Approximating Truncated LS and TLS Solutions by Rank Revealing Two-Sided Orthogonal Decompositions

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APPROXIMATING TRUNCATED LS AND TLS SOLUTIONS BY
RANK REVEALING TWO-SIDED ORTHOGONAL
DECOMPOSITIONS

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Abstract. Two-sided orthogonal decompositions generally do not yield all the information that the singular value decomposition (SVD) does, but they yield enough information to solve various problems because they provide accurate bases for the relevant subspaces. In this paper we consider two-sided orthogonal decompositions in computing approximations to the SVD-based truncated least squares and total least squares solutions to the overdetermined system of linear equations $Ax \approx b$, where $A$ is numerically rank deficient. We derive analytical bounds which show how the accuracy of the solution is intimately connected to the quality of the subspaces.

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1. Introduction. Algorithms based on orthogonal decompositions are playing an important role in many signal processing applications, cf. [1, 2, 19, 24]. There are several reasons for this. Orthogonal transformations are numerically stable, which is particularly important when the dimension $n$ (or the condition number) of the matrix involved increases. Orthogonal decompositions are sometimes easy to update, which usually reduces the computational burden from $O(n^3)$—associated with recomputation of the decomposition—to $O(n^2)$ flops for an updating. Orthogonal decomposition and updating algorithms can often be implemented in parallel on systolic architectures, cf. [13, 17]. And, finally, orthogonal decompositions immediately yield information about subspaces defined on the matrix which often play an essential role in noise suppression techniques and other signal processing applications.

One of the main numerical tools in signal processing is the singular value decomposition (SVD), which is very accurate and also yields detailed subspace information. However, the SVD is burdensome to compute, and it is also computationally demanding and difficult to update [3]. This is a drawback in recursive algorithms that rely on a simple updating of the coefficient matrix (such as appending a row or a column). In other problems, such as constrained least squares with inequality constraints [23], a sequence of full SVDs have to be computed and therefore the disadvantages or difficulties associated with the SVD algorithm are multiplied.

Depending on the application, the difficulties with the SVD make alternative algorithms attractive, provided they are nearly as reliable, more efficient, and easier to update.

Recently, a new SVD-like updating scheme was presented in [16], in which a QR factorization is updated and modified in order to produce an “acceptable” approximation to the SVD. This algorithm is suited for subspace tracking applications [16].

Another alternative to the SVD is the rank revealing QR factorization by Foster [10] and Chan [4] which can be used to solve many problems almost as accurate as the SVD, but faster [6]. The RRQR factorization is guaranteed to provide lower and upper bounds for the small singular values, as well as approximations to the numerical null space, whenever the rank deficiency of the matrix is small compared

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to the size of the problem. The RRQR factorization is particularly suited for subset selection problems. However, the RRQR factorization and, in particular, its subspace information are not so easy to update.

In this paper we focus on the use of an alternative orthogonal decomposition to the RRQR factorization, namely, a rank revealing two-sided orthogonal decomposition. Two examples of decompositions of this type are the rank revealing URV and ULV algorithms proposed by Stewart [20, 22], which require condition estimation and strategic plane rotations. The theoretical analysis that we present in this paper applies generally to any two-sided orthogonal decomposition, but frequently we will discuss what the results mean in relation to the URV and ULV algorithms proposed by Stewart [20, 22] since—except for the SVD—the URV and ULV algorithms are the only known rank-revealing two-sided orthogonal decomposition (to date).

The URV and ULV factorizations are more computationally demanding than the RRQR factorization, but they have several advantages. First, the URV/ULV-based approximations to the numerical null space are cheaper to update [6]. Second, numerical experiments in [8] indicate that the URV/ULV-decompositions generally offer better approximations to the numerical null space than the RRQR factorization. Third, unlike the RRQR factorization, the quality of the URV and ULV subspaces does not depend very much on the gap in the singular value spectrum.

Thus, when updating and/or accurate subspaces are of issue, then the URV and ULV decompositions are more appealing alternatives to the SVD than the RRQR factorization. For this reason, it is worthwhile to explore the merits of the rank revealing URV and ULV decompositions in computing truncated SVD (TSVD) and truncated total least squares (T-TLS) solutions to the overdetermined system $Ax \approx b$ with numerically rank deficient coefficient matrix $A$. By this, we mean problems where the matrix $A$ has a large condition number and where there is a well-defined gap between the large and small singular values. For such problems, it makes good sense to use rank revealing decompositions, because the numerical rank of the matrix is well defined, namely, as the number of large singular values of $A$.

Throughout the paper we shall consider both the URV and the ULV decomposition as the basic tools without favoring one for the other. This analysis will help to enlighten the advantages and disadvantages of these two similar decompositions. In fact, our analysis is a step beyond Stewart's remark in [22] that "only experience with real-life problems will tell us under what circumstances one decomposition is to be preferred to the other."

The aim of this paper is essentially to obtain insight about the accuracy of approximations to the TSVD and T-TLS solutions computed by rank revealing URV/ULV decompositions. In our analysis, the subspace angles between the "exact" numerical range and null space of $A$, defined via the SVD of $A$, and the approximate subspaces produced by the URV and ULV decompositions, play an essential role. We use these subspace angles to obtain insight into the URV/ULV-based solutions that would otherwise be difficult to get.

Other investigations of URV/ULV-based algorithms have appeared in [16, 20, 25]. However, these papers have mainly focused on implementations and hence the results do not give as much insight as the results presented in this paper. A major reason for this is that in the above papers the role played by the subspace angles has not been investigated.

Our paper is organized as follows. In §2 we review the SVD and its role in connection with numerically rank deficient least squares problems. In §3 we establish our
notation for the URV and ULV decompositions. In §4 we discuss the approximating properties of the subspaces computed from the two-sided orthogonal decompositions, in relation to the relevant SVD-based subspaces. We also show how the TSVD and T-TLS solutions can be replaced by alternative nearby solutions based on the URV and ULV decompositions, which can be computed more efficiently, and we present error bounds for these solutions. The theoretical results show how the accuracy of the solutions is intimately connected to the quality of the subspaces. In §5 we address the subproblem of determining the numerical rank from the two-sided decompositions.

