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

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Abstract

In this work we obtain results related to 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 case 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 \( p = \min\{m, n\} \)). To do this, we develop a novel perspective for the convergence analysis of the classical deterministic block Krylov methods in this context. Indeed, starting with a 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 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 \( h \) (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 [19]). It is well known that truncated singular value decompositions (SVD) 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, 10, 14, 19]). 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 \( 1 \leq h \leq \text{rank}(A) \), recall that the 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 \( \Sigma_h \) 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 \( \text{rank}(B) \leq h \), where \( \| \cdot \|_{2,F} \) stand for spectral and Frobenius norms respectively. Nevertheless, it is well known that (in general) computation of the SVD of a matrix is expensive. In turn, this last fact is one of the motivations for the efficient numerical computation of approximations of truncated SVD of matrices [5, 11, 12, 18, 19, 22, 23].

A closer look at these 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 subspace \( \mathcal{U}_h \), spanned by the top \( h \) columns of \( U \). Hence, one of the main strategies for computing low-rank approximations is the computation of \( h \)-dimensional subspaces \( \mathcal{S}' \subset \mathbb{K}^m \) that are related (in some sense) to the left dominant subspaces \( \mathcal{U}_h \) of \( A \) corresponding to SVD’s of \( A \).

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 of convenient \( h \)-dimensional subspaces \( R(P) = \mathcal{S}' \) (equivalently, orthonormal sets of \( h \) vectors); here \( R(B) \) denotes the range of a matrix \( B \). Among others, implementations of the block power and block Krylov methods have become very popular. The applications of these methods are based on deterministic and randomized approaches. Randomized methods [6, 7, 11, 12, 18] 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 compatibility assumptions with the structure of \( A \), regardless of the particular choice of \( A \) (see [4]).

Yet, even if \( PA \) is a good low-rank approximation of \( A \), the range \( R(PA) \subset \mathbb{K}^m \) might actually not be close to the subspaces \( \mathcal{U}_h \subset \mathbb{K}^m \); here, the distance between subspaces is measured in terms of the principal angles between them. To derive low-rank approximations that also share some other features with \( A \), it seems natural to consider subspaces \( \mathcal{S}' \) that are close to the subspaces \( \mathcal{U}_h \). Moreover, these subspaces can be used to construct approximated truncated SVD and are also relevant in the study of principal component analysis [14]. As opposed to the low-rank approximation problem, there is an obstruction to consider the approximation of the subspaces \( \mathcal{U}_h \), namely that they are not uniquely determined unless there is a singular gap \( \sigma_h > \sigma_{h+1} \). In case there is a singular gap, then \( \mathcal{U}_h \) has structural relations with \( A \), and there are several positive results (both deterministic and randomized) in this setting. Indeed, subspaces \( \mathcal{S}' \) that are close to \( \mathcal{U}_h \) can be obtained in terms of the block power or block Krylov methods, and a starting guess matrix \( X \in \mathbb{K}^{n \times r} \) for \( r \geq h \), that satisfies some compatibility assumptions in terms of \( V_h^* \) [5, 20, 22].

In this work, we adopt a deterministic approach and adapt some of the main ideas of [5], to deal with the approximation of \( \mathcal{U}_h \), in case there is no singular gap at the index \( h \) (i.e. \( \sigma_h = \sigma_{h+1} \)). Thus, our results complement the convergence analysis in [5] (that was obtained under the assumption of the singular gap \( \sigma_h > \sigma_{h+1} \)). On the other hand, the no singular gap case is of interest due to the common occurrence of repeated singular values in applications with some degree of symmetry.

To do this, 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 with \( r = h \) (i.e. for a minimal choice of \( r \)). Our approach is based on enclosing \( \sigma_j > \sigma_h = \sigma_{h+1} = \sigma_k > \sigma_{k+1} \) in such a way that \( j < h \) and \( k \geq h \).
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 \( h \)-dimensional approximations of left and right \( h \)-dominant subspaces. Moreover, we show that block Krylov spaces can also be used to compute arbitrarily good low-rank approximations of \( A \), even if there is no singular gap (see Section 2.2 for a detailed description of the problems mentioned above).

The paper is organized as follows. In Section 2.1 we recall the notions of principal angles and principal vectors between subspaces, that play a central role in our work. In Section 2.2 we describe the context and main problems considered in this work. In Section 3 we include some of the main results from [5] related to the convergence analysis of the block Krylov methods, assuming the existence of a singular gap at a prescribed index. In Sections 3.1 and 3.2 we state our main results on \( h \)-dimensional dominant subspace approximations and low-rank approximations by matrices of rank \( h \), when there is no singular gap at the index \( h \). In Section 3.3 we include some remarks and comments on the results herein and previous work on these matters. We also include a brief discussion of some open problems. 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. Finally we include a description of some of the main results in [5]. These results, which are obtained under the assumption of a singular gap at a prescribed index, also serve as a model for the type of convergence analysis that we are interested in.

### 2.1 Principal angles between subspaces

**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 [10], we define the principal angles between \( S \) and \( T \), denoted

\[
0 \leq \theta_1(S, T) \leq \ldots \leq \theta_k(S, T) \leq \frac{\pi}{2} \quad \text{where} \quad k = \min\{s, t\},
\]

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

\[
\sin(\theta_{s-j+1}(S, T)) = \sigma_j((I - TT^*)S) = \sigma_j((I - TT^*)SS^*) = \sigma_j((I - P_T)PS)
\]

for \( 1 \leq j \leq s \), where \( P_H \in \mathbb{K}^{n \times n} \) denotes the orthogonal projection onto a subspace \( H \subset \mathbb{K}^n \); it is worth noticing that in this last case the roles of \( S \) and \( T \) (equivalently the roles of \( P_T \) and \( P_T \)) 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 [21] we let \( \Theta(S, T) = \text{diag}(\theta_1(S, T), \ldots, \theta_s(S, T)) \) denote the diagonal matrix with the principal angles in its main diagonal. In particular,

\[
\| \sin(\Theta(S, T)) \|_{2,F} = \| (I - P_T)PS \|_{2,F}
\]

are scalar measures of the (angular) distance between \( S \) and \( T \) (see [10, 21]).

We mention some properties of the principal angles between subspaces that we will need in what follows. With the previous notation, we point out that if \( S' \subset S \) and \( T \subset T' \) are subspaces with dimensions \( s' \) and \( t' \) respectively, then (recall that \( s = \dim S \leq \dim T = t \))

\[
\| \Theta(S, T') \|_{2,F} \leq \| \Theta(S, T) \|_{2,F} \quad , \quad \| \sin(\Theta(S, T')) \|_{2,F} \leq \| \sin(\Theta(S, T)) \|_{2,F}
\]
and similarly
\[ \|\Theta(S', T)\|_{2,F} \leq \|\Theta(S, T)\|_{2,F} , \quad \|\sin \Theta(S', T)\|_{2,F} \leq \|\sin \Theta(S, T)\|_{2,F} , \]
which follow from Eq. (1). On the other hand, \( \dim S^\perp = n - s \geq n - t = \dim T^\perp \) and therefore,
\[ \sin(\theta_{(n-t)-j+1}(S^\perp, T^\perp)) = \sigma_j((I - P_{S^\perp})P_{T^\perp}) = \sigma_j(P_{S}(I - P_{T})) , \quad 1 \leq j \leq n - t. \]

By comparing the previous identity with Eq. (1), if \( \theta_1(S, T), \ldots, \theta_d(S, T) > 0 \) are the positive angles between \( S \) and \( T \) (for some \( 0 \leq d \leq \min\{s, n - t\} \)) then these coincide with the positive angles between \( S^\perp \) and \( T^\perp \) i.e.
\[ \theta_j(S, T) = \theta_j(S^\perp, T^\perp) \quad \text{for} \quad 1 \leq j \leq d. \]

Notice that as a consequence of Eq. (2) we get that
\[ \|\Theta(S, T)\|_{2,F} = \|\Theta(S^\perp, T^\perp)\|_{2,F}. \]

**Principal vectors between subspaces.** In what follows we shall also make use of the principal vectors associated with the subspaces \( S \) and \( T \): indeed, by construction of the principal angles, we get that there exist orthonormal systems \( \{u_1, \ldots, u_s\} \subset S \) and \( \{v_1, \ldots, v_s\} \subset T \) such that
\[ \langle u_i, v_j \rangle = \delta_{ij} \cos(\theta_j(S, T)) \quad \text{for} \quad 1 \leq i, j \leq s, \]
where \( \delta_{ij} \) 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 \( S \) and \( T \). Notice that the previous facts imply, in particular, that the subspaces \( S_j = \text{Span}\{u_1, \ldots, u_j\} \subset S \) and \( T_j = \text{Span}\{v_1, \ldots, v_j\} \subset T \) are such that
\[ \Theta(S_j, T_j) = \text{diag}(\theta_1(S, T), \ldots, \theta_j(S, T)) \in \mathbb{R}^{j \times j} \quad \text{for} \quad 1 \leq j \leq s. \]
Moreover, if \( \tilde{S} \subset S \) and \( \tilde{T} \subset T \) are two \( j \)-dimensional subspaces then, it follows that \( \Theta(S_j, T_j) \leq \Theta(\tilde{S}, \tilde{T}) \); that is, \( S_j \) and \( T_j \) are \( j \)-dimensional subspaces of \( S \) and \( T \) respectively, that are at minimal angular (vector-valued) length.

2.2 Setting the context and problems

We begin with a formal description of the class of dominant subspaces of a matrix, without assuming a singular gap. Then, we describe the context and main problems considered in this work.

**Dominant subspaces and low-rank approximations.** 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 \( S' \subset \mathbb{K}^m \) be a subspace of dimension \( 1 \leq h \leq \text{rank}(A) \leq p \). We say that \( S' \) is a left dominant subspace for \( A \) if \( S' \) 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, \( S' \) is a left dominant subspace for \( A \) if the \( h \) largest singular values of \( P_{S'}A \) are \( \sigma_1 \geq \ldots \geq \sigma_h \). Hence, in this case we have that
\[ \|P_{S'}A - A\| \leq \|QA - A\| \]
for every orthogonal projection \( Q \in \mathbb{K}^{m \times m} \) with \( \text{rank}(Q) = h \) and every unitarily invariant norm; that is, \( P_{S'}A \) 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.
Dominant subspaces and SVD. 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 $\Sigma$ is a (rectangular) diagonal matrix, with diagonal entries given by the singular values of $A$. In what follows we let $u_j$ (respectively $v_j$) denote the columns of $U$ (respectively of $V$).

Given $1 \leq h \leq m$, we define the subspace $U_h = \text{Span}\{u_1, \ldots, u_h\} \subset \mathbb{K}^m$; similarly, if $1 \leq h \leq n$, we let $V_h = \text{Span}\{v_1, \ldots, v_h\} \subset \mathbb{K}^n$. Then, $U_h$ and $V_h$ 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 $U_h$ and $V_h$ 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 $0 \leq j = j(h) < h < k = k(h)$ be given by $j(h) = \max\{0 \leq j < h : \sigma_j > \sigma_h\}$, where we set $\sigma_0 = +\infty$ and $k = k(h) = \max\{1 \leq j \leq \text{rank}(A) : \sigma_j = \sigma_h\}$. If we further let $U_0 = \{0\}$ then, it is straightforward to check that an $h$-dimensional subspace $S'$ is a left dominant subspace for $A$ if and only if there exists an $(h-j)$-dimensional subspace $U \subset U_h \ominus U_j := U_h \cap U_j^\perp \subset \mathbb{K}^m$ such that

$$S' = U \oplus U_j.$$ 

Therefore, we have a natural parametrization of $h$-dimensional left dominant subspaces in terms of subspaces $U$ that vary over the Grassmann manifold of $(h-j)$-dimensional subspaces of $U_h \ominus U_j < \mathbb{K}^m$.

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 $S' = U_h$, i.e. the subspace spanned by the top $h$ columns of $U$; and a similar fact also holds for right dominant subspaces.

**Main problems.** Consider $A$ as above and a matrix $X \in \mathbb{K}^{n \times r}$ (a starting guess). From $A$ and $X$ we construct the block Krylov space $K_q(A, X)$, for $q \geq 0$, that is

$$K_q = K_q(A, X) = R((AX \ (AA^*)AX \ \ldots \ (AA^*)^qAX) \ ) \subset \mathbb{K}^m,$$

(recall that $R(B)$ denotes the range of a matrix $B$).

