## RANK DECISIONS IN MATRIX QUOTIENT DECOMPOSITIONS\*

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Abstract. This paper describes an orthogonal, fully rank revealing generalized (quotient) URV decomposition for a pair of rectangular matrices. The algorithm for computing the decomposition is fully rank revealing in the sense that it makes rank decisions in an order that is guaranteed to reliably determine if the pair of matrices is close to a pair with a prescribed generalized SVD (GSVD) structure. Numerical experiments are presented that show enhanced numerical reliability when using the decomposition as a preprocessing step for a GSVD.

Key words. generalized SVD, generalized URV, quotient SVD, generalized singular values

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1. Introduction. Let  $A \in \mathbb{R}^{m_a \times n}$  and  $B \in \mathbb{R}^{m_b \times n}$ . Define

(1.1) 
$$C = \begin{bmatrix} A \\ B \end{bmatrix}.$$

If we let

$$r_a = \operatorname{rank}(A), \qquad r_b = \operatorname{rank}(B), \qquad \text{and} \qquad r_c = \operatorname{rank}(C),$$

then the dimension of the intersection of the row subspaces of A and B is given by

$$(1.2) d_i = r_a + r_b - r_c.$$

The ranks and the dimension  $d_i$  satisfy the inequalities

(1.3) 
$$0 \le r_a \le \min(m_a, n), \quad 0 \le r_b \le \min(m_b, n), \quad \text{and} \quad \max(r_a + r_b - n, 0) \le d_i \le \min(r_a, r_b).$$

For given  $m_a$ ,  $m_b$ , and n, it is easily seen that if  $r_a$ ,  $r_b$ , and  $d_i$  satisfy (1.3), then there exist matrices  $A \in \mathbb{R}^{m_a \times n}$  and  $B \in \mathbb{R}^{m_b \times n}$  with ranks  $r_a$  and  $r_b$  and row subspace intersection of dimension  $d_i$ .

The quotient or generalized SVD (GSVD) [18, 13, 11, 2], is a decomposition that reveals these ranks. The decomposition has been defined in several different ways. One appropriate definition is

(1.4)

$$\left[ \begin{array}{c|cccc} U^{\mathrm{T}} & 0 \\ \hline 0 & V^{\mathrm{T}} \end{array} \right] \left[ \begin{array}{c|cccc} A \\ \hline B \end{array} \right] Q \left[ \begin{array}{ccccc} I_{n-r_c} & 0 \\ 0 & R^{-1} \end{array} \right] = \begin{array}{c|cccc} n_a - d_i & d_i & r_b - d_i \\ d_i & 0 & I_{r_a - d_i} & 0 & 0 \\ 0 & 0 & S_A & 0 \\ \hline 0 & 0 & 0 & 0 \\ \hline 0 & 0 & S_B & 0 \\ \hline 0 & 0 & 0 & I_{r_b - d_i} \\ m_b - r_b & 0 & 0 & 0 & 0 \end{array} \right]$$

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where  $R \in \mathbb{R}^{r_c \times r_c}$  is nonsingular and upper triangular; U, V, and Q are square and orthogonal; and  $S_A$  and  $S_B$  are real,  $d_i \times d_i$ , diagonal, and positive definite. If

$$S_A = \operatorname{diag}(\alpha_{r_a - d_i + 1}, \dots, \alpha_{r_a})$$
 and  $S_B = \operatorname{diag}(\beta_{r_a - d_i + 1}, \dots, \beta_{r_a}),$ 

then  $\alpha_j^2 + \beta_j^2 = 1$  for  $j = r_a - d_i + 1, \ldots, r_a$ . For  $j = 1, \ldots, r_a - d_i$  we let  $\alpha_j = 1$  and  $\beta_j = 0$ . For  $j = r_a + 1, \ldots, r_c$  we let  $\alpha_j = 0$  and  $\beta_j = 1$ . Aside from minor details associated with performing the decomposition in place and storing R in the storage allocated for A and B, this is the decomposition computed by the LAPACK routine dggsvd3  $[1]^1$ .

The pairs  $(\alpha_j, \beta_j)$  for  $j = 1, \ldots, r_c$  are generalized singular value pairs and the quantities  $\alpha_j/\beta_j$  are the generalized singular values of A and B. The block  $I_{r_a-d_i}$  corresponds to the pair (1,0), or the generalized singular value  $\infty$ , with multiplicity  $r_a - d_i$ . The block  $I_{r_b-d_i}$  corresponds to the pair (0,1), or the generalized singular value 0, with multiplicity  $r_b - d_i$ . The total number of generalized singular values, when defined in this way to include zero and infinite singular values, is equal to  $r_c$ . The number of finite, nonzero generalized singular values is the dimension of the intersection of the row subspaces of A and B.

The GSVD has a number of applications, including the computation of a common null space for A and B, computation of the Kronecker form of a rectangular pencil  $A - \lambda B$  [6], computation of the intersection of the row subspaces of A and B, linearly constrained least squares problems [19], the general Gauss-Markov linear model [10], and generalized total least squares [17].

If we limit ourselves to orthogonal transformations by requiring that R=I then we can still compute

$$\begin{bmatrix}
U^{\mathrm{T}} & 0 \\
0 & V^{\mathrm{T}}
\end{bmatrix} \begin{bmatrix} A \\
B \end{bmatrix} Q = \begin{pmatrix} m_a - r_a \\
m_b - r_b \\
m_b - r_b \end{pmatrix} \begin{pmatrix} n - r_c & r_a - d_i & r_b - d_i & d_i \\
0 & A_{12} & A_{13} & A_{14} \\
0 & 0 & 0 & A_{24} \\
0 & 0 & 0 & 0 \\
0 & 0 & B_{13} & B_{14} \\
0 & 0 & 0 & 0 & B_{24} \\
0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

where the square blocks  $A_{12}$ ,  $A_{24}$ ,  $B_{13}$ , and  $B_{24}$  are all upper triangular with full rank. This decomposition reveals all three ranks associated with the GSVD and is a complete orthogonal variant of a generalized QR factorization as defined in [12], which also reveals three ranks. We refer to (1.5) as a generalized URV (GURV) decomposition.

Variants of generalized QR or GURV decompositions have a number of applications and have been described many times in many different contexts [4, 7, 8, 12, 14, 15]. In many cases, the decompositions do not make all three rank decisions required to obtain all the block sizes in (1.4) or (1.5), possibly because one of the matrices is assumed to have full rank or because it is not necessary for the application at hand to guarantee nonsingularity of a particular triangular block. Such a decomposition can typically be viewed as either a special case of (1.5) or as an intermediate stage in the computation of (1.5). For an example of the former, we note that if A has full row rank then the block of  $m_a - r_a$  zero rows in the decomposition is absent. As an example of the latter, the LAPACK GSVD preprocessing step dggsvp3 computes a related decomposition, but determines only  $r_a - d_i$  and  $r_b$ . We will give more details below on the connection between the LAPACK decomposition and (1.5).

<sup>&</sup>lt;sup>1</sup>References to LAPACK routines are to the routines from LAPACK 3.6.0.

The rank decisions required to determine the block sizes in a GSVD or GURV decomposition can be difficult. For the ordinary SVD, the singular values determine the distance of a given  $m \times n$  matrix A from a matrix with prescribed rank r, making it relatively easy to determine the numerical rank of A and partition the SVD of A as

$$U^{\mathrm{T}}AV = {r \atop m-r} \left[ \begin{array}{cc} r & n-r \\ \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{array} \right],$$

where  $\Sigma_2$  contains small singular values. The Eckhart–Young theorem guarantees that  $\|\Sigma_2\|_2$  is the 2-norm distance of A from a matrix of rank r. The situation is not so simple with a GSVD. While the number of zero, infinite, and finite non-zero generalized singular values fully determine the partitioning of (1.4), the singular values can be sensitive to errors in A and B and there is no equivalent of the Eckhart–Young theorem that connects generalized singular values to the distance from a pair with a prescribed GSVD structure. An alternative to trying to partition a GSVD by looking at the magnitudes of the generalized singular values is to make rank decisions to partition a GURV decomposition before iteratively computing the generalized singular values. The decomposition can then serve as a preprocessing step to the full GSVD.

