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BOUNDING THE SUBSPACES FROM RANK REVEALING TWO-SIDED ORTHOGONAL DECOMPOSITIONS

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Abstract. The singular value decomposition (SVD) is a widely used computational tool in various applications. However, in some applications the SVD is viewed as computationally demanding or difficult to update. The rank revealing QR ($RRQR$) factorization and the recently-proposed rank revealing two-sided orthogonal (URV or ULV) decompositions are promising alternatives for determining the numerical rank of a matrix and approximating its singular subspaces. In this paper we prove sharp *a posteriori* bounds for assessing the quality of the subspaces obtained by two-sided orthogonal decompositions. Our analysis shows that the quality of the subspaces obtained by URV or ULV algorithm depends on the quality of the estimated start vectors and not on a gap condition. From our analysis we conclude that these decompositions may be more accurate alternatives to the SVD than the $RRQR$ factorization. Finally, we implement the algorithms in an adaptive manner, which is particularly useful for applications where the "noise" subspace must be computed, such as in signal processing or total least squares.

1. Introduction. The singular value decomposition (SVD) is a widely used computational tool and is the most reliable tool for detecting near rank-deficiency in a matrix [13, p. 246]. It has important applications, for instance, in matrix approximation, subset selection, spectral estimation, direction of arrival estimation, optimization, rank-deficient least squares (LS), total least squares (TLS), etc. [1, 4, 11, 19, 20, 4, 21].

In particular, the SVD can be used to characterize the solutions or solve the matrix approximation problems in the LS and TLS methods. These methods are used to solve the overdetermined system of linear equations

$$AX = B, \tag{1}$$

where $A \in \Re^{m\times n}$, $B \in \Re^{m\times d}$, and $m \geq n$. Due to various sources of errors, the system usually lacks a solution and the relationship between the columns of A and B must be *estimated*. To estimate the relationship, many direct methods solve a *nearby* compatible system $CX = D$, and this is a plausible strategy when $\|[A\ B] - [C\ D]\|$ is small. For stability reasons, when A is ill-conditioned with numerical rank k, it makes sense to require that C be of rank k. In some applications, due to the potential instability, the LS problem

$$\min_{x\in\Re^n} \|AX - B\|_2 \tag{2}$$

is replaced by the "stabilized" LS problem

$$\min_{x\in\Re^n} \|A_k X - B\|_2 \tag{3}$$

where A_k is the nearest rank-k matrix approximation to A in the 2-norm. This is essentially the same as solving the compatible system $A_k X = B_k$ where B_k is the orthogonal projection of B on the range (column space) of A_k. The TLS approach to (1) requires the minimum norm solution of

$$\hat{A}X = \hat{B} \tag{4}$$

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where $[\hat{A}\ \hat{B}]$ is the nearest rank-k matrix approximation to $[A\ B]$ in the 2-norm. The SVD is a convenient tool in solving the matrix approximation problem associated with these two methods, as well as providing elegant formulas for the solutions. A comprehensive treatment of TLS is given in [27]. The LS and TLS methods can be viewed as orthogonal projection methods, and a sensitivity analysis for the LS and TLS solutions is presented in [10]. The subspace angle is a key factor in the analysis.

For applications where a sequence of LS or TLS problems must be solved, or a "noise" subspace must be adaptively estimated, the SVD is viewed as computationally demanding or difficult to update. Therefore, alternative factorizations have been considered which yield the numerical rank, subspace information, or matrix approximations that are nearly as reliable as the powerful but computationally demanding SVD.

The rank revealing QR ($RRQR$) factorization of Chan [5] is a potentially useful alternative to the SVD. In this algorithm the rectangular matrix A is preprocessed by an initial QR factorization, and then condition estimation, careful column pivoting, and plane rotations on the left side are employed to produce a rank revealing factorization. Some applications of $RRQR$ are discussed in [3, 7, 16].

G.W. Stewart [23, 24] introduced rank-revealing "two-sided" orthogonal (or complete) factorizations, so-called URV and ULV factorizations, as alternatives. While complete orthogonal decompositions have been around for some time (e.g., see [15]), Stewart's technique for achieving such a factorization is quite novel and promising. In this algorithm the rectangular matrix A is preprocessed by a QR factorization, and then condition estimation and plane rotations on both sides are employed to produce a rank revealing factorization. Recently, Park and Eldén [18] presented an accurate algorithm for downdating a row in the URV.

For the URV decomposition of A, there exist orthogonal matrices $U_R \in \Re^{m\times m}$ and $V_R \in \Re^{n\times n}$ such that

$$\begin{aligned} A &= U_R R V_R^T \\ &= [U_{Rk}\ U_{R0}\ U_R^{\perp}]\, R\, [V_{Rk}\ V_{R0}]^T \end{aligned} \tag{5}$$

where

$$R = \begin{array}{cc} \begin{array}{cc} k & n-k \end{array} & \\ \left[\begin{array}{cc} R_k & F \\ 0 & G \\ 0 & 0 \end{array}\right] & \begin{array}{l} k \\ n-k \\ m-k \end{array} \end{array}$$

is upper triangular and $k \leq n$. Based on this factorization,

$$A = U_{Rk} R_k V_{Rk}^T + U_{Rk} F V_{R0}^T + U_{R0} G V_{R0}^T. \tag{6}$$

Also, $A_{Rk} \equiv U_{Rk} R_k V_{Rk}^T$ is a rank-k matrix approximation to A satisfying

$$||A - A_{Rk}|| = \left\| \begin{bmatrix} F \\ G \end{bmatrix} \right\|.$$

$||\cdot|| = ||\cdot||_2$ unless otherwise indicated. For the ULV decomposition of A, there exist orthogonal matrices $U_L \in \Re^{m\times m}$ and $V_L \in \Re^{n\times n}$ such that

$$\begin{aligned} A &= U_L\, L V_L^T \\ &= [U_{Lk}\ U_{L0}\ U_{\perp}]\, L\, [V_{Lk}\ V_{L0}]^T \end{aligned} \tag{7}$$

where

$$L = \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \left[\begin{array}{cc} L_k & 0 \\ H & E \\ 0 & 0 \end{array} \right] \end{array} \begin{array}{l} \\ k \\ n-k \\ m-k \end{array}$$

is lower triangular. Based on this factorization,

$$A = U_{Lk} L_k V_{Lk}^T + U_{L0} H V_{Lk}^T + U_{L0} E V_{L0}^T. \tag{8}$$

$A_{Lk} \equiv U_{Lk} L_k V_{Lk}^T$ denotes a rank-k matrix approximation to A satisfying

$$\|A - A_{Lk}\| = \|[H\ E]\|.$$

These factorizations may be refined using various schemes. In [23] it is shown how so-called "left" and "right" iterations may be used to iteratively refine the decompositions. Based on this refinement strategy, error bounds for estimating the singular values of the matrix A are also provided. In [26] a refinement procedure is based on inverse iteration.

Ideally, it would be useful for the user to have some kind of a diagnostic measure to assess the quality of subspaces obtained by a two-sided orthogonal decomposition as compared to the reliable *SVD*. This has important applications in areas where the *SVD* might be used, for instance, in matrix approximation, subset selection, signal processing, least squares, and total least squares problems.

The objectives of this paper are (i) to provide error bounds for the subspaces determined by two-sided orthogonal decompositions and to incorporate them into the *URV* and *ULV* algorithms in an adaptive manner, (ii) show the importance of a good condition estimator, and (iii) show how these decompositions may be more accurate alternatives to the *SVD* than *RRQR*.

