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NEW FAST AND ACCURATE JACOBI SVD ALGORITHM. I*

ZLATKO DRMAČ† AND KREŠIMIR VESELIĆ‡

Dedicated to the memory of Patricia J. Eberlein, whose enthusiasm and belief in the powers of the Jacobi methods were a constant inspiration

Abstract. This paper is the result of concerted efforts to break the barrier between numerical accuracy and run-time efficiency in computing the fundamental decomposition of numerical linear algebra—the singular value decomposition (SVD) of general dense matrices. It is an unfortunate fact that the numerically most accurate one-sided Jacobi SVD algorithm is several times slower than generally less accurate bidiagonalization-based methods such as the QR or the divide-and-conquer algorithm. Our quest for a highly accurate and efficient SVD algorithm has led us to a new, superior variant of the Jacobi algorithm. The new algorithm has inherited all good high accuracy properties of the Jacobi algorithm, and it can outperform the QR algorithm.

Key words. Jacobi method, singular value decomposition, eigenvalues

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1. Introduction.

In 1846, Jacobi [25] introduced a new simple and accurate algorithm for diagonalization of symmetric matrices. The algorithm starts with symmetric matrix $H^{(0)} = H \in \mathbb{R}^{n\times n}$ and then generates a sequence of congruences, $H^{(k+1)} = (V^{(k)})^T H^{(k)} V^{(k)}$, where $V^{(k)}$ is plane rotation; i.e., $V^{(k)}$ differs from the identity only at the cleverly chosen positions (p_k, p_k), (p_k, q_k), (q_k, p_k), (q_k, q_k), where

$$\begin{pmatrix} V^{(k)}_{p_k,p_k} & V^{(k)}_{p_k,q_k} \\ V^{(k)}_{q_k,p_k} & V^{(k)}_{q_k,q_k} \end{pmatrix} = \begin{pmatrix} \cos\phi_k & \sin\phi_k \\ -\sin\phi_k & \cos\phi_k \end{pmatrix}.$$

The angle ϕ_k is determined to annihilate the (p_k, q_k) and (q_k, p_k) positions in $H^{(k)}$. Simple trigonometry reveals that in the nontrivial case ($H^{(k)}_{p_kq_k} \neq 0$) we can take

$$\cot 2\phi_k = \frac{H^{(k)}_{q_kq_k} - H^{(k)}_{p_kp_k}}{2H^{(k)}_{p_kq_k}} \quad \text{and} \quad \tan\phi_k = \frac{\operatorname{sign}(\cot 2\phi_k)}{|\cot 2\phi_k| + \sqrt{1+\cot^2 2\phi_k}} \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right],$$

where ϕ_k is the smaller of two angles satisfying the requirements. (If $H^{(k)}_{p_kq_k} = 0$, then $V^{(k)} = I$, the identity.) Under suitable pivot strategies $k \mapsto (p_k, q_k)$, the sequence $(H^{(k)})_{k=0}^{\infty}$ converges to diagonal matrix Λ, and the product $V^{(0)}V^{(1)}\cdots V^{(k)}\cdots$ converges to the orthogonal matrix V of eigenvectors of H, $HV = V\Lambda$. The convergence is monitored using the off-norm, $\Omega(H) = \sqrt{\sum_{i\neq j} H_{ij}^2}$, for which one easily shows the monotonicity $\Omega^2(H^{(k+1)}) = \Omega^2(H^{(k)}) - 2(H^{(k)})^2_{p_k,q_k} \leq \Omega^2(H^{(k)})$.

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†Department of Mathematics, University of Zagreb, Bijenička 30, 10000 Zagreb, Croatia (drmac@math.hr). The work of this author was supported by the Croatian Ministry of Science and Technology under grant 0037120 (*Numerical Analysis and Matrix Theory*).

‡Lehrgebiet Mathematische Physik, Fernuniversität Hagen, Postfach 940, D-58084 Hagen, Germany (kresimir.veselic@FernUni-Hagen.de).

Hestenes [23] noted that the Jacobi method can be used to compute the SVD of general matrices. If A is of full column rank[1] and if we define $H = A^TA$, then the application of the method to H, $H^{(k+1)} = (V^{(k)})^T H^{(k)} V^{(k)}$, can be represented by the sequence $A^{(k+1)} = A^{(k)}V^{(k)}$. To determine the parameters of $V^{(k)}$ we only need the four pivot elements of $H^{(k)}$, that is, the 2×2 Gram matrix of the p_kth and the q_kth column of $A^{(k)}$. The limit matrix of $(A^{(k)})_{k=0}^{\infty}$ is $U\Sigma$, where the columns of orthonormal U are the left singular vectors and the diagonal matrix Σ carries the singular values along its diagonal. The accumulated product of Jacobi rotations is orthogonal matrix V of the eigenvectors of H. The SVD of A is $A = U\Sigma V^T$.

The development of fast methods based on reduction of A to bidiagonal form shifted interest away from the Jacobi SVD method—bidiagonalization-based routines xGESVD [11] and xGESDD [21] from LAPACK [1] can in some cases be ten or even fifteen times faster than the Jacobi SVD. However, Demmel and Veselić [12] showed that the Jacobi algorithm is more accurate than any other algorithm that first reduces the matrix to bidiagonal form. Some classes of matrices that appear ill-conditioned with respect to SVD computation in fact define the SVD perfectly well, and the ill-conditioning is artificial. For instance, if $A \in \mathbb{R}^{m\times n}$ is such that $\min_{D=\mathrm{diag}} \kappa_2(AD)$ is moderate, then the Jacobi SVD algorithm computes all singular values $\sigma_1 \geq \cdots \geq \sigma_n$ with guaranteed number of correct digits independent of the size of $\kappa_2(A) = \sigma_{\max}(A)/\sigma_{\min}(A) \equiv \sigma_1/\sigma_n$. The Jacobi method correctly deals with artificial ill-conditioning (e.g., grading), while the bidiagonalization-based methods do not.

In this paper we present a new preconditioned Jacobi SVD algorithm which provides higher accuracy with efficiency comparable to the bidiagonalization-based methods. In section 2 we show that rank revealing QR factorization can be used as an efficient preconditioner for the Jacobi SVD algorithm, and we reduce the problem to SVD computation of structured triangular matrices. Important detail of choosing A or A^T as input to the new algorithm is discussed in section 3. The dilemma "A or A^T" generates interesting mathematical questions leading us to study entropy of the set of normalized diagonals of the adjoint orbit of a positive definite matrix. The basic structure of the new Jacobi SVD algorithm is developed in section 4. Numerical properties are analyzed in section 5. It is shown that the backward perturbation has structure which allows scaling invariance of the condition number for the forward error. Implementation details of a new Jacobi SVD for triangular matrices and results of numerical testing of the preconditioned Jacobi SVD are given in the second part of this paper [18], where we demonstrate the potential of the new approach.

2. QR factorization as preconditioner for the Jacobi SVD algorithm. In the case $m \gg n$, the QR factorization $A = Q\,(\,R^T \quad 0\,)^T$ is an attractive preprocessor for the Jacobi SVD algorithm, because Jacobi rotations can be applied to $R \in \mathbb{R}^{n\times n}$ instead of $A \in \mathbb{R}^{m\times n}$. If the QR factorization is computed with a rank revealing column pivoting, $A\Pi = Q\,(\,R^T \quad 0\,)^T$, then the additional structure of R opens quite a few possibilities for more efficient SVD computation by the Jacobi algorithm.

2.1. Faster convergence. Veselić and Hari [34] noted that the eigenvalues of symmetric positive definite H can be computed more efficiently if the Jacobi SVD method is applied to the lower triangular factor L from the pivoted Cholesky factorization $P^THP = LL^T$. If $H = A^TA$, $\mathrm{rank}(A) = n$, then Cholesky factorization with pivoting of H corresponds to the QR factorization with column pivoting

[1] This is only a temporary assumption for the sake of simplicity.

$A\Pi = Q\,(\,R^T \quad 0\,)^T$, $L = R^T$. Hence, the Jacobi SVD on R^T should have better convergence than if applied to R, and the preconditioning is performed simply by taking R^T instead of R as input. Implicitly, this is one step of the Rutishauser [31] LR diagonalization method $R^TR \rightsquigarrow RR^T$, which has a nontrivial diagonalizing effect.

Let $R = \left(\begin{smallmatrix} R_{[11]} & R_{[12]} \\ 0 & R_{[22]} \end{smallmatrix}\right)$, where the diagonal blocks are $k \times k$ and $(n-k)\times(n-k)$, and consider the corresponding block partitions of $H = R^TR$ and $M = RR^T$:

$$H = \begin{pmatrix} H_{[11]} & H_{[12]} \\ H_{[21]} & H_{[22]} \end{pmatrix} = \left(\begin{array}{c|c} R_{[11]}^T R_{[11]} & R_{[11]}^T R_{[12]} \\ \hline R_{[12]}^T R_{[11]} & R_{[12]}^T R_{[12]} + R_{[22]}^T R_{[22]} \end{array}\right),$$

$$M = \begin{pmatrix} M_{[11]} & M_{[12]} \\ M_{[21]} & M_{[22]} \end{pmatrix} = \left(\begin{array}{c|c} R_{[11]}R_{[11]}^T + R_{[12]}R_{[12]}^T & R_{[12]}R_{[22]}^T \\ \hline R_{[22]}R_{[12]}^T & R_{[22]}R_{[22]}^T \end{array}\right). \tag{2.1}$$

Note that the $(1,1)$ block in M is increased, and the $(2,2)$ block is decreased, i.e., $\mathrm{Trace}(M_{[11]}) = \mathrm{Trace}(H_{[11]}) + \|R_{[12]}\|_F^2$, $\mathrm{Trace}(M_{[22]}) = \mathrm{Trace}(H_{[22]}) - \|R_{[12]}\|_F^2$.

This redistribution of the mass of the diagonal blocks makes the gap between the dominant and subdominant parts of the spectrum more visible on the diagonal. Using the monotonicity of the spectrum, we also conclude that properly ordered eigenvalues $\lambda_i(\cdot)$ of the diagonal blocks satisfy $\lambda_i(M_{[11]}) \geq \lambda_i(H_{[11]})$, $\lambda_j(M_{[22]}) \leq \lambda_j(H_{[22]})$, $1 \leq i \leq k$, $1 \leq j \leq n-k$. With suitable pivot strategy, this has positive impact on the structure of Jacobi rotations (smaller angles) in the off-diagonal blocks in (2.1). Moreover, the off-diagonal blocks of M are expected to be smaller than those in H.

PROPOSITION 2.1. *With the partition of R and* (2.1) *define* $R_{[1:]} = (\,R_{[11]} \quad R_{[12]}\,)$, $R_{[:2]} = \left(\begin{smallmatrix} R_{[12]} \\ R_{[22]} \end{smallmatrix}\right)$, $\cos\Phi = H_{[11]}^{-1/2} H_{[12]} H_{[22]}^{-1/2}$, *and* $\cos\Psi = M_{[11]}^{-1/2} M_{[12]} M_{[22]}^{-1/2}$. *Then, with* $\|\cdot\| \in \{\|\cdot\|_2 \equiv \sigma_{\max}(\cdot), \|\cdot\|_F\}$,

$$\text{(i)}\quad \|M_{[12]}\| \leq \frac{\sigma_{\max}(R_{[22]})}{\sigma_{\min}(R_{[11]})}\|H_{[12]}\|\,; \quad \text{(ii)}\quad \|\cos\Psi\| \leq \frac{\sigma_{\max}(R_{[:2]})}{\sigma_{\min}(R_{[1:]})}\|\cos\Phi\|. \tag{2.2}$$

Proof. To prove the well-known relation (i), one notes that $M_{[12]} = R_{[11]}^{-T} H_{[12]} R_{[22]}^T$. For the new estimate (ii), we use the connections between the LQ factorization, Cholesky factorization and the positive definite matrix square root to conclude that there exist orthogonal matrices S_1, S_2 such that

$$\cos\Psi = (R_{[1:]}R_{[1:]}^T)^{-1/2}\, S_1\, \cos\Phi\, (R_{[:2]}^T R_{[:2]})^{1/2}\, S_2.$$

Taking the norm completes the proof. ∎

Let $\xi = \xi(R,k) = \sigma_{\max}(R_{[22]})/\sigma_{\min}(R_{[11]})$. If $\xi < 1$, then $\|M_{[12]}\|_F \leq \xi\|H_{[12]}\|_F < \|H_{[12]}\|_F$. Thus, a smaller value of ξ implies more block diagonal structure in M than in H. Now, it is the task of the rank revealing pivoting in the QR factorization to find index k for which $\xi \ll 1$. If the pivoting is done right, and if the singular values of R are distributed so that $\sigma_k \gg \sigma_{k+1}$ for some k, then ξ will be much smaller than one. See [7], [8] for a detailed analysis related to (2.2(i)).

