ROW HOUSEHOLDER TRANSFORMATIONS FOR RANK-k CHOLESKY INVERSE MODIFICATIONS

By

Adam W. Bojanczyk
James G. Nagy
and
Robert J. Plemmons

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Adam W. Bojanczyk,* James G. Nagy,† and Robert J. Plemmons ‡

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Abstract

Householder transformations applied from the left are generally used to zero a contiguous sequence of entries in a column of a matrix A. Our purpose in this paper is to introduce new *row Householder* and *row hyperbolic Householder* transformations which are also applied from the left, but now zero a contiguous sequence of entries in a row of A. We then show how these row Householder transformations can be used to design efficient sliding data window recursive least squares covariance algorithms, which are base upon rank-k modifications to the inverse Cholesky factor, R^{-1}, of the covariance matrix. The algorithms are rich in matrix-matrix BLAS-3 computations, making them efficient on vector and parallel architectures. Preliminary numerical experiments are reported, comparing these row Householder-based rank-k modification schemes with k applications of the classical updating and downdating covariance schemes which use Givens and hyperbolic rotations.

Abbreviated Title. Row Householder Transformations

Key Words. (Row) Householder transformations, Cholesky updating and downdating, recursive least squares, BLAS-3 computations.

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*School of Electrical Engineering, Cornell University, E&TC Building, Ithaca, NY 14850-3801.

†Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, MN 55455.

‡Department of Mathematics and Computer Science, Wake Forest University, P.O. Box 7388, Winston-Salem, NC 27109. Research supported in part by the US Air Force under grant AFOSR-91-0163.

1 Introduction

In this paper we introduce new *row Householder* and *row hyperbolic Householder* transformations, which zero one *row* of a matrix at a time when applied from the left. These transformations are a generalization of an idea first proposed by Bartels and Kaufman [3] and, as in classical Householder transformations, are rank-1 modifications to the identity matrix. We will discuss their use in developing efficient algorithms for recursive least squares problems of the sliding window type.

In [3], Bartels and Kaufman consider schemes for modifying R, where $X = QR$ and X is the given data matrix, subject to rank-2 updates of X. To solve these problems efficiently, they introduce a modified Householder transformation which, when applied from the left, can zero entries simultaneously in two column vectors. Here we suggest a generalization to this transformation which, when applied from the left, can eliminate all elements in a row of a matrix. We then illustrate how these transformations can be very useful in developing efficient algorithms for modifying R^{-1} (rather than R) subject to rank-k changes in X. (Algorithms for modifying R subject to rank-k changes in X were considered in [15] and analyzed in [6]). We show, in terms of operations counts, that our algorithms are more efficient for modifying R^{-1} than k applications of the classical algorithms based on Givens and hyperbolic rotations (see, for example, Pan and Plemmons [12].) Moreover, as Bartels and Kaufman show for rank-2 modifications, our algorithms are rich in matrix-matrix BLAS-3 computations, making them even more economical on high performance architectures than k applications of the rank-1 modification schemes.

The outline of this paper is as follows. In Section 1 we introduce the new row Householder transformations. In Section 2 we show how these transformations can be used to efficiently update least squares solutions when observations are added and/or deleted from the linear system. In Section 4 we consider downdating computations. In Section 5 we discuss compact WY representation of products of row Householder transformations, and in Section 6 we provide some numerical experiments and some concluding remarks.

2 Row Householder Transformations

In this section we introduce a row Householder transformation, which is a rank 1 modification to the identity matrix, that when applied from the left will eliminate k elements in a row of a matrix at once. We will split our discussion into two subsections. The first will consider row Householder transformations which are orthogonal, and the second subsection will consider transformations which are pseudo orthogonal with respect to a signature matrix Φ.

2.1 Orthogonal Row Householder Transformations

The row Householder transformation we introduce in this section is a generalization of an idea first proposed by Bartels and Kaufman [3]. Let B be a $(k+1) \times k$ matrix of the form

$$B = \begin{bmatrix} b^T \\ D \end{bmatrix},$$

where D is nonsingular.

Suppose we wish to eliminate the first row of B (*i.e.,* b^T) by premultiplying by an orthogonal matrix. (Note that this discussion applies, in general, to the case where we want to eliminate the j^{th} row of B. In this case we simply permute the j^{th} row to the top of B.) In order to accomplish this we construct a Householder transformation

$$P = I - \frac{1}{\lambda} pp^T, \tag{1}$$

where $p \in \Re^{k+1}$ and $\lambda = p^T p/2$, such that

$$PB = \begin{bmatrix} 0^T \\ \tilde{D} \end{bmatrix}. \tag{2}$$

In order to illustrate how this can be done let

$$p = \begin{bmatrix} \pi \\ q \end{bmatrix}$$

where π is the first component of p and q is the vector consisting of the last k components of p.

If P has the form (1) and satisfies (2), then we obtain the relation

$$\begin{bmatrix} b^T \\ D \end{bmatrix} - \frac{1}{\lambda} p(\pi b^T + q^T D) = \begin{bmatrix} 0 \\ \tilde{D} \end{bmatrix}.$$

That is,

$$D^T q = \mu b, \tag{3}$$

where $\mu = (\lambda/\pi - \pi)$. We note that we have one degree of freedom here. That is, if we choose μ, then we can solve (3) for q. Once q is known, we can use $\mu = (\lambda/\pi - \pi)$ to find π. Specifically,

$$\pi = -\mu - \text{sgn}(\mu)\sqrt{\mu^2 + q^T q}.$$

Since μ is a free variable, we suggest choosing $\mu = 1/\|b\|_2$. If $\|b\|_2 = 0$, we simply set $P = I$.

In general, we have the following algorithm.

Algorithm ROWHT

Input: $B^T = [b \;\; D^T]$, where $D \in \Re^{k\times k}$ is nonsingular.

Output: $p \in \Re^{k+1}$, where $P = I - \frac{1}{\lambda}pp^T$, $\lambda = p^T p/2$, has the property that the first row of PB is all zeros.

if $\|b\|_2 = 0$
- $p = 0$, $P = I$

else
- $\mu = 1/\|b\|_2$
- solve $D^T q = \mu b$
- $\pi = -\mu - \sqrt{\mu^2 + q^T q}$
- $p^T = [\pi \;\; q^T]$

A Householder transformation (computed by algorithm ROWHT) which zeros elements in a row vector will be called a *row* Householder transformation to differentiate it from the classical *column* Householder transformation which zeros elements in a column vector.

Note that finding p requires solving a $k \times k$ system of linear equations which in general amounts to $O(k^3)$ operations. However, if the QR decomposition of D is available, the cost of finding p is decreased to $O(k^2)$ operations.

In the sequel we will encounter the problem of annihilating r rows, $r \geq 1$, of a $(k+r) \times k$ matrix by finding an orthogonal P such that

$$P \begin{bmatrix} b_1^T \\ \vdots \\ b_r^T \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{D} \end{bmatrix}.$$

Such a P can be constructed as a product of r row Householder transformations P_i, $P = P_r P_{r-1} \cdots P_1$, with P_i annihilating row i of the matrix. As the major cost of determining such transformations is in solving systems of linear equations, it is worthwhile to attempt to decrease this cost. This can be done by maintaining and updating the QR decomposition of the bottom $k \times k$ submatrix. For the sake of illustration we show the first step of this process. Let

$$B = \begin{bmatrix} b_1^T \\ \vdots \\ b_r^T \\ D \end{bmatrix},$$

and let

$$D_0 \equiv D = Q_0 R_0$$

be the QR decomposition of D which is assumed to be given. Let $P_1 = I - p_1 p_1^T/\lambda_1$ be a modified Householder transformation such that

$$P_1 \begin{bmatrix} b_1^T \\ b_2^T \\ \vdots \\ b_r^T \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ b_2^T \\ \vdots \\ b_r^T \\ D_1 \end{bmatrix}.$$

Then the form of P_1 implies that

$$D_1 = D_0 - \frac{1}{\lambda_1} p_1 b_1^T = Q_0 R_0 - \frac{1}{\lambda_1} p_1 b_1^T \tag{4}$$

Thus the QR factorization of D_1 can be obtained at the cost of $13k^2$ multiplications (and $13k^2$ additions) by updating the QR factorization of D_0 after a rank-1 change of D_0, [9]. This has to be repeated $r-1$ times resulting in the total of $O(rk^2)$ operations for the overall process of computing all transformations P_i, $i = 1, \cdots, r$.