In this setting, our first main problem is to show the existence of some $h$-dimensional subspace $T \subseteq K_q$ that is close to some $h$-dimensional left dominant subspace $U_h$ of $A$. In this context, proximity between subspaces is measured by $\|\sin \Theta(U_h, T)\|_{2,F}$ i.e. in terms of (the spectral or Frobenius norm of) the sines of the principal angles between the subspaces $U_h$ and $T$ (see Section 3.1). Once we establish the existence of $T \subseteq K_q$ as above, we get the low-rank approximation $P_T A$ of $A$. We point out that our approach does not provide an effective way (algorithm) to compute $T$.

Therefore our second main problem is to compute, in an algorithmic way, an $h$-dimensional subspace $T' \subset K_q$ together with a corresponding upper bound for the approximation error

$$\|A - P_{T'} A\|_{2,F}.$$ 

Further, we require that the upper bound for the approximation error of $A$ by $P_{T'} A$ becomes arbitrarily close to $\|A - A_h\|_{2,F}$, i.e. the error in approximating $A$ by the (optimal) low-rank matrix $A_h$ obtained from truncated SVD’s of $A$ (as described at the beginning of Section 1). Hence, by solving this second problem, we obtain (in an effective way) the low-rank approximation $P_{T'} A$ of $A$ (see Section 3.2) that behaves much like the optimal low-rank approximations of $A$.

In case there is a singular gap i.e. $\sigma_h > \sigma_{h+1}$ these problems have been recently solved in [5] (see Section 2.3 below). In this work we adapt the approach considered in [5] to construct approximations of dominant spaces and low-rank approximation of $A$, based on the block Krylov subspaces $K_q$, in the case that there is no singular gap at the index $h$. 
2.3 DIKM-I theory with prescribed singular gaps: structural results

In [5] P. Drineas, I.C.F. Ipsen, E.M. Kontopoulou and M. Magdon-Ismail 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 [5] has a deep influence on our present work; indeed, we shall follow some of the lines developed in that work, which 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. Next, we include some of the features of the DIKM-I theory that we need in what follows.

In this section we keep using the notation considered so far: \( A \in \mathbb{K}^{m \times n} \), \( A = U \Sigma V^* \) its SVD, its singular values \( \sigma_1 \geq \ldots \geq \sigma_p \), \( p = \min\{m, n\} \), and so on. In case \( 1 \leq k < \text{rank}(A) \leq p \) then we consider the partitions

\[
\Sigma = \begin{pmatrix} \Sigma_k & \Sigma_{k,\perp} \\ \Sigma_{k,\perp} & 0 \end{pmatrix}, \quad U = (U_k \ U_{k,\perp}) , \quad V = (V_k \ V_{k,\perp}) .
\]

The following is one of the main results of the DIKM-I theory. In what follows, given a matrix \( Z \) we let \( Z^\dagger \) denote its Moore-Penrose pseudo-inverse.

**Theorem 2.1** ([5]). Assume that \( \sigma_k > \sigma_{k+1} \), let \( \phi(x) \) be a polynomial of degree at most \( 2q + 1 \) with odd powers only, such that \( \phi(\Sigma_k) \) is non-singular. Let \( \tilde{X} \in \mathbb{K}^{n \times r} \) be such that \( \text{rank}(V_k^* \tilde{X}) = k \) (so \( r \geq k \)) and let \( K_q = K_q(A, \tilde{X}) \). Then,

\[
\| \sin \Theta(K_q, U_k) \|_{2,F} \leq \| \phi(\Sigma_{k,\perp}) \|_2 \| \phi(\Sigma_k)^{-1} \|_2 \| V_k^* \tilde{X}(V_k^* \tilde{X})^\dagger \|_{2,F} .
\]

\[ \square \]

Theorem 2.1 provides an upper bound for the (angular) distance between the subspaces \( \tilde{K}_q \) and \( U_k \). By choosing polynomials \( \phi \in \mathbb{K}[x] \) as above in a convenient way, we can make the upper bound in Theorem 2.1 arbitrarily small for sufficiently large \( q \geq 0 \) (see Theorem 2.2 below). Thus we consider Theorem 2.1 as part of the convergence analysis of the block Krylov method.

In the next result we make use of the following well known proto-algorithm (see for example [5]). We will make use of this algorithm again in Section 3.2.

**Algorithm 2.1** (Proto-algorithm for low-rank approximation)

**Require:** \( A \in \mathbb{K}^{m \times n} \), starting guess \( X \in \mathbb{K}^{n \times r} \); rank parameter \( k \leq \text{rank}(A) \); power parameter \( \ell \geq 0 \).

1. Set \( K_\ell = (AX \ (AA^*)AX \ \ldots \ (AA^*)^\ell AX) \in \mathbb{K}^{m \times (\ell + 1) \cdot r} \);
2. Test that \( d := \dim R(K_\ell) \geq k \). In this case:
3. Compute \( U_{W,k} \in \mathbb{K}^{d \times k} \) isometry, such that \( R(U_{W,k}) \) is a left dominant subspace of \( W \).
4. Return \( \hat{U}_k = U_K U_{W,k} \in \mathbb{K}^{m \times k} \).

Once the Algorithm 2.1 is performed, we describe the output matrix in terms of its columns \( \hat{U}_k = (\hat{u}_1, \ldots, \hat{u}_k) \). We also consider the matrices \( \hat{U}_i = (\hat{u}_1, \ldots, \hat{u}_i) \in \mathbb{K}^{m \times i} \), for \( 1 \leq i \leq k \).

**Theorem 2.2** ([5]). Assume that \( \sigma_k > \sigma_{k+1} \), let \( \phi(x) \) be a polynomial of degree at most \( 2q + 1 \) with odd powers only, such that \( \phi(\sigma_i) \geq \sigma_i \) for \( 1 \leq i \leq k \). Consider the output of Algorithm 2.1
with starting guess $\tilde{X} \in \mathbb{K}^{n \times r}$ such that \( \text{rank}(V_k^* \tilde{X}) = k \), rank parameter $k$ and power parameter $q$. Then, for $1 \leq i \leq k$,

$$
\| A - \hat{U}_i \hat{U}_i^* A \|_{2,F} \leq \| A - A_i \|_{2,F} + \Delta
$$

$$
\sigma_i - \Delta \leq \| \hat{u}_i^* A \|_2 \leq \sigma_i
$$

where $A_i \in \mathbb{K}^{m \times n}$ is a best rank-$i$ approximation of $A$ and $\Delta = \| \phi(\Sigma_{k,i}) \|_2 \| V_k^* \tilde{X} (V_k^* \tilde{X})^\dagger \|_F$. □

The following result from [5] complements Theorems 2.1 and 2.2 above, in the sense that it implies that the upper bounds in those theorems can be made arbitrarily small. This result corresponds to a generalization of the Chebyshev-based gap-amplifying polynomials developed in [18].

**Lemma 2.3 ([5])**. Assume that $k < \text{rank}(A)$, so that $\sigma_k > \sigma_{k+1} > 0$, and let

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

Then, there exists a polynomial (with odd powers only and with degree $2q + 1$)

$$
\phi(x) = \sum_{i=0}^{q} a_{2i+1} x^{2i+1}
$$

with $a_{2i+1} \neq 0$, for $0 \leq i \leq q$, such that

$$
\phi(\sigma_1) \geq \ldots \geq \phi(\sigma_k) \quad , \quad \phi(\sigma_i) \geq \sigma_i > 0 \quad , \quad \text{for } 1 \leq i \leq k,
$$

and

$$
|\phi(\sigma_i)| \leq \frac{4\gamma_k}{2(2q+1) \min\{\sqrt{\gamma_k}, 1\}} \quad , \quad \text{for } i \geq k + 1.
$$

Hence, $\|\phi(\Sigma_k)^{-1}\|_2 \leq \gamma_k^{-1}$ and $\|\phi(\Sigma_{k,i})\|_2 \leq \frac{4\gamma_k}{2(2q+1) \min\{\sqrt{\gamma_k}, 1\}}$. □

We point out that the inequalities $\phi(\sigma_1) \geq \ldots \geq \phi(\sigma_k)$ 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 [5]).

To describe the following result from the DIKM-I theory (that follows from Theorems 2.1 2.2 and Lemma 2.3), assume that $\text{rank}(A) > k$; then we consider

$$
\gamma_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_{k+1}} > 0 \quad \text{and} \quad \Delta(W,q,k)_{2,F} = 4 \frac{\| V_k^* W (V_k^* W)^\dagger \|_{2,F}}{2(2q+1) \min\{\sqrt{\gamma_k}, 1\}},
$$

where $W \in \mathbb{K}^{n \times \ell}$, for some $\ell \geq 1$ and $q \geq 0$. Notice that in case $\sigma_k > \sigma_{k+1}$ then then expressions in Eq. (6) do not depend on the particular SVD of $A$.

**Theorem 2.4 ([5])**. Assume that $\sigma_k > \sigma_{k+1} > 0$. Let $\tilde{X} \in \mathbb{K}^{n \times r}$ be such that $\text{rank}(V_k^* \tilde{X}) = k$ and let $\tilde{K}_q = \mathcal{K}_q(A, \tilde{X})$. Consider the output of Algorithm 2.1 with starting guess $\tilde{X}$ such that $\text{rank}(V_k^* \tilde{X}) = k$, rank parameter $k$ and power parameter $q \geq 0$. Then we have that

$$
\| \sin \Theta(\tilde{K}_q, \hat{U}_k) \|_{2,F} \leq \Delta(\tilde{X}, q,k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k},
$$

$$
\| A - \hat{U}_i \hat{U}_i^* A \|_{2,F} \leq \| A - A_i \|_{2,F} + \Delta(\tilde{X}, q,k)_{F} \sigma_{k+1} \quad , \quad 1 \leq i \leq k,
$$

$$
\sigma_i - \Delta(\tilde{X}, q,k)_{F} \sigma_{k+1} \leq \sigma_i (\hat{U}_k \hat{U}_k^* A) \leq \sigma_i \quad \text{for } 1 \leq i \leq k.
$$

□
Theorem 2.4 shows the type of convergence analysis obtained in \[5\] for the deterministic block Krylov methods. On the one hand, it provides an upper bound for the distance between the subspaces \( \mathcal{K}_q \) and \( U_k \), that becomes arbitrarily small for sufficiently large \( q \geq 0 \). Similarly, this result also provides an upper bound for the error in the approximation of \( A \) by the low-rank matrix \( \hat{U}_k \hat{U}_k^* A \) that is arbitrarily close to the optimal error \( \|A - A_k\|_2, F \) (obtained using exact truncated singular value decomposition) for sufficiently large \( q \geq 0 \). Moreover, it is also possible to obtain bounds for the error in the approximation of the singular values of \( A \) by the (computable) singular values of \( \hat{U}_k \hat{U}_k^* A \), obtained from the Algorithm 2.1.

In the next section we complement Theorem 2.4 by developing upper bounds for the error of \( h \)-dimensional dominant subspace approximation, for the error in low-rank approximation and the error in singular values approximation, in case there is no singular gap at the index \( h \) (that is, when Theorem 2.4 can not be applied).

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. Our results are motivated by the structural results of the DIKM-I theory described in Section 2.3. At the end of this section we include some comments and further research problems related to the present work.

3.1 Approximation of dominant subspaces by block Krylov spaces

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 \( 1 \leq h \leq \text{rank}(A) \leq p \), we let \( 0 \leq j(h) < h \) be given by

\[
  j = j(h) = \max\{0 \leq \ell < h : \sigma_\ell > \sigma_h\} \quad (10)
\]

where we set \( \sigma_0 = +\infty \) and

\[
  k = k(h) = \max\{1 \leq \ell \leq \text{rank}(A) : \sigma_\ell = \sigma_h\} \quad (11)
\]

Since \( h \leq \text{rank}(A) \), we get that \( \sigma_k > 0 \). As mentioned in the preceding sections, we will focus on the case when \( h < k \) (i.e. when \( \sigma_h = \sigma_{h+1} \)). Let \( A = U \Sigma V^* \) be a full SVD of \( A \). In case \( 1 \leq k < \text{rank}(A) \leq p \) then we consider the partitioning of \( U \), \( \Sigma \) and \( V \) as in Eq. \[4\] that is,

\[
  \Sigma = \begin{pmatrix} \Sigma_k & \Sigma_{k,\perp} \\ \Sigma_{k,\perp}^\top & 0 \end{pmatrix}, \quad U = \begin{pmatrix} U_k & U_{k,\perp} \end{pmatrix}, \quad V = \begin{pmatrix} V_k & V_{k,\perp} \end{pmatrix}.
\]

**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

\[
  \Theta(S, R(X)) < \frac{\pi}{2} I,
\]

where \( \Theta(S, R(X)) \in \mathbb{R}^{h \times h} \) denotes the diagonal matrix with the principal angles between \( S \) and \( R(X) \) in its main diagonal (see Section 2.4).

