## 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 show that the problem of computing the singular values of A' is well-conditioned when the left singular vectors of A are given and can be ill-conditioned when they are not. Previous algorithms are based on an unstable algorithm for the ill-conditioned problem.

## Downdating the Singular Value Decomposition<sup>†</sup>

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## 1. Introduction

The singular value decomposition (SVD) of a matrix  $A \in \mathbf{R}^{m \times n}$  is

$$A = U\Sigma V^T, \tag{1.1}$$

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 non-negative entries in decreasing order. The columns of U and V are the *left singular vectors* and the *right singular vectors* of A, respectively; the diagonal entries of  $\Sigma$  are the *singular values* of A.

In many least squares and signal processing applications (see [3, 15, 20] 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. In [13] we consider the problem of updating the SVD. In this paper we consider the problem of downdating the SVD. This problem is also related to the problem of downdating the URV and ULV decompositions (see [17]).

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

$$A = \begin{pmatrix} A' \\ a^T \end{pmatrix}, \tag{1.2}$$

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

$$A' = U' \Sigma' {V'}^T, \tag{1.3}$$

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 non-negative entries in decreasing order. We would like to take advantage of our knowledge of the SVD of A when computing the SVD of A'.

First consider the case m > n. We write

$$U = (U_1 \ U_2), \ \Sigma = \begin{pmatrix} D \\ 0 \end{pmatrix}$$
 and  $U' = (U'_1 \ U'_2), \ \Sigma' = \begin{pmatrix} D' \\ 0 \end{pmatrix}$ ,

where  $U_1 \in \mathbf{R}^{m \times n}$ ,  $U_2 \in \mathbf{R}^{m \times (m-n)}$  and  $D \in \mathbf{R}^{n \times n}$ ; and  $U'_1 \in \mathbf{R}^{(m-1) \times n}$ ,  $U'_2 \in \mathbf{R}^{(m-1) \times (m-n-1)}$ and  $D' \in \mathbf{R}^{n \times n}$ . Equations (1.1) and (1.3) can be rewritten as

$$A = U\Sigma V^{T} = (U_{1} \ U_{2}) \begin{pmatrix} D \\ 0 \end{pmatrix} V^{T} = U_{1}DV^{T}$$
(1.4)

and

$$A' = U' \Sigma' {V'}^{T} = (U'_{1} \ U'_{2}) \ \begin{pmatrix} D'\\ 0 \end{pmatrix} {V'}^{T} = U'_{1} D' {V'}^{T}.$$
(1.5)

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 SVD (1.4). We show that

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

where  $z = V^T a \in \mathbb{R}^n$ . Thus the eigenvalues of  $D^2 - zz^T$  must be non-negative<sup>1</sup>. The singular values of A' can be computed by 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 non-negative diagonal. The right singular vector matrix V' can be computed as VS. The diagonal elements of  $D' = \Omega$  are the singular values. We present Algorithm I to solve Problem 1 stably in Section 2.1.

Since Problem 1 requires computing the eigendecomposition of  $D^2 - zz^T$ , small perturbations in V, D and a can cause large perturbations in D' and V'. We analyze the ill-conditioning of the singular values in Section 6.1. Our perturbation results are similar to those of Stewart [19] 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

$$A' = XC_1 V^T, (1.6)$$

where  $C_1 \in \mathbf{R}^{n \times n}$  is given by

$$C_1 = \left(I - \frac{1}{1+\mu}u_1u_1^T\right)D,$$

with  $u_1$  a vector and  $\mu \ge 0$  a scalar. The singular values of A' can be computed by the SVD

$$C_1 = Q_1 \Omega W_1^T,$$

where  $Q_1, W_1 \in \mathbf{R}^{n \times n}$  are orthogonal and  $\Omega \in \mathbf{R}^{n \times n}$  is non-negative diagonal. The left singular vector matrix  $U'_1$  can be computed as  $XQ_1$ . The right singular vector matrix V' can be computed as  $VW_1$ . The diagonal elements of  $D' = \Omega$  are the singular values. We present Algorithm II to solve Problems 2 and 3 stably in Section 4.1.

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 Section 4.1).

The case  $m \leq n$  is similar. We write

$$V = (V_1 \ V_2), \ \Sigma = (D \ 0) \text{ and } V' = (V'_1 \ V'_2), \ \Sigma' = (D' \ 0),$$

<sup>&</sup>lt;sup>1</sup> In general the eigenvalues of  $D^2 - zz^T$  can be negative.

where  $V_1 \in \mathbf{R}^{n \times m}$ ,  $V_2 \in \mathbf{R}^{n \times (n-m)}$  and  $D \in \mathbf{R}^{m \times m}$ ; and  $V'_1 \in \mathbf{R}^{n \times (m-1)}$ ,  $V'_2 \in \mathbf{R}^{n \times (n-m+1)}$ and  $D' \in \mathbf{R}^{(m-1) \times (m-1)}$ . Equations (1.1) and (1.3) can be rewritten as

$$A = U\Sigma V^{T} = U(D \ 0) \begin{pmatrix} V_{1}^{T} \\ V_{2}^{T} \end{pmatrix} = UDV_{1}^{T}$$
(1.7)

and

$$A' = U' \Sigma' {V'}^T = U' (D' \ 0) \left( \begin{array}{c} {V_1'}^T \\ {V_2'}^T \end{array} \right) = U' D' {V_1'}^T.$$
(1.8)

There are three downdating problems to consider:

- 1. Given V (or  $V_1$ ), D and a, compute V' (or  $V'_1$ ) and D'.
- 2. Given U, V (or  $V_1$ ) and D, compute U', V' (or  $V'_1$ ) and D'.
- 3. Given U and D, compute U' and D'.

We assume that Problem 1 has a solution as before. We extend Algorithm I to solve Problem 1 stably for  $m \leq n$  in Section 2.2. Both the singular values and the singular vectors can be ill-conditioned. We analyze the ill-conditioning of the singular values in Section 6.2.

Problems 2 and 3 always have a solution. We extend Algorithm II to solve Problems 2 and 3 stably for  $m \leq n$  in Section 4.3. 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 Section 4.3).

Both cases of Problems 1 and 2 were considered by Bunch and Nielsen [3], using results from [4, 8]. They also reduced Problem 1 to computing the eigendecomposition of  $D^2 - zz^T$ , but their scheme for finding this eigendecomposition can be unstable [3, 4]. They solve Problem 2 by reducing it to Problem 1. This risks solving a well-conditioned problem using an ill-conditioned process.

Let  $k = \min(m, n)$ . Algorithm I solves Problem 1 in  $O(nk^2)$  time, and Algorithm II solves Problems 2 and 3 in  $O((m+n)k^2)$  and  $O(mk^2)$  time, respectively. As with the *SVD* updating algorithm in [13], Algorithm I can be accelerated by the fast multipole method of Carrier, Greengard and Rokhlin [5, 11] to solve Problem 1 in  $O(nk \log_2^2 \epsilon)$  time, and Algorithm II can be accelerated to solve Problems 2 and 3 in  $O((m+n)k \log_2^2 \epsilon)$  and  $O(mk \log_2^2 \epsilon)$  time, respectively, where  $\epsilon$  is the machine precision. This is an important advantage for large matrices. Since the techniques are essentially the same as those in [13], we do not elaborate on this issue.

We take the usual model of arithmetic<sup>2</sup>

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

<sup>&</sup>lt;sup>2</sup> This model excludes machines like CRAYs and CDC Cybers that do not have a guard digit. Algorithms I and II can easily be modified for such machines.

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

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

for any positive floating point number  $\alpha$ . For simplicity, we ignore the possibility of overflow and underflow.

We use the definition of stability in Stewart [18, pages 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* [1, 2] and is used in the context of downdating least squares solutions and Cholesky/QR factorizations [1, 2, 16, 19].

Section 2 introduces Algorithm I; Section 3 gives an algorithm for finding the eigendecomposition of  $D^2 - zz^T$ ; Section 4 introduces Algorithm II; Section 5 gives an algorithm for finding the *SVD* of  $C_1$ ; and Section 6 analyzes the ill-conditioning of Problem 1 for the singular values.

## 2. Algorithm I

## **2.1.** The case m > n

Combining (1.2) and (1.4), we get

$$\left(\begin{array}{c}A'\\a^{T}\end{array}\right)=U\left(\begin{array}{c}D\\0\end{array}\right)\ V^{T},$$

where  $U \in \mathbf{R}^{m \times m}$  and  $V \in \mathbf{R}^{n \times n}$  are orthogonal; and  $D \in \mathbf{R}^{n \times n}$  is non-negative diagonal, with diagonal entries in decreasing order. From (1.5), we have

$$A' = U' \begin{pmatrix} D' \\ 0 \end{pmatrix} V'^T,$$

where  $U' \in \mathbf{R}^{(m-1)\times(m-1)}$  and  $V' \in \mathbf{R}^{n\times n}$  are orthogonal; and  $\Omega \in \mathbf{R}^{n\times n}$  is non-negative diagonal, with diagonal entries in decreasing order. Thus

$$A'^T A' + aa^T = V D^2 V^T$$

and

$$V'D'^{2}V'^{T} = A'^{T}A' = VD^{2}V^{T} - aa^{T}.$$

Letting  $z = V^T a$ , this can be rewritten as

$$V'D'^{2}V'^{T} = V\left(D^{2} - zz^{T}\right)V^{T}.$$
(2.1)

The eigenvalues of  $D^2 - zz^T$  must be non-negative and are the diagonal elements of  $D'^2$ . Let  $S\Omega^2 S^T$  be the eigendecomposition of  $D^2 - zz^T$ . Then we have V' = VS and  $D' = \Omega$ .

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

$$\tilde{S} = \bar{S} + O(\epsilon) \quad \text{and} \quad \tilde{D}' = \bar{\Omega} + O(\epsilon \|D\|_2),$$
(2.2)

where the eigendecomposition

$$\bar{D}^2 - \bar{z}\bar{z}^T = \bar{S}\bar{\Omega}^2\bar{S}^T$$

is exact and

$$\bar{D} = D + O(\epsilon ||D||_2) \text{ and } \bar{z} = z + O(\epsilon ||D||_2).$$
 (2.3)

It then computes a right singular vector matrix satisfying

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

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

$$\bar{a} = V\bar{z} = a + O(\epsilon \|D\|_2). \tag{2.4}$$

Thus  $\overline{D}'$  and  $V\overline{S}$  are the exact solution to Problem 1 with slightly perturbed input data V,  $\overline{D}$  and  $\overline{a}$ . Hence Algorithm I is stable (see Section 1).

Problem 1 requires computing the eigendecomposition of  $D^2 - zz^T$ . Small perturbations in D and a can cause large perturbations in D' and V' = VS; in other words,  $\overline{D}'$  and  $\overline{S}$  can be very different from D' and S, respectively. Thus  $\widetilde{D}'$  and  $\widetilde{S}$  can be very different from D'and S, respectively. We analyze the ill-conditioning of the singular values in Section 6.1.

