Electronic Transactions on Numerical Analysis.
Volume 43, pp. 163-187, 2015.
Copyright © 2015, Kent State University.
ISSN 1068-9613.

BLOCK GRAM-SCHMIDT DOWNDATING[*]

JESSE L. BARLOW[†]

Abstract. Given positive integers m, n, and p, where $m \geq n+p$ and $p \ll n$. A method is proposed to modify the QR decomposition of $X \in \mathbb{R}^{m\times n}$ to produce a QR decomposition of X with p rows deleted. The algorithm is based upon the classical block Gram-Schmidt method, requires an approximation of the norm of the inverse of a triangular matrix, has $\mathcal{O}(mnp)$ operations, and achieves an accuracy in the matrix 2-norm that is comparable to similar bounds for related procedures for $p = 1$ in the vector 2-norm. Since the algorithm is based upon matrix-matrix operations, it is appropriate for modern cache oriented computer architectures.

Key words. QR decomposition, singular value decomposition, orthogonality, downdating, matrix-matrix operations.

AMS subject classifications. 65F25, 65F20, 65F35

1. Introduction.

Given a matrix $X \in \mathbb{R}^{m\times n}$ and an integer p, where $m \geq n+p$ and $p \ll n$. Suppose that we have the orthogonal decomposition (i.e., QR decomposition)

$$X = UR, \tag{1.1}$$

where $U \in \mathbb{R}^{m\times n}$ is left orthogonal and $R \in \mathbb{R}^{n\times n}$ is upper triangular. Let X be partitioned as

$$X = \begin{bmatrix} X_0 \\ \overline{X} \end{bmatrix} \begin{matrix} \}p \\ \}m-p \end{matrix} , \tag{1.2}$$

and suppose that we wish to produce the QR decomposition

$$\overline{X} = \overline{U}\,\overline{R}, \tag{1.3}$$

where $\overline{U} \in \mathbb{R}^{(m-p)\times\bar{n}}$ is left orthogonal, $\overline{R} \in \mathbb{R}^{\bar{n}\times n}$ is upper trapezoidal, and $\bar{n} \leq n$. Obtaining (1.3) inexpensively from (1.1), called the *block downdating* problem, is important in the context of solving recursive least squares problems where observations are added or deleted over time. It also arises as an intermediate computation in a recent null space algorithm by Overton et al. [18]. In (1.2), the first p observations are deleted, but, by simply applying a row permutation to X, any p observations can be deleted. Without changing the algorithm, we could assume that $U \in \mathbb{R}^{m\times n_0}$ and $R \in \mathbb{R}^{n_0\times n}$ is upper trapezoidal, where $n_0 \leq n$, but, for simplicity, we assume $n_0 = n$.

For $p = 1$, the block downdating problem (or simply the *downdating* problem) has an extensive literature [4, 9, 20]. A block downdating algorithm for the Cholesky decomposition based upon hyperbolic transformations was described by Q. Liu [17]. Our block CGS algorithm, closely related to the BCGS2 algorithm in [3] and the CGS2 algorithm in [1, 12], has matrix-matrix operations substituted for the matrix-vector operations, orthogonal decompositions—either the QR or the singular value decomposition—substituted for normalizations along with inverse norm estimates and singular values used in orthogonality tests instead of the size of vector norms. This leads to a BLAS-3 [10] or matrix-matrix operation oriented algorithm, which is more suited to modern computer architectures as it makes more effective use of caching. It requires $\mathcal{O}(mnp)$ operations.

---

[*] Received December 5, 2013. Accepted November 5, 2014. Published online on January 23, 2015. Recommended by L. Reichel. The research of Jesse L. Barlow was sponsored by the National Science Foundation under contract no. CCF-1115704.

[†] Department of Computer Science and Engineering, The Pennsylvania State University, University Park, PA, 16802–6822, USA (`barlow@cse.psu.edu`).

The downdating problem for $p = 1$ is solved by adding the column $\mathbf{b} = \mathbf{e}_1$, the first column of the identity, to X in (1.1), updating its QR factorization, and obtaining the matrices $\overline{U}$ and $\overline{R}$ in (1.3) as "by-products" of that updating process.

For $p > 1$ we substitute for $\mathbf{b} = \mathbf{e}_1$ the left orthogonal matrix $B \in \mathbb{R}^{m\times p}$ given by

$$B = \begin{bmatrix} V \\ 0 \end{bmatrix} \begin{matrix} \}p \\ \}m-p \end{matrix} , \tag{1.4}$$

where $V \in \mathbb{R}^{p\times p}$ is orthogonal.

Following a script in [3] for adding a block of columns B, we seek an integer $k \leq p$, a left orthogonal matrix $Q_B \in \mathbb{R}^{m\times k}$, an upper trapezoidal matrix $R_B \in \mathbb{R}^{k\times p}$, and a matrix $S_B \in \mathbb{R}^{n\times p}$ such that

$$B = US_B + Q_B R_B, \tag{1.5}$$

$$U^T Q_B = 0. \tag{1.6}$$

Once the problem (1.5)–(1.6) is solved, we have the decomposition

$$\begin{bmatrix} V & X_0 \\ 0 & \overline{X} \end{bmatrix} = \begin{bmatrix} Q_B & U \end{bmatrix} \begin{bmatrix} R_B & 0 \\ S_B & R \end{bmatrix}.$$

We then let $Z \in \mathbb{R}^{(n+k)\times(n+k)}$ be an orthogonal matrix such that

$$Z^T \begin{bmatrix} R_B & 0 \\ S_B & R \end{bmatrix} = \begin{bmatrix} \underbrace{\begin{matrix} R_V \\ 0 \end{matrix}}_{p} & \underbrace{\begin{matrix} Y_0 \\ \overline{R} \end{matrix}}_{n} \end{bmatrix} \begin{matrix} \}p \\ \}\bar{n} \end{matrix} , \tag{1.7}$$

where $\bar{n} = n - p + k$ and $\overline{R} \in \mathbb{R}^{\bar{n}\times n}$ remains upper trapezoidal. Applying Z to $\begin{bmatrix} Q_B & U \end{bmatrix}$, we obtain

$$\widetilde{U} = \begin{bmatrix} Q_B & U \end{bmatrix} Z = \begin{bmatrix} \underbrace{\widetilde{U}_1}_{p} & \underbrace{\widetilde{U}_2}_{\bar{n}} \end{bmatrix}, \tag{1.8}$$

where we note that

$$\begin{bmatrix} V & X_0 \\ 0 & \overline{X} \end{bmatrix} = \widetilde{U} \begin{bmatrix} R_V & Y_0 \\ 0 & \overline{R} \end{bmatrix}. \tag{1.9}$$

Thus,

$$\begin{bmatrix} V \\ 0 \end{bmatrix} = \widetilde{U}_1 R_V,$$

requiring that the matrix $\widetilde{U}_1$ in (1.8) has the form

$$\widetilde{U}_1 = \begin{bmatrix} U_V \\ 0 \end{bmatrix} \begin{matrix} \}p \\ \}m-p \end{matrix} \tag{1.10}$$

and implying that $U_V, R_V \in \mathbb{R}^{p\times p}$ must be orthogonal.

Since $\widetilde{U}$ is left orthogonal, $\widetilde{U}_2 \in \mathbb{R}^{m\times\bar{n}}$ has the form

$$\widetilde{U}_2 = \begin{bmatrix} 0 \\ \hline \overline{U} \end{bmatrix} \begin{matrix} \}p \\ \}m-p \end{matrix} \tag{1.11}$$

so that $\overline{U}$ in (1.11) and $\overline{R}$ in (1.9) satisfy (1.3). Once Q_B, S_B, and R_B are obtained, the decomposition (1.7) can be constructed efficiently as the product of 2×2 orthogonal transformations.

Unfortunately, if the matrix

$$C = \begin{bmatrix} B & U \end{bmatrix} \tag{1.12}$$

is rank deficient, the problem of obtaining Q_B, R_B, and S_B in (1.5)–(1.6) is ill-posed; the left orthogonal matrix Q_B is not unique, R_B is rank deficient, and the resulting factorization in (1.3) is rank deficient. From (1.5)–(1.6), C in (1.12) can be factored into

$$C = \begin{bmatrix} Q_B & U \end{bmatrix} \begin{bmatrix} S_B & I_n \\ R_B & 0 \end{bmatrix}.$$

Since $\begin{bmatrix} Q_B & U \end{bmatrix}$ is left orthogonal and the matrix on the right is quasi-upper triangular, C is rank deficient (ill-conditioned) only if R_B is.

There is little difficulty in obtaining Q_B, R_B, and S_B that satisfy (1.5) with a small residual, i.e., where $\|B - US_B - Q_BR_B\|_2$ is small. However, if C is (near) rank deficient, the ill-conditioning in R_B can make it difficult to obtain Q_B such that $\left\|U^TQ_B\right\|_2$ is small, i.e., such that (1.6) has a small residual. Understanding this issue and constructing an algorithm that addresses it are the main themes of the text below.

To develop block CGS downdating, we relax the assumption that U is left orthogonal and instead assume that

$$\left\|I_n - U^TU\right\|_2 \le \xi \ll 1 \tag{1.13}$$

for some small and unknown value ξ. In some contexts (as in, say, [3]), we may assume that $\xi \le f(m,n)\varepsilon_M$ where ε_M is machine precision and $f(m,n)$ is a modestly growing function, but, in our discussion, we simply assume that it is "small." It is possible that ξ depends on the condition number of R, for example, when it is the result of a modified Gram-Schmidt QR factorization [6]. Using the assumption (1.13), in Section 2 we design our algorithm with the goal of computing $Q_B \in \mathbb{R}^{m\times k}$, $R_B \in \mathbb{R}^{k\times p}$ upper trapezoidal, and $S_B \in \mathbb{R}^{n\times p}$, $k \le p$, such that

$$\|B - US_B - Q_BR_B\|_2 \le \sqrt{5}\xi + \mathcal{O}(\xi^2), \tag{1.14}$$

$$\left\|U^TQ_B\right\|_2 \le 0.5\xi + \mathcal{O}(\xi^2). \tag{1.15}$$

When $k < p$, i.e., when R_B is strictly upper trapezoidal, the algorithm produces a lower bound estimate ξ_{est} for ξ in (1.13).

The algorithm we develop and the bounds associated with it, (1.14)–(1.15), assume the reliability of an $\mathcal{O}(p^2 \log\, p)$ operation heuristic that, for an upper triangular matrix R_2, finds the largest integer k such that, for a prescribed constant β_{orth}, $\left\|R_2^{-1}(1\colon k, 1\colon k)\right\|_2 \le \beta_{orth}$.