2.2 Row Hyperbolic Householder Transformations

Let Φ =diag(± 1) be an $(k+1) \times (k+1)$ diagonal matrix, and suppose p is a vector of length $k+1$ with $p^T \Phi p > 0$. Then a Hyperbolic Householder transformation is a matrix of the form

$$P = \Phi - \frac{1}{\lambda} p p^T \tag{5}$$

where $\lambda = \frac{1}{2} p^T \Phi p$. The matrix P is a *pseudo orthogonal* matrix with respect to Φ, *i.e.,*

$$P^T \Phi P = \Phi.$$

Hyperbolic Householder transformations are typically used to introduce zeros into a column of a matrix, and were studied in detail by Rader and Steinhardt [15]. Here we introduce a *row Hyperbolic Householder* transformation which eliminates entries in a row of a matrix. The discussion in this subsection is similar to that given in §2.1 for the (orthogonal) row Householder transformations.

Let B be a $(k+1) \times k$ matrix of the form

$$B = \begin{bmatrix} b^T \\ D \end{bmatrix},$$

where D is nonsingular. Suppose we wish to eliminate the first row of B using a transformation of the form (5). As in §2.1 this can be illustrated as follows. Let

$$p = \begin{bmatrix} \pi \\ q \end{bmatrix}$$

where π is the first component of p and q is a vector consisting of the last k components of p. Now suppose

$$P\begin{bmatrix} b^T \\ D \end{bmatrix} = \begin{bmatrix} 0^T \\ \tilde{D} \end{bmatrix}.$$

Then, assuming P has the form (5), where

$$\Phi = \begin{bmatrix} \phi_1 & 0 \\ 0 & \tilde{\Phi} \end{bmatrix},$$

we have

$$\begin{bmatrix} \phi_1 & 0 \\ 0 & \tilde{\Phi} \end{bmatrix}\begin{bmatrix} b^T \\ D \end{bmatrix} - \frac{1}{\lambda}\begin{bmatrix} \pi \\ q \end{bmatrix}(\pi b^T + q^T D) = \begin{bmatrix} 0^T \\ \tilde{D} \end{bmatrix}.$$

Thus, we obtain

$$D^T q = \mu b \tag{6}$$

where $\mu = (\lambda\phi_1/\pi - \pi)$.

Now, if we fix μ, then we can solve (6) for q. Once q is known, then, using $\mu = (\lambda\phi_1/\pi - \pi)$, we have

$$\pi^2 + \pi\mu - \phi_1\lambda = 0.$$

Thus, since

$$\lambda = \frac{1}{2}p^T\Phi p = \frac{1}{2}(\phi_1\pi^2 + q^T\tilde{\Phi}q),$$

and since $\phi_1^2 = 1$, we obtain the relation

$$\pi^2 + 2\pi\mu - \phi_1 q^T\tilde{\Phi}q = 0.$$

Thus, if

$$\mu^2 + \phi_1 q^T\tilde{\Phi}q \geq 0, \tag{7}$$

we have

$$\pi = -\mu - \operatorname{sgn}(\mu)\sqrt{\mu^2 + \phi_1 q^T\tilde{\Phi}q}.$$

We point out that the requirement $\mu^2 + \phi_1 q^T\tilde{\Phi}q \geq 0$ is satisfied for our problem of inverse matrix modifications. This will be discussed in further detail in Section 4.

As for the (orthogonal) row Householder transformations, we suggest choosing $\mu = 1/\|b\|_2$, and $P = \Phi$ if $\|b\|_2 = 0$. The following algorithm summarizes the above discussion.

Algorithm ROWHHT

Input: $B^T = [b \;\; D^T]$, where $D \in \Re^{k \times k}$ is nonsingular.

Output: $p \in \Re^{k+1}$, where $P = \Phi - \frac{1}{\lambda} pp^T$, $\lambda = p^T \Phi p/2$, has the property that the first row of PB is all zeros.

if $\|b\|_2 = 0$
  $p = 0$, $P = \Phi$
else
  $\mu = 1/\|b\|_2$
  solve $D^T q = \mu b$
  $\pi = -\mu - \sqrt{\mu^2 + \phi_1 q^T \tilde{\Phi} q}$
  $p^T = [\pi \;\; q^T]$

Similarly as for the orthogonal case, a hyperbolic Householder transformation (computed by algorithm ROWHHT) which zeros elements in a row vector will be called a *row* hyperbolic Householder transformation. If the QR decomposition of D is available the cost of finding p is of the order of $O(k^2)$ operations. For the problem of annihilating r rows, $r \geq 1$, of a $(k+r) \times k$ matrix B that cost is of the order of $O(rk^2)$ operations (see the discussion at the end of Section 2.1).

3 Modifying the Inverse Cholesky Factor

Let X be a real $m \times n$ matrix with full column rank, and let s be a real vector of length m. Consider the least squares problem

$$\min \|s - Xw\|_2. \tag{8}$$

It is well known (see, for instance [10]) that this problem can be solved by finding the QR factorization of X. Specifically, let $X = QR$, where Q is an $m \times n$ matrix with orthonormal columns, and R is an $n \times n$ upper triangular matrix. Then the solution to (8) is given by

$$w = R^{-1} Q^T s.$$

In many applications, such as signal processing, it is often required to recalculate w when successive observations (*i.e.*, equations) are added to and/or deleted from (8). In this section we consider *updating* the solution w to $\hat{w}$ when k new observations are added to the system, and *downdating* w to $\check{w}$ when k observations are removed from the system. This method is called *recursive least squares* (RLS), and can be reformulated as a k-step process of k successive modifications of w after addition/deletion of a single observation. Such rank-1 modifications are most often realized by plane rotations and have been studied by many authors. In this paper we treat multiple addition/deletion of observation as a block process in a manner analogous to that presented in [15]. However, unlike in [15] where the the upper triangular factor in the QR decomposition of X was modified, this paper proposes algorithms for direct modification of the inverse of the triangular factor. This procedure is called the covariance method in RLS computations. We will show how the row Householder transformations described in Section 2 can be used to design efficient sliding data window RLS covariance algorithms.

3.1 Inverse Updating

We now describe a method for updating w to $\hat{w}$ after the addition of k new observations. Let w be the solution to

$$\min \|s - Xw\|_2$$

and let R be the upper triangular factor in the QR factorization of X. Suppose k new observations

$$\left[\begin{array}{cc} Y^T & u \end{array} \right],$$

where $Y^T \in \Re^{k \times n}$ and $u \in \Re^k$, are added to the system. We first show how R^{-1} can be updated to $\hat{R}^{-1}$, where

$$\hat{X} = \left[\begin{array}{c} X \\ Y^T \end{array} \right] = \hat{Q}\hat{R}.$$

Using this $\hat{R}^{-1}$, we then show how the solution w of

$$\min \|s - Xw\|_2 \tag{9}$$

can be updated to the solution $\hat{w}$ of

$$\min \left\| \left[\begin{array}{c} s \\ u \end{array} \right] - \left[\begin{array}{c} X \\ Y^T \end{array} \right] \hat{w} \right\|_2 . \tag{10}$$

3.2 Updating of R^{-1}

Let $X = QR$, with R known, and suppose we wish to find $\hat{R}$ where

$$\hat{X} = \left[\begin{array}{c} X \\ Y^T \end{array} \right] = \hat{Q}\hat{R}$$

is the QR factorization of $\hat{X}$. It is well known that this can be accomplished by finding an orthogonal matrix H such that

$$H \left[\begin{array}{c} R \\ Y^T \end{array} \right] = \left[\begin{array}{c} \hat{R} \\ 0^T \end{array} \right] . \tag{11}$$

We pick H to be a product of $(n+k) \times (n+k)$ Householder transformations H_i, $i = 1, \cdots, n$, such that H_i annihilates subdiagonal elements in column i, $i = 1, \cdots, n$, of the matrix

$$H_{i-1} \cdots H_2 H_1 \left[\begin{array}{c} R \\ Y^T \end{array} \right] .$$

It is known that if H is orthogonal and satisfies (11), then H also updates the inverse of R, namely

$$H\begin{bmatrix} R^{-T} \\ 0^T \end{bmatrix} = \begin{bmatrix} \hat{R}^{-T} \\ E^T \end{bmatrix}, \tag{12}$$

where E is an $n \times k$ matrix. To see this, note that

$$I = \begin{bmatrix} R^{-1} & 0 \end{bmatrix}\begin{bmatrix} R \\ Y^T \end{bmatrix} = \begin{bmatrix} R^{-1} & 0 \end{bmatrix} H^T H \begin{bmatrix} R \\ Y^T \end{bmatrix} = \begin{bmatrix} U & E \end{bmatrix}\begin{bmatrix} \hat{R} \\ 0^T \end{bmatrix}.$$

Thus $U = R^{-1}$.

