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DOWNDATING THE SINGULAR VALUE DECOMPOSITION*

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Abstract. Let A be a matrix with known singular values and left and/or right singular vectors, and let A' be the matrix obtained by deleting a row from A. We present efficient and stable algorithms for computing the singular values and left and/or right singular vectors of A'. We also show that the problem of computing the singular values of A' is well conditioned when the left singular vectors of A are given, but can be ill conditioned when they are not. Our algorithms reduce the problem to computing the eigendecomposition or singular value decomposition of a matrix that has a simple structure, and solve the reduced problem via finding the roots of a secular equation. Previous algorithms of this type can be unstable and always solve the ill-conditioned problem.

Key words. singular value decomposition, downdating, secular equation

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1. Introduction.

Let

$$A = U\Sigma V^T \tag{1}$$

be the *singular value decomposition* (SVD) of a matrix $A \in \mathbf{R}^{m\times n}$, where $U \in \mathbf{R}^{m\times m}$ and $V \in \mathbf{R}^{n\times n}$ are orthogonal and $\Sigma \in \mathbf{R}^{m\times n}$ is zero except on the main diagonal, which has nonnegative entries in nonincreasing order. The columns of U and V are the *left singular vectors* and the *right singular vectors* of A, respectively, and the diagonal entries of Σ are the *singular values* of A.

In many least squares and signal processing applications (see [5], [21], and [27] and the references therein) we repeatedly update A by appending a row or a column or downdate A by deleting a row or a column. After each update or downdate we must compute the SVD of the resulting matrix. We consider the updating problem in [15] and [17]; here we consider the downdating problem.

Since deleting a column of A is tantamount to deleting a row of A^T, we only consider row deletions. Without loss of generality we further assume that the last row is deleted. Thus we can write

$$A = \begin{pmatrix} A' \\ a^T \end{pmatrix}, \tag{2}$$

where $A' \in \mathbf{R}^{(m-1)\times n}$ is the downdated matrix. Let the SVD of A' be

$$A' = U'\Sigma' V'^T, \tag{3}$$

where $U' \in \mathbf{R}^{(m-1)\times(m-1)}$ and $V' \in \mathbf{R}^{n\times n}$ are orthogonal and $\Sigma' \in \mathbf{R}^{(m-1)\times n}$ is zero except on the main diagonal, which has nonnegative entries in nonincreasing order. We would like to take advantage of our knowledge of the SVD of A when computing the SVD of A'.

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We assume that $m > n$; the case $m \le n$ is similar and is treated in detail in [15] and [16]. We write

$$U = (\,U_1 \quad U_2\,), \quad \Sigma = \begin{pmatrix} D \\ 0 \end{pmatrix} \qquad \text{and} \qquad U' = (\,U_1' \quad U_2'\,), \quad \Sigma' = \begin{pmatrix} D' \\ 0 \end{pmatrix},$$

where $U_1 \in \mathbf{R}^{m\times n}$, $U_2 \in \mathbf{R}^{m\times(m-n)}$, $U_1' \in \mathbf{R}^{(m-1)\times n}$, $U_2' \in \mathbf{R}^{(m-1)\times(m-n-1)}$, and $D, D' \in \mathbf{R}^{n\times n}$ are diagonal matrices. Then (1) and (3) can be rewritten as

$$A = U\Sigma V^T = (\,U_1 \quad U_2\,)\begin{pmatrix} D \\ 0 \end{pmatrix} V^T = U_1 D V^T \tag{4}$$

and

$$A' = U'\Sigma' V'^T = (\,U_1' \quad U_2'\,)\begin{pmatrix} D' \\ 0 \end{pmatrix} V'^T = U_1' D' V'^T. \tag{5}$$

There are three downdating problems to consider.

1. Given V, D, and a, compute V' and D'.
2. Given U (or U_1), V, and D, compute U' (or U_1'), V', and D'.
3. Given U (or U_1) and D, compute U' (or U_1') and D'.

We assume that Problem 1 has a solution, i.e., that a is the last row of some matrix A with singular value decomposition (4). Equations (1) and (2) imply that

$$A'^T A' = V' D'^2 V'^T = V(D^2 - zz^T)V^T,$$

where $z = V^T a \in \mathbf{R}^n$. Thus the singular values of A' can found by computing the eigendecomposition $D^2 - zz^T = S\,\Omega^2 S^T$, where $S \in \mathbf{R}^{n\times n}$ is orthogonal and $\Omega \in \mathbf{R}^{n\times n}$ is nonnegative and diagonal. The diagonal elements of $D' = \Omega$ are the singular values. The right singular vector matrix V' can be computed as VS. We present Algorithm I to solve Problem 1 stably[1] in §§2–3.

Since Problem 1 requires computing the eigendecomposition of $D^2 - zz^T$, small perturbations in V, D, and a can cause large perturbations in V' and D'. We analyze the ill-conditioning of the singular values in §6. Our perturbation results are similar to those of Stewart [26] in the context of downdating the Cholesky/QR factorization.

Problems 2 and 3 always have a solution. We show that there exists a column orthogonal matrix $X \in \mathbf{R}^{(m-1)\times n}$ such that

$$A' = XCV^T,$$

where $C \in \mathbf{R}^{n\times n}$ is given by

$$C = \left(I - \frac{1}{1+\mu} u_1 u_1^T\right) D,$$

with u_1 a vector and $\mu \ge 0$ a scalar. The singular values of A' can found by computing the singular value decomposition $C = Q\,\Omega\,W^T$, where Q, $W \in \mathbf{R}^{n\times n}$ are orthogonal

[1] We use the definition of stability in Stewart [25, pp. 75–76]. Let $\mathcal{F}(\mathcal{X})$ be a function of the input data $\mathcal{X}$. We say that an algorithm for computing $\mathcal{F}(\mathcal{X})$ is *stable* if its output is a small perturbation of $\mathcal{F}(\bar{\mathcal{X}})$, where $\bar{\mathcal{X}}$ is a small perturbation of $\mathcal{X}$. This notion of stability is similar to that of *mixed stability* [2], [3] and is used in the context of downdating least squares solutions and Cholesky/QR factorizations [2], [3], [22], [26].

and $\Omega \in \mathbf{R}^{n\times n}$ is nonnegative and diagonal. The diagonal elements of $D' = \Omega$ are the singular values. The left singular vector matrix U_1' can be computed as XQ. The right singular vector matrix V' can be computed as VW. We present Algorithm II to solve Problems 2 and 3 stably in §§4–5.

For Problems 2 and 3 the singular values are well conditioned with respect to perturbations in the input data, whereas the singular vectors can be very sensitive to such perturbations (see §4.1).

Bunch and Nielsen [5] also reduce Problem 1 to computing the eigendecomposition of $D^2 - zz^T$, but their scheme for finding this eigendecomposition is based on results from [6] and [11] and can be unstable [5], [6]. They solve Problem 2 by reducing it to Problem 1, which risks solving a well-conditioned problem using an ill-conditioned process.

Algorithm I solves Problem 1 in $O(n^3)$ time, and Algorithm II solves Problems 2 and 3 in $O(mn^2)$ time when U_1 is given. As with the SVD updating algorithm in [15] and [17], Algorithm I can be accelerated using the fast multipole method of Carrier, Greengard, and Rokhlin [7], [14] to solve Problem 1 in $O(n^2 \log_2^2 \epsilon)$ time, and Algorithm II can be accelerated to solve Problems 2 and 3 in $O(mn \log_2^2 \epsilon)$ time, where ϵ is the machine precision. This is an important advantage for large matrices. Since the techniques are essentially the same as those in [15] and [17], we do not elaborate on this issue.

We take the usual model of arithmetic:[2]

$$fl(\alpha \circ \beta) = (\alpha \circ \beta)\,(1 + \nu),$$

where α and β are floating point numbers; $\circ$ is one of $+$, $-$, $\times$, and $\div$; $fl(\alpha \circ \beta)$ is the floating point result of the operation $\circ$; and $|\nu| \le \epsilon$. We also require that

$$fl(\sqrt{\alpha}) = \sqrt{\alpha}\,(1 + \nu)$$

for any positive floating point number α. For simplicity we ignore the possibility of overflow and underflow.

