A mixed precision Jacobi SVD algorithm

Weiguo Gao$^{1,2,3}$, Yuxin Ma$^4$, and Meiyue Shao$^{2,3}$

$^1$School of Mathematical Sciences, Fudan University, Shanghai 200433, China
$^2$School of Data Science, Fudan University, Shanghai 200433, China
$^3$MOE Key Laboratory for Computational Physical Sciences, Fudan University, Shanghai 200433, China
$^4$Department of Numerical Mathematics, Faculty of Mathematics and Physics, Charles University, Sokolovská 49/83, 186 75 Praha 8, Czechia

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Abstract

We propose a mixed precision Jacobi algorithm for computing the singular value decomposition (SVD) of a dense matrix. After appropriate preconditioning, the proposed algorithm computes the SVD in a lower precision as an initial guess, and then performs one-sided Jacobi rotations in the working precision as iterative refinement. By carefully transforming a lower precision solution to a higher precision one, our algorithm achieves about $2\times$ speedup on the x86-64 architecture compared to the usual one-sided Jacobi SVD algorithm in LAPACK, without sacrificing the accuracy.

Keywords: Singular value decomposition, Jacobi algorithm, mixed precision algorithm, high relative accuracy

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1 Introduction

In recent years, partly because of the quick development of machine learning, low precision arithmetic becomes more and more widely supported by hardware on various computational units such as GPUs. Since lower precision arithmetic is in general faster than higher precision arithmetic, the availability of low precision arithmetic motivates researchers to rethink about efficiency and accuracy of existing numerical algorithms. It is possible to make significant speedup if an algorithm can make clever use of low precision arithmetic. As a consequence, mixed precision algorithms have attracted a lot of attention, especially in numerical linear algebra and high performance computing [1, 2, 22].

There are mainly two classes of mixed precision algorithms. Traditional mixed precision algorithms, such as classical iterative refinement for linear systems [24, 26] and Cholesky QR algorithm [33], improve the numerical stability of the algorithm by temporarily using a higher precision at certain points. In contrast with traditional ones, modern mixed precision algorithms use a lower precision to perform part of the computations in order to reduce the execution time of programs, while preserving accuracy of the final solution the same as that of fixed precision algorithms.
There are a number of works in the literature focusing on mixed precision linear solvers. In 2018, a general framework for solving a nonsingular linear system $Ax = b$ based on iterative refinement with three precisions was proposed by Carson and Higham [6]. By computing the most expensive operation, LU factorization of $A$, in a lower precision, a mixed precision algorithm can solve linear systems up to twice as fast as traditional dense linear solvers without loss of accuracy. Refinement through GMRES (GMRES-IR) utilizing lower precision LU factorization as the preconditioner is also developed for ill-conditioned linear system, in order to obtain higher performance than traditional dense linear solvers. More recently, Carson and Khan [8] proposed that mixed precision GMRES-IR can be further accelerated by sparse approximate inverse preconditioners. Carson, Higham, and Pranesh also proposed three-precision GMRES-IR with QR preconditioning to solve linear least squares problems through augmented systems [7].

Compared to dense linear solvers, iterative refinement for dense eigensolvers (that computes a large number of eigenpairs) is more complicated, though most eigensolvers are essentially iterative. Since several popular algorithms (such as the QR algorithm) are highly structured, and cannot make full use of a near diagonal or near upper triangular input, it seems difficult to use these algorithms directly for iterative refinement. Ogita and Aishima recently published several papers on Newton-like methods for refining the solution of symmetric eigenvalue problems, including singular value decomposition [28, 29, 30]. A similar but more complicated algorithm was proposed by Bujanović, Kressner, and Schröder to refine the Schur decomposition for non-symmetric eigenvalue problems [4]. This refinement algorithm also leads to a mixed precision nonsymmetric eigensolver. There is another recent algorithm called iterative perturbative theory (IPT) developed by Kenmoe, Kriemann, Smerlak, and Zadorin in [25] that works for both symmetric and nonsymmetric eigenvalue problems.