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

We can now state our main results. We begin with the next technical result that will allow us to show that block Krylov methods produce arbitrary good approximations of right and left dominant subspaces. Recall that given a matrix \( Z \) we let \( Z^\dagger \) denote its Moore-Penrose pseudo-inverse.

Throughout the rest of the work, we fix \( 1 \leq h \leq \text{rank}(A) \leq p = \min\{m, n\} \) and we let let \( 0 \leq j = j(h) < h \leq k = k(h) \leq \text{rank}(A) \) be defined as in Eqs. \[10\] and \[11\].
**Theorem 3.2.** Let $q \geq 0$ and let $\phi(x)$ be a polynomial of degree at most $2q + 1$ with odd powers only, such that $\phi(\sigma_1) \geq \ldots \geq \phi(\sigma_k) > 0$. Let $(A, X)$ be $h$-compatible and let $K_q = K_q(A, X)$. Then, there exists an $h$-dimensional left dominant subspace $S'$ for $A$ such that

$$
\| \sin \Theta(K_q, S') \|_{2,F} \leq 4 \| \sin \Theta(R(V^*_k X), V^*_k \mathcal{V}_j) \|_{2,F} + \| \phi(\Sigma_{k,1}) \|_2 \| \phi(\Sigma_k)^{-1} \|_2 \| V_{k,1}^* X (V^*_k X) \|^2_{2,F} .
$$

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

$$
\Theta(R(V^*_k X), V^*_k \mathcal{V}_j) \leq \Theta(R(X), \mathcal{V}_j) .
$$

**Proof.** See Section 4.1.

We point out that Theorem 3.2 above is related to 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. On the other hand, since our assumptions are based on non-structural choices, there is a price to pay: we need a priori partial knowledge of the relative position of the subspaces $R(V^*_k X)$ and $R(V^*_k \mathcal{V}_j)$ to have control on the upper bound above (notice that Theorem 2.1 does not require such partial knowledge). We remark that the second inequality in Theorem 3.2 provides an alternative method to have a control of the relative position of the subspaces $R(V^*_k X)$ and $V^*_k \mathcal{V}_j$.

To state the following result, recall the notation from Eq. (6) above from the DIKM-I theory; hence, given a SVD $A = U \Sigma V^*$ then

$$
\gamma_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_{k+1}} > 0 \quad \text{and} \quad \Delta(W, q, k)_{2,F} = 4 \frac{\| V_{k+1} W (V^*_k W) \|_{2,F}}{2(2q+1) \min\{\sqrt{\gamma_k}, 1\} } ,
$$

where $W \in \mathbb{K}^{n \times \ell}$, for some $\ell \geq 1$ and $q \geq 0$.

**Corollary 3.3.** Let $(A, X)$ be $h$-compatible and let $K_q = K_q(A, X)$ for some $q \geq 0$. Then, there exists an $h$-dimensional left dominant subspace $S'$ for $A$ such that

$$
\| \sin \Theta(K_q, S') \|_{2,F} \leq 4 \| \sin \Theta(R(X), \mathcal{V}_j) \|_{2,F} + \Delta(X, q, k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k} .
$$

In case $j = 0$ (respectively $k = \text{rank}(A)$) the first term (respectively the second term) should be omitted in the previous upper bound.  

**Proof.** See Section 4.1.

The following result can be regarded as a convenient algorithmic augmentation process of the initial subspace $R(X) = X \subset \mathbb{K}^n$; that is, we begin with $X$ that satisfies a compatibility assumption with some $h$-dimensional right dominant subspace of $A$ and we construct an associated (auxiliary) subspace $K_{q,t} \subset \mathbb{K}^n$ that is (arbitrarily) close to an $h$-dimensional right dominant subspace (see Theorem 3.6 below).

Let $(A, X)$ be $h$-compatible and consider $A = U \Sigma V^*$ a SVD of $A$. For the next result we recall the notation in Eq. (6) and further introduce

$$
\Delta(X, q, j)_{2,F} = 4 \frac{\| V_{j+1}^* X (V_j^* X) \|_{2,F} }{2(2q+1) \min\{\sqrt{\gamma_j}, 1\} } , \quad \Delta^*(Y, t, k)_{2,F} := 4 \frac{\| U_{k+1}^* Y (U_k^* Y) \|_{2,F} }{2(2t+1) \min\{\sqrt{\gamma_k}, 1\} } ,
$$

(12)

where $\gamma_j = \frac{\sigma_j - \sigma_{j+1}}{\sigma_{j+1}} > 0$, $Y \in \mathbb{K}^{m \times \ell}$, for some $\ell \geq 1$ and $t \geq 0$. Notice that expressions in Eq. (12) do not depend on the particular SVD of $A$, since by construction $\sigma_j > \sigma_{j+1}$ and $\sigma_k > \sigma_{k+1}$.
Theorem 3.4. Let \((A, X)\) be \(h\)-compatible, let \(K_q = K_q(A, X) \subset \mathbb{K}^m\) and let \(Y_q\) be such that \(Y_q Y_q^*\) is the orthogonal projection onto \(K_q\), for some \(q \geq 0\). For \(t \geq 0\) we let
\[
K_{q,t} = R((A^* A)X) + R((A^* A)^2 X) + \cdots + R((A^* A)^{q+t+1} X) \subset \mathbb{K}^n.
\] (13)

Then, there exists an \(h\)-dimensional right dominant subspace \(\tilde{S}\) for \(A\) such that
\[
\|\sin \Theta(K_{q,t}^*, \tilde{S})\|_{2,F} \leq 4 \Delta(X, q, j)_{2,F} \frac{\sigma_{j+1}}{\sigma_j} + \Delta^*(Y_q, t, k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k}.
\] (14)

In case \(j = 0\) (respectively \(k = \text{rank}(A)\)) the first term (respectively the second term) should be omitted in the previous upper bound.

Proof. See section 4.2.

Using the correspondence between left and right dominant subspaces of \(A\) we can derive the existence of (arbitrarily good) approximates of left dominant subspaces obtained from the block Krylov method in case there is no singular gap.

In the next result we consider the notation in Eq. (12).

Theorem 3.5. Let \((A, X)\) be \(h\)-compatible. Given \(q, t \geq 0\), consider \(K_{q+t+1} = K_{q+t+1}(A, X) \subset \mathbb{K}^m\). Then, there exists an \(h\)-dimensional left dominant subspace \(\tilde{S}\) for \(A\) such that
\[
\|\sin \Theta(K_{q+t+1}^*, \tilde{S})\|_{2,F} \leq 4 \Delta^*(AX, q, j)_{2,F} \frac{\sigma_{j+1}}{\sigma_j} + \Delta^*(W_q, t, k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k},
\] (15)

where \(W_q\) is such that \(W_q W_q^*\) is the orthogonal projection onto \(K_q(A^*, AX) \subset \mathbb{K}^n\). In case \(j = 0\) (respectively \(k = \text{rank}(A)\)) the first term (respectively the second term) should be omitted in the previous upper bound.

Proof. Since the pair \((A, X)\) is \(h\)-compatible, there exists an \(h\)-dimensional right dominant subspace \(S \subset \mathbb{K}^n\) for \(A\), such that \(\dim(X^* S) = h\). Set \(Z = AX\) and let \(S' = AS \subset \mathbb{K}^m\). Hence, \(S'\) is a left dominant subspace for \(A\) and then, a right dominant subspace of \(A^*\) with \(\dim S' = h\). Moreover, \(Z^* S' = X^* A^* AS = X^* S\), since \(A^* AS = S\). In particular, \(\dim Z^* S' = h\) and hence \(\Theta(R(Z), S') < \frac{\pi}{2} I\). Therefore, we can apply Theorem 3.4 to \(A^*\) and \(Z\); in this case, we consider the (auxiliary) subspace
\[
K_{q,t}^*(A^*, Z) = R((AA^*)Z) + R((AA^*)^2 Z) + \cdots + R((AA^*)^{q+t+1} Z) \subset \mathbb{K}^n.
\]
It is clear that \(K_{q,t}^*(A, Z) \subset K_{q+t+1}^*\). Then, by Theorem 3.4 there exists an \(h\)-dimensional right dominant \(\tilde{S}\) for \(A^*\) (and therefore a left dominant subspace for \(A\)) such that
\[
\|\sin \Theta(K_{q+t+1}^*, \tilde{S})\|_{2,F} \leq \|\sin \Theta(K_{q,t}^*(A^*, Z), \tilde{S})\|_{2,F} \leq 4 \Delta^*(AX, q, j)_{2,F} \frac{\sigma_{j+1}}{\sigma_j} + \Delta(W_q, t, k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k},
\]
where we used that if \(A = USV^*\) is a SVD for \(A\) then \(A^* = V \Sigma U^*\) is a SVD for \(A^*\).

With the notation of Theorems 3.4 and 3.5, it seems useful to obtain upper bounds for
\[
\|U_{k,\perp}^* Y_q(U_k^* Y_q)^\dagger\|_{2,F} \quad \text{and} \quad \|V_{k,\perp}^* W_q(V_k^* W_q)^\dagger\|_{2,F}
\]
in case \(k < \text{rank}(A)\). Theorem 3.6 together with Remark 3.9 show that we can obtain such upper bounds. In turn, these results will allow us to have a better control over the upper bounds in Eqs. (14) and (15).
Theorem 3.6. Let \((A, X)\) be h-compatible, let \(K_q = K_q(A, X) \subset \mathbb{K}^m\) and let \(Y_q\) be such that \(Y_q Y_q^\dagger\) is the orthogonal projection onto \(K_q\). Assume that \(k < \text{rank}(A)\). Then, we have that

\[
\|U_{k,\perp}^\dagger Y_q (U_k^\dagger Y_q)^\dagger\|_2 \leq \min \left\{ \frac{2 \|V_{k,\perp} X (V_k^\dagger X)^\dagger\|_2}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)} \frac{\sigma_{k+1}}{\sigma_k}, \frac{\|V_{k,\perp}^\dagger X (V_k^\dagger X)^\dagger\|_2}{(1 + \gamma_k)^{2q+1}} \right\}
\]

and

\[
\|U_{k,\perp}^\dagger Y_q (U_k^\dagger Y_q)^\dagger\|_F \leq \sqrt{q + 1} \cdot \min \left\{ \frac{2 \|V_{k,\perp} X (V_k^\dagger X)^\dagger\|_F}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)} \frac{\sigma_{k+1}}{\sigma_k}, \frac{\|V_{k,\perp}^\dagger X (V_k^\dagger X)^\dagger\|_F}{(1 + \gamma_k)^{2q+1}} \right\}.
\]

Proof. See Section 3.2.

The previous result motivates the following.

Definition 3.7. Let \((A, X)\) be h-compatible and assume that \(k < \text{rank}(A)\). Given \(q, t \geq 0\) we set:

1. The quantity \(\Pi(q, t, k) = \Pi_2\) given by

\[
\Pi_2 = \frac{1}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)} \min \left\{ \frac{2}{1 + \gamma_k} \frac{1}{1 + \gamma_k} \right\}.
\]

2. The quantity \(\Pi(q, t, k)_F = \Pi_F\) given by \(\Pi_F = \sqrt{q + 1} \cdot \Pi_2\).

The quantities \(\Pi_2\) and \(\Pi_F\) together with Theorem 3.4 allow us to obtain explicit upper bounds for the angular distance between \(K_{q,t}^*\) (defined in Eq. (13)) and right dominant subspaces for \(A\). We summarize these facts in the following corollary, which will play a central role in the proofs of the results in Section 3.2.

Corollary 3.8. Let \((A, X)\) be h-compatible, and for \(q, t \geq 0\) let \(K_{q,t}^*\) be defined as in Eq. (13). Then, there exists an h-dimensional right dominant subspace \(\tilde{S}\) for \(A\) such that

\[
\|\sin \Theta(K_{q,t}^*, \tilde{S})\|_{2,F} \leq \frac{16 \|V_{k,\perp}^\dagger X (V_k^\dagger X)^\dagger\|_{2,F}^{2q+1} + 4 \Pi_2 \|V_{k,\perp}^\dagger X (V_k^\dagger X)^\dagger\|_{2,F}}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)}.
\]

In case \(j = 0\) (respectively \(k = \text{rank}(A)\)) the first term (respectively the second term) should be omitted in the previous upper bound.