The outline of this paper is as follows. The algorithm for computing Q_B, R_B, and S_B that satisfy (1.14)–(1.15) is assembled in Section 2. It is based firmly upon the function `block_CGS2_step` from [3, Function 2.2], which we restate as Function 2.1. Our modification, given as `block_CGS2_down` (Function 2.2), is justified by Theorems 2.1 and 2.2, FUNCTION 2.1 (Function `block_CGS2_step` from [3]).

```
function [$Q_B, S_B, R_B$]=block_CGS2_step($U, B$)
%
% First block Gram-Schmidt step
% Produces $Y_1 = (I - UU^T)B$
% Left orthogonal $Q_1$ satisfies $\mathrm{Range}(Q_1) = \mathrm{Range}(Y_1) = \mathrm{Range}((I_m - UU^T)B)$
% if $R_1$ nonsingular
%
(1) $S_1 = U^T B$;
(2) $Y_1 = B - US_1$;
(3) $Q_1 R_1 = Y_1$;        % QR decomposition of $Y_1$
%
% Second block Gram-Schmidt step
% Produces $Y_2 = (I - UU^T)Q_1$
% Left orthogonal $Q_B$ satisfies $\mathrm{Range}(Q_B) = \mathrm{Range}(Y_2) = \mathrm{Range}((I_m - UU^T)^2 B)$
% if $R_1$ and $R_2$ nonsingular
%
(4) $S_2 = U^T Q_1$;
(5) $Y_2 = Q_1 - US_2$;
(6) $Q_B R_2 = Y_2$;        % QR decomposition of $Y_2$
%
% Assemble $R_B$ and $S_B$ to satisfy (1.5)
%
(7) $S_B = S_1 + S_2 R_1$; $R_B = R_2 R_1$;
end block_CGS2_step
```

requires a condition number estimate to determine the appropriate value k for the dimensions of Q_B and R_B and leads to the function `block_downdate_info` (Function 2.4). We forgo a backward error analysis of `block_downdate_info`, but this could also be established from the backward error analysis of `block_CGS2_step` in [3, Section 3.2].

In Section 3.1, we perform a sequence of Givens rotations to produce Z in (1.7) that results in the factorization (1.3). In Section 3.2, we give an analysis of the relationship between $\left\| I_{\bar{n}} - \overline{U}^T \overline{U} \right\|_F$ and $\left\| I_n - U^T U \right\|_F$ and show how, in practice, $\widetilde{U}_1$ and $\widetilde{U}_2$ deviate from structural orthogonality in (1.10)–(1.11). Numerical tests are presented in Section 4 along with a Householder-based algorithm for adding a block of rows in Section 4.1. Proofs of important theorems are given in Section 5, and we summarize with a brief conclusion in Section 6.

2. A block Gram-Schmidt algorithm for downdating.

2.1. The functions `block_CGS2_step` and `block_CGS2_down`. We begin our development by examining the function `block_CGS2_step` from [3, Function 2.2] (given as Function 2.1 here) applied to a general matrix $B \in \mathbb{R}^{m \times p}$ with the intention of producing matrices Q_B, R_B, and S_B to solve (1.5)–(1.6). The function performs two classical Gram-Schmidt (BCGS) steps on B. The resulting matrices Q_B and R_B satisfy

$$Q_B R_B = (I_m - UU^T)^2 B,$$

and Q_B, S_B, and R_B satisfy (1.5). The remaining issue is the extent to which (1.6) or at least (1.15) can be satisfied. In [3], Function 2.1 is part of a QR factorization of a larger matrix, and the conditions on that QR factorization implicitly impose conditions on R_B relative to the loss of orthogonality in U.

Assuming U satisfies (1.13) and that R_B is nonsingular, we have that

$$\begin{aligned} U^T Q_B &= (I_n - U^T U)^2 U^T B R_B^{-1}, \\ \|U\|_2 &\leq (1+\xi)^{1/2}. \end{aligned}$$

A crude norm bound is

$$\begin{aligned} \left\|U^T Q_B\right\|_2 &\leq \left\|I_n - U^T U\right\|_2^2 \|U\|_2 \|B\|_2 \left\|R_B^{-1}\right\|_2 \\ &\leq \xi^2 (1+\xi)^{1/2} \|B\|_2 \left\|R_B^{-1}\right\|_2 . \end{aligned}$$

If

$$\xi \|B\|_2 \left\|R_B^{-1}\right\|_2 \leq c_{orth} \tag{2.1}$$

for some constant c_{orth}, then

$$\left\|U^T Q_B\right\|_2 \leq c_{orth}\xi + \mathcal{O}(\xi^2). \tag{2.2}$$

The inequality (2.1) poses two problems: we cannot always guarantee that R_B is nonsingular much less that it satisfies (2.1), and ξ is not necessarily known. The relationship (2.1)–(2.2) can be made columnwise in that for any positive integer $k \leq p$,

$$\left\|U^T Q_B(:,1\colon k)\right\|_2 \leq c_{orth}\xi + \mathcal{O}(\xi^2) \tag{2.3}$$

if

$$\xi \left\|B(:,1\colon k)\right\|_2 \left\|R_B^{-1}(1\colon k, 1\colon k)\right\|_2 \leq c_{orth}. \tag{2.4}$$

Unfortunately, (2.3)–(2.4) does not lead to such a bound as in (1.14).

The downdating problem (1.3) demands that we choose B of the form (1.4), but our ideas for choosing Q_B, R_B, and S_B apply to the situation in [3] where B is more general, provided that we normalize it as $\|B\|_2 = 1$. For the downdating problem, R_B and S_B are discarded once the decomposition (1.3) is computed, whereas for the application in [3], these quantities are needed in subsequent computations.

To delete the first p rows from the QR decomposition (1.1), we let

$$B_0 = \begin{bmatrix} I_p \\ 0 \end{bmatrix}$$

and look at the application of the Function 2.1 to B_0. Steps (1)–(2) of Function 2.1 read

$$\begin{aligned} S_1 &= U^T B_0 = U(1\colon p, :)^T, \\ Y_1 &= B_0 - U S_1. \end{aligned}$$

Instead of computing the QR decomposition in step (3), we compute the singular value decomposition (SVD) of Y_1. Thus, we have

$$\begin{aligned} Y_1 &= Q_1 R_1 V^T, && \qquad (2.5)\\ Q_1 &\in \mathbb{R}^{m\times p}, \text{ left orthogonal}, \\ V &\in \mathbb{R}^{p\times p}, \text{ orthogonal}, \\ R_1 &= \operatorname{diag}(\rho_1,\ldots,\rho_p), \quad \rho_1 \geq \cdots \geq \rho_p \geq 0. && \qquad (2.6) \end{aligned}$$

REMARK 2.1. In (2.5), the matrix R_1 in the statement (3) of Function 2.1 is replaced by the diagonal matrix of Y_1's singular values rather than its upper triangular factor. We use the same notation for it since it is the matrix R_1 obtained by Function 2.1 with B given by (1.4) and V being the right singular vector matrix in (2.5). Moreover, R_1 is used in the same way in the algorithm described below as it is in Function 2.1. We substitute the SVD because it sets us up to extract useful information for solving the problem (1.14)–(1.15).

To obtain a matrix Q_B that is near orthogonal to U, the second BCGS step, steps (4)–(5) in Function 2.1, reads

$$\begin{aligned} S_2 &= U^T Q_1, \\ Y_2 &= Q_1 - U S_2, \\ \widehat{Q}_B R_2 &= Y_2, \quad \text{QR decomposition}, \\ \widehat{Q}_B &\in \mathbb{R}^{m\times p}, \text{ left orthogonal}, \\ R_2 &\in \mathbb{R}^{p\times p}, \text{ upper triangular}. \end{aligned} \tag{2.7}$$

To guarantee that Q_1 and $\widehat{Q}_B$ are left orthogonal to near machine accuracy, that is,

$$\left\| I_p - Q^T Q \right\|_F \le \varepsilon_M L(m,p) \le \xi, \quad Q \in \{Q_1, \widehat{Q}_B\}, \tag{2.8}$$

where $L(m,p) = \mathcal{O}(mp^{3/2})$, ε_M is the machine unit, and ξ is defined in (1.13), we recommend that (2.5) is computed with either the Golub-Kahan-Householder (GKH) SVD [13] or the Lawson-Hanson-Chan (LHC) SVD [16, Section 18.5], [8] and that the QR factorization (2.7) may be computed using the Householder QR factorization [7].

Step (6) of Function 2.1 becomes

$$S_B = S_1 V + S_2 R_1, \quad \widehat{R}_B = R_2 R_1. \tag{2.9}$$

Equations (2.7) and (2.9) yield $\widehat{Q}_B$, $\widehat{R}_B$, and S_B such that

$$B = U S_B + \widehat{Q}_B \widehat{R}_B. \tag{2.10}$$

We write $\widehat{Q}_B$ and $\widehat{R}_B$ because we are not yet ready to accept these matrices as solutions to (1.14)–(1.15), however, S_B will not be further modified by our algorithms. The only difference between (2.9) and step (6) of Function 2.1 is the presence of V in the computation of S_B.

The modifications (2.5) and (2.9) to `block_CGS2_step` produce `block_CGS2_down` given in Function 2.2. This function produces the same $\widehat{Q}_B$, $\widehat{R}_B$, and S_B as Function 2.1 applied to U and B in (1.4). Note that it also outputs R_1, the diagonal matrix of singular values from the SVD in (2.5)–(2.6), and the upper triangular matrix R_2.

REMARK 2.2. Function 2.2 requires three matrix multiplications with U, one SVD of Y_1 using the GKH or LHC SVD, one QR decomposition of Y_2, two matrix multiplications and one matrix addition to form S_B, and one multiplication of a triangular matrix by a diagonal matrix to form R_B. This totals to $6mnp + 10mp^2 + (20/3)p^3 + 2np^2 + \mathcal{O}(m+n)$ operations. The dominant cost is the matrix multiplication with U.