Briefly, we introduce our notations. All norms are 2-norms unless otherwise specified. Usually, Greek letters represent scalars, lower case letters represent vectors, and upper case letters represent matrices. \( R(C) \) denotes the range (column space) of the matrix \( C \). The superscript \( T \) represents the transpose operator.

2. Truncated SVD and TLS Solutions. In this section we briefly review the SVD and its role in connection with numerically rank deficient LS and TLS problems.

2.1. Truncated SVD. The ordinary LS problem

\[
\min_{x \in \mathbb{R}^n} \|Ax - b\|, \ A \in \mathbb{R}^{m \times n} \quad (m \geq n)
\]

arises in a wide variety of applications. Denote the SVD of \( A \) by (cf. [12, §2.3])

\[
A = U \Sigma V^T = [U_1 \ U_2 \ U_2^T] \Sigma [V_1 \ V_2]^T
\]

where

\[
\Sigma = \begin{bmatrix} k & n-k \\ \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} = \begin{bmatrix} k \\ n-k \\ m-n \end{bmatrix}
\]

The parameter \( k \) is the numerical rank of \( A \) and the singular values of \( A \), denoted \( \sigma_i \), are the diagonal elements of \( \Sigma \). They are ordered such that \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0 \), and we assume that \( \sigma_k \gg \sigma_{k+1} \). From the SVD of \( A \) it follows,

\[
A = U_1 \Sigma_1 V_1^T + U_2 \Sigma_2 V_2^T
\]

and the ordinary LS solution of minimum norm can be expressed in terms of the SVD components by

\[
x_{LS} = A^T b = V_1 \Sigma_1^{-1} U_1^T b + V_2 \Sigma_2^{-1} U_2^T b.
\]

Here, \( A^T \) denotes the pseudoinverse of \( A \) [12, §5.5.4]. However, when \( A \) is ill-conditioned the ordinary LS solution has a very large norm due to the inversion of small (nonzero) singular values in \( \Sigma_2 \). Therefore, the minimum norm LS solution to the "regularized" or stabilized LS problem

\[
\min_{x \in \mathbb{R}^n} \|A_k x - b\|
\]

is often computed, where \( A_k \) is the rank-\( k \) matrix nearest to \( A \) in the 2-norm. It is well known that \( A_k \) can be expressed in terms of SVD components by \( A_k \equiv U_1 \Sigma_1 V_1^T \). This amounts to truncating the sum in (3). The minimum norm LS solution to (4) is called the truncated SVD (TSVD) solution \( x_k \) because it can be expressed conveniently as

\[
x_k = A_k^T b = V_1 \Sigma_1^{-1} U_1^T b.
\]

The reader is referred to [9, 14, 15] and [27, Theorem 5.1] for a perturbation analysis of the TSVD solution.
2.2. Truncated TLS. Alternatively, the TLS technique may be used, especially if the errors in $A$ and $b$ are independently and identically distributed. A comprehensive treatment of the classical TLS problem, including computational aspects, is given in \cite{26}. The ill-conditioning in $A$ translates to instability of the TLS solution, and stability may be restored by solving a related matrix approximation problem that resembles the TSVD technique described above. Specifically, the matrix approximation problem is

$$\min_{[A \ b]} ||[A \ b] - [C \ d]||_F \text{ subject to rank}(C) = \text{rank}([C \ d]) = k.$$ 

If $[\tilde{A} \ \tilde{b}]$ solves this matrix approximation problem, then we will denote the minimum norm solution to $\tilde{A}x = \tilde{b}$ by $\tilde{z}_k$, called the truncated TLS (T-TLS) solution. A sensitivity analysis of the truncated TLS solution is given by Fierro and Bunch in \cite{9}. Denote the SVD of the compound matrix $[A \ b]$ by

$$[A \ b] = U \Sigma V^T = [U_1 \ U_2 \ U_2^T] \Sigma [V_1 \ V_2]^T$$

where

$$\Sigma = \begin{bmatrix} k & n-k+1 \\ 0 & \Sigma_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} k \\ n-k+1 \\ m-n-1 \end{bmatrix}$$

and $V_2 = \begin{bmatrix} 1 \\ n \end{bmatrix}$.

The singular values of $[A \ b]$, denoted $\sigma_i$, are the diagonal elements of $\Sigma$ and $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{n+1} \geq 0$. If $\sigma_k > \sigma_{k+1}$ then the solution $[\tilde{A} \ \tilde{b}]$ to (6) can be expressed in terms of the SVD components of $[A \ b]$ by

$$[\tilde{A} \ \tilde{b}] = U_1 \Sigma_1 V_1^T$$

and the minimum norm T-TLS solution $\tilde{z}_k$ may be expressed \cite{11, 26, 28}

$$\tilde{z}_k = -V_{12} V_{22}^T = -V_{12} V_{22}^T \|V_{22}\|^{-2}.$$ 

3. The URV and ULV Decompositions. The SVD discussed above belongs to a whole class of two-sided orthogonal decomposition—but the SVD is special because the "middle matrix" in the decomposition, $\Sigma$, is diagonal, and this is what makes the algorithm so computationally demanding. However, in many circumstances one can sacrifice the diagonal structure for more efficient algorithms that provide the same rank information and nearly the same subspace information. This is the motivation behind the development of the rank revealing URV and ULV decompositions.

The rank revealing URV and ULV decompositions—as well as efficient algorithms to compute them—were originally proposed by Stewart in \cite{20, 22}. Here, we summarize the definitions and properties of these decompositions. The URV and ULV decompositions are denoted

$$A = U_R L V_R^T = [U_{Rk} \ U_{R0} \ U_{R0}] \ R [V_{Rk} \ V_{R0}]^T$$

and

$$A = U_L L V_L^T = [U_{Lk} \ U_{L0} \ U_{L0}] \ L [V_{Lk} \ V_{L0}]^T$$
where \( R \) and \( L \) have the following structure

\[
R = \begin{bmatrix} R_k & F \\ 0 & G \end{bmatrix} \quad \text{and} \quad L = \begin{bmatrix} L_k & 0 \\ H & E \end{bmatrix}
\]