Note that (2.2(ii)) estimates scaled off-diagonal blocks, which is relevant for the convergence of the Jacobi algorithm. Relevant separation is given by $\zeta = \zeta(R,k) = \sigma_{\max}(R_{[:2]})/\sigma_{\min}(R_{[1:]})$. In general, $\xi < 1$ does not imply $\zeta < 1$, but an additional factorization will provide that stronger separation.

THEOREM 2.2. *Let $R = LQ_L$ be the LQ factorization of R,*

$$\begin{pmatrix} R_{[11]} & R_{[12]} \\ 0 & R_{[22]} \end{pmatrix} = \begin{pmatrix} L_{[11]} & 0 \\ L_{[21]} & L_{[22]} \end{pmatrix} Q_L = LQ_L.$$

Then we have the following monotonicity relations:

$$\sigma_i\left(\begin{pmatrix} L_{[11]} \\ L_{[21]} \end{pmatrix}\right) \geq \sigma_i(L_{[11]}) = \sigma_i(R_{[1:]}) \geq \sigma_i(R_{[11]}), \quad i = 1, \ldots, k; \tag{2.3}$$

$$\sigma_j(L_{[22]}) \leq \sigma_j(\begin{pmatrix} L_{[21]} & L_{[22]} \end{pmatrix}) = \sigma_j(R_{[22]}) \leq \sigma_j(R_{[:2]}), \quad j = 1, \ldots, n-k. \tag{2.4}$$

In particular, if $\sigma_{\min}(R_{[1:]}) > \sigma_{\max}(R_{[22]})$, *then* $\xi(L^T, k) < 1$, $\zeta(L^T, k) < 1$, *and* $\|L_{[21]}\| < \|R_{[12]}\|$. *In that case,* $M = RR^T$ *is a shifted quasi-definite matrix.*

Proof. The inequalities (2.3) and (2.4) are obtained by an application of the monotonicity principle to the corresponding eigenvalues. Combination of the inequalities with the assumption $\sigma_{\min}(R_{[1:]}) > \sigma_{\max}(R_{[22]})$ gives the bounds on ξ and ζ. Since $L_{[21]} = R_{[22]}R_{[12]}^T L_{[11]}^{-T}$ we have, for $\|\cdot\| \in \{\|\cdot\|_2, \|\cdot\|_F\}$, $\|L_{[21]}\| \leq \frac{\sigma_{\max}(R_{[22]})}{\sigma_{\min}(R_{[1:]})}\|R_{[12]}\| < \|R_{[12]}\|$. Finally, note that $M - s^2 I$ is quasi-definite for any $s \in (\sigma_{\max}(R_{[22]}), \sigma_{\min}(R_{[1:]}))$. ∎

Remark 2.1. Theorem 2.2 introduces gap $\gamma(R, k) = \sigma_{\max}(R_{[22]})/\sigma_{\min}(R_{[1:]})$, which from the pivoted QR factorization requires less than the condition $\sigma_{\max}(R_{[22]}) < \sigma_{\min}(R_{[11]})$. If $\gamma < 1$, then the off-diagonal block in $M^{(1)} = L^T L$ satisfies $\|M_{[21]}^{(1)}\| \leq (\sigma_{\max}(L_{[22]})/\sigma_{\min}(L_{[11]}))(\sigma_{\max}(R_{[22]})/\sigma_{\min}(R_{[11]}))\|H_{21}\|$.

Now, it is reasonable to expect that the one-sided Jacobi SVD algorithm applied to L runs quite differently than if applied to the initial A. The structure of L calls for modifications, and the result is a new Jacobi-type algorithm designed for triangular matrices. Its complete description is in the second part of this report [18].

Remark 2.2. It is well known that repeated application of the step "do QR factorization and transpose R" is actually a simple way to approximate the SVD; see [29], [20], [32]. Fernando and Parlett [20] first realized that "the use of a preconditioner for cyclic Jacobi is not a futile effort." Here we stress the term *preconditioner* and use of the implicit Cholesky SVD as preconditioner for Jacobi iterations.

2.2. Rank deficient cases. Consider the case of A with low numerical rank. The task is to compute the singular values with standard error bound. In a rank revealing QR factorization, the computed $\tilde{R}$, $\tilde{Q}$ satisfy backward stability relations

$$(A + \delta A)\Pi = \hat{Q}\begin{pmatrix} \tilde{R} \\ 0 \end{pmatrix}, \quad \|\delta A(:,i)\|_2 \leq \varepsilon_{qr}\|A(:,i)\|_2, \quad i = 1, \ldots, n; \quad \|\tilde{Q} - \hat{Q}\|_F \leq \varepsilon_{qr},$$

where $\hat{Q}$ is orthogonal and ε_{qr} is bounded by a moderate $f(m,n)$ times the round-off $\boldsymbol{\varepsilon}$. Suppose there is an index $k \in \{1, \ldots, n\}$ such that $\tilde{R}$ can be partitioned as

$$\tilde{R} = \begin{pmatrix} \tilde{R}_{[11]} & \tilde{R}_{[12]} \\ 0 & \tilde{R}_{[22]} \end{pmatrix}, \quad \text{where } \tilde{R}_{[22]} \in \mathbb{R}^{(n-k)\times(n-k)} \text{ is sufficiently small.} \tag{2.5}$$

If we set $\tilde{R}_{[22]}$ to zero, then we will implicitly continue working with the matrix

$$\hat{Q}\begin{pmatrix} \tilde{R}_{[11]} & \tilde{R}_{[12]} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \left(A + \delta A - \hat{Q}\begin{pmatrix} 0 & 0 \\ 0 & \tilde{R}_{[22]} \\ 0 & 0 \end{pmatrix}\Pi^T\right)\Pi \equiv (A + \Delta A)\Pi. \tag{2.6}$$

If $\|\tilde{R}_{[22]}\|_2/\|A\|_2$ is of the order of ε_{qr}, then replacing $\tilde{R}_{[22]}$ with zero is in the matrix norm a backward stable operation for singular value computation with classical error bound—the perturbation in each singular value is small compared to $\|A\|_2 = \sigma_{\max}(A)$.

Further, (2.6) is the QR factorization of $(A+\Delta A)\Pi$, where for the computed orthogonal factor we can keep $\tilde{Q}$. If we compute the LQ factorization of the $k \times n$ matrix, $\hat{R} \equiv (\,\tilde{R}_{[11]} \quad \tilde{R}_{[12]}\,) = LQ_1$, then the Jacobi iterations work on substantially smaller $k \times k$ lower triangular matrix L. Thus, a rank revealing ULV decomposition is in this case an excellent preprocessor for the Jacobi SVD algorithm.

THEOREM 2.3. *Let the block $\tilde{R}_{[11]}$ in (2.6) be nonsingular and let $\tilde{R}_{[11]} = DT$, where D is diagonal with $\sigma_{\min}(D) = |\tilde{r}_{kk}|$. Further, let the truncated block $\tilde{R}_{[22]}$ satisfy $\|\tilde{R}_{[22]}\|_2 \le \tau|\tilde{r}_{kk}|$. If $\tilde{\sigma}_1 \ge \cdots \ge \tilde{\sigma}_k$ and $\hat{\sigma}_1 \ge \cdots \ge \hat{\sigma}_k$ are the nonzero singular values of $\tilde{R}$ and $\hat{R}$, respectively, then for $i = 1, \ldots, k$*

$$0 \le \frac{\tilde{\sigma}_i - \hat{\sigma}_i}{\tilde{\sigma}_i} \le \left(\frac{\hat{\sigma}_k}{\tilde{\sigma}_i}\right) \tau \|T^{-1}\|_2.$$

Proof. We first note that $\max_{i=1:k} |\tilde{\sigma}_i - \hat{\sigma}_i| \le \|\tilde{R}_{[22]}\|_2 \le \tau|\tilde{r}_{kk}| \le \tau\tilde{\sigma}_1$, which estimates truncation error relative to the matrix norm. This bound actually contains better estimate because $|\tilde{r}_{kk}|$ is related to $\tilde{\sigma}_k$. From the Courant–Fisher minimax theorem we conclude $|\tilde{r}_{kk}| \le \|T^{-1}\|_2 \sigma_k(\tilde{R}_{[11]})$, where $\sigma_k(\tilde{R}_{[11]})$ is the kth largest singular value of $\tilde{R}_{[11]}$. The proof is completed by the Cauchy interlacing theorem, which yields $\sigma_k(\tilde{R}_{[11]}) \le \hat{\sigma}_k \le \tilde{\sigma}_k$. ∎

Consider, for example, the classical Businger–Golub pivoting [6],

$$A\Pi = Q \begin{pmatrix} R \\ 0 \end{pmatrix}, \quad |r_{ii}| \ge \sum_{k=i}^{j} r_{kj}^2, \quad 1 \le i < j \le n. \tag{2.7}$$

With careful implementation [16], the computed $\tilde{R}$ has the structure (2.7) up to small round-off. The index k can be determined, for example, by looking for a gap between two consecutive diagonals of $\tilde{R}$, i.e., $|\tilde{r}_{k+1,k+1}| \le \epsilon|\tilde{r}_{kk}|$. In that case, $\|\tilde{R}_{[22]}\|_2 \le \sqrt{n-k}\epsilon|\tilde{r}_{kk}|$. Further, with $D = \mathrm{diag}(\|\tilde{R}_{[11]}(i,:)\|_2)_{i=1}^{k}$, the condition number $\|T^{-1}\|_2$ in Theorem 2.3 is usually smaller than $O(k)$. (Its theoretical upper bound contains 2^k factor, and it is attained at the Kahan matrix.) We refer to [14] for more details.

To conclude, in cases of low numerical rank, we can always use best available rank revealing QR factorization to reduce the dimension, if necessary with an additional LQ factorization, as described above.

3. A or A^T? If $A \in \mathbb{R}^{m\times n}$ with $m > n$, then the QR factorization of A is an efficient preprocessor and preconditioner for the Jacobi algorithm. If $m < n$, then we start with the QR factorization of A^T. But what if A is a square nonsingular $n \times n$ matrix? For example, let $A = DQ$, where D is diagonal and Q is orthogonal. In that case working with A is implicit diagonalization of $A^TA = Q^TD^2Q$, while taking A^T implicitly diagonalizes diagonal matrix $AA^T = D^2$. For a nonnormal A, a better choice between A^TA and AA^T has a smaller off-diagonal part and the diagonals reveal the spectrum in the sense that their distribution reveals the distribution of the spectrum as closely as possible. This desirable spectrum revealing property implies that we prefer A with less equilibrated column norms. Otherwise, the effect of preconditioning is weaker, and larger angles of Jacobi rotations are more likely to appear during the process, thus causing slower convergence. In an efficient computation, the decision "A or A^T" has to be based on at most $O(n^2)$ flops. This complexity corresponds to computing the diagonal entries of $H = A^TA$ and $M = AA^T$.