Besides Newton-like algorithms, the Jacobi algorithm [23] is also suitable for iterative refinement [3, 32] since it converges locally quadratically [19]. A natural idea is to quickly compute the solution in lower precision, and then use the Jacobi algorithm to improve the accuracy to working precision. This leads to a basic mixed precision eigensolver. However, it is challenging to achieve high performance in this manner, as both preprocessing and refinement stages require $O(n^3)$ work. We observe that a basic mixed precision eigensolver usually has relatively low performance (see Section 7.2). In order to accelerate the computation—this is the motivation of exploiting low precision arithmetic—it is crucial to carefully design the algorithm so that the Jacobi algorithm can quickly refine the low-precision solution.

In this work we propose a mixed precision Jacobi SVD algorithm. Our algorithm makes use of low precision arithmetic as a preconditioning step, and then refines the solution by the one-sided Jacobi algorithm developed by Drmač and Veselić in [17, 18]. On the x86-64 architecture our mixed precision algorithm is in general about twice as fast as the fixed precision one in LAPACK. Moreover, the mixed precision algorithm inherits high accuracy properties of the Jacobi algorithm even if a large amount of work is performed in a lower precision. As an eigensolver, the Jacobi algorithm is usually not the first choice since it is often slower than alternatives such as the divide and conquer algorithm [3, 25]. However, when high relative accuracy is desired, the Jacobi algorithm seems the best candidate by far [14, 13].

The rest of this paper is organized as follows. In Section 2 we briefly review the one-sided Jacobi SVD algorithm. Then in Section 3 we propose a mixed precision Jacobi SVD algorithm and discuss algorithmic details. Theoretical analyses on the mixed precision Jacobi SVD algorithm are provided in Sections 4–6: in Section 4 we show that our mixed precision Jacobi SVD algorithm is backward stable, and is as accurate as the fixed precision Jacobi SVD algorithm; in Sections 5 we analyze the quality of conditioning in a lower precision; in Section 6 we discuss the accuracy of different methods for switching precisions. Numerical experiments are provided in Section 7 to demonstrate the efficiency of our mixed precision algorithm.
2 The one-sided Jacobi SVD algorithm

In this section, we briefly review the one-sided Jacobi SVD algorithm developed by Drmač and Veselić in [17, 18]. Compared with other variants of the Jacobi SVD algorithm, this one is superior in performance while preserving high accuracy. Implementation of this Jacobi SVD algorithm has been available in LAPACK starting from versions 3.2.¹

2.1 Jacobi rotations

For any column vectors \( x_1, x_2 \in \mathbb{C}^m \), there exists a unitary matrix \( J = \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \) with \( c \in \mathbb{R} \) such that the columns of \([x_1, x_2]J\) are orthogonal to each other.² This orthogonal transformation plays a key role in the one-sided Jacobi SVD algorithm. To compute the SVD of a matrix \( X \in \mathbb{C}^{m \times n} \) with \( m \geq n \), the one-sided Jacobi SVD algorithm repeatedly orthogonalizes a pair of columns of \( X \) until \( X^*X \) becomes numerically diagonal, i.e., all off-diagonal entries of \( X^*X \) have negligible magnitudes. In other words, a sequence of matrices \( X^{(k)} = X^{(k-1)}J^{(k)}, \quad (k = 1, 2, \ldots, N) \), with \( X^{(0)} = X \) is computed until \( X^{(N)} \) has numerically orthogonal columns after \( N \) steps, where the unitary matrix \( J^{(k)} \) is a so-called Jacobi plane rotation matrix of the form

\[
J^{(k)} = \begin{bmatrix}
I_{p_k-1} & c_k & s_k \\
-s_k & I_{q_k-p_k-1} & c_k \\
& & I_{n-q_k}
\end{bmatrix}
\]

that orthogonalizes \( p_k \)-th and \( q_k \)-th columns of \( X^{(k-1)} \). Then by normalizing the columns of \( X^{(N)} \) (i.e., \( X^{(N)} = U_X \Sigma \) where \( U_X^*U_X = I_m \) and \( \Sigma \) is diagonal and positive definite) and setting \( V_X = J^{(1)}J^{(2)} \cdots J^{(N)} \), we obtain \( X = U_X \Sigma V_X^* \) as the computed SVD of \( X \).³

Notice that the choice of \((p_k, q_k)\)'s largely affects the convergence of the Jacobi SVD algorithm. One popular strategy that guarantees the convergence is the cyclic strategy that periodically performs sweeps of the following sequence of \((p_k, q_k)\)'s:

\[
(1, 2), (1, 3), \ldots, (1, n), \quad (2, 3), \ldots, (2, n), \quad (3, 4), \ldots, (3, n), \quad \ldots, \quad (n-1, n). \quad (1)
\]

Algorithm 1 summarizes the basic one-sided Jacobi SVD algorithm.