Proof. This is a straightforward consequence of Theorem 3.4, Theorem 3.6, Definition 3.7, the inequality \(\sigma_{j+1}/\sigma_j \leq 1\) and the identity \(\sigma_{k+1}/\sigma_k = (1 + \gamma_k)^{-1}\).

Remark 3.9. Consider the notation and hypothesis in Theorem 3.5 and assume that \(k < \text{rank}(A)\). Thus, \(W_q\) is such that \(W_q W_q^\dagger\) is the orthogonal projection onto \(K_q(A^*, AX) \subset \mathbb{K}^n\). We can apply Theorem 3.6 to the matrix \(A^*\) and initial guess matrix \(AX \in \mathbb{K}^{m \times r}\), and get that

\[
\|V_{k,\perp}^\dagger W_q (V_k^\dagger W_q)^\dagger\|_2 \leq \min \left\{ \frac{2 \|U_{k,\perp}^\dagger AX (U_k^\dagger AX)^\dagger\|_2}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)} \frac{\sigma_{k+1}}{\sigma_k}, \frac{\|U_{k,\perp}^\dagger AX (U_k^\dagger AX)^\dagger\|_2}{(1 + \gamma_k)^{2q+1}} \right\}.
\]

Similarly, we also get that

\[
\|V_{k,\perp}^\dagger W_q (V_k^\dagger W_q)^\dagger\|_F \leq \sqrt{q + 1} \cdot \min \left\{ \frac{2 \|U_{k,\perp}^\dagger AX (U_k^\dagger AX)^\dagger\|_F}{2(2q+1) \min(\sqrt{\gamma_k}/2, 1/2)} \frac{\sigma_{k+1}}{\sigma_k}, \frac{\|U_{k,\perp}^\dagger AX (U_k^\dagger AX)^\dagger\|_F}{(1 + \gamma_k)^{2q+1}} \right\}.
\]

Furthermore, we can also apply Theorem 3.6 to the matrix \(A\) and initial guess \(X\) and \(q = 0\), and conclude that

\[
\|U_{k,\perp}^\dagger AX (U_k^\dagger AX)^\dagger\|_2, F \leq \|V_{k,\perp}^\dagger X (V_k^\dagger X)^\dagger\|_{2,F}.
\]

In turn, these inequalities can be used to obtain upper bounds for the expressions \(\Delta^*(AX, q, j)_{2,F}\) and \(\Delta(W_q, t, k)_{2,F}\) that appear in Eq. (15) in terms of the parameters \(t, q \geq 0\).
In the following result we apply the estimates from Remark 3.9 in Theorem 3.5 with the particular choice \( t = 0 \) and for the spectral norm (the Frobenius norm case can be handled similarly); to simplify the statement below, we consider the following constant: given an \( h \)-compatible pair \((A,X)\) set \( C(A,X,j,k)_2 = C_2 \) determined as follows: if \( 1 \leq j < h \leq k < \text{rank}(A) \) then

\[
C_2 = \max \left\{ 16 \| V_{j;k}^* X (V_{j;k}^* X)^\dagger \|_2 , 4 \| V_{k;j}^* X (V_{k;j}^* X)^\dagger \|_2 \right\}.
\]  

(17)

If \( j = 0 \) we let \( C_2 = 4 \| V_{k;j}^* X (V_{k;j}^* X)^\dagger \|_2 \); if \( k = \text{rank}(A) \) then we set \( C_2 = 16 \| V_{k;j}^* X (V_{k;j}^* X)^\dagger \|_2 \).

**Theorem 3.10.** Let \((A,X)\) be \( h \)-compatible and let \( C_2 \) be defined as in Eq. (17). Given \( q \geq 0 \) let \( K_{q+1} = K_{q+1}(A,X) \subset \mathbb{K}^m \). We follow the conventions: \( \gamma_0 = \gamma_{\text{rank}(A)} = +\infty \) in case \( j = 0 \) or \( k = \text{rank}(A) \). Then, there exists an \( h \)-dimensional left dominant subspace \( \hat{S} \) for \( A \) such that:

1. If \( \gamma_k \geq 1 \) (and hence \( 2^{(2q+1)\min(\sqrt{\gamma_j},1)} = 2^{(2q+1)} \leq (1 + \gamma_k)^{2q+1} \) we have that

\[
\| \sin \Theta(K_{q+1},\hat{S}) \|_2 \leq \frac{2C_2}{2^{(2q+1)} \min(\sqrt{\gamma_j},1)}.
\]  

(18)

2. If \( \gamma_k < 1 \) (and hence \( \min\{\sqrt{\gamma_j}, \sqrt{\gamma_k}/2, 1/2\} \leq \min\{\sqrt{\gamma_j}, 1\}, \min\{\sqrt{\gamma_k}/2, 1/2\} \) we have that

\[
\| \sin \Theta(K_{q+1},\hat{S}) \|_2 \leq \frac{3C_2}{2^{(2q+1)} \min(\sqrt{\gamma_j}, \sqrt{\gamma_k}/2, 1/2)}.
\]  

(19)

**Proof.** See Section 4.3.

We point out that Theorem 3.10 complements the convergence analysis described in Theorem 2.4 from the DIKM-I theory (see Eq. (7)) for the spectral norm. That is, this result can be applied in contexts in which Theorem 2.4 cannot be applied; moreover, Theorem 3.10 shows the existence of \( h \)-dimensional subspaces \( T \subseteq K_{q+1}(A,X) \) that are arbitrarily good approximations of some \( h \)-dimensional left dominant subspace \( \hat{S} \) of \( A \) (for sufficiently large \( q \geq 0 \)). As opposed to Theorem 3.2 Theorem 3.10 does not require a priori (strict) control of the relative position of the subspaces \( R(V_{k;j}^* X) \) and \( R(V_{j;k}^* V_j) \) (see the comments after Theorem 3.2). On the other hand, the speeds at which the upper bounds in Eqs. (18) and (19) decrease depending on both gaps \( \gamma_j \) and \( \gamma_k \); 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 3.10 can be made arbitrarily small. 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 such low-rank approximations. Our approach to deal with this problem is based on approximate right dominant subspaces of a matrix \( A \); indeed, we follow arguments from 22.

For the next result, we consider Algorithm 2.1 with input: \( A \in \mathbb{K}^{m \times n} \), starting guess \( X \in \mathbb{K}^{n \times r} \); we set our target rank to \( 1 \leq h \leq \text{rank}(A) \). Once the algorithm stops, we describe the output matrix in terms of its columns, \( \hat{U}_h = (\hat{u}_1, \ldots, \hat{u}_h) \in \mathbb{K}^{m \times h} \). In this case we set

\[
\hat{U}_i = (\hat{u}_1, \ldots, \hat{u}_i) \in \mathbb{K}^{m \times i}, \quad \text{for} \quad 1 \leq i \leq h.
\]  

(20)

As before, we let \( j = j(h) < h \leq k = k(h) \) be defined as in Eqs. (10) and (11), and we consider the notation used so far. Further, given \( 1 \leq i \leq h \) we let \( A_i \in \mathbb{K}^{m \times n} \) denote a best rank-\( i \) approximation of \( A \) (so that \( \| A - A_i \|_2 = \sigma_{i+1} \)).
Definition 3.11. Let \((A,X)\) be \(h\)-compatible and let \(t,q \geq 0\). We consider the constants 
\(\delta(A,X,q,t,j,k)_2,F = \delta_2,F\) defined by
\[
\delta_2,F := \sqrt{2} \left( \frac{16 \|V_{j,1}^* X (V_j^* X)^\dagger\|_{2,F}}{2^{(2q+1) \min\{\sqrt{\gamma},1\}}} + 4 \Pi_{2,F}(q,t,k) \|V_{k,1}^* X (V_k^* X)^\dagger\|_{2,F} \right),
\]
where \(\Pi_{2,F}(q,t,k)\) are as in Definition 3.7 in case \(j = 0\) (respectively \(k = \text{rank}(A)\)) the first term (respectively the second term) in Eq. (21) should be omitted. \(\triangle\)

Theorem 3.12. Let \((A,X)\) be \(h\)-compatible and let \(q,t \geq 0\) be such that \(\delta_2 \leq 1\) (see Eq. (21)). Let \(U_K\) be the output of Algorithm 2.7 with the power parameter set to \(q+t+1 \geq 1\). There exists an \(h\)-dimensional right dominant subspace \(\tilde{S}\) of \(A\) such that
\[
\|AP_{\tilde{S}} - U_KU_K^*AP_{\tilde{S}}\|_{2,F} \leq \sigma_{h+1} \cdot \delta_2,F.
\]

Proof. See Section 4.4.

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

Theorem 3.13. Let \((A,X)\) be \(h\)-compatible and let \(q,t \geq 0\) be such that \(\delta_2 \leq 1\) (see Eq. (21)). Let \(\hat{A}_h = \hat{U}_h\hat{U}_h^* A\), where \(\hat{U}_h\) is the output of Algorithm 2.7 with the power parameter set to \(q+t+1 \geq 1\). Then,
\[
\sigma_i - \sigma_{i+1} \cdot \delta_2 \leq \sigma_i(\hat{A}_h) \leq \sigma_i \quad \text{for} \quad 1 \leq i \leq h.
\]

Proof. See Section 4.4.

Theorem 3.14. Let \((A,X)\) be \(h\)-compatible and let \(q,t \geq 0\) be such that \(\delta_2 \leq 1\). Let \(\hat{U}_h\) be the output of Algorithm 2.7 with the power parameter set to \(q+t+1 \geq 1\). Then, for every \(1 \leq i \leq h\) we have that
\[
\|A - \hat{U}_h\hat{U}_h^* A\|_{2,F} \leq \|A - A_i\|_{2,F} + \sigma_{i+1} \cdot \delta_2,F,
\]
where \(\delta_{2,F}\) are defined in Eq. (21).

Proof. See Section 4.4.

The previous results show that it would be interesting to understand the way that the expression
\[
\delta(q,t)_2,F = \delta(A,X,q,t,j,k)_2,F
\]
decreases, as a function of the indices \(q, t \geq 0\). Hence, we consider the following

Remark 3.15. Let us fix an \(h\)-compatible pair \((A,X)\). Let \(0 \leq j < h \leq k \leq \text{rank}(A)\) be the indices satisfying Eqs. (10) and (11). We follow the conventions: \(\gamma_0 = \gamma_{\text{rank}(A)} = +\infty\) in case \(j = 0\) or \(k = \text{rank}(A)\). We extend the definition of the constant \(C_2\) (see before Theorem 3.10) and consider the constants \(C(A,X,j,k)_2,F = C_{2,F}\) determined as follows: if \(1 \leq j < h \leq k < \text{rank}(A)\) then
\[
C_{2,F} = \max \left\{16 \|V_{j,1}^* X (V_j^* X)^\dagger\|_{2,F}, 4 \|V_{k,1}^* X (V_k^* X)^\dagger\|_{2,F} \right\}.
\]
If \(j = 0\) we let \(C_{2,F} = 4 \|V_{k,1}^* X (V_k^* X)^\dagger\|_{2,F}\); if \(k = \text{rank}(A)\) then we set \(C_2 = 16 \|V_{j,1}^* X (V_j^* X)^\dagger\|_{2,F}\). We consider the following cases:

1. Assume that \(\gamma_k \geq 1\). Then \(2^{(2q+1) \min\{\sqrt{\gamma},1\}} = 2^{2q+1} \leq (1 + \gamma_k)^{2q+1}\). Hence, if we take \(q \geq 0\) and set \(t = 0\) we get that
\[
\Pi_2(q,0,k) \leq \frac{1}{(1 + \gamma_k)^{2q+1}} \leq \frac{1}{2^{(2q+1)}} \quad \Rightarrow \quad \delta(q,0)_2 \leq \sqrt{2} \cdot \frac{2C_2}{2^{(2q+1) \min\{\sqrt{\gamma},1\}}}.
\]
and similarly
\[
\Pi_F(q, 0, k) \leq \frac{\sqrt{q + 1}}{(1 + 7k)^{(q+1)/2}} \leq \frac{\sqrt{q + 1}}{2^{q+1}} \implies \delta(q, 0)_F \leq \sqrt{2(q + 1)} \cdot \frac{2 C_F}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}}.
\]

2. Assume that \(\gamma_k < 1\). Hence, if we take \(q \geq 0\) and set \(t = 0\) we get that
\[
\Pi_2(q, 0, k) \leq \frac{2}{2^{(q+1)} \min\{\sqrt{\gamma_k/2}, 1/2\}} \implies \delta(q, 0)_2 \leq \sqrt{2} \cdot \frac{3 C_2}{2^{(q+1)} \min\{\sqrt{\gamma_k^2/2, 1/2}\}}
\]
and similarly
\[
\Pi_F(q, 0, k) \leq \frac{2 \sqrt{q + 1}}{2^{(q+1)} \min\{\sqrt{\gamma_k/2}, 1/2\}} \implies \delta(q, 0)_F \leq \sqrt{2(q + 1)} \cdot \frac{3 C_F}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}, \min\{\sqrt{\gamma_k}, 1\}}.
\]

The following result summarizes the above facts. Notice that the power parameter of the block Krylov method is described only in terms of the parameter \(q \geq 0\) (that is, setting \(t = 0\) in Theorems 3.13 and 3.14).