Although equation (2.10) guarantees that $\widehat{Q}_B$, $\widehat{R}_B$, and S_B satisfy (1.5) (and thus also (1.14)), we cannot guarantee that $Q_B = \widehat{Q}_B$ satisfies (1.15). However, we are able to identify a subset of the columns of $\widehat{Q}_B$ that are sufficiently orthogonal to U. More precisely, for a given constant c_{orth} such that $0 < c_{orth} \le 1$, we intend to find the largest

FUNCTION 2.2 (The function `block_CGS2_down`).

```
function [$\widehat{Q}_B, S_B, \widehat{R}_B, R_2, R_1$]=block_CGS2_down($U, p$)
%
% First orthogonalization of $B_0$ against $U$
%
(1) $S_1 = U^T \begin{bmatrix} I_p \\ 0 \end{bmatrix} \quad (= U(1\colon p, :\,)^T)$;
(2) $Y_1 = \begin{bmatrix} I_p \\ 0 \end{bmatrix} - US_1$;
(3) $Q_1 R_1 V^T = Y_1$;        % SVD of $Y_1$
%
% Second orthogonalization
%
(4) $S_2 = U^T Q_1$; $Y_2 = Q_1 - US_2$;
(5) $\widehat{Q}_B R_2 = Y_2$;        % QR decomposition of $Y_2$
(6) $S_B = S_1 V + S_2 R_1$; $\widehat{R}_B = R_2 R_1$;
end block_CGS2_down
```

integer k such that

$$\left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_2 \leq c_{orth}\xi + \mathcal{O}(\xi^2), \tag{2.11}$$

$$\left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_F \leq c_{orth}\xi_F + \mathcal{O}(\xi^2), \qquad \xi_F \geq \max\{\left\| I_n - U^T U \right\|_F, \xi\}. \tag{2.12}$$

In this paper, we default to $c_{orth} = 0.5$ as it was used in [4] for the case $p = 1$. Daniel et al. [9] used $c_{orth} = 1$ for the case $p = 1$ since it maintains roughly the same level of orthogonality. Values of $c_{orth} > 1$ are not desirable since that would make the bound in (2.11) larger than the bound in (1.13). On the other hand, we do not want the restriction (2.11) to be too harsh, thus we recommend c_{orth} to be bounded away from zero.

To assure the bound (1.15), we need two theorems both of which require the definition

$$\beta_j = \left\| R_2^{-1}(1\colon j, 1\colon j) \right\|_2, \quad j = 1, \ldots, p, \quad \beta_0 = 0 \tag{2.13}$$

and both of which are proved in Section 5.1. Equation (2.13) defines the norms of the inverses of the leading principal submatrices of R_2 in (2.7). The first theorem relates the values β_j in (2.13) to the singular values in the diagonal matrix R_1 in (2.5).

THEOREM 2.1. *Assume that U satisfies (1.13). Let Q_1 in (2.5) be left orthogonal and β_j, $j = 1, \ldots, p$, be given by (2.13). Let ρ_j, $j = 1, \ldots, p$, be the singular values of Y_1 in (2.5). If, for a given constant c_{orth} with $0 < c_{orth} \leq 1$, k is the largest integer such that*

$$\beta_k \leq \beta_{orth} = \left(1 + c_{orth}^2\right)^{1/2} \tag{2.14}$$

and $k < p$, then

$$\rho_j \leq \alpha_{orth}\xi + \mathcal{O}(\xi^2), \qquad \alpha_{orth} = \frac{\left(1 + c_{orth}^2\right)^{1/2}}{c_{orth}}, \tag{2.15}$$

for $j = k+1, \ldots, p$.

Using $c_{orth} = 0.5$, the two constants in Theorem 2.1 are $\beta_{orth} = \sqrt{5}/2$ and $\alpha_{orth} = \sqrt{5}$. If $k < p$, then the inequality

$$\rho_{k+1} \leq \alpha_{orth}\xi + \mathcal{O}(\xi^2)$$

yields the lower bound estimate of ξ given by

$$\xi_{est} = \rho_{k+1}/\alpha_{orth}. \tag{2.16}$$

This estimate may be useful in determining if U has become too far off from being left orthogonal after a sequence of modifications to the QR factorization.

A second theorem, which follows from Theorem 2.1, shows that establishing k in (2.14) leads to an algorithm to produce Q_B, S_B, and R_B satisfying (1.14)–(1.15).

THEOREM 2.2. *Assume the hypothesis and terminology of Theorem 2.1 including the assumption that k satisfies (2.14). Let $\widehat{Q}_B$, $\widehat{R}_B$, and S_B be the output of Function 2.2. Then, we have (2.11)–(2.12) and*

$$B = US_B + \widehat{Q}_B(:,1\colon k)\widehat{R}_B(1\colon k,:) + D_k, \tag{2.17}$$

where $D_p = 0_{m\times p}$,

$$D_k = \widehat{Q}_B(:,k+1\colon p)\widehat{R}_B(k+1\colon p, k+1\colon p), \quad k < p, \tag{2.18}$$

and

$$\|D_k\|_2 \le \begin{cases} 0 & k = p, \\ \rho_{k+1} & k < p. \end{cases} \tag{2.19}$$

Thus, using the bound for ρ_{k+1} in (2.15), for $c_{orth} = 0.5$, we have that $Q_B = \widehat{Q}_B(:,1\colon k)$, $R_B = \widehat{R}_B(1\colon k,:)$, and S_B satisfy (1.14)–(1.15).

In the next section, to find the integer k that satisfies (2.14), we give an $\mathcal{O}(p^2 \log\ p)$ operation algorithm.

2.2. Finding the largest k such that $\widehat{Q}_B(:,1\colon k)$ is near orthogonal to U. To produce an algorithm to find the largest k satisfying (2.14), for the upper triangular matrix R_2 in step (5) of Function 2.2, we need an algorithm to compute $\left\|R_2^{-1}(1\colon j,1\colon j)\right\|_2$ with reasonable accuracy for a given j, and we need a binary search.

To produce the first, we compute $\mathbf{z}_j, \mathbf{w}_j \in \mathbb{R}^j$ such that

$$\begin{aligned} R_2^{-1}(1\colon j,1\colon j)\mathbf{w}_j &= \beta_j \mathbf{z}_j, \\ R_2^{-T}(1\colon j,1\colon j)\mathbf{z}_j &= \beta_j \mathbf{w}_j + \mathbf{f}_j, \end{aligned}$$

thus yielding the approximate leading singular triplet $(\beta_j, \mathbf{z}_j, \mathbf{w}_j)$ of $R_2^{-1}(1\colon j,1\colon j)$. The vector $\mathbf{f}_j$ is a residual that satisfies

$$\mathbf{w}_j^T \mathbf{f}_j = 0, \quad \|\mathbf{f}_j\|_2 \le tol * \beta_j$$

for some tolerance tol. This can easily be done with a few steps of a Golub-Kahan-Lanczos (GKL) bidiagonal reduction followed by an algorithm to find the largest singular triplet of a bidiagonal matrix. This approach is related to ideas in Ferng, Golub, and Plemmons [11] and ideas that have been used in ULV decompositions [2, 5]. If we are seeking the leading singular value of $R_2^{-1}(1\colon j,1\colon j)$, such a procedure is akin to finding the leading eigenvalue of a symmetric, positive definite matrix by the Lanczos algorithm, and no reorthogonalization is necessary in this circumstance [19]. Since the details of GKL bidiagonal reduction and the process of extracting the leading singular triplet is explored in detail elsewhere (see, for instance, [14, Chapters 8 and 9]), we skip these here and simply assume that the triplet $(\beta_j, \mathbf{z}_j, \mathbf{w}_j)$ can be delivered by the "black box" call

$$[\beta_j, \mathbf{z}_j, \mathbf{w}_j] = \texttt{GKL\_inv\_norm}(R_2(1\colon j,1\colon j)).$$

FUNCTION 2.3 (Lanczos-based routine for finding k satisfying (2.14)).

```
function $k$ = max_col_orth($R_2, \beta_{orth}$)
$n$=length($R_2$);
if $\beta_{orth}|R_2(1,1)| < 1$
%
% All of $R_2$ is too small, no columns are guaranteed orthogonal
%
    $k = 0$;
else
    $[\beta, \mathbf{z}, \mathbf{w}]$=GKL_inv_norm($R_2$);
    if $\beta <= \beta_{orth}$
%
% $\left\|R_2^{-1}\right\|_2 \leq \beta_{orth}$, all columns are guarantee orthogonal
%
        $k = p$;
    else
%
% Do binary search
%
        $first = 1$; $last = p$;
%
% At any given point in this loop
% $first \leq k < last$
%
        while $last - first > 1$
                $middle = \lfloor (first + last)/2 \rfloor$;
                $cols = 1\colon middle$;
                $[\beta, \mathbf{z}, \mathbf{w}]$ = GKL_inv_norm($R_2(cols, cols)$);
                if $\beta > \beta_{orth}$
                    $last = middle$;
                else
                    $first = middle$;
                end;
        end;
        $k = first$;
    end;
end;
end max_col_orth
```

Coupling `GKL_inv_norm` with a binary search that successively brackets k in the interval

$$first \leq k < last$$

that starts with $first = 1$ and $last = p$ and converges when $k = first = last - 1$, yields the function `max_col_orth` (Function 2.3) that produces k in (2.14).

2.3. The necessary information for a block downdate. The following function, Function 2.4, uses `block_CGS2_down` (Function 2.2) to produce $\widehat{Q}_B$, S_B, and $\widehat{R}_B$ and then uses `max_col_orth` (Function 2.3) to find k such that $Q_B = \widehat{Q}_B(:, 1\colon k)$, S_B, and $R_B = \widehat{R}_B(:, 1\colon k)$ satisfy (1.14)–(1.15) as shown by Theorem 2.2.

FUNCTION 2.4 (Block Downdate Information).

```
function $[Q_B, S_B, R_B, k, \xi_{est}]$=block_downdate_info $(U, p)$
%
% Produces information for a Block Downdate Operation for deleting the first $p$ rows
% from a QR decomposition where $U$ is a near left orthogonal matrix.
% Function max_orth_cols from Section 2.2 is called to find the largest integer $k$
% such that $\left\|R_2^{-1}(1\colon k, 1\colon k)\right\|_2 \leq \beta_{orth}$ for $1 \leq j \leq p$.
%
% Define constants used in the function. Specify $c_{orth} = 0.5$ to get
% the bounds (1.14)–(1.15).
%
$c_{orth} = 0.5$; $\beta_{orth} = \left(1 + c_{orth}^2\right)^{1/2}$; $\alpha_{orth} = \beta_{orth}/c_{orth}$;
$[\widehat{Q}_B, S_B, \widehat{R}_B, R_2, R_1]$=block_CGS2_down$(U, p)$;
%
% Determine “rank =k”, the number of columns of $\widehat{Q}_B$ guaranteed orthogonal to $U$.
%
$k$=max_orth_cols$(R_2, \beta_{orth})$
%
% Give lower bound estimate, $\xi_{est}$ in (2.16), for $\xi$.
% Note that $\rho_{k+1} = R_1(k+1, k+1)$.
%
if $k < p$
    $\xi_{est} = R_1(k+1, k+1)/\alpha_{orth}$;
else
    $\xi_{est} = 0$;
end;
%
% Produce rank $k$ solution to satisfy (1.14)–(1.15).
%
$R_B = \widehat{R}_B(1\colon k, :\,)$;
$Q_B = \widehat{Q}_B(:\,, 1\colon k)$;
end block_downdate_info
```

REMARK 2.3. Except for $\mathcal{O}(p^2 \log p)$ operations for `max_orth_cols`, almost all of the operations for Function 2.4 are from `block_CGS2_down`, thus it requires $6mnp + 10mp^2 + (20/3)p^3 + 2np^2 + \mathcal{O}(m + n + p^2 \log\ p)$ operations.