2. Solving Problem 1.

From (2), (4), and (5) we have

$$A \equiv \begin{pmatrix} A' \\ a^T \end{pmatrix} = U \begin{pmatrix} D \\ 0 \end{pmatrix} V^T \quad \text{and} \quad A' = U' \begin{pmatrix} D' \\ 0 \end{pmatrix} V'^T,$$

so that

$$VD^2V^T = A^TA = A'^TA' + aa^T = V'D'^2V'^T + aa^T.$$

Letting $z = V^Ta$, this equation can be rewritten as

$$V'D'^2V'^T = V\left(D^2 - zz^T\right)V^T. \tag{6}$$

Thus the eigenvalues of $D^2 - zz^T$ are the diagonal elements of D'^2 and must be nonnegative. If $S\Omega^2S^T$ is the eigendecomposition of $D^2 - zz^T$, then $V' = VS$ and $D' = \Omega$.

[2] This model excludes machines like the CRAY and CDC Cyber that do not have a guard digit. Algorithms I and II can easily be modified for such machines.

Algorithm I uses the scheme in §3 to compute a *numerical eigendecomposition* $\tilde{S}\tilde{D}'^2\tilde{S}^T$ satisfying

$$\tilde{S} = \bar{S} + O(\epsilon) \quad \text{and} \quad \tilde{D}' = \bar{D}' + O(\epsilon\|D\|_2),$$

where the eigendecomposition

$$\bar{D}^2 - \bar{z}\bar{z}^T = \bar{S}\bar{D}'^2\bar{S}^T$$

is exact and

$$\bar{D} = D + O(\epsilon\|D\|_2) \quad \text{and} \quad \bar{z} = z + O(\epsilon\|D\|_2).$$

It then computes a right singular vector matrix satisfying

$$\tilde{V}' = V\bar{S} + O(\epsilon).$$

Since V is orthogonal, the error in z can be attributed to an error in a:

$$\bar{a} = V\bar{z} = a + O(\epsilon\|D\|_2).$$

Thus $\bar{D}'$ and $V\bar{S}$ are the exact solution to Problem 1 with slightly perturbed input data V, $\bar{D}$, and $\bar{a}$, so that Algorithm I is stable.

Since small perturbations in D and a can cause large perturbations in D' and S, it follows that $\tilde{D}'$ and $\tilde{S}$ can be very different from D' and S, respectively. We analyze the ill-conditioning of the singular values in §6.

The scheme in §3 takes $O(n^2)$ time, and computing VS takes $O(n^3)$ time. Thus the total time for Algorithm I is $O(n^3)$.

Barlow, Zha, and Yoon [1] compute the eigendecomposition of $D^2 - zz^T$ by using a variant of the LINPACK downdating procedure [10] to "reduce" D to bidiagonal form and then solving the bidiagonal singular value problem. The total time appears to be at least as large as that for Algorithm I.

3. Computing the eigendecomposition of $D^2 - zz^T$. In this section we present an algorithm for computing the eigendecomposition of $D^2 - zz^T$, where $D = \operatorname{diag}(d_1, \ldots, d_k)$, with $d_1 \geq \cdots \geq d_k \geq 0$, and $z = (\zeta_1, \ldots, \zeta_k)^T$. In light of (6) we assume that the eigenvalues of $D^2 - zz^T$ are nonnegative.

We further assume that D and z satisfy

$$d_k > 0, \quad d_i - d_{i+1} \geq \theta\|D\|_2, \quad \text{and} \quad |\zeta_i| \geq \theta\|D\|_2, \tag{7}$$

where θ is a small multiple of ϵ to be specified in §3.4. Any matrix of the form $D^2 - zz^T$ can be stably reduced to one that satisfies these conditions by using the deflation procedure described in §3.5.

3.1. Properties of the eigendecomposition. The following lemma characterizes the eigenvalues and eigenvectors of $D^2 - zz^T$.

LEMMA 3.1 (Bunch and Nielsen [5]). *The eigenvalues of $D^2 - zz^T$ are nonnegative if and only if $z^TD^{-2}z \leq 1$.*

Assume that $z^TD^{-2}z \leq 1$. Then the eigendecomposition of $D^2 - zz^T$ can be written as $S\Omega^2S^T$, where $S = (s_1, \ldots, s_k)$ and $\Omega = \operatorname{diag}(\omega_1, \ldots, \omega_k)$. The eigenvalues $\{\omega_i^2\}_{i=1}^k$ satisfy the secular equation

$$f_1(\omega) \equiv -1 + \sum_{j=1}^{k} \frac{\zeta_j^2}{d_j^2 - \omega^2} = 0 \tag{8}$$

and the interlacing property

$$d_1 > \omega_1 > d_2 > \cdots > d_k > \omega_k \geq 0. \tag{9}$$

The eigenvectors are given by

$$s_i = \left(\frac{\zeta_1}{d_1^2 - \omega_i^2}, \ldots, \frac{\zeta_k}{d_k^2 - \omega_i^2} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{k} \frac{\zeta_j^2}{(d_j^2 - \omega_i^2)^2}} \, . \tag{10}$$

Conversely, given D and the eigenvalues of $D^2 - \hat{z}\hat{z}^T$, we can reconstruct $\hat{z}$.

LEMMA 3.2. *Given a diagonal matrix* $D = \mathrm{diag}(d_1, \ldots, d_k)$ *and a set of numbers* $\{\hat{\omega}_i\}_{i=1}^k$ *satisfying the interlacing property*

$$d_1 > \hat{\omega}_1 > d_2 > \cdots > d_k > \hat{\omega}_k \geq 0, \tag{11}$$

there exists a vector $\hat{z} = (\hat{\zeta}_1, \ldots, \hat{\zeta}_k)^T$ *such that the eigenvalues of* $D^2 - \hat{z}\hat{z}^T$ *are* $\{\hat{\omega}_i^2\}_{i=1}^k$. *The components of* $\hat{z}$ *are given by*

$$|\hat{\zeta}_i| = \sqrt{(d_i^2 - \hat{\omega}_k^2) \prod_{j=1}^{i-1} \frac{\hat{\omega}_j^2 - d_i^2}{d_j^2 - d_i^2} \prod_{j=i}^{k-1} \frac{\hat{\omega}_j^2 - d_i^2}{d_{j+1}^2 - d_i^2}}, \qquad 1 \leq i \leq k, \tag{12}$$

where the sign of $\hat{\zeta}_i$ *can be chosen arbitrarily.*

Proof. This is Löwner's construction [20] of $\hat{z}$ given $-D^2$ and the eigenvalues of $(-D^2) + \hat{z}\hat{z}^T$. □

3.2. Computing the eigenvectors. In practice we can only hope to compute an approximation $\hat{\omega}_i$ to ω_i. But problems can arise if we approximate s_i by

$$\hat{s}_i = \left(\frac{\zeta_1}{d_1^2 - \hat{\omega}_i^2}, \ldots, \frac{\zeta_k}{d_k^2 - \hat{\omega}_i^2} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{k} \frac{\zeta_j^2}{(d_j^2 - \hat{\omega}_i^2)^2}}$$

(i.e., replace ω_i by $\hat{\omega}_i$ in (10), as in [5]). For even if $\hat{\omega}_i$ is close to ω_i, the approximate ratio $\zeta_j/(d_j^2 - \hat{\omega}_i^2)$ can still be very different from the exact ratio $\zeta_j/(d_j^2 - \omega_i^2)$, resulting in a unit eigenvector very different from s_i. After all the $\{\hat{\omega}_i\}_{i=1}^k$ are computed and all the corresponding eigenvectors are approximated in this manner, the resulting eigenvector matrix may not be orthogonal.