**Theorem 3.16.** Let \((A, X)\) be \(h\)-compatible and let \(C_{2, F}\) be defined as in Eq. (25). We follow the conventions: \(\gamma_0 = \gamma_{\text{rank}(A)} = +\infty \) in case \(j = 0\) or \(k = \text{rank}(A)\).

1. If \(\gamma_k \geq 1\), assume that \(q \geq 0\) is such that \(\sqrt{2} \cdot \frac{2 C_2}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}} \leq 1\).
2. If \(\gamma_k < 1\), assume that \(q \geq 0\) is such that \(\sqrt{2} \cdot \frac{3 C_2}{2^{(q+1)} \min\{\sqrt{\gamma_k^2/2, 1/2}\}} \leq 1\).

Let \(\hat{U}_h\) be the output of Algorithm (2.1) with power parameter set to \(q + 1 \geq 1\); Let 
\[
\hat{A}_i = \hat{U}_i \hat{U}_i^* A \quad \text{for } 1 \leq i \leq h,
\]
be the rank-1 approximation of \(A\) obtained from Algorithm 2.1 Then, we have that
1. If \(\gamma_k \geq 1\),
\[
\sigma_i - \sigma_{i+1} \cdot \sqrt{2} \cdot \frac{2 C_2}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}} \leq \sigma_i(\hat{A}_h) \leq \sigma_i \quad \text{for } 1 \leq i \leq h
\]
and
\[
\|A - \hat{U}_i \hat{U}_i^* A\|_{2, F} \leq \|A - A_i\|_{2, F} + \sigma_{i+1} \cdot \sqrt{2(q + 1)} \cdot \frac{2 C_F}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}}.
\]
2. If \(\gamma_k < 1\),
\[
\sigma_i - \sigma_{h+1} \cdot \sqrt{2} \cdot \frac{3 C_2}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}} \leq \sigma_i(\hat{A}_h) \leq \sigma_i \quad \text{for } 1 \leq i \leq h
\]
and
\[
\|A - \hat{U}_i \hat{U}_i^* A\|_{2, F} \leq \|A - A_i\|_{2, F} + \sigma_{i+1} \cdot \sqrt{2(q + 1)} \cdot \frac{3 C_F}{2^{(q+1)} \min\{\sqrt{\gamma_j}, 1\}}.
\]

**Proof.** This is a straightforward consequence of Theorems 3.13 and 3.14 and Remark 3.15.
3.3 Comments and final remarks

Our present work deals with two different (yet related) topics: dominant subspace approximation and low-rank matrix approximation. On the one hand, 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.

**Algorithmic low-rank approximations.** We point out that our approach is deterministic, and does not assume a singular gap at a prescribed index. Instead, we take advantage of existing singular gaps at enveloping indices. Our convergence analysis now relies on the singular gaps at these enveloping indices, as described in Theorem 3.16. Numerical implementations (including randomized starting guess matrices, dealing with efficiency and stability, etc) are beyond the scope of our present work. We plan to consider these problems elsewhere.

**Dominant subspace approximation by block Krylov subspaces.** On the other hand, the results related to $h$-dimensional dominant subspace approximation without a singular gap at the index $h$ (in terms of initial compatible matrices $X \in \mathbb{K}^{n \times r}$ with $r = h$) seem to be new; in this context, we deal with the approximation of left and right dominant subspaces, adapting some of the main techniques of [5] to this setting. In case there is no singular gap, then an interesting problem arises: namely, that there is no uniquely determined target subspace to approximate; to deal with this last fact, we are required to develop some geometric arguments related to subspace approximation. Our convergence analysis also relies on the singular gaps at enveloping indices, as described in Corollary 3.8 and Theorem 3.10. We believe that our approach can be extended to deal with randomized methods. We plan to consider the analysis of randomized methods elsewhere.

**Further research directions.** As a final remark, we point out that the present results together with the results from [5] do not seem to 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 case there is a small singular gap $\sigma_h > \sigma_{h+1}$, for which $\gamma_h \approx 0$ (so $\sigma_h / \sigma_{h+1} \approx 1$). This situation corresponds, for example, to the case where $\sigma_h$ lies in a cluster of singular values $\sigma_j \geq \ldots \geq \sigma_h \geq \ldots \geq \sigma_k$, for $j < h < k$ and $\sigma_j / \sigma_k \approx 1$. In this case the methods of our present work do not apply. On the other hand, Theorem 2.1 from [5] does apply, but it exhibits a rather slow speed of convergence with respect to the power parameter (number of iterations) $q \geq 0$. We will consider these and other related problems 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, which 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 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 $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$, with $p = \min\{m, n\}$.

2. $1 \leq h \leq \text{rank}(A) \leq p$; moreover, we let $0 \leq j(h) < h$ be given by

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

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

   $$k = k(h) = \max\{1 \leq \ell \leq \text{rank}(A) : \sigma_\ell = \sigma_h\} \geq h.$$
3. An 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 $r \geq \text{rank}(X) \geq h$.

4. The block Krylov space $\mathcal{K}_q = \mathcal{K}_q(A,X)$ constructed in terms of $A$ and $X$ as in Eq. (4), that is

$$\mathcal{K}_q = \mathcal{K}_q(A,X) = R(AX, (AA^*)AX \ldots (AA^*)^qAX) \subset \mathbb{K}^m.$$ 

Moreover, we consider $Y_q$ an isometry (that is, a matrix with orthonormal columns) such that $Y_q^*Y_q$ is the orthogonal projection onto $\mathcal{K}_q$.

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

$$\Sigma = \begin{pmatrix} \Sigma_{\ell} & \Sigma_{\ell,\perp} \\ \Sigma_{\ell,\perp}^T & 0 \end{pmatrix}, \quad U = (U_{\ell} \ U_{\ell,\perp}), \quad V = (V_{\ell} \ V_{\ell,\perp}). \quad (26)$$

Notice that the vectors in $\mathcal{K}_q$ can be described in terms of the vectors in the range of matrices $\psi(AA^*)AX \in \mathbb{K}^{m \times r}$, where $\psi(x) \in \mathbb{K}[x]$ is a polynomial of degree at most $q$. In terms of SVD of $A$, we get that

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

where $\phi(x) = x \psi(x^2) \in \mathbb{K}[x]$ is a polynomial of degree at most $2q + 1$ with odd powers only, and represents a generalized matrix function (see [11, 13]). Here $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_p) \in \mathbb{R}^{m \times n}$, where $p = \min\{m, n\}$; hence,

$$\phi(\Sigma) = \text{diag}(\phi(\sigma_1), \ldots, \phi(\sigma_p)) \in \mathbb{R}^{m \times n}.$$ 

In this case we write

$$\Phi := U\phi(\Sigma)V^*X \in \mathbb{K}^{m \times r}, \quad (27)$$

so by the previous facts, $R(\Phi) \subset \mathcal{K}_q$. Let $S$ be an $h$-dimensional right dominant subspace $S$ of $A$ such that $\Theta(R(X),S) < \frac{\pi}{2}I$ as above. As already mentioned, we can consider a SVD of $A = U\Sigma V^*$ in such a way that $S = V_k$. In this case, $R(V_k^*X) = R(V_k^*)$: if we assume further that $\phi(\sigma_j) \geq 0$ for $1 \leq j \leq h$ (so $\phi(S_h) \subset \mathbb{K}^{h \times h}$ is an invertible matrix) then $\dim R(\Phi) \geq h$, where $\Phi$ is defined as in Eq. (27). We will further consider similar facts related to convenient block decompositions of the SVD of $A$.

### 4.1 Proof of Theorem 3.2 and Corollary 3.3

We begin this section with a proof of Theorem 3.2. We present our arguments divided 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 $k < \text{rank}(A) \leq p = \min\{m, n\}$. Since $k < \text{rank}(A)$ then $\sigma_h = \sigma_k > \sigma_{k+1} > 0$.

We consider $X \in \mathbb{K}^{n \times r}$ such $\dim(D_X) = s \geq h$ and such that there exists a right dominant subspace $S \subset \mathbb{K}^n$ of dimension $h$ with $\Theta(S, X) < \pi/2I$, where $X = R(X) \subset \mathbb{K}^n$ 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 $1 \leq k \leq \text{rank}(A)$. It is worth noticing that $\Sigma_k$, $R(U_k) = U_k$ and $R(V_k) = V_k$ do not depend on the particular choice of SVD of $A$; also notice that the partition is well defined since $k < \text{rank}(A)$. Let $\phi(x)$ be a polynomial of degree $2q + 1$ with odd powers only, such that $\phi(\sigma_1) \geq \ldots \geq \phi(\sigma_k) > 0$; hence $\phi(\Sigma_k)$ is invertible.

**Step 2: Applying the DIKM-I theory to the adapted model.** Let $\mathcal{K}_q = \mathcal{K}_q(A,X)$ denote the block Krylov subspace and let $P_q \in \mathbb{K}^{m \times m}$ denote the orthogonal projection onto $\mathcal{K}_q$. Notice that if we let $\Phi \in \mathbb{K}^{m \times r}$ be as in Eq. (27) then $R(\Phi) \subset \mathcal{K}_q$. Consider for now an arbitrary $h$-dimensional subspace $S' \subset \mathbb{K}^m$. Then

$$\|\sin \Theta(\mathcal{K}_q, S')\|_{2,F} = \|(I - P_q)P_{S'}\|_{2,F} \leq \|(I - \Phi^\dagger)P_{S'}\|_{2,F}, \quad (28)$$
where we have used that \( \dim K_q \geq \dim R(\Phi) \geq \dim S' = h \). We now consider the decomposition \( \Phi = \Phi_k + \Phi_{k, \perp} \), where

\[
\Phi_k \equiv U_k \phi(\Sigma_k) V_k^* X \quad \text{and} \quad \Phi_{k, \perp} \equiv U_k, \perp \phi(\Sigma_{k, \perp}) V_{k, \perp} X.
\]

By [3] Lemma 4.2| (see also [10]) we get that

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

By the previous inequality we get that

\[
\|(I - \Phi \Phi^\dagger) P_{S'}\|_{2,F} \leq \|(I - \Phi \Phi_k^\dagger) P_{S'}\|_{2,F}.
\]

We can further estimate

\[
\|(I - \Phi \Phi_k^\dagger) P_{S'}\|_{2,F} \leq \|(I - \Phi \Phi_k^\dagger) P_{S'}\|_{2,F} + \|\Phi_{k, \perp} \Phi_k^\dagger P_{S'}\|_{2,F}.
\]

**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. (30). 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 \( \Theta(S, \mathcal{X}) < \pi/2 \) 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 \( k \geq \dim(\mathcal{W}) := t \geq h \). Let

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

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

\[
\Phi_k \Phi_k^\dagger = U_k P_{\mathcal{T}} U_k^*.
\]

We now consider \( \mathcal{H}' = \text{Span}\{e_1, \ldots, e_j\} \subset \mathbb{K}^k \), where \( j = j(h) \geq 1 \) and \( \{e_1, \ldots, e_k\} \) denotes the canonical basis of \( \mathbb{K}^k \); we also consider the principal angles

\[
\Theta(\mathcal{W}, \mathcal{H}') = \text{diag}(\theta_1(\mathcal{W}, \mathcal{H}'), \ldots, \theta_j(\mathcal{W}, \mathcal{H}')) \in \mathbb{R}^{j \times j}.
\]

By Proposition 5.1 we get that

\[
\Theta(\mathcal{W}, \mathcal{H}') \leq \Theta(\mathcal{X}, \mathcal{V}_j) < \pi/2,
\]

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

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

\[
\|\sin \Theta(\mathcal{T}', \mathcal{H}')\|_{2,F} \leq \|\sin \Theta(\mathcal{W}', \mathcal{H}')\|_{2,F} = \|\sin \Theta(\mathcal{W}, \mathcal{H}')\|_{2,F}
\]

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

Let \( \mathcal{T}'' = \mathcal{T} \ominus \mathcal{T}' \) so \( \dim(\mathcal{T}'') = t - j \) and \( \mathcal{T}' \subset (\mathcal{T}')^\perp \). Since \( \dim((\mathcal{T}')^\perp) = \dim((\mathcal{H}')^\perp) \), by Eq. (3) 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 \( \{y_1, \ldots, y_{t-j}\} \subset T'' \) and \( \{z_1, \ldots, z_{t-j}\} \subset (H')^\perp \) be the principal vectors associated to \( T'' \) and \( (H')^\perp \). Then, if we let \( H'' = \text{Span}\{z_1, \ldots, z_{t-j}\} \) we have that \( \dim H'' = h - j \),

\[
\| \sin\Theta(T'', H'') \|_{2,F} \leq \| \sin\Theta(T'', (H')^\perp) \|_{2,F} \leq \| \Theta(W, H') \|_{2,F}.
\]

On the one hand, we have that \( T = T' \oplus T'' \); on the other hand, we have that \( S' := U_k(H' \oplus H'') = U_j \oplus U_k H'' \subseteq U_k \subseteq K^m \) is an \( h \)-dimensional left dominant subspace of \( A \) (see Section 2.2).