3. Producing a new QR factorization.

3.1. The algorithm to produce a new QR factorization. The remaining step in performing the block downdate is to find an orthogonal matrix Z such that

$$Z^T \begin{array}{c}\left[\begin{array}{cc} R_B & 0 \\ S_B & R \end{array}\right] \\ \underbrace{\hphantom{R_B}}_{p}\;\underbrace{\hphantom{R_B}}_{n}\end{array} \begin{array}{l} \}k \\ \}n \\ \end{array} = \begin{array}{c}\left[\begin{array}{cc} R_V & Y_0 \\ 0 & \overline{R} \end{array}\right] \\ \underbrace{\hphantom{R_V}}_{p}\;\underbrace{\hphantom{R_V}}_{n}\end{array} \begin{array}{l} \}p \\ \}\bar{n} \\ \end{array}, \quad \bar{n} = n - p + k, \tag{3.1}$$

where $\overline{R}$ remains upper trapezoidal. First, permute the rows of the above matrix so that

$$P^T \begin{array}{c}\left[\begin{array}{cc} R_B & 0 \\ S_B & R \end{array}\right] \\ \underbrace{\hphantom{R_B}}_{p}\;\underbrace{\hphantom{R_B}}_{n}\end{array} \begin{array}{l} \}k \\ \}n \\ \end{array} = \begin{bmatrix} R_B & 0 \\ S_B(\bar{n}+1\colon n, :\,) & R(\bar{n}+1\colon n, :\,) \\ S_B(1\colon \bar{n}, :\,) & R(1\colon \bar{n}, :\,) \end{bmatrix}.$$

We then let $\breve{Z}_0$ be a product of Householder transformations such that

$$\breve{Z}_0^T \begin{bmatrix} R_B \\ S_B(\bar{n}+1\colon n,\,:\,) \end{bmatrix} = \breve{R}_B,$$

where $\breve{R}_B$ is upper triangular. Letting $Z_0 = \begin{bmatrix} \breve{Z}_0 & 0 \\ 0 & I_{\bar{n}} \end{bmatrix}$, we have

$$Z_0^T \begin{bmatrix} R_B & 0 \\ S_B(\bar{n}+1\colon n,\,:\,) & R(\bar{n}+1\colon n,\,:\,) \\ S_B(1\colon \bar{n},\,:\,) & R(1\colon \bar{n},\,:\,) \end{bmatrix} = \left[\begin{matrix} \underbrace{\begin{matrix} \breve{R}_B \\ \breve{S}_B \end{matrix}}_{p} & \underbrace{\begin{matrix} \breve{Y}_0 \\ \breve{R} \end{matrix}}_{n} \end{matrix}\right] \begin{matrix} \}p \\ \}\bar{n} \end{matrix} .$$

Note that $\breve{R}$ is upper trapezoidal and $\breve{Y}_0$ is nonzero only in the columns $\bar{n}+1, \ldots, n$.

The remaining orthogonal transformations in Z are either Givens rotations or Householder transformations applied to only two rows. For simplicity, we just refer to both kinds as “Givens rotations”.

Since $\breve{R}_B$ is upper triangular, we let

$$\breve{Z} = Z_1 \cdots Z_p, \tag{3.2}$$

where each $Z_j, j = 1, \ldots, p$, is given by

$$Z_j = G_{j,p+\bar{n}} \cdots G_{j,p+1}$$

and $G_{j,\ell}$ is a Givens rotation rotating rows j and ℓ and inserting a zero in position (j, ℓ) so that

$$\breve{Z}^T \begin{bmatrix} \breve{R}_B \\ \breve{S}_B \end{bmatrix} = \begin{bmatrix} R_V \\ 0 \end{bmatrix}.$$

In terms of data movement, (3.2) is a poor Givens ordering. A better one is to let

$$\breve{Z} = \widehat{Z}_1 \cdots \widehat{Z}_{p-1} \widehat{Z}_p \cdots \widehat{Z}_n \cdots \widehat{Z}_{\bar{n}+p-1}.$$

Here we have

$$\widehat{Z}_j = \begin{cases} G_{j,\bar{n}+p} \cdots G_{1,n+p-j+1} & j < p, \\ G_{p,\bar{n}+2p-j} \cdots G_{1,\bar{n}+p-j+1} & p \le j \le \bar{n}, \\ G_{p,\bar{n}+2p-j} \cdots G_{j-\bar{n}+1,p+1} & \bar{n} < k < \bar{n}+p. \end{cases}$$

On its set of “active rows,” each of these $\widehat{Z}_j$ has the form

$$\widehat{Z}_j = \begin{bmatrix} \Gamma_j & \Delta_j \\ -\Delta_j & \Gamma_j \end{bmatrix}, \quad \Gamma_j^2 + \Delta_j^2 = I,$$

where Γ_j and Δ_j are diagonal. The orthogonal factor Z in the operation above is given by

$$Z = P Z_0 \widehat{Z}_1 \ldots \widehat{Z}_{\bar{n}+p-1}.$$

REMARK 3.1. Ignoring terms of $\mathcal{O}(mn)$, the algorithm described in this section requires $2mp^2 + (10/3)p^3 - 2kp^2$ operations to calculate and apply Z_0 and $6m\bar{n}p + 3n\bar{n}p + 3\bar{n}p^2$ operations to calculate and apply $\breve{Z}$, with a total of $6m\bar{n}p + 3n\bar{n}p + 3\bar{n}p^2 + 2mp^2 + (10/3)p^3 - 2kp^2$ operations. The dominant cost in this algorithm is the operation of updating the orthogonal factor as in (1.8).

3.2. Properties of the new QR factorization. In our new QR factorization, we have $\widetilde{U}$ given in (1.8) with

$$\widetilde{U} = \Bigg[\begin{array}{cc} \underbrace{\begin{matrix} U_V \\ \Delta U_V \end{matrix}}_{p} & \underbrace{\begin{matrix} \Delta\overline{U} \\ \overline{U} \end{matrix}}_{\bar{n}} \end{array}\Bigg] \begin{matrix} \}p \\ \}m-p \end{matrix} \quad , \tag{3.3}$$

where, if $\xi = 0$, $\Delta\overline{U} = 0_{p\times\bar{n}}$ and $\Delta U_V = 0_{(m-p)\times p}$. In practice, this will not necessarily be the case. Given the QR factorization (1.1), our downdate algorithm has produced

$$\begin{aligned}
\begin{bmatrix} V & X_0 \\ 0 & \overline{X} \end{bmatrix} &= \begin{bmatrix} Q_B & U \end{bmatrix} \begin{bmatrix} R_B & 0 \\ S_B & R \end{bmatrix} + \begin{bmatrix} D_k & 0 \end{bmatrix} \\
&= \begin{bmatrix} Q_B & U \end{bmatrix} ZZ^T \begin{bmatrix} R_B & 0 \\ S_B & R \end{bmatrix} + \begin{bmatrix} D_k & 0 \end{bmatrix} \\
&= \widetilde{U} \begin{bmatrix} R_V & Y_0 \\ 0 & \overline{R} \end{bmatrix} + \begin{bmatrix} D_k & 0 \end{bmatrix} \\
&= \begin{bmatrix} U_V & \Delta\overline{U} \\ \Delta U_V & \overline{U} \end{bmatrix} \begin{bmatrix} R_V & Y_0 \\ 0 & \overline{R} \end{bmatrix} + \begin{bmatrix} D_k & 0 \end{bmatrix} . \qquad (3.4)
\end{aligned}$$

Blockwise that is

$$\begin{aligned}
\begin{bmatrix} V \\ 0 \end{bmatrix} &= \begin{bmatrix} U_V \\ \Delta U_V \end{bmatrix} R_V + D_k, \\
X_0 &= U_V Y_0 + (\Delta\overline{U})\overline{R}, \\
\overline{X} &= (\Delta U_V) Y_0 + \overline{U}\,\overline{R}. \qquad (3.5)
\end{aligned}$$

We accept $\overline{U}$ above to produce (1.3). Thus we need bounds for

$$\left\|\overline{X} - \overline{U}\,\overline{R}\right\|_F \tag{3.6}$$

and

$$\left\|I_{\bar{n}} - \overline{U}^T\overline{U}\right\|_F . \tag{3.7}$$

For the quantity in (3.6), we could use an identical argument to obtain a bound in the 2-norm, but for the quantity in (3.7), the Frobenius norm yields a more meaningful bound.

Bounds for $\left\|\Delta\overline{U}\right\|_2$ and $\|\Delta U_V\|_2$ are also desirable. Theorems 3.1 and 3.3 are proved in Section 5.2. The short proof of Corollary 3.2 following from Theorem 3.1 is given in this section.

THEOREM 3.1. *Let $\widetilde{U}$ be the result of the matrix Z defined to perform the operation* (1.7) *using Q_B, R_B, and S_B produced by Function* 2.4 *with input U satisfying* (1.13) *and Q_B satisfying* (2.8). *Assume that Q_B is exactly left orthogonal. If $\widetilde{U}$ is partitioned according to* (3.3), *then*

$$\|\Delta U_V\|_2 \le \alpha_{orth}\xi + \mathcal{O}(\xi^2), \tag{3.8}$$

$$\left\|\Delta\overline{U}\right\|_2 \le (\alpha_{orth} + \gamma_{orth})\xi + \mathcal{O}(\xi^2), \tag{3.9}$$

$$\left\|I_{n+k} - \widetilde{U}^T\widetilde{U}\right\|_2 \le \gamma_{orth}\xi + \mathcal{O}(\xi^2), \tag{3.10}$$

where

$$\gamma_{orth} = 1 + c_{orth}.$$

COROLLARY 3.2. *Assume the terminology and hypothesis of Theorem 3.1. Then*

$$\left\|\overline{X} - \overline{U}\,\overline{R}\right\|_F \le \|\Delta U_V\|_2 \|X\|_F \tag{3.11}$$

$$\le \alpha_{orth}\xi \|X\|_F + \mathcal{O}(\xi^2). \tag{3.12}$$

Proof. From (3.5), we have

$$\overline{X} - \overline{U}\,\overline{R} = \overline{X} - \overline{UR} = (\Delta U_V)Y_0,$$

where

$$Y_0 = Z(:\,,1\colon p)^T \begin{bmatrix} 0 \\ R \end{bmatrix}.$$

Thus,

$$\left\|\overline{X} - \overline{UR}\right\|_F = \|(\Delta U_V)Y_0\|_F \le \|\Delta U_V\|_2 \|Y_0\|_F\,.$$

Since

$$\|Y_0\|_F = \left\| Z(:\,,1\colon p)^T \begin{bmatrix} 0 \\ R \end{bmatrix} \right\|_F \le \|X\|_F\,,$$

we have (3.11). The bound (3.8) gives us (3.12). □

We now let

$$\widetilde{U}_1 = \begin{bmatrix} U_V \\ \Delta U_V \end{bmatrix}\begin{matrix} \}p \\ \}m-p \end{matrix}\,, \qquad \widetilde{U}_2 = \begin{bmatrix} \Delta\overline{U} \\ \overline{U} \end{bmatrix}\begin{matrix} \}p \\ \}m-p \end{matrix}$$

and present a theorem bounding the quantity in (3.7).