But Lemma 3.2 allows us to overcome this problem (cf. [18]). After we have computed all the approximations $\{\hat{\omega}_i\}_{i=1}^k$, we find a *new* vector $\hat{z}$ such that $\{\hat{\omega}_i^2\}_{i=1}^k$ are the *exact* eigenvalues of $D^2 - \hat{z}\hat{z}^T$ and then use (10) to compute the eigenvectors of $D^2 - \hat{z}\hat{z}^T$. Note that each difference

$$\hat{\omega}_j^2 - d_i^2 = (\hat{\omega}_j - d_i)(\hat{\omega}_j + d_i) \quad \text{and} \quad d_j^2 - d_i^2 = (d_j - d_i)(d_j + d_i)$$

in (12) can be computed to high relative accuracy, as can each ratio and each product. Thus $|\hat{\zeta}_i|$ can be computed to high relative accuracy. We choose the sign of $\hat{\zeta}_i$ to be the sign of ζ_i. Substituting the *exact* eigenvalues $\{\hat{\omega}_i^2\}_{i=1}^k$ and the computed $\hat{z}$ into (10), each eigenvector of $D^2 - \hat{z}\hat{z}^T$ can also be computed to componentwise high relative accuracy. Consequently, after all the singular vectors of $D^2 - \hat{z}\hat{z}^T$ are computed, the eigenvector matrix will be numerically orthogonal.

To ensure the existence of $\hat{z}$, we need $\{\hat{\omega}_i\}_{i=1}^k$ to satisfy the interlacing property (11). But since $\{\omega_i\}_{i=1}^k$ satisfy the same interlacing property (see (9)), this is only an accuracy requirement on $\{\hat{\omega}_i\}_{i=1}^k$ and is not an additional restriction on $D^2 - zz^T$.

We use the eigendecomposition of $D^2 - \hat{z}\hat{z}^T$ as an approximation to the eigendecomposition of $D^2 - zz^T$. This is stable as long as $\hat{z}$ is close to z.

3.3. Finding the eigenvalues. To guarantee that $\hat{z}$ is close to z, we must ensure that the approximations $\{\hat{\omega}_i\}_{i=1}^k$ to the singular values are sufficiently accurate. The key is the stopping criterion for the root-finder, which requires a slight reformulation of the secular equation (cf. [5], [18]).

Consider the root $\omega_i \in (d_{i+1}, d_i)$, for $1 \le i \le k-1$; the root $\omega_k \in [0, d_k)$ is treated in a similar manner.

First assume that[3] $\omega_i \in \left(d_{i+1}, \frac{d_i+d_{i+1}}{2}\right)$. Let $\delta_j = d_j - d_{i+1}$, and let

$$\psi_i(\xi) \equiv \sum_{j=1}^{i} \frac{\zeta_j^2}{(\delta_j - \xi)(d_j + d_{i+1} + \xi)} \quad \text{and} \quad \phi_i(\xi) \equiv \sum_{j=i+1}^{k} \frac{\zeta_j^2}{(\delta_j - \xi)(d_j + d_{i+1} + \xi)}.$$

Setting $\omega = d_{i+1} + \xi$, we seek the root $\xi_i = \omega_i - d_{i+1} \in (0, \delta_i/2)$ of the reformulated secular equation

$$g_i(\xi) \equiv f_1(\xi + d_{i+1}) = -1 + \psi_i(\xi) + \phi_i(\xi) = 0.$$

Note that we can compute each ratio $\zeta_j^2/((\delta_j - \xi)(d_j + d_{i+1} + \xi))$ in $g_i(\xi)$ to high relative accuracy for any $\xi \in (0, \delta_i/2)$. Indeed, either $\delta_j - \xi$ is a sum of negative terms or $|\xi| \le |\delta_j|/2$, and $d_j + d_{i+1} + \xi$ is a sum of positive terms. Thus, since both $\psi_i(\xi)$ and $\phi_i(\xi)$ are sums of terms of the same sign, we can bound the error in computing $g_i(\xi)$ by

$$\eta k(1 + |\psi_i(\xi)| + |\phi_i(\xi)|),$$

where η is a small multiple of ϵ that is independent of k and ξ.

Next we assume that $\omega_i \in \left[\frac{d_i+d_{i+1}}{2}, d_i\right)$. Let $\delta_j = d_j - d_i$, and let

$$\psi_i(\xi) \equiv \sum_{j=1}^{i} \frac{\zeta_j^2}{(\delta_j - \xi)(d_j + d_i + \xi)} \quad \text{and} \quad \phi_i(\xi) \equiv \sum_{j=i+1}^{k} \frac{\zeta_j^2}{(\delta_j - \xi)(d_j + d_i + \xi)}.$$

Setting $\omega = d_i + \xi$, we seek the root $\xi_i = \omega_i - d_i \in [\delta_{i+1}/2, 0)$ of the equation

$$g_i(\xi) \equiv f_1(\xi + d_i) = -1 + \psi_i(\xi) + \phi_i(\xi) = 0.$$

For any $\xi \in [\delta_{i+1}/2, 0)$, we can compute each ratio $\zeta_j^2/((\delta_j - \xi)(d_j + d_i + \xi))$ to high relative accuracy (either $\delta_j - \xi$ is a sum of positive terms or $|\xi| \le |\delta_j|/2$, and $d_j + d_i + \xi = d_j + (d_i + \xi)$, where $|\xi| \le d_i/2$), and we can bound the error in computing $g_i(\xi)$ as before.

In practice a root-finder cannot make any progress at a point ξ where it is impossible to determine the sign of $g_i(\xi)$ numerically. Thus we propose the stopping criterion

$$|g_i(\xi)| \le \eta k(1 + |\psi_i(\xi)| + |\phi_i(\xi)|), \tag{13}$$

[3] This condition can easily be checked by computing $f_1\left(\frac{d_i+d_{i+1}}{2}\right)$. If $f_1\left(\frac{d_i+d_{i+1}}{2}\right) > 0$, then $\omega_i \in \left(d_{i+1}, \frac{d_i+d_{i+1}}{2}\right)$, otherwise $\omega_i \in \left[\frac{d_i+d_{i+1}}{2}, d_i\right)$.

where, as before, the right-hand side is an upper bound on the round-off error in computing $g_i(\xi)$. Note that for each i there is at least one floating point number that satisfies this stopping criterion numerically, namely, $fl(\xi_i)$.

We have not specified the scheme for finding the root of $g(\xi)$. We can use the bisection method or the rational interpolation strategies in [4], [5], [13], and [19]. What is most important is the stopping criterion and the fact that, with the reformulation of the secular equation given above, we can find a ξ that satisfies it.

3.4. Numerical stability. We now show that the vector $\hat{z}$ defined in (12) is close to z.

THEOREM 3.3. *If* $\theta = 2\eta k^2$ *in* (7) *and each* $\hat{\xi}_i$ *satisfies* (13), *then*

$$|\hat{\zeta}_i - \zeta_i| \leq 4\eta k^2 \|z\|_2, \qquad 1 \leq i \leq k. \tag{14}$$

The proof is nearly identical to that of the analogous result in [18]. As argued there, the factor k^2 in θ and (14) is likely to be $O(k)$ in practice.

3.5. Deflation. We now show that we can stably reduce $D^2 - zz^T$ to a matrix of the same form that further satisfies

$$d_k > 0, \quad d_i - d_{i+1} \geq \theta\|D\|_2, \quad \text{and} \quad |\zeta_i| \geq \theta\|D\|_2,$$

where θ is specified in §3.4. Similar reductions appear in [5] and [9].

Partition D and z as

$$D = \begin{pmatrix} D_1 & \\ & d_k \end{pmatrix} \quad \text{and} \quad z = \begin{pmatrix} z_1 \\ \zeta_k \end{pmatrix}.$$

First assume that $d_k = 0$. Since $D^2 - zz^T$ is nonnegative definite, its diagonal elements must be nonnegative, so that $d_k^2 - \zeta_k^2 \geq 0$. Thus $\zeta_k = 0$ and

$$D^2 - zz^T = \begin{pmatrix} D_1^2 - z_1 z_1^T & \\ & 0 \end{pmatrix}.$$

The eigenvalue 0 can be deflated, and the matrix $D_1^2 - z_1 z_1^T$ has nonnegative eigenvalues and is of the same form but of smaller dimensions. This reduction is exact.