\( R_k \) and \( G \) are upper triangular matrices, while \( L_k \) and \( E \) are lower triangular. Moreover, \( R_k \) and \( L_k \) are nonsingular. It follows that

\[
A = U_{Rk} R_k V_{Rk}^T + U_{Rk} F V_{R0}^T + U_{R0} G V_{R0}^T
\]

and

\[
A = U_{Lk} L_k V_{Lk}^T + U_{Lk} H V_{L0}^T + U_{L0} E V_{L0}^T.
\]

These decompositions are said to be rank revealing if \( R_k \) and \( L_k \) are well conditioned, \( \|G\| = O(\sigma_{k+1}) \), and \( \|E\| = O(\sigma_{k+1}) \). Based on the above expressions, two potentially useful rank-k matrix approximations to \( A \) are given by

\[
A_{Rk} = U_{Rk} R_k V_{Rk}^T \quad \text{and} \quad A_{Lk} = U_{Lk} L_k V_{Lk}^T.
\]

As an alternative to the TSVD approach in (4), one may now wish to use the URV and ULV decompositions instead to estimate the relationship between \( b \) and the columns of \( A \) by solving the LS problems

\[
\min_{x \in \mathbb{R}^n} \|A_{Rk} x - b\|_2 \quad \text{and} \quad \min_{x \in \mathbb{R}^n} \|A_{Lk} x - b\|_2.
\]

If \( x_{URV} \) and \( x_{ULV} \) denote the minimum norm LS solutions to these two problems, then

\[
x_{URV} = A_{Rk}^{+} b = V_{Rk} L_k^{-1} U_{Rk}^T b \quad \text{and} \quad x_{ULV} = A_{Lk}^{+} b = V_{Lk} L_k^{-1} U_{Rk}^T b.
\]

Approximate T-TLS solutions, similar to \( x_{URV} \) and \( x_{ULV} \), can also be defined in terms of the URV and ULV decompositions (cf. §4.3).

Moreover, the columns of the matrices \( V_{R0}, V_{L0}, U_{Rk} \) and \( U_{Lk} \) approximate the numerical null space and range as defined via the SVD of \( A \). All these approximations are investigated in the next sections. We postpone the discussion of the rank-revealing properties of the URV and ULV decompositions to §5.

4. Approximation Properties of the URV and ULV Decompositions.

The purpose of this section is to investigate the approximation properties of several quantities computed from the rank revealing URV and ULV decompositions described in the previous section. We start with an investigation of the accuracy of the approximate range and null spaces, since these bounds are going to play a crucial role in the rest of the paper. Then we investigate the accuracy of the approximate TSVD and T-TLS solutions computed by essentially substituting the URV and ULV decompositions for the SVD, thus replacing one problem with a similar, nearby problem that can be solved more efficiently.
4.1. Approximate Subspaces. From the SVD of $A$ we know $\|AV_2\| = \|\Sigma_2\| = \sigma_{k+1}$. From the definitions of the URV and ULV decompositions, it follows immediately that $\|AV_{R0}\| = \|[FT^T G^T]^T\|$ and $\|AV_{L0}\| = \|E\|$, which imply that if $E$, $F$ and $G$ have small elements in absolute value then the columns of $V_{L0}$ and $V_{R0}$ should span an approximation to the numerical null space $\mathcal{R}(V_2)$.

We shall now prove that under suitable conditions, the subspaces $\mathcal{R}(V_{R0})$ and $\mathcal{R}(V_{L0})$ indeed approximate the numerical null space $\mathcal{R}(V_2)$, while the subspaces $\mathcal{R}(U_{Rk})$ and $\mathcal{R}(U_{Lk})$ approximate the numerical range $\mathcal{R}(U_1)$. The quality of the approximation is measured by the “distance” between the subspaces, which is the largest principal angle between the subspaces. Let $\text{dist}(S_1, S_2)$ denote the distance between the subspaces $S_1$ and $S_2$. The following definition from [12, p. 76] quantifies this notion.

**Definition:** Let $W = [W_1 \ W_2]$ and $Z = [Z_1 \ Z_2]$ be orthogonal matrices where $W_1, Z_1 \in \mathbb{R}^{p \times (p-s)}$ and $W_2, Z_2 \in \mathbb{R}^{p \times t}$. Then $\text{dist}(S_1, S_2) = \|W_2^T Z_1\|$.

The following notation is convenient. From the above definition we have

\[
\sin \theta_{URV} \equiv \text{dist}(\mathcal{R}(V_2), \mathcal{R}(V_{R0})) = \|V_2^T V_{R0}\| = \|V_2^T V_{Rk}\|
\]

\[
\sin \theta_{ULV} \equiv \text{dist}(\mathcal{R}(V_2), \mathcal{R}(V_{L0})) = \|V_2^T V_{L0}\| = \|V_2^T V_{Lk}\|
\]

and from the definition plus [8, Lemma 2.1] we have

\[
\sin \phi_{URV} \equiv \text{dist}(\mathcal{R}(U_1), \mathcal{R}(U_{Rk})) = \|U_1^T U_{Rk}\|
\]

\[
\sin \phi_{ULV} \equiv \text{dist}(\mathcal{R}(U_1), \mathcal{R}(U_{Lk})) = \|U_1^T U_{Lk}\|
\]

The following result by Fierro and Bunch [8] provides a posteriori bounds on the distance between these subspaces.

**Theorem 4.1. (A Posteriori Subspace Bounds)** Let $A$ have the SVD in (2) and the URV and ULV decompositions as in (10) and (11). If $\|E\| < \sigma_{\min}(L_k)$ then

\[
\frac{\|H\|}{\|L\| + \|E\|} \leq \sin \theta_{ULV} \leq \frac{\|H\|}{\sigma_{\min}(L_k) - \|E\|}
\]

and if $\|G\| < \sigma_{\min}(R_k)$ then

\[
\frac{\|F\|}{\|R\| + \|G\|} \leq \sin \theta_{URV} \leq \frac{\|F\|}{\sigma_{\min}(R_k) - \|G\|}
\]

\[
\sin \phi_{URV} \leq \frac{\|F\| \|G\|}{\sigma_{\min}^2(R_k) - \|G\|^2}
\]

This theorem shows how the size of the off-diagonal block of the triangular matrix is related to the quality, i.e., accuracy, of the URV and ULV-subspaces as approximations to the singular subspaces. Hence we conclude that the quality of the subspaces does not really depend on the gap in the singular value spectrum, but rather on the size of the off-diagonal block of the triangular matrix. Presently there are no known lower bounds for $\sin \theta_{ULV}$ and $\sin \phi_{URV}$.
The two angles associated with each decomposition are interrelated as follows.