The paper is organized as follows. In §2 we derive *a posteriori* error bounds for decompositions of the form (5) and (7). The bounds suggest that the *ULV* decomposition yields a more accurate estimate of the numerical nullspace than the *URV* decomposition, while the *URV* decomposition yields a better estimate of the numerical range. In §3 our theoretical results show that the quality of the subspaces obtained by the aforementioned *URV* and *ULV* algorithms depend on the quality of the estimated singular vectors, not on the gap in the singular values. This is verified in our numerical simulations. This motivates us to implement the rank revealing two-sided orthogonal factorizations in an adaptive manner. In our simulations the refinement procedure is based on the repeated estimation of the singular vectors using the Cline-Conn-Van Loan (CCVL) condition estimator [8]. Our experimental evidence shows that this process has the tendency to reduce the nearest off-diagonal elements when estimating a small singular value in a cluster of small singular values. This improves the subsequent estimation step by the CCVL condition estimator. In §4 we compare the subspaces obtained by the *RRQR* factorization and the *URV*/*ULV* factorizations. The analysis implies that the rank revealing two-sided orthogonal factorizations may be more accurate alternatives to the *SVD* than the *RRQR* factorization. In §5 we summarize our conclusions.

Finally, $C(1:i, 1:i)$ denotes the leading submatrix of C of order i, and superscripts $\dagger$ and T denote the pseudoinverse and transpose, respectively. Also, $\eta \equiv \sigma_{k+1}/\sigma_k$, and the "gap" in the singular values of A is large when $1 - \eta$ is close to 1.

The SVD of A (see [13, §2.3]) is denoted

$$A = U\Sigma V^T \tag{9}$$

where, for $m \geq n$,

$$U = [U_k \; U_0 \; U^{\perp}], \quad V = [V_k \; V_0]$$

and

$$\Sigma = \begin{array}{cc} & \begin{array}{cc} k & n-k \end{array} \\ & \left[\begin{array}{cc} \Sigma_k & 0 \\ 0 & \Sigma_0 \\ 0 & 0 \end{array} \right] \begin{array}{l} k \\ n-k \, . \\ m-n \end{array} \end{array}$$

Therefore

$$A = U_k \Sigma_k V_k^T + U_0 \Sigma_0 V_0^T . \tag{10}$$

The nonnegative diagonal elements of Σ, denoted σ_i, are the singular values of A and are arranged in decreasing order. In accordance with [12], given a user-supplied threshhold parameter tol such that

$$\sigma_k > tol > \sigma_{k+1},$$

then the numerical rank of A is k (with respect to threshhold tol).

2. Subspace Bounds. It is well known [22, 28] that a singular vector corresponding to a singular value in a cluster is extremely sensitive to small perturbations, but that the span of the singular vectors corresponding to the cluster is well determined, i.e., relatively insensitive to small perturbations. Thus we provide bounds for the error in approximating the span. The following definition defines subspaces associated with the SVD.

Definition [22] Let $A \in \Re^{m \times n}$ and let $\mathbf{X} \subset \Re^n$ and $\mathbf{Y} \subset \Re^m$ be subspaces of dimension l. Then $\mathbf{X}$ and $\mathbf{Y}$ form a pair of *singular subspaces for* A if

$$\begin{array}{ll} \text{(i)} & A\mathbf{X} \subset \mathbf{Y} \\ \text{(ii)} & A^T\mathbf{Y} \subset \mathbf{X}. \end{array}$$

$R(V_k)$ and $R(U_k)$ are subspace pairs of dimension k, and $R(V_0)$ and $R(U_0)$ are subspace pairs of dimension $n-k$, where $R(C)$ denote the range of matrix C. $R(V_0)$ is termed the numerical nullspace of A, sometimes referred to as the "noise" subspace. $R(U_k)$ is termed the numerical range of A.

For the (nonunique) URV decomposition in (5), there exist matrices Q and P (see [22]) such that $R(U_{Rk} + U_{R0}Q)$ and $R(V_{Rk} + V_{R0}P)$ form a pair of singular subspaces for A with

$$\|[Q \; P]\|_F \leq \frac{2\|F\|_F}{\sigma_{\min}(R_k) - \|G\|},$$

where $\|\cdot\|_F$ denotes the Frobenius norm and $\sigma_{\min}(C)$ denotes the smallest singular value of the matrix C. If $F = 0$ then $R(U_{Rk})$ and $R(V_{Rk})$ form a pair of singular subspaces for A as well as $R(U_{R0})$ and $R(V_{R0})$. If $||F||$ is small then $R(U_i)$ and $R(V_i)$ $(i = Rk, R0)$ nearly form a pair of singular subspaces for A (similar statements can be made for the *ULV*).

However, we wish to determine the "distance" between the subspaces $R(V_0)$ and $R(V_{R0})$ (and $R(V_0)$ and $R(V_{L0})$), as well as $R(U_k)$ and $R(U_{Rk})$ (and $R(U_k)$ and $R(U_{Lk})$). We will need the following definition for the distance between two subspaces.

Definition [13, p.76] Let $W = [W_1\ W_2]$ and $Z = [Z_1\ Z_2]$ be orthogonal matrices where $W_1, Z_1 \in \Re^{p\times(p-q)}$ and $W_2, Z_2 \in \Re^{p\times q}$. If $\mathcal{S}_1 = R(W_1)$ and $\mathcal{S}_2 = R(Z_1)$ then $\text{dist}(\mathcal{S}_1, \mathcal{S}_2) = ||W_2^T Z_1||$.

2.1. Subspace Bounds for the *URV* and *SVD*. If $\sin\theta \equiv \text{dist}(\mathcal{S}_1, \mathcal{S}_2)$ then θ is the (largest) subspace angle between $\mathcal{S}_1$ and $\mathcal{S}_2$. Let $\sin\theta_{URV} \equiv \text{dist}(R(V_0), R(V_{R0}))$ and let $\sin\phi_{URV} \equiv \text{dist}(R(U_k), R(U_{Rk}))$. Based on the definition, it easily follows that

$$\sin\theta_{URV} = ||V_k^T V_{R0}|| = ||V_{Rk}^T V_0|| \quad \text{and} \quad \sin\phi_{URV} = ||{U_k^{\perp}}^T U_{Rk}|| = ||{U_{Rk}^{\perp}}^T U_k||,$$

where $U_k^{\perp} \equiv [U_0\ U^{\perp}]$ and $U_{Rk}^{\perp} \equiv [U_{R0}\ U_{\perp}]$. However, for our analysis in §2 a more useful expression for $\sin\phi_{URV}$ is needed and requires some preliminary work since it is advantageous to deal with orthogonal complements. We will use the following result throughout the paper.

