Analysis of the Unified Transformations*

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Abstract

We show the singular values of the unified transformations [6], propose pivoting strategies for downdating, and present a stability analysis.

Keywords: Hyperbolic transformations, downdating, stability, error analysis.

1 Introduction

In [6], we presented the unified transformations by unifying and generalizing unitary and hyperbolic rotations and Householder transformations. Note that we use the term "unitary rotation" as it is an extention of Givens rotation to the complex case although it is not really a rotation in geometrical sense. Unified transformations provide a single type of transformation for both Cholesky updating and downdating. Moreover, they can be applied to general downdating where the downdated matrix can be indefinite. They can be used in fast triangularization of structured matrices [6].

Definition 1 (Rotation) *Given a signature matrix* $S = \mathrm{diag}(\sigma_1, \sigma_2)$*, a unified rotation has the form:*

$$Q = \begin{pmatrix} c^* & (\sigma_2/\sigma_1)s^* \\ -s & c \end{pmatrix} \tag{1}$$

where the pair (c, s) *satisfies*

$$\sigma_1|c|^2 + \sigma_2|s|^2 = \hat{\sigma}_1, \quad \hat{\sigma}_1 = \pm 1.$$

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The unified rotation Q defined above satisfies

$$Q^{\mathrm{H}}\hat{S}Q = S$$

where $\hat{S} = \mathrm{diag}(\hat{\sigma}_1, \hat{\sigma}_2)$ $(\hat{\sigma}_2/\hat{\sigma}_1 = \sigma_2/\sigma_1)$. When $\sigma_1 = \sigma_2 = 1$ and $\hat{\sigma}_1 = 1$, Q is a unitary rotation (Givens rotation generalized to the complex case). When $\sigma_2 = -\sigma_1 = -1$ and $\hat{\sigma}_1 = 1$, Q is a hyperbolic rotation (real hyperbolic rotation generalized to the complex case). The following algorithm [6] computes a unified rotation to eliminate the second component a 2-by-1 vector.

Algorithm 1 (Rotation) *Given the updating or general downdating problem:*

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{\mathrm{H}} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

this algorithm computes a unified rotation

$$Q = \begin{pmatrix} c^* & (\sigma_2/\sigma_1)s^* \\ -s & c \end{pmatrix}$$

and a signature matrix $\hat{S} = \mathrm{diag}(\hat{\sigma}_1, \hat{\sigma}_2)$ *so that*

$$Q \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \rho \\ 0 \end{pmatrix} \quad \textit{and} \quad Q^{\mathrm{H}}\hat{S}Q = \mathrm{diag}(\sigma_1, \sigma_2).$$

if $x_2 = 0$
    $c = 1$; $s = 0$; $\hat{\sigma}_1 = \sigma_1$; $\hat{\sigma}_2 = \sigma_2$; return
end
if $\sigma_1|x_1| = -\sigma_2|x_2|$
    error("No hyperbolic rotation when $|x_1| = |x_2|$")
end
if $|x_1| > |x_2|$
    $\tau = x_2/x_1$; $\delta = 1 + (\sigma_2/\sigma_1)|\tau|^2$;
    $c = \mathrm{sign}(x_1)/\sqrt{|\delta|}$; $s = \tau c$;
else
    $\tau = x_1/x_2$; $\delta = \sigma_2/\sigma_1 + |\tau|^2$;
    $s = \mathrm{sign}(x_2)/\sqrt{|\delta|}$; $c = \tau s$;
end
if $\delta > 0$
    $\hat{\sigma}_1 = \sigma_1$; $\hat{\sigma}_2 = \sigma_2$;
else
    $\hat{\sigma}_1 = -\sigma_1$; $\hat{\sigma}_2 = -\sigma_2$;
end

The unified Householder transformation unifies and generalizes unitary Householder transformation [5] and hyperbolic Householder transformation [7, 8].

Definition 2 (Householder Transformation) *Given a signature matrix* $S = \mathrm{diag}(\sigma_i)$ *and a complex vector* u *such that* $u^{\mathrm{H}}Su \neq 0$ *and it is scaled so that* $|u^{\mathrm{H}}Su| = 2$*, a unified Householder transformation is of the form* PJ *where*

$$P = S - \mathrm{sign}(u^{\mathrm{H}}Su)uu^{\mathrm{H}} \tag{2}$$

and J *is the matrix representing the permutation* $(1, j)$ *for some index* j*.*

The following algorithm shows how to construct a unified Householder transformation to introduce a sequence of zeros into a complex vector.