The convergence of the one-sided Jacobi SVD algorithm can be accelerated by de Rijk’s pivoting strategy [12]. This pivoting strategy splits each sweep into \( n-1 \) subsweeps—in the \( i \)-th subsweep, it identifies the column of \( X_{i:n} \) with largest Euclidean norm and interchanges this dominant column with \( X_{i} \), and then orthogonalizes the column pairs \((p, q)\) for \( q = p + 1, \ldots, n \).⁴

¹Real versions were released in LAPACK version 3.2, while complex versions were released later in LAPACK version 3.6.0.
²Actually, the choice of \( J \) is not unique for the purpose of orthogonalizing \( x_1 \) and \( x_2 \). The Jacobi SVD algorithm always chooses the one that is closest to the identity matrix to ensure convergence.
³In practice, appropriate reordering of \( U_X \) and \( \Sigma \) is required so that the diagonal entries of \( \Sigma \) are descending.
⁴Throughout the paper we adopt the MATLAB colon notation to denote indices that describe submatrices.
Algorithm 1 One-sided Jacobi SVD algorithm (without preconditioning)

**Input:** A matrix $A \in \mathbb{C}^{m \times n}$, the convergence threshold $\epsilon_{tol} \in (0, +\infty)$, maximal iteration count $\text{maxiter}$.

**Output:** The singular value decomposition $X = U_X \Sigma V_X^*$.

1: \[ V_X \leftarrow I. \]
2: converged $\leftarrow$ false, iter $\leftarrow 1.$
3: while iter $< \text{maxiter}$ and converged $= false$ do
4:     converged $\leftarrow$ true.
5:     for each pair $(p, q)$ with $p < q$ in (1) do
6:         if $|X(:,q)^*X(:,p)| > \epsilon_{tol}\|X(:,p)\|_2\|X(:,q)\|_2$ then
7:             Choose a Jacobi rotation matrix $J$ that orthogonalizes $X(:,p)$ and $X(:,q)$.
8:             $X \leftarrow XJ.$
9:             $V_X \leftarrow V_XJ.$
10:        converged $\leftarrow$ false.
11:    end if
12:  end for
13:  iter $\leftarrow$ iter + 1.
14: end while
15: for $i \leftarrow 1 : n$ do
16:    $\Sigma(i,i) \leftarrow \|X(:,i)\|_2.$
17:    $U_X(:,i) \leftarrow X(:,i)/\Sigma(i,i).$
18: end for
19: Sort the diagonal entries of $\Sigma$, and permute the columns of $U_X$ and $V_X$ accordingly.

2.2 Preconditioning

In [17], Drmač and Veselić discussed a carefully designed preconditioning strategy for the one-sided Jacobi SVD algorithm. Roughly speaking, the key idea is to transform $A$ to a “more diagonally dominant” matrix $X$, so that the column norms of $X$ are good approximations of the singular values.

First, a rank-revealing QR (RRQR) factorization $AP = Q_1R$ is computed, where $Q_1 \in \mathbb{C}^{m \times n}$ has orthonormal columns, $R \in \mathbb{C}^{n \times n}$ is upper triangular, and $P \in \mathbb{R}^{n \times n}$ is a permutation matrix. If the columns of $R$ are close to diagonally dominant, we set $X = R$; otherwise, an LQ factorization, $R = LQ_2$, is performed, and we set $X = L$. Finally, the matrix $X$ is fed to the one-sided Jacobi SVD algorithm. The preconditioned algorithm is shown in Algorithm 2.

The preconditioning strategy has been observed to effectively accelerate the convergence of the one-sided Jacobi SVD algorithm. Moreover, it provides opportunities for fast implementations without explicitly accumulating the Jacobi plane rotations. For instance, if $X$ is expressed as $X = D_rZ_r$, where $D_r$ is diagonal and $Z_r$ has normalized rows, then $V_X$ can be constructed using $V_X = X^{-1}U_X\Sigma$ when $Z_r$ is reasonably well-conditioned (this often occurs after preconditioning). Consequently, Step 9 in Algorithm 1 can be omitted. This strategy improves the computational efficiency because accumulating rotations is usually very time-consuming.