Let $s^2(H) = \sum_{i=1}^{n} h_{ii}^2 = \mathrm{Trace}(H \circ H)$, $s^2(M) = \mathrm{Trace}(M \circ M)$. (Here $\circ$ denotes the Hadamard matrix product.) Since H and M are orthogonally similar,

$\|H\|_F = \|M\|_F$, a larger value ($s^2(H)$ or $s^2(M)$) implies smaller corresponding off-norm $\Omega(H)$ or $\Omega(M)$. In fact, $s^2(\cdot)$ attains its maximum over the set of matrices orthogonally similar to H only at diagonal matrices. In the standard symmetric Jacobi algorithm the value of $\frac{\Omega^2(H)}{\|H\|_F^2} = 1 - \frac{\mathrm{Trace}(H\circ H)}{\mathrm{Trace}(HH)} = 1 - \frac{s^2(H)}{\|H\|_F^2}$ is used to measure numerical convergence. Hence, $s^2(\cdot)$ is one possible choice for the decision between A and A^T, but with respect to the standard matrix off-norm. Note, however, that in floating point computation $s^2(\cdot)$ may ignore tiny diagonal entries, and that it does not provide any information about the distributions of the diagonal entries of H and M. The latter is crucial for the success of both the preconditioner and the Jacobi iterations. In the next section we address that issue by a novel application of well-known tools.[2]

3.1. Entropy of the diagonal of the adjoint orbit. Let $H = H^T$ be positive semidefinite. From the spectral decomposition $H = U\Lambda U^T$, $h_{ii} = \sum_{j=1}^n |u_{ij}|^2\lambda_j$, $i = 1, \ldots, n$. If we define vectors $d(H) = (\, h_{11}, \ldots, h_{nn}\,)^T$, $\lambda(H) = (\, \lambda_1, \ldots, \lambda_n\,)^T$, then $d(H) = (U \circ U)\lambda(H)$, where the matrix $S = U \circ U$ is doubly stochastic, in fact, orthostochastic. Thus, $d(H)$ is majorized by $\lambda(H)$ ($d(H) \prec \lambda(H)$), which is known as the Schur theorem; see, e.g., [3]. If we use normalization[3] by the trace,

$$\frac{d(H)}{\mathrm{Trace}(H)} = S\frac{\lambda(H)}{\mathrm{Trace}(H)}, \text{ and define } d'(H) = \frac{d(H)}{\mathrm{Trace}(H)}, \ \lambda'(H) = \frac{\lambda(H)}{\mathrm{Trace}(H)},$$

then $d'(H)$ and $\lambda'(H)$ are two finite probability distributions connected by the doubly stochastic matrix S. Thus, $d'(H)$ has larger entropy than $\lambda'(H)$. Recall that for a probability distribution $p = (\, p_1, \ldots, p_n\,)^T$ ($p_i \geq 0$, $\sum_i p_i = 1$) the entropy of p is $\eta(p) = -\frac{1}{\log n}\sum_{i=1}^n p_i \log p_i \in [0, 1]$. For any doubly stochastic matrix S we have $\eta(Sp) \geq \eta(p)$ with the equality if and only if S is a permutation matrix. The entropy is a symmetric concave function on the compact and convex set of finite probability distributions. It is maximal, $\eta(p) = 1$, if and only if $p_i = 1/n$ for all i. Also, $\eta(p) = 0$ if and only if the probability distribution degenerates to $p_k = 1$, $p_i = 0$, $i \neq k$.

Definition 3.1. *The d-entropy of positive semidefinite H is defined as the entropy of its diagonal normalized by the trace, $\eta_d(H) \equiv \eta(d'(H))$.*

Proposition 3.2. *The d-entropy η_d is strictly positive on the open cone of positive definite matrices. It always attains its maximum 1 on the real adjoint orbit $\mathcal{O}(H) = \{W^THW : W \ \ orthogonal\}$. Further, it holds $\eta_d(\mathcal{O}(H)) = \{1\}$ if and only if H is a scalar ($H = scalar \cdot I$). If H has s different eigenvalues with multiplicities $n_1, \ldots, n_s$, then η_d attains its minimal value on $\mathcal{O}(H)$ at each of $\frac{n!}{\prod_{i=1}^s n_i!}$ different diagonal matrices in $\mathcal{O}(H)$, and nowhere else.*

Proof. There always exists an orthogonal W such that W^THW has constant diagonal. The fact that the entropy $\eta_d(\cdot)$ of the diagonal of H is larger than the entropy of the vector of the eigenvalues holds for any symmetric concave function. To see that, recall the relation $d'(H) = S\lambda'(H)$, where S is doubly stochastic. By the Birkhoff theorem [3, Theorem II.2.3], S is from the convex hull of permutation matrices, thus $S = \sum_k \alpha_k P_k$, where the P_k's are permutation matrices and the α_k's are nonnegative with sum one. Thus, $d'(H)$ belongs to the convex polyhedral set spanned by permutations of the vector $\lambda'(H)$. Hence, a concave function on $d'(H)$

[2] For the sake of brevity, we will just illustrate the main idea and leave the details for a forthcoming paper.

[3] By definition, $0/0 = 0$ and $0 \log 0 = 0$.

cannot have smaller value than its minimal value on the vectors $P_k\lambda'(H)$. Note that the number of minimal points represents the number of possible affiliations of n diagonal entries with s different eigenvalues. ∎

Example 3.1. The following example illustrates the preceding discussion on the relation between the entropy and the spectral information along the diagonal of the matrix. Let A be the upper triangular factor from the QR factorization of the 4×4 Hilbert matrix, and let $H = A^TA$, $M = AA^T$. The $d(H)$, $\lambda(H)$, and $d(M)$ are

$$\begin{aligned} h_{11} &\approx 1.4236e{+}00, \quad h_{22} \approx 4.6361e{-}01, \quad h_{33} \approx 2.4138e{-}01, \quad h_{44} \approx 1.5068e{-}01, \\ \lambda_1 &\approx 2.2506e{+}00, \quad \lambda_2 \approx 2.8608e{-}02, \quad \lambda_3 \approx 4.5404e{-}05, \quad \lambda_4 \approx 9.3513e{-}09, \\ m_{11} &\approx 2.2355e{+}00, \quad m_{22} \approx 4.3655e{-}02, \quad m_{33} \approx 1.3022e{-}04, \quad m_{44} \approx 3.5308e{-}08. \end{aligned}$$

If we look at only the diagonal entries of the matrix, we cannot say how close the diagonal is to the spectrum. After all, the matrix can be diagonal, that is, with minimum entropy in its orbit, and we cannot detect that. But if we have the diagonals of two orthogonally similar matrices, then we see the difference between the two diagonals. If we compute the entropies, $\eta_d(H) \approx 7.788e-001 > \eta_d(M) \approx 8.678e-002$.

Remark 3.1. Just looking at $d(H)$ and $d(M)$ in Example 3.1 and knowing that they are diagonals of unitarily similar matrices is enough to choose $d(M)$ as a better approximation of the spectrum since if H were close to diagonal, then $\kappa_2(H)$ would be $O(1)$, while $\kappa_2(M) \geq 10^8$. In other words, orthogonal similarity can hide the high spectral condition number of diagonal matrix (so that it is not seen on the diagonal of the similar matrix), but it cannot produce it starting from a well-conditioned, almost diagonal matrix. In some sense, with respect to the problem of guessing the spectrum, the diagonal of M has less uncertainty than the diagonal of H. Our algorithm can better utilize diagonals with a smaller entropy.

4. The algorithm. We now describe the new preconditioned Jacobi SVD algorithm with rank revealing QR factorization as preconditioner. At this point we do not consider the details of the application of the one-sided Jacobi rotations to triangular matrix. Instead, we use triangular Jacobi SVD as a black box and give the details in [18]. On input to the black box we have triangular nonsingular matrix X, and the box computes $X_\infty = XV_x$, where $X_\infty = U_x\Sigma$, $X = U_x\Sigma V_x^T$ is the SVD of X, and V_x is the product of the Jacobi rotations. If V_x is not computed, we write $X_\infty = X\,\langle V_x\rangle$. We keep this notation in other situations as well. If in a relation some matrix is enclosed in $\langle\cdot\rangle$, then that matrix is not computed and no information about it is stored. For example, $A = \langle Q\rangle\,(\,R^T \quad 0\,)^T$ means computing only R in the QR factorization of A.

4.1. Computing only Σ. We first describe the algorithm for computing only the singular values of A. In Algorithm 1 we use two QR factorizations with pivoting and then apply the one-sided Jacobi SVD algorithm. We do not specify which rank revealing QR factorization is used—the rule is to use the best available; see, e.g., [5], [4]. In some cases, the rows of A can be sorted to get more structured backward error; see section 5.3.

Remark 4.1. The pivoting in the second QR factorization is optional, and $P_1 = I$ works well. If efficient QR factorization with local pivoting is available, it can be used to compute R_1. If $\max_{i=2:n} \|R(1:i-1,i)\|_2/|r_{ii}| \leq O(n)\boldsymbol{\varepsilon}$, then the columns of A are nearly orthogonal, and the second QR factorization is unnecessary, $X = R^T$.

Algorithm 1 $\sigma = SVD(A)$.

$(P_r A)P = \langle Q \rangle \begin{pmatrix} R \\ 0 \end{pmatrix}$; $\rho = \mathrm{rank}(R)$; [optional deflation, section 2.2][optional P_r, section 5.3]
$R(1:\rho, 1:n)^T P_1 = \langle Q_1 \rangle R_1$; $X = R_1^T$; [optional pivoting P_1]
$X_\infty = X \langle V_x \rangle$; {Use section 5.4 for sharp stopping criterion.}
$\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, \rho$; $\boxed{\sigma = (\sigma_1, \ldots, \sigma_\rho, 0, \ldots, 0)}$.

Algorithm 2 $(\sigma, V) = SVD(A)$.

$(P_r A)P = \langle Q \rangle \begin{pmatrix} R \\ 0 \end{pmatrix}$; $\rho = \mathrm{rank}(R)$; [optional deflation, section 2.2][optional P_r, section 5.3]
$X = R(1:\rho, 1:n)^T$; $X_\infty = X \langle V_x \rangle$;
$\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, \rho$; $\boxed{\sigma = (\sigma_1, \ldots, \sigma_\rho, 0, \ldots, 0)}$;
$U_x(:,i) = \dfrac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, \rho$; $\boxed{V = PU_x}$.

4.2. Computing Σ and V. If we need the singular values and the right singular vectors, a direct application of Jacobi rotations to A or R requires the accumulated product of rotations to construct the right singular vector matrix V. To avoid the explicit multiplication of Jacobi rotations, in this case we use Algorithm 2. The beauty of the preconditioning $R \rightsquigarrow R^T$ in Algorithm 2 is in the fact that the set of the right singular vectors is computed without the product of the Jacobi rotations, and at the same time, due to preconditioning, fewer rotations are needed to reach the numerical convergence. If $\rho \ll n$, an additional LQ factorization of $R(1:\rho, 1:n)$ is advisable. In that case, the accumulation of rotations can be avoided, as described in section 4.4.2.

4.3. Computing Σ and U. If Σ and U are needed and if we apply the Jacobi SVD on $X = A$ or $X = R$, then we do not need the product of Jacobi rotations. The problem is that in the case $m \gg n$ the rotations on A are too expensive, and that in both cases (A or R) the convergence is slower than in the case $X = R^T$.

In the case $X = R^T$, we need the accumulated product of the Jacobi rotations, and the cost of the product of only one sweep of fast rotations is $2n\rho(\rho - 1) = 2n\rho^2 - 2n\rho$. To this we should also add the cost of heavier memory traffic and increased cache miss probability because two square arrays are transformed. All this is avoided by an extra QR factorization followed by transposition of the triangular factor, which is computed in $2n\rho^2 - 2\rho^3/3$ flops on BLAS 3 level.

In some cases $X = A$ is the perfect choice. For instance, if H is a symmetric positive definite matrix and $P^T H P = AA^T$ its pivoted Cholesky factorization with lower triangular matrix A, then A^T has the same properties as R in (2.7). Thus $A \langle V \rangle = U\Sigma$ will be an efficient Jacobi SVD and, since $H = (PU)\Sigma^2(PU)^T$, we obtain the spectral decomposition of H without computing V.