THEOREM 3.3. *Assume the terminology and hypothesis of Theorem 3.1. Let* Q_B *satisfy* (2.8), *and define* $\xi_F = \max\{\left\|I_n - U^T U\right\|_F, \xi\}$. *Then*

$$\left\|I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2\right\|_F^2 \le \xi_F^2 + 2\left(\left\|U^T Q_B\right\|_F^2 - \left\|\widetilde{U}_1^T \widetilde{U}_2\right\|_F^2\right)$$

$$+ \left\|I_p - Q_B^T Q_B\right\|_F^2 - \left\|I_p - \widetilde{U}_1^T \widetilde{U}_1\right\|_F^2, \tag{3.13}$$

$$\left\|I_{\bar{n}} - \overline{U}^T \overline{U}\right\|_F \le \left\|I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2\right\|_F + \left\|(\Delta\overline{U})^T(\Delta\overline{U})\right\|_F, \tag{3.14}$$

$$\le \left\|I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2\right\|_F + \sqrt{p}(\alpha_{orth} + \gamma_{orth})^2\xi^2 + \mathcal{O}(\xi_F^3). \tag{3.15}$$

Thus,

$$\left\|I_{\bar{n}} - \overline{U}^T \overline{U}\right\|_F^2 \le \frac{5}{2}\xi_F^2 - 2\left\|\widetilde{U}_1^T \widetilde{U}_2\right\|_F^2 - \left\|I_p - \widetilde{U}_1^T \widetilde{U}_1\right\|_F^2 + \mathcal{O}(\xi_F^3). \tag{3.16}$$

Theorem 3.3 establishes that a loss of orthogonality in $\overline{U}$ will not be significantly worse than that in U. Moreover, it is possible that $\overline{U}$ is closer to a left orthogonal matrix than U since $\left\|I_p - \widetilde{U}_1^T \widetilde{U}_1\right\|_F$ and $\left\|\widetilde{U}_1^T \widetilde{U}_2\right\|_F$ may contain a significant portion of the loss of orthogonality in $\widetilde{U}$ while $\left\|I_p - Q_B^T Q_B\right\|_F$ will be near machine accuracy and our implied bound from (1.15) for $\left\|U^T Q_B\right\|_F$ could be quite pessimistic. In the next section, our numerical tests on a sliding window problem bear out this observation.

4. Numerical tests.

We consider a classic “sliding window” problem from statistics. Here, we compute the QR decomposition of a matrix $X(t) \in \mathbb{R}^{m\times n}$ which is a slice of a large matrix $X_{big} \in \mathbb{R}^{M\times n}$. The results displayed are for $M = 4000$, $m = 300$, $n = 250$. At step t,

$$X(t) = X_{big}\left(p * (t-1) + 1 \colon p(t-1) + m, \colon\right),$$

where, in the example shown, $p = 40$. The matrix X_{big} is constructed by generating a random $M \times n$ matrix using MATLAB’s `randn` function that simulates a standard normal distribution and then multiplying the rows at random by factors of 1, 10^{-7}, 10^{-14}, and 10^{-21}. Thus X_{big} is a random matrix with rows that have large and small entries.

4.1. Adding a block of rows to a QR factorization.

For the purposes of our numerical tests in Section 4.2, we also need an algorithm that adds a block of rows to a QR factorization. Again, supposing that we already have the factorization (1.1) and we wish to add a $p\times n$ block of rows given by X_{new}, then we simply compute the QR factorization

$$\begin{bmatrix} R \\ X_{new} \end{bmatrix} = Q_{new} \begin{bmatrix} R_{new} \\ 0 \end{bmatrix},$$

where Q_{new} is the product of n Householder transformations. Thus, the new QR factorization is

$$\begin{bmatrix} X \\ X_{new} \end{bmatrix} = U_{new} R_{new},$$

where

$$U_{new} = \begin{bmatrix} U & 0 \\ 0 & I_p \end{bmatrix} Q_{new}(\colon, 1 \colon n).$$

4.2. The sliding window experiment.

Given the QR factorization

$$X(t) = U(t)R(t)$$

at step t, the QR factorization of $X(t+1)$ is produced by adding p rows at the bottom of $X(t)$ using the algorithm in Section 4.1 to produce its QR factorization, deleting the p rows at the top of $X(t)$, and updating its QR factorization using Function 2.4 followed by the algorithm in Section 3.1 to obtain

$$X(t+1) = U(t+1)R(t+1).$$

For $t = 1, 2, \ldots,$ rank, changes were frequent because of the wild scaling of X_{big}.

At $t = 1$, we produce the QR decomposition

$$X(1) = U(1)R(1)$$

using the modified Gram-Schmidt algorithm. Since $X(1)$ is ill-conditioned, consistent with the bound in [6], we expect that

$$\left\| I - U(1)^T U(1) \right\|_2$$

will be significantly larger than the IEEE double precision machine unit $\varepsilon_M = 2^{-53} \approx 1.1102 \times 10^{-16}$.

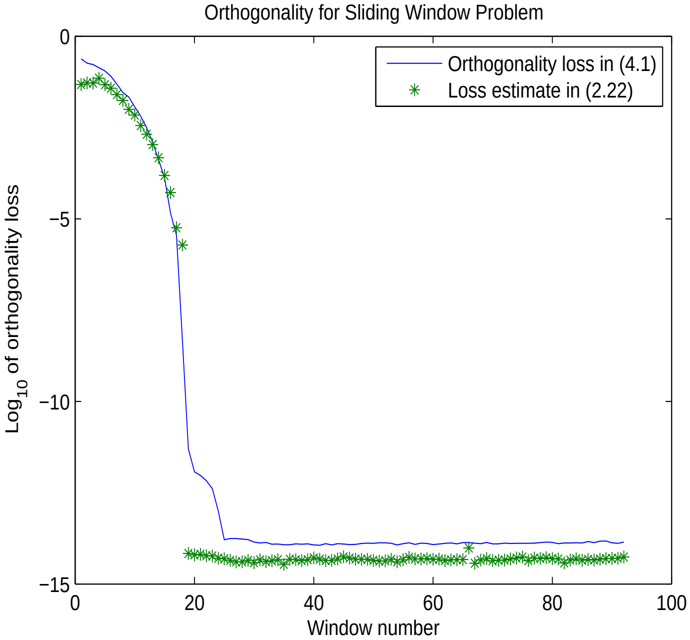

FIG. 4.1. *Loss of orthogonality for the sliding window example.*

We produce two graphs. The first, Figure 4.1, is the graph of

$$\xi = \left\| I - U(t)^T U(t) \right\|_2 . \tag{4.1}$$

The symbol ”+” in the graph indicates the estimate of ξ given by ξ_{est} in (2.16) from the function `block_downdate_info` whenever $k < p$ holds in Theorem 2.2. As can see be observed, ξ_{est} is a fairly accurate estimate of ξ.

The second, Figure 4.2, is the graph of

$$\frac{\|X(t) - U(t)R(t)\|_2}{\|X(t)\|_2} . \tag{4.2}$$

The value of ”*” is graphed whenever $k < p$ hold in Function 2.4, which makes $\overline{R}$ having smaller rank than R.

Note that in Figure 4.1, the value of $\left\| I - U(t)^T U(t) \right\|_2$ improves to near machine precision after about 10–20 steps, and this improvement persists. A similar pattern can be observed for the relative residual $\|X(t) - U(t)R(t)\|_2 / \|X(t)\|_2$, that is, it also improves to near machine precision and remains at this level. If we compute the QR factorization of $X(1)$ with Householder transformations instead of the modified Gram-Schmidt method, the loss of orthogonality starts out at near machine precision and stays there. The residuals, graphed in Figure 4.2, follow the same pattern.

We have repeated this test with different values of M, m, n, and p many times. If $U(1)$ satisfied the fundamental assumption (1.13), the result was always similar. However, if the matrix $U(1)$ in the initial MGS factorization of $X(1)$ did not satisfy the assumption (1.13), meaning that $U(1)$ could not be considered “near left orthogonal” and thus did not meet a fundamental assumption of this work, the residuals still self-corrected, but the loss of orthogonality either did not self-correct or took significantly longer to do so.

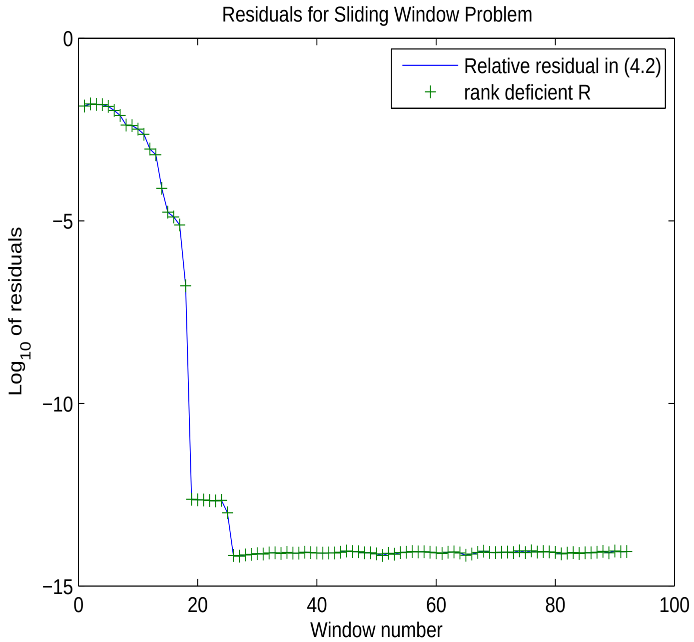

FIG. 4.2. *Residuals for the sliding window example.*

5. Proofs of the key theorems.

5.1. Proofs of Theorems 2.1 and 2.2. Using the form of R_1 in (2.6), we have that if for some $\ell \leq p$ it hold that $\rho_\ell = \cdots = \rho_p = 0$, then

$$(I - UU^T)\begin{bmatrix} V(:,\ell\colon p) \\ 0 \end{bmatrix} = 0,$$

thus concluding that $\begin{bmatrix} V(:,\ell\colon p) \\ 0 \end{bmatrix}$ is linearly dependent upon the columns of U and thereby allowing us to immediately reduce the dimension of this problem. Therefore, without loss of generality, we assume that

$$\rho_1 \geq \ldots \geq \rho_p > 0 \tag{5.1}$$

and thus that R_1 is nonsingular.