The goal of this paper is to illustrate a potential problem with a commonly used sequence of rank decisions for computing a GURV decomposition and to describe an alternate sequence of rank decisions that more reliably determines the partitioning of a GSVD. The main observation is that correctly determining the rank of C is critically important to recovering accurately from a perturbed pair of matrices both the GSVD rank structure and the generalized singular values. The rank of C should be determined in as direct and reliable a way as possible. It should not be determined indirectly through a sequence of other rank decisions. For an example of an indirect determination of  $r_c$ , we describe an algorithm in section 2 that computes  $r_b$  and  $r_a-d_i$  in sequence, so that  $r_c$  is determined by the relation  $r_c = r_b + (r_a - d_i)$ .

This paper is organized as follows. In section 2, we describe a quotient URV decomposition that suffers from sensitivity of rank decisions and define the idea of a fully rank revealing GURV decomposition that can be used to reliably determine the distance of a pair from a pair with a prescribed GSVD block structure. In section 3 we describe a sequencing of rank decisions that gives a fully rank revealing GURV decomposition. In section 4 we give the results of numerical experiments. Finally, in section 5 we summarize the results.

**2. Sensitive rank decisions.** We now describe one common approach to computing a GURV decomposition. The computation involves truncating small elements introduced by applying rank revealing factorizations to various blocks of C. We use E and F to denote small blocks in A and B respectively. The numerical or computed ranks of A, B, and C are  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$ , with  $\tilde{d}_i$  determined from the numerical ranks as in (1.2). We start by computing a rank revealing decomposition of B:

(2.1) 
$$\left[ \begin{array}{c|c} I_{m_a} & 0 \\ \hline 0 & V^{(1)\mathrm{T}} \end{array} \right] \left[ \begin{array}{c|c} A \\ \hline B \end{array} \right] P^{(1)} = \begin{array}{c} m_a \\ \tilde{r}_b \end{array} \left[ \begin{array}{c|c} A_1^{(1)} & A_2^{(1)} \\ \hline B_{11}^{(1)} & B_{12}^{(1)} \\ \hline F_{21}^{(1)} & F_{22}^{(1)} \end{array} \right],$$

where the rank of  $\begin{bmatrix} B_{11}^{(1)} & B_{12}^{(1)} \end{bmatrix}$  is  $\tilde{r}_b$ . The transformations  $V^{(1)}$  and  $P^{(1)}$  are orthogonal, as are all the transformations we apply when computing (1.5). It might be

convenient to use a QR factorization with column pivoting, in which case  $P^{(1)}$  would be a permutation matrix. Next we compute an RQ factorization of  $\begin{bmatrix} B_{11}^{(1)} & B_{12}^{(1)} \end{bmatrix}$  to get

(2.2) 
$$\begin{bmatrix} A_1^{(1)} & A_2^{(1)} \\ \hline B_{11}^{(1)} & B_{12}^{(1)} \\ F_{21}^{(1)} & F_{22}^{(1)} \end{bmatrix} Q^{(2)} = \begin{bmatrix} m_a \\ \tilde{r}_b \\ m_b - \tilde{r}_b \end{bmatrix} \begin{bmatrix} A_1^{(2)} & A_2^{(2)} \\ \hline 0 & B_{12}^{(2)} \\ F_{21}^{(2)} & F_{22}^{(2)} \end{bmatrix},$$

where we have repartitioned so that  $B_{12}^{(2)}$  is square, upper triangular, and nonsingular. A rank revealing decomposition paired with an RQ factorization is a basic operation that we use repeatedly. If we do the same thing to  $A_1^{(2)}$ , we obtain

$$\begin{bmatrix}
U^{(3)^{\mathrm{T}}} & 0 \\
\hline
0 & I_{m_b}
\end{bmatrix}
\begin{bmatrix}
A_1^{(2)} & A_2^{(2)} \\
\hline
0 & B_{12}^{(2)} \\
F_{21}^{(2)} & F_{22}^{(2)}
\end{bmatrix}
\begin{bmatrix}
P^{(3)^{\mathrm{T}}}Q^{(3)} & 0 \\
0 & I_{\tilde{r}_b}
\end{bmatrix} = \begin{bmatrix}
\tilde{r}_a - \tilde{d}_i & \tilde{r}_b \\
\tilde{r}_a - \tilde{d}_i & 0 & A_{12}^{(3)} & A_{13}^{(3)} \\
m_a - \tilde{r}_a + \tilde{d}_i & 0 & B_{13}^{(3)} \\
\tilde{r}_b & 0 & 0 & B_{13}^{(3)} \\
m_b - \tilde{r}_b & F_{21}^{(3)} & F_{22}^{(3)} & F_{23}^{(3)}
\end{bmatrix},$$

where  $A_{12}^{(3)}$  is nonsingular and upper triangular. At this point, the computed multiplicity  $\tilde{r}_a - \tilde{d}_i$  of the generalized singular value  $\infty$  has been determined. The finite generalized singular values are the generalized singular values of  $A_{23}^{(3)}$  and  $B_{13}^{(3)}$ . If QR with column pivoting is used for the rank revealing decompositions, all the E and F blocks are set to zero, and an additional QR factorization is performed on  $A_{23}^{(3)}$  when  $m_a - \tilde{r}_a + \tilde{d}_i > \tilde{r}_b$ , then this is the decomposition computed by the LAPACK GSVD preprocessing routine dggsvp3. The algorithm is described in [3]. A decomposition of this form can then be passed to the routine dtgsja which implements a variant of the Kogbetliantz algorithm to compute a GSVD diagonalization of  $A_{23}^{(3)}$  and  $B_{13}^{(3)}$ . The iteration computes R and the finite generalized singular values. The dimension  $\tilde{d}_i$  can be determined by making a judgment as to how many of the finite generalized singular values are nonzero, although this might be a numerically difficult decision.

If we want a decomposition of the form (1.5), we can continue by computing a rank revealing decomposition and then an RQ factorization of  $A_{23}^{(3)}$ , which results in

where  $A_{24}^{(4)}$  is upper triangular and nonsingular. At this point the  $\tilde{r}_b \times \tilde{r}_b$  block  $\begin{bmatrix} B_{13}^{(4)} & B_{14}^{(4)} \end{bmatrix}$  has lost its triangular structure. An additional QR factorization of this block gives

If we set the E and F blocks to zero, then this is (1.5). The procedure makes three rank decisions, determining  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$ , as well as  $\tilde{d}_i$ , fully determining the sizes of all blocks in the GSVD. The finite, nonzero generalized singular values are the singular values of  $A_{24}B_{24}^{-1}$ .

The SVD is a rank revealing decomposition in the sense that for a given rank  $\tilde{r}$ , it can be used to determine a perturbation E with minimal 2-norm such that  $\operatorname{rank}(A-E) \leq \tilde{r}$ . Various weaker rank revealing decompositions might find perturbations that are only close to minimal. We wish to extend the idea of a rank revealing decomposition to the GURV decomposition. For a given set of prescribed ranks  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$ , let

$$(2.5) \qquad \mathcal{S}(\tilde{r}_a,\tilde{r}_b,\tilde{r}_c) = \left\{ (\tilde{A},\tilde{B}) : \operatorname{rank}(\tilde{A}) \leq \tilde{r}_a, \ \operatorname{rank}(\tilde{B}) \leq \tilde{r}_b, \ \operatorname{rank}(\tilde{C}) \leq \tilde{r}_c \right\},$$

where in this definition we assume  $\tilde{A}$  is  $m_a \times n$ ,  $\tilde{B}$  is  $m_b \times n$ , and  $\tilde{C}$  is defined in terms of  $\tilde{A}$  and  $\tilde{B}$  in a manner similar to (1.1). Given any set of prescribed ranks  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$  satisfying (1.2), there exist perturbations E and F such that  $(A - E, B - F) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$ . We would like to find E and F that give the GSVD structure  $(A - E, B - F) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$  while also approximately minimizing

$$\|(E,F)\|_{a,b} = \left\| \left[ \begin{array}{c} aE \\ bF \end{array} \right] \right\|_{2}.$$

Since A and B might be scaled differently, we have defined a norm on matrix pairs that includes weights a > 0 and b > 0.