**Theorem 4.2.** If $\|C\| < \sigma_{\min}(R_k)$ and $\|E\| < \sigma_{\min}(L_k)$ then

$$
\sin \phi_{URV} \leq \frac{\|C\|}{\sigma_{\min}(R_k)} \sin \theta_{URV} \quad \text{and} \quad \sin \theta_{ULV} \leq \frac{\|E\|}{\sigma_{\min}(L_k)} \sin \phi_{ULV}.
$$

**Proof.** The proof follows from the proof of Theorem 4.1 in [8]; we omit the details here. \(\square\)

The above theorems have interesting implications for the URV and ULV algorithms suggested by Stewart. As proven in [25, Theorem 1] the off-diagonal block \(F\) (\(H\)) is exactly zero when at each step the estimated singular vector \(v_{\min}^i (u_{\min}^i)\) is equal to the corresponding true right (left) singular vector of the current \(R(1 : i, 1 : i)\) (\(L(1 : i, 1 : i)\)). While this may not be achieved in practice, Fierro and Bunch [8] showed by numerical experiments that

1. good estimates of the singular vectors lead to correspondingly small subspace angles \(\theta_{URV}\) and \(\phi_{ULV}\), and
2. the size of \(\|F\|\) or \(\|H\|\) is related to the quality of estimated singular vectors, as described by Theorem 4.1.

The reader should keep this in mind to interpret \(\|H\|\), \(\|F\|\), \(\theta\), or \(\phi\) (especially since we will determine bounds in terms of these parameters): high quality approximations to the singular vectors used in the algorithm make these parameters correspondingly small, and there is an intimate relationship, as described in Theorems 4.1 and 4.2, between \(\|H\|\) and \(\sin \phi_{ULV}\), as well \(\|F\|\) and \(\sin \theta_{ULV}\). We are not aware of a similar result for the RRQR algorithm, and further, it is not supported by numerical experiments, if [8, Table 6], or current theory.

Note that the bounds for the \(\theta\)-angles in Theorem 4.1 are not symmetric; \(\sin \theta_{ULV}\) can be roughly \(\sigma_{k+1}/\sigma_k\) times smaller than \(\sin \theta_{URV}\), and hence the ULV decomposition can be expected to produce a better approximation to the null space than URV when the gap is significant; cf. [8]. However, the URV decomposition can be expected to produce a better approximation to the numerical range of \(A\).

### 4.2. Approximate TSVD Solutions

Now we investigate the quality of the approximate TSVD solutions \(x_{URV}\) and \(x_{ULV}\) defined in (15).

First we will need a perturbation result for pseudoinverses by Wedin [27].

**Lemma 4.3.** If \(C\) is an acute perturbation of \(D\), with \(D = C + \delta C\), and \(\mu \equiv (1 + \sqrt{5})/2\) then

$$
\|C^T - D^T\| \leq \mu \|C^T\| \|D^T\| \|\delta C\|.
$$

To apply this lemma for our purpose we assume the mild conditions \(\|HE\| < \sigma_k\) and \(\|F^T G^T F^T\| < \sigma_k\) are satisfied.

In order to motivate the use of the URV and ULV decompositions, we will first show that when \(\|H\|\) is sufficiently small (\(\Rightarrow\) small subspace angle) then \(A_{L_k} = U_{L_k} L_k V_{L_k}^T\) closely approximates the TSVD matrix \(A_k = U_1 \Sigma_1 V_1^T\).

$$
\|A_k - A_{L_k}\| = \|U_1 U_1^T A - U_{L_k} U_{L_k}^T A\| \leq \|A\| \sin \phi_{ULV}
$$

and thus from Theorem 4.1 it follows

$$
\frac{\|A_k - A_{L_k}\|}{\|A_k\|} \leq \sin \phi_{ULV} \leq \frac{\|H\| \|E\|}{\sigma_{\min}(L_k) - \|E\|^2}.
$$

Furthermore, from Lemma 1 and (16) it follows

$$
\frac{\|A_k^i - A_{L_k}^i\|}{\|A_k^i\|} \leq \mu \Psi_{ULV} \sin \phi_{ULV} \leq \mu \Psi_{ULV} \frac{\|H\| \|E\|}{\sigma_{\min}(L_k) - \|E\|^2}.
$$
where $\Psi_{ULV} \equiv ||L|| ||L_k^\perp||$ is a condition number for $x_{ULV}$. In particular, if $||H|| = 0$, then the TSVD matrix $A_k$ in (4) can be alternatively expressed as $A_k = U_k L_k V_k^T$. Usually, $||H|| \neq 0$ and we see that the difference between $A_k^1$ and $A_k^\perp$ is proportional to $||H||$. It is interesting to notice that $||H||$ can be made very small using refinement procedures as discussed in [8, 21, 25].

For the URV decomposition, a similar analysis leads to the results

$$\frac{||A_k - A_{R_k}||}{||A_k||} \leq \sin \theta_{URV} \leq \frac{||F||}{\sigma_{\min}(R_k) - ||G||},$$

and

$$\frac{||A_k^1 - A_{R_k}^1||}{||A_k^1||} \leq \mu \Psi_{URV} \sin \theta_{URV} \leq \mu \Psi_{URV} \frac{||F||}{\sigma_{\min}(R_k) - ||G||}.$$

where $\Psi_{URV} \equiv ||R|| ||R_k^1||$ is a condition number for $x_{URV}$. As with the ULV, the norm of the off-diagonal block $F$ in $R$ can be reduced by the abovementioned refinement procedures if higher quality subspaces are required.

Intuitively, from (17)–(18) and (19)–(20) and the fact that $A_k$ and $A_{L_k}$, as well as $A_k$ and $A_{R_k}$, are acute matrices, small subspace angles should mean good approximations to the truncated LS solution $x_k$. The following result quantifies this with error bounds for the solutions $x_{URV}$ and $x_{ULV}$ as approximations to the TSVD solution $x_k$.