Using (5.1), we note that

$$\begin{aligned} U^T Q_1 &= (I - U^T U)U^T B R_1^{-1}, \\ &= (I - U^T U)F_1, \end{aligned} \tag{5.2}$$

where $F_1 = U^T B R_1^{-1}$. This allows us to rewrite Q_1 as

$$Q_1 = BR_1^{-1} - UF_1 \tag{5.3}$$

leading to the following lemma.

LEMMA 5.1. *Let* $U \in \mathbb{R}^{m\times n}$ *and* ξ *satisfy* (1.13). *Let* $B, Q_1 \in \mathbb{R}^{m\times p}$ *be left orthogonal matrices and be as in* (5.3), $n + p \leq m$, $R_1 \in \mathbb{R}^{p\times p}$ *be nonsingular, and* $F_1 = U^T B R_1^{-1}$. *Then for any unit vector* $\mathbf{w} \in \mathbb{R}^p$,

$$\left\|R_1^{-1}\mathbf{w}\right\|_2^2 = 1 + \|F_1\mathbf{w}\|_2^2 (1 + \delta_w), \quad |\delta_w| \leq \xi, \tag{5.4}$$

where δ_w *depends upon* $\mathbf{w}$.

Proof. Using the fact that Q_1 and B are left orthogonal and computing the normal equation's matrix of both sides of (5.3) yields

$$\begin{aligned} I &= R_1^{-T}R_1^{-1} - R_1^{-T}B^TUF_1 - F_1^TU^TBR_1^{-1} + F_1^TU^TUF_1 \\ &= R_1^{-T}R_1^{-1} - 2F_1^TF_1 + F_1^TU^TUF_1 \\ &= R_1^{-T}R_1^{-1} - F_1^TF_1 - F_1^T(I - U^TU)F_1. \end{aligned}$$

Thus,

$$R_1^{-T}R_1^{-1} = I + F_1^TF_1 + F_1^T(I - U^TU)F_1$$

so that for any unit vector $\mathbf{w} \in \mathbb{R}^p$, $\|\mathbf{w}\|_2 = 1$, the use of norm inequalities yields

$$\begin{aligned} \left\|R_1^{-1}\mathbf{w}\right\|_2^2 &= 1 + \|F_1\mathbf{w}\|_2^2 + \mathbf{w}^TF_1^T(I - U^TU)F_1\mathbf{w} \\ &\leq 1 + \|F_1\mathbf{w}\|_2^2 + \left\|I - U^TU\right\|_2 \|F_1\mathbf{w}\|_2^2 \\ &= 1 + (1 + \xi)\|F_1\mathbf{w}\|_2^2. \end{aligned}$$

By a similar argument,

$$\left\|R_1^{-1}\mathbf{w}\right\|_2^2 \geq 1 + (1 - \xi)\|F_1\mathbf{w}\|_2^2.$$

Thus, for some $|\delta_w| \leq \xi$ that depends upon $\mathbf{w}$, we have (5.4). □

REMARK 5.1. Note that Lemma 5.1 does not depend upon R_1 being diagonal, but R_1 only needs to be nonsingular.

From (5.4), using the definition of the 2-norm yields

$$\|F_1(:,1:k)\|_2 \leq \frac{\left(\left\|R_1^{-1}(1:k,1:k)\right\|_2^2 - 1\right)^{1/2}}{(1-\xi)^{1/2}}.$$

From the definition of R_1 in (2.5)–(2.6), i.e., as a diagonal matrix of singular values, we have that

$$\|F_1(:,1:k)\|_2 \leq \frac{\left(1-\rho_k^2\right)^{1/2}}{\rho_k}(1-\xi)^{-1/2}, \tag{5.5}$$

and thus from (5.2) it follows that

$$\begin{aligned} \left\|U^TQ_1(:,1:k)\right\|_2 &\leq \left\|I - U^TU\right\|_2 \|F_1(:,1:k)\|_2 \\ &\leq \xi\frac{\left(1-\rho_k^2\right)^{1/2}}{\rho_k} + \mathcal{O}(\xi^2). \end{aligned}$$

The following lemma allows us to assume that R_2 in (2.7) is nonsingular.

LEMMA 5.2. *Assume the hypothesis and terminology of Lemma 5.1. Let the left orthogonal matrix $\widehat{Q}_B \in \mathbb{R}^{m\times p}$ and the upper triangular matrix $R_2 \in \mathbb{R}^{p\times p}$ be given by (2.7). If $R_2(1\colon k, 1\colon k)$ is singular, then*

$$\rho_k \leq \xi(1+\xi). \tag{5.6}$$

Proof. If $\rho_k = 0$, the theorem holds trivially, so we assume that $\rho_k > 0$. For the left orthogonal matrix B in (1.4),

$$\begin{aligned} Q_1 R_1 &= (I - UU^T)B, \\ \widehat{Q}_B R_2 R_1 &= (I - UU^T)^2 B. \end{aligned}$$

If $R_2(1\colon k, 1\colon k)$ is singular, there is a vector $\mathbf{v} \neq 0$ such that

$$R_2(1\colon k, 1\colon k)\mathbf{v} = 0.$$

Since $\rho_1 \geq \cdots \geq \rho_k > 0$ and $R_1(1\colon k, 1\colon k) = \operatorname{diag}(\rho_1, \ldots, \rho_k)$, we can choose $\mathbf{v}$ so that

$$\mathbf{v} = R_1(1\colon k, 1\colon k)\mathbf{w},$$

where $\mathbf{w}$ is a unit vector. Thus,

$$\widehat{Q}_B(:, 1\colon k)R_2(1\colon k, 1\colon k)R_1(1\colon k, 1\colon k)\mathbf{w} = (I - UU^T)^2 B(:, 1\colon k)\mathbf{w} = 0.$$

Since

$$(I - UU^T)^2 = I - UU^T - U(I - U^T U)U^T,$$

this implies

$$\begin{aligned} Q_1(:, 1\colon k)R_1(1\colon k, 1\colon k)\mathbf{w} &= (I - UU^T)B(:, 1\colon k)\mathbf{w} \\ &= U(I - U^T U)U^T B(:, 1\colon k)\mathbf{w}. \end{aligned}$$

Thus, by the definition of ρ_k and using the fact that $\|\mathbf{w}\|_2 = 1$,

$$\begin{aligned} \rho_k &\leq \|R_1(1\colon k, 1\colon k)\mathbf{w}\|_2 \leq \left\|U(I - U^T U)U^T B(:, 1\colon k)\mathbf{w}\right\|_2 \\ &\leq \left\|U(I - U^T U)U^T B(:, 1\colon k)\right\|_2. \end{aligned}$$

Since B is left orthogonal, we have

$$\rho_k \leq \|U\|_2^2 \left\|I - U^T U\right\|_2 \leq \xi \|U\|_2^2.$$

From the assumption (1.13),

$$\|U\|_2^2 = \left\|U^T U\right\|_2 \leq 1 + \left\|I - U^T U\right\|_2 = 1 + \xi,$$

thus ρ_k satisfies (5.6). ☐

Assuming R_2 is nonsingular, we have that

$$U^T \widehat{Q}_B = (I - U^T U)F_2, \quad F_2 = U^T Q_1 R_2^{-1}$$

so that

$$\begin{aligned} \left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_2 &\le \xi \left\| F_2(:\,, 1\colon k) \right\|_2 , \\ \left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_F &\le \xi_F \left\| F_2(:\,, 1\colon k) \right\|_2 . \end{aligned}$$

Invoking Lemma 5.1, for any unit vector $\mathbf{w} \in \mathbb{R}^p$, we obtain

$$\left\| R_2^{-1} \mathbf{w} \right\|_2^2 = 1 + \left\| F_2 \mathbf{w} \right\|_2^2 (1 + \delta_w), \quad |\delta_w| \le \xi$$

so that, again from the definition of the matrix 2-norm,

$$\begin{aligned} \left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_2 &\le \xi \left(\beta_k^2 - 1 \right)^{1/2} + \mathcal{O}(\xi^2), \\ \left\| U^T \widehat{Q}_B(:\,, 1\colon k) \right\|_F &\le \xi_F \left(\beta_k^2 - 1 \right)^{1/2} + \mathcal{O}(\xi_F^2), \end{aligned}$$

where $\beta_k = \left\| R_2^{-1}(1\colon k, 1\colon k) \right\|_2$.

Proof of Theorem 2.1. We note that F_1 and F_2 are related according to

$$\begin{aligned} F_2 = U^T Q_1 R_2^{-1} &= (I - U^T U) U^T B R_1^{-1} R_2^{-1} \\ &= (I - U^T U) F_1 R_2^{-1} . \end{aligned} \tag{5.7}$$

We now exploit (5.7) to show an important relationship between $\beta_j = \left\| R_1^{-1}(1\colon j, 1\colon j) \right\|_2$ and ρ_j, the jth singular value of R_1. Applying norm inequalities to (5.7) and (5.5), we have

$$\begin{aligned} \left\| F_2(:\,, 1\colon j) \right\|_2 &\le \left\| I - U^T U \right\|_2 \left\| F_1(:\,, 1\colon j) \right\|_2 \left\| R_2^{-1}(1\colon j, 1\colon j) \right\|_2 \\ &\le \xi \left(\frac{\left(1 - \rho_j^2\right)^{1/2}}{\rho_j} \right) \left(1 + \left\| F_2(:\,, 1\colon j) \right\|_2^2 \right)^{1/2} + \mathcal{O}(\xi^2), \end{aligned}$$

which yields

$$\frac{\left\| F_2(:\,, 1\colon j) \right\|_2}{\left(1 + \left\| F_2(:\,, 1\colon j) \right\|_2^2 \right)^{1/2}} \le \xi \frac{\left(1 - \rho_j^2\right)^{1/2}}{\rho_j} + \mathcal{O}(\xi^2).$$

Since $\beta_j > \beta_{orth}$ implies (2.15) and since $x / \left(1 + x^2\right)^{1/2}$ is a strictly increasing function for $x > 0$, $\left\| F_2(:\,, 1\colon j) \right\|_2 \le c_{orth}$ implies that

$$\frac{c_{orth}}{(1 + c_{orth}^2)^{1/2}} \le \xi \frac{\left(1 - \rho_j^2\right)^{1/2}}{\rho_j} + \mathcal{O}(\xi^2) \le \xi / \rho_j + \mathcal{O}(\xi^2),$$

which becomes

$$\rho_j \le \alpha_{orth} \xi + \mathcal{O}(\xi^2),$$

where α_{orth} is given in (2.15). □

We note that if k is the largest integer such that $\beta_k \le \left(1 + c_{orth}^2\right)^{1/2}$, then the matrix $Q_B = \widehat{Q}_B(:\,, 1\colon k)$ as defined in Theorem 2.2 satisfies

$$\begin{aligned} \left\| U^T Q_B \right\|_2 &\le c_{orth} \xi + \mathcal{O}(\xi^2), \\ \left\| U^T Q_B \right\|_F &\le c_{orth} \xi_F + \mathcal{O}(\xi^2). \end{aligned} \tag{5.8}$$

Some algebra shows that

$$\begin{aligned} B &= US_B + \widehat{Q}_B \widehat{R}_B \\ &= US_B + Q_B R_B + D_k, \end{aligned} \tag{5.9}$$

where D_k is given by (2.18).