We refer to a GURV decomposition as fully rank revealing if given matrices A and B, scaling parameters a > 0 and b > 0, and prescribed ranks  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$  satisfying (1.3), the decomposition can be used to compute E and F such that  $(A - E, B - F) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$  and

$$(2.6) ||(E,F)||_{a,b} \le g(m_a, m_b, n, \tilde{r}_a, \tilde{r}_b, \tilde{r}_c) \cdot \left( \min_{(A-\tilde{E}, B-\tilde{F}) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)} ||(\tilde{E}, \tilde{F})||_{a,b} \right),$$

where  $g(m_a, m_b, n, \tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$  is a factor that depends on the ranks and the problem size and reflects the quality of the rank decisions. We will write  $g = g(m_a, m_b, n, \tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$  with an understanding that this factor can depend on the problem size and the prescribed ranks.

Inequalities, instead of equalities, are used in the rank constraints in (2.5) to account for the fact that a minimal perturbation that exactly induces the structure  $\operatorname{rank}(A-E)=\tilde{r}_a$ ,  $\operatorname{rank}(B-F)=\tilde{r}_b$ , and

$$\operatorname{rank}\left(\left[\frac{A-E}{B-F}\right]\right) = \tilde{r}_c$$

might not exist. For example consider

$$C = \left[ \frac{A}{B} \right] = \left[ \frac{1 \quad 0}{0 \quad 1} \right]$$

with  $\tilde{r}_a = 1$ ,  $\tilde{r}_b = 1$ , and  $\tilde{r}_c = 1$ . A perturbation that minimizes  $||(E, F)||_{1,1}$  subject to  $(A - E, B - F) \in \mathcal{S}(1, 1, 1)$  is easily seen to be

$$\left[\begin{array}{c} E \\ \hline F \end{array}\right] = \left[\begin{array}{cc} 0 & 0 \\ \hline 0 & 1 \end{array}\right].$$

However this perturbation actually gives  $\operatorname{rank}(B-F)=0<1$ . Hence the degree of rank deficiency in B-F is greater than expected. This can happen with any of the three ranks. With  $\mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$  defined as above, the set

$$\left\{ (\tilde{E},\tilde{F}): (A-\tilde{E},B-\tilde{F}) \in \mathcal{S}(\tilde{r}_a,\tilde{r}_b,\tilde{r}_c), \ \|(\tilde{E},\tilde{F})\|_{a,b} \leq \|(A,B)\|_{a,b} \right\}$$

is compact and clearly contains the perturbations

$$(E,F) = \mathop{\arg\min}_{(A-\tilde{E},B-\tilde{F}) \in \mathcal{S}(\tilde{r}_a,\tilde{r}_b,\tilde{r}_c)} \| (\tilde{E},\tilde{F}) \|_{a,b}.$$

Unfortunately the decomposition (2.4), as computed by the above procedure, is not a fully rank revealing GURV decomposition. Ill-conditioning in the numerical row subspace of B can increase the magnitude of small elements that should be revealed by the second and third rank decisions. We illustrate the issue with a small example. Consider the matrix pair

(2.7) 
$$\left[ \frac{A}{B} \right] = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 0 \\ \epsilon & 0 & 0 & \delta \end{bmatrix},$$

where  $0 < \epsilon \ll \delta \ll 1$ . As given, this pair has  $r_a = 2$ ,  $r_b = 2$ , and  $r_c = 4$ . We assume that  $\delta$  is significantly smaller than 1 but that it is large enough that B can be considered to have numerical rank 2. We also assume that  $\epsilon$  is small enough that it is less than, but not much less than, the tolerance used in rank decisions. Thus, the given matrix pair is close to a pair  $(\tilde{A}, \tilde{B})$  for which  $\tilde{r}_a = 2$ ,  $\tilde{r}_b = 2$ , and  $\tilde{r}_c = 3$ . Simply setting  $\epsilon = 0$  achieves these ranks and, in fact, gives a pair that is already in the desired form (1.5). The modified matrix pair has generalized singular value pairs

(1,0),  $(1/\sqrt{1+\delta^2}, \delta/\sqrt{1+\delta^2})$ , and (0,1). The original matrix pair has generalized singular value pairs (1,0), (1,0), (0,1), and (0,1), including multiplicities.

Since we know that A and B are close to a pair for which  $\tilde{r}_a = 2$ ,  $\tilde{r}_b = 2$ , and  $\tilde{r}_c = 3$ , we might want to use the previously outlined algorithm to compute a decomposition (1.5) that has this rank structure. The first step would be a rank revealing factorization of B. However, B already has the desired form (2.1), with two numerically linearly independent rows. The next step would be an RQ factorization of B, which gives

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 0 \\ \epsilon & 0 & 0 & \delta \end{bmatrix} \begin{bmatrix} \frac{\delta}{\sqrt{\delta^2 + \epsilon^2}} & 0 & 0 & \frac{\epsilon}{\sqrt{\delta^2 + \epsilon^2}} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{-\epsilon}{\sqrt{\delta^2 + \epsilon^2}} & 0 & 0 & \frac{\delta}{\sqrt{\delta^2 + \epsilon^2}} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{-\epsilon}{\sqrt{\delta^2 + \epsilon^2}} & 0 & 0 & \frac{\delta}{\sqrt{\delta^2 + \epsilon^2}} \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{\delta^2 + \epsilon^2} \end{bmatrix}.$$

This is (2.2). The next step, leading to (2.3), would be the rank revealing decomposition and RQ factorization of

$$A_1^{(2)} = \left[ \begin{array}{cc} 0 & 1\\ \frac{-\epsilon}{\sqrt{\delta^2 + \epsilon^2}} & 0 \end{array} \right].$$

At this point we are faced with two unpleasant options. The desired rank of  $A_1^{(2)}$  is  $\tilde{r}_a - \tilde{d}_i = 1$ . To force  $A_1^{(2)}$  to have this rank, we need to use a perturbation with 2-norm at least  $\epsilon/\sqrt{\delta^2 + \epsilon^2}$ , which can be much larger than  $\epsilon$ . This is objectionable on grounds of backward stability: we end up with a decomposition of a pair that is not close to the original pair.

If we revise our expectations for the ranks, and instead decide that  $\tilde{r}_a - \tilde{d}_i = 2$ , then we end up with  $\tilde{d}_i = 0$  and no nonzero, finite generalized singular values. With this choice, in addition to failing to find a row subspace intersection, we also miss the presence of a common numerical right null space for A and B. While we have completely missed finding nearby matrices with the desired GSVD structure, we do get a fully backward stable decomposition.

Note that if we choose  $\tilde{r}_a - d_i = 2$ , we end up concluding that  $\tilde{r}_c = 4$ , when in fact C clearly has numerical rank equal to 3. Perturbation theory for generalized singular values from [9] is only applicable for perturbations that preserve the rank of C. For this reason, an incorrect estimate of  $r_c$  is potentially catastrophic. To elaborate on this point, let  $\tilde{C}$  be a perturbed version of C for which  $\mathrm{rank}(\tilde{C}) = \mathrm{rank}(C) = r_c$ . If we let

$$\boldsymbol{\alpha} = \begin{bmatrix} \alpha_1 & \cdots & \alpha_{r_c} \end{bmatrix}^{\mathrm{T}}$$
 and  $\boldsymbol{\beta} = \begin{bmatrix} \beta_1 & \cdots & \beta_{r_c} \end{bmatrix}^{\mathrm{T}}$ 

be the vectors of singular value pairs of C and define the vectors of perturbed singular value pairs  $\tilde{\alpha}$  and  $\tilde{\beta}$  similarly, then in [9] it is shown that

(2.8) 
$$\|\tilde{\alpha} - \alpha\|_{2}^{2} + \|\tilde{\beta} - \beta\|_{2}^{2} \leq 2\|C - \tilde{C}\|_{F}^{2} \min(\|C^{\dagger}\|_{2}, \|\tilde{C}^{\dagger}\|_{2}),$$

where  $C^{\dagger}$  denotes the pseudoinverse of C. This bound is adapted from the results of [16]. The assumption that  $\operatorname{rank}(\tilde{C}) = \operatorname{rank}(C)$  is essential. Given a matrix C that might have been generated by introducing errors into a matrix  $\hat{C}$  with some unknown rank  $\hat{r}_c$ , a backward stable algorithm might compute the GSVD of a matrix  $\tilde{C}$  that is close to C, and hence close to  $\hat{C}$ . But if the algorithm is not able to ensure that  $\operatorname{rank}(\tilde{C}) = \hat{r}_c$ , then the perturbation theory says nothing about accuracy

of the computed generalized singular values. In fact, as we will see in section 4, an incorrect estimate of the rank of C can produce computed singular values that have little resemblance to those of the original matrix  $\hat{C}$ .