3 A mixed precision Jacobi SVD algorithm

In this section, we propose a mixed precision Jacobi SVD algorithm. The basic idea is to perform SVD in a lower precision as a preconditioner, and then refine the solution by the one-sided Jacobi SVD algorithm in working precision. This idea yields a basic mixed precision Jacobi SVD
Algorithm 2 Preconditioned one-sided Jacobi SVD algorithm

**Input:** A matrix $A \in \mathbb{C}^{m \times n}$, the convergence threshold $\epsilon_{\text{tol}} \in (0, +\infty)$, maximal iteration count $\text{maxiter}$.

**Output:** The full singular value decomposition $A = U \Sigma V^*$.

1: Factorize $A$ such that $AP = Q_1 R$.
2: if the $R$ is almost diagonal then
3: \quad $X \leftarrow R, V \leftarrow P$.
4: else
5: \quad Factorize $R$ such that $R = LQ_2$.
6: \quad $X \leftarrow L, V \leftarrow PQ_2^*$.
7: end if
8: Compute the SVD $X = U_X \Sigma_X V_X^*$ by Algorithm 1.
9: $U \leftarrow Q_1 \cdot U_X, V \leftarrow V \cdot V_X$.

algorithm as shown in Algorithm 3. However, we shall see in Section 7.2 that the performance of this simple algorithm is far from satisfactory. The number of sweeps in Step 4 is not much lower than that of Algorithm 2 so that only limited speedup can be expected.

In order to achieve better performance, we need to redesign a mixed precision algorithm carefully. We split the algorithm into the following stages.

1. QR preconditioning is performed in order to accelerate the convergence and also avoid unnecessary complication for rectangular matrices.

2. The singular value decomposition is computed in a lower precision.

3. The solution in lower precision is transformed back to the working precision.

4. The one-sided Jacobi SVD algorithm without preconditioning (i.e., Algorithm 1) is applied to refine the solution in working precision.

The first three stages can be interpreted as a careful preconditioning strategy involving low precision arithmetic that produces a reasonably good initial guess for Algorithm 1. If the initial guess is of good quality, the last stage starts with nearly orthogonal columns and then quick convergence can be expected due to the asymptotic quadratic convergence of the Jacobi algorithm. Our mixed precision algorithm is briefly summarized as Algorithm 4. In the following we discuss the four stages of Algorithm 4 in details. We use $\text{working}(\cdot)$ and $\text{lower}(\cdot)$, respectively, to explicitly convert the data into working and lower precisions. In addition, $\text{fl}(\cdot)$ and $\text{fl}_\text{low}(\cdot)$, respectively, denote the computed results in working and lower precisions.

### 3.1 QR preconditioning

As mentioned in Section 2.2, preconditioning can simplify the computation and accelerate the convergence of the one-sided Jacobi SVD algorithm. The preconditioning strategy in Algorithm 4 is inherited from that in [17], with some minor changes. We remark that this preconditioning strategy is very effective so that the one-sided Jacobi SVD algorithm can often converge in a few sweeps. As a result the benefit for computing a low precision SVD may be limited in some special cases. In Section 3.5, we shall present additional techniques to handle these special cases.

When the input is a square matrix, we simply use the same preconditioning strategy as in [17]. For a rectangular matrix $A \in \mathbb{C}^{m \times n}$ with $m > n$, instead of performing a rank-revealing QR factorization as in [17], we perform a plain QR factorization $A = QR_1$ to obtain an $n \times n$
Algorithm 3 Basic mixed precision Jacobi SVD algorithm

**Input:** A matrix $A \in \mathbb{C}^{m \times n}$ with $m \geq n$, the threshold $\text{tol}_{\text{alg}} \in (0, +\infty)$ for choosing the lower precision SVD algorithm, the orthogonality threshold $\text{tol}_{\text{orth}} \in (0, +\infty)$, the condition number threshold $\text{tol}_{\text{cond}} \in (0, +\infty)$.