**Step 5: obtaining some more upper bounds.** Since

\[
\| \Theta(T', H') \|_{2,F} \leq \| \Theta(T'', H'') \|_{2,F} \leq \| \Theta(W, H') \|_{2,F}
\]

then Proposition 5.3 implies that \( \| \Theta(U_k T', S') \|_{2,F} \leq 4 \| \Theta(W, H') \|_{2,F} \). Hence

\[
\|(I - \Phi_k \Phi_k^\dagger) P_{S'} \|_{2,F} = \| \Theta(U_k T', S') \|_{2,F} \leq 4 \| \Theta(W, H') \|_{2,F},
\]

since \( U_k \) is an isometry and \( R(\Phi_k) = U_k T \) (see Eq. (31)).

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

\[
\Phi_k^\dagger = (V_k^* X)^\dagger (U_k \phi(\Sigma_k) P_W)^\dagger.
\]

Since \( U_k \in K^{m \times k} \) has trivial kernel, we get that

\[
(U_k \phi(\Sigma_k) P_W)^\dagger = (\phi(\Sigma_k) P_W)^\dagger (U_k P_T)^\dagger = (\phi(\Sigma_k) P_W)^\dagger P_T U_k^* = (\phi(\Sigma_k) P_W)^\dagger U_k^*
\]

where we have used Proposition 5.1 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 \( \ker((\phi(\Sigma_k) P_W)^\dagger) = T \). The previous facts show that

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

so then,

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

The result now follows from the estimates in Eqs. (28), (29) and (30) together with the bounds in Eqs. (32) and (33).

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

Now we consider a brief proof of Corollary 5.3.

**Proof.** By Lemma 2.3 we conclude that there exists a polynomial \( \phi(x) \) satisfying the hypothesis of Theorem 3.2 and such that

\[
\| \phi(\Sigma_{k,\perp}) \|_2 \| \phi(\Sigma_k)^{-1} \|_2 \| V_{k,\perp}^* X(V_k^* X)^\dagger \|_{2,F} \leq 4 \| V_{k,\perp}^* X(V_k^* X)^\dagger \|_{2,F} \frac{\sigma_{k+1}}{\sigma_k^2}.
\]

The result now follows from the previous inequality and the definition of \( \Delta(X, q, k)_{2,F} \).

**Remark 4.2.** Some comments related to the previous proof are in order. We have followed the general lines of the proof of [5, Theorem 2.1]. Nevertheless, the assumption in [5] (i.e., that \( R(V_k^* X) = R(V_k^* X) \)) automatically implies that \( \|(I - \Phi_k \Phi_k^\dagger) P_{S'} \|_{2,F} = 0 \) in Eq. (29). 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.

We can now see that the assumption that the pair \( (A, X) \) is \( h \)-compatible (for an arbitrary \( 1 \leq h \leq \text{rank}(A) \)) is weaker, at least from the point of view of our present approach, than the structural assumption that the pair \( (A, X) \) is \( k \)-compatible for an index \( k \) such that \( \sigma_k > \sigma_{k+1} \), as considered in [5].
4.2 Proof of Theorem 3.4

Proof. Consider Notation 4.1 and assume that $1 \leq j < h \leq k < \text{rank}(A)$. Notice that $\sigma_h = \sigma_k > 0$, since $h \leq \text{rank}(A)$.

**Step 1:** Applying the DIKM-I theory using the singular gap $\sigma > \sigma_{j+1}$. Let $X \in \mathbb{K}^{n \times r}$ be such that $\text{dim}(X) = s \geq h$ and $\Theta(S, X) < \frac{\pi}{2} I$, where $X = R(X) \subset \mathbb{K}^n$ denotes the range of $X$ and $S \subset \mathbb{K}^n$ is an $h$-dimensional right dominant subspace of $A$. Consider a full SVD $A = U\Sigma V^*$ in such a way that $S = V_h$.

We can now consider decompositions as in Eq. (20), using the index $j = j(h)$ that is,

$$\Sigma = \begin{pmatrix} \Sigma_j & \Sigma_{j,\perp} \\ \Sigma_{j,\perp}^* & \Sigma_{\perp} \end{pmatrix}, \quad U = \begin{pmatrix} U_j & U_{j,\perp} \end{pmatrix}, \quad V = \begin{pmatrix} V_j & V_{j,\perp} \end{pmatrix}. \quad (34)$$

As a consequence of our hypothesis, we get that $R(V_j^* X) = R(V_j^*)$ (notice that the subspace $R(V_j^*)$ is independent of our choice of SVD of $A$, since $\sigma_j > \sigma_{j+1}$). Hence, we can apply Theorem 2.1 and Lemma 2.3 (that correspond to the DIKM-I theory with singular gaps) and conclude that if we let

$$\gamma_j = \frac{\sigma_j - \sigma_{j+1}}{\sigma_{j+1}}$$

and

$$\Delta(X, q, j)_{2,F} = 4 \frac{\|V_j^* X (V_j^* X)^T\|_{2,F}}{\sqrt{\gamma_j} \gamma_j, I}$$

then, we have that

$$\|\sin \Theta(K_q, R(U_j))\|_{2,F} \leq \Delta(X, q, j)_{2,F} \frac{\sigma_{j+1}}{\sigma_j}, \quad (35)$$

where $K_q = K_q(A, X)$ denotes the Krylov space with power parameter $q \geq 0$.

**Step 2:** Applying Theorem 3.2 to $A^*$. Since $\sigma_h > 0$ and $\Theta(R(V_h), R(X)) < \pi/2 I$, we conclude that $R(V_h^* X) = R(V_h^*)$ and therefore $\text{rank}(U_h^* A X) = \text{rank}(\Sigma_h V_h^* X) = \text{rank}(V_h^* X) = h$. The previous facts show that

$$\text{dim}K_q \geq h \quad \text{and} \quad \Theta(K_q, R(U_h)) < \frac{\pi}{2} I.$$

Let $Y_q$ denote an isometry such that $Y_q Y_q^* \in \mathbb{K}^{m \times m}$ is the orthogonal projection onto $K_q$. We now consider $K_{q,t} = K_t(A^*, Y_q)$ which is the block Krylov space of order $t$ constructed in terms of $A^*$ and $Y_q$. Notice that $S^* = R(U_h)$ is an $h$-dimensional right dominant subspace of $A^*$ such that $\Theta(R(Y_q), S^*) < \frac{\pi}{2} I$. Moreover, the subspace $R(U_j)$ is a $j$-dimensional right dominant subspace of $A^*$, such that $\Theta(R(Y_q), R(U_j)) = \Theta(K_q, R(U_j))$. Hence, we can apply Theorem 3.2 and Lemma 2.3 to the matrices $A^*$ and $Y_q$ and conclude that if we let

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

and

$$\Delta^*(Y_q, t, k)_{2,F} = 4 \frac{\|U_{k,\perp} Y_q (U_k^* Y_q)^T\|_{2,F}}{\sqrt{\gamma_k} \gamma_{k,t}, I}$$

then, there exists an $h$-dimensional left dominant subspace $\tilde{S}$ of $A^*$ such that

$$\|\sin \Theta(K_{q,t}^*, \tilde{S})\|_{2,F} \leq 4 \Delta(X, q, j)_{2,F} \frac{\sigma_{j+1}}{\sigma_j} + \Delta^*(Y_q, t, k)_{2,F} \frac{\sigma_{k+1}}{\sigma_k},$$

where we have also applied Eq. (35). It is clear that $\tilde{S}$ is an $h$-dimensional right dominant subspace of $A$.

**Step 3:** Computing $K_{q,t}^*$. We end the proof by noticing the following facts: recall that

$$K_q = R(A X) + R((A^*) A X) + \cdots + R((A^*)^h A X) = R(Y_q). \quad (36)$$

Similarly, notice that

$$K_{q,t}^* = R(A^* Y_q) + R((A^* A) A^* Y_q) + \cdots + R((A^* A)^t A^* Y_q).$$
If we consider the identity in Eq. (36) and we let 0 ≤ ℓ ≤ t then

\[ R((A^*A)^{\ell}A^*Y_q) = R((A^*A)^{\ell+1}X) + R((A^*A)^{\ell+2}X) + \cdots + R((A^*A)^{\ell+q+1}X). \]

The previous facts show that

\[ K_{q,t}^* = R((A^*A)X) + R((A^*A)^2X) + \cdots + R((A^*A)^{q+t+1}X). \]

The cases j = 0 or k = rank(A) can be treated with similar arguments (the details are left to the reader).

4.3 Proofs of Theorems 3.6 and 3.10

Proof of Theorem 3.6. We assume that (A, X) is h-compatible, we let \( K_q = K_q(A, X) \subset \mathbb{K}^m \) and \( Y_q \) be such that \( Y_qY_q^* \) is the orthogonal projection onto \( K_q \). We first notice that given any \( Z \in \mathbb{K}^{n \times r} \), then the expression \( U_{k,1}^* Z(U_{k,1}^* Z)^d \) only depends on \( Z \) through its range. Indeed, by Proposition 3.4, we have that \( (U_{k,1}^* Z)^d = Z^d(U_{k,1}^* P_R(Z))^d \); hence

\[ U_{k,1}^* Z(U_{k,1}^* Z)^d = U_{k,1}^* ZZ^d(U_{k,1}^* P_R(Z))^d = U_{k,1} P_R(Z)(U_{k,1}^* P_R(Z))^d. \]

Given coefficients \( c_i \neq 0 \), for 0 ≤ i ≤ q, we consider

\[ K_q = (\sqrt{c_0}AX \sqrt{c_1}(AA^*)AX \cdots \sqrt{c_q}(AA^*)AX) \in \mathbb{C}^{n \times (q+1)r}, \]

Notice that by construction, \( R(K_q) = K_q = R(Y_q) \). Thus, in what follows we replace \( Y_q \) with the matrix \( K_q \) (based on the comments at the beginning of the proof). Notice that

\[ U_{k,1}^* K_q = (\sqrt{c_0}\Sigma_k \sqrt{c_1}\Sigma_k^3 \cdots \sqrt{c_q}\Sigma_k^{2q+1}) X_{q,1} \]

where \( X_{q,1} = \oplus_{q+1} V_q^* X \in \mathbb{K}^{k(q+1) \times r(q+1)} \) is the \((q + 1) \times (q + 1)\) block diagonal matrix with main diagonal blocks equal to \( V_q^* X \). By Proposition 3.3, we get that

\[ (U_{k,1}^* K_q)^d = X_{q,1}^d ((\sqrt{c_0} \Sigma_k \sqrt{c_1} \Sigma_k^3 \cdots \sqrt{c_q} \Sigma_k^{2q+1}) P_R(X_{q,1})^d). \]