3. The fully rank revealing decomposition. In this section we describe a procedure for computing a fully rank revealing GURV decomposition. The idea is very simple and is based on computing  $r_c$  prior to computing  $r_a$  and  $r_b$ . Since  $r_c$  is computed directly by a rank revealing decomposition of C, potentially even by the SVD of C, the decomposition achieves the most reliable possible estimate of  $r_c$  and thereby minimizes concerns about the effect of an incorrect estimate of  $r_c$  on the accuracy of computed generalized singular values.

Let A and B be given matrices and let  $\tilde{r}_a$ ,  $\tilde{r}_b$ , and  $\tilde{r}_c$  satisfy (1.3). We intend to make a rank decision directly on the matrix C. This might be complicated by different scalings in A and B. To compensate for this, we redefine

$$C = \left[ \frac{aA}{bB} \right]$$

to include the scaling parameters a > 0 and b > 0. The scaling parameters will be the same as the weights used in  $||(E, F)||_{a,b}$  in the previous section.

We assume that  $\tilde{E}$  and  $\tilde{F}$  are arbitrary perturbations for which

$$(3.1) (a\tilde{A}, b\tilde{B}) = (aA - \tilde{E}, bB - \tilde{F}) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c).$$

We will describe an algorithm for a GURV decomposition that can compute perturbations E and F such that

$$(3.2) (aA - E, bB - F) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c) \text{and} \|(E, F)\|_{1,1} \le g\|(\tilde{E}, \tilde{F})\|_{1,1},$$

where g reflects the quality of individual rank decisions for aA, bB, and C. If the SVD is used for these decisions, then we will show that  $g \leq 3$ . Thus, up to some factor dependent only on sizes and ranks, the pair (E,F) is no larger than any other perturbation to (aA,bB) that gives the desired GSVD structure. If we let E=aE', F=bF',  $\tilde{E}=a\tilde{E}'$ , and  $\tilde{F}=b\tilde{F}'$ , then (3.2) is equivalent to

$$(A - E', B - F') \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$$
 and  $\|(E', F')\|_{a,b} \le g\|(\tilde{E}', \tilde{F}')\|_{a,b}$ ,

where  $\tilde{E}'$  and  $\tilde{F}'$  are arbitrary perturbations for which  $(A - \tilde{E}', B - \tilde{F}') \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c)$ . It follows that

$$\|(E',F')\|_{a,b} \leq g \cdot \left( \min_{\substack{(A-\tilde{E}',B-\tilde{F}') \in \mathcal{S}(\tilde{r}_a,\tilde{r}_b,\tilde{r}_c)}} \|(\tilde{E}',\tilde{F}')\|_{a,b} \right).$$

Thus, by scaling C, we can apply any desired weight to the perturbations E and F. An algorithm that can produce perturbations satisfying (3.2) can be used to compute a fully rank revealing GURV decomposition with weights incorporated as in (2.6). A useful choice of scaling might be  $a = 1/\|A\|$  and  $b = 1/\|B\|$  for a suitable matrix norm  $\|\cdot\|$ . We now focus solely on describing an algorithm for constructing E and F satisfying (3.2).

We assume that we have available a basic rank revealing decomposition. Given an  $m \times n$  matrix X and a prescribed rank  $0 \le \tilde{r} \le \min(m, n)$ , we assume that we can compute an orthogonal matrix W such that

$$XW = X \left[ \begin{array}{cc} W_1 & W_2 \end{array} \right] = \left[ \begin{array}{cc} H_1 & X_2 \end{array} \right],$$

where  $H_1$  is  $m \times (n - \tilde{r})$  and satisfies

$$||H_1||_2 \le f(m, n, \tilde{r})\sigma_{\tilde{r}+1}(X)$$

for some  $f(m, n, \tilde{r}) \geq 1$  that reflects the quality of the rank revealing decomposition. If the SVD is used, then  $f(m, n, \tilde{r}) = 1$ . We assume that various transposed or permuted variants of the rank revealing factorization are available, so that we can, for example, introduce a block of rows with a small norm at the bottom part of X instead of a block of columns  $H_1$  with a small norm in the left part of X as above.

A general description of the procedure is as follows. Using the basic rank revealing decomposition we begin by computing

$$CQ = \begin{bmatrix} aA \\ \overline{bB} \end{bmatrix} \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} = \begin{pmatrix} m_a \\ m_b \end{pmatrix} \begin{bmatrix} E_1 & aA_2 \\ \overline{F_1} & bB_2 \end{bmatrix},$$

where

$$\left\| \left[ \frac{E_1}{F_1} \right] \right\|_2 \le f(m_a + m_b, n, \tilde{r}_c) \sigma_{\tilde{r}_c + 1}(C),$$

and Q is orthogonal. By setting the  $E_1$  and  $F_1$  blocks to zero, we get a perturbation that introduces the desired degree of rank deficiency in C. We again use a rank revealing factorization to construct  $E_2$  and  $F_2$  so that

$$rank(A_2 - E_2) \le \tilde{r}_a$$
 and  $rank(B_2 - F_2) \le \tilde{r}_b$ 

with

$$||E_2||_2 \le f(m_a, \tilde{r}_c, \tilde{r}_a)\sigma_{\tilde{r}_a+1}(aA_2)$$
 and  $||F_2||_2 \le f(m_b, \tilde{r}_c, \tilde{r}_b)\sigma_{\tilde{r}_b+1}(bB_2)$ .

Let

$$E = \begin{bmatrix} E_1 & E_2 \end{bmatrix} Q^{\mathrm{T}}$$
 and  $F = \begin{bmatrix} F_1 & F_2 \end{bmatrix} Q^{\mathrm{T}}$ .

Then

$$(aA - E, bB - F) \in \mathcal{S}(\tilde{r}_a, \tilde{r}_b, \tilde{r}_c).$$

The perturbation  $\|(E,F)\|_{1,1}$  is not much larger than the smallest perturbation that gives the desired rank structure. To see this, observe that if some other  $\tilde{E}$  and  $\tilde{F}$  give the desired degree of rank deficiency, then  $\|\tilde{E}\|_2 \geq \sigma_{\tilde{r}_a+1}(aA)$ ,  $\|\tilde{F}\|_2 \geq \sigma_{\tilde{r}_b+1}(bB)$ , and  $\|(\tilde{E},\tilde{F})\|_{1,1} \geq \sigma_{\tilde{r}_c+1}(C)$ . Thus

$$\|(\tilde{E}, \tilde{F})\|_{1,1} \ge \max(\sigma_{\tilde{r}_c+1}(C), \sigma_{\tilde{r}_a+1}(aA), \sigma_{\tilde{r}_b+1}(bB)).$$