We would like to be able to work with R^{-T}, and not with R explicitly, since the triangular solves needed in solving systems associated with R can then be replaced by matrix-vector or matrix-matrix multiplications. The following lemma shows how we can construct an orthogonal matrix H satisfying (11) and avoid using R explicitly.

Lemma 1 *Let $\hat{V} = -R^{-T}Y$, and let $\hat{H}$ be an orthogonal matrix such that*

$$\hat{H}\begin{bmatrix} \hat{V} \\ I_k \end{bmatrix} = \begin{bmatrix} 0 \\ \hat{D} \end{bmatrix}, \tag{13}$$

where I_k is the $k \times k$ identity matrix and $\hat{D}$ is a $k \times k$ matrix. Then

$$\hat{H}\begin{bmatrix} R \\ Y^T \end{bmatrix} = \begin{bmatrix} U \\ 0 \end{bmatrix} \tag{14}$$

If U is upper triangular then $U = \hat{R}$ and

$$\hat{H}\begin{bmatrix} R^{-T} \\ 0^T \end{bmatrix} = \begin{bmatrix} \hat{R}^{-T} \\ E^T \end{bmatrix}. \tag{15}$$

where $E = R^{-1}\hat{V}\hat{D}^{-1}$.

Proof: The proof for $k = 1$ can be found in [12]. For $k > 1$ one proceeds as follows. Let

$$\hat{H}\begin{bmatrix} \hat{V} & R \\ I_k & Y^T \end{bmatrix} = \begin{bmatrix} 0 & U \\ \hat{D} & \hat{Y}^T \end{bmatrix}. \tag{16}$$

From the orthogonality of $\hat{H}$, the definition of $\hat{V}$ and the fact that $\hat{D}$ is nonsingular, it follows that $\hat{Y} = 0$ and hence

$$R^T R + YY^T = U^T U .$$

Thus if U is upper triangular with positive diagonal elements then $U = \hat{R}$. From (12), for the inverse we have an analogous relation, namely

$$\hat{H}\begin{bmatrix} \hat{V} & R^{-T} \\ I_k & 0 \end{bmatrix} = \begin{bmatrix} 0 & \hat{R}^{-T} \\ \hat{D} & E^T \end{bmatrix}. \tag{17}$$

Now (17) implies

$$\begin{bmatrix} \hat{V}^T\hat{V}+I & \hat{V}^T R^{-T} \\ R^{-1}\hat{V} & R^{-1}R^{-T} \end{bmatrix} = \begin{bmatrix} \hat{D}^T\hat{D} & \hat{D}^T E^T \\ E\hat{D} & \hat{R}^{-1}\hat{R}^{-T}+EE^T \end{bmatrix}$$

from which one obtains that

$$E = -R^{-1}\hat{V}\hat{D}^{-1} .$$

This completes the proof. □

The relation (17) shows that it is possible to work with the inverses only. The condition that has to be satisfied is that application of the transformation $\hat{H}$ in (17) has to result in a lower triangular matrix U^{-T}.

We now show how to construct an orthogonal matrix $\hat{H}$ satisfying (13) and (14). To do this, we will use the row Householder transformation. More precisely, suppose that we have constructed row Householder transformations $P_1, P_2, \ldots, P_j$ such that

$$P_j \cdots P_2 P_1 \begin{bmatrix} \hat{V} \\ I \end{bmatrix} = \begin{bmatrix} 0_j \\ \hat{V}_j \\ \hat{D}_j \end{bmatrix},$$

where 0_j denotes the $j \times k$ matrix of all zeros, and $\hat{V}_j \in \Re^{(n-j)\times k}$ and $\hat{D}_j \in \Re^{k\times k}$. Then using Algorithm ROWHT, we find $\hat{p}_j^T = [\pi_j \ \ q_j]$ so that

$$\hat{P}_j \begin{bmatrix} \hat{v}_j^T \\ \hat{D}_j \end{bmatrix} = \begin{bmatrix} 0^T \\ \hat{D}_{j+1} \end{bmatrix},$$

where $\hat{v}_j^T$ is the first row of $\hat{V}_j$ and $\hat{P}_j = I - \frac{1}{\lambda_j}\hat{p}_j\hat{p}_j^T$. Then P_{j+1} is simply given by

$$P_{j+1} = I - \frac{1}{\lambda_j} p_j p_j^T,$$

where $p_j = [0, \cdots, 0, \ \pi_j, \ 0, \cdots, 0, \ q_j]$ (the j-th component of p_j is π_j, the last k components of p_j form the vector q_j, and all other components are zeros). That is,

$$P_{j+1} = \begin{bmatrix} I_j & 0 & 0 & 0 \\ 0 & -\frac{1}{\lambda_j}\pi_j^2 & 0 & -\frac{\pi_j}{\lambda_j} q_j^T \\ 0 & 0 & I_{n-j-1} & 0 \\ 0 & -\frac{\pi_j}{\lambda_j} q_j & 0 & -\frac{1}{\lambda_j} q_j q_j^T \end{bmatrix}.$$

It is now easy to see that $P = P_n \cdots P_2 P_1$ satisfies (13) and hence

$$P_n \cdots P_2 P_1 \begin{bmatrix} R^{-T} \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{R}^{-T} \\ E^T \end{bmatrix},$$

as $\hat{R}^{-T}$ is by construction lower triangular and hence the desired downdated factor.

Now that we have a scheme for updating R^{-T}, we need to use this information to efficiently update the least squares solution w to $\hat{w}$. The following theorem shows how this can be done.

Theorem 1 *Let $\hat{H}$ satisfies (17), that is*

$$\hat{H}\begin{bmatrix} \hat{V} & R^{-T} \\ I_k & 0 \end{bmatrix} = \begin{bmatrix} 0 & \hat{R}^{-T} \\ \hat{D} & E^T \end{bmatrix}.$$

If w is the solution to (9), then the solution to (10) is given by

$$\hat{w} = w - E\hat{D}^{-T}(u - Y^T w)$$

Moreover $E = -R^{-1}\hat{V}\hat{D}^{-1}$.

Proof: Let $\hat{s}^T = [s^T \;\; u^T]$. We know from the normal equations that

$$\hat{w} = (\hat{X}^T\hat{X})^{-1}\hat{X}^T\hat{s} = (X^TX + YY^T)^{-1}(X^Ts + Yu).$$

Using the Sherman-Morrison-Woodbury formula, we have

$$(X^TX + YY^T)^{-1} = C - CY(I + Y^TCY)^{-1}Y^TC$$

where $C = (X^TX)^{-1}$. Thus

$$\hat{w} = \left[C - CY(I + Y^TCY)^{-1}Y^TC\right](X^Ts + Yu).$$

But $X^TX = X^Ts$ implies that

$$\hat{w} = \left[C - CY(I + Y^TCY)^{-1}Y^TC\right](C^{-1}w + Yu).$$

Now from $\hat{V} = -R^{-T}Y$ it follows that

$$R^{-1}\hat{V} = -R^{-1}R^{-T}Y = -CY.$$

Thus

$$I + Y^TCY = I + \hat{V}^T\hat{V} = \hat{D}^T\hat{D}.$$

We now have

$$\begin{aligned} \hat{w} &= \left[C - CY(\hat{D}^T\hat{D})^{-1}Y^TC\right](C^{-1}w + Yu) \\ &= w + CYu - CY(\hat{D}^T\hat{D})^{-1}Y^Tw - CY(\hat{D}^T\hat{D})^{-1}Y^TCYu. \end{aligned}$$

Letting $E = R^{-1}\hat{V}\hat{D}^{-1} = -CY\hat{D}^{-1}$, and using the observation that $Y^TCY = \hat{D}^T\hat{D} - I$, we obtain

$$\begin{aligned} \hat{w} &= w - E\hat{D}u + E\hat{D}^{-T}Y^Tw + E\hat{D}^{-T}(\hat{D}^T\hat{D} - I)u \\ &= w + E\left[-\hat{D}^{-T}u + \hat{D}^{-T}Y^Tw\right] \\ &= w - E\hat{D}^{-T}(u - Y^Tw). \quad \square \end{aligned}$$

Thus, summarizing the results of this section, we obtain the following algorithm.

Algorithm IUP-k
Given: R^{-T} and w, where $X = QR$ and w solves (9).
Input: New set of k observations $[Y^T \ u]$.
Then this algorithm computes $\hat{R}^{-T}$ and $\hat{w}$, where

$$\hat{X} = \begin{bmatrix} X \\ Y^T \end{bmatrix} = \hat{Q}\hat{R}$$

and $\hat{w}$ solves (10).