LEMMA 2.1. *Given the usual* SVD *and* URV *factorizations of A, then*

$$\sin\phi_{URV} = ||U_k^T U_{R0}|| = ||U_{Rk}^T U_0||.$$

Proof: First we will find an expression for ${U_k^{\perp}}^T U_{Rk}$ and show $||{U_k^{\perp}}^T U_{Rk}|| = ||U_{Rk}^T U_0||$.

$$\begin{aligned}
{U_k^{\perp}}^T U_{Rk} &= {U_k^{\perp}}^T A V_{Rk} R_k^{-1} \\
&= \begin{bmatrix} U_0^T \\ {U^{\perp}}^T \end{bmatrix} [U_k\ U_0\ U^{\perp}] \begin{bmatrix} \Sigma_k & 0 \\ 0 & \Sigma_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_k \\ V_0 \end{bmatrix} V_{Rk} R_k^{-1} \\
&= \begin{bmatrix} 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \Sigma_k V_k^T & 0 \\ 0 & \Sigma_0 V_0^T \\ 0 & 0 \end{bmatrix} V_{Rk} R_k^{-1} \\
&= \begin{bmatrix} \Sigma_0 V_0^T V_{Rk} R_k^{-1} \\ 0 \end{bmatrix},
\end{aligned}$$

and thus $||{U_k^{\perp}}^T U_{Rk}|| = ||\Sigma_0 V_0^T V_{Rk} R_k^{-1}||$. Now, from the *URV* factorization of A, $U_{Rk}^T = R_k^{-T} V_{Rk}^T A^T$. Thus, $U_{Rk}^T U_0 = R_k^{-T} V_{Rk}^T A^T U_0 = R_k^{-T} V_{Rk}^T V_0 \Sigma_0$ and therefore $||U_{Rk}^T U_0|| = ||(U_{Rk}^T U_0)^T|| = ||{U_k^{\perp}}^T U_{Rk}||$. Similarly, one can show $||{U_{Rk}^{\perp}}^T U_k|| = ||G V_{R0}^T V_k \Sigma_k^{-1}|| = ||U_k^T U_{R0}||$.

A corresponding lemma can be proven for the *ULV* decomposition. Now we are ready for the main result of this section.

THEOREM 2.2. ***(URV Error Bounds)*** *Let $A \in R^{m\times n}$ have the usual* SVD *and* URV *factorizations, and define $\eta = \sigma_{k+1}/\sigma_k$. Then the distance between the numerical nullspace $R(V_0)$ and the* URV *approximate nullspace $R(V_{R0})$, and the distance between the numerical range $R(U_k)$ and its* URV *estimate $R(U_{Rk})$ are bounded by:*

$$(a) \quad \frac{||F||}{||R|| + \eta\,||G||} \;\leq\; dist(R(V_0), R(V_{R0})) \;\leq\; \frac{\sigma_{\min}(R_k)\,||F||}{\sigma_{\min}^2(R_k) - \sigma_{k+1}^2}$$

$$(b) \quad dist(R(U_k), R(U_{Rk})) \;\leq\; \frac{||F||\,||G||}{\sigma_k^2 - ||G||^2}.$$

Proof: To prove the upper bound in (a),

$$\begin{aligned} V_{Rk}^T V_0 &= R_k^{-1}(U_{Rk}^T A - F V_{R0}^T) V_0 \\ &= R_k^{-1}(U_{Rk}^T U_0 \Sigma_0 - F V_{R0}^T V_0). \end{aligned} \tag{11}$$

Now we need to find an expression for $U_{Rk}^T U_0$. First, $AV_{Rk} = U_{Rk} R_k$ implies $U_{Rk}^T = R_k^{-T} V_{Rk}^T A^T$. Second, $U_{Rk}^T U_0 = R_k^{-T} V_{Rk}^T V_0 \Sigma_0$. Substituting into (11),

$$\begin{aligned} V_{Rk}^T V_0 &= R_k^{-1}(R_k^{-T} V_{Rk}^T V_0 \Sigma_0^2 - F V_{R0}^T V_0) \\ &= R_k^{-1} R_k^{-T} V_{Rk}^T V_0 \Sigma_0^2 - R_k^{-1} F V_{R0}^T V_0. \end{aligned}$$

Taking norms,

$$\sin\theta_{URV} \leq ||R_k^{-1}||^2 \sin\theta_{URV}\, \sigma_{k+1}^2 + ||R_k^{-1}||\,||F||,$$

and solving for $\sin\theta_{URV}$ yields

$$\sin\theta_{URV} \leq \frac{||R_k^{-1}||\,||F||}{1 - \sigma_{\min}^{-2}(R_k)\,\sigma_{k+1}^2} = \frac{\sigma_{\min}(R_k)\,||F||}{\sigma_{\min}^2(R_k) - \Sigma_{k+1}^2}.$$

To prove (b), we use an argument similar to (a). Using $U_k^T U_{R0} = \Sigma_k^{-1}(V_k^T V_{R0}) G^T$, it remains to find an expression for $V_k^T V_{R0}$:

$$V_k^T V_{R0} = \Sigma_k^{-1} U_k^T A V_{R0} = \Sigma_k^{-1}(U_k^T U_{Rk} F + U_k^T U_{R0} G).$$

Upon substitution, $U_k^T U_{R0} = \Sigma_k^{-2}(U_k^T U_{Rk} F + U_k^T U_{R0} G) G^T$. It follows

$$\sin\phi_{URV} \leq \sigma_k^{-2}(||F||\,||G|| + \sin\phi_{URV} ||G||^2).$$

Solving for $\sin\phi_{URV}$ yields

$$\sin\phi_{URV} \leq \frac{\sigma_k^{-2}||F||\,||G||}{1 - ||G||^2\sigma_k^{-2}} = \frac{||F||\,||G||}{\sigma_k^2 - ||G||^2}.$$

To prove the lower bound in (a), it is straightforward to show

$$F = U_{Rk}^T U_1 \Sigma_1 V_k^T V_{R0} + U_{Rk}^T U_2 \Sigma_2 V_0^T V_{R0}.$$

Taking norms in an obvious manner,

$$\begin{aligned} ||F|| &\leq ||R||\,||V_k^T V_{R0}|| + ||U_{Rk}^T U_2||\,||\Sigma_2|| \\ &= ||R||\,\sin\theta_{URV} + ||U_k^T U_{R0}||\,\sigma_{k+1} \\ &\leq ||R||\,\sin\theta_{URV} + ||\Sigma_k^{-1}(V_k^T V_{R0}) G^T||\,||\Sigma_2|| \\ &\leq (||R|| + \eta||G||)\sin\theta_{URV}, \end{aligned}$$

hence the lower bound follows. This completes the proof of the theorem.

It can also be shown

$$\operatorname{dist}(R(V_0), R(V_{R0})) \leq \frac{\|F\|}{\sigma_{\min}(R_k) - \eta\|G\|} \quad \text{and} \quad \operatorname{dist}(R(U_k), R(U_{Rk})) \leq \frac{\|F\|\,\sigma_{k+1}}{\sigma^2_{\min}(R_k) - \sigma^2_{k+1}}.$$

Note that it is possible to find *a posteriori* upper bounds by using Theorem 2.2 together with the facts $\sigma_{\min}(R_k) \leq \sigma_k, , \eta \leq 1$, $\sigma_{\min}(R_k)/(\sigma_{\min}(R_k) + \|G\|) \leq 1$, and $\sigma_{k+1} \leq \|G\|$. Given the above, the following corollary is immediate.

COROLLARY 2.3. ***(A Posteriori Bounds for* URV*)*** *Under the assumptions of Theorem 2.2, the following a posteriori bounds hold:*

$$(a) \quad \frac{\|F\|}{\|R\|+\|G\|} \leq dist(R(V_0), R(V_{R0})) \leq \frac{\|F\|\,\sigma_{\min}(R_k)}{\sigma^2_{\min}(R_k) - \|G\|^2}$$

$$(b) \quad dist(R(U_k), R(U_{Rk})) \leq \frac{\|F\|\|G\|}{\sigma^2_{\min}(R_k) - \|G\|^2}.$$

These bounds show explicitly that when $\|F\|$ is small then the subspaces nearly coincide. In §3 we discuss a way to achieve a small $\|F\|$ so that high quality subspaces are obtained.

2.2. Subspace Bounds for the *ULV* and *SVD*. In this section we are concerned with the *ULV* decomposition. Let A have the usual *SVD* and *ULV* as in §1. Let $\sin\theta_{ULV} \equiv \operatorname{dist}(R(V_0), R(V_{L0}))$ and $\sin\phi_{ULV} \equiv \operatorname{dist}(R(U_k), R(U_{Lk}))$. After the *ULV* factorization is complete, we wish to determine upper bounds on the errors in the approximate subspaces.