In the following reductions we assume that $d_k > 0$. Recall from Lemma 3.1 that the eigenvalues of $D^2 - zz^T$ are nonnegative if and only if

$$\sum_{i=1}^{k} \frac{\zeta_i^2}{d_i^2} \leq 1. \tag{15}$$

Assume that $|\zeta_i| < \theta\|D\|_2$. We illustrate the reduction for $i = k$. Changing ζ_k to 0 perturbs z by $O(\theta\|D\|_2)$. In the perturbed matrix

$$\begin{pmatrix} D_1^2 - z_1 z_1^T & \\ & d_k^2 \end{pmatrix},$$

the eigenvalue d_k^2 can be deflated, and the matrix $D_1^2 - z_1 z_1^T$ satisfies (15) and is of the same form but of smaller dimensions. This reduction is stable.

Now assume that $d_i - d_{i+1} < \theta\|D\|_2$. We illustrate the reduction for $i = k - 1$. Changing d_k to d_{k-1} perturbs D by $O(\theta\|D\|_2)$. Let G be a Givens rotation in the

$(k-1, k)$ plane such that $(Gz)_k = 0$. Then when we symmetrically apply G to the perturbed matrix, we get

$$G\left(\begin{pmatrix} D_1 & \\ & d_{k-1} \end{pmatrix}^2 - \begin{pmatrix} z_1 \\ \zeta_k \end{pmatrix}\begin{pmatrix} z_1 \\ \zeta_k \end{pmatrix}^T\right) G^T = \begin{pmatrix} D_1^2 - \breve{z}_1 \breve{z}_1^T & \\ & d_{k-1}^2 \end{pmatrix},$$

where $\breve{z}_1 = \left(\zeta_1, \ldots, \zeta_{k-2}, \sqrt{\zeta_{k-1}^2 + \zeta_k^2}\right)^T$. The eigenvalue d_{k-1}^2 can be deflated, and the matrix $D_1^2 - \breve{z}_1 \breve{z}_1^T$ satisfies (15) and is of the same form but of smaller dimensions. This reduction is also stable.

4. Solving Problems 2 and 3. In this section we present an algorithm that solves Problems 2 and 3 by reducing them to the problem of finding the singular value decomposition of a simple matrix.

4.1. The algorithm. Partition U_1 and U_2 as

$$U_1 = \begin{pmatrix} U_{11} \\ u_1^T \end{pmatrix} \quad \text{and} \quad U_2 = \begin{pmatrix} U_{12} \\ u_2^T \end{pmatrix},$$

where $U_{11} \in \mathbf{R}^{(m-1)\times n}$, $u_1 \in \mathbf{R}^n$, $U_{12} \in \mathbf{R}^{(m-1)\times(m-n)}$, and $u_2 \in \mathbf{R}^{m-n}$. Then from (2) and (4) we get

$$A' = (\, U_{11} \quad U_{12}\,) \begin{pmatrix} D \\ 0 \end{pmatrix} V^T = U_{11} D V^T \quad \text{and} \quad a^T = u_1^T D V^T. \tag{16}$$

The decomposition of A' in (16) is almost a singular value decomposition — U_{11} is close to being column orthogonal since it is obtained by deleting the last row from U_1. In the following we decompose U_{11} into a product of an $(m-1) \times n$ column orthogonal matrix and a simple $n \times n$ matrix. To this end we will need a scalar $\mu \geq 0$ and a vector $x \in \mathbf{R}^{m-1}$ such that $\|u_1\|^2 + \mu^2 = 1$ and the matrix

$$Y = \begin{pmatrix} U_{11} & x \\ u_1^T & \mu \end{pmatrix} \tag{17}$$

is column orthogonal. We show how to compute Y in §4.2.

Note that if $\mu = 1$, then $u_1 = 0$ and $x = 0$, so that U_{11} is column orthogonal. In general $\mu \neq 1$, but we can orthogonally transform the rows of Y so that $\mu = 1$. The matrix

$$H = \begin{pmatrix} I - \dfrac{1}{1+\mu} u_1 u_1^T & u_1 \\ -u_1^T & \mu \end{pmatrix}$$

is orthogonal and $(u_1^T, \mu)H = (0, \ldots, 0, 1)^T$. Since YH is column orthogonal, it follows that

$$YH = \begin{pmatrix} U_{11}\left(I - \dfrac{1}{1+\mu} u_1 u_1^T\right) - x\, u_1^T & U_{11} u_1 + \mu\, x \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} X & 0 \\ 0 & 1 \end{pmatrix}, \tag{18}$$

where

$$X = U_{11}\left(I - \frac{1}{1+\mu} u_1 u_1^T\right) - x\, u_1^T$$

is column orthogonal.[4] Thus

$$(U_{11} \quad x) = (U_{11} \quad x)\, HH^T = (X \quad 0)\, H^T = X \begin{pmatrix} I - \frac{1}{1+\mu} u_1 u_1^T & -u_1 \end{pmatrix},$$

which implies that

$$U_{11} = X \left(I - \frac{1}{1+\mu} u_1 u_1^T \right). \tag{19}$$

Plugging (19) into (16), we get

$$A' = X \left(I - \frac{1}{1+\mu} u_1 u_1^T \right) D V^T \equiv X C V^T. \tag{20}$$

Let $Q\,\Omega\,W^T$ be the SVD of C, where Q, $W \in \mathbf{R}^{n\times n}$ are orthogonal and $\Omega \in \mathbf{R}^{n\times n}$ is nonnegative and diagonal. Substituting into (20), we get

$$A' = XQ\,\Omega\,W^T V^T = (XQ)\,\Omega\,(VW)^T. \tag{21}$$

Comparing with (5), we have $U_1' = XQ$, $D' = \Omega$, and $V' = VW$. We specify U_2' in §4.2.

Algorithm II computes a numerically column orthogonal matrix $\tilde{Y}$ and a *numerical* singular value decomposition $\tilde{Q}\,\tilde{\Omega}\,\tilde{W}^T$ satisfying (see §4.2 and §5)

$$\tilde{Y} = \bar{Y} + O(\epsilon), \quad \tilde{Q} = \bar{Q} + O(\epsilon), \quad \tilde{\Omega} = \bar{\Omega} + O(\epsilon\|D\|_2), \quad \tilde{W} = \bar{W} + O(\epsilon), \tag{22}$$

where

$$\bar{Y} = \begin{pmatrix} \bar{U}_{11} & \bar{x} \\ \bar{u}_1^T & \bar{\mu} \end{pmatrix}$$

is a column orthogonal matrix with

$$\bar{U}_{11} = U_{11} + O(\epsilon), \quad \bar{u}_1 = u_1 + O(\epsilon), \quad \text{and} \quad \bar{\mu} = \mu + O(\epsilon)$$

and

$$\bar{C} \equiv \left(I - \frac{1}{1+\bar{\mu}} \bar{u}_1 \bar{u}_1^T \right) \bar{D} = \bar{Q}\,\bar{\Omega}\,\bar{W}$$

is an exact SVD with

$$\bar{D} = D + O(\epsilon\|D\|_2).$$

Let

$$\bar{X} = \bar{U}_{11} \left(I - \frac{1}{1+\bar{\mu}} \bar{u}_1 \bar{u}_1^T \right) - \bar{x}\,\bar{u}_1^T.$$

Algorithm II then computes numerical approximations to U' and V' satisfying

$$\tilde{U}_1' = \bar{X}\bar{Q} + O(\epsilon), \quad \tilde{U}_2' = \bar{U}_2' + O(\epsilon), \quad \text{and} \quad \tilde{V}' = V\bar{W} + O(\epsilon), \tag{23}$$

[4] Paige [22] has proven similar relations.

where $(\bar{X}\bar{Q}, \bar{U}_2') \in \mathbf{R}^{(m-1)\times(m-1)}$ is orthogonal (see §4.2). Since $\bar{X}\bar{Q}$, $\bar{\Omega}$, and $V\bar{W}$ solve Problems 2 and 3 exactly for slightly perturbed input data $\bar{U}_1$, $\bar{D}$, and V, Algorithm II is stable.