Similarly, we have that

\[ U_{k,1}^* K_q = (\sqrt{c_0} \Sigma_{k,1} \sqrt{c_1} \Sigma_{k,1}^3 \cdots \sqrt{c_q} \Sigma_{k,1}^{2q+1}) X_{q,2}, \]

where \( X_{q,2} = \oplus_{q+1} V_{k,1}^* X \in \mathbb{K}^{k(n-k)(q+1) \times r(q+1)} \) is the \((q + 1) \times (q + 1)\) block diagonal matrix with main diagonal blocks equal to \( V_{k,1}^* X \). Therefore \( \|U_{k,1}^* K_q U_{k,1}^* K_q\|_{2,F} \) is bounded from above by

\[ \|(\sqrt{c_0} \Sigma_{k,1} \cdots \sqrt{c_q} \Sigma_{k,1}^{2q+1})\|_2 \|X_{q,2} X_{q,1}^d\|_{2,F} \|(\sqrt{c_0} \Sigma_k \cdots \sqrt{c_q} \Sigma_k^{2q+1})\|_2. \]

On the one hand, notice that \( X_{q,1}^d = \oplus_{q+1} (V_k^* X)^d \) is also a block diagonal matrix. Hence,

\[ X_{q,2} X_{q,1}^d = \oplus_{q+1} V_{k,1}^* X (V_k^* X)^d. \]

The previous facts show that

\[ \|X_{q,2} X_{q,1}^d\|_2 = \|V_{k,1}^* X (V_k^* X)^d\|_2 \quad \text{and} \quad \|X_{q,2} X_{q,1}^d\|_F = \sqrt{q + 1} \|V_{k,1}^* X (V_k^* X)^d\|_F. \]

On the other hand, notice that

\[ (\sqrt{c_0} \Sigma_{k,1} \cdots \sqrt{c_q} \Sigma_{k,1}^{2q+1}) (\sqrt{c_0} \Sigma_{k,1} \cdots \sqrt{c_q} \Sigma_{k,1}^{2q+1})^d = \sum_{i=0}^q c_i (\Sigma_{k,1}^2)^{2i+1} = \psi(\Sigma_{k,1}^2) \in \mathbb{R}^{(n-k) \times (n-k)}, \]

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where $\psi(x) = \sum_{i=0}^{q} c_i x^{2i+1}$ is a degree $2q + 1$ polynomial with odd powers only. Then, we conclude that
\[
\| \left( \sqrt{c_0} \Sigma_{k,\perp} \cdots \sqrt{c_q} \Sigma_{k,\perp}^2 \right) \|_2 \leq \| \psi(\Sigma_{k,\perp}^2) \|_2 ,
\]
where we have used that $\| C^* C \|_2 = \| CC^* \|_2 = \| C \|_2^2$ for any matrix $C$. Similarly, we get that
\[
\| (\sqrt{c_0} \Sigma_k \cdots \sqrt{c_q} \Sigma_k^2 \Sigma_{k,\perp}^2) \|_2 \leq \| \psi(\Sigma_k^2) \|_2 .
\]
We can now consider the degree $2q + 1$ polynomial of Lemma 23 constructed in terms of the squared singular numbers $\sigma_1^2 \geq \ldots \sigma_k^2 \geq \sigma_{k+1}^2 \geq \ldots \geq \sigma_p^2$. In this case, we get that
\[
\| \psi(\Sigma_k^2)^{-1} \|_2 \leq \sigma_k^{-2} \quad \text{and} \quad \| \psi(\Sigma_k^2 \Sigma_{k,\perp}) \|_2 \leq \frac{4 \sigma_{k+1}^2}{2(2q+1) \min(\sqrt{\mu_k},1)}
\]
where
\[
\mu_k = \frac{\sigma_k^2 - \sigma_{k+1}^2}{\sigma_{k+1}^2} = \frac{\sigma_k + \sigma_{k+1}}{\sigma_{k+1}} \cdot \gamma_k \geq 2 \gamma_k.
\]
Hence, by Eqs. (37)–(41) we get that
\[
\| U_{k,\perp}^* Y_q(U_k^* Y_q)^\dagger \|_{2,F} = \| U_{k,\perp}^* K_q(U_k^* K_q)^\dagger \|_{2,F} \leq 2 \| X_q,2(X_q,1)^\dagger \|_{2,F} \frac{\sigma_{k+1}}{\sigma_k} .
\]
Now, we argue as above, but choosing $c_i = c^i$ for $c > 0$ and $0 \leq i \leq q$. In this case,
\[
\| \psi(\Sigma_k^2)^{-1} \|_2 = \left( \sum_{i=0}^{q} c^i \sigma_k^{2(2i+1)} \right)^{-1} \quad \text{and} \quad \| \psi(\Sigma_k^2 \Sigma_{k,\perp}) \|_2 = \sum_{i=0}^{q} c^i \sigma_{k+1}^{2(2i+1)} .
\]
Since
\[
\lim_{c \to +\infty} \sum_{i=0}^{q} c^i \sigma_{k+1}^{2(2i+1)} = \left( \frac{\sigma_k}{\sigma_{k+1}} \right)^{2q+1} \frac{\sigma_{k+1}}{\sigma_k}
\]
we now see that
\[
\| U_{k,\perp}^* Y_q(U_k^* Y K_q)^\dagger \|_{2,F} = \| U_{k,\perp}^* K_q(U_k^* K_q)^\dagger \|_{2,F} \leq \| X_q,2(X_q,1)^\dagger \|_{2,F} \left( \frac{\sigma_{k+1}}{\sigma_k} \right)^{2q+1} .
\]
The result now follows from Eqs. (37), (38), (42), (43) and the fact that $\sigma_{k+1}/\sigma_k = (1 + \gamma_k)^{-1}$. \hfill \Box

**Proof of Theorem 5.10.** Assume first that $1 \leq j < h \leq k < \text{rank}(A)$; notice that $\sigma_h = \sigma_k > 0$, since $h \leq \text{rank}(A)$. Consider an $h$-compatible pair $(A, X)$ and let $C_2$ be defined as in Eq. (17). Let $K_{q+1} = K_{q+1}(A,X) \subset \mathbb{K}^m$ for a fixed $q \geq 0$. By setting $t = 0$ in Theorem 5.10, we see that there exists an $h$-dimensional left dominant subspace $\tilde{S}$ for $A$ such that
\[
\| \sin(\Theta(K_{q+1}, \tilde{S})) \|_2 \leq 16 \| U_{j,\perp}^* A X (U_{j,\perp}^* A X)^\dagger \|_{2,F} + 4 \| V_{k,\perp}^* W_q(V^* W_q)^\dagger \|_2 \frac{\sigma_{k+1}}{\sigma_k} ,
\]
where we used that $\sigma_{j+1}/\sigma_j$ and $1 \leq 2^{\min(\sqrt{\gamma_k},1)}$. By Remark 3.3 we get that
\[
\| U_{j,\perp}^* A X (U_{j,\perp}^* A X)^\dagger \|_{2,F} \leq \| V_{j,\perp}^* X (V_{j,\perp}^* X)^\dagger \|_{2,F}
\]
and then,
\[
\| V_{k,\perp}^* W_q(V^* W_q)^\dagger \|_2 \leq \min \left\{ \frac{2 \| V_{k,\perp}^* X (V_{k,\perp}^* X)^\dagger \|_2 \sigma_{k+1}}{2(2q+1) \min(\sqrt{\gamma_k}/2,1)} \sigma_k , \| V_{k,\perp}^* X (V_{k,\perp}^* X)^\dagger \|_2 \right\} .
\]
Assume first that $\gamma_k \geq 1$, so that $2^{(2q+1)\min\{\sqrt{\gamma_k}, 1\}} = 2^{2q+1} \leq (1 + \gamma_k)^{2q+1}$. Hence, Eq. (44) and the previous facts imply that

$$\| \sin \Theta(K_{q+1, \hat{S}}) \|_2 \leq \frac{16}{2^{(2q+1)\min\{\sqrt{\gamma_k}, 1\}} + 4} \frac{\| V_{k,\perp} X (V_k^* X)^\dagger \|_2}{2^{2q+1}}.$$

Eq. (18) now follows from the previous facts together with the definition of $C_2$.

Assume now that $\gamma_k < 1$; then $\min\{\sqrt{\gamma_k}, \sqrt{\gamma_k}/2, 1/2\} \leq \min\{\gamma_j, 1\}, \min\{\sqrt{\gamma_k}/2, 1/2\}$. Hence, the previous facts and Eq. (44) imply that

$$\| \sin \Theta(K_{q+1, \hat{S}}) \|_2 \leq \frac{16}{2^{(2q+1)\min\{\sqrt{\gamma_k}, 1\}} + 8} \frac{\| V_{k,\perp} X (V_k^* X)^\dagger \|_2}{2^{2q+1}}.$$

Eq. (19) now follows from the previous facts together with the definition of $C_2$.

The cases $j = 0$ or $k = \text{rank}(A)$ can be treated with similar arguments (the details are left to the reader).

4.4 Proof of Theorems 3.12, 3.13 and 3.14

Throughout this section we consider Notation 4.1 and the notation from Theorem 3.14. 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 $K_{q+t+1}$ constructed in terms of $A$ and $X$, for some fixed $q, t \geq 0$; further, we let $U_I \in \mathbb{K}^{m \times i}$ 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 further assume that $1 \leq j < h \leq k < \text{rank}(A)$; notice that $\sigma_k = \sigma_k > 0$, since $h \leq \text{rank}(A)$. The cases $j = 0$ or $k = \text{rank}(A)$ can be treated with similar arguments (the details are left to the reader).

**Proof of Theorem 3.12** Let $K^*_{q,t} \subseteq \mathbb{K}^{n}$ be the subspace defined in Theorem 3.4 that is

$$K^*_{q,t} = R((A^* A) X) + R((A^* A)^2 X) + \cdots + R((A^* A)^{q+t+1} X).$$

By Corollary 3.8 and Eq. (21), there exists an $h$-dimensional right dominant subspace $\hat{S}$ for $A$ such that

$$\| \sin \Theta(K^*_{q,t}, \hat{S}) \|_2 \leq \frac{16}{2^{(2q+1)\min\{\sqrt{\gamma_k}, 1\}} + 4} \frac{\| V_{k,\perp} X (V_k^* X)^\dagger \|_2}{2^{2q+1}} + 4 \Pi_{2,F} \| V_{k,\perp} X (V_k^* X)^\dagger \|_2 = \frac{1}{2} \cdot \frac{1}{\sqrt{2}} \cdot \frac{1}{\delta_2,F}. \quad (46)$$

By hypothesis we have that $\delta_2 \leq 1$; these last facts imply that $\| \sin \Theta(K^*_{q,t}, \hat{S}) \|_2 \leq \frac{1}{\sqrt{2}}$ and then,

$$\Theta(K^*_{q,t}, \hat{S}) \leq \frac{\pi}{4} I. \quad (47)$$

On the other hand, it is clear that $A(K^*_{q,t}) \subseteq K_{q+t+1}$. We now set $\hat{A} = AP_{\hat{S}}$, where $P_{\hat{S}}$ denotes the orthogonal projection onto $\hat{S} \subseteq \mathbb{K}^{n}$. In this case we get that $A = A_{\hat{S}} + (A - A_{\hat{S}})$ so that $A_{\hat{S}}(A - A_{\hat{S}})^* = AP_{\hat{S}}(I - P_{\hat{S}})A = 0$. If we let $V_{\hat{S}} \in \mathbb{K}^{n \times h}$ denote the right singular vectors of $A_{\hat{S}}$ then $R(V_{\hat{S}}) = \hat{S}$. Notice that Eq. (47) implies that $V_{\hat{S}}^* K^*_{q,t} = R(V_{\hat{S}}^*)$ so we can apply Lemma 5.6 in this context. Hence, we consider the principal vectors $\{w_1, \ldots, w_h\} \in K^*_{q,t}$, corresponding to the pair of subspaces $<K^*_{q,t}, \hat{S}>$; we also let $Q \in \mathbb{K}^{n \times h}$ be an isometry with columns $w_1, \ldots, w_h$ so that $R(AQ) \subseteq AK^*_{q,t} \subseteq K_{q+t+1}$. Recall that $U_K$ denotes the matrix whose columns form an orthonormal basis of the Krylov space $K_{q+t+1}$ (see Algorithm 2.1). Then, the previous facts together with Lemma 5.6 show that

$$\| A_{\hat{S}} - U_K U_K^* A_{\hat{S}} \|_{2,F} \leq \| (I - AQ(AQ)^\dagger) A_{\hat{S}} \|_{2,F} = \| A_{\hat{S}} - AQ(AQ)^\dagger A_{\hat{S}} \|_{2,F} \leq \| A - A_{\hat{S}} \|_2 \tan \Theta(K^*_{q,t}, \hat{S}) \|_2,F.$$
On the one hand, \(\|A - A_S\|_2 = \sigma_{h+1}\), since \(\tilde{S}\) is an \(h\)-dimensional right dominant subspace of \(A\). On the other hand, Eq. (47) also implies that

\[
\| A - A_S \|_2 \| \tan \Theta(K_{q,t}^*, \tilde{S}) \|_2, F \leq \sigma_{h+1} \sqrt{2} \| \sin \Theta(K_{q,t}^*, \tilde{S}) \|_2, F \leq \sigma_{h+1} \delta_2, F,
\]

where we have also used Eq. (46).