It follows that

$$||(E,F)||_{1,1} \leq f(m_a + m_b, n, \tilde{r}_c)\sigma_{\tilde{r}_c+1}(C) + f(m_a, \tilde{r}_c, \tilde{r}_a)\sigma_{\tilde{r}_a+1}(aA_2) + f(m_b, \tilde{r}_c, \tilde{r}_b)\sigma_{\tilde{r}_b+1}(bB_2) \leq \max(f(m_a + m_b, n, \tilde{r}_c), f(m_a, \tilde{r}_c, \tilde{r}_a), f(m_b, \tilde{r}_c, \tilde{r}_b)) \cdot [\sigma_{\tilde{r}_c+1}(C) + \sigma_{\tilde{r}_a+1}(aA) + \sigma_{\tilde{r}_b+1}(bB)] \leq 3\max(f(m_a + m_b, n, \tilde{r}_c), f(m_a, \tilde{r}_c, \tilde{r}_a), f(m_b, \tilde{r}_c, \tilde{r}_b)) ||(\tilde{E}, \tilde{F})||_{1,1}.$$

$$(3.3)$$

The use of aA and bB instead of  $aA_2$  and  $bB_2$  in the second inequality can be justified by standard interlacing results for singular values; see Corollary 8.6.3 of [5]. The inequality (3.3) is (3.2) with

$$g = 3 \max \left( f(m_a + m_b, n, \tilde{r}_c), f(m_a, \tilde{r}_c, \tilde{r}_a), f(m_b, \tilde{r}_c, \tilde{r}_b) \right).$$

For rank decisions using the SVD we have  $\|(E,F)\|_{1,1} \leq 3\|(\tilde{E},\tilde{F})\|_{1,1}$  so that

$$\|(E',F')\|_{a,b} \leq 3 \cdot \left( \min_{(A-\tilde{E}',B-\tilde{F}')\in\mathcal{S}(\tilde{r}_a,\tilde{r}_b,\tilde{r}_c)} \|(\tilde{E}',\tilde{F}')\|_{a,b} \right).$$

An implementation of this procedure, used to compute a GURV decomposition, might proceed as follows. We start with the rank revealing factorization

$$\begin{bmatrix}
aA \\
bB
\end{bmatrix} Q^{(1)} = \begin{bmatrix}
m_a \\
m_b
\end{bmatrix} \begin{bmatrix}
F_1^{(1)} & A_2^{(1)} \\
F_1^{(1)} & B_2^{(1)}
\end{bmatrix}.$$

An RQ decomposition with row pivoting might be used, in which case the decomposition could be done in place and the permutation of rows could be easily inverted after the decomposition has been computed. Applying a rank revealing decomposition to  $A_2^{(1)}$  and then both a rank revealing decomposition and RQ factorization to  $B_2^{(1)}$  give

$$\begin{bmatrix} U^{(2)\mathrm{T}} & 0 \\ \hline 0 & V^{(2)\mathrm{T}} \end{bmatrix} \begin{bmatrix} E_1^{(1)} & A_2^{(1)} \\ \hline F_1^{(1)} & B_2^{(1)} \end{bmatrix} \begin{bmatrix} I_{n-\tilde{r}_c} & 0 \\ 0 & P_A^{(2)} P_B^{(2)} Q_B^{(2)} \end{bmatrix} =$$

$$\begin{bmatrix} \tilde{r}_a \\ m_a - \tilde{r}_a \\ m_b - \tilde{r}_b \end{bmatrix} \begin{bmatrix} E_{11}^{(2)} & A_{12}^{(2)} & A_{13}^{(2)} \\ E_{21}^{(2)} & E_{22}^{(2)} & E_{23}^{(2)} \\ \hline F_{11}^{(2)} & 0 & B_{13}^{(2)} \\ F_{21}^{(2)} & F_{22}^{(2)} & F_{23}^{(2)} \end{bmatrix},$$

where  $B_{13}^{(2)}$  is upper triangular and nonsingular. At this point,  $\tilde{r}_c$ ,  $\tilde{r}_a$ , and  $\tilde{r}_b$  have been explicitly computed and the intersection dimension  $\tilde{d}_i$  can be computed from (1.2). The perturbation that gives the desired rank structure is obtained merely by subtracting off the E and F blocks. In proceeding on to compute a decomposition of the form (1.5), we make no further rank decisions and apply only orthogonal transformations that leave the 2-norm of the perturbation unchanged.

A QR factorization of  $A_{12}^{(2)}$  gives

(3.4)

$$\begin{bmatrix} U^{(3)\mathrm{T}} & 0 & 0 \\ 0 & I_{m_a - \tilde{r}_a} & 0 \\ \hline 0 & 0 & I_{m_b} \end{bmatrix} \begin{bmatrix} E_{11}^{(2)} & A_{12}^{(2)} & A_{13}^{(2)} \\ E_{21}^{(2)} & E_{22}^{(2)} & E_{23}^{(2)} \\ \hline F_{11}^{(2)} & 0 & B_{13}^{(2)} \\ F_{21}^{(2)} & F_{22}^{(2)} & F_{23}^{(2)} \end{bmatrix} = \begin{bmatrix} \tilde{r}_a - \tilde{d}_i \\ \tilde{d}_i \\ \tilde{d}_i \\ F_{a} \end{bmatrix} \begin{bmatrix} E_{11}^{(3)} & A_{12}^{(3)} & A_{13}^{(3)} \\ E_{21}^{(3)} & 0 & A_{23}^{(3)} \\ \hline F_{31}^{(3)} & E_{32}^{(3)} & E_{33}^{(3)} \\ \hline F_{11}^{(3)} & 0 & B_{13}^{(3)} \\ \hline F_{21}^{(3)} & F_{22}^{(3)} & F_{23}^{(3)} \end{bmatrix},$$

where  $A_{12}^{(3)}$  is nonsingular and upper triangular and  $A_{23}^{(3)}$  has linearly independent rows. An RQ factorization of  $A_{23}^{(3)}$  gives

where  $A_{24}^{(4)}$  is upper triangular and nonsingular. Finally, we can use a QR factorization to restore the upper triangular structure of the  $\tilde{r}_b \times \tilde{r}_b$  block  $\begin{bmatrix} B_{13}^{(4)} & B_{14}^{(4)} \end{bmatrix}$ , which

where  $B_{24}^{(5)}$  is upper triangular and full rank. After removing the E and F blocks, this decomposition is the same as (1.5). It is also a special case of (2.3) with  $A_{23}^{(3)}$  and  $B_{13}^{(3)}$  in (2.3) corresponding to

$$\begin{bmatrix} 0 & A_{24}^{(5)} \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} B_{13}^{(5)} & B_{14}^{(5)} \\ 0 & B_{24}^{(5)} \end{bmatrix}$$

in (3.5). It can then be passed directly to the LAPACK routine dtgsja.

4. Numerical experiments. In this section we present the results of numerical experiments in which the fully rank revealing GURV decomposition is compared with

(2.3), as computed by the LAPACK routine dggsvp3. Both routines are used as a preprocessing step for a generalized SVD as computed by the LAPACK routine dtgsja. The decomposition (3.5) has been implemented in Fortran 90 using calls to LAPACK  $3.6.0.^2$ 

For rank decisions, the code uses QR with column pivoting, truncating the decomposition at the first diagonal element to fall below a supplied tolerance. Three tolerances  $\tilde{\delta}_c$ ,  $\tilde{\delta}_a$ , and  $\tilde{\delta}_b$  are used for the rank decisions on C, aA, and bB. The scaling parameters are given by  $a = 1/\max_{jk} |a_{jk}|$  and  $b = 1/\max_{jk} |b_{jk}|$ . The tolerances  $\hat{\delta}_a$  and  $\hat{\delta}_b$  for dggsvp3 are independent of  $\tilde{\delta}_a$  and  $\tilde{\delta}_b$  and do not involve any scaling.

One point of comparison between the two algorithms is the accuracy of the computed row subspace intersection. An orthonormal basis for this subspace is not directly provided by the decomposition (1.4). However, if we let

$$R = \begin{pmatrix} r_a - d_i & d_i & r_b - d_i \\ R_{11} & R_{12} & R_{13} \\ d_i & 0 & R_{22} & R_{23} \\ 0 & 0 & R_{33} \end{pmatrix} \quad \text{and} \quad Q = \begin{bmatrix} n - r_c & r_a - d_i & d_i & r_b - d_i \\ Q_1 & Q_2 & Q_3 & Q_4 \end{bmatrix}$$

then it is easily seen that the rows of

$$\left[\begin{array}{cc}R_{22}&R_{23}\end{array}\right]\left[\begin{array}{c}Q_3^{\mathrm{T}}\\Q_4^{\mathrm{T}}\end{array}\right]$$

form a basis for the row subspace intersection. An RQ factorization of  $\begin{bmatrix} R_{22} & R_{23} \end{bmatrix}$  can be used to convert this to an orthonormal basis. This is what was done when computing row subspace intersections in the numerical experiments.

