

Deflation for the Half-Arrow Singular Value Decomposition

Jesse L. Barlow, Stanley Eisenstat, Nevena Jakovčević Stor, and Ivan Slapničar

Abstract

A half-arrow matrix F has the form

$$F = \begin{pmatrix} \Psi & \mathbf{g} \\ \mathbf{0}^T & \rho \end{pmatrix}, \quad \mathbf{g} \in \mathbf{R}^n, \quad \rho \in \mathbf{R}, \quad (1)$$

$$\Psi = \text{diag}(\psi_1, \dots, \psi_n), \quad \psi_1 \geq \psi_2 \geq \dots \geq \psi_n \geq 0. \quad (2)$$

We consider the problem of determining which of the diagonals of Ψ are close to singular values of F and how these values can be deflated efficiently. Such deflation techniques were explored in the “conquer” stage of the divide-and-conquer bidiagonal SVD algorithms given by Jessup and Sorensen [9] and Gu and Eisenstat [7].

A version of the algorithm in [9] is coded in the LAPACK [1] subroutine **dlasd2.f** [10] as a part of the bidiagonal SVD subroutine **dbdsbc.f** [1, p.208].

The SVD version of the Cauchy interlace theorem [6, Corollary 8.6.3] states that the singular values $\sigma_1, \dots, \sigma_{n+1}$ of F satisfy

$$\sigma_j \geq \psi_j \geq \sigma_{j+1}, \quad j = 1, \dots, n. \quad (3)$$

Interpretating a result in [13, p.95], Jessup and Sorensen [9] point to three cases where ψ_j is a singular value of F :

- **Case I:** $g_j = \mathbf{e}_j^T \mathbf{g} = 0$, then $(\psi_j, \mathbf{e}_j, \mathbf{e}_j)$ is a singular triplet of F ;
- **Case II:** $\psi_j = 0$, so we let $G_{n+1,j}$ be a Givens rotation affecting rows j and $n+1$ whose non-trivial part is defined by

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} g_j \\ \rho \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{\rho} \end{pmatrix}, \quad \begin{aligned} c^2 + s^2 &= 1, \\ \hat{\rho} &= \pm \sqrt{g_j^2 + \rho^2}, \end{aligned}$$

and we have that

$$\tilde{F} = G_{n+1,j} F$$

has the singular triplet $(0, \mathbf{e}_j, \mathbf{e}_j)$;

- **Case III:** $\psi_i = \psi_j$ for some $i \neq j$, so we let G_{ij} be a Givens rotation affecting rows i and j where the non-trivial part of G_{ij} is defined by

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} g_i \\ g_j \end{pmatrix} = \begin{pmatrix} \hat{g}_j \\ 0 \end{pmatrix}, \quad \begin{aligned} c^2 + s^2 &= 1 \\ \hat{g}_j &= \pm \sqrt{g_j^2 + g_{j+1}^2} \end{aligned}$$

and we have that

$$\tilde{F} = G_{ij} F G_{ij}^T$$

has the singular triplet $(\psi_j, \mathbf{e}_j, \mathbf{e}_j)$.

In all three cases, the computation of the SVD of F is reduced to that of computing the SVD of a lower dimensional half-arrow matrix. If none of these deflations is possible for any j , then from [13, p.95], we have the strict interlacing property

$$\sigma_j > \psi_j > \sigma_{j+1}, \quad j = 1, \dots, n. \quad (4)$$

The deflation strategies in [9, 7] are based upon the idea that one of these three cases applies to a matrix near F . We model these strategies as follows: we compute a value γ_F such that $\|F\|_2 \leq \gamma_F \leq \sqrt{2}\|F\|_2$, and let τ be a small value, usually $\mathcal{O}(\varepsilon_M)$ where ε_M is the machine unit. In some applications, τ may be an acceptable level of error.

Corresponding to the three cases for when ψ_j is a singular value of F , we can deflate g_j in the following three cases:

1. If

$$|g_j| \leq \tau\gamma_F \quad (5)$$

we simply set g_j to zero;

2. If

$$\frac{\psi_j |g_j|}{\sqrt{g_j^2 + \rho^2}} \leq \tau\gamma_F,$$

then we apply the Givens rotation $G_{n+1,j}$ to rows $n+1$ and j setting g_j to zero producing

$$\tilde{F} + \delta F_{n+1,j} = G_{n+1,j} F, \quad \|\delta F_{n+1,j}\|_2 \leq \sqrt{2}\tau\gamma_F \quad (6)$$

where \tilde{F} is a half-arrow matrix with Ψ unchanged;

3. If

$$|\delta_{ij}| \leq \tau\gamma_F, \quad \delta_{ij} = \frac{g_j g_i}{g_i^2 + g_j^2} (\psi_i - \psi_j) \quad (7)$$

and $|g_j| \leq |g_i|$, then we apply the Givens rotation G_{ij} to rows i and j setting g_j to zero producing

$$\tilde{F} + \delta F_{ij} = G_{ij} F G_{ij}^T, \quad \|\delta F_{ij}\|_2 \leq \sqrt{2}\tau\gamma_F \quad (8)$$

where \tilde{F} is again a half-arrow matrix with Ψ unchanged. If (7) holds and $|g_j| > |g_i|$, we set g_i to zero in an analogous manner.

The deflations (5) and (8) are discussed in [9, 7] and the deflation (6) is discussed in [9].

We enhance the approach in [9, 7] and in the LAPACK routine **dlasd2.f** [10] by producing a better deflation algorithm that is still $\mathcal{O}(n)$ operations. We also show that if for a particular value of j , g_j cannot be deflated by (5) or by (6) or by (8) for any $i \neq j$, then

$$\sigma_j - \sigma_{j+1} > \tau\gamma_F / \sqrt{2n+1}. \quad (9)$$

However, the only algorithm we give with that guarantee for all j has a worst case complexity proportional to n^2 . If we weaken these conditions, so that there is no index i such that $|i-j| < q$, and we have (8), then

$$\sigma_j - \sigma_{j+1} > \sqrt{2}\tau^2 q \gamma_F + \mathcal{O}(\tau^4 q^2 \gamma_F). \quad (10)$$

The algorithm we recommend is a heuristic proposed here with worst case complexity proportional to n , the same asymptotic complexity as the LAPACK procedure, but with better deflation guarantees. It achieves (10) with $q = 2$ for all j . Bounds similar to (9) and (10) are not possible for the singular values of deflated structure matrices, for instance, there are no such bounds for bidiagonal matrices.

In light of work by Demmel and Gragg [4] that formulated an algorithm to compute the nonzero singular values of F to near relative accuracy, we formulate and analyze versions of the deflations in (5) and (8) that preserve relative accuracy in the singular values.

By choosing γ_F to be within a constant factor of $\|F\|_2$, these deflations produce no more error in the singular values than would be expected of a normwise backward stable algorithm for finding the SVD of F . However, for algorithms to compute the SVD of F , deflation gives us dimension reduction and speeds up the algorithms in [9] and [7]. The LAPACK routine `dlasd2.f` uses only the first and third types of deflation.

Two other applications for this kind of deflation have been investigated. The first is in SVD-based regularization approaches given in [8, §4.3] and [11]. The second is in the implementation of a Krylov-Schur implementation [2, 12] of the Golub-Kahan-Lanczos SVD algorithm [5].

This is a continuation of work in [3].

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