1. Compute $\hat{V} = -R^{-T}Y$.
   Cost $kn^2/2$ multiplications.

2. Find $\hat{H} = P_n \cdots P_2 P_1$, where P_i are row Householder Transformations, such that
   $$\hat{H} \begin{bmatrix} \hat{V} \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ \hat{D} \end{bmatrix}$$
   Cost $13 \cdot k^2 n$ multiplications.

3. Update R^{-T} to $\hat{R}^{-T}$:
   $$\hat{H} \begin{bmatrix} R^{-T} \\ 0 \end{bmatrix} = \begin{bmatrix} \hat{R}^{-T} \\ E^T \end{bmatrix}$$
   Cost kn^2 multiplications.

4. Update w to $\hat{w}$:
   $$\hat{w} = w - E\hat{D}^{-T}(u - Y^T w)$$
   Cost $\frac{3}{2}k^2 + 2kn$ multiplications (as from (4) the QR decomposition of D is already available from step 2).

The total cost for Algorithm IUP-k is $\frac{3}{2} \cdot kn^2 + 13 \cdot k^2 n + 2 \cdot kn + \frac{3}{2}k^2$ multiplications. We note that the straight forward implementation of the rank-1 method of Pan and Plemmons [12] would require $\frac{5}{2}kn^2 + O(k^2 n)$ multiplications.

4 Inverse Downdating

We now describe a method for downdating w to $\breve{w}$ after the deletion of k observations. Let

$$s = \begin{bmatrix} \breve{s} \\ d \end{bmatrix}, \quad X = \begin{bmatrix} \breve{X} \\ Z^T \end{bmatrix}$$

and w be the solution to

$$\min \|s - Xw\|_2$$

Suppose further that R is the upper triangular factor in the QR factorization of X, and that the k observations

$$\begin{bmatrix} Z^T & d \end{bmatrix},$$

where $Z^T \in \Re^{k \times n}$ and $d \in \Re^k$, are to be deleted from the system. We first show how R^{-1} can be updated to $\breve{R}^{-1}$, where

$$\breve{X} = \breve{Q}\breve{R}$$

Using this $\breve{R}^{-1}$, we then show how the solution w of

$$\min \|s - Xw\|_2 \tag{18}$$

can be downdated to the solution $\breve{w}$ of

$$\min \|\breve{s} - \breve{X}\breve{w}\|_2. \tag{19}$$

For the $n \times n$ upper triangular factor R, where

$$X = \begin{bmatrix} \breve{X} \\ Z^T \end{bmatrix} = QR\,,$$

and for the $n \times k$ Z, $k + n < m$, such that

$$R^T R - ZZ^T > 0, \tag{20}$$

we want to determine the downdated Cholesky factor $\breve{R}$ of $\breve{X}$ by "removing" Z^T from R. That is we want $\breve{R}$ to satisfy

$$\breve{R}^T \breve{R} = R^T R - ZZ^T\,.$$

In [15] it is shown that this can be accomplished by finding a hyperbolic transformation $\breve{H}$ with respect to the signature Φ,

$$\Phi = \begin{bmatrix} I_n & 0 \\ 0 & -I_k \end{bmatrix},$$

such that

$$\breve{H} \begin{bmatrix} R \\ Z^T \end{bmatrix} = \begin{bmatrix} \breve{R} \\ 0^T \end{bmatrix}. \tag{21}$$

We pick $\check{H}$ to be a product of $(n+k)\times(n+k)$ Hyperbolic Householder transformations H_i, $i=1,\cdots,n$, such that H_i annihilates subdiagonal elements in column i, $i=1,\cdots,n$, of the matrix

$$H_{i-1}\cdots H_2H_1\begin{bmatrix} R \\ Z^T \end{bmatrix}.$$

Similarly as for orthogonal transformations, if the hyperbolic $\check{H}$ satisfies (21) then $\check{H}$ also downdates the inverse of R. To see this, note that

$$I=\begin{bmatrix} R^{-1} & 0 \end{bmatrix}\Phi\begin{bmatrix} R \\ Z^T \end{bmatrix}=\begin{bmatrix} R^{-1} & 0 \end{bmatrix}\check{H}^T\Phi\check{H}\begin{bmatrix} R \\ Z^T \end{bmatrix}=\begin{bmatrix} U & F \end{bmatrix}\begin{bmatrix} \check{R} \\ 0^T \end{bmatrix}.$$

Thus $U=\check{R}^{-1}$, and

$$\check{H}\begin{bmatrix} R^{-T} \\ 0 \end{bmatrix}=\begin{bmatrix} \check{R}^{-T} \\ F^T \end{bmatrix}. \tag{22}$$

We would like to work with the inverses directly and hence need a way for constructing H satisfying (21) without any explicit reference to R. The following lemma provides means just for that.

Lemma 2 *Assume $R^TR-ZZ^T>0$. Let $\check{V}=R^{-T}Z$, and let H be a hyperbolic (with respect to Φ) transformation such that*

$$\check{H}\begin{bmatrix} \check{V} \\ I_k \end{bmatrix}=\begin{bmatrix} 0 \\ \check{D} \end{bmatrix}, \tag{23}$$

where I_k is the $k\times k$ identity matrix and $\check{D}$ is a $k\times k$ matrix. Then

$$\check{H}\begin{bmatrix} R \\ Z^T \end{bmatrix}=\begin{bmatrix} \check{U} \\ 0 \end{bmatrix} \tag{24}$$

If $\check{U}$ is upper triangular, then $\check{U}=\check{R}$ and

$$\check{H}\begin{bmatrix} R^{-T} \\ 0^T \end{bmatrix}=\begin{bmatrix} \check{R}^{-T} \\ F^T \end{bmatrix}. \tag{25}$$

where $F=-R^{-1}\check{V}\check{D}^{-1}$.

Proof: The proof for $k=1$ can be found in [12]. For $k>1$ one proceeds as follows. Let

$$\check{H}\begin{bmatrix} \check{V} & R \\ I_k & Z^T \end{bmatrix}=\begin{bmatrix} 0 & \check{U} \\ \check{D} & \check{Z}^T \end{bmatrix}. \tag{26}$$

From the definition of $\check{V}$ and the that fact that H is hyperbolic (with respect to Φ) we obtain that

$$\begin{bmatrix} \check{V}^T\check{V}-I_k & 0 \\ 0 & R^TR-ZZ^T \end{bmatrix}=\begin{bmatrix} -\check{D}^T\check{D} & -\check{D}^T\check{Z}^T \\ -\check{Z}\check{D} & \check{U}^T\check{U}-\check{Z}\check{Z}^T \end{bmatrix}. \tag{27}$$

Comparing upper left entries on both sides we get

$$-\check{D}^T\check{D} = \check{V}^T\check{V} - I_k = Z^T R^{-1} R^{-T} Z - I_k \,.$$

Now, as $R^T R - ZZ^T > 0$ then $I_k - Z^T R^{-1} R^{-T} Z > 0$ and hence $\check{D}$ is nonsingular.

From (27) and the nonsingularity of $\check{D}$ it follows that $\check{Z} = 0$ and hence

$$R^T R - ZZ^T = \check{U}^T \check{U} \,.$$

Thus if $\check{U}$ is upper triangular (with positive diagonal elements) then $U = \check{R}$. From (22), for the inverse we have an analogous relation, namely

$$\check{H} \begin{bmatrix} \check{V} & R^{-T} \\ I_k & 0 \end{bmatrix} = \begin{bmatrix} 0 & \check{R}^{-T} \\ \check{D} & F^T \end{bmatrix} . \tag{28}$$

Now (28) implies

$$\begin{bmatrix} \check{V}^T\check{V} - I_k & \check{V}^T R^{-T} \\ R^{-1}\check{V} & R^{-1}R^{-T} \end{bmatrix} = \begin{bmatrix} -\check{D}^T\check{D} & -\check{D}^T F^T \\ -F\check{D} & \check{R}^{-1}\check{R}^{-T} - FF^T \end{bmatrix}$$

from which one obtains that

$$F = -R^{-1}\check{V}\check{D}^{-1} \,.$$

This completes the proof.

□

The relation (28) shows that, as for updating the inverse, it is also possible to downdate the inverse directly. The condition that has to be satisfied is that application of $\check{H}$ in (28) has to result in a lower triangular matrix U^{-T}.

The construction of $\check{H}$ satisfying (28) is analogous to that described at the end of Section 3.2. Now however $\check{H}$ is constructed as a product of row hyperbolic Householder transformations. The only thing that needs to be verified is that the condition (7) is always satisfied for each factor that makes up $\check{H}$.