It is well known that the singular values of A' are always well conditioned with respect to perturbations in A', but that the singular vectors of A' can be very sensitive to such perturbations [12], [25]. Since

$$A' = U_{11}DV^T = \bar{U}_{11}\bar{D}V^T + O(\epsilon\|D\|_2) = \bar{X}\bar{C}V^T + O(\epsilon\|D\|_2),$$

this guarantees that $\tilde{D}' = \tilde{\Omega}'$ is close to D'. However, $\tilde{Q}$ and $\tilde{W}$ can be very different from Q and W, respectively, and thus $\tilde{U}_1'$ and $\tilde{V}'$ can be very different from U_1' and V', respectively.

Consider the case where U_1 is given. It takes $O(mn)$ time to compute μ and x (see §4.2), it takes $O(mn)$ time to compute X, it takes $O(n^2)$ time to compute the SVD of C (see §5), and it takes $O(mn^2)$ and $O(n^3)$ time to compute XQ and VW, respectively. Algorithm II computes both XQ and VW for Problem 2 and computes XQ for Problem 3. Thus the total times for solving Problems 2 and 3 are $O((m+n)\,n^2)$ and $O(mn^2)$, respectively.

4.2. Computing Y. In this subsection we show how to compute the column orthogonal matrix Y (see (17)).

First we assume that U_2 is known. Let P be an orthogonal matrix such that $Pu_2 = \|u_2\|_2\, e_1$, where $e_1 = (1, 0, \ldots, 0)^T$, and define $(z_2, X_{12}) = U_{12}P^T$, where $z_2 \in \mathbf{R}^{m-1}$ and $X_{12} \in \mathbf{R}^{(m-1)\times(m-n-1)}$. Since

$$\begin{pmatrix} U_{11} & U_{12} \\ u_1^T & u_2^T \end{pmatrix} \begin{pmatrix} I_n & \\ & P^T \end{pmatrix} = \begin{pmatrix} U_{11} & z_2 & X_{12} \\ u_1^T & \|u_2\|_2 & 0 \end{pmatrix}$$

is orthogonal, the matrix

$$\begin{pmatrix} U_{11} & z_2 \\ u_1^T & \|u_2\|_2 \end{pmatrix}$$

is column orthogonal and $\|u_1\|_2^2 + \|u_2\|_2^2 = 1$. Thus we set $x = z_2$ and $\mu = \|u_2\|_2$. It takes $O(m\,(m-n))$ time to compute x and μ. This computation is stable (see (22)).

From (18) we have

$$\begin{pmatrix} U_{11} & x & X_{12} \\ u_1^T & \mu & 0 \end{pmatrix} \begin{pmatrix} H & \\ & I_{m-n-1} \end{pmatrix} = \begin{pmatrix} X & 0 & X_{12} \\ 0 & 1 & 0 \end{pmatrix},$$

and thus $(X, X_{12}) \in \mathbf{R}^{(m-1)\times(m-1)}$ is orthogonal. We set $U_2' = X_{12}$ (see (5) and (21)). It takes $O(m\,(m-n))$ time to compute X_{12}. This computation is also stable (see (23)).

Next we assume that U_2 is *not* known. Let $u = (x^T, \mu)$ be the result of applying the Gram–Schmidt procedure with reorthogonalization [8, §4] to orthonormalize $e_n = (0, \ldots, 0, 1)^T$ to the columns of U_1. If $u \neq 0$, then

$$Y = (\,U_1 \quad u\,) \equiv \begin{pmatrix} U_{11} & x \\ u_1^T & \mu \end{pmatrix}$$

is column orthogonal and $YY^Te_n = e_n$, so that

$$1 = (YY^Te_n)_n = u_1^Tu_1 + \mu^2.$$

If $u = 0$, then $U_1 U_1^T e_n = e_n$, so that $1 = (U_1 U_1^T e_n)_n = u_1^T u_1$, and we get a nonzero u by repeating the Gram–Schmidt procedure with a random unit vector in place of e_n (note that in this case $\mu = 0$).[5] The time for computing x and μ is $O(lmn)$, where l is the number of reorthogonalization steps, which is a small constant in practice [8]. These computations are stable (see (22)).

4.3. Another perspective. In this subsection we present another derivation of the decomposition $A' = XCV^T$, which relates Algorithm II to a method for downdating the QR decomposition (cf. [23]).

Consider the augmented matrix

$$\mathcal{A} = \begin{pmatrix} u_1 & D \\ \mu & 0 \end{pmatrix}.$$

From (18), (17), and (16) we have

$$Y \begin{pmatrix} u_1 & D \\ \mu & 0 \end{pmatrix} = \begin{pmatrix} 0 & U_{11} D \\ 1 & u_1^T D \end{pmatrix} = \begin{pmatrix} 0 & A'V \\ 1 & a^T V \end{pmatrix}.$$

On the other hand, from (18) we get

$$Y \begin{pmatrix} u_1 & D \\ \mu & 0 \end{pmatrix} = (YH)\, H^T \begin{pmatrix} u_1 & D \\ \mu & 0 \end{pmatrix} = \begin{pmatrix} X & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & C \\ 1 & u_1^T D \end{pmatrix} = \begin{pmatrix} 0 & XC \\ 1 & u_1^T D \end{pmatrix}.$$

Thus $A'V = XC$, and the result follows.

Park and Van Huffel [24] downdate by using plane rotations to reduce $\mathcal{A}$ to a matrix of the form

$$\begin{pmatrix} 0 & B \\ 1 & w^T \end{pmatrix},$$

where $B = {F'}^T A' V G'$ is bidiagonal and F' and G' are orthogonal, and then solving the bidiagonal singular value problem. The total time appears to be at least as large as that for Algorithm II.

5. Computing the SVD of C. In this section we present an algorithm for computing the singular value decomposition of the matrix $C \in \mathbf{R}^{k\times k}$ given by

$$C = \left(I - \frac{1}{1+\mu} u_1 u_1^T \right) D, \tag{24}$$

where $D = \mathrm{diag}(d_1, \ldots, d_k)$ with $d_1 \geq d_2 \geq \cdots \geq d_k \geq 0$, $u_1 = (\mu_1, \ldots, \mu_k)^T$ with $\|u_1\|_2 \leq 1$, and $\mu = \sqrt{1 - \|u_1\|_2^2}$. For convenience we define $d_{k+1} = 0$ and $\mu_{k+1} = \mu$.

We assume that

$$d_i - d_{i+1} \geq \theta \|D\|_2 \quad \text{and} \quad |\mu_i| \geq \theta, \tag{25}$$

where θ is a small multiple of ϵ to be specified in §5.3. Any matrix of the form (24) can be reduced to one that satisfies these conditions by using the deflation procedure described in §5.4.

[5] The same construction is used in downdating the QR decomposition [8].

5.1. Properties of the SVD. In this subsection we establish some properties of the singular value decomposition of C. The following lemma characterizes the singular values and singular vectors.