**Theorem 4.4.** (Error in Estimating the TSVD Solution) Let $A$ have the SVD in (2) and rank revealing URV and ULV decompositions in (10) and (11). Let $x_k$, $x_{URV}$ and $x_{ULV}$ denote minimum norm LS solutions as defined in (4) and (14), and define the residual $r_k = b - A_k x_k$. Further, define

$$\Psi_{ULV} \equiv ||L|| ||L_k^\perp|| \quad \text{and} \quad \Psi_{URV} \equiv ||R|| ||R_k^1||.$$

If $||E|| < \sigma_{\min}(L_k)$ then

$$\frac{||x_k - x_{ULV}||}{||x_k||} \leq \sin \theta_{ULV} + \Psi_{ULV} \frac{||r_k||}{||b||} \sin \phi_{ULV} \leq \frac{||H|| ||E||}{\sigma_{\min}(L_k) - ||E||^2} + \Psi_{ULV} \frac{||r_k||}{||b||} \frac{||H||}{\sigma_{\min}(L_k) - ||E||^2}.$$

Similarly, if $||G|| < \sigma_{\min}(R_k)$ then

$$\frac{||x_k - x_{URV}||}{||x_k||} \leq \sin \theta_{URV} \left(1 + \Psi_{URV}^2 \frac{||F||}{||R||} \right) + \Psi_{URV} \frac{||r_k||}{||b||} \sin \phi_{URV} \leq \frac{||F||}{\sigma_{\min}(R_k) - ||G||} \left(1 + \Psi_{URV}^2 \frac{||F||}{||R||} \right) + \Psi_{URV} \frac{||r_k||}{||b||} \frac{||F||}{\sigma_{\min}(R_k) - ||G||^2}.$$

**Proof.** The proof for the relative error in $x_{ULV}$ begins with

$$x_k - x_{ULV} = (A_k^1 - A_{L_k}^1) b = (A_k^1 - A_{L_k}^1) b - (A_k^1 A_k - A_{L_k}^1 A_{L_k}) x_k + (A_k^1 A_k - A_{L_k}^1 A_{L_k}) x_k$$

$$= (A_k^1 - A_{L_k}^1) b - (A_k^1 - A_{L_k}^1) A x_k + (A_k^1 - A_{L_k}^1) A x_k$$

$$= (A_k^1 - A_{L_k}^1) r_k + (A_k^1 - A_{L_k}^1) A x_k$$

$$= -A_{L_k}^1 r_k + (A_k^1 A_k - A_{L_k}^1 A_{L_k}) x_k$$

$$= -A_{L_k}^1 U_{L_k} U_{L_k}^T U_2 U_2 r_k + (A_k^1 A_k - A_{L_k}^1 A_{L_k}) x_k.$$
where we have used the facts \( A_k^T = A_k^T U_k U_k^T \) and \( r_k = U_2 U_2 r_k \). Noting that 
\[ \|U_k^T U_2\| = \sin \phi_{ULV} \], it follows
\[
\|x_k - x_{ULV}\| \leq \|A_k^T\| \|r_k\| \sin \phi_{ULV} + \sin \theta_{ULV} \|x_k\|.
\]
Using the fact \( 1 \leq \|A\| \|b\|/\|b\| \), we get
\[
\frac{\|x_k - x_{ULV}\|}{\|x_k\|} \leq \sin \theta_{ULV} + \Psi_{ULV} \frac{\|r_k\|}{\|b\|} \sin \phi_{ULV},
\]
which is the desired result. The second upper bound in the theorem follows immediately from Theorem 4.1. The proof for the relative error in \( x_{URV} \) is similar and begins with
\[
x_k - x_{URV} = (A_k^T - A_k^T) b
\]
\[
= (A_k^T - A_k^T) b - (A_k^T A_k - A_k^T A_k) x_k + (A_k^T A_k - A_k^T A_k) x_k.
\]
\[
= (A_k^T - A_k^T) b - (A_k^T A_k - A_k^T A_k) + (A_k^T A_k - A_k^T A_k) x_k + (A_k^T A_k - A_k^T A_k) x_k
\]
\[
= (A_k^T - A_k^T) r_k - V_k^T Z_k^{-1} F V_0^T x_k + (A_k^T - A_k^T) r_k.
\]
\[
= -A_k^T r_k - V_k^T Z_k^{-1} F V_0^T x_k + (A_k^T - A_k^T) r_k.
\]
\[\text{(22)}\]
where we have used the facts \( A_k^T = A_k^T U_k U_k^T \) and \( r_k = U_2 U_2^T r_k \). Note that
\( V_k^T Z_k^{-1} F V_0^T x_k = V_k^T Z_k^{-1} F V_0^T V k \Sigma^{-1} U_2^T b \), thus it follows
\[
\|V_k^T Z_k^{-1} F V_0^T x_k\| \leq \frac{\|F\|}{\text{min}(R_k)} \|V_0^T V k \| \|A_k^T\| \|U_2^T b\|
\]
\[\text{(23)}\]
Using this result and the fact \( \|b\|/\|A\| \leq \|x_k\| \), we get
\[
\frac{\|x_k - x_{URV}\|}{\|x_k\|} \leq \sin \theta_{URV} \left( 1 + \Psi_{URV} \frac{\|F\|}{\|R\|} \right) + \Psi_{URV} \frac{\|r_k\|}{\|b\|} \sin \phi_{URV},
\]
which is the desired result. The second bound follows from Theorem 4.1. This completes the proof of the theorem. \( \Box \)

The results show how the subspace angles \( \theta \) and \( \phi \) are related to the accuracy of the URV- and ULV-based approximations to the truncated LS solution to \( Ax \approx b \). Simply stated, small subspace angles translate to accurate solutions. The solutions \( x_{URV} \) and \( x_{ULV} \) will be good approximations to the TSVD solution whenever \( \|H\| \) and \( \|F\| \) are sufficiently small.