Suppose that we have constructed row hyperbolic (with respect to Φ) Householder transformations $P_1, P_2, \ldots, P_j$ such that

$$P_j \cdots P_2 P_1 \begin{bmatrix} \check{V} \\ I \end{bmatrix} = \begin{bmatrix} 0_j \\ \check{V}_j \\ \check{D}_j \end{bmatrix},$$

where 0_j denotes the $j \times k$ matrix of all zeros, $\check{V}_j \in \Re^{(n-j)\times k}$ and $\check{D}_j \in \Re^{k\times k}$. Let $\check{v}_j^T$ be the first row of $\check{V}_j$ and let

$$\check{\Phi} = \begin{bmatrix} 1 & 0 \\ 0 & -I_k \end{bmatrix}.$$

We wish to use Algorithm ROWHHT to find $\check{p}_j^T = [\check{\pi}_j \;\; \check{q}_j]$ so

$$\check{P}_{j+1} = \check{\Phi} - \frac{1}{\check{\lambda}_j}\check{p}_j\check{p}_j^T,$$

satisfies

$$\check{P}_{j+1}\begin{bmatrix}\check{v}_j^T\\ \check{D}_j\end{bmatrix}=\begin{bmatrix}0^T\\ \check{D}_{j+1}\end{bmatrix}.$$

Note first that $\check{D}_j$ is nonsingular. The condition (7) for P_j becomes

$$\check{\mu}_j^2-\check{q}_j^T\check{q}_j>0 \tag{29}$$

where from (6) $\check{q}_j$ is given by

$$\check{q}_j=\check{\mu}_j\check{D}_j^{-T}\check{v}_j\ . \tag{30}$$

Substituting (30) in to (29) we obtain

$$\check{\mu}_j^2(1-\check{v}_j^T\check{D}_j^{-1}\check{D}_j^{-T}\check{v}_j)>0 \tag{31}$$

Note however that from

$$\check{D}_j^T\check{D}_j-\check{v}_j\check{v}_j^T>0 \tag{32}$$

(which is satisfied because $\check{D}_j^T\check{D}_j-\check{V}_j^T\check{V}_j>0$) it follows that

$$1-\check{v}_j^T\check{D}_j^{-1}\check{D}_j^{-T}\check{v}_j>0\ ,$$

which shows that (7) is satisfied.

Now, the construction of $\check{H}$ proceeds in a straightforward manner, exactly as in the (orthogonal) updating case.

The scheme for downdating R^{-T} can be extended to downdating the least squares solution w to $\check{w}$. The following theorem shows how this can be done.

Theorem 2 *Let $\check{H}$ satisfy (23), that is*

$$\check{H}\begin{bmatrix}\check{V} & R^{-T}\\ I_k & 0\end{bmatrix}=\begin{bmatrix}0 & \check{R}^{-T}\\ \check{D} & F^T\end{bmatrix}.$$

If w is the solution to (9), then the solution to (19) is given by

$$\check{w}=w+F\check{D}^{-T}(d-Z^Tw)$$

Moreover $F=-R^{-1}\check{V}\check{D}^{-1}$.

Proof: The proof is analogous to that of Theorem 1 and hence is omitted.

□

Thus, summarizing the results of this section, we obtain the following algorithm.

Algorithm IDOWN-k

Given: R^{-T} and w, where $X = QR$ and w solves (9).

Input: Set of k observations $[Z^T \;\; d]$.

Then this algorithm computes $\check{R}^{-T}$ and $\check{w}$, where

$$X = \begin{bmatrix} \check{X} \\ Z^T \end{bmatrix} = QR,$$

$\check{X} = \check{Q}\check{R}$ and $\check{w}$ solves (19).

1. Compute $\check{V} = -R^{-T}Z$.

   Cost $kn^2/2$ multiplications.

2. Find $\check{H} = P_n \cdots P_2 P_1$, where P_i are row hyperbolic Householder transformations, such that

$$\check{H} \begin{bmatrix} \check{V} \\ I \end{bmatrix} = \begin{bmatrix} 0 \\ \check{D} \end{bmatrix}$$

   Cost $13 \cdot k^2 n$ multiplications.

3. Downdate R^{-T} to $\check{R}^{-T}$:

$$\check{H} \begin{bmatrix} R^{-T} \\ 0 \end{bmatrix} = \begin{bmatrix} \check{R}^{-T} \\ F^T \end{bmatrix}$$

   Cost kn^2 multiplications.

4. Downdate w to $\check{w}$:

$$\check{w} = w - F\check{D}^{-T}(d - Z^T w)$$

   Cost $\frac{3}{2}k^2 + 2kn$ multiplications (as from (4) the QR decomposition of D is already available from step 2).

It is easy to see that the complexity analysis for the above algorithm is the same as Algorithm IUP-k. That is, the total cost is $\frac{3}{2} \cdot kn^2 + 13 \cdot k^2 n + 2 \cdot kn + \frac{3}{2}k^2$ multiplications. Moreover, the straight forward implementation of the rank-1 downdating method of Pan and Plemmons [12] requires $\frac{5}{2}kn^2 + O(k^2 n)$ multiplications.

5 Block WY Representation for Products

We are interested in row Householder methods that are rich in matrix-matrix operations in order to increase the efficiency of our algorithms on vector and parallel machines. To that end, it is important to accumulate and apply products of Householder transformations in block form [10].

It is known (see e.g., Schreiber and Van Loan [16]), that products

$$Q = H_n H_{n-1} \cdots H_1$$

of column oriented Householder transformation matrices

$$H_i = I - w_i w_i^T, \quad i = 1, \cdots, n, \tag{33}$$

defined by m-vectors w_i with $w_i^T w_i = 2$, can be accumulated in a compact WY form

$$Q = I - YTY^T \tag{34}$$

where Y is an $m \times n$ rectangular matrix, and each of its columns is a Householder vector w_i, and T is a unit lower triangular $n \times n$ matrix. Obviously, then, if A is an $m \times n$ matrix then $H_n H_{n-1} \cdots H_1 A$ can be accumulated using matrix-matrix operations as

$$H_n H_{n-1} \cdots H_1 A = QA = A - YT(Y^T A).$$

An algorithm for constructing and applying Q in the form (34) is in the new LAPACK software system [1]. We remark that Puglisi [14] has extended the work in [16] by giving a scheme to compute and apply the product form (34) which involves more BLAS-3 matrix-matrix operations, but which also requires additional work and storage.

Clearly, since orthogonal row Householder transformation matrices P as given in (1) can also be written in the form (33), the same results on accumulation and application of products of Householder transformations in block form apply for our case. Thus the use of row Householder orthogonal transformations for modifying the inverse QR factorization is rich in level-3 BLAS operations, and the compact WY representation block algorithms in LAPACK can be used for our application.

The case of row hyperbolic Householder transformations, used for downdating, requires some further discussion. Recall that for an m-vector p_i and a signature matrix Φ, an $m \times m$ row (or column) hyperbolic Householder transformation matrix can be written in the form

$$P_i = \Phi - \frac{2}{p_i^T \Phi p_i} p_i p_i^T, \tag{35}$$

provided that $0 < p_i^T \Phi p_i$. The matrix P_i is pseudo orthogonal with respect to Φ, i.e., $P_i^T \Phi P_i = \Phi$. Observe also that $P = P^T$. We now proceed to show how to accumulate and apply products of hyperbolic Householder transformations in a compact WY-type representation block form similar to (34).

First, we write (35) in the form

$$P_i = \Phi - w_i w_i^T, \tag{36}$$

where w_i is an m-vector given by

$$w_i = \left(\sqrt{\frac{2}{p_i^T \Phi p_i}}\right) p_i.$$

Note that $w_i^T \Phi w_i = 2$.

It will be shown that products

$$Q_\Phi = P_n P_{n-1} \cdots P_1$$

of row or column oriented hyperbolic Householder transformation matrices (36), defined by m-vectors w_i, and associated with the same signature matrix Φ, can be accumulated in a compact WY form

$$Q_\Phi = \Phi^n - \Phi^{n-1} Y T Y^T. \tag{37}$$

A method for computing the block representation (37) is given by the following theorem.