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

#### **2.2.** The case $m \leq n$

Combining (1.2) and (1.7), we get

$$\begin{pmatrix} A'\\ a^T \end{pmatrix} = U (D \ 0) V^T = U (D \ 0) \begin{pmatrix} V_1^T\\ V_2^T \end{pmatrix},$$
(2.5)

where  $U \in \mathbf{R}^{m \times m}$  and  $V \in \mathbf{R}^{n \times n}$  are orthogonal;  $D \in \mathbf{R}^{m \times m}$  is non-negative diagonal, with diagonal entries in decreasing order; and  $V = (V_1 \ V_2)$ , with  $V_1 \in \mathbf{R}^{n \times m}$  and  $V_2 \in \mathbf{R}^{n \times (n-m)}$ . Multiplying both sides of (2.5) times  $V_2$ , we have

$$\begin{pmatrix} A'\\ a^T \end{pmatrix} V_2 = U \ (D \ 0) \ \begin{pmatrix} V_1^T\\ V_2^T \end{pmatrix} V_2 = 0,$$

and so  $V_2^T a = 0$ . Equation (2.5) also implies that

$$A'^{T}A' = (V_{1} \ V_{2}) \begin{pmatrix} D^{2} \ 0 \\ 0 \ 0 \end{pmatrix} \begin{pmatrix} V_{1}'^{T} \\ V_{2}'^{T} \end{pmatrix} - aa^{T}.$$
 (2.6)

From (1.8), we have

$$A' = U' (D' 0) {V'}^{T} = U' (D' 0) \begin{pmatrix} V_{1}'^{T} \\ V_{2}'^{T} \end{pmatrix},$$

where  $U' \in \mathbf{R}^{(m-1)\times(m-1)}$  and  $V' \in \mathbf{R}^{n\times n}$  are orthogonal;  $D' \in \mathbf{R}^{(m-1)\times(m-1)}$  is non-negative diagonal, with diagonal entries in decreasing order; and  $V' = (V'_1 \ V'_2)$ , with  $V'_1 \in \mathbf{R}^{n\times(m-1)}$  and  $V'_2 \in \mathbf{R}^{n\times(n-m+1)}$ . Let  $z = V_1^T a$ . Plugging the last relation into (2.6) we have

$$(V_1' \ V_2') \begin{pmatrix} D'^2 \ 0 \\ 0 \ 0 \end{pmatrix} \begin{pmatrix} V_1'^T \\ V_2'^T \end{pmatrix} = (V_1 \ V_2) \begin{pmatrix} D^2 - zz^T \ 0 \\ 0 \ 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix},$$
(2.7)

where we have used the fact that  $a = (V_1 \ V_2) \begin{pmatrix} z \\ 0 \end{pmatrix}$ .

Note that  $D'^2 \in \mathbf{R}^{(m-1)\times(m-1)}$  and  $D^2 - zz^T \in \mathbf{R}^{m\times m}$ . The eigenvalues of  $D^2 - zz^T$  must be non-negative and are the diagonal elements of  $D'^2$  and 0. Thus letting

$$D^2 - zz^T = S \left( \begin{array}{cc} \Omega^2 & 0 \\ 0 & 0 \end{array} \right) S^T,$$

we have  $D' = \Omega$ ,  $(V'_1 \ v) = V_1 S$  and  $V'_2 = (v \ V_2)$ , where  $v \in \mathbb{R}^n$  is the last column of the matrix  $V_1 S$ .

Algorithm I uses the scheme in Section 3 to compute the eigendecomposition of  $D^2 - zz^T$ . Similar to Section 2.1, Algorithm I is stable (see (2.2) and (2.4)). However, the computed singular values and singular vectors can be very different from the exact singular values and singular vectors of A', respectively. We analyze the ill-conditioning of the singular values in Section 6.2.

The scheme in Section 3 takes  $O(m^2)$  time, and the computation of  $V_1S$  takes  $O(nm^2)$  time. Thus the total time for Algorithm I is  $O(nm^2)$ .

# 3. Computing the Eigendecomposition of $D^2 - zz^T$

## 3.1. Relations for the Eigendecomposition of $D^2 - zz^T$

In this subsection we establish some relations for the eigendecomposition of  $D^2 - zz^T$ , where  $D = diag(d_1, \ldots, d_k) \in \mathbf{R}^{k \times k}$ , with  $d_1 \ge \ldots \ge d_k \ge 0$ ; and  $z = (\zeta_1, \ldots, \zeta_k)^T \in \mathbf{R}^k$ . In light of (2.1) and (2.7), we assume that the eigenvalues of  $D^2 - zz^T$  are non-negative. This implies that  $\|D\|_2 \ge \|z\|_2$ .

We further assume that D and z satisfy

$$d_k > 0, \quad d_i - d_{i+1} \ge \theta \|D\|_2 \quad \text{and} \quad |\zeta_i| \ge \theta \|D\|_2,$$
 (3.1)

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

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

LEMMA 1 (BUNCH AND NIELSEN [3]). The eigenvalues of  $D^2 - zz^T$  are non-negative if and only if  $z^T D^{-2}z \leq 1$ . Assume that  $z^T D^{-2}z \leq 1$ . Then the eigendecomposition of  $D^2 - zz^T$  can be written as  $S\Omega^2 S^T$ , where

$$S = (s_1, \ldots, s_k)$$
 and  $\Omega = \operatorname{diag}(\omega_1, \ldots, \omega_k)$ ,

with  $\omega_1 > \ldots > \omega_k \ge 0$ . The eigenvalues  $\{\omega_i^2\}_{i=1}^k$  of  $D^2 - zz^T$  satisfy the secular equation

$$f_1(\omega) \equiv -1 + \sum_{j=1}^k \frac{\zeta_j^2}{d_j^2 - \omega^2} = 0, \qquad (3.2)$$

and the interlacing property

$$d_1 > \omega_1 > \ldots > d_k > \omega_k \ge 0,$$

where  $\omega_k = 0$  if and only if  $z^T D^{-2} z = 1$ . The eigenvectors are given by

$$s_{i} = \left(\frac{\zeta_{1}}{d_{1}^{2} - \omega_{i}^{2}}, \dots, \frac{\zeta_{k}}{d_{k}^{2} - \omega_{i}^{2}}\right)^{T} / \sqrt{\sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{(d_{j}^{2} - \omega_{i}^{2})^{2}}}.$$
(3.3)

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

LEMMA 2. Given a diagonal matrix  $D = \text{diag}(d_1, \ldots, d_k)$  and a set of numbers  $\{\hat{\omega}_i\}_{i=1}^k$  satisfying the interlacing property

$$d_1 > \hat{\omega}_1 > \ldots > d_k > \hat{\omega}_k \ge 0, \tag{3.4}$$

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

$$|\hat{\zeta}_i| = \sqrt{(d_i^2 - \hat{\omega}_k^2)} \prod_{j=1}^{i-1} \frac{(\hat{\omega}_j^2 - d_i^2)}{(d_j^2 - d_i^2)} \prod_{j=i}^{k-1} \frac{(\hat{\omega}_j^2 - d_i^2)}{(d_{j+1}^2 - d_i^2)},$$
(3.5)

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

**Proof:** The existence of  $\hat{z}$  and equation (3.5) are established in [12].

## **3.2.** Computing the Eigenvectors of $D^2 - zz^T$

For each exact  $\omega_i$ , equation (3.3) gives the corresponding exact eigenvector. Observe that if  $\omega_i$  was given exactly, then each difference  $d_j^2 - \omega_i^2$  could be computed to high relative accuracy as  $(d_j - \omega_i)(d_j + \omega_i)$ . Each ratio and each product could also be computed to high relative accuracy. As a result, the corresponding eigenvector  $s_i$  could be computed to component-wise high relative accuracy. In practice we can only hope to compute an approximation  $\hat{\omega}_i$  to  $\omega_i$ . But problems can arise if we approximate  $s_i$  by

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

(i.e., replace  $\omega_i$  by  $\hat{\omega}_i$  in (3.3), as in [3]). For even if  $\hat{\omega}_i$  is close to  $\omega_i$ , 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  $\{\hat{\omega}_i\}_{i=1}^k$  are computed and all the corresponding eigenvectors are approximated in this manner, the resulting eigenvector matrix may not be orthogonal.

But Lemma 2 allows us to overcome this problem. 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 compute the eigenvectors of  $D^2 - \hat{z}\hat{z}^T$  using Lemma 1. Note that each difference

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

in (3.5) can be computed to high relative accuracy. Each ratio and each product can also be computed to high relative accuracy. Thus  $|\hat{\zeta}_i|$  can be computed to high relative accuracy. We choose the sign of  $\hat{\zeta}_i$  to be the sign of  $\zeta_i$ . Substituting the *exact* eigenvalues  $\{\hat{\omega}_i^2\}_{i=1}^k$  and the computed  $\hat{z}$  into (3.3), each eigenvector of  $D^2 - \hat{z}\hat{z}^T$  can again 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 (3.4). But since  $\{\omega_i\}_{i=1}^k$  satisfy the same interlacing property (see Lemma 1), 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 that of  $D^2 - zz^T$ . This is stable as long as  $\hat{z}$  is close to z (see (2.2) and (2.4)).

#### **3.3.** Finding the Roots of the Secular Equation

In this subsection, we show how to find the roots of the secular equation

$$f(\omega) = -\rho + \sum_{j=1}^{k} \frac{\zeta_j^2}{d_j^2 - \omega^2} = 0,$$

where  $\rho \ge 0$  is a scalar. Equation (3.2) is the special case<sup>3</sup> where  $\rho = 1$ .

<sup>&</sup>lt;sup>3</sup> Equation (5.3) is another special case.

Consider the root  $\omega_i \in (d_{i+1}, d_i)$  for  $1 \leq i \leq k-1$ ; the possible k-th root  $\omega_k$  is considered later. We first assume that  $\omega_i \in (d_{i+1}, \frac{d_i+d_{i+1}}{2})$ . Let  $\delta_j = d_j - d_{i+1}$  and

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

Since

$$f(\xi + d_{i+1}) = -\rho + \psi(\xi) + \phi(\xi) \equiv g(\xi),$$

we seek the root  $\xi_i = \omega_i - d_{i+1} \in (0, \delta_i/2)$  of  $g(\xi) = 0$ .

An important property of  $g(\xi)$  is that we can compute each difference  $\delta_j - \xi$  to high relative accuracy for any  $\xi \in (0, \delta_i/2)$ . Indeed, since  $\delta_{i+1} = 0$ , we have  $fl(\delta_{i+1} - \xi) = -fl(\xi)$ ; since  $fl(\delta_i) = fl(d_i - d_{i+1})$  and  $0 < \xi < (d_i - d_{i+1})/2$ , we can compute  $fl(\delta_i - \xi)$ as  $fl(fl(d_i - d_{i+1}) - fl(\xi))$ ; and in a similar fashion, we can compute  $\delta_j - \xi$  to high relative accuracy for any  $j \neq i, i + 1$ .

Because we can also compute  $d_j + d_{i+1} + \xi$  (a sum of positive terms) to high relative accuracy, we can compute each ratio  $\zeta_j^2/((\delta_j - \xi)(d_j + d_{i+1} + \xi))$  in  $g(\xi)$  to high relative accuracy for any  $\xi \in (0, \delta_i/2)$ . Thus, since both  $\psi(\xi)$  and  $\phi(\xi)$  are sums of terms of the same sign, we can bound the error in computing  $g(\xi)$  by

$$\eta k(\rho + |\psi(\xi)| + |\phi(\xi)|),$$

where  $\eta$  is a small multiple of  $\epsilon$  that is independent of k and  $\xi$ .