THEOREM 2.4. ***(*ULV *Error Bounds)*** *Let $A \in R^{m\times n}$ have the usual* SVD *and* ULV *factorizations, and define $\eta = \sigma_{k+1}/\sigma_k$. Then the distance between the numerical nullspace $R(V_0)$ and the* ULV *approximate nullspace $R(V_{L0})$, and the distance between the numerical range $R(U_k)$ and its* ULV *estimate $R(U_{Lk})$ are bounded by:*

$$(a) \quad dist(R(V_0), R(V_{L0})) \leq \frac{\sigma_{k+1}\|H\|}{\sigma^2_{\min}(L_k) - \sigma^2_{k+1}}$$

$$(b) \quad \frac{\|H\|}{\|L\| + \eta\|E\|} \leq dist(R(U_k), R(U_{Lk})) \leq \frac{\|H\|\sigma_{\min}(L_k)}{\sigma^2_{\min}(L_k) - \sigma^2_{k+1}}.$$

Proof: To prove the upper bound in (a), we have

$$V_{Lk}^T V_0 = L_k^{-1} U_{Lk}^T A V_0 = L_k^{-1} U_{Lk}^T U_0 \Sigma_0. \tag{12}$$

Now to find an expression for $U_{Lk}^T U_0$, $A = [U_{Lk}\ U_{L0}]L[V_{Lk}\ V_{L0}]^T$ implies $U_{Lk}^T = L_k^{-T}(V_{Lk}^T A^T - H^T U_{L0}^T)$. Hence,

$$\begin{aligned} U_{Lk}^T U_0 &= L_k^{-T}(V_{Lk}^T A^T - H^T U_{L0}^T) U_0 \\ &= L_k^{-T}(V_{Lk}^T A^T - H^T U_{L0}^T) U_0 \qquad (13) \\ &= L_k^{-T}(V_{Lk}^T V_0 \Sigma_0 - H^T U_{L0}^T U_0). \qquad (14) \end{aligned}$$

Substituting (14) into (12), it follows that

$$V_{Lk}^T V_0 = L_k^{-1}(L_k^{-T}(V_{Lk}^T V_0 \Sigma_0 - H^T U_{L0}^T U_0)\Sigma_0),$$

and taking norms,

$$\|V_{Lk}^T V_0\| \leq \|L_k^{-1}\|^2 \|\Sigma_0\| \, \|V_{Lk}^T V_0\| + \|L_k^{-1}\|^2 \|H\| \, \|\Sigma_0\|.$$

Solving for $\|V_{Lk}^T V_0\| = \sin \theta_{ULV}$, we get

$$\sin \theta_{ULV} \leq \frac{\|H\| \, \|L_k^{-1}\|^2 \, \sigma_{k+1}}{1 - \|L_k^{-1}\|^2 \sigma_{k+1}^2} = \frac{\|H\| \, \sigma_{k+1}}{\sigma_{\min}^2(L_k) - \sigma_{k+1}^2}.$$

To prove (b), substituting $V_{Lk}^T V_0 = L_k^{-1}(U_{Lk}^T U_0)\Sigma_0$ into

$$U_{Lk}^T U_0 = L_k^{-1}(V_{Lk}^T V_0 \Sigma_0 - H^T U_{L0}^T U_0),$$

it follows that

$$\begin{aligned} U_{Lk}^T U_0 &= L_k^{-T}(L_k^{-1}(U_{Lk}^T U_0)\Sigma_0^2 - H^T U_{L0}^T U_0) \\ &= L_k^{-T} L_k^{-1}(U_{Lk}^T U_0)\Sigma_0^2 - L_k^{-T} H^T U_{L0}^T U_0. \end{aligned}$$

Taking norms in the obvious way yields

$$\sin \phi_{ULV} \leq \|L_k^{-1}\|^2 \sigma_{k+1}^2 \sin \phi_{ULV} + \|L_k^{-1}\| \, \|H\|,$$

and solving for $\sin \phi_{ULV}$ yields

$$\sin \phi_{ULV} \leq \frac{\|L_{11}^{-1}\| \, \|H\|}{1 - \sigma_{k+1}^2 \|L_{11}^{-1}\|^2} = \frac{\sigma_{\min}(L_k) \|H\|}{\sigma_{\min}^2(L_k) - \sigma_{k+1}^2}.$$

The lower bound for $\sin \phi_{ULV}$ follows analogously to proof for the lower bound for $\sin \theta_{URV}$. This completes the proof of the theorem.

It can also be shown

$$\mathrm{dist}(R(V_0), R(V_{L0})) \leq \frac{\sigma_{k+1}\|H\|}{\sigma_{\min}^2(L_k) - \sigma_{k+1}^2} \quad \text{and } \mathrm{dist}(R(U_k), R(U_{Lk})) \leq \frac{\|H\|\sigma_{k+1}}{\sigma_k \sigma_{\min}(L_k) - \sigma_{k+1}\|E\|}.$$

As before, it is possible to generate *a posteriori* upper bounds for the subspace angles in terms of computed *ULV* factors. The necessary facts are $\sigma_{\min}(L_k) \leq \sigma_k$, $\eta < 1$, $\sigma_{\min}(L_k)/(\sigma_{\min}(L_k) + \|E\|) \leq 1$, and $\sigma_{k+1} \leq \|E\|$, as well as Theorem 2.4.

COROLLARY 2.5. ***(A Posteriori Bounds for* ULV** *Under the assumptions of Theorem 2.4, the following a posteriori bounds hold:*

$$(a) \quad dist(R(V_0), R(V_{L0})) \;\leq\; \frac{\|H\|\|E\|}{\sigma_{\min}^2(L_k) - \|E\|^2}$$

$$(b) \quad \frac{\|H\|}{\|L\| + \|E\|} \;\leq\; dist(R(U_k), R(U_{Lk})) \;\leq\; \frac{\sigma_{\min}(L_k)\,\|H\|}{\sigma_{\min}^2(L_k) - \|E\|^2}.$$

This shows a large $\|H\|$ translates to a large $\sin \phi_{ULV}$. In the next section we discuss a way to produce a small $\|H\|$. Comparing the *a posteriori* bounds for the *URV* and *ULV*, we may conclude that the *ULV* can be expected to yield a higher quality estimate of the numerical nullspace than the *URV*. Tables 1-4 summarize the results of some typical experiments that verify this conclusion.

3. Algorithm and Numerical Simulations. As mentioned earlier, the *URV* and *ULV* factorizations may be refined iteratively using various schemes. The purpose of refinement procedures is to concentrate less "energy" of R (or L) in the 1,2 (or 2,1) position so as to decouple the matrix as much as possible. Recall from §2 that when the triangular matrix is decoupled (i.e., off-diagonal blocks are zero matrices) then we have obtained singular subspaces for the matrix, and when the off-diagonal block is small then we have obtained good singular subspace approximations. In [23] it is shown how so-called "left" and "right" iterations ("shiftless" QR) may be used to iteratively refine the subspaces. Based on this particular refinement strategy, error bounds for estimating the singular values of the matrix A are also provided.