The upper bound for the relative error in \( x_{ULV} \) in terms of \( \sin \theta_{ULV} \) and \( \sin \phi_{ULV} \) is actually quite natural. Notice that \( x_{ULV} \in \mathcal{R}(U_k) \) and \( x_k \in \mathcal{R}(V_k) \), hence the distance between these subspaces plays an important role. In addition, \( x_{ULV} \) and \( x_k \) are unique minimum norm solutions to compatible systems where the right-hand sides are projected into \( \mathcal{R}(U_k) \) and \( \mathcal{R}(V_k) \), respectively, hence the distance between \( \mathcal{R}(U_k) \) and \( \mathcal{R}(V_k) \) appears in the upper bounds. Similar remarks hold for \( x_{URV} \).

Now we make some conclusions about the accuracy of the approximations based on the bounds in Theorem 4.4. Using Theorem 4.2, the URV upper bound can be slightly overestimated by
\[
\sin \theta_{URV} \left( 1 + \Psi_{URV} \frac{\|F\|}{\|R\|} \right) + \Psi_{URV} \frac{\|r_k\|}{\|b\|} \sin \phi_{URV},
\]
<table>
<thead>
<tr>
<th>$\sin \theta_{ULV}$</th>
<th>$\sin \phi_{ULV}$</th>
<th>$\sin \theta_{URV}$</th>
<th>$\sin \phi_{URV}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$8.99 \cdot 10^{-15}$</td>
<td>$2.13 \cdot 10^{-12}$</td>
<td>$2.71 \cdot 10^{-03}$</td>
<td>$2.71 \cdot 10^{-11}$</td>
</tr>
<tr>
<td>Upper bounds from Theorem 4.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$6.28 \cdot 10^{-14}$</td>
<td>$6.35 \cdot 10^{-13}$</td>
<td>$2.74 \cdot 10^{-2}$</td>
<td>$2.72 \cdot 10^{-11}$</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>$|r_k|_0$</th>
<th>$|x_k-x_{URV}|$</th>
<th>$\sin \theta_{ULV} + \Psi_{ULV} |r_k|<em>0 \sin \phi</em>{ULV}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.34 \cdot 10^{-4}$</td>
<td>$5.84 \cdot 10^{-15}$</td>
<td>$3.76 \cdot 10^{-14}$</td>
</tr>
<tr>
<td>$2.15 \cdot 10^{-2}$</td>
<td>$1.28 \cdot 10^{-13}$</td>
<td>$4.59 \cdot 10^{-12}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$|r_k|_0$</th>
<th>$|x_k-x_{URV}|$</th>
<th>$\sin \theta_{URV} \left(1 + \Psi_{URV} \frac{|r_k|<em>0}{|R|} \right) + \Psi</em>{URV} |r_k|<em>0 \sin \phi</em>{URV}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.34 \cdot 10^{-4}$</td>
<td>$1.31 \cdot 10^{-9}$</td>
<td>$2.71 \cdot 10^{-9}$</td>
</tr>
<tr>
<td>$2.15 \cdot 10^{-2}$</td>
<td>$1.55 \cdot 10^{-10}$</td>
<td>$2.77 \cdot 10^{-9}$</td>
</tr>
</tbody>
</table>

Table 1

Comparing the relative errors, upper bounds, and the subspace angles for the URV and ULV decomposition for $A \in \mathbb{R}^{30 \times 10}$ with numerical rank 7. Both $\Psi_{ULV}$ and $\Psi_{URV}$ are $O(10^{-2})$.

and we conclude that for most problems the upper bound for the relative error is dominated by

$$\sin \theta_{URV} \approx \frac{\|F\|}{\sigma_{\min}(R_k) - \|G\|}.$$  

On the other hand, the relative error in the ULV approximation is proportional to

$$\sin \theta_{ULV} \approx \frac{\|H\| \|E\|}{\sigma_{\min}(L_k) - \|E\|^2}$$

whenever $\|r_k\|_0 \ll 1$, since this tends to diminish the second term, and is proportional to

$$\sin \phi_{ULV} \approx \frac{\|H\|}{\sigma_{\min}(L_k) - \|E\|}$$

whenever $\Psi_{URV} \|r_k\|_0 \approx 1$. Numerical experiments in [8] indicate $\sin \phi_{ULV}$ is of the order $\sin \theta_{URV}$.

Hence, we can expect a ULV decomposition to yield a more accurate estimate of the TSVD solution, which is consequential of the fact that it yields a higher quality estimate of the numerical null space than the URV.

The error bounds are quite good, as illustrated by typical examples in Table 1. In these simple but illustrative Matlab experiments the singular values of $A \in \mathbb{R}^{30 \times 10}$ are

$$\sigma(A) = \{1, 0.5, 0.2, 0.1, 5 \cdot 10^{-2}, 3 \cdot 10^{-2}, 10^{-2}, 10^{-4}, 10^{-5}, 10^{-6}\},$$

and the numerical rank of $A$ is 7. We solved the LS problems given in (4) and (14) for two right-hand sides. In the first example we chose $b$ such that $\|r_k\|/\|b\| = 1.34 \cdot 10^{-4}$ and in the second example we chose $b$ such that $\|r_k\|/\|b\| = 2.15 \cdot 10^{-2}$.

4.3. Approximate Truncated TLS solutions. Now we analyze the accuracy of an approximate T-TLS solution that is computed by means of a rank revealing two-sided orthogonal decomposition of the compound matrix $[A \ b]$. This analysis is
similar to the analysis in the previous subsection in that the subspace bounds also play an important role here.