**Output:** The full singular value decomposition $A = U \Sigma V^*$. 

1: Apply the preconditioned one-sided Jacobi algorithm (Algorithm 2) in lower precision to obtain $\text{lower}(A) = U_{\text{low}} \Sigma_{\text{low}} V_{\text{low}}^*$.
2: Convert $V_{\text{low}}$ to the working precision and compute the QR factorization $\text{working}(V_{\text{low}}) = QR$.
3: $Y \leftarrow AQ$.
4: Apply the one-sided Jacobi algorithm (Algorithm 1) to $Y$, i.e., $Y = U \Sigma V_Y^*$. 
5: $V \leftarrow V_Y Q$.

matrix $R_1$ and then apply the preconditioning strategy for square matrices to $R_1$. Since RRQR is very costly, our revised strategy in general reduces the computational time unless $m$ is really close to $n$.

The RRQR algorithm\(^5\) can also be improved by using low precision arithmetic. Compared to the plain QR factorization, the RRQR algorithm requires a lot of effort to determine the column permutation. Hence pivoting is the dominant cost for RRQR in practice. Once the permutation is already known, computing a plain QR factorization on a permuted matrix is much cheaper than performing the RRQR algorithm. In order to determine the permutation, it suffices to apply the RRQR algorithm in a lower precision. This leads to a mixed precision RRQR algorithm as shown in Algorithm 5. Though this algorithm in fact computes QR factorizations twice, it is still observed to be faster than the usual RRQR algorithm in working precision on the x86-64 architecture since the most expensive part is performed using a lower precision. We use this mixed precision algorithm to compute the RRQR factorization in the preconditioning stage.

### 3.2 SVD in a lower precision

After the first stage, we have already transformed $A$ to a square matrix $X$ whose SVD is easier to compute. The goal of the second stage in our algorithm is to compute the singular value decomposition $X = U_X \Sigma_X V_X^*$ in a lower precision.

When computing the SVD in a lower precision, there are several possible choices, such as Jacobi algorithm, QR algorithm, and divide and conquer algorithm. The divide and conquer algorithm is not a good option for highly accurate computation [13, 14, 18] because we observed that the computed singular vectors are often not sufficiently accurate so that many sweeps will be needed by the subsequent one-sided Jacobi SVD algorithm after switching back to the working precision. Though the QR algorithm is in general less accurate than the Jacobi algorithm [13], Drmač pointed out in [16] that the QR algorithm can compute the SVD accurately as long as it is carefully preconditioned (using the strategy discussed in Section 3.1). Therefore we use either the Jacobi algorithm or the QR algorithm since they are relatively accurate. The choice mainly depends on the performance.

In order to determine which algorithm is used, we check the orthogonality of $X$ in the lower precision after QR preconditioning. When the computed result $\text{fl}_{\text{low}}(X)$ has nearly orthogonal columns (e.g., $\|\text{fl}_{\text{low}}(X)^* \text{fl}_{\text{low}}(X) - I\| = O(u_{\text{low}}^{1/2})$), the Jacobi algorithm is chosen as it converges

\(^5\)To be precise, the RRQR algorithm here refers to $XGEQP3$ in LAPACK, which implements the Businger–Golub QR factorization with column pivoting; see [5, 15].
Algorithm 4 Mixed precision Jacobi SVD algorithm

**Input:** A matrix $A \in \mathbb{C}^{m \times n}$ with $m \geq n$, the threshold $\text{tol}_{\text{alg}} \in (0, +\infty)$ for choosing the lower precision SVD algorithm, the orthogonality threshold $\text{tol}_{\text{orth}} \in (0, +\infty)$, the condition number threshold $\text{tol}_{\text{cond}} \in (0, +\infty)$.

