mathcal{H}' = V^* \mathcal{V}'$ then

$$\Theta(\mathcal{W}, \mathcal{H}') \leq \Theta(\mathcal{X}, \mathcal{V}') \in \mathbb{R}^{j \times j}$$
.

Proof. First notice that

$$P_{\mathcal{X}}P_{\mathcal{Y}'}P_{\mathcal{X}} < P_{\mathcal{X}}VV^*P_{\mathcal{X}}$$
.

By hypothesis $\operatorname{rank}(P_{\mathcal{X}}P_{\mathcal{V}'}P_{\mathcal{X}}) = j$ which shows that $\dim \mathcal{W} = \operatorname{rank}(V^*P_{\mathcal{X}}) \geq j$. On the other hand, since V is an isometry then $\Theta(\mathcal{W}, \mathcal{H}') = \Theta(V\mathcal{W}, V\mathcal{H}') = \Theta(VV^*\mathcal{X}, \mathcal{V}')$. Consider $D = VV^*P_{\mathcal{X}}VV^*$; then $R(D) = VV^*\mathcal{X}$, so $\dim R(D) = \dim \mathcal{W} \geq j$. Moreover,

$$0 \le D \le P_{R(D)} \implies P_{\mathcal{V}'} P_{\mathcal{X}} P_{\mathcal{V}'} = P_{\mathcal{V}'} D P_{\mathcal{V}'} \le P_{\mathcal{V}'} P_{R(D)} P_{\mathcal{V}'},$$

where we used that $P_{\mathcal{V}'}VV^* = P_{\mathcal{V}'}$. Then, $\cos^2\Theta(\mathcal{X},\mathcal{V}') \leq \cos^2\Theta(VV^*\mathcal{X},\mathcal{V}') \in \mathbb{R}^{j\times j}$ and the result follows from the fact that $f(x) = \cos^2(x)$ is a decreasing function on $[0,\pi/2]$.

Proposition 5.2. Let $B \in \mathbb{K}^{k \times k}$ be such that $B = B^*$ and let \mathcal{H}' , $\mathcal{W}' \subset \mathbb{K}^k$ be subspaces such that $P_{\mathcal{H}'}B = BP_{\mathcal{H}'}$, dim $\mathcal{H}' = \dim \mathcal{W}'$ and \mathcal{H}' , $\mathcal{W}' \subset \ker(B)^{\perp}$. If we let $B\mathcal{W}' = \mathcal{T}'$,

$$\|\sin\Theta(\mathcal{H}',\mathcal{T}')\|_{2,F} \le \|B(I-P_{\mathcal{H}'})\|_2 \|B^{\dagger}\|_2 \|\sin\Theta(\mathcal{H}',\mathcal{W}')\|_{2,F}$$
.

Proof. Notice that $(BP_{\mathcal{H}'})^{\dagger} = P_{\mathcal{H}'}B^{\dagger} = B^{\dagger}P_{\mathcal{H}'}$. Then,

$$(I - P_{\mathcal{H}'})P_{\mathcal{T}'} = (I - P_{\mathcal{H}'})(BP_{\mathcal{W}'})(BP_{\mathcal{W}'})^{\dagger} = (B(I - P_{\mathcal{H}'}))(I - P_{\mathcal{H}'})P_{\mathcal{W}'}(BP_{\mathcal{W}'})^{\dagger}.$$

Also, notice that $(BP_{\mathcal{W}'})^{\dagger} = P_{\mathcal{W}'}B^{\dagger}P_{\mathcal{T}'}$; in particular, $\|(BP_{\mathcal{W}'})^{\dagger}\|_2 \leq \|B^{\dagger}\|_2$. Finally, since dim $\mathcal{T}' = \dim \mathcal{W}' = \dim \mathcal{H}'$ the previous facts imply that

$$\|\sin\Theta(\mathcal{H}',\mathcal{T}')\|_{2,F} < \|B(I-P_{\mathcal{H}'})\|_2 \|B^{\dagger}\|_2 \|\sin\Theta(\mathcal{H}',\mathcal{W}')\|_{2,F}$$
.