The ULV and URV factorizations of \([A \ b]\) are denoted by
\[
[A \ b] = [\hat{U}_{Lk} \hat{U}_{L0} \hat{U}_1]L[V_{Lk} V_{L0}]^T \quad \text{and} \quad [A \ b] = [\hat{U}_{Rk} \hat{U}_{R0} \hat{U}_1]R[V_{Rk} V_{R0}]^T,
\]
where \(\hat{L}\) and \(\hat{R}\) are partitioned in accordance with (12) such that \(\hat{L}_k\) and \(\hat{R}_k\) are \(k \times k\) matrices, while \(\hat{H}\) is \((n - k + 1) \times k\) and \(\hat{F}^T\) is \(k \times (n - k + 1)\). We define two rank-\(k\) matrix approximations to \([A \ b]\) by
\[
[\hat{A}_{Lk} \hat{b}_{Lk}] = \hat{U}_{Lk} \hat{L}_k \hat{V}_{Lk}^T \quad \text{and} \quad [\hat{A}_{Rk} \hat{b}_{Rk}] = \hat{U}_{Rk} \hat{R}_k \hat{V}_{Rk}^T.
\]
Partition the matrices \(\hat{V}_{L0}\) and \(\hat{V}_{R0}\) as
\[
\hat{V}_{L0} = \begin{bmatrix} V_{L01} \\ V_{L02} \end{bmatrix}, \quad \hat{V}_{R0} = \begin{bmatrix} V_{R01} \\ V_{R02} \end{bmatrix}
\]
so that
\[
\hat{V}_{L0} = \begin{bmatrix} V_{L01} \\ V_{L02} \end{bmatrix} \quad \text{and} \quad \hat{V}_{R0} = \begin{bmatrix} V_{R01} \\ V_{R02} \end{bmatrix}.
\]
The related total least squares-like problems then become
\[
[\hat{A}_{Lk} \hat{b}_{Lk}] \begin{bmatrix} x \\ -1 \end{bmatrix} = 0 \quad \text{and} \quad [\hat{A}_{Rk} \hat{b}_{Rk}] \begin{bmatrix} x \\ -1 \end{bmatrix} = 0,
\]
and the corresponding T-TLS-like solutions are given by \([9, \S 2]\)
\[
\hat{x}_{ULV} = -\hat{V}_{L01} \hat{V}_{L02}^T \quad \text{and} \quad \hat{x}_{URV} = -\hat{V}_{R01} \hat{V}_{R02}^T.
\]
These solutions are guaranteed to exist whenever \([\|\hat{H} \hat{E}\| < \sigma_k\) and \(\|\hat{F}^T \hat{G}^T\| < \sigma_k\).

Further, let
\[
\sin \hat{\theta}_{ULV} = \text{dist}(N([\hat{A}_{Lk} \hat{b}_{Lk}]), N([\hat{A} \hat{b}])) \quad \text{and} \quad \sin \hat{\theta}_{URV} = \text{dist}(N([\hat{A}_{Rk} \hat{b}_{Rk}]), N([\hat{A} \hat{b}])),
\]
where the null space of a matrix \(C\) is denoted \(N(C)\). Recall that \([\hat{A} \hat{b}]\) is the nearest rank-\(k\) matrix approximation to \([A \ b]\) in the Frobenius norm.

An application of a result by Fierro and Bunch \([7]\) facilitates the following comparison between the T-TLS solution and its approximations \(\hat{x}_{ULV}\) and \(\hat{x}_{URV}\).

**Theorem 4.5.** Let \([A \ b]\) have the SVD as in (7) with the rank-\(k\) matrix approximations as in (24). Let \(\hat{x}_{ULV}\) and \(\hat{x}_{URV}\) denote the T-TLS-like solutions to the homogeneous systems in (25). If \(\|\hat{H} \hat{E}\| < \sigma_k\) then
\[
\sin \hat{\theta}_{ULV} \leq \|\hat{x}_k - \hat{x}_{ULV}\| \leq \sin \hat{\theta}_{ULV} \sqrt{1 + \|\hat{x}_k\|^2} \sqrt{1 + \|\hat{x}_{ULV}\|^2} \leq \frac{\|\hat{H}\| \|\hat{E}\|}{\sigma^2_{\text{min}}(\hat{L}_k) - \|\hat{E}\|^2} \sqrt{1 + \|\hat{x}_k\|^2} \sqrt{1 + \|\hat{x}_{ULV}\|^2}
\]
and if \(\|\hat{F}^T \hat{G}^T\| < \sigma_k\) then
\[
\sin \hat{\theta}_{URV} \leq \|\hat{x}_k - \hat{x}_{URV}\| \leq \sin \hat{\theta}_{URV} \sqrt{1 + \|\hat{x}_k\|^2} \sqrt{1 + \|\hat{x}_{URV}\|^2} \leq \frac{\|\hat{F}\| \|\hat{G}\|}{\sigma_{\text{min}}(\hat{R}_k) - \|\hat{G}\|^2} \sqrt{1 + \|\hat{x}_k\|^2} \sqrt{1 + \|\hat{x}_{URV}\|^2}.
\]
Note from Theorem 4.1 we have \( \| \tilde{F} \|_R + \| G \| \leq \| \tilde{x}_k - \tilde{x}_{URV} \| \), while no lower bound on \( \tilde{\theta}_{ULV} \) is currently available.

The square roots \( \sqrt{1 + \| \cdot \|^2} \) in the theorem are (atypical) condition numbers for the respective solutions, cf. [9]. Recall that each solution can be computed from an orthonormal basis of the null space of its corresponding rank-\( k \) matrix approximation to \([A \; b]\). Hence the traditional condition number \( \sigma_1 / \sigma_k \) does not appear, and instead the condition of the ULV and URV T-TLS-like problems can be conveniently determined from the norm of the solution (assuming that \( A \) and \( b \) are correctly scaled).

5. Assessing the Numerical Rank. In this section we take a closer look at the decision in the URV and ULV algorithms concerning the numerical rank-\( k \) of the matrix \( A \). We have postponed the discussion to this stage because we want to make use of the subspace bounds derived in the previous section.

Given a user-specified tolerance \( \tau \), we must determine the truncation parameter \( k \) such that \( \sigma_k > \tau > \sigma_{k+1} \). It is reasonable to assume that a small perturbation of the parameters \( \tau \), \( \sigma_{k+1} \), and \( \sigma_k \) will not alter the numerical rank. Otherwise, the determination of the numerical rank is a difficult and ill-posed problem, even for the SVD. On the other hand, we have seen that a large gap between \( \sigma_k \) and \( \sigma_{k+1} \) is not required to ensure good approximations from the URV and ULV. Hence, the URV and ULV decompositions can be expected to treat more general problems than the RRQR factorization, as long as \( \sigma_k \) and \( \sigma_{k+1} \) are not too close.