Algorithm 2 (Householder Transformation) *Given a complex vector* x *and a signature matrix* $S = \mathrm{diag}(\sigma_i)$*, this algorithm computes the vector* u*, scalars* α *and* δ*, and permutation* $(1, j)$ *in the unified Householder transformation*

$$P = \hat{S} - \delta^{-1}uu^{\mathrm{H}}.$$

Let matrix J *represent the permutation* $(1, j)$*, then* $\hat{S} = JSJ$*,*

$$(PJ)x = -\alpha e_1 \quad \text{and} \quad (PJ)^{\mathrm{H}}\hat{S}(PJ) = S.$$

$m = \max\{|x_i|\}$; $x = x/m$;
$J = I$;
if $\mathrm{sign}(x^{\mathrm{H}}Sx) \neq \sigma_1$
    find j so that $\sigma_j = \mathrm{sign}(x^{\mathrm{H}}Sx)$;
    $J =$ permutation $(1, j)$;
end
$y = Jx$; $\hat{S} = JSJ$;
$\alpha = \mathrm{sign}(\hat{\sigma}_1 y_1)\sqrt{|y^{\mathrm{H}}\hat{S}y|}$;
$u = \hat{S}y + \alpha e_1$;
$\delta = \hat{\sigma}_1 \alpha^* u_1$;
$\alpha = m\alpha$;

In this paper, we present an error analysis of the unified transformations. We derive the unified formulas for the condition numbers of the unified transformations and show that their condition numbers can be arbitrarily large. Then, we propose pivoting strategies for avoiding large condition numbers in mixed updating-downdating procedure. Finally, we present a unified stability analysis.

2 Householder Transformation

In this section, we first derive the singular values of the unified Householder transformation. We will show that all singular values, except possibly two, of a unified Householder transformation equal one. The other two are reciprocal each other and the ratio can be arbitrarily large (or small). Thus the condition number of a unified Householder transformation can be arbitrarily large. So, we propose a pivoting scheme to improve the stability. Then we present a unified error analysis, which includes unitary and hyperbolic Householder transformations as special cases.

2.1 Condition Number

We first show that P defined in (2) (or PJ) has at least $n-2$ unit singular values, where n is the order of P. Suppose that the diagonal of the signature matrix S has p positive elements and m negative elements. Partitioning $S = M + N$ where M is the positive part of S and N the negative part, we have

$$P = M + N - \xi uu^{\mathrm{H}} \quad \text{where} \quad \xi = \mathrm{sign}(u^{\mathrm{H}}Su)$$

and

$$\mathrm{rank}(M) = p, \quad \mathrm{rank}(N) = m, \quad \text{where } p + m = n.$$

Thus $\mathrm{rank}(N - \xi uu^{\mathrm{H}}) \leq m+1$ implying that P has at least $n-(m+1) = p-1$ eigenvalues equal to $+1$. Similarly, P has at least $m-1$ eigenvalues equal to -1 since $\mathrm{rank}(M - \xi uu^{\mathrm{H}}) \leq p+1$. It follows that P has at least $(m-1)+(p-1) = n-2$ unit singular values since P is Hermitian.

Next, we derive the other two possible non-unit singular values of P. Recall that the generating vector u in (2) is scaled so that $|u^{\mathrm{H}}Su| = 2$. Since P is S-unitary and Hermitian, we have $SPS = P^{-1}$. So, using $P = S - \xi uu^{\mathrm{H}}$, we get

$$P + P^{-1} = P + SPS = 2S - \xi uu^{\mathrm{H}} - \xi(Su)(Su)^{\mathrm{H}}.$$

Recalling that $\xi = \mathrm{sign}(u^{\mathrm{H}}Su)$ and $|u^{\mathrm{H}}Su| = 2$, we can verify that

$$(P + SPS)(u \pm Su) = -\xi(u^{\mathrm{H}}u)(u \pm Su).$$

One of $u + Su$ and $u - Su$ must be nonzero, because otherwise (both are zero) we have $u = 0$ leading to the trivial case of $P = S$. This implies that at least one of $u + Su$ and $u - Su$ is an eigenvector of $P + SPS$, which equals $P + P^{-1}$. However, all eigenvalues of $P + P^{-1}$ have the form $\lambda + \lambda^{-1}$ where λ is an eigenvalue of P. Thus

$$\lambda + \lambda^{-1} = -\xi u^{\mathrm{H}}u = -\mathrm{sign}(u^{\mathrm{H}}Su)(u^{\mathrm{H}}u).$$