3.1. Algorithm. Now we turn our attention to a brief discussion of the algorithms by Stewart. At the i^{th} step of the *URV* algorithm, we work with the upper triangular matrix

$$\begin{array}{cc} \begin{array}{cc} i & n-i \end{array} & \\ \begin{bmatrix} R^i & F_i \\ 0 & G_i \end{bmatrix} & \begin{array}{l} i \\ n-i \end{array} \end{array}$$

and a *unit estimate* v_{est}^i of the exact $i \times 1$ right singular vector $v_{\min}^i$ corresponding to $\sigma_{\min}(R^i)$. Using plane rotations, find an $i \times i$ orthogonal matrix Q^i such that $(Q^i)^T v_{est}^i = (0, \ldots, 0, 1)^T$ and $R^i Q^i$ is upper Hessenberg. Then determine an $i \times i$ orthogonal matrix P^i such that $(P^i)^T (R^i Q^i)$ is upper triangular. Represent the updated triangular matrix by

$$(P^i)^T (R^i Q^i) = \begin{array}{cc} \begin{array}{cc} i-1 & n-i+1 \end{array} & \\ \begin{bmatrix} R^{(i-1)} & F_{i-1} \\ 0 & G_{i-1} \end{bmatrix} & \begin{array}{l} i-1 \\ n-i+1 \end{array} \end{array} \equiv \begin{array}{cc} \begin{array}{ccc} i-1 & 1 & n-i \end{array} & \\ \begin{bmatrix} R^{(i-1)} & f_i & F_i' \\ 0 & r_{ii} & g_i^T \\ 0 & 0 & G_i' \end{bmatrix} & \begin{array}{l} i-1 \\ 1 \\ n-i. \end{array} \end{array}$$

Analogously, at the i^{th} step of the *ULV* algorithm we work with the lower triangular matrix

$$\begin{array}{cc} \begin{array}{cc} i & n-i \end{array} & \\ \begin{bmatrix} L^i & 0 \\ H_i & E_i \end{bmatrix} & \begin{array}{l} i \\ n-i \end{array} \end{array}$$

and a *unit estimate* u_{est}^i of the exact $i \times 1$ left singular vector $u_{\min}^i$ corresponding to $\sigma_{\min}(L^i)$. Using plane rotations, find an $i \times i$ orthogonal matrix P^i such that $P^i u_{est}^i = (0, \ldots, 0, 1)^T$ and $P^i L^i$ is lower Hessenberg. Then use plane rotations to determine an $i \times i$ orthogonal matrix Q^i such that $(P^i L^i)(Q^i)^T$ is lower triangular. Represent the updated triangular matrix by

$$(P^i L^i)(Q^i)^T = \begin{array}{cc} \begin{array}{cc} i-1 & n-i+1 \end{array} & \\ \begin{bmatrix} L^{(i-1)} & 0 \\ H_{i-1} & E_{i-1} \end{bmatrix} & \begin{array}{l} i-1 \\ n-i+1 \end{array} \end{array} \equiv \begin{array}{cc} \begin{array}{ccc} i-1 & 1 & n-i \end{array} & \\ \begin{bmatrix} L^{(i-1)} & 0 & 0 \\ h_i^T & l_{ii} & 0 \\ H_i' & e_i & E_i' \end{bmatrix} & \begin{array}{l} i-1 \\ 1 \\ n-i. \end{array} \end{array}$$

The following result shows how the accuracy of the estimate v_{est}^i is related to the norm of the column $f_i \equiv F_{i-1}(:,1)$ and the approximation of $\sigma_{\min}(R^i)$ by $|r_{ii}|$, as well as how the accuracy of the estimate u_{est}^i is related to the size of the row $h_i^T \equiv H_{i-1}(1,:)$ and the approximation of $\sigma_{\min}(L^i)$ by $|l_{ii}|$.

THEOREM 3.1. *Using the notation above, let v_{est}^i with unit 2-norm denote an estimate of $v_{\min}^i$, the right singular vector of R^i corresponding to $\sigma_{\min}(R^i)$. If θ_{URV}^i denotes the angle between v_{est}^i and $v_{\min}^i$, then*

$$\frac{\|f_i\|}{\|R^i\|} \le \sin\theta_{URV}^i \quad \text{and} \quad \frac{\sqrt{2}}{\kappa(R^i)}\sqrt{\frac{|r_{ii}| - \sigma_{\min}(R^i)}{\sigma_{\min}(R^i)}} \le \sin\theta_{URV}^i,$$

where $\kappa(R^i) = \frac{\|R^i\|}{\sigma_{\min}(R^i)}$. Analogously, using the notation above, let u_{est}^i with unit 2-norm denote an estimate of $u_{\min}^i$, the left singular vector of L^i corresponding to $\sigma_{\min}(L^i)$. If ϕ_{ULV}^i denotes the angle between u_{est}^i and $u_{\min}^i$, then

$$\frac{\|h_i\|}{\|L^i\|} \le \sin\phi_{ULV}^i \quad \text{and} \quad \frac{\sqrt{2}}{\kappa(L^i)}\sqrt{\frac{|l_{ii}| - \sigma_{\min}(L^i)}{\sigma_{\min}(L^i)}} \le \sin\phi_{ULV}^i,$$

where $\kappa(L^i) = \frac{\|L^i\|}{\sigma_{\min}(L^i)}$.

Proof: We begin with

$$\begin{aligned}\left\|R^i v_{est}^i\right\|^2 &= \left\|P^{i^T}\left(R^i Q^i\right) Q^{i^T} v_{est}^i\right\|^2 \\ &= \|f_i\|^2 + r_{ii}^2.\end{aligned}$$

Let R^i have the SVD

$$R^i = U_R \Sigma_R V_R^T + u_{\min}^i \sigma_{\min}(R^i)\left(v_{\min}^i\right)^T.$$

Then it follows

$$\begin{aligned}\left\|R^i v_{est}^i\right\|^2 &= \left\|U_R\Sigma_R V_R^T v_{est}^i\right\|^2 + \sigma_{\min}^2(R^i)\left|\left(v_{\min}^i\right)^T v_{est}^i\right|^2 \\ &\le \|R^i\|^2 \sin^2\theta_{URV}^i + \sigma_{\min}^2(R^i).\end{aligned}$$

Hence,

$$\|f_i\|^2 + r_{ii}^2 \le \|R^i\|^2 \sin^2\theta_{URV}^i + \sigma_{\min}^2(R^i),$$

which implies

$$\frac{\|f_i\|^2}{\|R^i\|^2} + \frac{r_{ii}^2 - \sigma_{\min}^2(R^i)}{\|R^i\|^2} \le \sin^2\theta_{URV}^i.$$

Since each term on the left is non-negative, then

$$\frac{\|f_i\|^2}{\|R^i\|^2} \le \sin^2\theta_{URV}^i \quad \text{and} \quad \frac{\sigma_{\min}^2(R^i)}{\|R^i\|^2} \times \frac{r_{ii}^2 - \sigma_{\min}^2(R^i)}{\sigma_{\min}^2(R^i)} \le \sin^2\theta_{URV}^i.$$

But $(r_{ii}^2 - \sigma_{\min}^2(R^i))/\sigma_{\min}^2(R^i) = (|r_{ii}| - \sigma_{\min}(R^i))(|r_{ii}| + \sigma_{\min}(R^i))/\sigma_{\min}^2(R^i) \ge 2(|r_{ii}| - \sigma_{\min}(R^i))/\sigma_{\min}(R^i)$, since $|r_{ii}| \ge \sigma_{\min}(R^i)$. Hence the desired result follows. Since the ULV results can be shown analogously, the theorem is proved.

This means good estimates of the right (left) singular vectors of R^i (L^i) for $i = n, \ldots, k+1$ lead to a small $\|F\|$ ($\|H\|$). By Corollaries 2.3 and 2.5 this means the quality of the subspaces depends on the quality of the estimated singular vectors. Theorem 3.1 extends [26, Theorem 1], where it is proven that if all the estimates $v^i_{\min}$ (or $u^i_{\min}$) are "exact" then $F = 0$ (or $H = 0$) and the relevant subspaces coincide.