We now assume that  $\omega_i \in [\frac{d_i+d_{i+1}}{2}, d_i)$ . Let  $\delta_j = d_j - d_i$  and

$$\psi(\xi)\equiv\sum_{j=1}^irac{\zeta_j^2}{(\delta_j-\xi)(d_j+d_i+\xi)}\quad ext{and}\quad \phi(\xi)\equiv\sum_{j=i+1}^krac{\zeta_j^2}{(\delta_j-\xi)(d_j+d_i+\xi)}.$$

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

$$g(\xi) \equiv f(\xi + d_i) = -\rho + \psi(\xi) + \phi(\xi) = 0.$$

For any  $\xi \in [\delta_{i+1}/2, 0)$ , we can compute each difference  $\delta_j - \xi$  to high relative accuracy. Since  $|\xi| \leq |\delta_{i+1}|/2 \leq d_i/2$ , we can compute each sum  $d_j + d_i + \xi$  to high relative accuracy as  $d_j + (d_i + \xi)$ . Thus we can again compute each ratio  $\zeta_j^2/((\delta_j - \xi)(d_j + d_i + \xi))$  to high relative accuracy and bound the error in computing  $g(\xi)$  as before.

Next we consider the case where  $\rho > 0$  and f(0) < 0 so that there is a root  $\omega_k \in (0, d_k)$ .

<sup>&</sup>lt;sup>4</sup> This can easily be checked by computing  $f(\frac{d_i+d_{i+1}}{2})$ . If  $f(\frac{d_i+d_{i+1}}{2}) > 0$ , then  $\omega_i \in (d_{i+1}, \frac{d_i+d_{i+1}}{2})$ , otherwise  $\omega_i \in [\frac{d_i+d_{i+1}}{2}, d_i)$ .

We first assume that<sup>5</sup>  $\omega_k < d_k/2$ . Let  $\delta_j = d_j$  and

$$\psi(\xi)\equiv\sum_{j=1}^krac{\zeta_j^2}{(\delta_j-\xi)(d_j+\xi)} \quad ext{and} \quad \phi(\xi)\equiv 0.$$

We seek the root  $\xi_i = \omega_i \in (0, \delta_k/2)$  of the equation

$$g(\xi) \equiv f(\xi) = -\rho + \psi(\xi) + \phi(\xi) = 0.$$

For any  $\xi \in (0, \delta_k/2)$ , we can compute each ratio  $\zeta_j^2/((\delta_j - \xi)(d_j + \xi))$  to high relative accuracy, and bound the error in computing  $g(\xi)$  as before.

We now assume that  $\omega_k \ge d_k/2$ . Let  $\delta_j = d_j - d_k$  and

$$\psi(\xi)\equiv\sum_{j=1}^krac{\zeta_j^2}{(\delta_j-\xi)(d_j+d_k+\xi)} \quad ext{and} \quad \phi(\xi)\equiv 0.$$

We seek the root  $\xi_i = \omega_i - d_k \in [-\delta_k/2, 0)$  of the equation

$$g(\xi) \equiv f(\xi + d_k) = -\rho + \psi(\xi) + \phi(\xi) = 0.$$

For any  $\xi \in [-d_k/2, 0)$ , we can compute each ratio  $\zeta_j^2/((\delta_j - \xi)(d_j + d_k + \xi))$  to high relative accuracy, and bound the error in computing  $g(\xi)$  as before.

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

$$|g(\xi)| \le \eta k(\rho + |\psi(\xi)| + |\phi(\xi)|), \tag{3.6}$$

where as before,  $\eta k(\rho + |\psi(\xi)| + |\phi(\xi)|)$  is an upper bound on the round-off error one would make in computing  $g(\xi)$ . 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 [3, 10, 14]. 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  $\xi$  that satisfies it.

#### **3.4.** Numerical Stability

In this subsection we first derive a bound on  $|\hat{\omega}_i^2 - \omega_i^2|$ , and then show that when  $\rho = 1$ , the  $\hat{z}$  defined in (3.5) is close to z.

Since  $f(\omega_i) = 0$ , we have

$$\rho = \left| \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{d_{j}^{2} - \omega_{i}^{2}} \right| \le \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|d_{j}^{2} - \omega_{i}^{2}|},$$

<sup>&</sup>lt;sup>5</sup> This can easily be checked by computing  $f(d_k/2)$ . If  $f(d_k/2) > 0$ , then  $\omega_k < d_k/2$ , otherwise  $\omega_k \ge d_k/2$ .

and the stopping criterion (3.6) implies that  $\hat{\omega}_i$  satisfies<sup>6</sup>

$$|f(\hat{\omega}_i)| \le \eta k \left( \sum_{j=1}^k \frac{\zeta_j^2}{|d_j^2 - \omega_i^2|} + \sum_{j=1}^k \frac{\zeta_j^2}{|d_j^2 - \hat{\omega}_i^2|} \right).$$

Since

$$f(\hat{\omega}_i) = f(\hat{\omega}_i) - f(\omega_i) = (\hat{\omega}_i^2 - \omega_i^2) \sum_{j=1}^k \frac{\zeta_j^2}{(d_j^2 - \hat{\omega}_i^2)(d_j^2 - \omega_i^2)},$$

it follows that

$$|\hat{\omega}_{i}^{2} - \omega_{i}^{2}| \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|} \leq \eta k \left( \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|d_{j}^{2} - \hat{\omega}_{i}^{2}|} + \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|d_{j}^{2} - \omega_{i}^{2}|} \right).$$
(3.7)

Note that for any j,

$$\frac{1}{|d_j^2 - \hat{\omega}_i^2|} + \frac{1}{|d_j^2 - \omega_i^2|} \le \frac{2}{|(d_j^2 - \hat{\omega}_i^2)(d_j^2 - \omega_i^2)|^{\frac{1}{2}}} + \frac{|\hat{\omega}_i^2 - \omega_i^2|}{|(d_j^2 - \hat{\omega}_i^2)(d_j^2 - \omega_i^2)|}.$$

Substituting this into (3.7) and using the Cauchy-Schwartz inequality, we get

$$\begin{split} |\hat{\omega}_{i}^{2} - \omega_{i}^{2}| \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|} \\ &\leq \frac{2\eta k}{1 - \eta k} \sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|^{\frac{1}{2}}} \\ &\leq \frac{2\eta k}{1 - \eta k} \|z\|_{2} \sqrt{\sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|}}, \end{split}$$

or

$$\begin{split} \hat{\omega}_{i}^{2} - \omega_{i}^{2} &| \leq \frac{2\eta k}{1 - \eta k} \|z\|_{2} / \sqrt{\sum_{j=1}^{k} \frac{\zeta_{j}^{2}}{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|}} \\ &\leq \frac{2\eta k \|z\|_{2}}{(1 - \eta k)|\zeta_{j}|} \sqrt{|(d_{j}^{2} - \hat{\omega}_{i}^{2})(d_{j}^{2} - \omega_{i}^{2})|} \\ &\leq \frac{2\eta k \|z\|_{2}}{(1 - \eta k)|\zeta_{j}|} \left(|d_{j}^{2} - \omega_{i}^{2}| + \frac{1}{2}|\hat{\omega}_{i}^{2} - \omega_{i}^{2}|\right). \end{split}$$

Letting  $\beta_j = 2\eta k ||z||_2/((1 - \eta k)|\zeta_j|)$ , this implies that

$$|\hat{\omega}_{i}^{2} - \omega_{i}^{2}| \leq \frac{\beta_{j}}{1 - \frac{1}{2}\beta_{j}} |d_{j}^{2} - \omega_{i}^{2}|$$
(3.8)

for every  $1 \le j \le k$ , provided that  $\beta_j < 2$ .

<sup>6</sup> This condition is also satisfied when  $\omega_k = 0$  is known to be a root as in (2.7).

Now consider the special case  $\rho = 1$ . Let  $\hat{\omega}_i^2 - \omega_i^2 = \alpha_{ij}(d_j^2 - \omega_i^2)/\zeta_j$  for all *i* and *j*. Suppose that we pick  $\theta = 2\eta k^2$  in (3.1). Then we have  $|\zeta_j| \ge 2\eta k^2 ||z||_2$ . Assume further that  $\eta k < 1/100$ . Then  $\beta_j \le 2/3$ , and (3.8) implies that  $|\alpha_{ij}| \le \alpha \equiv 4\eta k ||z||_2$  for all *i* and *j*. Thus, from (3.5),

$$|\hat{\zeta}_{i}| = \sqrt{-\frac{\prod_{j} (\hat{\omega}_{j}^{2} - d_{i}^{2})}{\prod_{j \neq i} (d_{j}^{2} - d_{i}^{2})}} = \sqrt{-\frac{\prod_{j} (\omega_{j}^{2} - d_{i}^{2})(1 + \alpha_{ji}/\zeta_{i})}{\prod_{j \neq i} (d_{j}^{2} - d_{i}^{2})}} = |\zeta_{i}| \sqrt{\prod_{j=1}^{k} \left(1 + \frac{\alpha_{ji}}{\zeta_{i}}\right)}$$

and, since  $\hat{\zeta}_i$  and  $\zeta_i$  have the same sign,

$$\begin{aligned} |\hat{\zeta}_{i} - \zeta_{i}| &= |\zeta_{i}| \left| \sqrt{\prod_{j=1}^{k} \left(1 + \frac{\alpha_{ji}}{\zeta_{i}}\right) - 1} \right| \leq |\zeta_{i}| \left( \left(1 + \frac{\alpha}{|\zeta_{i}|}\right)^{\frac{k}{2}} - 1 \right) \\ &\leq |\zeta_{i}| \left( \exp\left(\frac{\alpha k}{2|\zeta_{i}|}\right) - 1 \right) \leq (e - 1) \alpha k/2 \\ &\leq 4\eta k^{2} ||z||_{2}, \end{aligned}$$

$$(3.9)$$

where we have used the fact that  $\alpha k/(2|\zeta_i|) \leq 1$  and that  $e^{\gamma} - 1 \leq (e-1)\gamma$  for  $0 < \gamma \leq 1$ .

One factor of k in  $\theta$  and (3.9) comes from the stopping criterion (3.6). It can be reduced to  $\log_2 k$  by using a binary tree structure for summing up the terms in  $\psi(\xi)$  and  $\phi(\xi)$ . The other factor of k comes from the upper bound for  $\prod_j (1 + \alpha_{ji}/\zeta_i)$ . This also seems quite conservative. Thus we might expect the factor of  $k^2$  in  $\theta$  and (3.9) to be more like O(k) in practice.

#### 3.5. Deflation

Consider the matrix  $D^2 - zz^T$ , where  $D = diag(d_1, \ldots, d_k) \in \mathbf{R}^{k \times k}$ , with  $d_1 \ge \ldots \ge d_k \ge 0$ ; and  $z = (\zeta_1, \ldots, \zeta_k)^T \in \mathbf{R}^k$ . Assume that the eigenvalues of  $D^2 - zz^T$  are non-negative. We now show that we can reduce it to a matrix of the same form that further satisfies (see (3.1))

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

where  $\theta$  is specified in Section 3.4. Similar reductions appear in [3, 7].