Proposition 5.3. Let \mathcal{T}' , \mathcal{T}'' and \mathcal{H}' , \mathcal{H}'' be pairs of mutually orthogonal subspaces in \mathbb{K}^k , such that $\dim(\mathcal{H}') \leq \dim(\mathcal{T}')$ and $\dim(\mathcal{H}'') \leq \dim(\mathcal{T}'')$. Consider the subspaces in \mathbb{K}^k given by the (orthogonal) sums $\mathcal{T} = \mathcal{T}' \oplus \mathcal{T}''$ and $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}''$, so $\dim(\mathcal{H}) \leq \dim(\mathcal{T})$. In this case we have that

$$\|\sin\Theta(\mathcal{T},\mathcal{H})\|_{2,F} \le \|\sin\Theta(\mathcal{T}',\mathcal{H}')\|_{2,F} + \|\sin\Theta(\mathcal{T}'',\mathcal{H}'')\|_{2,F}$$
.

Proof. We will make use of the following fact: given two subspaces $\mathcal{R}, \mathcal{S} \subset \mathbb{K}^k$ of the same dimension d then the non-zero singular values of $P_{\mathcal{R}} - P_{\mathcal{S}}$ coincide with the non-zero entries of $(\sin(\theta_d), \sin(\theta_d), \ldots, \sin(\theta_1), \sin(\theta_1))$, where $\Theta(\mathcal{R}, \mathcal{S}) = \operatorname{diag}(\theta_1, \ldots, \theta_d)$. In particular, $\|\sin\Theta(\mathcal{R}, \mathcal{S})\|_2 = \|P_{\mathcal{R}} - P_{\mathcal{S}}\|_2$ and $\sqrt{2} \|\sin\Theta(\mathcal{R}, \mathcal{S})\|_F = \|P_{\mathcal{R}} - P_{\mathcal{S}}\|_F$.

Let $\mathcal{T}_0' \subset \mathcal{T}'$ and $\mathcal{T}_0'' \subset \mathcal{T}''$ be such that $\dim \mathcal{T}_0' = \dim \mathcal{H}'$, $\dim \mathcal{T}_0'' = \dim \mathcal{H}''$ and $\Theta(\mathcal{T}', \mathcal{H}') = \Theta(\mathcal{T}_0', \mathcal{H}')$, $\Theta(\mathcal{T}'', \mathcal{H}'') = \Theta(\mathcal{T}_0'', \mathcal{H}'')$. Let $\mathcal{T}_0 = \mathcal{T}_0' \oplus \mathcal{T}_0'' \subset \mathcal{T}$; since $\dim \mathcal{H} = \dim \mathcal{T}_0$ we get that $\Theta(\mathcal{H}, \mathcal{T}) \leq \Theta(\mathcal{H}, \mathcal{T}_0)$. The previous remarks show that we can assume further that $\dim \mathcal{T}' = \dim \mathcal{H}'$ and $\dim \mathcal{T}'' = \dim \mathcal{H}''$, so that $\dim \mathcal{T} = \dim \mathcal{H}$. In this case we have that

$$\|\sin\Theta(\mathcal{T},\mathcal{H})\|_{2} = \|P_{\mathcal{T}} - P_{\mathcal{H}}\|_{2} \le \|P_{\mathcal{T}'} - P_{\mathcal{H}'}\|_{2} + \|P_{\mathcal{T}''} - P_{\mathcal{H}''}\|_{2}$$
$$= \|\sin\Theta(\mathcal{T}',\mathcal{H}')\|_{2} + \|\sin\Theta(\mathcal{T}'',\mathcal{H}'')\|_{2},$$

where we used that $P_{\mathcal{T}} = P_{\mathcal{T}'} + P_{\mathcal{T}''}$ and $P_{\mathcal{H}} = P_{\mathcal{H}'} + P_{\mathcal{H}''}$. The Frobenius norm can be handled similarly.

Proposition 5.4. Let $B \in \mathbb{K}^{p \times q}$ and let $C \in \mathbb{K}^{q \times r}$ with $R(C) = \mathcal{V} \subset \mathbb{K}^q$ such that $\mathcal{V} \subset \ker B^{\perp}$.

$$(BC)^{\dagger} = C^{\dagger} (BP_{\mathcal{V}})^{\dagger} .$$

Proof. In this case R(BC) = BV and $\ker BC = \ker C$. Moreover,

$$BCC^{\dagger}(BP_{\mathcal{V}})^{\dagger} = BP_{\mathcal{V}}(BP_{\mathcal{V}})^{\dagger} = P_{B\mathcal{V}}$$
 and

$$C^{\dagger}(BP_{\mathcal{V}})^{\dagger}BC = C^{\dagger}(BP_{\mathcal{V}})^{\dagger}BP_{\mathcal{V}}C = C^{\dagger}P_{\ker(BP_{\mathcal{V}})^{\perp}}C = P_{\ker C^{\perp}}\,,$$

where we used that $\ker(BP_{\mathcal{V}}) = \mathcal{V}^{\perp}$, since $\mathcal{V} \subset \ker B^{\perp}$.