In the numerical experiments, we consider small and large problems, each with a fixed GSVD structure. The small problem has  $m_a = 50$ ,  $m_b = 40$ , n = 100,  $r_a = 15$ ,  $r_b = 18$ , and  $r_c = 30$ , so that  $d_i = 3$ . The large problem has  $m_a = 1000$ ,  $m_b = 1000$ , n = 2010,  $r_a = 400$ ,  $r_b = 400$ , and  $r_c = 750$ , so that  $d_i = 50$ . For both the large and small problems we let

$$\begin{bmatrix} D_A \\ \overline{D}_B \end{bmatrix} = \begin{pmatrix} r_a - d_i \\ d_i \\ d_i \\ m_b - r_a \\ m_b - r_b \end{pmatrix} \begin{pmatrix} 0 & I_{r_a - d_i} & 0 & 0 \\ 0 & 0 & S_A & 0 \\ 0 & 0 & 0 & 0 \\ \overline{0} & 0 & S_B & 0 \\ 0 & 0 & 0 & I_{r_b - d_i} \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where

$$S_A = \left[ \begin{array}{ccc} \sqrt{1-2^{-28}} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2}I_{d_i-2} & 0 \\ 0 & 0 & 2^{-14} \end{array} \right], \qquad S_B = \left[ \begin{array}{ccc} 2^{-14} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2}I_{d_i-2} & 0 \\ 0 & 0 & \sqrt{1-2^{-28}} \end{array} \right].$$

Then A and B were constructed from the formula

$$\begin{bmatrix} A \\ \hline B \end{bmatrix} = \begin{bmatrix} U & 0 \\ \hline 0 & V \end{bmatrix} \begin{bmatrix} D_A \\ \hline D_B \end{bmatrix} \begin{bmatrix} I_{n-r_c} & 0 \\ 0 & R \end{bmatrix} Q^{\mathrm{T}} + \begin{bmatrix} E \\ \hline F \end{bmatrix},$$

<sup>&</sup>lt;sup>2</sup>The code is available at http://saaz.mathstat.gsu.edu/rrqsvd/rrqsvd.html

where U, V, and Q were random uniformly distributed orthogonal matrices. These matrices were generated as the Q factor in the QR factorization of matrices of random numbers generated from a standard normal distribution. The triangular factor R was constructed in one of two ways: it was either the R factor in a QR factorization of an  $r_c \times r_c$  matrix of standard normal random numbers, or it was a triangular matrix containing standard normal random numbers. The former gives a well-conditioned R and the latter gives an ill-conditioned R. The perturbations E and F were matrices of normal random numbers of mean zero and standard deviation  $\sigma = 10^{-15}$ .

The matrices A and B have  $d_i$  nonzero, finite generalized singular values corresponding to the pairs

$$(\alpha_{r_a-d_i+1}, \beta_{r_a-d_i+1}) = (\sqrt{1-2^{-28}}, 2^{-14}),$$
  
$$(\alpha_{r_a-d_i+k}, \beta_{r_a-d_i+k}) = (\sqrt{2}/2, \sqrt{2}/2), \qquad k = 2, \dots, d_i - 1,$$

and

$$(\alpha_{r_a}, \beta_{r_a}) = (2^{-14}, \sqrt{1 - 2^{-28}}).$$

The experiments report results for both the code that computes the rank revealing decomposition (3.5) and the LAPACK routine dggsvp3 that computes a variant of (2.3). The two routines were used as preprocessing steps for the GSVD routine dgtsja and various computed quantities were compared. Each small experiment was run 20 times and each large experiment was run 10 times with different randomly generated U, V, Q, R, E, and F. Tolerances for rank decisions were chosen to obtain consistent, but not always correct, ranks over the course of the runs. Where appropriate, we give results in the form of intervals showing the largest and smallest values of each specific value observed in each experiment over the runs. When we need to distinguish between quantities associated with (3.5) and (2.3), the former are marked with a tilde and the latter with a hat. Descriptions in the tables of quantities associated with the LAPACK algorithm are marked with an "(L)."

The comparison of the algorithms is not entirely straightforward. The preprocessing decomposition (2.3) involves only two rank decisions, and it explicitly determines only  $\hat{r}_b$  and  $\hat{r}_a - \hat{d}_i$ . To provide a consistent basis of comparison, for the LAPACK algorithm we have simply assumed the known value of  $\hat{d}_i = 3$  for the small problem and  $\hat{d}_i = 50$  for the large problem and then taken the  $\hat{d}_i$  largest finite generalized singular values as the singular values associated with our estimates of the finite, nonzero singular values of A and B. It is possible that  $\hat{d}_i$  might actually be estimated by applying a threshold to the computed generalized singular values. However, it is not entirely clear how to set the threshold, especially if the generalized singular values are ill-conditioned. Another option would be to look at the numerical rank of  $A_{23}^{(3)}$ , which should be equal to  $d_i$ . Singular values  $\sigma_{d_i}(A_{23}^{(3)})$  and  $\sigma_{d_i+1}(A_{23}^{(3)})$  are reported in the tables and, at least for the well-conditioned problems, show a gap that would support setting  $\hat{d}_i$  to the nominal values  $d_i = 3$  and  $d_i = 50$ . In the case of ill-conditioned R, the gap between these singular values is less satisfactory. These concerns are not an issue for (3.5), which estimates all three ranks.

Table 1 shows the result of computations with two sets of tolerances applied to the small problem with well-conditioned R. Note that by construction A has numerical rank 15, B has numerical rank 18, and C has numerical rank 30. None of these ranks are difficult to estimate. In each case, there is a clear gap between numerically nonzero and numerically zero singular values. With the fully rank revealing algorithm, it was very easy to set  $\tilde{\delta}_a$ ,  $\tilde{\delta}_b$ , and  $\tilde{\delta}_c$  to reliably estimate these ranks. The third column of the

Table 1 Well-conditioned R,  $m_a = 50$ ,  $m_b = 40$ , n = 100,  $\sigma = 10^{-15}$ .

| Quantity  | Description                | Same tol.      | Different tol. |
|---|----------------------------|----------------|----------------|
| $	ilde{\delta}_{a,b,c}$   | Rank tol.                  | 2e-14          | 2e-14          |
| $\hat{\delta}_{a,b}$  | Rank tol. (L)              | 2e-14          | 5e-10          |
| $\kappa_2(R)$   | Condition of $R$           | [3e1, 1e3]     | [3e1, 1e3]     |
| $\ C^{\dagger}\ _2$   | Pseudoinverse norm         | [3, 9e1]       | [3, 9e1]       |
| $(\tilde{r}_c, \tilde{r}_a, \tilde{r}_b)$                                   | Computed ranks             | (30, 15, 18)   | (30, 15, 18)   |
| $(\hat{r}_c, \hat{r}_a, \hat{r}_b)$   | Computed ranks (L)         | (31, 16, 18)   | (30, 15, 18)   |
| $\ \tilde{E}\ _2$   | Error on $A$               | [3e-15, 7e-15] | [3e-15, 7e-15] |
| $\ \tilde{F}\ _2$   | Error on $B$               | [5e-15, 8e-15] | [4e-15, 8e-15] |
| $\ \hat{E}\ _2$   | Error on $A$ (L)           | [3e-15, 5e-15] | [1e-11, 2e-11] |
| $\ \hat{F}\ _2$   | Error on $B$ (L)           | [4e-15, 7e-15] | [4e-15, 7e-15] |
| $\ \tilde{P} - P\ _2$   | Intersection err.          | [1e-11, 3e-11] | [1e-11, 3e-11] |
| $\ \hat{P} - P\ _2$   | Intersection err. (L)      | [3e-11, 6e-11] | [3e-11, 5e-11] |
| $\sigma_{d_i}(A_{23}^{(3)})$  | SV Gap $d_i$ (L) (not      | [2e-4, 4e-4]   | [2e-4, 4e-4]   |
| $\sigma_{d_i+1}(A_{23}^{(3)})$  | used to compute $d_i$ )    | [2e-14, 5e-14] | [3e-14, 6e-14] |
| $d_{\hat{r}_a - \hat{d}_i}(A_1^{(2)})$                                      | Rank decision, $r_a - d_i$ | [3e-11, 9e-11] | [8e-1, 1]      |
| $d_{\hat{r}_a - \hat{d}_i + 1}(A_1^{(2)})$                                  | (L)                        | [1e-14, 2e-14] | [3e-11, 9e-11] |
| $ \tilde{\beta}_{\tilde{r}_a - \tilde{d}_i + 1} - \beta_{r_a - d_i + 1} $   | Gen. SV error              | [1e-17, 1e-15] | [1e-17, 1e-15] |
| $ \tilde{\alpha}_{\tilde{r}_a - \tilde{d}_i + 2} - \alpha_{r_a - d_i + 2} $ | Gen. SV error              | [0, 7e-16]     | [0, 7e-16]     |
| $ \tilde{\alpha}_{\tilde{r}_a - \tilde{d}_i + 3} - \alpha_{r_a - d_i + 3} $ | Gen. SV error              | [3e-17, 8e-16] | [3e-17, 8e-16] |
| $ \hat{\beta}_{\hat{r}_a - \hat{d}_i + 1} - \beta_{r_a - d_i + 1} $         | Gen. SV error (L)          | [2e-1, 5e-1]   | [7e-17, 1e-15] |
| $ \hat{\alpha}_{\hat{r}_a - \hat{d}_i + 2} - \alpha_{r_a - d_i + 2} $       | Gen. SV error (L)          | [3e-5, 8e-2]   | [1e-16, 1e-15] |
| $ \hat{\alpha}_{\hat{r}_a - \hat{d}_i + 3} - \alpha_{r_a - d_i + 3} $       | Gen. SV error (L)          | [6e-10, 4e-6]  | [3e-18, 1e-15] |