In Algorithm 3 we define for a matrix M its property $\tau(M)$ to be *true* if M is of full column rank and the Jacobi SVD algorithm applied to M converges quickly. For instance, if A is the Cholesky factor of positive definite matrix, computed with pivoting, then $\tau(A) = true$. If evaluation of $\tau(A)$ requires more than $O(mn)$ flops, or if we do not know how to judge A, then by definition $\tau(A) = false$.

Algorithm 3 $(\sigma, U) = SVD(A)$.

if $\tau(A)$ **then** {e.g., A computed by pivoted Cholesky factorization, $P^T H P = AA^T$}
  $X = A$; $X_\infty = X \langle V_x \rangle$;
  $\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, n$; $\boxed{\sigma = (\sigma_1, \ldots, \sigma_n)}$;
  $\boxed{U(:,i) = \frac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, n}$;
else
  $(P_r A)P = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$; $\rho = \mathrm{rank}(R)$; [optional deflation, section 2.2][optional P_r, section 5.3]
  if $\tau(R)$ **then** {e.g., $\max_{i=2:n} \|R(1:i-1,i)\|_2 / |r_{ii}|$ small}
    $X = R$; $X_\infty = X \langle V_x \rangle$;
    $\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, \rho$; $\boxed{\sigma = (\sigma_1, \ldots, \sigma_\rho, 0, \ldots, 0)}$;
    $U_x(:,i) = \frac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, \rho$; $\boxed{U = P_r^T Q \begin{pmatrix} U_x \\ 0_{(m-\rho)\times\rho} \end{pmatrix}}$;
  else
    $R(1:\rho, 1:n)^T P_1 = \langle Q_1 \rangle R_1$; [optional pivoting P_1]
    $X = R_1^T$; $X_\infty = X \langle V_x \rangle$;
    $\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, \rho$; $\boxed{\sigma = (\sigma_1, \ldots, \sigma_\rho, 0, \ldots, 0)}$;
    $U_x(:,i) = \frac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, \rho$; $\boxed{U = P_r^T Q \begin{pmatrix} P_1 U_x \\ 0_{(m-\rho)\times\rho} \end{pmatrix}}$;
  end if
end if

4.4. Computation of U, Σ, and V. In this section we describe an efficient implementation of the preconditioned Jacobi SVD algorithm for computing the full SVD. The classical implementation of the Jacobi SVD algorithm transforms two matrices, one approaching the matrix of the left singular vectors scaled by the corresponding singular values ($U\Sigma$), and the second being the accumulated product of the Jacobi rotations (V). We extend an idea from [14] and compute the product of Jacobi rotations a posteriori from a well-conditioned matrix equation. In this way, the expensive iterative part has fewer flops and needs less cache space. The rotations are explicitly accumulated only if none of four candidate matrix equations can guarantee an accurate solution.

4.4.1. Classical computation of V by accumulation. Let the Jacobi iterations stop at index $\overline{k}$ and let $\tilde{X}_\infty = \tilde{X}^{(\overline{k})}$. Let $\tilde{V}_x$ be the computed accumulated product of Jacobi rotations used to compute $\tilde{X}_\infty$. Rowwise backward stability implies that $\tilde{X}_\infty = (X + \delta X)\hat{V}_x$, where $\hat{V}_x$ is orthogonal, and $\|\delta X(i,:)\|_2 \leq \epsilon_J \|X(i,:)\|_2$, $\epsilon_J \leq O(n\boldsymbol{\varepsilon})$; see [13]. The matrix $\tilde{V}_x$ can be written as $\tilde{V}_x = (I + E_0)\hat{V}_x$, where $\|E_0\|_2$ is small. In fact, $\max_i \|E_0(i,:)\|_2 \leq \varepsilon_J$. Note that the matrix $\hat{V}_x$ is a purely theoretical entity—it exists only in the proof of the backward stability. If we want to recover $\hat{V}_x$, the best we can do is to compute

$$X^{-1}\tilde{X}_\infty = (I + E_1)\hat{V}_x, \quad E_1 = X^{-1}\delta X, \tag{4.1}$$

since we do not have δX. Thus, we can come $\|E_1\|_2$ close to $\hat{V}_x$. To estimate E_1, we write $X = DY$, where D is diagonal scaling, $D_{ii} = \|X(i,:)\|_2$, and Y has unit rows in the Euclidean norm. We obtain for $\|\cdot\| \in \{\|\cdot\|_2, \|\cdot\|_F\}$

$$\|E_1\| \leq \|Y^{-1}\|_2 \|D^{-1}\delta X\| \leq \|Y^{-1}\|_2 \sqrt{n}\epsilon_J \leq \|Y^{-1}\|_2 O(n^{3/2})\boldsymbol{\varepsilon}. \tag{4.2}$$

Finally, the matrix $\tilde{X}_\infty$ is written as $\tilde{U}_x\tilde{\Sigma}$. The diagonal entries of $\tilde{\Sigma}$ are computed as $\tilde{\Sigma}_{ii} = \tilde{\sigma}_i = \mathit{computed}(\|\tilde{X}_\infty(:,i)\|_2) = \|\tilde{X}_\infty(:,i)\|_2(1+\nu_i)$, $|\nu_i| \leq O(n\boldsymbol{\varepsilon})$, and then $\tilde{U}_x(:,i)$ is computed by dividing $\tilde{X}_\infty(:,i)$ by $\tilde{\sigma}_i$. Thus,

$$\tilde{U}_x\tilde{\Sigma} = \tilde{X}_\infty + \delta\tilde{X}_\infty, \quad |\delta\tilde{X}_\infty| \leq \boldsymbol{\varepsilon}|\tilde{X}_\infty|. \tag{4.3}$$

If $\tilde{\sigma}_i$ is computed using a double accumulated dot product, then $|\nu_i| \leq O(\boldsymbol{\varepsilon})$ and the columns of $\tilde{U}_x$ are of unit norm up to $O(\boldsymbol{\varepsilon})$. The following proposition explains how well the computed SVD resembles the matrix X.

PROPOSITION 4.1. *The matrices $\tilde{U}_x$, $\tilde{\Sigma}$, $\tilde{V}_x$, $\hat{V}_x$ satisfy residual relations*

$$\text{(i)} \quad \tilde{U}_x\tilde{\Sigma}\hat{V}_x^T = X + F = X(I + X^{-1}F); \quad \text{(ii)} \quad \tilde{U}_x\tilde{\Sigma}\tilde{V}_x^T = (X+F)(I+E_0^T),$$

where for all i, $\|F(i,:)\|_2 \leq \overline{\varepsilon_J}\|X(i,:)\|_2$, $\overline{\varepsilon_J} = \varepsilon_J + \boldsymbol{\varepsilon}(1+\varepsilon_J)$. Further, $\|E_0\|_2 \leq \sqrt{n}\varepsilon_J \leq O(n^{3/2}\boldsymbol{\varepsilon})$, and $\|X^{-1}F\|_2 \leq \|Y^{-1}\|_2\sqrt{n}\overline{\varepsilon_J}$.

Proof. From the relations $\tilde{X}_\infty = (X+\delta X)\hat{V}_x$ and (4.3) we obtain $\tilde{U}_x\tilde{\Sigma}\hat{V}_x^T = X+F$, $F = \delta X + \delta\tilde{X}_\infty\hat{V}_x^T$, and for (ii) we use $\tilde{V}_x = (I+E_0)\hat{V}_x$. ∎

4.4.2. Computation of V from matrix equation. Suppose that, instead of $\tilde{V}_x$, we decide to use some other approximation of $\hat{V}_x$. The matrix $X^{-1}\tilde{X}_\infty$ is a good candidate (it gets $\|E_1\|_2$ close to $\hat{V}_x$), but we cannot have the exact value of $X^{-1}\tilde{X}_\infty$. We can solve the matrix equation and take $\breve{V}_x = \mathit{computed}(X^{-1}\tilde{X}_\infty)$. Since X is triangular, the residual bound for $\breve{V}_x$ is

$$E_2 = X\breve{V}_x - \tilde{X}_\infty, \quad |E_2| \leq \epsilon_T|X||\breve{V}_x|, \quad \epsilon_T \leq \frac{n\boldsymbol{\varepsilon}}{1-n\boldsymbol{\varepsilon}}. \tag{4.4}$$

From (4.1) and (4.4) we conclude that

$$\breve{V}_x = (I+E_3)\hat{V}_x = \hat{V}_x(I + \hat{V}_x^T E_3 \hat{V}_x), \quad E_3 = E_1 + X^{-1}E_2\hat{V}_x^T, \tag{4.5}$$

where only the symmetric part $Sym(E_3) = 0.5(E_3 + E_3^T)$ contributes to the first order departure from orthogonality of $\breve{V}_x$, $\|\breve{V}_x^T\breve{V}_x - I\|_2 \leq 2\|Sym(E_3)\|_2 + \|E_3\|_2^2$.

The following proposition shows that we have also computed a rank revealing decomposition of X (in the sense of [10]).

PROPOSITION 4.2. *The matrices $\tilde{U}_x$, $\tilde{\Sigma}$, $\breve{V}_x$ satisfy the residual relations*

$$\tilde{U}_x\tilde{\Sigma}\breve{V}_x^T = (X+F)(I+E_3^T), \quad E_3 = E_1 + X^{-1}E_2\hat{V}_x^T; \tag{4.6}$$

$$\tilde{U}_x\tilde{\Sigma}\breve{V}_x^{-1} = X + F_1, \quad F_1 = E_2\breve{V}_x^{-1} + \delta\tilde{X}_\infty\breve{V}_x^{-1}, \tag{4.7}$$

where F is as in Proposition 4.1, *$\|E_3\|_2 \leq \|Y^{-1}\|_2(\sqrt{n}\varepsilon_J + n\epsilon_T)$, and it holds for all i that $\|F_1(i,:)\|_2 \leq (\varepsilon_T\||\breve{V}_x|\|_2 + \boldsymbol{\varepsilon}(1+\varepsilon_J))\|\breve{V}_x^{-1}\|_2\|X(i,:)\|_2$.*

This analysis shows that the quality of the computed right singular vector matrix $\breve{V}_x$ depends on the condition number $\|Y^{-1}\|_2$, where $X = DY$. Hence, the rows of the triangular matrix X must be well-conditioned in the scaled sense. If X is computed from the initial A using the QR factorization with column pivoting, $AP = Q\,(\,R^T \quad 0\,)^T$, then $X = R$ can be written as $X = DY$ with well-conditioned Y.

Thus, we expect that $\breve{V}_x$ can be computed accurately, but immediately notice a drawback. The Jacobi rotations implicitly transform the matrix $P^T(A^TA)P$, which means that we do not have the preconditioning effect—for that the input matrix to Jacobi procedure should be $X^T = Y^TD$.

We conclude that the initial matrix should be of the form $X = DY = ZC$, where D, C are diagonal and both Y and Z are well-conditioned. Well-conditioned Z implies fast convergence, while well-conditioned Y ensures stable a posteriori computation of the right singular vectors. Therefore, we define X in the following way:

(i) $AP = Q\,(\,R^T \quad 0\,)^T$;
(ii) $R^TP_1 = Q_1R_1$;
(iii) $X = R_1^T$.

The matrix R can be written as $R = D_rR_r$ with well-conditioned R_r, and if we write $R_1 = (R_1)_c(D_1)_c$, then $\kappa((R_1)_c) = \kappa(R_r)$; thus $X = DY$ with $D = (D_1)_c$, $Y = (R_1)_c^T$. Further, $R_1 = (D_1)_r(R_1)_r$ with the expected value of $\kappa((R_1)_r)$ smaller than $\kappa((R_1)_c)$, and thus $X = ZD_c$ with well-conditioned Z. In fact, Z^TZ is very strongly diagonally dominant. We have strong numerical evidence that the pivoting in the second QR factorization is not worth the overhead. If we have an efficient QR factorization with local pivoting, such overhead is negligible. Note that $X = R_1$ also has the required properties. Without column pivoting in the second QR factorization ($P_1 = I$) we cannot give any theoretical bound on the condition number of Y, and condition estimators must be used. Putting all of this together, we obtain Algorithm 4.