First assume that  $d_k = 0$ . Since  $D^2 - zz^T$  is non-negative definite, its diagonal elements must all be non-negative. Thus  $d_k^2 - \zeta_k^2 \ge 0$  and  $\zeta_k = 0$ . Writing

$$D = \begin{pmatrix} D_1 \\ 0 \end{pmatrix}$$
 and  $z = \begin{pmatrix} z_1 \\ 0 \end{pmatrix}$ ,

we have

$$D^2 - zz^T = \left(\begin{array}{cc} D_1^2 - z_1 z_1^T \\ 0 \end{array}\right).$$

The eigenvalue 0 can be deflated, and the matrix  $D_1^2 - z_1 z_1^T$  has no negative 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 1 that the eigenvalues of  $D^2 - zz^T$  are non-negative if and only if

$$\sum_{i=1}^{k} \frac{\zeta_i^2}{d_i^2} \le 1.$$
(3.10)

Assume that  $|\zeta_i| < \theta ||D||_2$ . We illustrate the reduction for i = k. Let

$$D = \begin{pmatrix} D_1 \\ d_k \end{pmatrix}, \quad z = \begin{pmatrix} z_1 \\ \zeta_k \end{pmatrix} \quad ext{and} \quad \check{z} = \begin{pmatrix} z_1 \\ 0 \end{pmatrix}.$$

We perturb  $\zeta_i$  to 0. The matrix  $D^2 - zz^T$  is perturbed to

$$D^{2} - \breve{z}\breve{z}^{T} = \begin{pmatrix} D_{1}^{2} - z_{1}z_{1}^{T} \\ & d_{k}^{2} \end{pmatrix}.$$
(3.11)

The eigenvalue  $d_k^2$  can be deflated, and the matrix  $D_1^2 - z_1 z_1^T$  satisfies (3.10) and is of the same form but of smaller dimensions. This reduction is stable (see (2.3)).

Now assume that  $d_i - d_{i+1} \leq \theta \|D\|_2$ . We illustrate the reduction for i = k - 1. Let

$$D = \begin{pmatrix} D_1 \\ d_k \end{pmatrix}$$
 and  $\check{D} = \begin{pmatrix} D_1 \\ d_{k-1} \end{pmatrix}$ .

We perturb  $d_{i+1}$  to  $d_i$ . The matrix  $D^2 - zz^T$  is perturbed to  $\check{D}^2 - zz^T$ , which also satisfies (3.10). Let G be a Givens rotation in the (k-1,k) plane that zeroes the k-th component of z; in other words,  $Gz = \check{z}$ , where  $\check{z} = (\check{z}_1^T, 0)^T$  with  $\check{z}_1 = (\zeta_1, \ldots, \zeta_{k-2}, \sqrt{\zeta_{k-1}^2 + \zeta_k^2})^T$ . Since  $G\check{D}G^T = \check{D}$ , we have

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

The eigenvalue  $d_{k-1}^2$  can be deflated, and the matrix  $D_1^2 - \check{z}_1 \check{z}_1^T$  satisfies (3.10) and is of the same form but of smaller dimensions. This reduction is stable (see (2.3)).

## 4. Algorithm II

### 4.1. The case m > n

From (1.2) and (1.4)

$$\begin{pmatrix} A'\\ a^T \end{pmatrix} = (U_1 \ U_2) \begin{pmatrix} D\\ 0 \end{pmatrix} V^T,$$

where  $U_1 \in \mathbf{R}^{m \times n}$  and  $U_2 \in \mathbf{R}^{m \times (m-n)}$  are column orthogonal;  $V \in \mathbf{R}^{n \times n}$  is orthogonal; and  $D \in \mathbf{R}^{n \times n}$  is non-negative diagonal. Partition  $U_1$  and  $U_2$  as

$$U_1 = \begin{pmatrix} U_{11} \\ u_1^T \end{pmatrix} \quad \text{and} \quad U_2 = \begin{pmatrix} U_{12} \\ u_2^T \end{pmatrix}, \tag{4.1}$$

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

$$\begin{pmatrix} A'\\ a^T \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12}\\ u_1^T & u_2^T \end{pmatrix} \begin{pmatrix} D\\ 0 \end{pmatrix} V^T,$$

or

$$A' = (U_{11} \ U_{12}) \begin{pmatrix} D \\ 0 \end{pmatrix} V^T = U_{11} D V^T \quad \text{and} \quad a = V D u_1.$$
(4.2)

The decomposition of A' in (4.2) is almost an SVD.  $U_{11}$  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  $x \in \mathbb{R}^{m-1}$  such that  $||u_1||^2 + \mu^2 = 1$  and

$$Y = \begin{pmatrix} U_{11} & x \\ u_1^T & \mu \end{pmatrix}$$
(4.3)

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

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

$$H = \left(\begin{array}{cc} I - \frac{1}{1+\mu} u_1 u_1^T & u_1 \\ -u_1^T & \mu \end{array}\right)$$

is orthogonal and  $(u_1^T \ \mu)H = (0, \dots, 0, 1)^T$ . Since

$$YH = \begin{pmatrix} U_{11}(I - \frac{1}{1+\mu}u_1u_1^T) - x \ u_1^T \ U_{11}u_1 + \mu \ x \\ 0 \ 1 \end{pmatrix}$$

is column orthogonal, it follows that

$$U_{11}u_1 + \mu \ x = 0,$$

so that

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

is column orthogonal<sup>7</sup>. Thus

$$YH = \begin{pmatrix} U_{11} & x \\ u_1^T & \mu \end{pmatrix} \begin{pmatrix} I - \frac{1}{1+\mu} u_1 u_1^T & u_1 \\ -u_1^T & \mu \end{pmatrix} = \begin{pmatrix} X & 0 \\ 0 & 1 \end{pmatrix},$$
(4.4)

and

$$(U_{11} \ x) = (U_{11} \ x)HH^{T} = (X \ 0)H^{T} = X\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T} - u_{1}\right),$$

which implies that

$$U_{11} = X \left( I - \frac{1}{1+\mu} u_1 u_1^T \right).$$
(4.5)

The first matrix on the right-hand side of (4.5) is column orthogonal and the second is simple. Plugging (4.5) into (4.2), we have

$$A' = X \left( I - \frac{1}{1+\mu} u_1 u_1^T \right) DV^T = X C_1 V^T,$$
(4.6)

where  $C_1 \in \mathbf{R}^{n \times n}$  is given by

$$C_1 \equiv \left(I - \frac{1}{1+\mu} u_1 u_1^T\right) D.$$

Let  $Q_1 \Omega W_1^T$  be the *SVD* of  $C_1$ , where  $Q_1, W_1 \in \mathbf{R}^{n \times n}$  are orthogonal and  $\Omega \in \mathbf{R}^{n \times n}$  is non-negative diagonal. Substituting this into (4.6), we have

$$A' = XQ_1 \Omega W_1^T V^T = (XQ_1) \Omega (VW_1)^T.$$
(4.7)

Comparing this with (1.5), we have  $D' = \Omega$ ,  $U'_1 = XQ_1$  and  $V' = VW_1$ . We specify  $U'_2$  in Section 4.2.

Algorithm II computes a numerically column orthogonal matrix  $\tilde{Y}$  and a numerical SVD  $\tilde{Q}_1 \tilde{\Omega} \tilde{W}_1^T$  satisfying (see Sections 4.2 and 5)

$$\tilde{Y} = \bar{Y} + O(\epsilon), \quad \tilde{Q}_1 = \bar{Q}_1 + O(\epsilon), \quad \tilde{\Omega} = \bar{\Omega} + O(\epsilon \|D\|_2) \text{ and } \quad \tilde{W}_1 = \bar{W}_1 + O(\epsilon), \quad (4.8)$$

where

$$\bar{Y} = \left(\begin{array}{cc} \bar{U}_{11} & \bar{x} \\ \bar{u}_1^T & \bar{\mu} \end{array}\right)$$

is an exact column orthogonal matrix with

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

and

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

<sup>&</sup>lt;sup>7</sup> Paige [16] has proven similar relations.

is an exact SVD with  $\overline{D} = D + O(\epsilon ||D||_2)$ .

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

$$\tilde{U}'_{1} = \bar{X}\bar{Q}_{1} + O(\epsilon), \quad \tilde{U}'_{2} = \bar{U}'_{2} + O(\epsilon) \text{ and } \tilde{V}' = V\bar{W}_{1} + O(\epsilon), \quad (4.9)$$

for Problems 2 and 3, where  $(\bar{X}\bar{Q}_1 \ \bar{U}'_2) \in \mathbf{R}^{(m-1)\times(m-1)}$  is exactly orthogonal (see Section 4.2.1). Since  $\bar{X}\bar{Q}_1$ ,  $\bar{\Omega}$  and  $V\bar{W}_1$  solve Problems 2 and 3 exactly for slightly perturbed input data  $\bar{U}_1$ ,  $\bar{D}$  and V, Algorithm II is stable (see Section 1).

Because  $\overline{U}'$  is column orthogonal, we have (see (4.5))

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

and thus from (4.2), we have

$$A' = U_{11}DV^T = \bar{U}_{11}\bar{D}V^T + O(\epsilon \|D\|_2) = \bar{X}\bar{C}_1V^T + O(\epsilon \|D\|_2).$$
(4.10)

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 [9, 18]. Thus (4.10) guarantees that  $\overline{D}'$  and  $\widetilde{D}'$  are close to D'; in other words, for Problems 2 and 3, the singular values are well-conditioned. But  $\overline{Q}_1$  and  $\overline{W}_1$  can be very different from  $Q_1$  and  $W_1$ , respectively, and thus  $\tilde{U}'_1$  and  $\tilde{V}'$  can be very different from  $U'_1$ and V', respectively.

It takes O(mn) time to compute X. It takes O(mn) time to compute  $\mu$ , x and  $U'_2$  (see Section 4.2). It takes  $O(n^2)$  time to compute the SVD of  $C_1$  (see Section 5). And it takes  $O(mn^2)$  and  $O(n^3)$  time to compute  $XQ_1$  and  $VW_1$ , respectively. Algorithm II computes  $FQ_1$  for Problem 3 and computes both  $XQ_1$  and  $VW_1$  for Problem 2. 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 and $U'_2$

Given a vector t, we will need an orthogonal matrix P(t) such that

$$P(t)t = ||t||_2 e_1,$$

where  $e_1 = (1, 0, ..., 0)^T$ . We define P(t) = sign(t) if t is a non-zero one-dimensional vector; P(t) = I if t = 0;

$$P(t) = \begin{pmatrix} \tau & t_1^T \\ -sign(\tau)t_1 & I - \frac{1}{1+|\tau|}t_1t_1^T \end{pmatrix}$$

if  $t = (\tau \ t_1^T)^T$  and  $||t||_2 = 1$ ; and  $P(t) = P(t/||t||_2)$  otherwise.