**Proof of Theorem 3.14.** We keep using the notation from the proof of Theorem 3.12 above. As a consequence of Theorem 3.12 and Lidskii’s inequality for singular values, we get that

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

Therefore, for \(1 \leq i \leq h\), we have that

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

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

**Proof of Theorem 3.14.** We keep using the notation from the proof of Theorem 3.12 above. In particular, we consider the existence of an \(h\)-dimensional right dominant subspace \(\tilde{S}\) for \(A\) that satisfies Eq. (46). We now argue as in the proof of [4] Theorem 2.3] and consider the estimate for the Frobenius norm first. Indeed, by [3] Lemma 8 we have that

\[
A - \tilde{U}_i \tilde{U}_i^* A = A - U_K(U_K^* A) \quad \text{for} \quad 1 \leq i \leq h,
\]

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.

\[
\| A - U_K(U_K^* A)_i \|_F = \min_{\text{rank}(Y) \leq i} \| A - U_K Y \|_F. \tag{48}
\]

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

\[
A = A_i + A_{i,\perp} \quad \text{where} \quad A_i = U_i \Sigma_i V_i^* \quad \text{and} \quad A_{i,\perp} = A - A_i.
\]

Then, by [4] Lemma 7.2 we get that

\[
\| A - \tilde{U}_i \tilde{U}_i^* A \|_F^2 \leq \| A - A_i \|_F^2 + \| A_i - U_K U_K^* A_i \|_F^2. \tag{49}
\]

Now we bound the second term in Eq. (49). Since \(\Theta(R(V_i), K_{q,t}^*) \leq \frac{\pi}{4} I_h\) then \(\Theta(R(V_i), K_{q,t}^*) \leq \frac{\pi}{4} I_i\) (see Section 2.1) and we see that \(V_i^*(K_{q,t}^*) = R(V_i^*)\). Thus, we can apply Lemma 5.6 in this context. Hence, we consider the principal vectors \(\{w_1, \ldots, w_4\} \subset K_{q,t}^*\) corresponding to the pair \((K_{q,t}^*, R(V_i))\). Moreover, we let \(Q \in \mathbb{R}^{n \times 4}\) be an isometry with \(R(Q) = \text{Span}\{w_1, \ldots, w_4\}\) so that \(R(AQ) \subset A(K_{q,t}^*) \subset K_{q,t+1}\). The previous facts together with Lemma 5.6 show that

\[
\| A_i - U_K U_K^* A_i \|_F \leq \| (I - AQ(AQ)^\dagger) A_i \|_F = \| A_i - AQ(AQ)^\dagger A_i \|_F \leq \| A - A_i \|_2 \| \tan \Theta(K_{q,t}^*, R(V_i)) \|_F \leq \| A - A_i \|_2 \| \tan \Theta(K_{q,t}^*, R(V_h)) \|_F.
\]

By Eq. (47) we get that \(\Theta(R(V_h), K_{q,t}^*) = \Theta(\tilde{S}, K_{q,t}^*) \leq \frac{\pi}{4} I;\) then,

\[
\| \tan \Theta(K_{q,t}^*, R(V_h)) \|_F \leq \sqrt{2} \| \sin \Theta(K_{q,t}^*, R(V_h)) \|_F \leq \delta_F
\]
where we have used Corollary 3.8 and Eq. (21). Therefore, the previous inequalities imply that
\[
\|A - \hat{U}_i \hat{U}_i^* A\|_F^2 \leq \|A - A_i\|_F^2 + (\sigma_{i+1} \cdot \delta_F)^2.
\] (50)

This proves the upper bound in Eq. (21) for the Frobenius norm. To prove the bound for the spectral norm, recall that by [11, Theorem 3.4.] we get that Eq. (50) implies that
\[
\|A - \hat{U}_i \hat{U}_i^* A\|_2 \leq \|A - A_i\|_2 + (\sigma_{i+1} \cdot \delta_F)^2,
\]
since \(\text{rank}(\hat{U}_i \hat{U}_i^* A) \leq i\). The upper bound in (21) for the spectral norm follows from this last fact.

5 Appendix

In this section we include a number of technical results that are needed for the proofs of the main results. Most of these 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 \( \dim \mathcal{X} \geq \dim \mathcal{V} = j \), \( \mathcal{V} \subset \ker(V^* V) \) and \( \Theta(\mathcal{X}, \mathcal{V}) < \pi/2 \). Then \( W = V^* \mathcal{X} \subset \mathbb{K}^k \) is such that \( \dim W \geq j \) and if we let \( \mathcal{H}' = V^* \mathcal{V}' \) then

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

**Proof.** First notice that

\[P_{\mathcal{X}} P_{\mathcal{V}} P_{\mathcal{X}} \leq P_{\mathcal{X}} V V^* P_{\mathcal{X}}.\]

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

\[0 \leq D \leq P_{R(D)} \implies P_{\mathcal{V}} P_{\mathcal{X}} P_{\mathcal{V}} = P_{\mathcal{V}} D P_{\mathcal{V}} \leq P_{\mathcal{V}} P_{R(D)} P_{\mathcal{V}},\]

where we used that \(P_{\mathcal{V}} V V^* = P_{\mathcal{V}}\). Then, \(\cos^2 \Theta(\mathcal{X}, \mathcal{V}') \leq \cos^2 \Theta(V V^* \mathcal{X}, \mathcal{V}') \in \mathbb{R}^{j \times j}\) 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 \(P_{\mathcal{H}'} B = B P_{\mathcal{H}'}\), \(\dim \mathcal{H}' = \dim \mathcal{W}'\) and \(\mathcal{W}' \subset \ker(B)^\perp\). If we let \(B W' = \mathcal{T}'\),

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

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

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

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

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

**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

\[\|\sin \Theta(\mathcal{T}, \mathcal{H})\|_{2,F} \leq 2(\|\sin \Theta(\mathcal{T}', \mathcal{H}')\|_{2,F} + \|\sin \Theta(\mathcal{T}'', \mathcal{H}'')\|_{2,F}).\]
Proof. As usual, we compute the sines of the principal angles in terms of singular values of products of projections: in this case, using that \( P_{\mathcal{H}} = P_{\mathcal{H}'} + P_{\mathcal{H}''} \) and \( P_{\mathcal{T}} = P_{\mathcal{T}'} + P_{\mathcal{T}''} \) we have that
\[
\| \sin \Theta(\mathcal{T}, \mathcal{H}) \|_{2,F} = \| (I - P_{\mathcal{T}}) P_{\mathcal{H}} \|_{2,F} = \| (P_{\mathcal{H}} - P_{\mathcal{T}}) P_{\mathcal{H}} \|_{2,F} = \| (P_{\mathcal{H}'} - P_{\mathcal{T}'} + P_{\mathcal{H}''} - P_{\mathcal{T}''}) (P_{\mathcal{H}'} + P_{\mathcal{H}''}) \|_{2,F} \leq \| (I - P_{\mathcal{T}'} P_{\mathcal{H}'}) \|_{2,F} + \| (I - P_{\mathcal{T}''} P_{\mathcal{H}''}) \|_{2,F}.
\]
Now, notice that \( P_{\mathcal{T}'} \leq I - P_{\mathcal{T}''} \) so
\[
\| P_{\mathcal{T}'} P_{\mathcal{H}'} \|_{2,F} \leq \| (I - P_{\mathcal{T}''}) P_{\mathcal{H}'} \|_{2,F} = \| \sin \Theta(\mathcal{T}'', \mathcal{H}'') \|_{2,F}.
\]
Similarly, \( \| P_{\mathcal{T}''} P_{\mathcal{H}''} \|_{2,F} \leq \| (I - P_{\mathcal{T}'}) P_{\mathcal{H}''} \|_{2,F} = \| \sin \Theta(\mathcal{T}', \mathcal{H}') \|_{2,F}. \]

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

Then
\[
(BC)^\dagger = C\dagger (BP_B)^\dagger.
\]
Proof. In this case \( R(BC) = BV \) and \( \ker BC = \ker C. \) Moreover,
\[
BCC\dagger (BP_B)^\dagger = BP_B (BP_B)\dagger = P_{BV} \quad \text{and}
\]
\[
C\dagger (BP_B)^\dagger BC = C\dagger (BP_B)^\dagger BP_V C = C\dagger P_{\ker (BP_B)^\dagger} C = P_{\ker C^\perp},
\]
where we used that \( \ker (BP_B) = \mathcal{V}^\perp \), 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
\[
\mathcal{P}_{C, i}^\xi(A) = C \cdot \arg \min_{\text{rank}(Y) \leq i} \| A - CY \|_\xi \quad \text{for} \quad \xi = 2, F.
\]
Due to the optimality properties of the projection \( C\dagger \) (see (11)) we get that
\[
\| A - CC\dagger A \|_\xi \leq \| A - \mathcal{P}_{C, i}^\xi(A) \|_\xi \quad \text{for} \quad \xi = 2, F. \tag{51}
\]
The following result is [22, Lemma C.5] (see also [3]).

Lemma 5.5 ([22]). Let \( A \in \mathbb{K}^{m \times n} \) and consider a decomposition \( A = A_1 + A_2 \), with \( \text{rank}(A_1) = i \). Let \( V_1 \in \mathbb{K}^{n \times i} \) denote the top right singular vectors of \( A_1 \). Let \( Z \in \mathbb{K}^{n \times p} \) such that \( \text{rank}(V_1^* Z) = i \) and let \( C = AZ \). Then \( \text{rank}(C) \geq i \) and
\[
\| A_1 - \mathcal{P}_{C, i}^\xi(A_1) \|_\xi \leq \| A_2 Z (V_1^* Z)^\dagger \|_\xi \quad \text{for} \quad \xi = 2, F.
\]

The following is a small variation of [22, 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 \( \text{rank}(A_1) = i \). 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 \( \mathcal{K}^* \subset \mathbb{K}^n \) be a subspace such that \( V_1^* (\mathcal{K}^*) = R(V_1^*) \). Let \( \{x_1, \ldots, x_i\} \subset \mathcal{K}^* \) denote the principal vectors corresponding to the pair \((\mathcal{K}^*, R(V_1))\) and let \( Q \in \mathbb{K}^{n \times i} \) be an isometry with \( R(Q) = \text{Span}(\{x_1, \ldots, x_i\}) \subset \mathcal{K}^* \). Then,
\[
\| A_1 - (AQ)(AQ)^\dagger A_1 \|_{2,F} \leq \| A - A_1 \|_2 \| \tan(\Theta(\mathcal{K}^*, R(V_1))) \|_{2,F}.
\]
Proof. Notice that by construction
\[ \Theta(R(Q), R(V_1)) = \Theta(K^*, R(V_1)) < \frac{\pi}{2} I. \]

Then, we get that rank\((AQ) = i\). Hence, we have that
\[
\|A_1 - (AQ)(AQ)\|_{2,F} \leq \|A_1 - \mathcal{P}^F_{AQ,i}(A_1)\|_{2,F} \leq \|A_2Q(V_1^*Q)\|_{2,F}
\]
\[
\leq \|A_2\|_2 \|V_2^*Q(V_1^*Q)\|_{2,F}
\]
\[
= \|A_2\|_2 \|\tan \Theta(R(Q), R(V_1))\|_{2,F}
\]
\[
= \|A - A_1\|_2 \|\tan \Theta(K^*, R(V_1))\|_{2,F},
\]
where we have used Eq. (51), Lemma 5.5, that the isometry \(V_2\) satisfies that \(A_2 = A_2V_2V_2^*\) and the identity \(\|V_2^*Q(V_1^*Q)\|_{2,F} = \|\tan \Theta(R(Q), R(V_1))\|_{2,F}\), that holds by [5, Lemma 4.3], since \(\text{rank}(V_1^*Q) = i\).

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