Theorem 3 *Suppose $Q_\Phi = \Phi^i - \Phi^{i-1} Y T Y^T$ is an $m \times m$ matrix, pseudo orthogonal with respect to Φ, with Y $m \times i$ and with T a unit lower triangular $i \times i$ matrix. If $P = \Phi - w w^T$, with w an n-vector such that $0 < w^T \Phi w$, and $z^T = -w^T \Phi^{i-1} Y T$, then the product PQ_Φ is given by*

$$PQ_\Phi = \Phi^{i+1} - \Phi^i Y_+ T_+ Y_+^T, \tag{38}$$

where

$$Y_+ = \left[Y, \Phi^i w\right], \quad T_+ = \begin{bmatrix} T & 0 \\ z^T & 1 \end{bmatrix}. \tag{39}$$

Proof: It can be seen that

$$\begin{gathered} PQ_\Phi = \left(\Phi - w w^T\right)\left(\Phi^i - \Phi^{i-1} Y T Y^T\right) = \\ \Phi^{i+1} - \Phi^i Y T Y^T + w w^T \Phi^{i-1} Y T Y^T - w w^T \Phi^i = \\ \Phi^{i+1} - \Phi^i Y T Y^T - w z^T Y^T - w w^T \Phi^i = \\ \Phi^{i+1} - \Phi^i \left[Y, \Phi^i w\right] \begin{bmatrix} T & 0 \\ z^T & 1 \end{bmatrix} \begin{bmatrix} Y^T \\ w^T \Phi^i \end{bmatrix} = \\ \Phi^{i+1} - \Phi^i Y_+ T_+ Y_+^T. \end{gathered}$$

□

Notice that $Q_\Phi = P_n P_{n-1} \cdots P_1$ reduces to $\Phi - YTY^Y$ if n is odd, and to $I - \Phi Y T Y^T$ if n is even.

The scheme described in Theorem 3 for accumulating products of hyperbolic Householder transformation matrices has the same advantages as the storage-efficient compact WY representation scheme for the orthogonal case given in [16]. In summary, the row orthogonal and row hyperbolic Householder methods considered in this paper are rich in matrix-matrix operations, and this fact can be used to increase the efficiency of our algorithms on vector and parallel machines.

6 Numerical Experiments

In this section we provide numerical experiments which consist of sliding window recursive least squares problems (RLS), and are designed to compare the accuracy of our block method with k applications of the rank-1 covariance inverse factorization RLS method of Pan and Plemmons [12]. In each of the examples given below, we indicate the length of the window used, and the number of observations which will be added and deleted.

The set of examples we use here have been used to test the effectiveness of condition estimators [7,8,13], and have also been used by Björck, Park and Eldén [5] to illustrate how the corrected semi-normal equations can be used to stablize rank-1 downdating. These examples are described as follows.

Example 1: In this example we construct a 100×10 data matrix whose entries are generated randomly from a uniform distribution in (-50,50). We then scale the first column of this matrix by multiplying the entries in the first column by 10^{-3}. This causes the windowed data to have a condition number on the order of 10^3. Here we choose the window length to be 20, and the number of observations added and deleted is $k = 5$.

Example 2: In this example we construct a 50×5 data matrix from a uniform distribution in (0,1). In this case, though, we add an outlier of the form $r \times 10^3$, where r is again a random number in (0,1), to the (18,3) entry. The effect of this outlier causes the data to become ill-conditioned when the 18^{th} row is added to the system. Here we choose the window length to be 8, and the number of observations added and deleted is $k = 3$.

Example 3: In this example we construct a 50×5 matrix. The first 25 rows are the first 25 rows of the Hilbert matrix. The second 25 rows are simply the first 25 rows given in reverse order. We then add a random number, δ, to all the entries in order to control the degree of ill-conditioning of the data. The smaller the value of δ, the more ill-conditioned is the data. As is done in [5], we use $\delta = 10^{-5}$ and $\delta = 10^{-9}$. Here, we again take the window length to be 8, and $k = 3$.

The numerical tests for the above examples were performed using Matlab, and the right hand side vector was chosen to be the row sums of the data matrix. Thus the exact solution is known, and is the vector of all ones. The quantities reported are the relative errors and residuals for our block method, and the rank-1 rotation based method of Pan and Plemmons [12]. The results are summarized in Figures 1-8, where the solid line is the plot of the rank-1 method and the dashed line is a plot of our block method. Also shown in the figures is a plot of $1/cond(X)$ for each window, indicated by + signs.

We see from the figures that numerically our block method performs in a similar manner to k applications of the rank-1 method of Pan and Plemmons. But since our methods are rich in BLAS-3 computations, our block method is better suited for vector and parallel architectures.

We note that, as for the rank-1 method of Pan and Plemmons, our block method can give

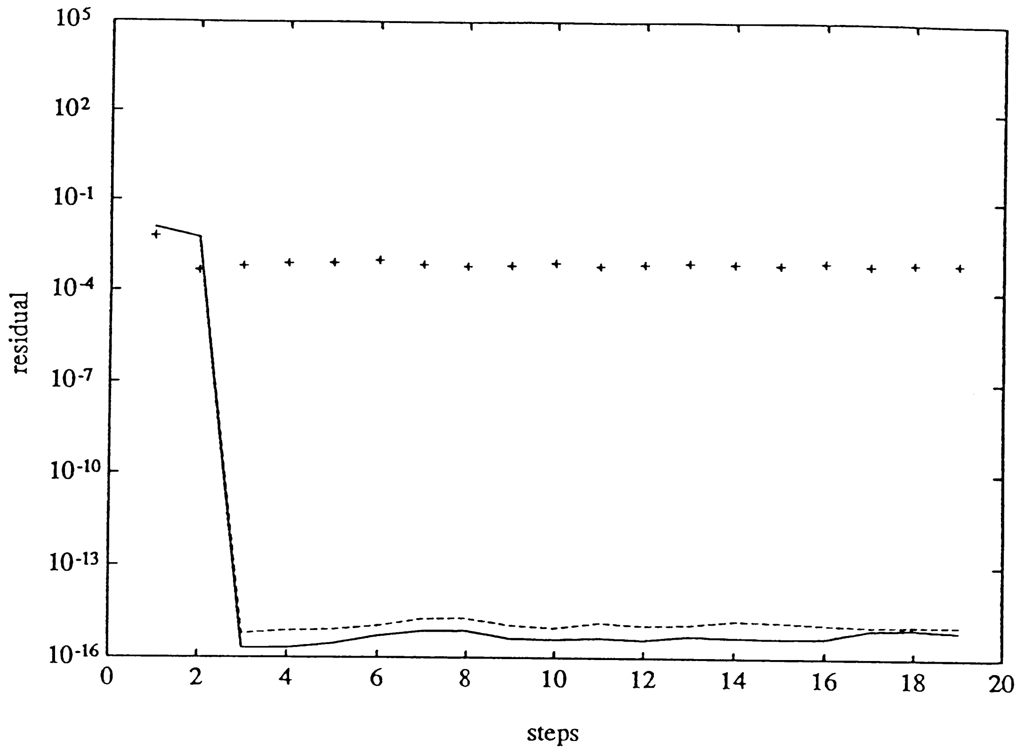

Figure 1: Residuals for Example 1.

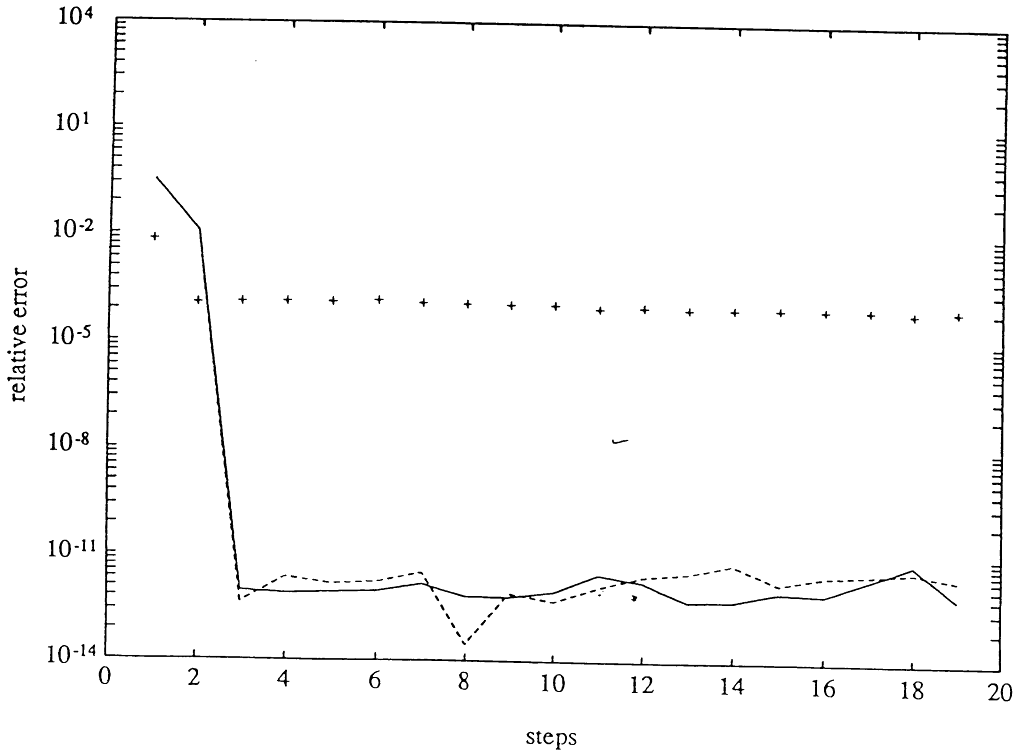

Figure 2: Relative errors for Example 1.