Motivated by these results, we consider a refinement strategy that monitors the columns (rows) of the off-diagonal block of the triangular matrix as it is generated one column (row) at a time. We proceed to the next step (a deflation step) provided the newly generated column (row) of the off-diagonal block is sufficiently small. Our refinement step is based on the repeated estimation of the singular vector using the Cline-Conn-Van Loan (CCVL) condition estimator [8]. The following algorithms modify Stewart's algorithms [23, 24] by incorporating the *a posteriori* bounds for the subspace angles, giving the algorithm an adaptive flavor.

An adaptive version of the *URV* decomposition Input: An $m \times n$ data matrix A, parameter *tol* for numerical rank determination, integer *max_iter* to control the maximum number of refinement steps per iteration, *est_sigk* an estimate of the k^{th} singular value of A, and subspace tolerance δ to determine the accuracy of the near-singular subspace pairs.

Step 1: Compute a QR factorization $A = QR$, where $Q \in \Re^{m\times n}$ has orthonormal columns and $R \in \Re^{n\times n}$ is upper triangular.

Step 2. Initialize $i \leftarrow n$, $V \leftarrow I$, $U \leftarrow Q$.

Step 3. Compute a unit estimate v^n_{est} of the right singular vector corresponding to $\sigma_{\min}(R)$ using condition estimator CCVL.

Step 4. While $(\|R(1:i, 1:i)\, v^i_{est}\| < tol)$ do

For $t = 1 : max\_iter$

(4a) Compute a sequence of plane rotations $Q_1, \ldots, Q_{i-1}$ so that $Q^T_{i-1} \cdots Q^T_1 v^i_{\min} = (0, 0, .., 0, 1)^T$. Update V: $V \leftarrow V \begin{bmatrix} Q^i & 0 \\ 0 & I_{n-i} \end{bmatrix}$, where $Q^i \equiv Q_1 \cdots Q_{i-1}$.

(4b) Determine a sequence of plane rotations $P_1, \ldots, P_{i-1}$ so that $P^T_{i-1} \cdots P^T_1 (R(1:i, 1:i)Q^i)$ is upper triangular. Update U and R: $U \leftarrow U \begin{bmatrix} P^i & 0 \\ 0 & I_{n-i} \end{bmatrix}$ and $R \leftarrow \begin{bmatrix} P^{iT} & 0 \\ 0 & I_{n-i} \end{bmatrix} R \begin{bmatrix} Q^i & 0 \\ 0 & I_{n-i} \end{bmatrix}$, where $P^i \equiv P_1 \cdots P_{i-1}$.

(4c) If $(max\_iter > 1)$ then

compute $est\_upbd = \|f_i\|/est\_sigk$, where $f_i = R(1:i-1, i)$.

if $(est\_upbd < \delta)$ then

DEFLATE: set $i \leftarrow i - 1$, and compute a unit estimate $v^i_{\min}$ of $R(1:i, 1:i)$ using condition estimator CCVL. Go to Step 4.

else

REFINE: recompute an estimate $v^i_{\min}$ of $R(1:i, 1:i)$ using condition estimator CCVL.

End ifs

End for

End while.

Step 5. Output: Numerical rank $k \leftarrow i$, *a posteriori* upper bounds $\|F\|/(\sigma_{\min}(R_k) -$

$\|G\|), \|F\| \|G\|/(\sigma_{\min}^2(R_k)-\|G\|^2)$, and an estimate of the gap $\sigma_{\min}(R_k)/\|G\|$.

END.

It is important to remember that when *max_iter* =1 then this algorithm does not incorporate refinement. When *max_iter* > 1, our experiments show this refinement process has the tendency to reduce the nearest off-diagonal elements when working in a cluster of small singular values, which improves the subsequent estimation step by the CCVL condition estimator. See [14] for an excellent survey on condition estimators.

For the *ULV* algorithm we implemented, the following changes were made in the *URV* algorithm described above:

- Given an initial QR factorization of A, initialize $U \leftarrow QZ$, $V \leftarrow Z$, and $L \leftarrow ZRZ$ where Z is the anti-identity matrix (zeros everywhere except for ones in the $j, n-j+1$ position).
- Compute an estimate $u_{\min}^i$ of the left singular vector corresponding to the smallest singular value of $L(1:i,1:i)$. Transform $u_{\min}^i$ to $(0,...,0,1)$, thereby transforming $L(1:i,1:i)$ to lower Hessenberg using $i-1$ plane rotations on the left. Accumulate the left plane rotations. Then restore lower triangularity to L using $i-1$ plane rotations on the right. Accumulate the right plane rotations.
- The subspace quality was iteratively estimated by $est\_upbd = n \cdot \|h_i^T\| \cdot \|E_i\|/(est\_sigk)^2$, where $h_i^T = L(i,1:i-1)$ and $E_i = L(i+1:n, i+1:n)$.

The numerical results herein indeed verify that the quality of the subspaces is independent of the gap in the singular value spectrum of A, but instead depend on the quality of the start vector (for example, see Tables 4-5).

However, the gap may have an indirect effect in the practical implementation – in the absence of privileged knowledge it can affect the ability of the condition estimator to deliver a good initial guess or start vector. Although refinement procedures are designed to help overcome this, a poor gap can hamper the rate of convergence when improving the start vector using inverse iteration or using repeated condition estimation as described in the algorithm, and a few extra refinement steps may be needed. This is illustrated by the following numerical simulations.

3.2. Numerical Simulations. The matrices $\{A_i\}_{i=1}^6$ of dimensions $m = 25$, $n = 10$ with numerical rank $k = 7$ are created by generating random matrices and replacing the singular values by the following values as in [6, §7]. The first seven singular values are fixed at

$$\sigma_1 = 1,\ \sigma_2 = 0.5,\ \sigma_3 = 0.2,\ \sigma_4 = 0.1,\ \sigma_5 = 0.05,\ \sigma_6 = 0.02,\ \sigma_7 = 0.01,$$

with the remaining singular values varying as follows:

σ	A_1	A_2	A_3	A_4	A_5	A_6
σ_8	$1.0 \cdot 10^{-18}$	$1.0 \cdot 10^{-6}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-4}$
σ_9	$1.0 \cdot 10^{-18}$	$1.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-6}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$	$5.0 \cdot 10^{-4}$
σ_{10}	$1.0 \cdot 10^{-18}$	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-6}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$.

We implemented the adaptive algorithms (as described earlier) in Matlab [17] with machine precision $\approx 2.2 \times 10^{-16}$. We

- compared the quality of the approximate subspaces and
- verified the *a posteriori* bounds.

The *a posteriori* bounds strongly suggest that the two-sided orthogonal decompositions do not depend on the gap and that the ULV decomposition yields a more accurate estimate of the numerical nullspace, while the URV decomposition yields a more accurate estimate of the numerical range. This is verified in the numerical simulations (see Tables 1-7). with $max\_iter = 1$ and 2, where the experiments also illustrate the quality of the *a posteriori* bounds. The bounds are not overly pessimistic and in most cases provide an extremely accurate indication of the quality of the subspace. Note that when $max\_iter = 2$ then CCVL provides improved estimates of the singular vectors resulting in higher quality subspaces, which confirms that this strategy is a good refinement strategy. In addition, Table 5 confirms the theoretical implications of [26, Theorem 1], which proves that exact estimates of the singular vectors yield singular subspaces ($\theta = 0$ and $\phi = 0$).