LEMMA 5.1. *Let $Q\,(\Omega, 0)\,W^T$ be the* SVD *of C with*

$$Q = (q_1, \ldots, q_k), \quad \Omega = \operatorname{diag}(\omega_1, \ldots, \omega_k), \quad \text{and} \quad W = (w_1, \ldots, w_k).$$

Then the singular values $\{\omega_i\}_{i=1}^k$ satisfy the secular equation

$$f_2(\omega) \equiv \sum_{j=1}^{k+1} \frac{\mu_j^2}{d_j^2 - \omega^2} = 0 \tag{26}$$

and the interlacing property

$$d_1 > \omega_1 > d_2 > \cdots > d_k > \omega_k > 0. \tag{27}$$

The singular vectors are given by

$$q_i = \left(\frac{\gamma_{i,1}\mu_1}{d_1^2 - \omega_i^2}, \ldots, \frac{\gamma_{i,k}\mu_k}{d_k^2 - \omega_i^2} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{k} \left(\frac{\gamma_{i,j}\mu_j}{d_j^2 - \omega_i^2} \right)^2}, \tag{28}$$

where $\gamma_{i,j} = \omega_i^2 + \mu d_j^2$, and

$$w_i = \left(\frac{d_1\mu_1}{d_1^2 - \omega_i^2}, \ldots, \frac{d_k\mu_k}{d_k^2 - \omega_i^2} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{k} \left(\frac{d_j\mu_j}{d_j^2 - \omega_i^2} \right)^2}. \tag{29}$$

Proof. Since $\mu > 0$ and $d_k > 0$ (see (25)), C is nonsingular and $\omega_k > 0$. Since C is square and $C^TC = D(I - u_1u_1^T)D$, the squares of the singular values $\{\omega_i^2\}_{i=1}^k$ and the right singular vectors $\{q_i\}_{i=1}^k$ are the eigenvalues and eigenvectors, respectively, of $D^2 - (Du_1)(Du_1)^T$. Relations (27) and (29) follow immediately from Lemma 3.1 with $z = Du_1$. Moreover, the singular values satisfy the secular equation

$$0 = f_1(\omega) = -1 + \sum_{j=1}^{k} \frac{(d_j\mu_j)^2}{d_j^2 - \omega^2} = -\sum_{j=1}^{k+1} \mu_i^2 + \sum_{j=1}^{k+1} \frac{d_j^2\mu_j^2}{d_j^2 - \omega^2} = \omega^2 \sum_{j=1}^{k+1} \frac{\mu_j^2}{d_j^2 - \omega^2}, \tag{30}$$

which implies that they satisfy (26) as well.

From (29) we see that w_i is a multiple of $(D^2 - \omega_i^2 I)^{-1}Du_1$. Since $\omega_i q_i = Cw_i$, it follows that q_i is a multiple of $C(D^2 - \omega_i^2 I)^{-1}Du_1$. Simplifying,

$$C(D^2 - \omega_i^2 I)^{-1}Du_1 = D(D^2 - \omega_i^2 I)^{-1}Du_1 - \frac{u_1^T D(D^2 - \omega_i^2 I)^{-1}Du_1}{1 + \mu} u_1. \tag{31}$$

Because ω_i satisfies (30), we have

$$u_1^T D(D^2 - \omega_i^2 I)^{-1}Du_1 = \sum_{j=1}^{k} \frac{d_j^2\mu_j^2}{d_j^2 - \omega_i^2} = 1.$$

Plugging this into (31), we have

$$
\begin{aligned}
C(D^2 - \omega_i^2 I)^{-1} D u_1 &= \left(\omega_i^2 I + (D^2 - \omega_i^2 I)\right)(D^2 - \omega_i^2 I)^{-1} u_1 - \frac{1}{1+\mu} u_1 \\
&= \omega_i^2 (D^2 - \omega_i^2 I)^{-1} u_1 + \frac{\mu}{1+\mu} u_1 \\
&= \frac{1}{1+\mu}\left(\omega_i^2 I + \mu D^2\right)(D^2 - \omega_i^2 I)^{-1} u_1.
\end{aligned}
$$

Ignoring the first factor and normalizing, we get (28). □

The following lemma allows one to construct a matrix of the form (24) using D and all the singular values.

LEMMA 5.2. *Given a diagonal matrix* $D = \mathrm{diag}(d_1, \ldots, d_k)$ *and a set of numbers* $\{\hat{\omega}_i\}_{i=1}^k$ *satisfying the interlacing property*

$$
d_1 > \hat{\omega}_1 > d_2 > \cdots > d_k > \hat{\omega}_k > d_{k+1} \equiv 0, \tag{32}
$$

there exists a vector $\hat{u}_1$ *and a scalar* $\hat{\mu} \ge 0$ *with* $\|\hat{u}_1\|_2^2 + \hat{\mu}^2 = 1$ *such that* $\{\hat{\omega}_i\}_{i=1}^k$ *are the singular values of*

$$
\hat{C} = \left(I - \frac{1}{1+\hat{\mu}} \hat{u}_1 \hat{u}_1^T\right) D.
$$

The vector $\hat{u}_1 = (\hat{\mu}_1, \ldots, \hat{\mu}_k)^T$ *and scalar* $\hat{\mu} = \hat{\mu}_{k+1}$ *are given by*

$$
|\hat{\mu}_i| = \sqrt{\prod_{j=1}^{i-1} \frac{\hat{\omega}_j^2 - d_i^2}{d_j^2 - d_i^2} \prod_{j=i}^{k} \frac{\hat{\omega}_j^2 - d_i^2}{d_{j+1}^2 - d_i^2}}, \qquad 1 \le i \le k+1, \tag{33}
$$

where the sign of $\hat{\mu}_i$ *can be chosen arbitrarily for* $1 \le i \le k$.

Proof. The numbers $\{\hat{\omega}_i\}_{i=1}^k$ satisfy the interlacing property (11). By Lemma 3.2 there exists a vector $\hat{z} = (\hat{\zeta}_1, \ldots, \hat{\zeta}_k)^T$ satisfying (12) such that the eigenvalues of $D^2 - \hat{z}\hat{z}^T$ are $\{\hat{\omega}_i^2\}_{i=1}^k$. Defining $\hat{u}_1 = D^{-1}\hat{z}$, it follows that $\hat{\mu}_i$ satisfies (33) for $1 \le i \le k$. The first result of Lemma 3.1 implies that $\hat{u}_1^T \hat{u}_1 = \hat{z}^T D^{-2} \hat{z} \le 1$, so that we can define $\hat{\mu} \equiv \hat{\mu}_{k+1} = \sqrt{1 - \|\hat{u}_1\|_2^2}$. It then follows that

$$
\hat{C}^T \hat{C} = D^2 - D\hat{u}_1 \hat{u}_1^T D = D^2 - \hat{z}\hat{z}^T,
$$

so that $\{\hat{\omega}_i\}_{i=1}^k$ are the singular values of $\hat{C}$. Consequently,

$$
\prod_{j=1}^k \hat{\omega}_j = \det(\hat{C}) = \det\left(I - \frac{1}{1+\hat{\mu}} \hat{u}_1 \hat{u}_1^T\right) \det(D) = \hat{\mu} \prod_{j=1}^k d_j,
$$

and hence

$$
\hat{\mu}_{k+1} = \prod_{j=1}^k \frac{\hat{\omega}_j}{d_j},
$$

which is (33) for $i = k+1$. □

5.2. Computing the singular vectors. In practice we can only hope to compute an approximation $\hat{\omega}_i$ to ω_i. Yet it is well known that equations similar to (28) and (29) can be very sensitive to small errors in ω_i (see §3.2). Lemma 5.2 allows us to overcome this problem. After we have computed all the approximate singular values $\{\hat{\omega}_i\}_{i=1}^k$ of C, we find a *new* matrix $\hat{C}$ whose *exact* singular values are $\{\hat{\omega}_i\}_{i=1}^k$ and then compute the singular vectors of $\hat{C}$ using Lemma 5.1. Note that each difference, each product, and each ratio in (33) can be computed to high relative accuracy.[6] Thus $|\hat{\mu}_i|$ can be computed to high relative accuracy. We choose the sign of $\hat{\mu}_i$ to be the sign of μ_i. Substituting the computed $\hat{u}_1$ and $\hat{\mu}$ and the *exact* singular values $\{\hat{\omega}_i\}_{i=1}^k$ into (28) and (29), each singular vector of $\hat{C}$ can also be computed to componentwise high relative accuracy. Consequently, after all the singular vectors are computed, the singular vector matrices of $\hat{C}$ will be numerically orthogonal.

To ensure the existence of $\hat{C}$, we need $\{\hat{\omega}_i\}_{i=1}^k$ to satisfy the interlacing property (32). But since the exact singular values of C satisfy the same interlacing property (see (27)), this is only an accuracy requirement on the computed singular values and is not an additional restriction on C. We can use the SVD of $\hat{C}$ as an approximation to the SVD of C. This is stable as long as $\hat{u}_1$ and $\hat{\mu}$ are close to u_1 and μ, respectively.