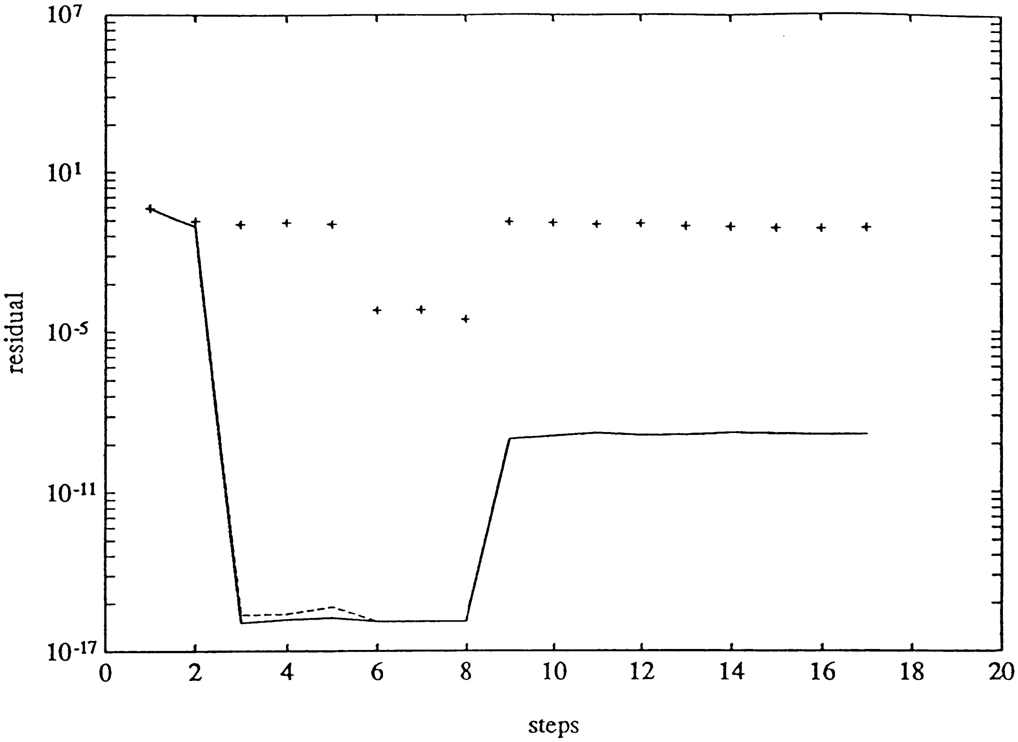

Figure 3: Residuals for Example 2.

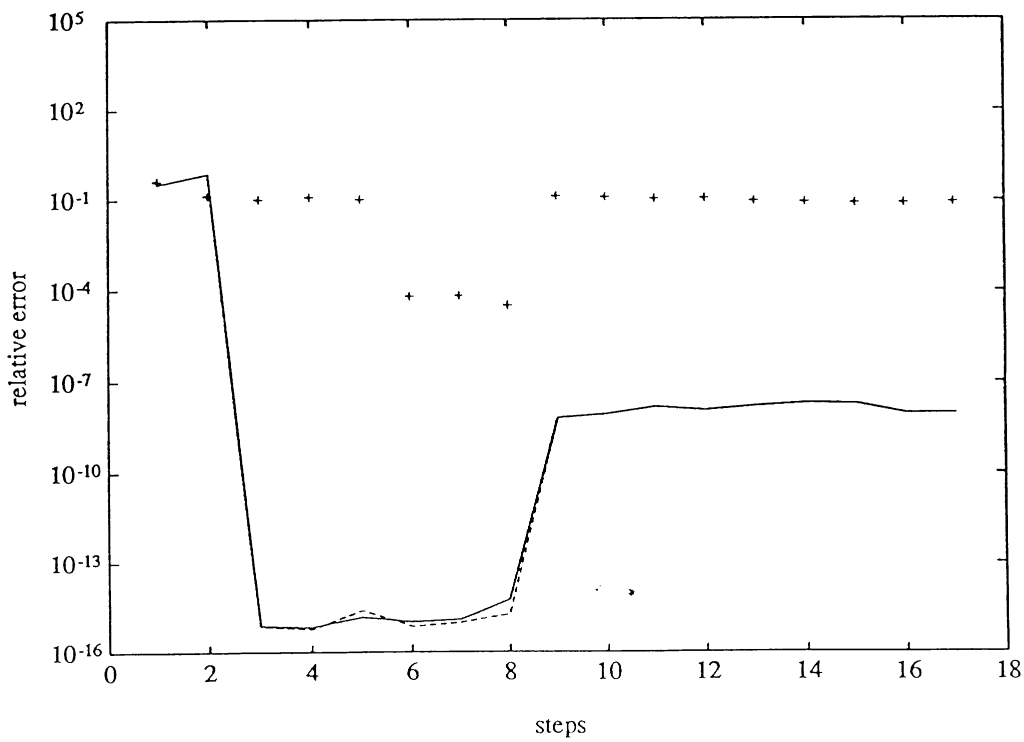

Figure 4: Relative errors for Example 2.

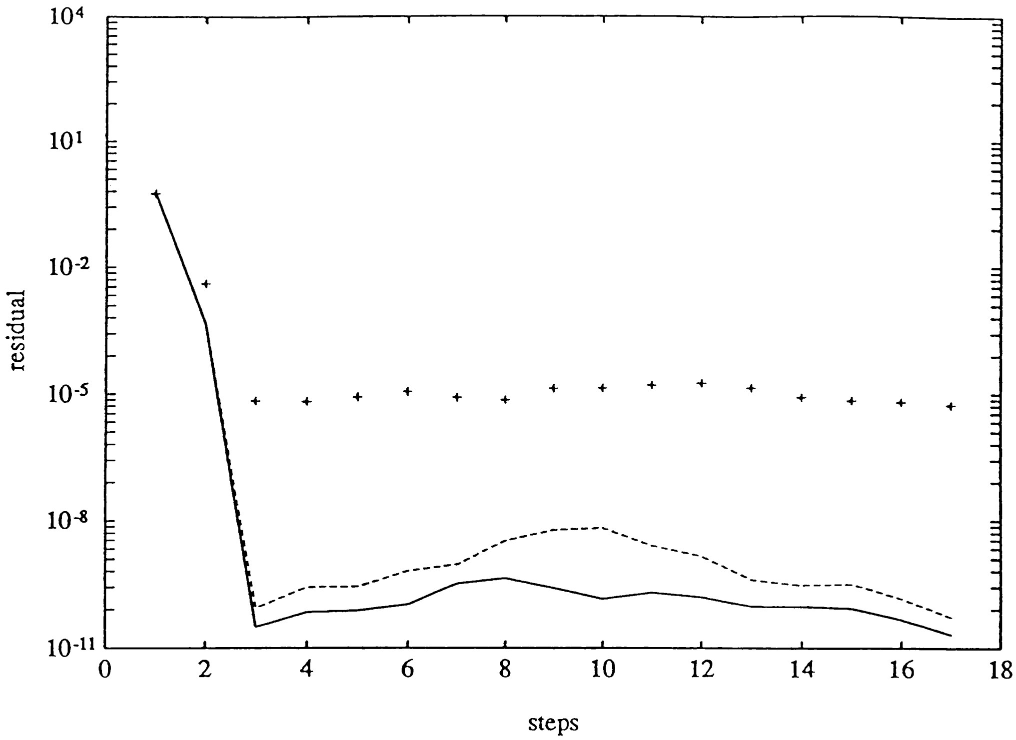

Figure 5: Residuals for Example 3, with $\delta = 10^{-5}$.