### **4.2.1.** Computing Y and $U'_2$ with $U_2$

Recall from (4.1) that

$$U_2 = \left(\begin{array}{c} U_{12} \\ u_2^T \end{array}\right),$$

where  $U_{12} \in \mathbf{R}^{(m-1)\times(m-n)}$  and  $u_2 \in \mathbf{R}^{m-n}$ . Define  $(z_2, X_{12}) = U_{12}P(u_2)^T$ , where  $z_2 \in \mathbf{R}^{m-1}$ and  $X_{12} \in \mathbf{R}^{(m-1)\times(m-n-1)}$  is column orthogonal. Since

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

is orthogonal,

$$\left(\begin{array}{cc} U_{11} & z_2 \\ u_1^T & \|u_2\|_2 \end{array}\right)$$

is column orthogonal and  $||u_1||_2^2 + ||u_2||_2^2 = 1$ . We set  $x = z_2$  and  $\mu = ||u_2||_2$ . This shows how to compute Y when  $U_2$  is available. These computations are stable (see (4.8)).

From (4.4) we have

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

and thus  $(X \ X_{12}) \in \mathbf{R}^{(m-1)\times(m-1)}$  is orthogonal. We set  $X_{12} = U'_2$  (see (1.5) and (4.7)). It takes O(n(m-n)) time to compute  $X_{12}$ . These computations are stable (see (4.8) and (4.9)).

#### 4.2.2. Computing Y without $U_2$

Recall from (4.1) that

$$U_1 = \left(\begin{array}{c} U_{11} \\ u_1^T \end{array}\right),$$

where  $U_{11} \in \mathbf{R}^{(m-1)\times n}$  and  $u_1 \in \mathbf{R}^n$ . Define  $(z_1, X_{11}) = U_{11}P(u_1)^T$ , where  $z_1 \in \mathbf{R}^{m-1}$  and  $X_{11} \in \mathbf{R}^{(m-1)\times (n-1)}$  is column orthogonal. Since

$$\begin{pmatrix} U_{11} \\ u_1^T \end{pmatrix} P(u_1)^T = \begin{pmatrix} z_1 & X_{11} \\ \|u_1\|_2 & 0 \end{pmatrix}$$

is column orthogonal, it follows that  $X_{11}^T z_1 = 0$  and that  $||z_1||_2^2 + ||u_1||_2^2 = 1$ . In finite precision arithmetic the computed  $X_{11}$  and  $z_1$  satisfy

$$X_{11}^T z_1 = O(\epsilon)$$
 and  $||z_1||_2^2 + ||u_1||_2^2 = 1 + O(\epsilon).$ 

By using a scheme similar to the iterative reorthogonalization scheme developed in [6, Section 4], Algorithm II finds a vector  $\tilde{z}$  with norm near unity that satisfies

$$z_1 = ||z_1||_2 \tilde{z} + O(\epsilon) \text{ and } X_{11}^T \tilde{z} = O(\epsilon),$$

Since the matrix

$$\begin{pmatrix} U_{11} & -\|u_1\|_2 \tilde{z} \\ u_1^T & \|z_1\|_2 \end{pmatrix} = \begin{pmatrix} \|z_1\|_2 \tilde{z} & X_{11} & -\|u_1\|_2 \tilde{z} \\ \|u_1\|_2 & 0 & \|z_1\|_2 \end{pmatrix} \begin{pmatrix} P(u_1)^T & \\ & 1 \end{pmatrix} + O(\epsilon)$$

is numerically column orthogonal, we can set  $x = -||u_1||_2 z$  and  $\mu = ||z_1||_2$ . These computations are stable (see (4.8)). The time for computing  $\tilde{z}$  is O(lmk), where *l* is the number of reorthogonalization steps, which is a small constant in practice [6].

#### 4.3. The case $m \leq n$

From (1.2) and (1.7), we get

$$\begin{pmatrix} A'\\ a^T \end{pmatrix} = U \left( D \ 0 \right) \begin{pmatrix} V_1^T\\ V_2^T \end{pmatrix},$$

where  $U \in \mathbf{R}^{n \times m}$  is orthogonal;  $D \in \mathbf{R}^{m \times m}$  is non-negative diagonal; and  $V_1 \in \mathbf{R}^{n \times m}$  and  $V_2 \in \mathbf{R}^{n \times (n-m)}$  are column orthogonal. Partition U and D as

$$U = \begin{pmatrix} U_{11} & x \\ u_1^T & \mu \end{pmatrix}$$
 and  $D = \begin{pmatrix} D_1 \\ d \end{pmatrix}$ ,

where  $x, u_1 \in \mathbb{R}^{m-1}$  are vectors;  $D_1 \in \mathbb{R}^{(m-1)\times(m-1)}$  is diagonal; and d is the smallest diagonal element of D. Note that  $u \equiv (u_1^T \ \mu)^T \in \mathbb{R}^m$  is a unit vector so that  $||u_1||_2^2 + \mu^2 = 1$ . We further assume that<sup>8</sup>  $\mu \geq 0$ . Then

$$A' = (U_{11} \ x) \begin{pmatrix} D_1 & 0 \\ & d & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} = (U_{11} \ x) \begin{pmatrix} D_1 \\ & d \end{pmatrix} V_1^T,$$
(4.11)

and

$$a = (V_1 \ V_2) \begin{pmatrix} D \\ 0 \end{pmatrix} u = V_1 D u.$$
(4.12)

The decomposition of A' in (4.11) is almost an SVD.  $(U_{11} \ x)$  is close to being orthogonal since it is obtained by deleting the last row from U. In the following we decompose it into a product of an  $(m-1) \times (m-1)$  orthogonal matrix and a simple  $(m-1) \times m$  matrix.

Note that if  $\mu = 1$ , then  $u_1 = 0$ , x = 0 and  $U_{11}$  is column orthogonal. In general,  $\mu \neq 1$ , but we can orthogonally transform the rows of U such that  $\mu = 1$ . From Section 4.1, the matrix

H =	( I –	$\frac{1}{1+\mu}u_1u_1^T$	$u_1$	
		$-u_1^T$	μ	)

<sup>8</sup> If  $\mu < 0$ , we multiply both U and V by -1. The result is an SVD of A with  $\mu > 0$ .

is orthogonal and  $(u_1^T \ \mu)H = (0, \dots, 0, 1)^T$ . Since

$$UH = \begin{pmatrix} U_{11}(I - \frac{1}{1+\mu}u_1u_1^T) - x \ u_1^T & U_{11}u_1 + \mu \ x \\ 0 & 1 \end{pmatrix}$$

is orthogonal, it follows that

$$U_{11}u_1 + \mu \ x = 0,$$

so that

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

is orthogonal. Thus

$$(U_{11} \ x) = (U_{11} \ x)HH^{T} = (X \ 0)H^{T} = X\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T} - u_{1}\right).$$

Plugging this into (4.11), we have

$$A' = X \left( I - \frac{1}{1+\mu} u_1 u_1^T - u_1 \right) \begin{pmatrix} D_1 & 0 \\ d & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}$$
$$= X(C \quad 0) \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} = XCV_1^T,$$
(4.13)

where  $C \in \mathbf{R}^{(m-1) \times m}$  is given by

$$C \equiv \left( I - \frac{1}{1+\mu} u_1 u_1^T - u_1 \right) \left( \begin{array}{c} D_1 \\ d \end{array} \right).$$

Let  $Q(\Omega \ 0)W^T$  be the *SVD* of *C*, where  $Q \in \mathbf{R}^{(m-1)\times(m-1)}$  and  $W \in \mathbf{R}^{m\times m}$  are orthogonal, and  $\Omega \in \mathbf{R}^{(m-1)\times(m-1)}$  is non-negative diagonal. Substituting this into (4.13), we have

$$A' = (XQ) \left( \begin{pmatrix} \Omega & 0 \end{pmatrix} & 0 \right) \begin{pmatrix} (V_1W)^T \\ V_2^T \end{pmatrix} = (XQ) \left( \Omega & 0 \right) (V_1W)^T.$$

Comparing this with (1.8), we have

$$D' = \Omega, \quad U' = XQ, \quad (V'_1 \ v) = V_1W \quad \text{and} \quad V'_2 = (v \ V_2),$$

where v is the last column of  $V_1W$ .

Algorithm II uses the stable scheme in Section 5 to compute the SVD of C. As in Section 4.1, Algorithm II is stable. The computed singular values are close to the exact singular values of A', but the computed singular vectors can be very different from the exact singular vectors.

It takes  $O(m^2)$  time to compute X. It takes  $O(m^2)$  time to compute the SVD of C (see Section 5). And it takes  $O(m^3)$  and  $O(nm^2)$  time to compute XQ and  $V_1W$ , respectively. Algorithm II computes XQ for both Problems 2 and 3 and computes  $V_1W$  for Problem 2. Thus the total times for solving Problems 2 and 3 are  $O((m+n)m^2)$  and  $O(m^3)$ , respectively.

## 5. Computing the SVD of C and $C_1$

### 5.1. Relations for the SVD of C and $C_1$

In this subsection we establish some relations for the SVD of the matrix  $C \in \mathbf{R}^{(k-1) \times k}$  given by

$$C = \left(I - \frac{1}{1+\mu}u_1u_1^T - u_1\right) \begin{pmatrix} D_1 \\ d \end{pmatrix},$$
(5.1)

where  $D = diag(D_1, d) = diag(d_1, \ldots, d_{k-1}, d_k) \in \mathbf{R}^{k \times k}$ , with  $d_1 \ge \ldots \ge d_{k-1} \ge d_k = d \ge 0$ ; and  $u \equiv (u_1^T, \mu)^T = (\mu_1, \ldots, \mu_{k-1}, \mu_k)^T \in \mathbf{R}^k$  is a unit vector. When d = 0, C simplifies to

$$\left( \left( I - \frac{1}{1+\mu} u_1 u_1^T \right) D_1 \quad 0 \right) \equiv \left( C_1 \quad 0 \right).$$

The results also apply to  $C_1$ .

We assume that

 $d_i - d_{i+1} \ge \theta \|D\|_2 \quad \text{and} \quad |\mu_i| \ge \theta, \tag{5.2}$ 

where  $\theta$  is a small multiple of  $\epsilon$  to be specified in Section 5.3. Any matrix of the form (5.1) can be reduced to one that satisfies these conditions by using the deflation procedure described in Section 5.4. This deflation procedure also applies to  $C_1$ .

The following lemma characterizes the singular values and singular vectors of C.