Since the key matrices in the algorithm are all triangular, condition estimators can be used to control the program flow. We can decide which matrix is the best input to the one-sided Jacobi algorithm, or which matrix equation to solve. For instance, in the case $\rho = n$ and small κ_1, the SVD $R_1^T = U_x\Sigma V_x^T$ implies $V_x = R_1^{-T}(U_x\Sigma)$, but we also note that $R(Q_1V_x) = (U_x\Sigma)$. It can be shown (as in section 4.4.2) that computing $W = Q_1V_x$ very efficiently as $R^{-1}X_\infty$ is numerically as accurate as first computing $V_x = R_1^{-T}X_\infty$ and then multiplying Q_1V_x. (Similar situations occur in the case of well-conditioned Y and $X = L_2$, where $Q_2^TV_x$ is computed directly as $R_1^{-1}X_\infty$.) Since in each major step we have estimates of relevant condition number (of scaled matrices), the algorithm can be authorized (an input option) to drop some small singular values if the condition number test shows that they are highly sensitive.

The last line of defense in Algorithm 4 computes with explicit accumulation of Jacobi rotations. So far, we know of no example in which accumulation of Jacobi rotation is needed, because the previous three preconditioning steps failed to produce X, which is structured as $X = DY$ with moderate $\|Y^{-1}\|_2$. In fact, we never had the case that required $X = L_2^T$. The worst-case example, which probably already has crossed the reader's mind, is Kahan's matrix [26].

Example 4.1. It is instructive to see how our algorithm deals with the upper triangular Kahan's matrix $K = K(m, c)$ with $K_{ii} = s^{i-1}$ and $K_{ij} = -c\cdot s^{i-1}$ for $i < j$, where $s^2 + c^2 = 1$. Using MATLAB, we generate $K(100, 0.9998)$. It is estimated that $\kappa_1 \approx \|R_r^{-1}\|$ is bigger than 10^{16}. Now, the trick here is that our entropy test will transpose the matrix automatically and take $A = K^T$ instead of $A = K$. In that case the estimated κ_1 is around one. Suppose now that the transposing mechanism is switched off, or that, e.g., $A = K(1 : m, 1 : n)$, $n < m$, so that no transposition is allowed. Let A be equal to the first 90 columns of K. Again, $\kappa_1 > 10^{16}$, but $\kappa_Y \approx 1$.

5. Assessing the accuracy of the computed SVD. In this section we analyze numerical properties of the new algorithm. To simplify the notation, we drop the permutation matrices, thus assuming that A is replaced with the permuted matrix

Algorithm 4 $(U, \sigma, V) = \mathrm{SVD}(A)$.

$(P_r A)P = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$; $\rho = \mathrm{rank}(R)$; [optional deflation, section 2.2][optional P_r, section 5.3]

if $\max_{i=2:n} \|R(1:i-1,i)\|/|r_{ii}|$ small **then** {columns of A almost orthogonal}

$X = R$; $\boxed{\kappa_0 = estimate(\|A_c^{\dagger}\|_2)}$; {At this point, $\kappa_0 \ll n$. $A^T A$ is γ-s.d.d.}

$X_\infty = X \langle V_x \rangle$; $V_x = R^{-1} X_\infty$; $\boxed{\sigma_i = \|X_\infty(:,i)\|_2, \quad i = 1, \ldots, n}$; $\boxed{V = PV_x}$;

$U_x(:,i) = \dfrac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, n$; $\boxed{U = P_r^T Q \begin{pmatrix} U_x & 0 \\ 0 & I_{m-n} \end{pmatrix}}$;

else

$\boxed{\kappa_0 = estimate(\|A_c^{\dagger}\|_2)}$; $\kappa_1 = estimate(\|R_r^{\dagger}\|_2)$;

if κ_1 small **then** {e.g., κ_1 small $\Longleftrightarrow \kappa_1 < \sqrt{n}$, or, e.g., $\kappa_1 < n$}

$R(1:\rho, 1:n)^T = Q_1 \begin{pmatrix} R_1 \\ 0 \end{pmatrix}$ {second preconditioning}; $X = R_1^T$;

else

$R(1:\rho, 1:n)^T P_1 = Q_1 \begin{pmatrix} R_1 \\ 0 \end{pmatrix}$ {second preconditioning};

$R_1 = L_2 \langle Q_2 \rangle$ {third preconditioning: LQ factorization}; $X = L_2$;

$\kappa_Y = estimate(\|Y^{-1}\|_2)$; **if** $\kappa_Y \geq n$ **then** $\kappa_Z = estimate(\|Z^{-1}\|_2)$; **end if**

end if

if Y well conditioned **then**

$X_\infty = X \langle V_x \rangle$; $\boxed{\sigma_i = \|X_\infty(:,i)\|_2}$; $U_x(:,i) = \dfrac{1}{\sigma_i} X_\infty(:,i), \quad i = 1, \ldots, \rho$;

if $\rho = n$ and κ_1 small **then**

$W = R^{-1} X_\infty$; {here $W \equiv Q_1 V_x$}; $\boxed{V = PW}$; $\boxed{U = P_r^T Q \begin{pmatrix} U_x & 0 \\ 0 & I_{m-\rho} \end{pmatrix}}$;

else if κ_1 small **then** {R rectangular, $\rho < n$}

$V_x = R_1^{-T} X_\infty$; $\boxed{V = PQ_1 \begin{pmatrix} V_x & 0 \\ 0 & I_{n-\rho} \end{pmatrix}}$; $\boxed{U = P_r^T Q \begin{pmatrix} U_x & 0 \\ 0 & I_{m-\rho} \end{pmatrix}}$;

else {here $X = L_2$ and $W \equiv Q_2^T V_x$}

$W = R_1^{-1} X_\infty$; $\boxed{V = PQ_1 \begin{pmatrix} U_x & 0 \\ 0 & I_{n-\rho} \end{pmatrix}}$; $\boxed{U = P_r^T Q \begin{pmatrix} P_1 W & 0 \\ 0 & I_{m-\rho} \end{pmatrix}}$;

end if

else if $\kappa_Z < n$ **then**

$X = L_2^T$; $X_\infty = X \langle V_x \rangle$; $\boxed{\sigma_i = \|X_\infty(:,i)\|_2}$; $U_x(:,i) = \dfrac{1}{\sigma_i} X_\infty(:,i)$, $i = 1, \ldots, \rho$;

$V_x = L_2^{-T} X_\infty$; $\boxed{V = PQ_1 \begin{pmatrix} V_x & 0 \\ 0 & I_{n-\rho} \end{pmatrix}}$; $\boxed{U = P_r^T Q \begin{pmatrix} P_1 Q_2^T U_x & 0 \\ 0 & I_{m-\rho} \end{pmatrix}}$;

else {last line of defense: use $X = L_2$ and accumulate Jacobi rotations}

$X_\infty = XV_x$; $\boxed{\sigma_i = \|X_\infty(:,i)\|_2}$; $U_x(:,i) = \dfrac{1}{\sigma_i} X_\infty(:,i)$, $i = 1, \ldots, \rho$;

$\boxed{V = PQ_1 \begin{pmatrix} U_x & 0 \\ 0 & I_{n-\rho} \end{pmatrix}}$; $\boxed{U = P_r^T Q \begin{pmatrix} P_1 Q_2^T V_x & 0 \\ 0 & I_{m-\rho} \end{pmatrix}}$;

end if

end if

P_rAP. The computed matrices are marked by *tildes*, and by *hats* we denote matrices whose existence is obtained during backward error analysis (they are usually close to the corresponding matrices marked with tildes). We note that detailed analysis is given without the details of the triangular SVD computation $X_\infty = XV_x$. We only need the fact that the computed $\tilde{X}_\infty$, $\tilde{V}_x$ satisfy $\tilde{X}_\infty = (X + \delta X)\hat{V}_x$, where for all i $\|\delta X(i,:)\|_2 \le \varepsilon_J \|X(i,:)\|_2$, $\varepsilon_J \le O(n\boldsymbol{\varepsilon})$, and $\hat{V}_x$ is exactly orthogonal, close to $\tilde{V}_x$. This is independent of the pivot strategy. For the sake of brevity we will not analyze all variants of algorithms given in section 4.

5.1. Backward error analysis. The following proposition is central to the analysis of Algorithms 1 and 2. It gives backward stability with a rather strong columnwise estimate of the relative backward error.

PROPOSITION 5.1. *Let the SVD of the real $m \times n$ matrix A be computed by reducing A to triangular form, $A = Q\,(\,R^T \quad 0\,)^T$, and then applying the Jacobi SVD algorithm to $X = R^T$. If only the singular values or singular values and the right singular vectors are needed (Algorithms* 1 *or* 2*), then the backward stability of the computation can be described as follows:*

(i) *Let $X \approx \tilde{U}_x \tilde{\Sigma} \langle \tilde{V}_x^T \rangle$ be the computed SVD of the computed matrix X. Then there exist a columnwise small perturbation ΔA and orthogonal matrices $\hat{Q}$, $\hat{V}_x$ such that*

$$A + \Delta A = \hat{Q} \begin{pmatrix} \hat{V}_x & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix} \tilde{U}_x^T, \quad \textit{where} \tag{5.1}$$

$$\|\Delta A(:,i)\|_2 \le \tilde{\eta} \|A(:,i)\|_2, \;\; i = 1, \ldots, n, \;\; \tilde{\eta} = \varepsilon_{qr} + \overline{\varepsilon_J} + \varepsilon_{qr}\overline{\varepsilon_J}. \tag{5.2}$$

(ii) *Furthermore, let $\varepsilon_u \equiv \|\tilde{U}_x^T \tilde{U}_x - I\|_F < 1/2$. There exist a backward perturbation $\mathcal{E}$ and orthogonal matrix $\hat{U}$ such that $\|\tilde{U}_x - \hat{U}\|_F \le \sqrt{2}\varepsilon_u$ and the SVD of $A + \mathcal{E}$ is*

$$A + \mathcal{E} = \hat{Q} \begin{pmatrix} \hat{V}_x & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix} \hat{U} \equiv \hat{U}_a \begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix} \hat{V}_a^T, \quad \textit{where} \tag{5.3}$$

$$\|\mathcal{E}(:,i)\|_2 \le \hat{\eta} \|A(:,i)\|_2, \;\; \hat{\eta} = \tilde{\eta} + \sqrt{2n}\varepsilon_u + O(\boldsymbol{\varepsilon}^2) \quad \textit{for all } i. \tag{5.4}$$

Proof. Let $\tilde{Q}$ and $\tilde{R}$ be the computed numerically orthogonal and the triangular factor of A, respectively. Then there exist an orthogonal matrix $\hat{Q}$ and backward perturbation δA such that $A + \delta A = \hat{Q}\,(\,\tilde{R}^T \quad 0\,)^T$, where for all column indices $\|\delta A(:,i)\|_2 \le \varepsilon_{qr} \|A(:,i)\|_2$. Let the one-sided Jacobi SVD be applied to $X = \tilde{R}^T$. By Proposition 4.1, $X + F = \tilde{U}_x \tilde{\Sigma} \hat{V}_x^T$, $\|F(i,:)\|_2 \le \overline{\varepsilon_J} \|X(i,:)\|_2$, and therefore

$$A + \delta A + \hat{Q} \begin{pmatrix} F^T \\ 0 \end{pmatrix} = \hat{Q} \begin{pmatrix} \hat{V}_x & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix} \tilde{U}_x^T, \;\; \Delta A = \delta A + \hat{Q} \begin{pmatrix} F^T \\ 0 \end{pmatrix}, \tag{5.5}$$

where $\|\Delta A(:,i)\|_2 \le \varepsilon_{qr} \|A(:,i)\|_2 + \overline{\varepsilon_J} \|\tilde{R}(:,i)\|_2$, $\|\tilde{R}(:,i)\|_2 \le (1 + \varepsilon_{qr}) \|A(:,i)\|_2$, and (5.1), (5.2) follow. Note that the right-hand side of relation (5.1) is not an SVD. To obtain a relation with the SVD of a matrix in the vicinity of A, we need to replace $\tilde{U}_x$ with a nearby orthogonal matrix. However, since the backward error ΔA is columnwise small, we need to do this carefully and preserve this fine structure of the backward error. Since $\tilde{U}_x$ is on the right-hand side, correcting its departure from orthogonality implies certain linear combinations of the columns of $A + \Delta A$. If A has very large and very small columns, then such linear combinations may introduce large perturbations into the small ones. This is why we cannot use the orthogonal polar

factor of $\tilde{U}_x$ as the closest orthogonal matrix. We proceed with the following thought experiment.