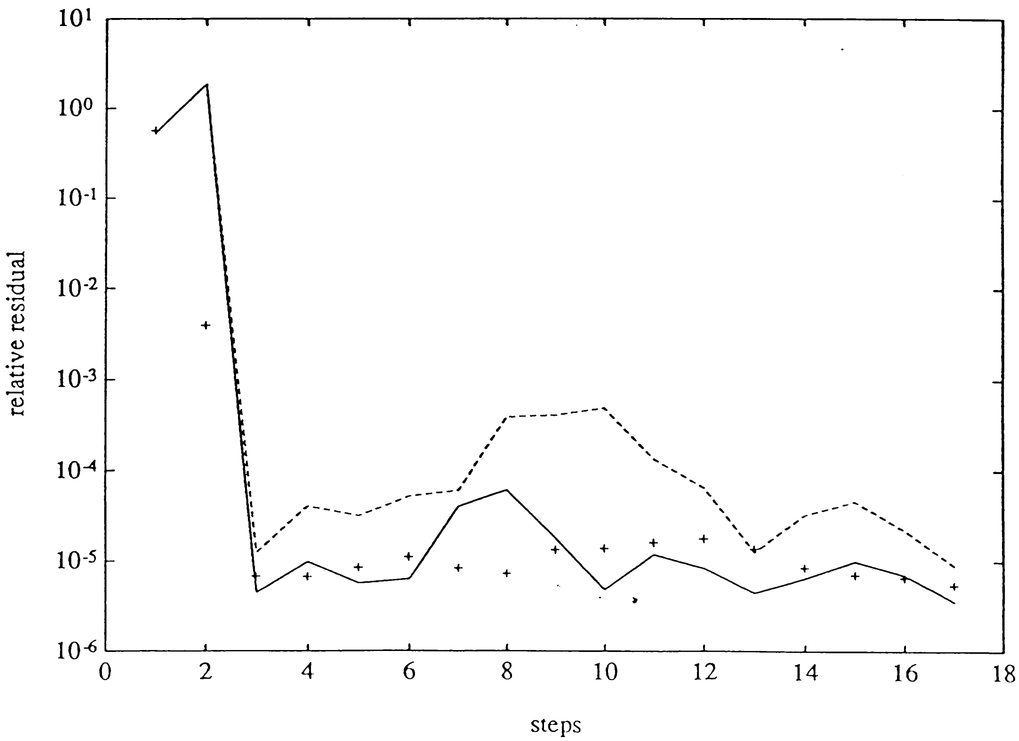

Figure 6: Relative errors for Example 3, with $\delta = 10^{-5}$.

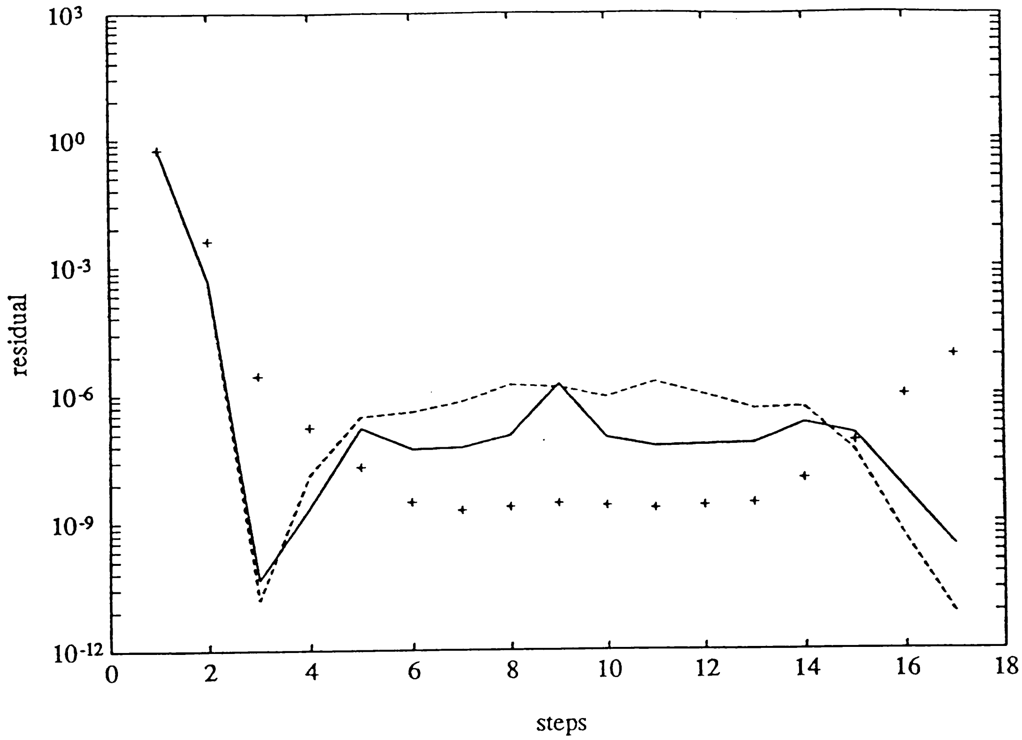

Figure 7: Residuals for Example 3, with $\delta = 10^{-9}$.

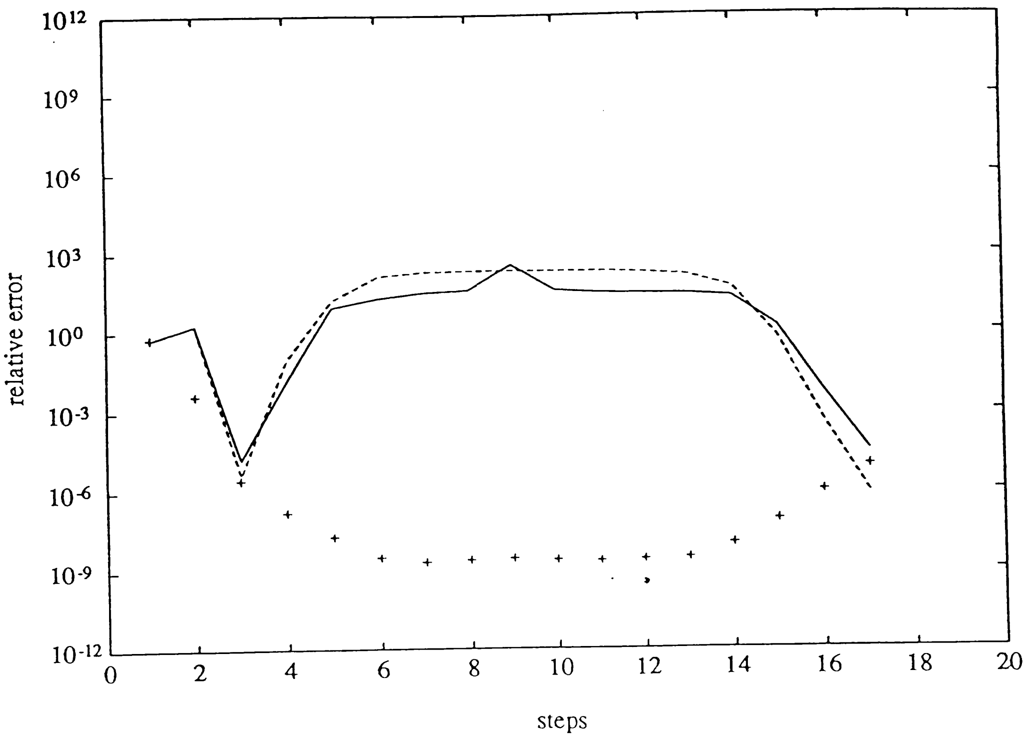

Figure 8: Relative errors for Example 3, with $\delta = 10^{-9}$.

inaccurate results if the data becomes too ill-conditioned. This is to be expected, though, since the downdating is sensitive to ill-conditioning. To obtain a more reliable block method when the data is ill-conditioned, one can apply schemes which also modify the Q factor, such as a block Gram-Schmidt method. Another approach is to use the original data, X. This could be done by extending the work of Björck, Park and Eldén [5], which uses the corrected semi-normal equations for rank-1 modifications, to the rank-k case.

Perhaps a more straight forward approach is to use a condition estimation technique, such as ACE [13], and, if the problem becomes ill-conditioned, re-initialize by computing a new inverse orthogonal factorization, producing a new R^{-1}. That is, ACE could be used to monitor the conditioning of the data, which can be done in $O(n) + O(k^3)$ operations per time step. The $O(k^3)$ comes from solving an eigenvalue problem required in ACE. If the data becomes ill-conditioned, one would then compute an explicit QR factorization of the current data, to re-initialize the RLS process, and continue with the updating and downdating. This approach would be most useful for problems such as Example 2, where the data is well conditioned except for a small number of windows, made ill-conditioned by outliers. Of course, if the problem is well conditioned, then our scheme is very efficient and needs no stabilizing modifications.

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