4. Rank Revealing QR Factorizations. A rank revealing QR factorization of A (with numerical rank k) is any factorization

$$A\Pi = QR \tag{15}$$

$$= [Q_1\ Q_2] \begin{array}{cc} \begin{array}{cc} k & n-k \end{array} & \\ \left[\begin{array}{cc} R_{11} & R_{12} \\ 0 & R_{22} \end{array}\right] & \begin{array}{l} k \\ n-k \end{array} \end{array} \tag{16}$$

where R is upper triangular, $\|R_{22}\|$ is order σ_{k+1}, R_{11} is well conditioned, and Π is a permutation matrix. In this factorization the approximate nullspace is not exhibited explicitly since the 1,2 position of R, namely R_{12}, is generally not small. In [5] Chan presents a rank revealing QR ($RRQR$) algorithm where the matrix A is preprocessed by an initial QR factorization followed by condition estimation, strategic column pivoting, and plane rotations applied on the left to restore triangularity. When the algorithm runs to completion, it can be shown [6] that

$$\|A(\Pi W)\| \le \sqrt{n-k}\,\sigma_{k+1}, \tag{17}$$

where the columns of $W = \begin{array}{cc} \left[\begin{array}{c} W_1 \\ W_2 \end{array}\right] & \begin{array}{l} k \\ n-k \end{array} \end{array}$ store the estimated $n-k$ right singular vectors. Hence $R(\Pi W)$ is an approximate nullspace for A. More rigorously, from [6, Theorem 4.1], if θ_{QR} denotes the subspace angle between $R(\Pi W)$ and $R(V_0)$ and $\sin\theta_{QR} \equiv \mathrm{dist}(R(\Pi W), R(V_0))$, then

$$\mathrm{dist}(R(\Pi W), R(V_0)) \le \eta\,(1 + \|W_2^{-1}\|\sqrt{n-k}). \tag{18}$$

In addition, it can be shown [7] that if ϕ_{RRQR} denotes the subspace angle between $R(U_k)$ and $R(Q_1)$ and $\sin\phi_{RRQR} \equiv \mathrm{dist}(R(Q_1), R(U_k))$, then

$$\mathrm{dist}(R(Q_1), R(U_k)) \le \eta\,\|W_2^{-1}\|\sqrt{n-k}. \tag{19}$$

The $RRQR$ bounds show that if

- η is small (large gap in the singular value spectrum of A)
- A has low rank-deficiency (k not too much smaller than n)
- W_2 is well-conditioned ($\|W_2^{-1}\|$ not too large)

then $R(\Pi W)$ $(R(Q_1))$ is a good approximation to the numerical nullspace (range) in the sense that the subspace angle is small. Hence, from these bounds and the numerical evidence in [6] the quality of the $RRQR$-based subspaces depends on a gap condition. This contrasts with the upper bounds we derived in Theorems 2.2 and 2.4 for rank revealing URV and ULV factorizations; for these factorizations η is *not* required to be small (cf. Theorem 3.1 in §3) Table 5 demonstrates this property. In practice, we need only a good estimate of the singular vector to which the plane rotations are applied! The condition estimator CCVL is well suited for this purpose as demonstrated in §4; so is inverse iteration as demonstrated in [26].

The numerical results in Tables 5-7 illustrate that the rank revealing URV and ULV factorizations may be more accurate alternatives to the SVD than $RRQR$. Using the same simulation setup as described in §4, Tables 5-7 compare the subspace angles θ_{RRQR}, θ_{URV}, θ_{ULV} and ϕ_{RRQR}, ϕ_{URV}, ϕ_{ULV} as computed by the URV and ULV algorithms we implemented and by Chan's $RRQR$ algorithm.

The results in Table 5 confirm that the URV and ULV decompositions do not depend on the gap, unlike the $RRQR$ factorization. For these results the exact singular vectors were supplied to the algorithms. However, in Table 6 we supply the algorithms with estimates obtained from CCVL. In the absence of refinement, the results show θ_{URV} is comparable to θ_{RRQR}. θ_{URV} could be better as suggested by theory if we used a better estimate; however, in fairness we supply both of these factorizations with the same estimated right singular vector. Note that θ_{ULV} is superior to both. Both ϕ_{URV} and ϕ_{ULV} are conspicuously better than ϕ_{RRQR}. Note that ϕ_{RRQR} exhibits the dependence on η as in (19) and that decreasing the gap (i.e., decreasing $1/\eta$) affects the ability of CCVL to deliver a good estimate of the right (or left) singular vector of R (or L) in the first pass.

However, when CCVL makes an additional pass per iteration ($max\_iter = 2$), it delivers a markedly improved estimate of the singular vectors, as indicated by the smaller subspace angles in Table 7 For $max\_iter = 2$, the URV and ULV decompositions make more appreciable gains in estimating the singular subspaces of A than the $RRQR$ factorization with one step of simultaneous inverse iteration.

5. Conclusion. In this paper we derived sharp *a posteriori* error bounds (§2) for assessing the quality of subspaces obtained by a rank revealing two-sided orthogonal decomposition, which is a product of an orthogonal matrix, a triangular matrix, and another orthogonal matrix. The theoretical results show how the quality of the subspaces depend on the size of the off-diagonal block of the triangular factor, and that the ULV provides a better estimate of the numerical nullspace than the URV decomposition. Specifically, we considered the promising rank revealing URV and ULV decompositions introduced by G.W. Stewart. The analysis shows that the quality of the subspaces depend on the quality of the estimated singular vectors and not on a gap condition (Theorem 3.1, §3) and that the ULV provides a better estimate of the numerical nullspace than the URV decomposition. We implemented the algorithms in an adaptive manner using the *a posteriori* error bounds and the incremental condition estimator CCVL. Based on our analysis in §4, we conclude that the URV and ULV decompositions may be more accurate alternatives to the SVD than the $RRQR$ factorization. Finally, we provided numerical examples to substantiate our conclusions.

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A_i	gap	$\frac{\|F\|}{\|R\|+\|G\|}$	$\sin\theta_{URV}$	$\frac{\|F\|\sigma_{\min}(R_k)}{\sigma^2_{\min}(R_k)-\|G\|^2}$	$\sin\theta_{ULV}$	$\frac{\|H\|\|E\|}{\sigma^2_{\min}(L_{11})-\|E\|^2}$
A_1	10^{16}	1.2221e-16	4.3106e-15	1.2221e-14	3.7295e-15	8.5223e-30
A_2	10^4	3.0310e-11	2.7514e-09	3.0310e-09	2.8326e-15	2.1900e-12
A_3	10^3	3.0310e-09	2.7514e-07	3.0310e-07	6.7910e-13	2.1900e-10
A_4	10^2	3.0305e-07	2.7514e-05	3.0311e-05	6.7681e-09	2.1952e-08
A_5	10^1	3.0047e-05	2.7534e-03	3.0381e-03	6.6288e-05	6.8643e-05
A_6	10^1	2.2016e-05	2.1912e-03	2.2082e-03	4.6321e-06	6.2003e-06

TABLE 1

Results of typical experiments verifying the a posteriori error bounds for the URV *and* ULV *subspace angles* θ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see Section 5). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$ *and* max_iter $= 1$.