**Output:** The full singular value decomposition $A = U\Sigma V^*$.

1: if $m > n$ then
2: Compute the QR factorization of $A$ such that $A = Q_0 R_1$.
3: $A_1 \leftarrow R_1$.
4: else
5: $Q_0 \leftarrow I$.
6: $A_1 \leftarrow A$.
7: end if
8: Apply the QR preconditioning like Algorithm 2 to $A$ such that $X = Q_1^* A_1 P Q_2^*$, where $Q_2$ could be the identity matrix.
9: if $\text{cond}_R \leq \text{tol}_{\text{cond}}$ and many trailing columns of $X$ have small norms then
10: $Q \leftarrow I$.
11: else
12: $X^* \leftarrow \text{lower}(X) D^{-1}$, where $D$ is a diagonal matrix and $D_{ii}$ is 2-norm of the $i$-th column of $\text{lower}(X)$.
13: $\text{orth} \leftarrow \|X^* X_t - I\|_{\text{max}}$.
14: if $\text{orth} \leq \text{tol}_{\text{orth}}$ then
15: $Q \leftarrow I$.
16: else
17: if $\text{orth} \leq \text{tol}_{\text{alg}}$ then
18: Apply the one-sided Jacobi SVD algorithm (Algorithm 1) in lower precision to obtain $\text{lower}(X) = U_{\text{low}} \Sigma_{\text{low}} V_{\text{low}}^*$ without generating $V_{\text{low}}$ explicitly.
19: else
20: Apply the QR SVD algorithm in lower precision to obtain $\text{lower}(X) = U_{\text{low}} \Sigma_{\text{low}} V_{\text{low}}^*$ without generating $V_{\text{low}}$ explicitly.
21: end if
22: Convert $U_{\text{low}}$ back to the working precision and compute the QR factorization $X^* \text{working}(U_{\text{low}}) = QR_2$.
23: end if
24: end if
25: $Y \leftarrow X Q$.
26: Apply the one-sided Jacobi algorithm (Algorithm 1) to $Y$, i.e., $Y = U_X \Sigma V_Y^*$ ($V_Y$ is not explicitly generated unless $V$ is needed).
27: $U \leftarrow Q_0 Q_1 U_X$, and optionally $V \leftarrow P Q_2^* V_Y Q$ if $V$ is needed.

Algorithm 5 Mixed precision RRQR algorithm

**Input:** A matrix $A \in \mathbb{C}^{m \times n}$.

**Output:** The RRQR factorization $AP = QR$.

1: Convert $A$ to a lower precision one: $A_{\text{low}} \leftarrow \text{lower}(A)$.
2: Compute the RRQR factorization $A_{\text{low}} P = Q_{\text{low}} R_{\text{low}}$ in a lower precision.
3: Use $P$ to permute the columns of $A$, i.e., $A \leftarrow AP$.
4: Compute the QR factorization (of the permuted matrix) $A = QR$ in working precision.
very rapidly due to the quadratic convergence; otherwise the QR algorithm is used because it is in general faster.

Finally, we remark that there is no need to compute both left and right singular vectors of $X$ in this stage. In the subsequent subsection we shall see that it suffices to compute $U_X$ only.

### 3.3 Switching precisions

Once the singular value decomposition $X = U_X \Sigma V_X^*$ is determined in a lower precision, it is necessary to transform $V_X$ into a unitary matrix $Q$ in working precision. This ensures that $Y = XQ$ has nearly orthogonal columns, allowing it to be processed efficiently by the Jacobi SVD algorithm in the final stage. We will outline the methods to build the unitary $Q$ in working precision.

Note that directly converting the computed result of $V_X$, i.e., $\text{fl}_{\text{low}}(V_X)$, from lower precision to working precision is problematic since the result is far from unitary in working precision, i.e., $\|\text{fl}_{\text{low}}(V_X)^* \text{fl}_{\text{low}}(V_X) - I\| = O(\text{u}_{\text{low}}) \gg u$, where $u$ and $\text{u}_{\text{low}}$, respectively, are the unit round-off of working and lower precisions. Hence a QR factorization of $\text{fl}_{\text{low}}(V_X) = QR_2$ in working precision is required to improve the orthogonality. Then the matrix $XQ$ can be fed to the one-sided Jacobi SVD algorithm in the last stage.

There is an alternative approach to construct the unitary matrix $Q$ in the working precision. Instead of working on the right singular vectors $\text{fl}_{\text{low}}(V_X)$, we convert the computed left singular vectors $\text{fl}_{\text{low}}(U_X)$ to working precision. Then a QR factorization $X^* \text{fl}_{\text{low}}(U_X) = QR_2$ is computed in working precision, so that theoretically the $Q$-factor of $X^*U_X$ is $V_X$ if computing $U_X$, the product $X^*U_X$ and this QR factorization are all in exact arithmetic. Finally, the matrix $XQ$ is fed to the one-sided Jacobi SVD algorithm in the last stage. We prefer this approach in practice because forming $V_X$ in the lower precision is a very expensive operation. For the one-sided Jacobi SVD algorithm, accumulating $V_X$ is clearly very costly; for the QR SVD algorithm, generating $V_X$ is observed to be much more expensive than generating $U_X$ in LAPACK’s subroutine $xGESVD$.