Let Π be a permutation matrix such that the columns of $A\Pi$ have decreasing Euclidean lengths.[4] Let $\Pi^T\tilde{U}_x = (I + G_0^T)\hat{U}_x$ be the RQ factorization of $\Pi^T\tilde{U}_x$, with lower triangular G_0 and orthogonal $\hat{U}_x$. Since $\tilde{U}_x$ is numerically orthogonal, we can nicely estimate G_0. First, $I + G_0$ is regular.

From the Cholesky factorization $(I + G_0)(I + G_0)^T = I + \hat{U}_x(\tilde{U}_x^T\tilde{U}_x - I)\hat{U}_x^T$, we conclude, using [17], that $\|G_0\|_F \leq \sqrt{2}\varepsilon_u$. Let $I + G = (I + G_0)^{-1}$. Obviously, G is lower triangular. Since $G = -G_0 + G_0^2(I + G_0)^{-1}$, it holds that $\|G\|_1 \leq \|G_0\|_1 + \|G_0\|_1^2/(1 - \|G_0\|_1)$. From (5.5) we obtain the SVD

$$(A + \Delta A)(I + \Pi G\Pi^T) = \hat{Q}\begin{pmatrix} \hat{V}_x & 0 \\ 0 & I \end{pmatrix}\begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix}(\Pi\hat{U}_x)^T. \tag{5.6}$$

Note that small $\|\Pi G\Pi^T\|_1 = \|G\|_1 \approx \|G_0\|_1$ does not automatically mean columnwise small backward perturbation in A. Let us estimate the columns of $A\Pi G\Pi^T$. Note that in the multiplication $A\Pi G$ each column of A gets a contribution only from columns that are smaller in norm, i.e., $A\Pi G(:,i) = \sum_{k=i}^n g_{ki}(A\Pi)(:,k)$, and thus $\|A\Pi G(:,i)\|_2 \leq \|G\|_1\|(A\Pi)(:,i)\|_2$. Since Π^T redistributes the columns back to the original order, we have $\|(A\Pi G\Pi^T)(:,i)\|_2 \leq \|G\|_1\|A(:,i)\|_2$.

Similarly, $\|(\Delta A\Pi G\Pi^T)(:,i)\|_2 \leq \tilde{\eta}\|G\|_1\|A(:,i)\|_2$. Note that from the relation $\tilde{U}_x = (I + \Pi G_0^T\Pi^T)(\Pi\hat{U}_x)$ we easily find that the matrix $\hat{U} = \Pi\hat{U}_x$ satisfies $\|\hat{U} - \tilde{U}_x\|_F \leq \|G_0\|_F$. Finally, note that (5.6) defines $\mathcal{E}$ in relation (5.3). ∎

Consider now the computation of the full SVD with a single preconditioning step.

PROPOSITION 5.2. *Let $A \approx \tilde{Q}\binom{\tilde{R}}{0}$ be the computed QR factorization of A. Let the computed SVD of $X = \tilde{R}^T$ be $X \approx \tilde{U}_x\tilde{\Sigma}\overline{V}_x$, where the following hold.*

(a) *$\overline{V}_x = \tilde{V}_x$ if $\overline{V}_x$ is computed as the accumulated product of Jacobi rotations (Proposition 4.1). In that case $\|\overline{V}_x - \hat{V}_x\|_F \leq \sqrt{n}\varepsilon_J$.*

(b) *$\overline{V}_x = \tilde{V}_x$ if $\overline{V}_x$ is computed from the triangular matrix equation (Proposition 4.2). In that case $\|\overline{V}_x - \hat{V}_x\|_F \leq \|Y^{-1}\|_2(\sqrt{n}\varepsilon_J + n\varepsilon_T)$, where $Y = \mathrm{diag}(1/\|X(i,:)\|_2)X$.*

Let $\tilde{V}_a = \tilde{U}_x$, $\hat{V}_a = \hat{U}$, where $\hat{U}$ is as in Proposition 5.1 and let

$$\hat{U}_a = \hat{Q}\begin{pmatrix} \hat{V}_x & 0 \\ 0 & I \end{pmatrix}, \quad \tilde{U}_a = \textit{computed}\left(\tilde{Q}\begin{pmatrix} \overline{V}_x & 0 \\ 0 & I \end{pmatrix}\right).$$

Then $\|\tilde{U}_a - \hat{U}_a\|_2 \leq \sqrt{m}\varepsilon_{qr} + \|\overline{V}_x - \hat{V}_x\|_2 + O(\boldsymbol{\varepsilon}^2)$, $\|\tilde{V}_a - \hat{V}_a\|_F \leq \sqrt{2}\varepsilon_u$, and the residual (that is, the backward error)

$$\Delta' A = \tilde{U}_a\begin{pmatrix} \tilde{\Sigma} \\ 0 \end{pmatrix}\tilde{V}_a^T - A = (I + (\tilde{U}_a - \hat{U}_a)\hat{U}_a^T)(A + \Delta A) - A \tag{5.7}$$

satisfies $\|\Delta' A(:,i)\|_2 \leq \tilde{\eta}'\|A(:,i)\|_2$, $\tilde{\eta}' = \tilde{\eta} + \|\tilde{U}_a - \hat{U}_a\|_2 + \tilde{\eta}\|\tilde{U}_a - \hat{U}_a\|_2$.

Proof. In addition to the proof of Proposition 5.1, we need an estimate for $\tilde{U}_a - \hat{U}_a$. Note that $\tilde{U}_a$ is computed using Householder vectors computed in the QR factorization, and then replace $\overline{V}_x$ with $\hat{V}_x + (\overline{V}_x - \hat{V}_x)$. ∎

[4] One should keep in mind that Π is an object in our thought experiment, unrelated to actual pivoting in the algorithm.

5.2. Backward errors for two preconditionings. In the case $X = R^T$ all transformations are applied to A from the same side, $\binom{\Sigma}{0} U_x^T = (V_x^T \oplus I) Q^T A$. This fact is the key for columnwise small backward error. In the case of two QR factorizations in the preconditioning phase, where $X = R_1^T$, columnwise small backward error in A is not obvious, because in that case we compute ULV decomposition by transforming A from both sides.

THEOREM 5.3. *For the computed matrix $\tilde{X}_\infty \approx \tilde{U}_x \tilde{\Sigma}$, there exist backward perturbation ΔA, permutation $\tilde{P}_1$, and orthogonal $\hat{Q}$, $\hat{Q}_1$, $\hat{V}_x$, S such that*

$$\begin{pmatrix} \tilde{U}_x \tilde{\Sigma} \\ 0 \end{pmatrix} \approx \begin{pmatrix} \tilde{X}_\infty \\ 0 \end{pmatrix} = \begin{pmatrix} \tilde{P}_1^T & 0 \\ 0 & I_{m-n} \end{pmatrix} \hat{Q}^T (A + \Delta A) S \hat{Q}_1 \hat{V}_x^T. \tag{5.8}$$

For each i, $\Delta A(:,i)$ is a small relative perturbation of $A(:,i)$, and S is close to identity.

Proof. The second factorization $R^T P_1 = Q_1 R_1$ is computed as $(\tilde{R}^T + \delta\tilde{R}^T)\tilde{P}_1 = \hat{Q}_1 \tilde{R}_1$, where $\|\delta\tilde{R}(i,:)\|_2 \le \varepsilon_{qr} \|\tilde{R}(i,:)\|_2$. Jacobi rotations are applied to $X = \tilde{R}_1^T$, which yields $\tilde{X}_\infty = (X + \delta X)\hat{V}_x$, $\|\delta X(i,:)\|_2 \le \varepsilon_J \|X(i,:)\|_2$. This means that $\tilde{R}_1$ is changed backward to $\tilde{R}_1 + \delta\tilde{R}_1$ with columnwise bound $\|\delta\tilde{R}_1(:,i)\|_2 \le \varepsilon_J \|\tilde{R}_1(:,i)\|_2$. To push $\delta\tilde{R}_1$ further backward we have to change $\tilde{R}$. It is easy to check that $\Delta\tilde{R} = \delta\tilde{R} + \tilde{P}_1 \delta\tilde{R}_1^T \hat{Q}_1^T$ is a rowwise small perturbation of $\tilde{R}$ with the property

$$(\tilde{R}^T + \Delta\tilde{R}^T)\tilde{P}_1 = \hat{Q}_1 (\tilde{R}_1 + \delta\tilde{R}_1). \tag{5.9}$$

Write $\tilde{R} + \Delta\tilde{R} = \tilde{R}(I+E)$ with $E = \tilde{R}^{-1}\Delta\tilde{R}$, and let $\tilde{R} = D_r \tilde{R}_r$ with $D_r = \mathrm{diag}(\|\tilde{R}(i,:)\|_2)_{i=1}^n$. It is easily shown that $\|E\|_F \le \sqrt{n}(\varepsilon_{qr} + \varepsilon_J(1+\varepsilon_{qr}))\|\tilde{R}_r^{-1}\|_2$. Note that this bound depends on $\|\tilde{R}_r^{-1}\|_2$, which in our case is at most $O(n)$.

Let $\Delta A_0 = \delta A + \hat{Q} \begin{pmatrix} (\Delta\tilde{R})^T & 0 \end{pmatrix}^T$. Then we almost have the explicit backward relationship (5.8) with columnwise bound. The backward perturbed matrix is

$$A + \Delta_0 A = (A + \delta A)(I + E) \;\; (= (I + \delta A A^\dagger) A (I + E) \;\text{ if }\; \mathrm{rank}(A) = n). \tag{5.10}$$

Note that $I + E$ represents multiplicative backward perturbation, which immediately and cleanly exposes its corresponding forward error. However, additive backward perturbation might be more desirable and interpretable. Therefore, we are going to transform the multiplicative part into an additive one. If the columns of $A + \delta A$ are not ordered from large to small in the Euclidean norm, then we order them using permutation Π and write $(A + \delta A)(I + E) = (A + \delta A)\Pi(I + \Pi^T E \Pi)\Pi^T$.

If $I + \Pi^T E \Pi = L S_0$ is the LQ factorization, then we can write $L = I + F$ with lower triangular F and $\|F\|_F \le O(1)\|E\|_F$. The orthogonal matrix S_0 is close to identity. Then we have

$$(A + \delta A)(I + E) = (A + \delta A)\Pi(I + F) S_0 \Pi^T = ((A + \delta A)\Pi + (A + \delta A)\Pi F) S_0 \Pi^T,$$

where $\|((A + \delta A)\Pi F)(:,i)\|_2 \le \|F\|_1 \|((A + \delta A)\Pi)(:,i)\|_2$. If we permute the columns of $A + \delta A$ back to the original order, we obtain

$$A + \Delta A_0 = (A + \delta A)(I + E) = (A + \delta A + \delta_1 A)\Pi S_0 \Pi^T, \tag{5.11}$$

where $\|\delta_1 A(:,i)\|_2 \le (1 + \varepsilon_{qr}(A))\|F\|_1 \|A(:,i)\|_2$, $i = 1, \ldots, n$. Using this in (5.8), we conclude that $\tilde{U}_x \tilde{\Sigma}$ is computed by orthogonal transformations on $A + \delta A + \delta_1 A$, where the perturbation $\Delta A = \delta A + \delta_1 A$ is columnwise small, and $S = \Pi S_0 \Pi^T$. ∎

The practical value of this is that no matter how the columns of A are scaled, the algorithm computes the SVD of A with columnwise small backward relative error.