Let $C \in \mathbb{K}^{m \times c}$ have rank p. For $1 \leq i \leq p$ we define

$$\mathcal{P}^{\xi}_{C,i}(A) = C \cdot \operatorname{argmin}_{\operatorname{rank}(Y) \le i} ||A - CY||_{\xi} \quad \text{ for } \quad \xi = 2, F.$$

Due to the optimality properties of the projection CC^{\dagger} (see [12]) we get that

$$||A - CC^{\dagger}A||_{\xi} \le ||A - \mathcal{P}_{C,i}^{\xi}(A)||_{\xi} \quad \text{for} \quad \xi = 2, F.$$
 (40)

The following result is [26, Lemma C.5] (see also [3]).

Lemma 5.5 ([26]). Let $A \in \mathbb{K}^{m \times n}$ and consider a decomposition $A = A_1 + A_2$, with $rank(A_1) = i$. Let $V_1 \in \mathbb{K}^{n \times i}$ denote the top right singular vectors of A_1 . Let $Z \in \mathbb{K}^{n \times p}$ be such that $rank(V_1^*Z) = i$ and let C = AZ. Then $rank(C) \geq i$ and

$$||A_1 - \mathcal{P}_{C,i}^{\xi}(A_1)||_{\xi} \le ||A_2 Z(V_1^* Z)^{\dagger}||_{\xi} \quad \text{for} \quad \xi = 2, F.$$

The following is a small variation of [26, Lemma C.1]

Lemma 5.6. Let $A \in \mathbb{K}^{m \times n}$ and consider the decomposition $A = A_1 + A_2$, with $A_1 A_2^* = 0$ and $rank(A_1) = i$. Let $V_1 \in \mathbb{K}^{n \times i}$ and $V_2 \in \mathbb{K}^{n \times (n-i)}$ denote the top right singular vectors of A_1 and A_2 respectively. Let $\tilde{\mathcal{K}} \subset \mathbb{K}^n$ be a subspace such that $V_1^*(\tilde{\mathcal{K}}) = R(V_1^*)$. Let $\{x_1, \ldots, x_i\} \subset \tilde{\mathcal{K}}$ denote the principal vectors corresponding to the pair $(\tilde{\mathcal{K}}, R(V_1))$ and let $Q \in \mathbb{K}^{n \times i}$ be an isometry with $R(Q) = Span(\{x_1, \ldots, x_i\}) \subset \tilde{\mathcal{K}}$. Then,

$$||A_1 - (AQ)(AQ)^{\dagger} A_1||_{2,F} \le ||A - A_1||_2 || \tan \Theta(\tilde{\mathcal{K}}, R(V_1))||_{2,F}.$$

Proof. Notice that by construction

$$\Theta(R(Q), R(V_1)) = \Theta(\tilde{\mathcal{K}}, R(V_1)) < \frac{\pi}{2} I.$$

Then, we get that rank(AQ) = i. Hence, we have that

$$\begin{split} \|A_1 - (AQ)(AQ)^{\dagger} A_1\|_{2,F} & \leq \|A_1 - \mathcal{P}_{AQ,i}^{2,F}(A_1)\|_{2,F} \leq \|A_2 Q(V_1^* Q)^{\dagger}\|_{2,F} \\ & \leq \|A_2\|_2 \|V_2^* Q(V_1^* Q)^{\dagger}\|_{2,F} \\ & = \|A_2\|_2 \|\tan\Theta(R(Q),R(V_1))\|_{2,F} \\ & = \|A - A_1\|_2 \|\tan\Theta(\tilde{\mathcal{K}},R(V_1))\|_{2,F} \,, \end{split}$$

where we have used Eq. (40), Lemma 5.5, that the isometry V_2 satisfies that $A_2 = A_2 V_2 V_2^*$ and the identity $||V_2^*Q(V_1^*Q)^{\dagger}||_{2,F} = ||\tan\Theta(R(Q),R(V_1))||_{2,F}V_1))||_{2,F}$, that holds by [6, Lemma 4.3], since $\operatorname{rank}(V_1^*Q) = i$.

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