Thus, we have that

$$\begin{aligned} \|B - US_B - Q_B R_B\|_2 &= \|D_k\|_2 \\ &= \left\| \widehat{Q}_B(:\, ,k+1\colon p)\widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2 \\ &= \left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2 . \end{aligned} \tag{5.10}$$

To prove a bound for $\left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2$ and thus to bound the residual in (5.10), we need the following lemma proved in [3].

LEMMA 5.3 ([3, Lemma 3.2]). *If* $U \in \mathbb{R}^{m\times n}$ *satisfies* (1.13), *then*

$$\left\| I_m - UU^T \right\| \leq 1.$$

Proof of Theorem 2.2. From (5.8), we have that $Q_B = \widehat{Q}_B(:\, ,1\colon k)$ satisfies (2.11). For $k = p$, we have $D_k = 0$, and (2.19) is trivially satisfied. For $k < p$, from (5.9), we have (2.17)–(2.18), thus by orthogonal equivalence,

$$\|D_k\|_2 = \left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2 .$$

Thus, we only need to establish a bound for $\left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2$ to prove the theorem.

Since

$$\widehat{R}_B(k+1\colon p, k+1\colon p) = R_2(k+1\colon p, k+1\colon p) R_1(k+1\colon p, k+1\colon p),$$

by a standard norm inequality and the SVD structure (2.5)–(2.6), it follows that

$$\begin{aligned} &\left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2 \\ &\quad \leq \|R_2(k+1\colon p, k+1\colon p)\|_2 \, \|R_1(k+1\colon p, k+1\colon p)\|_2 \\ &\quad = \rho_{k+1} \, \|R_2(k+1\colon p)\|_2 \leq \rho_{k+1} \, \|R_2\|_2 . \end{aligned} \tag{5.11}$$

A bit of algebra shows that

$$R_2 = \widehat{Q}_B^T (I - UU^T) Q_1,$$

thus we can use orthogonal equivalence and Lemma 5.3 to show

$$\|R_2\|_2 \leq \left\| I - UU^T \right\|_2 \leq 1.$$

Thus, from (5.11),

$$\|D_k\|_2 = \left\| \widehat{R}_B(k+1\colon p, k+1\colon p) \right\|_2 \leq \rho_{k+1} \, \|R_2\|_2 \leq \rho_{k+1},$$

which establishes (2.19). $\square$

5.2. Proofs of Theorems 3.1 and 3.3. We begin with the proof of Theorem 3.1. First, we need two lemmas.

LEMMA 5.4. *Let* $\widetilde{U}$ *and* γ_{orth} *be as in Theorem 3.1. Then*

$$\left\| I_{n+k} - \widetilde{U}^T \widetilde{U} \right\|_2 \overset{def}{=} \tilde{\xi} \leq \gamma_{orth} \xi + \mathcal{O}(\xi^2).$$

Proof. We have that

$$\begin{aligned} I_{n+k} - \widetilde{U}^T \widetilde{U} &= Z^T [I_{n+k} - \begin{bmatrix} Q_B & U \end{bmatrix}^T \begin{bmatrix} Q_B & U \end{bmatrix}] Z \\ &= Z^T \begin{bmatrix} I_k - Q_B^T Q_B & Q_B^T U \\ U^T Q_B & I_n - U^T U \end{bmatrix} Z. \end{aligned}$$

Thus using standard norm inequalities, we have

$$\begin{aligned} \left\| I_{n+k} - \widetilde{U}^T \widetilde{U} \right\|_2 &= \left\| \begin{bmatrix} I_k - Q_B^T Q_B & Q_B^T U \\ U^T Q_B & I_n - U^T U \end{bmatrix} \right\|_2 \\ &\leq \left\| \begin{bmatrix} \left\| I_k - Q_B^T Q_B \right\|_2 & \left\| U^T Q_B \right\|_2 \\ \left\| U^T Q_B \right\|_2 & \left\| I_n - U^T U \right\|_2 \end{bmatrix} \right\|_2 . \end{aligned}$$

Since Q_B satisfies (2.8) and since Theorem 2.2 implies that Function 2.4 produces a matrix Q_B satisfying

$$\left\| U^T Q_B \right\|_2 \leq c_{orth} \xi + \mathcal{O}(\xi^2), \qquad \left\| I_k - Q_B^T Q_B \right\|_2 \leq \xi$$

and moreover U is assumed to satisfy (1.13), it follows that

$$\left\| I_{n+k} - \widetilde{U}^T \widetilde{U} \right\|_2 \leq \left\| \begin{bmatrix} 1 & c_{orth} \\ c_{orth} & 1 \end{bmatrix} \right\|_2 \xi + \mathcal{O}(\xi^2) = \gamma_{orth} \xi + \mathcal{O}(\xi^2). \qquad \square$$

LEMMA 5.5. *Let* $R_V \in \mathbb{R}^{p \times p}$ *be the upper triangular matrix defined in (3.1). Using the terminology in Theorem 2.1 and Lemma 5.4 with the convention that* $\rho_{p+1} = 0$*, we have*

$$\begin{aligned} \left\| R_V^{-1} \right\|_2 &\leq (1 + \tilde{\xi})^{1/2} (1 - \rho_{k+1})^{-1} \\ &\leq 1 + (\alpha_{orth} + \gamma_{orth}/2)\xi + \mathcal{O}(\xi^2), && (5.12) \\ \left\| R_V \right\|_2 &\leq 1 + (\alpha_{orth} + \gamma_{orth}/2)\xi + \mathcal{O}(\xi^2). && (5.13) \end{aligned}$$

Proof. Theorem 2.2 implies

$$\widetilde{U}_1 R_V = \begin{bmatrix} V \\ 0 \end{bmatrix} - D_k, \tag{5.14}$$

where D_k is bounded as in (2.19). Through the use of a singular value inequality in [15, Problem 7.3.P16], we conclude that

$$\sigma_p(\widetilde{U}_1)\sigma_j(R_V) \leq \sigma_j(\widetilde{U}_1 R_V) \leq \sigma_1(\widetilde{U}_1)\sigma_j(R_V).$$

Thus, using standard norm inequalities,

$$\sigma_p(R_V) \left\| \widetilde{U}_1 \right\|_2 \geq \sigma_p \begin{bmatrix} V \\ 0 \end{bmatrix} - \left\| D_k \right\|_2 .$$

Since V is orthogonal and

$$\left\|\widetilde{U}_1\right\|_2 \leq \left\|\widetilde{U}\right\|_2 \leq (1+\tilde{\xi})^{1/2} + \mathcal{O}(\xi^2),$$

we have that within a margin of $\mathcal{O}(\xi^2)$,

$$\sigma_p(R_V)(1+\tilde{\xi})^{1/2} \geq 1 - \|D_k\|_2 .$$

Invoking Theorem 2.2 yields

$$\sigma_p(R_V) \geq (1+\tilde{\xi})^{-1/2}(1-\rho_{k+1}).$$

Thus,

$$\|R_V^{-1}\|_2 = \sigma_p(R_V)^{-1} \leq (1+\tilde{\xi})^{1/2}(1-\rho_{k+1})^{-1} + \mathcal{O}(\xi^2).$$

From the bound for $\tilde{\xi}$ in Lemma 5.4 and the bound for ρ_{k+1} in Theorem 2.1, we have

$$\|R_V^{-1}\|_2 \leq (1+\alpha_{orth}+\gamma_{orth}/2)\xi + \mathcal{O}(\xi^2).$$

To establish the bound for $\|R_V\|_2$, simply note that

$$R_V = \widetilde{U}_1^{\dagger}\left(\begin{bmatrix} V \\ 0 \end{bmatrix} - D_k\right)$$

so that

$$\|R_V\|_2 \leq \left\|\widetilde{U}_1^{\dagger}\right\|_2 (1+\rho_{k+1}) \leq (1-\tilde{\xi})^{-1/2}(1+\rho_{k+1}).$$

The bound (5.13) follows from an argument similar to that for (5.12). ☐

We are now ready to prove Theorem 3.1.

Proof of Theorem 3.1. We have already proved (3.10). Next we bound $\|\Delta U_V\|_2$. From (1.8), (3.1), (3.3), and (5.14), we have

$$\Delta U_V = -D_k(p+1\colon m, :\,)R_V^{-1}.$$

Thus, from Theorem 2.1 and Lemma 5.5,

$$\begin{aligned}\|\Delta U_V\|_2 &\leq \|D_k(p+1\colon m, :\,)\|_2 \left\|R_V^{-1}\right\|_2 \\ &\leq \rho_{k+1}(1+(\alpha_{orth}+\gamma_{orth}/2)\xi + \mathcal{O}(\xi^2) \\ &= \alpha_{orth}\xi + \mathcal{O}(\xi^2),\end{aligned}$$

which is (3.8).