5.3. Complete pivoting and two-sided scaling. In [14], we recommended that the rows of A be sorted before the first QR factorization with column pivoting, thus having the effect of complete pivoting suggested by Powell and Reid [30]. The reason was more structured backward error, as shown in [9]. It is important that the whole algorithm preserves this structured perturbation.

THEOREM 5.4. *Let $A = D_1 C D_2$, where D_1, D_2 are diagonal matrices, be pre-pivoted so that the computed QR factorization satisfies*

$$D_1(C+\delta C)D_2 = \hat{Q}\begin{pmatrix}\tilde{R}\\ 0\end{pmatrix}, \quad \hat{Q}^T\hat{Q} = I_m. \tag{5.12}$$

Let $q = \max_{i\geq j} |(D_2)_{ii}/(D_2)_{jj}|$. There exists an orthogonal matrix S, close to identity, such that the backward perturbation in Theorem 5.3 can be written as

$$\begin{pmatrix}\tilde{U}_x\tilde{\Sigma}\\ 0\end{pmatrix} \approx \begin{pmatrix}\tilde{X}_\infty\\ 0\end{pmatrix} = \begin{pmatrix}\tilde{P}_1^T & 0\\ 0 & I_{m-n}\end{pmatrix}\hat{Q}^T D_1(C+\Delta C)D_2 S\hat{Q}_1\hat{V}_x^T. \tag{5.13}$$

It holds that $\|\Delta C\|_F \leq \|\delta C\|_F + q\sqrt{8}\|E\|_F(\|C\|_2 + \|\delta C\|_2) + O(\|E\|_F^2)$.

Proof. We go back to relation (5.10) and rewrite it as

$$A+\Delta A = (A+\delta A)(I+E) = D_1(C+\delta C)D_2(I+E). \tag{5.14}$$

If $I+E = (I+F)S$ is the LQ factorization, then $\|F\|_F \leq \sqrt{8}\|E\|_F + \sqrt{2}\|E\|_F^2$, provided that $\|E\|_F \leq 1/5$; see [17]. Further, $\|I-S\|_2 \leq \|E\|_2 + \|F\|_2$, and

$$A+\Delta A = D_1(C+\delta C)(I+F_1)D_2 S, \;\; F_1 = D_2 F D_2^{-1}, \;\; \|F_1\|_F \leq q\|F\|_F. \tag{5.15}$$

If we let $\Delta C = \delta C + CF_1 + \delta C F_1$, then using (5.8) we obtain (5.13). ∎

For SVD perturbation under this backward error with two-sided scaling we refer to [33], [9], [14], [10], [15], [24].

5.4. Forward relative errors in the computed SVD. Since the Jacobi SVD algorithm has columnwise small backward error, the condition number for the errors in the singular values of $A+\delta A = (I+\delta A A^\dagger)A$ is up to a $\sqrt{n}$ factor $\min_{D=\mathrm{diag}}\kappa_2(AD)$. This is in sharp contrast with bidiagonalization-based methods where the backward error has no columnwise structure and the condition number is $\kappa_2(A)$.

THEOREM 5.5. *Consider $A \in \mathbb{R}^{m\times n}$ with the SVD $A = U\left(\begin{smallmatrix}\Sigma\\ 0\end{smallmatrix}\right)V^T$ and singular values $\sigma_1 \geq \cdots \geq \sigma_n > 0$. Let $\tilde{\sigma}_1 \geq \cdots \geq \tilde{\sigma}_n$ be the singular values of the perturbed matrix $\tilde{A} = A+\delta A = (I+\Gamma)A$, $\Gamma = \delta A A^\dagger$, and let $\|\Gamma\|_2 < 1$.*

(i) *It holds that*

$$\max_{j=1:n}\frac{|\tilde{\sigma}_j - \sigma_j|}{\sqrt{\tilde{\sigma}_j\sigma_j}} \leq \|Sym(\Gamma)\|_2 + \frac{1}{2}\frac{\|\Gamma\|_2^2}{1-\|\Gamma\|_2} \leq \|\Gamma\|_2 + O(\|\Gamma\|_2^2). \tag{5.16}$$

(ii) *Let $I+\Xi = \mathrm{diag}(\|(I+\Gamma)U(:,i)\|_2)_{i=1}^n$, $\breve{U} = (I+\Gamma)U(I+\Xi)^{-1}$, $\breve{U}^T\breve{U} = I+\Omega$, and $\hat{\Omega} = \Omega(1:n,1:n)$. Let the singular values of $\tilde{A}$ be written with multiplicities as*

$$\tilde{\sigma}_1 = \cdots = \tilde{\sigma}_{\tilde{s}_1} > \tilde{\sigma}_{\tilde{s}_1+1} = \cdots = \tilde{\sigma}_{\tilde{s}_2} > \cdots > \tilde{\sigma}_{\tilde{s}_{\tilde{\ell}-1}+1} = \cdots = \tilde{\sigma}_{\tilde{s}_{\tilde{\ell}}}, \;\; \tilde{s}_{\tilde{\ell}} = n, \;\; \tilde{s}_0 \equiv 0,$$

and let the relative gaps be defined by $\tilde{\gamma}_i = \min_{j\neq i}\frac{|\tilde{\sigma}_{\tilde{s}_i}^2 - \tilde{\sigma}_{\tilde{s}_j}^2|}{\tilde{\sigma}_{\tilde{s}_i}^2 + \tilde{\sigma}_{\tilde{s}_j}^2}$, $i = 1,\ldots,\tilde{\ell}$, $\tilde{\gamma} = \min_i\tilde{\gamma}_i$. If $\|\hat{\Omega}\|_2 < \tilde{\gamma}/3$, then for all i and $\breve{\sigma}_j = \sigma_j\|(I+\Gamma)U(:,j)\|_2 = \sigma_j(1+\Xi_{jj})$

$$\sqrt{\sum_{j=\tilde{s}_{i-1}+1}^{\tilde{s}_i}\left|\frac{\tilde{\sigma}_{\tilde{s}_i} - \breve{\sigma}_j}{\breve{\sigma}_j}\right|^2} \leq \sqrt{\sum_{j=\tilde{s}_{i-1}+1}^{\tilde{s}_i}\left|1-\frac{\tilde{\sigma}_{\tilde{s}_i}^2}{\breve{\sigma}_j^2}\right|^2} \leq \frac{2}{\tilde{\gamma}_i}\|\hat{\Omega}\|_2^2.$$

In particular, $\max_{j=1:n} \frac{|\tilde\sigma_j-\breve\sigma_j|}{\breve\sigma_j} \le \frac{2}{\tilde\gamma}\|\hat\Omega\|_2^2$.

(iii) *For columnwise small* δA, $\|\Gamma\|_F \le \sqrt{n}\max_{i=1:n}(\|\delta A(:,i)\|_2/\|A(:,i)\|_2)\|A_c^\dagger\|_2$, *where* A_c *is obtained by scaling the columns of* A *to have unit norm.*

Proof. Since $I+\Gamma$ is nonsingular, we can use [27] and relation $(I+\Gamma)^{-1} = (I-\Gamma)+\Gamma^2(I+\Gamma)^{-1}$ to conclude that

$$\max_{1\le j\le n}\frac{|\tilde\sigma_j-\sigma_j|}{\sqrt{\tilde\sigma_j\sigma_j}} \le \frac{1}{2}\|(I+\Gamma)^{-1}-(I+\Gamma)^T\|_2 = \frac{1}{2}\|-2Sym(\Gamma)+\Gamma^2(I+\Gamma)^{-1}\|_2.$$

Relation (5.16) follows using the fact that $\|\Gamma\|_2<1$. Write

$$\tilde A = (I+\Gamma)U\begin{pmatrix}\Sigma\\0\end{pmatrix}V^T = \breve U(I+\Xi)\begin{pmatrix}\Sigma\\0\end{pmatrix}V^T, \tag{5.17}$$

where $(I+\Gamma)U = \breve U(I+\Xi)$ with diagonal matrix Ξ determined so that $\breve U$ has unit columns. Obviously, $|\Xi_{ii}| \le \|\Gamma U(:,i)\|_2$ for all i, and $\|\Xi\|_2 \le \|\Gamma\|_2$. Write $\tilde A$ as

$$\tilde A = \breve U\begin{pmatrix}\breve\Sigma\\0\end{pmatrix}V^T,\quad \begin{pmatrix}\breve\Sigma\\0\end{pmatrix} = (I+\Xi)\begin{pmatrix}\Sigma\\0\end{pmatrix},\quad \breve\Sigma = \mathrm{diag}(\breve\sigma_j)_{j=1}^n, \tag{5.18}$$

and note that $\breve U^T\breve U = I+\Omega$ with $\Omega_{ii}=0$ for all i. Now,

$$\tilde A^T\tilde A = V\,(\,\breve\Sigma\quad 0\,)\,(I+\Omega)\begin{pmatrix}\breve\Sigma\\0\end{pmatrix}V^T = V\breve\Sigma(I_n+\hat\Omega)\breve\Sigma V^T, \tag{5.19}$$

where $\hat\Omega = \Omega(1:n,1:n)$. Using the orthogonal similarity in the last relation, we can compare the eigenvalues of $\tilde A^T\tilde A$ and the corresponding eigenvalues of the matrix $M \equiv \breve\Sigma(I_n+\hat\Omega)\breve\Sigma$. A second look at the relations (5.17)–(5.19) reveals the transformation of the multiplicative perturbation $I+\Gamma$ of A into the nonorthogonality of the left singular vector matrix U and then the splitting of the nonorthogonality of $(I+\Gamma)U$ into the column length changes and angle changes. The changes of the unit lengths of the columns of U are then taken as perturbation of Σ, thus defining $\breve\Sigma$.

Note that the matrix M is $\|\hat\Omega\|_2$—scaled diagonally dominant (s.d.d.) [2] with eigenvalues $\tilde\sigma_1^2\ge\cdots\ge\tilde\sigma_n^2$ and diagonal entries $\breve\sigma_1^2\ge\cdots\ge\breve\sigma_n^2$. Using [22, Corollary 3.2] we conclude that

$$\sum_{j=\tilde s_{i-1}+1}^{\tilde s_i}\left|1-\frac{\tilde\sigma_{\tilde s_i}^2}{(\breve\sigma_j)^2}\right|^2 + \sum_{j=\tilde s_{i-1}+1}^{\tilde s_i}\sum_{k=\tilde s_{i-1}+1}^{\tilde s_i}\hat\Omega_{jk}^2 \le \frac{4}{\tilde\gamma_i^2}\left(\sum_{j=\tilde s_{i-1}+1}^{\tilde s_i}\Big(\sum_{k=1}^{\tilde s_{i-1}}\hat\Omega_{jk}^2+\sum_{k=\tilde s_i+1}^{n}\hat\Omega_{jk}^2\Big)\right)^2. \qquad \square$$

Remark 5.1. Consider the right-handed Jacobi SVD algorithm on $X\in\mathbb{R}^{n\times n}$. Let $\tilde X_\infty \equiv \tilde X^{(\tilde k)} = (X+\delta X)\hat V$ be the computed matrix and $\tilde X_\infty+\delta\tilde X_\infty = \tilde U\tilde\Sigma$ as in relation (4.3). Let $\max_{i\ne j}\left|(\tilde U^T\tilde U)_{ij}\right|\le\tau$, $\max_i\left|1-\|\tilde U(:,i)\|_2\right|\le\nu$. We wish to know how the sizes of τ and ν influence the relative distance between the $\tilde\sigma_i=\tilde\Sigma_{ii}$ and the corresponding exact singular value $\hat\sigma_i$ of $\tilde U\tilde\Sigma$. As in the proof of Theorem 5.5, we split the perturbation (the departure from orthogonality of $\tilde U$) into two parts. Let $\tilde U = \breve U(I+\Xi)$, where $\breve U$ has unit columns and Ξ is a diagonal matrix with