### 3.4 Refinement for nearly orthogonal matrices

After preconditioning and switching precisions, we eventually obtain $\text{fl}(Y) \approx U_X \Sigma$ with nearly orthogonal columns, while columns of $\text{fl}(Y)$ are orthogonal at the level of $\text{u}_{\text{low}}$. In this stage, we apply the one-sided Jacobi SVD algorithm on $\text{fl}(Y)$ to compute the SVD in the working precision, because the Jacobi SVD algorithm can take advantage of the property that $\text{fl}(Y)$ has nearly orthogonal columns. Typically it takes three sweeps for our mixed precision algorithm to refine the solution if $\text{u}_{\text{low}}$ is close to $u^{1/2}$ (which holds for IEEE single and double precisions).

After switching precisions, trailing columns of $\text{fl}(Y)$, that correspond to small singular values, can occasionally be less accurate compared to leading columns that correspond to large singular values. We test the orthogonality of $\text{fl}(Y)$ and partition $\text{fl}(Y)$ into two blocks $\text{fl}(Y) = [Y_1, Y_2]$ so that $\|Y_1^*Y_1 - I\| = O(\text{u}_{\text{low}})$ while $\max\{\|Y_2^*Y_1\|, \|Y_2^*Y_2 - I\|\} \gg \text{u}_{\text{low}}$. If the $Y_2$ block is non-empty, we apply Jacobi rotations in $Y_2$ first, and then apply Jacobi rotations between $Y_1$ and $Y_2$ in one sweep. Thanks to careful QR preconditioning, the solution from lower precision usually has good relative accuracy. We have observed that in most cases the $Y_2$ block is empty, i.e., the orthogonality of $Y$ is satisfactory. Our strategy for handling $Y_2$ is only a safeguard, and is rarely activated. We remark that in the final stage it is safe to skip several techniques of the one-sided Jacobi SVD algorithm proposed in [18] that aim at handling difficult cases as the solution from the lower precision is reasonably accurate.
The computation of right singular vectors $V_X$ is also adjusted compared to the algorithm in [18]. When the problem is reasonably well-conditioned, $V_X$ can be formed through $V_X = \Sigma^{-1}U_X^*X$; otherwise, $V_X$ is computed by accumulating Jacobi rotations, which is expensive. In the latter case, instead of directly accumulating Jacobi rotations, we first compute $U_X$ without accumulating $V_X$. Then similar to the strategy of switching precisions, we form $V_X$ from the QR factorization of $X^*U_X$. These left and right singular vectors are used as the initial guess of another round of the one-sided Jacobi SVD algorithm by accumulating Jacobi rotations. Since such an initial guess is highly accurate, the final Jacobi SVD algorithm always converges in one sweep. The cost of computing $V_X$ is much lower compared to that by the original strategy in [18] since we avoid accumulating Jacobi rotations for many sweeps.

3.5 Handling special cases

The purpose of computing SVD in a lower precision is to reduce the number of sweeps required by the one-sided Jacobi SVD algorithm in working precision. As we mentioned in Section 3.4, the accuracy of the solution from lower precision is at the level of $O(u_{low})$, and it still requires about three sweeps to refine the solution in working precision. However, there exist matrices for which the benefit of computing SVD in a lower precision is limited. For these matrices our mixed precision Jacobi SVD algorithm can be even slower than the fixed precision algorithm. Since the ultimate purpose of developing a mixed precision Jacobi SVD algorithm is to improve the computational efficiency, it is necessary to detect this type of matrices and avoid the overhead caused by the additional work performed in lower precision. In the following, we identify three special cases in which computing SVD in lower precision needs to be avoided.