LEMMA 3. Let  $Q(\Omega \ 0)W^T$  be the SVD of C with

$$Q = (q_1, \ldots, q_{k-1}), \quad \Omega = \text{diag}(\omega_1, \ldots, \omega_{k-1}) \text{ and } W = (w_1, \ldots, w_{k-1}, w_k),$$

where  $\omega_1 > \ldots > \omega_{k-1} > 0$ . Then the singular values  $\{\omega_i\}_{i=1}^{k-1}$  satisfy the secular equation

$$f_2(\omega) = \sum_{j=1}^k \frac{\mu_j^2}{d_j^2 - \omega^2} = 0$$
(5.3)

and the interlacing property

$$d_1 > \omega_1 > \ldots > d_{k-1} > \omega_{k-1} > d_k = d.$$

The singular vectors are given by

$$q_{i} = \left(\frac{\gamma_{i,1}^{2}\mu_{1}}{d_{1}^{2} - \omega_{i}^{2}}, \dots, \frac{\gamma_{i,k-1}^{2}\mu_{k-1}}{d_{k-1}^{2} - \omega_{i}^{2}}\right)^{T} / \sqrt{\sum_{j=1}^{k-1} \frac{(\gamma_{i,j}^{2}\mu_{j})^{2}}{(d_{j}^{2} - \omega_{i}^{2})^{2}}},$$
(5.4)

where  $\gamma_{i,j}^2 = (\omega_i^2 - d^2) + \mu(\omega_j^2 - d^2)$ , and

$$w_i = \left(\frac{d_1\mu_1}{d_1^2 - \omega_i^2}, \dots, \frac{d_{k-1}\mu_{k-1}}{d_{k-1}^2 - \omega_i^2}, \frac{d_k\mu_k}{d_k^2 - \omega_i^2}\right)^T / \sqrt{\sum_{j=1}^k \frac{(d_j\mu_j)^2}{(d_j^2 - \omega_i^2)^2}}, \quad (5.5)$$

$$w_{k} = \begin{cases} \left(\frac{\mu_{1}}{d_{1}}, \dots, \frac{\mu_{k-1}}{d_{k-1}}, \frac{\mu_{k}}{d_{k}}\right)^{T} / \sqrt{\sum_{j=1}^{k} \left(\frac{\mu_{j}}{d_{j}}\right)^{2}} & \text{if } d_{k} > 0, \\ (0, \dots, 0, 1)^{T} & \text{if } d_{k} = 0. \end{cases}$$
(5.6)

**Proof:** Since

$$C^{T}C = \begin{pmatrix} D_{1} \\ d \end{pmatrix} \begin{pmatrix} \left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T}\right)^{2} & -\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T}\right)u_{1} \\ -u_{1}^{T}\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T}\right) & u_{1}^{T}u_{1} \end{pmatrix} \begin{pmatrix} D_{1} \\ d \end{pmatrix} \\ = \begin{pmatrix} D_{1} \\ d \end{pmatrix} \begin{pmatrix} I - u_{1}u_{1}^{T} & -\mu u_{1} \\ -\mu u_{1}^{T} & 1 - \mu^{2} \end{pmatrix} \begin{pmatrix} D_{1} \\ d \end{pmatrix} \\ = D(I - uu^{T})D,$$

we have

$$det(C^{T}C - \omega^{2}I) = det(D^{2} - \omega^{2}I - Duu^{T}D)$$

$$= det(D^{2} - \omega^{2}I) (1 - u^{T}D(D^{2} - \omega^{2})^{-1}Du)$$

$$= -\omega^{2} det(D^{2} - \omega^{2}I) u^{T}(D^{2} - \omega^{2})^{-1}u$$

$$= -\omega^{2} \prod_{j=1}^{k} (d_{j}^{2} - \omega^{2}) \sum_{j=1}^{k} \frac{\mu_{j}^{2}}{d_{j}^{2} - \omega^{2}},$$
(5.7)

where we have assumed that  $d_j^2 - \omega^2 \neq 0$ . The sum on the right-hand side is  $f_2(\omega)$ , which has exactly one zero in each interval  $(d_{i+1}, d_i)$  for  $1 \leq i \leq k-1$ . These k-1 positive zeros of det $(C^T C - \omega^2 I)$  must be the singular values of C.

For  $1 \leq i \leq k-1$ , the right singular vector  $w_i$  is a unit vector satisfying

$$C^T C w_i = D(I - uu^T) D w_i = \omega_i^2 w_i.$$

Solving this equation we get (5.5). Because  $w_k$  is a unit vector satisfying  $Cw_k = 0$ , we have

$$C^T C w_k = D(I - uu^T) D w_k = 0.$$

Solving this equation we get (5.6).

From (5.5) we see that  $w_i$  is the normalized eigenvector of  $(D^2 - \omega_i^2 I)^{-1} Du$ . Since  $\omega_i q_i = Cw_i$ , it follows that  $q_i$  is the normalized eigenvector of  $C(D^2 - \omega_i^2 I)^{-1} Du$ . Simplifying,

$$C(D^{2} - \omega_{i}^{2}I)^{-1}Du$$

$$= \left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T} - u_{1}\right) \left(\begin{array}{c}D_{1}^{2}(D_{1}^{2} - \omega_{i}^{2}I)^{-1}u_{1}\\d^{2}(d^{2} - \omega_{i}^{2})^{-1}\mu\end{array}\right)$$

$$= D_{1}^{2}(D_{1}^{2} - \omega_{i}^{2}I)^{-1}u_{1} - \left(\frac{u_{1}^{T}D_{1}^{2}(D_{1}^{2} - \omega_{i}^{2}I)^{-1}u_{1}}{1+\mu} + d^{2}(d^{2} - \omega_{i}^{2})^{-1}\mu\right)u_{1}.$$
 (5.8)

Because  $\omega_i$  satisfies the secular equation (5.3), we have

$$u^{T}(D^{2}-\omega_{i}^{2}I)^{-1}u=\sum_{j=1}^{k}rac{\mu_{j}^{2}}{d_{j}^{2}-\omega_{i}^{2}}=0.$$

Since  $||u||_2 = 1$ , this implies that

$$u_1^T D_1^2 (D_1^2 - \omega_i^2 I)^{-1} u_1 = 1 - \mu^2 d^2 (d^2 - \omega_i^2)^{-1}.$$

Plugging this into (5.8), we have

$$\begin{split} C(D^2 - \omega_i^2 I)^{-1} Du \\ &= \omega_i^2 (D_1^2 - \omega_i^2 I)^{-1} u_1 + u_1 - \left(\frac{1 + \mu d^2 (d^2 - \omega_i^2)^{-1}}{1 + \mu}\right) u_1 \\ &= \omega_i^2 (D_1^2 - \omega_i^2 I)^{-1} u_1 + \left(\frac{\mu \omega_i^2 (\omega_i^2 - d^2)^{-1}}{1 + \mu}\right) u_1 \\ &= \frac{\omega_i^2 (\omega_i^2 - d^2)^{-1}}{1 + \mu} \left((1 + \mu)(\omega_i^2 - d^2)I + \mu (D_1^2 - \omega_i^2 I)\right) (D_1^2 - \omega_i^2 I)^{-1} u_1 \\ &= \frac{\omega_i^2 (\omega_i^2 - d^2)^{-1}}{1 + \mu} \left((\omega_i^2 - d^2)I + \mu (D_1^2 - d^2 I)\right) (D_1^2 - \omega_i^2 I)^{-1} u_1. \end{split}$$

Ignoring the leading positive factor and normalizing, we get (5.4).

When  $d = d_k = 0$ , the k-th component of  $w_i$  is 0 for  $1 \le i \le k-1$ , and  $w_k = (0, \ldots, 0, 1)^T$ . Thus W can be written as  $diag(W_1, 1)$ , and the SVD of

$$C_1 = \left(I - \frac{1}{1+\mu}u_1u_1^T\right)D_1$$

is  $Q\Omega W_1^T$ .

The following lemma allows one to construct a matrix of the form (5.1) using D and all the singular values.

LEMMA 4. Given a diagonal matrix  $D = \text{diag}(D_1, d) = \text{diag}(d_1, \ldots, d_{k-1}, d_k)$  and a set of numbers  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  satisfying the interlacing property

$$d_1 > \hat{\omega}_1 > \ldots > d_{k-1} > \hat{\omega}_{k-1} > d_k = d \ge 0, \tag{5.9}$$

there exists a unit vector  $\hat{u}^T \equiv (\hat{u}_1^T, \hat{\mu}) = (\hat{\mu}_1, \dots, \hat{\mu}_{k-1}, \hat{\mu}_k)$  with  $\hat{\mu}_k = \hat{\mu} > 0$ , such that  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  are the singular values of

$$\hat{C} = \left(I - \frac{1}{1+\hat{\mu}}\hat{u}_1\hat{u}_1^T - \hat{u}_1\right) \begin{pmatrix} D_1 \\ d \end{pmatrix}.$$

The vector  $\hat{u}$  is determined by

$$|\hat{\mu}_i| = \sqrt{\prod_{j=1}^{i-1} \frac{(\hat{\omega}_j^2 - d_i^2)}{(d_j^2 - d_i^2)}} \prod_{j=i}^{k-1} \frac{(\hat{\omega}_j^2 - d_i^2)}{(d_{j+1}^2 - d_i^2)}, \quad 1 \le i \le k,$$
(5.10)

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

**Proof:** Assume that  $\hat{C}$  exists. By definition,

$$\det(\hat{C}^T \hat{C} - \omega^2 I) = -\omega^2 \prod_{j=1}^{k-1} (\hat{\omega}_j^2 - \omega^2).$$

As in the proof of Lemma 3, we also have

$$\det(\hat{C}^T\hat{C} - \omega^2 I) = -\omega^2 \prod_{j=1}^k (d_j^2 - \omega^2) \sum_{j=1}^k \frac{\hat{\mu}_j^2}{d_j^2 - \omega^2}.$$

Combining these two equations,

$$\prod_{j=1}^{k-1} \left( \hat{\omega}_j^2 - \omega^2 \right) = \prod_{j=1}^k \left( d_j^2 - \omega^2 \right) \sum_{j=1}^k \frac{\hat{\mu}_j^2}{d_j^2 - \omega^2}$$

Setting  $\omega = d_i$ , we get

$$\hat{\mu}_{i}^{2} = rac{\prod_{j}{(\hat{\omega}_{j}^{2} - d_{i}^{2})}}{\prod_{j 
eq i}{(d_{j}^{2} - d_{i}^{2})}}.$$

Because of the interlacing property (5.9), the expression on the right-hand side is positive. Taking square roots we get (5.10).

On the other hand, if  $\hat{u}$  is given by (5.10), then  $\hat{u}$  is a unit vector (see [9]). Working the above process backward, the singular values of  $\hat{C}$  are  $\{\hat{\omega}_i\}_{i=1}^{k-1}$ .

In the special case d = 0, Lemma 4 reconstructs a matrix

$$\hat{C}_1 = \left(I - \frac{1}{1+\hat{\mu}}\hat{u}_1\hat{u}_1^T\right)D_1$$

with given singular values.

#### **5.2.** Computing the Singular Vectors of C

By (5.2) and Lemma 3,  $\mu > 0$ ,  $\omega_i - d > 0$  and  $d_i - d \ge 0$  for any *i*. Thus if the singular value  $\omega_i$  of C was given exactly, then each difference

$$d_j^2 - \omega_i^2 = (d_j - \omega_i)(d_j + \omega_i)$$

in (5.4) and (5.5) could be computed to high relative accuracy; and each sum

$$\gamma_{i,j}^2 = (\omega_i^2 - d^2) + \mu(d_j^2 - d^2) = (\omega_i - d)(\omega_i + d) + \mu(d_j - d)(d_j + d)$$

in (5.4) could be computed to high relative accuracy (each factor in the products is positive). Each product and each ratio in (5.4) and (5.5) could also be computed to high relative accuracy. As a result, the corresponding singular vectors  $q_i$  and  $w_i$  could be computed to computed to component-wise high relative accuracy.