table gives results for the use of the same tolerance  $\delta = 5\mathrm{e}{-14}$  for all rank decisions in both algorithms. The fourth column gives results in which the tolerance for rank decisions was varied for the LAPACK algorithm to attempt to force determination of the correct ranks.

When the same tolerance of 5e-14 was used in both algorithms, the decomposition (2.3) consistently overestimated  $r_a-d_i$ , leading to an overestimate of both  $r_a$  and  $r_c$ . The estimate of  $r_a-d_i$  was made by looking at the diagonal elements of a QR factorization with column pivoting of  $A_1^{(2)}$ . The last untruncated diagonal and first truncated diagonal are reported in the table as  $d_{\hat{r}_a-\hat{d}_i}(A_1^{(2)})$  and  $d_{\hat{r}_a-\hat{d}_i+1}(A_1^{(2)})$ . Note that there is a large gap between these values. While the true value is  $r_a-d_i=15-3=12$ , in the first experiment, the algorithm is forced to make the decision  $\hat{r}_a-\hat{d}_i=13$ . With  $\hat{d}_i=3$  and the rank of B correctly estimated as  $\hat{r}_b=18$ , this leads to the conclusion that  $\hat{r}_a=16$  and  $\hat{r}_c=31$ .

The relative backward errors associated with the full GSVD computation for the rank revealing algorithm are given by

$$\tilde{E} = \frac{\tilde{A} - A}{\|A\|_2}, \qquad \tilde{F} = \frac{\tilde{B} - B}{\|B\|_2}$$

with  $\hat{E}$  and  $\hat{F}$  defined similarly. For the case in which the tolerance is set to  $5\mathrm{e}{-14}$ , the backwards errors are consistent with backward stability.

The effect of the overestimate of  $r_c$  is clear for the generalized singular values computed using (2.3), which are much less accurate than those computed by the fully rank revealing preprocessing algorithm. The latter have errors that are consistent with the backward errors and the perturbation bound (2.8). For the former, the perturbation bound (2.8) cannot be applied, since  $r_c$  has not been correctly estimated. Note that singular value errors are only reported for the smaller of  $\alpha$  or  $\beta$ . Normalization enforces a similar error in the other component of each pair.

Finally, we formed the orthogonal projector P for the row subspace intersection computed by each method and have given the errors in the computed subspaces relative to a subspace determined from the original randomly generated Q and R. Perhaps surprisingly, the rank revealing algorithm is better in this respect only by a relatively small margin. Recall however, that as (2.7) shows, it is easy to get the dimension for this subspace completely wrong. This experiment does not illustrate the fact, but it is easy to construct examples for which the LAPACK approach computes a substantially worse row subspace intersection relative to the fully rank revealing decomposition.

The fourth column of Table 1 is the same as the first, except that the threshold for the rank decisions in (2.3) is increased to force dggsvp3 to correctly estimate  $r_a - d_i$ . The result is an increase in backward error, but a dramatic improvement in the quality of the computed generalized singular values. If  $r_c$  is known in advance, it can sometimes be better to accept a larger backward error if it is necessary to force a correct estimate of  $\hat{r}_c$ .

Table 2 is similar to Table 1, but with ill-conditioned R, leading to larger  $C^{\dagger}$  and, by (2.8), greater sensitivity in the generalized singular values. In the case of different tolerances, we had to choose different values of  $\hat{\delta}_a$  and  $\hat{\delta}_b$  to ensure consistently correct rank estimates for the LAPACK algorithm. In these experiments, the ill-conditioned singular values display an expected loss of accuracy. Increasing the tolerance for rank decisions in (2.3) was not as consistently successful in improving the accuracy of the computed singular values as in the second experiment.

One potential objection to the results is that the computation using dggsvp3 gives  $\hat{r}_c = 31$  and therefore returns 31 singular value pairs, while the original problem had  $r_c = 30$  and only 30 singular value pairs. In Table 1, we have chosen to match the 3 singular values corresponding to the computed row subspace intersection with the 3 singular values associated with the exact row subspace intersection. That is, we compare  $\hat{\alpha}_{\hat{r}_a - \hat{d}_i + j} = \hat{\alpha}_{r_a - d_i + j + 1}$  to  $\alpha_{r_a - d_i + j}$  for j = 1, 2, 3. One could also try comparing  $\hat{\alpha}_{r_a - d_i + j}$  to  $\alpha_{r_a - d_i + j}$ . However doing so makes very little difference to the overall conclusion that an incorrect value of  $\hat{r}_c$  dramatically undermines accuracy of computed singular value pairs. In the first three runs for Table 1, column 3, the LAPACK generalized singular values that were closest to  $\sqrt{2}/2$  were approximately 0.7061, 0.6321, and 0.7060. There is no way to match the computed and exact singular value pairs that gives more than about two correct digits.

Finally, Table 3 is analogous to Table 1, but for the larger problem. Given the larger number of generalized singular values, we have given only the maximum errors observed in any  $\alpha_k$  or  $\beta_k$  over all the runs. As before, the use of a smaller tolerance for dggsvp3 gives consistent overestimates of  $r_c$  and correspondingly inaccurate generalized singular values. The relaxed tolerance estimates the ranks correctly and restores accuracy to the singular values, but at the cost of greater backward error. The tolerances used in these experiments are somewhat larger than in the small problem experiments, which should not be surprising considering the fact that backward errors due to rounding are somewhat larger for this problem.