Now proceed to prove (3.9). We have that

$$\widetilde{U}_1^T\widetilde{U}_2 = U_V^T\Delta\overline{U} + (\Delta U_V)^T\overline{U}$$

so that

$$\left\|U_V^T\Delta\overline{U}\right\|_2 \leq \left\|\widetilde{U}_1^T\widetilde{U}_2\right\|_2 + \left\|(\Delta U_V)^T\overline{U}\right\|_2 . \tag{5.15}$$

To bound the first term in (5.15), note that

$$\left\|\widetilde{U}_1^T\widetilde{U}_2\right\|_2 \leq \left\|I_{n+k} - \widetilde{U}^T\widetilde{U}\right\|_2 = \tilde{\xi},$$

and thus

$$\left\|U_V^T \Delta \overline{U}\right\|_2 \leq \tilde{\xi} + \left\|\Delta U_V\right\|_2 \left\|\overline{U}\right\|_2 . \tag{5.16}$$

Since $\overline{U}$ is just the lower right block of $\widetilde{U}$,

$$\left\|\overline{U}\right\|_2 \leq \left\|\widetilde{U}\right\|_2 \leq (1+\tilde{\xi})^{1/2}$$

so that (5.16) becomes

$$\left\|U_V^T \Delta \overline{U}\right\|_2 \leq \tilde{\xi} + \left\|\Delta U_V\right\|_2 (1+\tilde{\xi})^{1/2}.$$

Again using the singular value result in [15, Problem 7.3.P16], we have

$$\sigma_p(U_V) \left\|\Delta \overline{U}\right\|_2 \leq (\tilde{\xi} + \left\|\Delta U_V\right\|_2)(1+\tilde{\xi})^{1/2}.$$

We note that from (3.4) it follows that

$$U_V = (V + D_k(1\colon p, :))R_V^{-1},$$

hence

$$\sigma_p(U_V) \geq \sigma_p(V + D_k(1\colon p, :))\sigma_p(R_V^{-1}).$$

Using the orthogonality of V and the bound for $\left\|D_k\right\|_2$ from Theorem 2.2, we have

$$\sigma_p(U_V) \geq (1-\rho_{k+1}) \left\|R_V\right\|_2^{-1} .$$

Therefore, using (5.13) yields

$$\begin{aligned}\left\|\Delta \overline{U}\right\|_2 &\leq (\tilde{\xi} + \left\|\Delta U_V\right\|_2)(1+\tilde{\xi})^{1/2}(1-\rho_{k+1})^{-1} \left\|R_V\right\|_2 \\ &= (\tilde{\xi} + \left\|\Delta U_V\right\|_2)(1+\tilde{\xi})^{1/2}(1+\rho_{k+1})(1-\rho_{k+1})^{-1} \\ &\leq (\alpha_{orth} + \gamma_{orth})\xi + \mathcal{O}(\xi^2). \qquad \square\end{aligned}$$

We now prove Theorem 3.3.

Proof of Theorem 3.3. We note that

$$\begin{aligned}\left\|I_{n+k} - \widetilde{U}^T \widetilde{U}\right\|_F^2 &= \left\|\begin{bmatrix} I_p - \widetilde{U}_1^T \widetilde{U}_1 & \widetilde{U}_1^T \widetilde{U}_2 \\ \widetilde{U}_2^T \widetilde{U}_1 & I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \end{bmatrix}\right\|_F^2 \\ &= \left\|I_p - \widetilde{U}_1^T \widetilde{U}_1\right\|_F^2 + 2\left\|\widetilde{U}_1^T \widetilde{U}_2\right\|_F^2 + \left\|I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2\right\|_F^2 \end{aligned} \tag{5.17}$$

and that by orthogonal equivalence

$$\begin{aligned}\left\|I_{n+k} - \widetilde{U}^T \widetilde{U}\right\|_F^2 &= \left\|Z^T (I_{n+k} - \begin{bmatrix} Q_B & U\end{bmatrix}^T \begin{bmatrix} Q_B & U\end{bmatrix})Z\right\|_F^2 \\ &= \left\|I_{n+k} - \begin{bmatrix} Q_B & U\end{bmatrix}^T \begin{bmatrix} Q_B & U\end{bmatrix}\right\|_F^2 \\ &= \left\|I_k - Q_B^T Q_B\right\|_F^2 + 2\left\|U^T Q_B\right\|_F^2 + \left\|I_n - U^T U\right\|_F^2 . \end{aligned} \tag{5.18}$$

Equating (5.17) and (5.18) and solving for $\left\|I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2\right\|_F^2$ obtains (3.13).

To obtain (3.15), we note that

$$\widetilde{U}_2 = \begin{bmatrix} \Delta\overline{U} \\ \overline{U} \end{bmatrix},$$

thus

$$I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 = (\Delta\overline{U})^T (\Delta\overline{U}) + I_{\bar{n}} - \overline{U}^T \overline{U}.$$

Thus,

$$\left\| I_{\bar{n}} - \overline{U}^T \overline{U} \right\|_F \leq \left\| I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \right\|_F + \left\| (\Delta\overline{U})^T (\Delta\overline{U}) \right\|_F,$$

which is (3.14). From the inequalities

$$\left\| (\Delta\overline{U})^T (\Delta\overline{U}) \right\|_F \leq \sqrt{p} \left\| (\Delta\overline{U})^T (\Delta\overline{U}) \right\|_2 \leq \sqrt{p} \left\| \Delta\overline{U} \right\|_2^2$$

and the bound (3.9), we obtain (3.15). To get (3.16), we note that

$$\left\| I_n - U^T U \right\|_F, \left\| I_k - Q_B^T Q_B \right\|_F \leq \xi_F \tag{5.19}$$

and that

$$\left\| U^T Q_B \right\|_F \leq c_{orth} \xi_F + \mathcal{O}(\xi_F^2) = \frac{1}{2} \xi_F + \mathcal{O}(\xi_F^2), \tag{5.20}$$

thus

$$\begin{aligned} \left\| I_{\bar{n}} - \overline{U}^T \overline{U} \right\|_F^2 &\leq (\left\| I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \right\|_F + \sqrt{p}(\alpha_{orth} + \gamma_{orth})^2 \xi^2)^2 + \mathcal{O}(\xi_F^4) \\ &\leq \left\| I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \right\|_F^2 + \sqrt{p}(\alpha_{orth} + \gamma_{orth})^2 \xi^2 \left\| I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \right\|_F + \mathcal{O}(\xi_F). \end{aligned}$$

From (3.13) and (5.19)–(5.20), we have

$$\left\| I_{\bar{n}} - \widetilde{U}_2^T \widetilde{U}_2 \right\|_F^2 \leq \frac{5}{2} \xi_F - 2 \left\| \widetilde{U}_1^T \widetilde{U}_2 \right\|_F^2 - \left\| I_p - \widetilde{U}_1^T \widetilde{U}_1 \right\|_F^2 + \mathcal{O}(\xi_F^3),$$

which is (3.16). □

6. Conclusion. We have taken the 2-norm formulation of the downdating algorithms in [4, 9, 20] for deleting a single row from a QR factorization and fashioned the matrix 2-norm formulation for a block downdating algorithm designed to delete p rows from a matrix. Similar to results shown in [4], if we are asked to delete p rows from a QR decomposition with a near left orthogonal factor U satisfying (1.13), we can obtain a QR decomposition for the remaining $m - p$ rows that has a new left orthogonal factor $\overline{U}$ whose loss of orthogonality can be bounded as in Theorem 3.3. Our numerical tests indicate that repeated block updates and downdates often have a correcting effect on the loss of orthogonality.

Acknowledgments. The author completed much of this work while visiting the University of California at Berkeley as the guest of James Demmel. That visit provided a stimulating and helpful atmosphere to work on the ideas in this paper as well as some other ideas. During that time, a conversation with Ming Gu had an important influence on this work. Thanks also to Lothar Reichel and to two careful referees for helpful suggestions that improved this manuscript.

REFERENCES

[1] N. ABDELMALEK, *Round off error analysis for Gram–Schmidt method and solution of linear least squares problems*, Nordisk Tidskr. Informationsbehandling (BIT), 11 (1971), pp. 354–367.

[2] J. BARLOW, H. ERBAY, AND I. SLAPNIČAR, *An allternative algorithm for the refinement of ULV decomposition*, SIAM J. Matrix Anal. Appl., 27 (2005), pp. 198–211.

[3] J. BARLOW AND A. SMOKTUNOWICZ, *Reorthogonalized block classical Gram-Schmidt*, Numer. Math., 123 (2013), pp. 395–423.

[4] J. BARLOW, A. SMOKTUNOWICZ, AND H. ERBAY, *Improved Gram–Schmidt downdating methods*, BIT, 45 (2005), pp. 259–285.

[5] J. BARLOW, P. YOON, AND H. ZHA, *An algorithm and a stability theory for downdating the ULV decomposition*, BIT, 36 (1996), pp. 14–40.

[6] A. BJÖRCK, *Solving linear least squares problems by Gram–Schmidt orthogonalization*, Nordisk Tidskr. Informationsbehandling (BIT), 7 (1967), pp. 1–21.

[7] P. BUSINGER AND G. GOLUB, *Linear least squares solutions by Householder transformations*, Numer. Math., 7 (1965), pp. 269–278.

[8] T. CHAN, *An improved algorithm for computing the singular value decomposition*, ACM Trans. Math. Software, 8 (1982), pp. 72–83.

[9] J. W. DANIEL, W. B. GRAGG, L. KAUFMAN, AND G. W. STEWART, *Reorthogonalization and stable algorithms for updating the Gram-Schmidt QR factorization*, Math. Comp., 30 (1976), pp. 772–795.

[10] J. DONGARRA, J. DUCROZ, I. DUFF, AND S. HAMMARLING, *A set of level 3 basic linear algebra subprograms*, ACM Trans. Math. Software, 16 (1990), pp. 1–17.

[11] W. FERNG, G. GOLUB, AND R. PLEMMONS, *Adaptive Lanczos methods for recursive condition estimation*, Numer. Algorithms, 1 (1991), pp. 1–20.

[12] L. GIRAUD, J. LANGOU, M. ROZLOŽNIK, AND J. VAN DEN ESHOF, *Rounding error analysis of the classical Gram–Schmidt orthogonalization process*, Numer. Math., 101 (2005), pp. 87–100.

[13] G. GOLUB AND W. KAHAN, *Calculating the singular values and pseudoinverse of a matrix*, Soc. Indust. Appl. Math. Ser. B Numer. Anal., 2 (1965), pp. 205–224.

[14] G. GOLUB AND C. VAN LOAN, *Matrix Computations*, 4th ed., Johns Hopkins University Press, Baltimore, 2013.

[15] R. HORN AND C. JOHNSON, *Matrix Analysis*, 2nd ed., Cambridge University Press, Cambridge, 2013.

[16] C. LAWSON AND R. HANSON, *Solving Least Squares Problems*, Prentice-Hall, Englewood Cliff, 1974.

[17] Q. LIU, *Modified Gram-Schmidt-based methods for block downdating the Cholesky factorization*, J. Comput. Appl. Math., 235 (2011), pp. 1897–1905.

[18] M. OVERTON, N. GUGLIELMI, AND G. STEWART, *An efficient algorithm for generalized null space decomposition*, SIAM J. Matrix Anal. Appl., to appear.

[19] B. PARLETT, H. SIMON, AND L. STRINGER, *On estimating the largest eigenvalue with the Lanczos algorithm*, Math. Comp., 38 (1982), pp. 153–166.

[20] K. YOO AND H. PARK, *Accurate downdating of a modified Gram–Schmidt QR decomposition*, BIT, 36 (1996), pp. 166–181.