In practice we can only hope to compute an approximation  $\hat{\omega}_i$  to  $\omega_i$ . It is well known that equations similar to (5.4) and (5.5) can be very sensitive to small errors in  $\omega_i$  (see Section 3.2). But Lemma 4 allows us to overcome this problem. After we have computed all the approximate singular values  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  of C, we use Lemma 4 to find a *new* matrix  $\hat{C}$ whose *exact* singular values are  $\{\hat{\omega}_i\}_{i=1}^{k-1}$ , and then compute the singular vectors of  $\hat{C}$  using Lemma 3. Note that each difference

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

in (5.10) can be computed to high relative accuracy. Each product and each ratio can also be computed to high relative accuracy. Thus  $|\hat{\mu}_i|$  can be computed to high relative accuracy. We choose the sign of  $\hat{\mu}_i$  to be the sign of  $\mu_i$ . Substituting the computed  $\hat{u}$  and the *exact* singular values  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  into (5.4), (5.5) and (5.6), each singular vector of  $\hat{C}$  can again be computed to component-wise 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  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  to satisfy the interlacing property (5.9). But since the exact singular values of C satisfy the same interlacing property (see Lemma 3), 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  $\hat{u}$  is close to u (see (4.8)).

#### 5.3. Stably Computing the Singular Values of C and $C_1$

In Section 3.3 we showed how to find the roots of a secular equation of the form

$$f(\omega) = -\rho + \sum_{j=1}^{k} \frac{\zeta_j^2}{d_j^2 - \omega^2} = 0,$$

where  $z = (\zeta_1, \ldots, \zeta_k)^T$  is a vector and  $\rho \ge 0$  is a scalar. Since equation (5.3) is the special case  $\rho = 0$  and  $z = u = (\mu_1, \ldots, \mu_k)^T$  with  $||u||_2 = 1$ , all that remains is to show that the approximations  $\{\hat{\omega}_i\}_{i=1}^{k-1}$  to  $\{\omega_i\}_{i=1}^{k-1}$  are sufficiently accurate that  $\hat{u}$  is close to u.

Applying (3.8) with  $\rho = 0$  and z = u, we get

$$|\hat{\omega}_{i}^{2} - \omega_{i}^{2}| \leq \frac{\beta_{j}}{1 - \frac{1}{2}\beta_{j}} |d_{j}^{2} - \omega_{i}^{2}|$$
(5.11)

for every i and j, provided that  $\beta_j = 2\eta k \|u\|_2/((1 - \eta k)|\mu_j|) < 2$ .

Let  $\hat{\omega}_i^2 - \omega_i^2 = \alpha_{ij}(d_j^2 - \omega_i^2)/\mu_j$  for all *i* and *j*. Suppose that we pick  $\theta = 2\eta k^2$  in (5.2). Then we have  $|\mu_j| \ge 2\eta k^2 ||u||_2$ . Assume further that  $\eta k < 1/100$ . Then  $\beta_j \le 2/3$ , and (5.11) implies that  $|\alpha_{ij}| \le \alpha \equiv 4\eta k ||u||_2$  for all *i* and *j*. Thus, from (5.10),

$$|\hat{\mu}_i| = \sqrt{\frac{\prod_j \left(\hat{\omega}_j^2 - d_i^2\right)}{\prod_{j \neq i} \left(d_j^2 - d_i^2\right)}} = \sqrt{\frac{\prod_j \left(\omega_j^2 - d_i^2\right) \left(1 + \alpha_{ji}/\mu_i\right)}{\prod_{j \neq i} \left(d_j^2 - d_i^2\right)}} = |\mu_i| \sqrt{\prod_{j=1}^{k-1} \left(1 + \frac{\alpha_{ji}}{\mu_i}\right)}$$

and, since  $\hat{\mu}_i$  and  $\mu_i$  have the same sign,

$$\begin{aligned} |\hat{\mu}_{i} - \mu_{i}| &= |\mu_{i}| \left| \sqrt{\prod_{j=1}^{k-1} \left( 1 + \frac{\alpha_{ji}}{\mu_{i}} \right)} - 1 \right| &\leq |\mu_{i}| \left( \left( 1 + \frac{\alpha}{|\mu_{i}|} \right)^{\frac{k}{2}} - 1 \right) \\ &\leq |\mu_{i}| \left( \exp\left( \frac{\alpha k}{2|\mu_{i}|} \right) - 1 \right) \leq (e-1) \alpha k/2 \\ &\leq 4\eta k^{2} ||u||_{2}, \end{aligned}$$
(5.12)

where we have used the fact that  $\alpha k/(2|\mu_i|) \leq 1$  and that  $e^{\gamma} - 1 \leq (e-1)\gamma$  for  $0 < \gamma \leq 1$ . As in the discussion following (3.9), we might expect the factor of  $k^2$  in  $\theta$  and (5.12) to be more like O(k) in practice.

We have been assuming that  $||u||_2 = 1$ . In practice this is not always true due to roundoff errors. However, since a vector with norm near unity is close to an *exact* unit vector to component-wise high relative accuracy, in practice u is given to component-wise high relative accuracy. This implies that each term in the secular equation (5.3) is still computed to high relative accuracy after the reformulation of Section 3.3. Hence the stopping criterion (3.6) holds and  $\hat{u}$  is close to u.

### **5.4.** Deflation for C and $C_1$

Consider the matrix

$$C = \left(I - \frac{1}{1+\mu}u_1u_1^T - u_1\right) \left(\begin{array}{c} D_1 \\ & d \end{array}\right),$$

where  $D = diag(D_1, d) = diag(d_1, ..., d_{k-1}, d_k) \in \mathbf{R}^{k \times k}$ , with  $d_1 \ge ... \ge d_{k-1} \ge d_k = d \ge 0$ ; and  $u_1 = (\mu_1, ..., \mu_{k-1})^T \in \mathbf{R}^{k-1}$ ,  $\mu = \mu_k \ge 0$  is a scalar, and  $u = (u_1^T \ \mu)^T$  is a unit vector<sup>9</sup>. We now show that we can reduce C to a matrix of the same form which further satisfies (see (5.2))

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

where  $\theta$  is specified in Section 5.3. We only discuss deflation procedures for C; the deflation procedures for  $C_1$  are the same with d = 0 and  $D_1$  replaced by D.

Assume that  $\mu < \theta$ . Then

$$C = \left(I - \frac{1}{1+\theta}u_1u_1^T - u_1\right) \begin{pmatrix} D_1 \\ d \end{pmatrix} + \left(\frac{\mu-\theta}{(1+\theta)(1+\mu)}u_1u_1^T - 0\right) \begin{pmatrix} D_1 \\ d \end{pmatrix}$$
$$= \check{C} + O(\theta \|D\|_2),$$

where

$$\check{C} = \left(I - \frac{1}{1+\theta}u_1u_1^T - u_1\right) \begin{pmatrix} D_1 \\ d \end{pmatrix}.$$

We perturb  $\mu$  to  $\theta$ . The perturbed matrix  $\check{C}$  has the same form but with  $\mu \geq \theta$ . This reduction is stable (see Section 4.1).

Next assume that  $|\mu_i| < \theta$  for some  $i \le k - 1$ . We illustrate the case i = 1. Let

$$u_1 = \begin{pmatrix} \mu_1 \\ \breve{u}_1 \end{pmatrix}$$
 and  $D_1 = \begin{pmatrix} d_1 \\ \breve{D}_1 \end{pmatrix}$ .

Then

$$\begin{split} C &= \left( \begin{array}{c} 1 - \frac{\mu_{1}^{2}}{1 + \mu} & -\frac{\mu_{1}}{1 + \mu} \breve{u}_{1}^{T} & -\mu_{1} \\ -\frac{\mu_{1}}{1 + \mu} \breve{u}_{1} & I - \frac{1}{1 + \mu} \breve{u}_{1} \breve{u}_{1}^{T} & -\breve{u}_{1} \end{array} \right) \left( \begin{array}{c} d_{1} \\ \breve{D}_{1} \\ d \end{array} \right) \\ &= \left( \begin{array}{c} 1 & 0 & 0 \\ 0 & I - \frac{1}{1 + \mu} \breve{u}_{1} \breve{u}_{1}^{T} & -\breve{u}_{1} \end{array} \right) \left( \begin{array}{c} d_{1} \\ \breve{D}_{1} \\ d \end{array} \right) \\ &+ \left( \begin{array}{c} -\frac{\mu_{1}^{2}}{1 + \mu} & -\frac{\mu_{1}}{1 + \mu} \breve{u}_{1}^{T} & -\mu_{1} \\ -\frac{\mu_{1}}{1 + \mu} \breve{u}_{1} & 0 & 0 \end{array} \right) \left( \begin{array}{c} d_{1} \\ \breve{D}_{1} \\ d \end{array} \right) \\ &= \left( \begin{array}{c} d_{1} \\ \breve{C} \end{array} \right) + O(\theta \| D \|_{2}), \end{split}$$

where

$$\breve{C} = \left(I - \frac{1}{1+\mu}\breve{u}_1\breve{u}_1^T - \breve{u}_1\right) \left(\begin{array}{c}\breve{D}_1\\ & d\end{array}\right).$$

<sup>&</sup>lt;sup>9</sup> As noted above, we only need to require u to have norm *near* unity.

We perturb  $\mu_i$  to 0. The perturbed matrix  $\begin{pmatrix} d_1 \\ \check{C} \end{pmatrix}$  has  $d_1$  as a singular value, and  $\check{C}$  is another matrix with the same form but smaller dimensions. This reduction is stable (see Section 4.1).

Now assume that  $d_i - d_{i+1} < \theta \|D\|_2$  for some  $i \le k-2$ . We illustrate the reduction for i = 1. Let  $G_{2,l} = diag(G, I_{l-2})$ , with G being a Givens rotation that zeroes the first component of  $\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$ , and let  $\check{u}_1 = \left(\sqrt{\mu_1^2 + \mu_2^2}, \mu_3, \dots, \mu_{k-1}\right)^T$  and  $\check{D} = diag(\check{D}_1, d_k) = diag(d_2, d_3, \dots, d_{k-1}, d_k).$ 

Then

$$G_{2,k-1} u_1 = \begin{pmatrix} 0 \\ \breve{u}_1 \end{pmatrix}$$
 and  $G_{2,k}^T \begin{pmatrix} d_2 \\ \breve{D} \end{pmatrix} = \begin{pmatrix} d_2 \\ \breve{D} \end{pmatrix} G_{2,k}^T$ .

Since

$$D = \begin{pmatrix} d_2 \\ \breve{D} \end{pmatrix} + O(\theta \|D\|_2),$$

we have

$$\begin{split} &G_{2,k-1}CG_{2,k}^{T} \\ &= G_{2,k-1}\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T} - u_{1}\right)D\ G_{2,k}^{T} \\ &= G_{2,k-1}\left(I - \frac{1}{1+\mu}u_{1}u_{1}^{T} - u_{1}\right)G_{2,k}^{T}\left(\begin{array}{c}d_{2}\\\check{D}\end{array}\right) + O(\theta||D||_{2}) \\ &= \left(I - \frac{1}{1+\mu}(G_{2,k-1}\ u_{1})\left(G_{2,k-1}\ u_{1}\right)^{T} - (G_{2,k-1}\ u_{1})\right)\left(\begin{array}{c}d_{2}\\\check{D}\end{array}\right) + O(\theta||D||_{2}) \\ &= \left(\begin{array}{c}1 & 0 & 0\\ 0 & I - \frac{1}{1+\mu}\check{u}_{1}\check{u}_{1}^{T} - \check{u}_{1}\end{array}\right)\left(\begin{array}{c}d_{2}\\\check{D}_{1}\\d\end{array}\right) + O(\theta||D||_{2}) \\ &= \left(\begin{array}{c}d_{2}\\\check{C}\end{array}\right) + O(\theta\,||D||_{2}), \end{split}$$

where

$$\check{C} = \left(I - \frac{1}{1+\mu}\check{u}_1\check{u}_1^T - \check{u}_1\right) \left( egin{array}{c} \check{D}_1 \\ & d \end{array} 
ight).$$

We perturb  $d_i$  to  $d_{i+1}$ . The perturbed matrix  $\begin{pmatrix} d_2 \\ \check{C} \end{pmatrix}$  has  $d_2$  as a singular value and  $\check{C}$  is another matrix with the same form but smaller dimensions. This reduction is stable (see

Section 4.1).