5.3. Stably computing the singular values. To guarantee that $\hat{u}_1$ and $\hat{\mu}$ are close to u_1 and μ, respectively, we must ensure that the approximations $\{\hat{\omega}_i\}_{i=1}^k$ to the singular values are sufficiently accurate. As in §3.3, the key is the stopping criterion for the root-finder, namely,

$$|g_i(\xi)| \le \eta k(|\psi_i(\xi)| + |\phi_i(\xi)|), \tag{34}$$

where the secular equation (26) has been reformulated as $g_i(\xi) \equiv \psi_i(\xi) + \phi_i(\xi) = 0$ in the analogous manner.

THEOREM 5.3. *If $\theta = 2\eta k^2$ in* (25) *and each $\hat{\xi}_i$ satisfies* (34), *then*

$$|\hat{\mu}_i - \mu_i| \le 4\eta k^2 \|u\|_2, \qquad 1 \le i \le k+1. \tag{35}$$

The proof is again nearly identical to that of the corresponding result in [18]. As argued there, the factor k^2 in θ and (35) is likely to be $O(k)$ in practice.

We have been assuming that $\|u_1\|_2 + \mu^2 = 1$. In practice this is not always true due to round-off errors. However, since a vector with norm near unity is close to an *exact* unit vector to componentwise high relative accuracy, in practice u_1 and μ are given to componentwise high relative accuracy. This implies that each term in the secular equation (26) is still computed to high relative accuracy after the reformulation. Hence the stopping criterion (34) holds, and $\hat{u}_1$ and $\hat{\mu}$ are close to u_1 and μ, respectively.

5.4. Deflation. We now show that we can reduce C to a matrix of the same form that further satisfies

$$d_i - d_{i+1} \ge \theta \|D\|_2 \quad \text{and} \quad |\mu_i| \ge \theta,$$

where θ is specified in §5.3.

[6] Note that $\hat{\mu} = \hat{\mu}_{k+1}$ is *not* computed from $\hat{\mu} = \sqrt{1 - \|\hat{u}_1\|_2^2}$, which might not give high relative accuracy.

Assume that $\mu \equiv \mu_{k+1} < \theta$. Changing μ to θ perturbs μ by $O(\theta)$. The perturbed matrix

$$\left(I - \frac{1}{1+\theta} u_1 u_1^T\right) D$$

has the same form but with $\mu \geq \theta$. This reduction is stable (see §5.3).

Next assume that $|\mu_i| < \theta$ for some $i \leq k$. We illustrate the case $i = 1$. Changing μ_1 to 0 perturbs u_1 by $O(\theta)$. Partition u_1 and D as

$$u_1 = \begin{pmatrix} \mu_1 \\ \breve{u}_1 \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} d_1 & \\ & \breve{D} \end{pmatrix}.$$

Then in the perturbed matrix

$$\begin{pmatrix} 1 & \\ & I - \frac{1}{1+\mu} \breve{u}_1 \breve{u}_1^T \end{pmatrix} \begin{pmatrix} d_1 & \\ & \breve{D} \end{pmatrix} \equiv \begin{pmatrix} d_1 & \\ & \breve{C} \end{pmatrix},$$

the singular value d_1 can be deflated, and $\breve{C}$ is another matrix with the same form but smaller dimensions. This reduction is also stable (see §5.3).

Now assume that $d_i - d_{i+1} < \theta \|D\|_2$ for some $i \leq k-1$. We illustrate the reduction for $i = 1$. Changing d_1 to d_2 perturbs D by $O(\theta \|D\|_2)$. Let G be a Givens rotation in the $(1, 2)$ plane such that $(Gu)_1 = 0$, and let

$$\breve{u}_1 = \left(\sqrt{\mu_1^2 + \mu_2^2}, \mu_3, \ldots, \mu_k\right)^T \quad \text{and} \quad \breve{D} = \mathrm{diag}(d_2, d_3, \ldots, d_k).$$

Then symmetrically applying G to the perturbed matrix, we get

$$\begin{aligned} &G\left(I - \frac{1}{1+\mu} u_1 u_1^T\right) \begin{pmatrix} d_2 & \\ & \breve{D} \end{pmatrix} G^T \\ &= \left(G - \frac{1}{1+\mu} G u_1 u_1^T\right) G^T \begin{pmatrix} d_2 & \\ & \breve{D} \end{pmatrix} \\ &= \left(I - \frac{1}{1+\mu} \begin{pmatrix} 0 \\ \breve{u}_1 \end{pmatrix} \begin{pmatrix} 0 \\ \breve{u}_1 \end{pmatrix}^T\right) \begin{pmatrix} d_2 & \\ & \breve{D}_1 \end{pmatrix} \\ &= \begin{pmatrix} d_2 & \\ & \left(I - \frac{1}{1+\mu} \breve{u}_1 \breve{u}_1^T\right) \breve{D}_1 \end{pmatrix}. \end{aligned}$$

The singular value d_2 can be deflated, and the remaining matrix has the same form but smaller dimensions. This reduction is stable as well.

Finally assume that $d_k < \theta \|D\|_2$ and $d_{k-1} - d_k \geq \theta \|D\|_2$. Changing d_k to $\theta \|D\|_2$ perturbs D by $O(\theta \|D\|_2)$. Let

$$\breve{D} = \mathrm{diag}\left(d_1, \ldots, d_{k-2}, d_{k-1}, \theta \|D\|_2\right).$$

Then the perturbed matrix

$$\left(I - \frac{1}{1+\mu} u_1 u_1^T\right) \breve{D}$$

has the same form but with $d_k \geq \theta \|D\|_2$. If the relation $d_{k-1} - d_k \geq \theta \|D\|_2$ no longer holds, then we can apply the previous reduction to reduce the matrix size. This reduction is again stable.

6. Ill-conditioning of Problem 1. In this section we bound the effect of perturbations in a on the singular values of A'. The effect of perturbations in V and D is similar. We assume that D is nonsingular.

From (20) and the second relation in (16), we have $A' = XCV^T$, where X is column orthogonal and

$$C = D - \frac{1}{1+\mu} u_1 u_1^T D,$$

with $u_1 = D^{-1}V^T a$ and $\mu = \sqrt{1 - \|u_1\|_2^2}$.

Let $\bar{a}$ be a vector slightly perturbed from a with $\|D^{-1}V^T\bar{a}\|_2 \le 1$, and let $\bar{A}'$ be the downdated matrix for the input data V, D, and $\bar{a}$. As before, we have $\bar{A}' = \bar{X}\bar{C}V^T$, where $\bar{X}$ is column orthogonal and

$$\bar{C} = D - \frac{1}{1+\bar{\mu}} \bar{u}_1 \, \bar{u}_1^T D,$$

with $\bar{u}_1 = D^{-1}V^T\bar{a}$ and $\bar{\mu} = \sqrt{1 - \|\bar{u}_1\|_2^2}$.

Let ω_i and $\bar{\omega}_i$ be the ith largest singular values of A and $\bar{A}$, respectively. Since the singular values of A' and $\bar{A}'$ are the singular values of C and $\bar{C}$, respectively, we have $|\bar{\omega}_i - \omega_i| \le \|\bar{C} - C\|_2$ (see [12, p. 428]).