A_i	gap	$\sin\phi_{URV}$	$\frac{\|F\|\|G\|}{\sigma^2_{\min}(R_k)-\|G\|^2}$	$\frac{\|H\|}{\|L\|+\|E\|}$	$\sin\phi_{ULV}$	$\frac{\|H\|\sigma_{\min}(L_{11})}{\sigma^2_{\min}(L_{11})-\|E\|^2}$
A_1	10^{16}	1.6706e-15	1.1875e-28	8.8184e-18	1.6964e-15	8.8184e-16
A_1	10^4	2.7034e-13	3.0310e-13	2.1900e-10	8.0259e-09	2.1900e-08
A_1	10^3	2.7215e-10	3.0310e-10	2.1899e-09	2.3561e-08	2.1900e-07
A_1	10^2	1.9571e-07	3.0311e-07	2.1947e-08	6.7894e-07	2.1952e-06
A_1	10^1	1.9258e-04	3.0381e-04	6.7889e-06	6.6499e-04	6.8643e-04
A_1	10^1	7.7421e-05	1.1041e-04	1.2362e-06	9.2929e-05	1.2400e-04

TABLE 2

Results of typical experiments verifying the a posteriori error bounds for the URV *and* ULV *subspace angles* ϕ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see Section 5). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$ *and* max_iter $= 1$.

A_i	gap	$\frac{\|F\|}{\|R\|+\|G\|}$	$\sin\theta_{URV}$	$\frac{\|F\|\sigma_{\min}(R_k)}{\sigma^2_{\min}(R_k)-\|G\|^2}$	$\sin\theta_{ULV}$	$\frac{\|H\|\|E\|}{\sigma^2_{\min}(L_{11})-\|E\|^2}$
A_1	10^{16}	1.2221e-16	4.3106e-15	1.2221e-14	3.7295e-15	8.5223e-30
A_2	10^4	2.0136e-18	2.5643e-15	2.0136e-16	2.8326e-15	2.1900e-12
A_3	10^3	2.0356e-16	9.8745e-15	2.0356e-14	3.2867e-15	1.5936e-11
A_4	10^2	2.0164e-14	1.1063e-12	2.0168e-12	6.8860e-15	9.1098e-14
A_5	10^1	6.6786e-12	2.2196e-10	6.7528e-10	2.4034e-10	2.1825e-09
A_6	10^1	1.3848e-09	9.8235e-08	1.3890e-07	9.7530e-11	9.3290e-08

TABLE 3

Results of typical experiments verifying the a posteriori error bounds for the URV *and* ULV *subspace angles* θ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see Section 5). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$, max_iter $= 2$, $\delta = 1e\text{-}09$.

A_i	gap	$\sin\phi_{URV}$	$\frac{\|F\|\|G\|}{\sigma^2_{\min}(R_k)-\|G\|^2}$	$\frac{\|H\|}{\|L\|+\|E\|}$	$\sin\phi_{ULV}$	$\frac{\|H\|\sigma_{\min}(L_{11})}{\sigma^2_{\min}(L_{11})-\|E\|^2}$
A_1	10^{16}	1.6706e-15	1.1875e-28	8.8184e-18	1.6964e-15	8.8184e-16
A_2	10^4	2.4484e-15	2.0136e-20	2.1900e-10	8.0259e-09	2.1900e-08
A_3	10^3	1.5391e-15	2.0356e-17	1.5936e-10	4.7849e-10	1.5936e-08
A_4	10^2	1.5281e-15	2.0168e-14	9.1080e-14	8.5146e-12	9.1098e-12
A_5	10^1	7.6490e-12	6.7528e-11	2.1585e-10	7.2083e-09	2.1825e-08
A_6	10^1	9.9386e-10	6.9449e-09	1.8602e-08	2.1073e-08	1.8658e-06

TABLE 4

Results of typical experiments verifying the a posteriori error bounds for the URV *and* ULV *subspace angles* ϕ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see Section 5). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$, max_iter $= 2$, *and* $\delta = 1e\text{-}09$.

A_i	$\sin\theta_{RRQR}$	$\sin\theta_{URV}$	$\sin\theta_{ULV}$	$\sin\phi_{RRQR}$	$\sin\phi_{URV}$	$\sin\phi_{ULV}$
A_1	5.6861e-15	2.7846e-15	3.6910e-15	2.7010e-14	1.6871e-15	2.9126e-15
A_2	5.2541e-10	3.7177e-15	3.3077e-15	1.8372e-04	2.4332e-15	5.0195e-15
A_3	5.2541e-08	2.3045e-15	3.2493e-15	1.8372e-03	1.5029e-15	3.1826e-15
A_4	5.2541e-06	4.1955e-15	2.3565e-15	1.8369e-02	1.5318e-15	6.4979e-15
A_5	5.2598e-04	4.5027e-15	4.5145e-15	1.8070e-01	1.8536e-15	5.8246e-15
A_6	2.4305e-04	1.6924e-15	1.3442e-15	9.4604e-02	8.4914e-16	5.1436e-15

TABLE 5

Results of typical experiments for the error bounds for the RRQR, URV, *and* ULV *subspace angles* θ *and* ϕ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see* §5*). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$, max_iter $= 1$. *The exact singular vectors were supplied in this experiment. No subspace refinement for any factorization.*

A_i	$\sin\theta_{RRQR}$	$\sin\theta_{URV}$	$\sin\theta_{ULV}$	$\sin\phi_{RRQR}$	$\sin\phi_{URV}$	$\sin\phi_{ULV}$
A_1	5.6861e-15	4.3106e-15	3.7295e-15	2.7010e-14	1.6706e-15	1.6964e-15
A_2	5.2541e-10	2.7514e-09	2.8326e-15	1.8372e-04	2.7034e-13	8.0259e-09
A_3	5.2541e-08	2.7514e-07	6.7910e-13	1.8372e-03	2.7215e-10	2.3561e-08
A_4	5.2541e-06	2.7514e-05	6.7681e-09	1.8369e-02	1.9571e-07	6.7894e-07
A_5	5.2598e-04	2.7534e-03	6.6288e-05	1.8070e-01	1.9258e-04	6.6499e-04
A_6	2.4305e-04	2.1912e-03	4.6321e-06	9.4604e-02	7.7421e-05	9.2929e-05

TABLE 6

Results of typical experiments for the error bounds for the RRQR, URV, *and* ULV *subspace angles* θ *and* ϕ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see* §5*). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$, max_iter $= 1$. *The singular vectors were estimated by the CCVL condition estimator. No subspace refinement for any factorization.*

A_i	$\sin\theta_{RRQR}$	$\sin\theta_{URV}$	$\sin\theta_{ULV}$	$\sin\phi_{RRQR}$	$\sin\phi_{URV}$	$\sin\phi_{ULV}$
A_1	5.2048e-15	4.3210e-15	3.7295e-15	2.7010e-14	1.6798e-15	1.6964e-15
A_2	5.8684e-13	2.5579e-15	2.6261e-15	1.8372e-04	2.4484e-15	2.3743e-15
A_3	4.6403e-13	9.9815e-15	3.3961e-15	1.8372e-03	1.5391e-15	1.4432e-15
A_4	1.4888e-10	1.1063e-12	2.9583e-15	1.8369e-02	1.5281e-15	7.1581e-14
A_5	1.4931e-06	2.2196e-10	2.4034e-10	1.8070e-01	7.6490e-12	7.2083e-09
A_6	9.6430e-08	9.8235e-08	9.7530e-11	9.4604e-02	9.9386e-10	2.1073e-08

TABLE 7

Results of typical experiments for the error bounds for the RRQR, URV, *and* ULV *subspace angles* θ *and* ϕ. *The matrices* $\{A_i\}$ *have various singular value spectrums (see* §5*). The numerical rank of the matrices was* $k = 7$ *for tol* $= 0.003$, max_iter $= 2$. *The singular vectors were estimated by the CCVL condition estimator. The* RRQR *approximate nullspace was improved by one step of simultaneous inverse iteration.*