In other words,

$$|u^{\mathrm{H}}u| = \sigma + \sigma^{-1}$$

where σ is a singular value of P. Solving for σ in the above equation, we obtain

$$\sigma_{\max} = \frac{|u^{\mathrm{H}}u| + \sqrt{(u^{\mathrm{H}}u)^2 - 4}}{2} = \sigma_{\min}^{-1}. \tag{3}$$

These are the two possible non-unit singular values. For a general (unscaled) u, the two possible non-unit singular values are:

$$\sigma_{\min}^{-1} = \sigma_{\max} = \frac{u^{\mathrm{H}}u}{|u^{\mathrm{H}}Su|} + \sqrt{\left(\frac{u^{\mathrm{H}}u}{u^{\mathrm{H}}Su}\right)^2 - 1}.$$

When $S = \pm I$, then $\sigma_{\min} = \sigma_{\max} = 1$, $J = I$, and PJ is the unitary Householder matrix. In the case when $S \neq \pm I$ and $J = I$ and P is the hyperbolic Householder defined in [7, 8], the above result on the condition number coincides with [2]. For a general signature matrix S, the ratio $(u^{\mathrm{H}}u)/|u^{\mathrm{H}}Su|$ can be arbitrarily large. In other words, $\mathrm{cond}(PJ)$ can be arbitrarily large. In the following, analogous to [11], we propose a pivoting scheme.

2.2 Pivoting

As shown in Algorithm 2, when a Householder transformation is constructed to introduce zeros into a given vector x, we have some freedom of choosing the permutation J. We propose the following pivoting scheme in which J is chosen to minimize the condition number of the Householder transformation.

Algorithm 3 (Householder with pivoting) *Given a complex vector x and a signature matrix $S = \mathrm{diag}(\sigma_i)$, this algorithm computes the vector u, scalars α and δ, and permutation $(1, j)$ in the unified Householder transformation PJ where*

$$P = \hat{S} - \delta^{-1}uu^{\mathrm{H}}.$$

Let matrix J represent the permutation $(1, j)$, then $\hat{S} = JSJ$,

$$(PJ)x = -\alpha e_1 \quad \textit{and} \quad (PJ)^{\mathrm{H}}\hat{S}(PJ) = S.$$

This algorithm incorporates pivoting to minimize the condition number of P.

$m = \max\{|x_i|\}$; $x = x/m$;
$J = I$;
if $S \neq \pm I$
    find j so that $\sigma_j = \mathrm{sign}(x^{\mathrm{H}}Sx)$ and $|x_j|$ is maximized;
    $J =$ permutation $(1, j)$;
end
$y = Jx$; $\hat{S} = JSJ$;
$\alpha = \mathrm{sign}(\hat{\sigma}_1 y_1)\sqrt{|y^{\mathrm{H}}\hat{S}y|}$;

$$u = \hat{S}y + \alpha e_1;$$
$$\delta = \hat{\sigma}_1 \alpha^* u_1;$$
$$\alpha = m\alpha;$$

2.3 Stability

Now, we present a stability analysis of the direct application of a unified Householder transformation. Our analysis includes both the unitary and hyperbolic Householder transformations as special cases. Since the permutation J in the unified Householder transformation PJ does not cause any rounding errors, we only consider the direct application of the S-unitary P to a vector z:

$$\hat{z} \equiv \mathrm{fl}(Pz). \tag{4}$$

Suppose that G is a permutation matrix such that

$$\breve{S} \equiv GSG = \mathrm{diag}(I_p, -I_m).$$

Again, if we partition $S = M + N$ where M is the positive part of S and N the negative part, then

$$GMG = \mathrm{diag}(I_p, 0) \quad \text{and} \quad GNG = \mathrm{diag}(0, -I_m). \tag{5}$$

Thus $\breve{P} \equiv GPG$ is $\breve{S}$-unitary. Rewriting (4) as $\hat{z} = \mathrm{fl}(Pz) = \mathrm{fl}(G\breve{P}Gz)$, we obtain

$$G\hat{z} = \mathrm{fl}(\breve{P}(Gz)).$$

In other words, $G\hat{z}$ is the result of the direct application of a hyperbolic Householder transformation $\breve{P}$ to the vector Gz. It is shown in [11] that the direct application of a hyperbolic Householder is relationally stable. Specifically, if we partition

$$G\hat{z} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} \quad \text{and} \quad Gz = \begin{pmatrix} x \\ y \end{pmatrix}, \tag{6}$$

then there exists a unitary Householder matrix H such that

$$H \begin{pmatrix} \hat{x} \\ y \end{pmatrix} = \begin{pmatrix} x \\ \hat{y} \end{pmatrix} + \breve{f} \tag{7}$$

with a suitably small $\breve{f}$. Using the partition (6), it follows that

$$GHG \left[G \begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} G\hat{z} - G \begin{pmatrix} 0 & 0 \\ 0 & -I_m \end{pmatrix} Gz \right] = G \begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} Gz - G \begin{pmatrix} 0 & 0 \\ 0 & -I_m \end{pmatrix} G\hat{z} + \breve{f}.$$