Since we want to avoid the explicit computation of the SVD to compute the numerical rank, a logical condition to check via the ULV decomposition is \( \sigma_{\min}(L_k) > \tau > \| E \| \), as

\[
(28) \quad \sigma_k > \sigma_{\min}(L_k) \quad \text{and} \quad \| E \| > \sigma_{k+1}.
\]

Hence, we are interested in assessing the quality of the singular values of \( L_k \) and \( E \) as approximations to the large and small singular values of \( A \), respectively. In [21], Stewart derived the following result in connection with a block analysis of left and right iterations for refining (10) or (11). Denote the singular values of \( L_k \) by \( \sigma_1(L_k), \ldots, \sigma_k(L_k) \) arranged in nonincreasing order and let \( \delta_j = \sigma_{j-1}(L_k) - 2\| H \| > \sigma_j(L_k), \rho_j = \sigma_j(L_k)/\delta_j \), and \( \delta = \sigma_k - \| H \| \).

**Theorem 5.1.** *(A Posteriori Bounds for Singular Values)* Let \( A \) have the SVD in (2) and rank revealing ULV decomposition in (11). If \( \rho_j < 1 \) and \( \| E \| < \sigma_{\min}(L_k) - \| H \| \) then

\[
|\sigma_j - \sigma_j(L_k)| \leq \frac{\sigma_j(L_k) \| H \|^2}{1 - \rho_j^2} \cdot \frac{\delta_j^2}{\delta_j} \quad \text{for} \quad j = 1, \ldots, k
\]

and

\[
|\sigma_j - \sigma_{j-k}(E)| \leq \frac{\| E \| \| H \|^2}{\delta^2 (1 - (\| E \| / \delta)^2)} \quad \text{for} \quad j = k + 1, \ldots, n.
\]

The same results hold for the URV decomposition by substituting the corresponding URV quantities.

Below we give an alternative theorem, based on subspace angles, that also assesses the numerical rank. In particular, we show that if \( \tilde{\theta}_{ULV} \) is sufficiently small, then
\[ \sigma_{\min}(L_k) \] and \[ ||E|| \] can be viewed as slight perturbations of \[ \sigma_k \] and \[ \sigma_{k+1} \], respectively, with similar results holding for the URV decomposition.

**Theorem 5.2.** Let \( A \) have the SVD in (9) and rank revealing \( ULV \) and \( URV \) decompositions as in (11) and (10). Let \( k \) denote the numerical rank of \( A \). If \( ||E|| < \sigma_{\min}(L_k) \) then

\[
\sigma_{\min}(L_k) \leq \sigma_k \leq \sigma_{\min}(L_k) + ||L|| \sin \phi_{ULV}
\]

\[
||E|| (1 - \Psi_{ULV} \sin \phi_{ULV}) \leq \sigma_{k+1} \leq ||E||
\]

and if \( ||G|| < \sigma_{\min}(R_k) \) then

\[
\sigma_{\min}(R_k) \leq \sigma_k \leq \sigma_{\min}(R_k) + ||R|| \sin \theta_{URV}
\]

\[
||G|| (1 - \Psi_{URV} \sin \theta_{URV}) \leq \sigma_{k+1} \leq ||G||
\]

**Proof.** Arrange the singular values of \( L_k \), denoted \( \sigma_1(L_k), \ldots, \sigma_{\min}(L_k) \), in non-increasing order. From (10) and standard perturbation theory for singular values we have

\[
|\sigma_i - \sigma_i(L_k)| \leq ||L|| \sin \phi_{ULV}.
\]

Now we wish to find bounds for the smaller singular values in terms of a subspace angle. Note that \( U_0 E V_0^T = A(I - V_k V_k^T), \sigma(E) = \sigma(U_0 E V_0^T), \) and \( \sigma(\Sigma_2) = \sigma(U_2 \Sigma_2 V_2^T) \), where \( \sigma(D) \) denotes the set of singular values of matrix \( D \). Then

\[
||U_2 \Sigma_2 V_2^T - U_0 E V_0^T|| = ||A(I - V_1 V_1^T) - A(I - V_k V_k^T)||
\]

\[
\leq ||A|| ||V_1 V_1^T - V_k V_k^T||
\]

\[
\leq ||A|| \frac{\sigma_{k+1}}{\sigma_{\min}(L_k)} \sin \phi_{ULV},
\]

where we have used the fact (cf. Theorem 4.2)

\[
||V_1 V_1^T - V_k V_k^T|| \leq \frac{\sigma_{k+1}}{\sigma_{\min}(L_k)} \sin \phi_{ULV}.
\]

Arrange the \( n-k \) singular values of \( E \), denoted \( ||E|| \equiv \sigma_1(E), \ldots, \sigma_{n-k}(E) \), in non-increasing order. Then from (30) and standard perturbation theory for singular values it follows

\[
|\sigma_{k+i} - \sigma_i(E)| \leq \Psi_{ULV} ||E|| \sin \phi.
\]

The situation is similar, as expected, for the URV decomposition. Denote the singular values of \( R_k \) by \( \sigma_1(R_k), \ldots, \sigma_{k}(R_k) \) in nonincreasing order. From \( ||A_k - \tilde{A}|| \leq ||A|| \sin \theta \) and the perturbation property of singular values we get

\[
|\sigma_i - \sigma_i(R_k)| \leq ||R|| \sin \theta.
\]

Also,

\[
||U_2 \Sigma_2 V_2^T - U_0 G V_0^T|| = ||U_1 U_1^T A - U_0 U_0^T A||
\]

\[
\leq ||A|| \sin \phi
\]

\[
\leq \Psi_{URV} ||G|| \sin \theta,
\]

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where we have used the fact \( \sin \phi \leq \frac{\|G\|}{\sigma_{\text{max}}(H)} \sin \phi \). Denote the singular values of \( G \) by \( \sigma_1(G), \ldots, \sigma_{n-k}(G) \) in nondecreasing order. Then we have

\[
|\sigma_{k+1} - \sigma_i(G)| \leq \Psi_{URV} \|G\| \sin \theta.
\]

Thus we have proved the theorem. \( \square \)

We see that small subspace angles mean we are guaranteed to capture the numerical rank of \( A \), because the bounds become tighter as the subspace angles decrease.

6. Conclusion. The truncated LS and TLS solutions can be computed by means of the SVD. In this paper we investigated the use of two-sided orthogonal decompositions, which can be computed more efficiently, to produce approximations to the truncated solutions. We derived error bounds for URV and ULV-based approximations to the TSV and T-TLS solutions which show how the accuracy of the approximate solutions is intimately connected to the quality of the URV and ULV-based subspaces.

REFERENCES