$\|\Xi\|_2 \le \nu$. Write $\tilde{U}\tilde{\Sigma}$ as $\breve{U}\breve{\Sigma}$, where $\breve{\Sigma}$ is the diagonal matrix with diagonal entries $\breve{\sigma}_i = \tilde{\sigma}_i(1+\Xi_{ii})$. Note that ν can be as small as $O(\boldsymbol{\varepsilon})$ with the cost of doubly accumulated dot products, and $O(n\boldsymbol{\varepsilon})$ if no extra precision is used. The potentially larger and harder to control value τ enters the estimate quadratically, and that opens a possibility for better stopping criteria. As in Theorem 5.5, we note that $\breve{\Sigma}\breve{U}^T\breve{U}\breve{\Sigma}$ has diagonal entries $\breve{\sigma}_i^2$ and eigenvalues $\hat{\sigma}_i^2$, $i = 1, \ldots, n$. Further, $\Omega = \breve{U}^T\breve{U} - I$ satisfies $\max_{ij}|\Omega_{ij}| \le \tau/(1-\nu)^2$. Let $\|\Omega\|_2 < \hat{\gamma}/3$, where the gap $\hat{\gamma}$ between the $\hat{\sigma}_i^2$'s is analogous to $\tilde{\gamma}$ in Theorem 5.5. Then, if $\hat{k}_i$ is the multiplicity of $\hat{\sigma}_i$, it holds that

$$\frac{|\hat{\sigma}_i - \breve{\sigma}_i|}{\breve{\sigma}_i} \le \frac{2}{\hat{\gamma}_i}\hat{k}_i(n-\hat{k}_i)\frac{\tau^2}{(1-\nu)^4} \le \frac{1}{\hat{\gamma}_i}\frac{n^2\tau^2}{2(1-\nu)^4}. \tag{5.20}$$

Example 5.1. We illustrate the application of the relation (5.20) in stopping the Jacobi SVD algorithm. Let $\boldsymbol{\varepsilon} \approx 2.22 \cdot 10^{-16}$, $n = 1000$, and $\tau = 10^{-8}$. Since we do not have the $\hat{\sigma}_i$'s, the relative gaps will be estimated using the computed $\tilde{\sigma}_i$'s. Let $\tilde{U}^T\tilde{U} = I + \tilde{\Omega}$. Then $\|\tilde{\Omega}\|_F \le \omega \equiv \sqrt{n(n-1)\tau^2 + n\nu^2} < 9.9950 \cdot 10^{-6}$ and

$$\max_{i=1:n}\frac{|\hat{\sigma}_i - \tilde{\sigma}_i|}{\sqrt{\hat{\sigma}_i\tilde{\sigma}_i}} \le \|(I+\tilde{\Omega})^{-1/2} - (I+\tilde{\Omega})^{1/2}\|_2 \le \omega_1 \equiv \frac{\omega}{\sqrt{1-\omega}} < 9.9951 \cdot 10^{-6}.$$

From this we conclude that for all i

$$\frac{|\hat{\sigma}_i - \tilde{\sigma}_i|}{\min\{\hat{\sigma}_i, \tilde{\sigma}_i\}} \le \omega_2 \equiv \frac{\omega_1}{1-\omega_1} < 9.996 \cdot 10^{-6}, \quad \frac{|\hat{\sigma}_i - \tilde{\sigma}_i|}{\hat{\sigma}_i + \tilde{\sigma}_i} \le \frac{\omega_1}{2} < 4.998 \cdot 10^{-6}.$$

Suppose that we have n different values $\tilde{\sigma}_1 > \cdots > \tilde{\sigma}_n > 0$ and that they are well separated relative to their uncertainty in approximating the $\hat{\sigma}_i$'s, i.e., let

$$\max_{i\ne j}\frac{|\tilde{\sigma}_i - \tilde{\sigma}_j|}{\tilde{\sigma}_i + \tilde{\sigma}_j} > 5\omega > 4.997 \cdot 10^{-5}. \text{ Then } \tilde{\gamma}_i \equiv \min_{j\ne i}\frac{|\tilde{\sigma}_i^2 - \tilde{\sigma}_j^2|}{\tilde{\sigma}_i^2 + \tilde{\sigma}_j^2} > 5\omega.$$

Since the $\hat{\sigma}_i$'s are $O(\omega)$ close to the $\tilde{\sigma}_i$'s, we know that the $\hat{\sigma}_i$'s are simple and that $\hat{\gamma}_i \equiv \min_{j\ne i}\frac{|\hat{\sigma}_i^2 - \hat{\sigma}_j^2|}{\hat{\sigma}_i^2 + \hat{\sigma}_j^2} \ge \tilde{\gamma}_i\big(1 - \frac{\omega_2}{5\omega}\big)\frac{1-\omega_2}{(1+\omega_2)^2} > 0.7999\tilde{\gamma}_i > 3.999\omega > 3\|\Omega\|_2$. Since $\breve{\sigma}_i = \tilde{\sigma}_i(1 + O(10^{-13}))$, we have $\breve{\sigma}_1 > \cdots > \breve{\sigma}_i > \breve{\sigma}_{i+1} > \cdots > \breve{\sigma}_n > 0$. We can now apply the quadratic bound, which yields for each i

$$\frac{|\hat{\sigma}_i - \breve{\sigma}_i|}{\breve{\sigma}_i} \le \frac{2}{0.7999}\frac{1}{\tilde{\gamma}_i}(n-1)\frac{\tau^2}{(1-\nu)^4} \le \frac{1}{\tilde{\gamma}_i}2.498 \cdot 10^{-13}. \tag{5.21}$$

Thus, if for instance $\tilde{\gamma}_i > 10^{-3}$, we can claim that $\tilde{\sigma}_i$ coincides with the corresponding $\hat{\sigma}_i$ to about ten decimal places, which actually doubles the previous number by about five known correct digits.

5.5. Accuracy of the singular vectors. The structure of the backward error in our algorithm is such that we can use well-developed and sharp perturbation theory [19], [28]. Our starting point is the relation (5.3) in Proposition 5.1, which is the SVD of $A+\mathcal{E}$ with the computed singular values in diagonal $\tilde{\Sigma}$, and exactly orthogonal matrices $\hat{Q}$, $\hat{V}_x$, $\hat{U}$ which are close to the corresponding computed approximations $\tilde{Q}$, $\overline{V}_x$, $\tilde{U}_x$, respectively. We first deal with the singular vector perturbations in the case of simple well-separated singular values. If $\sigma_1 \ge \cdots \ge \sigma_n$ are the singular values of $A = U\left(\begin{smallmatrix}\Sigma\\0\end{smallmatrix}\right)V^T$, then the relative separation is defined as $\rho_i = \min\big\{2, \min_{j\ne i}\frac{|\sigma_j - \sigma_i|}{\sigma_i}\big\}$, $i = 1, \ldots, n$. If the singular values are simple, then each ρ_i is positive and the singular

vectors define one-dimensional singular subspaces. If the perturbed matrix also has only simple singular values, then we can use the angles between the original and the perturbed subspaces as a natural error measure. Let θ_i and ϑ_i denote the error angles in the ith left and right singular vector, respectively. In the case of the perturbation from relation (5.3), $\theta_i = \angle(U(:,i), \hat{U}_a(:,i))$, $\vartheta_i = \angle(V(:,i), \hat{V}_a(:,i))$.

PROPOSITION 5.6. *Let $A = U\left(\begin{smallmatrix}\Sigma\\0\end{smallmatrix}\right)V^T$ be the SVD of A and let* (5.3) *be the SVD of a perturbed matrix with $\|\mathcal{E}(:,i)\|_2 \le \hat{\eta}\|A(:,i)\|_2$, $i = 1,\ldots,n$ (cf. Proposition* 5.1*). Let $\Phi = \mathcal{E}A^\dagger$, $\phi = \|\Phi + \Phi^T + \Phi\Phi^T\|_2$, $\phi \le 2\|Sym(\Phi)\|_2 + \|\Phi\|_2^2$. If $\phi < \rho_i$, then*

$$\max\{\sin\theta_i, \sin\vartheta_i\} \le \sqrt{2}\left\{\frac{\xi}{\rho_i - \phi} + \|\Phi\|_2\right\}, \tag{5.22}$$

where $\xi \le 2\|Sym(\Phi)\|_2 + O(\|\Phi\|_2^2)$ and $\|\Phi\|_2 \le \sqrt{n}\hat{\eta}\|A_c^\dagger\|_2$.

Proof. We obtain the proof by applying [19, Theorem 3.3]. ∎

Application of the above estimates to the actually computed matrices $\tilde{U}_a$, $\tilde{V}_a$ follows by combining Propositions 5.6 and 5.2, since the angles $\angle(\tilde{U}_a(:,i), \hat{U}_a(:,i))$ and $\angle(\tilde{V}_a(:,i), \hat{V}_a(:,i))$ are small, with bounds sharper than those in (5.22).

In cases of clustered or multiple singular values, the singular vectors are not the right objects to be approximated numerically. Instead, we try to compute well-defined singular subspaces, belonging to multiple or tightly grouped singular values. The structure of the backward perturbation in the Jacobi SVD algorithm fits nicely into the perturbation estimates. For the sake of simplicity, we will give only one perturbation result, following [28]. Other interesting bounds can be derived from the fact that $A + \mathcal{E} = (I + \Phi)A$, where $\|\Phi\|$ is independent of the column scaling of A.

PROPOSITION 5.7. *Let $\Sigma = \Sigma_1 \oplus \Sigma_2$, $\tilde{\Sigma} = \tilde{\Sigma}_1 \oplus \tilde{\Sigma}_2$ with $\Sigma_1 = \mathrm{diag}(\sigma_1,\ldots,\sigma_k)$, $\Sigma_2 = \mathrm{diag}(\sigma_{k+1},\ldots,\sigma_n)$, $\tilde{\Sigma}_1 = \mathrm{diag}(\tilde{\sigma}_1,\ldots,\tilde{\sigma}_k)$, $\tilde{\Sigma}_2 = \mathrm{diag}(\tilde{\sigma}_{k+1},\ldots,\tilde{\sigma}_n)$. Let $\varrho = \min_{i=1:k;j=1:n-k} |\sigma_i - \tilde{\sigma}_{k+j}|/\sqrt{\sigma_i^2 + \tilde{\sigma}_{k+j}^2}$. In the rectangular case, $m > n$, replace ϱ with $\min\{\varrho, 1\}$. Let $\mathcal{U}_1$, $\hat{\mathcal{U}}_1$, $\mathcal{V}_1$, $\hat{\mathcal{V}}_1$ be the subspaces spanned by the columns of $U_1 \equiv U(:,1:k)$, $\hat{U}_a(:,1:k)$, $V(:,1:k)$, $\hat{V}_a(:,1:k)$, respectively. If $\varrho > 0$, then*

$$\left\| \begin{pmatrix} \|\sin\Theta(\mathcal{U}_1, \hat{\mathcal{U}}_1)\|_F \\ \|\sin\Theta(\mathcal{V}_1, \hat{\mathcal{V}}_1)\|_F \end{pmatrix} \right\|_F \le \frac{\sqrt{\|\Phi^T U_1\|_F^2 + \|-\Phi U_1 + \Phi^2(I-\Phi)^{-1}U_1\|_F^2}}{\varrho}. \tag{5.23}$$

Thus, the error angles are bounded by $O(\|\Phi\|_F/\varrho)$.

This concludes the first part of our report. We have defined the global structure of a new preconditioned Jacobi SVD algorithm, which uses pivoted QR factorization as the preconditioner and reduces the computation to the SVD of structured triangular matrices. We have shown that the new algorithm computes the SVD with columnwise small backward error and with condition number independent of column scaling. Reliable implementation of the preconditioner is given in [16]. The new implementation of the Jacobi SVD on triangular matrices and the results of numerical testing are presented in [18], where we show that the new method can reach the efficiency of less accurate bidiagonalization-based methods (SGESVD and SGESDD from LAPACK). The speedup over the equally accurate standard one-sided Jacobi SVD can be a factor of ten or more.

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