Finally, using (5), we have the following equation for the stability:

$$GHG\,(M\hat{z} - Nz) = Mz - N\hat{z} + f \tag{8}$$

with a suitably small f. Note that Mz (or $M\hat{z}$) is the vector obtained by setting the elements of z (or $\hat{z}$)corresponding to -1 in S to zero and Nz (or $N\hat{z}$) can be obtained similarly. When $G = I$ ($S = \mathrm{diag}(I_p, -I_m)$), the equation (8) above becomes (7) showing the relational stability of the hyperbolic Householder transformation presented in [11]. When $S = I = M$ (or $S = -I = N$), the above equation (8) becomes

$$H\hat{z} = z + f \quad \text{or} \quad Hz = \hat{z} + f,$$

which shows the backward stability of the unitary Householder transformation.

3 Rotation

Now we turn to the unified rotation defined in (1). Similar to the previous section, we first derive the condition number of a unified rotation. Then we propose a pivoting strategy. Finally, we discuss the stability.

3.1 Condition Number

It can be verified that the two eigenvalues of

$$Q^H Q = \begin{pmatrix} |c|^2 + |s|^2 & (\sigma_2/\sigma_1 - 1)cs^* \\ (\sigma_2/\sigma_1 - 1)c^*s & |c|^2 + |s|^2 \end{pmatrix},$$

where Q is defined in (1), are:

$$\lambda = |c|^2 + |s|^2 \pm |\sigma_2/\sigma_1 - 1|\, |c|\, |s|.$$

It then follows that the condition number of Q is

$$\mathrm{cond}(Q) = \sqrt{\frac{|c|^2 + |s|^2 + |\sigma_2/\sigma_1 - 1|\, |c|\, |s|}{|c|^2 + |s|^2 - |\sigma_2/\sigma_1 - 1|\, |c|\, |s|}}.$$

In particular, when $\sigma_2 = \sigma_1$, then Q is unitary and $\mathrm{cond}(Q) = 1$; when $\sigma_2 = -\sigma_1 = -1$ and $|c|^2 - |s|^2 = \hat{\sigma}_1 = 1$, then Q is hyperbolic and $\mathrm{cond}(Q) = (|c| + |s|)/(|c| - |s|)$. In general, when $\sigma_2 = -\sigma_1 = -1$,

$$\mathrm{cond}(Q) = \frac{|c| + |s|}{||c| - |s||} \tag{9}$$

which can be arbitrarily large.

3.2 Pivoting

To avoid rotations with large condition numbers during mixed updating-downdating, we can apply the following pivoting strategy. If $\sigma_2 = -\sigma_1$ when a rotation is computed to eliminate an element, we can choose, if possible, the element to be eliminated so that the condition number (9) is minimized. In particular, if the rotation is computed by Algorithm 1, we choose x_2 so that $(|x_1| + |x_2|)/\,|\,|x_1| - |x_2|\,|$ is minimized.

3.3 Stability

Finally, we discuss the stability of the unified rotation. It is shown [10] that the direct application of a hyperbolic rotation is neither backward stable nor relationally stable. However, Chambers' algorithm [3] and the LINPACK algorithm [4] are relationally stable [1, 9], but not backward stable. It is also shown [10] that the relational stability extends to a sequence of mixed updating-downdating. In the following, we present a unified algorithm which performs a direct application when the unified rotation Q is unitary and LINPACK method when Q is hyperbolic. Thus it is backward stable when Q is unitary and relationally stable when Q is hyperbolic.