Since

$$\bar{u}_1 - u_1 = D^{-1}V^T(\bar{a} - a),$$

we have

$$\|\bar{u}_1 - u_1\|_2 \le \|D^{-1}\|_2 \, \|\bar{a} - a\|_2.$$

Similarly,

$$\bar{\mu} - \mu = \frac{(1 - \|\bar{u}_1\|_2^2) - (1 - \|u_1\|_2^2)}{\sqrt{1 - \|\bar{u}_1\|_2^2} + \sqrt{1 - \|u_1\|_2^2}} = -\frac{(\bar{u}_1 + u_1)^T \, (\bar{u}_1 - u_1)}{\sqrt{1 - \|\bar{u}_1\|_2^2} + \sqrt{1 - \|u_1\|_2^2}},$$

so that

$$|\bar{\mu} - \mu| \le \frac{2 \, \|\bar{u}_1 - u_1\|_2}{\sqrt{1 - \|u_1\|_2^2}} \le \frac{2 \, \|D^{-1}\|_2 \|\bar{a} - a\|_2}{\sqrt{1 - \|u_1\|_2^2}}.$$

Since

$$\begin{aligned} \bar{C} - C &= \frac{1}{1+\mu} u_1 a^T V - \frac{1}{1+\bar{\mu}} \bar{u}_1 \bar{a}^T V \\ &= \left(\frac{(\bar{\mu} - \mu)\, u_1}{(1+\mu)(1+\bar{\mu})} - \frac{\bar{u}_1 - u_1}{1+\bar{\mu}} \right) a^T V - \frac{\bar{u}_1}{1+\bar{\mu}} \, (\bar{a} - a)^T V, \end{aligned}$$

we have

$$\begin{aligned} |\bar{\omega}_i - \omega_i| &\le \|\bar{C} - C\|_2 \\ &\le \frac{\|(\bar{\mu} - \mu)\, u_1\|_2}{(1+\mu)(1+\bar{\mu})} \, \|a\|_2 + \frac{\|\bar{u}_1 - u_1\|_2}{1+\bar{\mu}} \, \|a\|_2 + \frac{\|\bar{u}_1\|_2}{1+\bar{\mu}} \, \|\bar{a} - a\|_2 \\ &\le |\bar{\mu} - \mu| \, \|a\|_2 + \|\bar{u}_1 - u_1\|_2 \, \|a\|_2 + \|\bar{a} - a\|_2 \\ &\le \frac{4 \max\left\{ \|D^{-1}\|_2 \, \|a\|_2, 1 \right\}}{\sqrt{1 - \|u_1\|_2^2}} \, \|\bar{a} - a\|_2. \end{aligned}$$

When the factor $\|D^{-1}\|_2\|a\|_2$ is very large, or when $\|u_1\|_2$ is near unity, we cannot guarantee that $\bar{\omega}_i$ is close to ω_i. This result parallels that of Stewart [26, p. 205] in the context of downdating the Cholesky/QR factorization.

To better explain the role of $\|u_1\|_2$, Stewart [26] also shows that

$$\omega_n \leq \|D\|_2 \sqrt{1 - \|u_1\|_2^2} \quad \text{and} \quad \|u_1\|_2^2 \geq \frac{(d_i/\omega_i)^2 - 1}{(d_i/\omega_i)^2 + 1}.$$

Thus if $\|u_1\|_2$ is near unity, then ω_n is close to zero and C (and hence A') is close to being singular. And if any d_i is reduced (to ω_i) by a large factor, then $\|u_1\|_2$ is near unity.

REFERENCES

[1] J. L. Barlow, H. Zha, and P. A. Yoon, *Stable chasing algorithms for modifying complete and partial singular value decompositions*, Tech. Report CSE-93-19, Dept. of Computer Science, The Pennsylvania State University, University Park, PA, Sept. 1993.

[2] Å. Björck, H. Park, and L. Eldén, *Accurate downdating of least squares solutions*, SIAM J. Matrix Anal. Appl., 15 (1994), pp. 549–568.

[3] A. W. Bojanczyk, R. P. Brent, P. van Dooren, and F. R. de Hoog, *A note on downdating the Cholesky factorization*, SIAM J. Sci. Statist. Comput., 8 (1987), pp. 210–221.

[4] C. F. Borges and W. B. Gragg, *A parallel divide and conquer algorithm for the generalized real symmetric definite tridiagonal eigenproblem*, in Numerical Linear Algebra and Scientific Computing, L. Reichel, A. Ruttan, and R. S. Varga, eds., de Gruyter, Berlin, 1993, pp. 10–28.

[5] J. R. Bunch and C. P. Nielsen, *Updating the singular value decomposition*, Numer. Math., 31 (1978), pp. 111–129.

[6] J. R. Bunch, C. P. Nielsen, and D. C. Sorensen, *Rank-one modification of the symmetric eigenproblem*, Numer. Math., 31 (1978), pp. 31–48.

[7] J. Carrier, L. Greengard, and V. Rokhlin, *A fast adaptive multipole algorithm for particle simulations*, SIAM J. Sci. Statist. Comput., 9 (1988), pp. 669–686.

[8] 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.

[9] J. J. Dongarra and D. C. Sorensen, *A fully parallel algorithm for the symmetric eigenvalue problem*, SIAM J. Sci. Statist. Comput., 8 (1987), pp. s139–s154.

[10] P. E. Gill, G. H. Golub, W. Murray, and M. A. Saunders, *Methods for modifying matrix factorizations*, Math. Comp., 28 (1974), pp. 505–535.

[11] G. H. Golub, *Some modified matrix eigenvalue problems*, SIAM Rev., 15 (1973), pp. 318–334.

[12] G. H. Golub and C. F. Van Loan, *Matrix Computations*, second ed., The Johns Hopkins University Press, Baltimore, MD, 1989.

[13] W. B. Gragg, J. R. Thornton, and D. D. Warner, *Parallel divide and conquer algorithms for the symmetric tridiagonal eigenproblem and bidiagonal singular value problem*, in Proc. 23rd Annual Pittsburgh Conference, University of Pittsburgh School of Engineering, Vol. 23, Modelling and Simulation, Pittsburgh, 1992.

[14] L. Greengard and V. Rokhlin, *A fast algorithm for particle simulations*, J. Comput. Phys., 73 (1987), pp. 325–348.

[15] M. Gu, *Studies in Numerical Linear Algebra*, Ph.D. thesis, Department of Computer Science, Yale University, New Haven, CT, 1993.

[16] M. Gu and S. C. Eisenstat, *Downdating the singular value decomposition*, Research Report YALEU/DCS/RR-939, Dept. of Computer Science, Yale University, New Haven, CT, May 1993.

[17] ———, *A stable and fast algorithm for updating the singular value decomposition*, Research Report YALEU/DCS/RR-966, Dept. of Computer Science, Yale University, New Haven, CT, June 1993.

[18] ———, *A stable and efficient algorithm for the rank-one modification of the symmetric eigenproblem*, SIAM J. Matrix Anal. Appl., 15 (1994), pp. 1266–1276.

[19] R.-C. Li, *Solving secular equations stably and efficiently*, Working paper, Dept. of Mathematics, University of California at Berkeley, Oct. 1992.

[20] K. LÖWNER, *Über monotone matrixfunktionen*, Math. Z., 38 (1934), pp. 177–216.

[21] M. MOONEN, P. VAN DOOREN, AND J. VANDEWALLE, *A singular value decomposition updating algorithm for subspace tracking*, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 1015–1038.

[22] C. C. PAIGE, *Error analysis of some techniques for updating orthogonal decompositions*, Math. Comp., 34 (1980), pp. 465–471.

[23] H. PARK AND L. ELDÉN, *Downdating the rank-revealing URV decomposition*, Tech. Report LiTH-MAT-R-1992-47, Dept. of Mathematics, Linköping University, Linköping, Sweden, Dec. 1992.

[24] H. PARK AND S. VAN HUFFEL, *Two-way bidiagonalization scheme for downdating the singular value decomposition*, Preprint 93-035, Army High Performance Computing Research Center, University of Minnesota, Minneapolis, MN, Apr. 1993.

[25] G. W. STEWART, *Introduction to Matrix Computations*, Academic Press, New York, 1973.

[26] ———, *The effects of rounding error on an algorithm for downdating a Cholesky factorization*, J. Inst. Maths. Applics., 23 (1979), pp. 203–213.

[27] ———, *Determining rank in the presence of error*, Tech. Report CS TR–2972 and UMIACS TR–92–108, Dept. of Computer Science and Institute for Advanced Computer Studies, University of Maryland, College Park, MD, Oct. 1992.