Finally assume that  $d_{k-1} - d < \theta ||D||_2$  and  $d_{k-2} - d_{k-1} \ge \theta ||D||_2$ . Let

$$\dot{D} = diag (d_1, \ldots, d_{k-2}, d_{k-1} + \theta \|D\|_2, d) = D + O(\theta \|D\|_2).$$

Then

$$C = \left( I - \frac{1}{1+\mu} u_1 u_1^T - u_1 \right) D = \breve{C} + O(\theta \| D \|_2),$$

where

$$\breve{C} = \left(I - \frac{1}{1+\mu}u_1u_1^T - u_1\right)\breve{D}.$$

We perturb  $d_{k-1}$  to  $d_{k-1} + \theta \|D\|_2$ . The perturbed matrix  $\check{C}$  has the same form but with  $d_{k-1} - d \ge \theta \|D\|_2$ . If the relation  $d_{k-2} - d_{k-1} \ge \theta \|D\|_2$  no longer holds, we can apply the previous reduction to reduce the matrix size again. This reduction is stable (see Section 4.1).

# 6. Ill-conditioning of Problem 1 for Singular Values

In this section we analyze the ill-conditioning of the singular values for Problem 1 by bounding the effect of perturbations in a on the singular values of A'. The effect of perturbations in V and D is similar.

#### 6.1. The Case m > n

From (4.6), we have

$$A' = XC_1 V^T,$$

where X is column orthogonal and  $C_1 \in \mathbf{R}^{n \times n}$  is given by

$$C_1 = \left(I - \frac{1}{1+\mu}u_1u_1^T\right)D,$$

with  $\mu \ge 0$  and  $||u_1||_2^2 + \mu^2 = 1$ .

Assume that D is non-singular. The second relation in equation (4.2) implies that  $u_1 = D^{-1}V^T a$ , whence  $\mu = \sqrt{1 - \|u_1\|_2^2}$ . Thus  $C_1$  can be rewritten as

$$C_1 = D - \frac{1}{1+\mu} u_1 \ z^T,$$

where  $z = V^T a$ .

Assume that  $\bar{a}$  is a vector slightly perturbed from a with  $\|D^{-1}V^T\bar{a}\|_2 \leq 1$ . Define

$$ar{z} = V^T ar{a}, \quad ar{u}_1 = D^{-1} V^T ar{a} \quad ext{and} \quad ar{\mu} = \sqrt{1 - \|ar{u}_1\|_2^2}.$$

Let

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

 $\bar{A}' = \bar{X}\bar{C}_1 V^T,$ 

where  $\bar{X}$  is a column orthogonal matrix. Thus the singular values of A' and  $\bar{A}'$  are the singular values of  $C_1$  and  $\bar{C}_1$ , respectively. Let  $\omega_i$  and  $\bar{\omega}_i$  be the *i*-th largest singular values of  $C_1$  and  $\bar{C}_1$ , respectively. Then  $|\bar{\omega}_i - \omega_i| \leq ||\bar{C}_1 - C_1||_2$  (see [9, page 428]).

Since

$$ar{z} - z = V^T(ar{a} - a)$$
 and  $ar{u}_1 - u_1 = D^{-1}V^T(ar{a} - a),$ 

we have

$$\|ar{z}-z\|_2 \leq \|ar{a}-a\|_2$$
 and  $\|ar{u}_1-u_1\|_2 \leq \|D^{-1}\|_2 \|ar{a}-a\|_2.$ 

Similarly,

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

so that

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

Since

$$\begin{split} \bar{C}_1 - C_1 &= -\frac{1}{1+\bar{\mu}}\bar{u}_1 \ \bar{z}^T + \frac{1}{1+\mu}u_1 \ z^T \\ &= \left(\frac{(\bar{\mu}-\mu) \ u_1}{(1+\mu)(1+\bar{\mu})} - \frac{\bar{u}_1 - u_1}{1+\bar{\mu}}\right) \ z^T - \frac{\bar{u}_1}{1+\bar{\mu}} \ (\bar{z}-z)^T, \end{split}$$

we have

$$\begin{aligned} |\bar{\omega}_{i} - \omega_{i}| &\leq \|\bar{C}_{1} - C_{1}\|_{2} \\ &\leq \left\|\frac{(\bar{\mu} - \mu) u_{1}}{(1 + \mu)(1 + \bar{\mu})} - \frac{\bar{u}_{1} - u_{1}}{1 + \bar{\mu}}\right\|_{2} \|z\|_{2} + \frac{\|\bar{u}_{1}\|_{2}}{1 + \bar{\mu}} \|\bar{z} - z\|_{2} \\ &\leq (|\bar{\mu} - \mu| + \|\bar{u}_{1} - u_{1}\|_{2})\|z\|_{2} + \|\bar{z} - z\|_{2} \\ &\leq \left(\frac{2\|\bar{u}_{1} - u_{1}\|_{2}}{\sqrt{1 - \|u_{1}\|_{2}^{2}}} + \|\bar{u}_{1} - u_{1}\|_{2}\right) \|a\|_{2} + \|\bar{z} - z\|_{2} \\ &\leq \frac{4 \max\left(\|D^{-1}\|_{2} \|a\|_{2}, 1\right)}{\sqrt{1 - \|u_{1}\|_{2}^{2}}} \|\bar{a} - a\|_{2}. \end{aligned}$$

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  $\omega_i$ . This result parallels that of Stewart [19, page 205] in the context of downdating the Cholesky/QR factorizations.

To better explain the role of  $||u_1||_2$ , Stewart [19] shows that

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

Thus if  $||u_1||_2$  is near unity, then  $\omega_n$  is close to zero and  $C_1$  (and hence A') is close to being singular. And if any  $d_i$  is reduced (to  $\omega_i$ ) by a big factor, then  $||u_1||_2$  is near unity.

### **6.2.** The Case $m \leq n$

From (4.13), we have

$$A' = X C V_1^T,$$

where X is orthogonal and  $C \in \mathbf{R}^{(m-1) \times m}$  is given by

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

with  $\mu \ge 0$  and  $||u_1||_2^2 + \mu^2 = 1$ .

Assume that D is non-singular. By (4.12),  $u = (u_1^T, \mu)^T = D^{-1}V_1^T a$ . Let

$$D = \begin{pmatrix} D_1 \\ d \end{pmatrix}$$
 and  $V_1^T a = \begin{pmatrix} z_1 \\ \zeta \end{pmatrix}$ .

Then  $u_1 = D_1^{-1} z_1$ ,  $\mu = \zeta/d$  and

$$C = \left(I - \frac{1}{1+\mu}u_1 z_1^T - d u_1\right).$$

Assume that  $\bar{a}$  is a vector slightly perturbed from a such that Problem 1 with input data  $V_1$ , D and  $\bar{a}$  has a solution (see Section 1). Define

$$\begin{pmatrix} \bar{z}_1 \\ \bar{\zeta} \end{pmatrix} = V_1^T \bar{a} \quad \text{and} \quad \begin{pmatrix} \bar{u}_1 \\ \bar{\mu} \end{pmatrix} = \begin{pmatrix} D_1 \ \bar{z}_1 \\ d^{-1} \ \bar{\zeta} \end{pmatrix}.$$

Let

$$ar{C} = \left(I - rac{1}{1+ar{\mu}}ar{u}_1\ ar{z}_1^T \quad -d\ ar{u}_1
ight),$$

and let  $\bar{A}'$  be the downdated matrix for the input data  $V_1$ , D and  $\bar{a}$ . Then by (4.13), we have

$$\bar{A}' = \bar{X}\bar{C}V^T,$$

where  $\bar{X}$  is an orthogonal matrix. Thus the singular values of A' and  $\bar{A}'$  are the singular values of C and  $\bar{C}$ , respectively. Let  $\omega_i$  and  $\bar{\omega}_i$  be the *i*-th largest singular values of C and  $\bar{C}$ , respectively. Then  $|\bar{\omega}_i - \omega_i| \leq ||\bar{C} - C||_2$  (see [9, page 428]).

Since

$$\left( \begin{array}{c} \bar{z}_1 - z_1 \\ \bar{\zeta} - \zeta \end{array} \right) = V_1^T (\bar{a} - a) \quad \text{and} \quad \left( \begin{array}{c} \bar{u}_1 - u_1 \\ \bar{\mu} - \mu \end{array} \right) = D^{-1} V^T (\bar{a} - a),$$

we have

$$\max\left(\|\bar{z}_1-z_1\|_2,|\bar{\zeta}-\zeta|\right) \le \|\bar{a}-a\|_2,$$

and

$$\max\left(\|\bar{u}_1 - u_1\|_2, |\bar{\mu} - \mu|\right) \le \left\|D^{-1}\right\|_2 \|\bar{a} - a\|_2$$

Similar to Section 6.1, we have

$$\bar{C} - C = \left(\frac{\bar{\mu} - \mu}{(1+\mu)(1+\bar{\mu})}u_1 \ z_1^T - \frac{u_1 \ (\bar{z}_1 - z_1)^T}{1+\bar{\mu}} - \frac{(\bar{u}_1 - u_1) \ \bar{z}_1^T}{1+\bar{\mu}} - d \ (\bar{u}_1 - u_1)\right).$$

Thus

$$\begin{aligned} &|\bar{\omega}_{i} - \omega_{i}| \\ &\leq \|\bar{C} - C\|_{2} \\ &\leq \left\|\frac{\bar{\mu} - \mu}{(1+\mu)(1+\bar{\mu})}u_{1} z_{1}^{T}\right\|_{2} + \left\|\frac{u_{1} (\bar{z}_{1} - z_{1})^{T}}{1+\bar{\mu}}\right\|_{2} + \left\|\frac{(\bar{u}_{1} - u_{1}) \bar{z}_{1}^{T}}{1+\bar{\mu}}\right\|_{2} + \|d (\bar{u}_{1} - u_{1})\|_{2} \\ &\leq |\bar{\mu} - \mu| \|z_{1}\|_{2} + \|\bar{z}_{1} - z_{1}\|_{2} + \|\bar{u}_{1} - u_{1}\|_{2} \|\bar{z}_{1}\|_{2} + d \|\bar{u}_{1} - u_{1}\|_{2} \\ &\leq 4 \max\left(\left\|D^{-1}\right\|_{2} \|a\|_{2}, \left\|D^{-1}\right\|_{2} \|\bar{a}\|_{2}, 1\right) \|\bar{a} - a\|_{2}. \end{aligned}$$

When the factor  $||D^{-1}||_2 ||a||_2$  is very large, we cannot guarantee that  $\bar{\omega}_i$  is close to  $\omega_i$  (cf. [19, page 205]).

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