The unified rotation Q satisfies

$$Q^{\mathrm{H}} \begin{pmatrix} \hat{\sigma}_1 & 0 \\ 0 & \hat{\sigma}_2 \end{pmatrix} Q = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \tag{10}$$

where $\sigma_1|c|^2 + \sigma_2|s|^2 = \hat{\sigma}_1$ ($\hat{\sigma}_1 = \pm 1$) and $\hat{\sigma}_2 = (\sigma_2/\sigma_1)\hat{\sigma}_1$. Consider the direct application of Q to a 2-by-1 vector:

$$\begin{pmatrix} \breve{x} \\ \breve{y} \end{pmatrix} \equiv Q \begin{pmatrix} x \\ y \end{pmatrix}. \tag{11}$$

It follows from (10) that

$$\begin{pmatrix} \breve{x} \\ \breve{y} \end{pmatrix}^{\mathrm{H}} \begin{pmatrix} \hat{\sigma}_1 & 0 \\ 0 & \hat{\sigma}_2 \end{pmatrix} \begin{pmatrix} \breve{x} \\ \breve{y} \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}^{\mathrm{H}} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

and

$$|\breve{x}|^2 + \frac{\sigma_1}{\sigma_2}|\breve{y}|^2 = \frac{\sigma_1}{\hat{\sigma}_1}\left(|x|^2 + \frac{\sigma_1}{\sigma_2}|y|^2\right). \tag{12}$$

When $\sigma_1 = \sigma_2$, thus $\hat{\sigma}_1 = \hat{\sigma}_2$, Q is unitary. When $\sigma_1 = -\sigma_2$ and $\sigma_1 = \hat{\sigma}_1$, (12) becomes $|\breve{x}|^2 + |y|^2 = |x|^2 + |\breve{y}|^2$ and there exists a unitary $\breve{Q}$ such that

$$\breve{Q} \begin{pmatrix} \breve{x} \\ y \end{pmatrix} = \begin{pmatrix} x \\ \breve{y} \end{pmatrix}. \tag{13}$$

When $\sigma_1 = -\sigma_2$ and $\sigma_1 = -\hat{\sigma}_1$, (12) becomes $|\breve{x}|^2 + |x|^2 = |y|^2 + |\breve{y}|^2$ and there exists a unitary $\tilde{Q}$ so that

$$\tilde{Q} \begin{pmatrix} \breve{x} \\ x \end{pmatrix} = \begin{pmatrix} y \\ \breve{y} \end{pmatrix}. \tag{14}$$

Suppose the (c, s)-pair in the unified rotation Q has been computed, we first use (1) and (11) to compute $\breve{x}$:

$$\breve{x} = c^* x + \frac{\sigma_2}{\sigma_1} s^* y. \tag{15}$$

Also, from (1) and (11), we have

$$\breve{y} = -sx + cy. \tag{16}$$

If $\sigma_1 = -\sigma_2$ and $\sigma_1 = \hat{\sigma}_1$, we compute $\breve{y}$ from $\breve{x}$ and y using (13). Solving for x in (15), we have

$$x = \frac{1}{c^*}\left(\breve{x} - \frac{\sigma_1}{\sigma_2}s^*y\right) = \frac{1}{c^*}\left(\breve{x} + s^*y\right).$$

Substituting x in (16) with the above equation, we get

$$\breve{y} = \frac{1}{c^*}(-s\breve{x} + y).$$

Note that in this case $|c|^2 - |s|^2 = 1$. Explicitly, the unitary $\breve{Q}$ in (13) is given by

$$\breve{Q} = \frac{1}{c^*}\begin{pmatrix} 1 & s^* \\ -s & 1 \end{pmatrix}.$$

Similarly, if $\sigma_1 = -\sigma_2$ and $\sigma_1 = -\hat{\sigma}_1$, we compute $\breve{y}$ from $\breve{x}$ and x using (14). From (15) and (16), we obtain

$$\breve{y} = -\frac{1}{s^*}(c\breve{x} + x),$$

noting that in this case $|c|^2 - |s|^2 = -1$. The unitary matrix $\tilde{Q}$ in (14) is

$$\tilde{Q} = \frac{1}{s^*}\begin{pmatrix} -1 & c^* \\ -c & -1 \end{pmatrix}.$$

In summary, we have the following algorithm.

Algorithm 4 (Application of a unified rotation) *Given the (c, s)-pair in a unified rotation Q with its associated σ_i and $\hat{\sigma}_i$ $(i = 1, 2)$ and a vector $(x, y)^T$, this algorithm computes the vector $(\breve{x}, \breve{y})^T = Q(x, y)^T$.*

$\breve{x} = c^*x + (\sigma_2/\sigma_1)s^*y$;
if $\sigma_1 = \sigma_2$
  $\breve{y} = -sx + cy$;
elseif $\sigma_1 = \hat{\sigma}_1$
  $\breve{y} = (-s\breve{x} + y)/c^*$;
else
  $\breve{y} = -(c\breve{x} + x)/s^*$;
end

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