| Quantity  | Description                | Same tol.      | Different tol. |
|---|----------------------------|----------------|----------------|
| $	ilde{\delta}_{a,b,c}$   | Rank tol.                  | 5e-14          | 5e-14          |
| $\hat{\delta}_{a,b}$  | Rank tol. (L)              | 5e-14          | 5e-10, 1e-12   |
| $\kappa_2(R)$   | Condition of $R$           | [4e7, 4e18]    | [4e7, 4e18]    |
| $\ C^{\dagger}\ _2$   | Pseudoinverse norm         | [5e6, 7e13]    | [5e6, 7e13]    |
| $(\tilde{r}_c, \tilde{r}_a, \tilde{r}_b)$                                   | Computed ranks             | (30, 15, 18)   | (30, 15, 18)   |
| $(\hat{r}_c, \hat{r}_a, \hat{r}_b)$   | Computed ranks (L)         | (31, 16, 18)   | (30, 15, 18)   |
| $\ \tilde{E}\ _2$   | Error on $A$               | [5e-15, 1e-14] | [5e-15, 1e-14] |
| $\ \tilde{F}\ _2$   | Error on $B$               | [4e-15, 1e-14] | [4e-15, 1e-14] |
| $\ \hat{E}\ _2$   | Error on $A$ (L)           | [4e-15, 7e-15] | [2e-11, 5e-11] |
| $\ \hat{F}\ _2$   | Error on $B$ (L)           | [5e-15, 1e-14] | [5e-15, 1e-14] |
| $\ \tilde{P} - P\ _2$   | Intersection err.          | [2e-9, 1e-4]   | [2e-9, 1e-4]   |
| $\ \hat{P} - P\ _2$   | Intersection err. (L)      | [6e-9, 2e-2]   | [6e-9, 8e-3]   |
| $\sigma_{d_i}(A_{23}^{(3)})$  | SV Gap $d_i$ (L) (not      | [2e-4, 3e-4]   | [2e-4, 3e-4]   |
| $\sigma_{d_i+1}(A_{23}^{(3)})$  | used to compute $d_i$ )    | [6e-12, 3e-7]  | [6e-12, 3e-7]  |
| $d_{\hat{r}_a - \hat{d}_i}(A_1^{(2)})$                                      | Rank decision, $r_a - d_i$ | [5e-11, 1e-10] | [2e-7, 7e-3]   |
| $d_{\hat{r}_a - \hat{d}_i + 1}(A_1^{(2)})$                                  | (L)                        | [1e-14, 2e-14] | [5e-11, 1e-10] |
| $ \tilde{\beta}_{\tilde{r}_a-\tilde{d}_i+1} - \beta_{r_a-d_i+1} $           | Gen. SV error              | [9e-15, 4e-5]  | [1e-14, 4e-5]  |
| $ \tilde{\alpha}_{\tilde{r}_a - \tilde{d}_i + 2} - \alpha_{r_a - d_i + 2} $ | Gen. SV error              | [2e-14, 5e-3]  | [2e-14, 5e-3]  |
| $ \tilde{\alpha}_{\tilde{r}_a-\tilde{d}_i+3}-\alpha_{r_a-d_i+3} $           | Gen. SV error              | [3e-12, 1e-1]  | [3e-12, 1e-1]  |
| $ \hat{\beta}_{\hat{r}_a - \hat{d}_i + 1} - \beta_{r_a - d_i + 1} $         | Gen. SV error (L)          | [2e-1, 5e-1]   | [5e-15, 4e-6]  |
| $ \hat{\alpha}_{\hat{r}_a - \hat{d}_i + 2} - \alpha_{r_a - d_i + 2} $       | Gen. SV error (L)          | [3e-4, 1e-1]   | [1e-13, 2e-1]  |
| $ \hat{\alpha}_{\hat{r}_a - \hat{d}_i + 3} - \alpha_{r_a - d_i + 3} $       | Gen. SV error (L)          | [5e-9, 7e-1]   | [1e-1, 7e-1]   |

The experiments were attempted for the large problem with ill-conditioned R, but we found that the LAPACK routine  $\tt dtgsja$  often failed to converge for numerically singular R unless it was given a very relaxed tolerance for convergence. With large errors introduced by  $\tt dtgsja$ , it was difficult to separate the effects of errors in  $\tt dtgsja$  from errors introduced as a result of preprocessing and partitioning of the decomposition. For this reason, we have chosen to omit the results of these experiments.

While we do not include a table, experiments were also done for larger perturbations E and F. With  $\sigma = 10^{-8}$  and well-conditioned R the results are similar, but with tolerances and errors increased in proportion to the increase in  $\sigma$ . For the ill-conditioned R, the perturbation theory suggests the potential for a near complete loss of accuracy in computed singular values. This is what was observed for both algorithms.

5. Conclusions. By enforcing a simple ordering of rank decisions in which  $\operatorname{rank}(C)$  is determined prior to computing  $\operatorname{rank}(A)$  and  $\operatorname{rank}(B)$ , we have developed a  $\operatorname{GURV}$  decomposition that is fully rank revealing in that it can, up to a small constant factor, determine the distance of a matrix pair from a pair with a prescribed GSVD structure. The decomposition can be used as a preprocessing step that determines all block sizes in the GSVD prior to the application of an iterative method for computing the generalized singular values. Numerical experiments suggest that it is more reliable than dggsvp3 in allowing for the recovery of a GSVD rank structure from a perturbed matrix pair. By increasing the reliability of the estimation of  $\operatorname{rank}(C)$ , the algorithm also increases the likelihood that perturbation theory for generalized singular values is

 $\begin{tabular}{ll} Table 3 \\ Well-conditioned $R$, $m_a=1000$, $m_b=1000$, $n=2010$, $d_i=50$, $\sigma=10^{-15}$. \end{tabular}$ 

| Quantity                                   | Description                                   | Same tol.       | Different tol.  |
|--|---|-----------------|-----------------|
| - "  |   |                 |                 |
| $\tilde{\delta}_{a,b,c}$                   | Rank tol.                                     | 5e-13           | 5e-13           |
| $\hat{\delta}_{a,b}$                       | Rank tol. (L)                                 | 5e-13           | 1e-9            |
| $\kappa_2(R)$                              | Condition of $R$                              | [9e2, 7e3]      | [9e2, 7e3]      |
| $\ C^{\dagger}\ _2$                        | Pseudoinverse norm                            | [2e1, 1e2]      | [2e1, 1e2]      |
| $(\tilde{r}_c, \tilde{r}_a, \tilde{r}_b)$  | Computed ranks                                | (750, 400, 400) | (750, 400, 400) |
| $(\hat{r}_c, \hat{r}_a, \hat{r}_b)$        | Computed ranks (L)                            | (751, 400, 401) | (750, 400, 400) |
| $\ \tilde{E}\ _2$                          | Error on $A$                                  | [5e-14, 8e-14]  | [5e-14, 8e-14]  |
| $\ \tilde{F}\ _2$                          | Error on $B$                                  | [5e-14, 7e-14]  | [5e-14, 7e-14]  |
| $\ \hat{E}\ _2$                            | Error on $A$ (L)                              | [3e-14, 5e-14]  | [4e-11, 7e-11]  |
| $\ \hat{F}\ _2$                            | Error on $B$ (L)                              | [5e-14, 9e-14]  | [5e-14, 6e-14]  |
| $\ \tilde{P} - P\ _2$                      | Intersection error                            | [2e-11, 2e-11]  | [2e-11, 2e-11]  |
| $\ \hat{P} - P\ _2$                        | Intersection error (L)                        | [8e-11, 2e-10]  | [1e-10, 2e-10]  |
| $\sigma_{d_i}(A_{23}^{(3)})$               | SV Gap $d_i$ (L) (not used to compute $d_i$ ) | [1e-3, 2e-3]    | [1e-3, 2e-3]    |
| $\sigma_{d_i+1}(A_{23}^{(3)})$             |   | [1e-12, 2e-12]  | [2e-12, 2e-12]  |
| $d_{\hat{r}_a - \hat{d}_i}(A_1^{(2)})$     | Rank decision, $r_a - d_i$                    | [2e-10, 3e-10]  | [1, 2]          |
| $d_{\hat{r}_a - \hat{d}_i + 1}(A_1^{(2)})$ | (L)   | [2e-13, 3e-13]  | [2e-10, 3e-10]  |
| $\max_k,  \tilde{\alpha}_k - \alpha_k $    | Gen. SV error                                 | 2e-15           | 1e-15           |
| $\max_k,  \tilde{\beta}_k - \beta_k $      | Gen. SV error                                 | 2e-15           | 2e-15           |
| $\max_k,  \hat{\alpha}_k - \alpha_k $      | Gen. SV error (L)                             | 7e-2            | 4e-15           |
| $\max_k,  \hat{\beta}_k - \beta_k $        | Gen. SV error (L)                             | 1e-1            | 6e-15           |

applicable, leading to more reliable approximation of the generalized singular values of the unperturbed pair.

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