One special case can be easily detected after QR preconditioning. After computing the RRQR factorization of $A$, if the condition number of $R$, denoted by $\text{cond}_R$ in Algorithm 4, is relatively small (e.g., $\kappa(R) \leq \text{tol}_{\text{cond}}$ with $\text{tol}_{\text{cond}} = O(n^{1/4})$ based on our experience of numerical experiments), QR preconditioning often leads to quick convergence of the one-sided Jacobi SVD algorithm in working precision, and hence we do not compute the SVD in lower precision; see Lines 9–10 in Algorithm 4.

Another special case occurs when the columns of $X$ are almost orthogonal in lower precision after QR preconditioning. In this case, computing SVD in lower precision becomes totally needless because it cannot further accelerate the convergence of the Jacobi SVD algorithm in working precision. To detect this case, we first scale the columns of $X$ so that they have unit column norms. Then we check whether $\|X^*X - I\|_{\text{max}}$ is below a prescribed threshold $\text{tol}_{\text{orth}}$, where $\|\cdot\|_{\text{max}}$ represents the largest absolute value of matrix elements. If $\|X^*X - I\|_{\text{max}} \leq \text{tol}_{\text{orth}}$ is detected, we simply skip the SVD in lower precision and directly use the one-sided Jacobi SVD algorithm in working precision to solve this problem; see Lines 12–15 in Algorithm 4. The test is relatively cheap compared to the entire SVD algorithm since it only requires one matrix–matrix multiplication in lower precision.

The third special case often (but not always) occurs for columnwise graded matrices of the form $A = BD$, where $D$ is an ill-conditioned diagonal matrix. When most singular values of $A$ are relatively small, it is not appropriate to compute SVD in lower precision as the benefit is limited. It is often possible to detect this case after QR preconditioning: if many trailing columns of $X$ have small norms, then the trailing singular values are also small; see Line 9 in Algorithm 4. In this case we skip the SVD in lower precision and move on to the one-sided Jacobi SVD algorithm in working precision.

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6For instance, for $u_{low} = 2^{-24} \approx 6 \times 10^{-8}$, we can choose $\text{tol}_{\text{orth}} \approx 10^{-5}$.

7A heuristic criterion is to check $1/4 \sim 1/3$ of the columns.
4 Accuracy of the computed SVD

In this section, we show that Algorithm 4 is numerically stable in the sense that it inherits nice high accuracy properties from usual one-sided Jacobi SVD algorithms. We use $\tilde{\cdot}$ and $\hat{\cdot}$ to denote theoretical and computed results, respectively.

In the following we make two assumptions on orthogonal transformations. We first assume that a computed QR factorization (possibly with column exchange) is columnwise backward stable, in the sense that

\[ (A + \Delta A)P = \tilde{Q}_0\tilde{R}_0, \quad \|\Delta A(:,i)\|_2 \leq \varepsilon_{\text{rrqr}}\|A(:,i)\|_2 \]  \hfill (2)

holds for each $i$, where $\varepsilon_{\text{rrqr}}$ is bounded by a low degree polynomial of the matrix dimension times the unit round-off $u$. We also assume that steps 1–14 of Algorithm 1 produces

\[ \hat{X}_\infty = (X + \Delta X_0)\hat{V}_X \]

with a rowwise backward error

\[ \|\Delta X_0(i,:,\cdot)\|_2 \leq \varepsilon_X\|X(i,:,\cdot)\|_2, \]

where $\varepsilon_X = O(nu)$. These assumptions are plausible in practice because applying orthogonal transformations from the left/right only introduces columnwise/rowwise backward error in floating-point arithmetic. The same notation and assumptions are used by the analysis in [17].

Steps 1–25 of Algorithm 4 produces an initial guess, which will be iteratively refined by the one-sided Jacobi SVD algorithm in working precision (i.e., steps 26–27). The accuracy of the final solution is mainly determined by the Jacobi SVD algorithm in working precision, as long as the initial guess is reasonably accurate. Since the numerical stability of steps 26–27 has already been analyzed in [17], we shall only focus on the difference between our algorithm and that in [17].

Our preconditioning strategy is similar to that in [17]. For rectangular matrices, Algorithm 4 performs an extra QR factorization in the preprocessing stage. Theoretically, this additional QR factorization can be merged with the subsequent RRQR factorization, because $A = Q_1R_1$ and $R_1P = Q_2R_2$ can be interpreted as $AP = (Q_1Q_2)R_2$. According to (2), this RRQR factorization is columnwise stable. \(^8\) In [17], the analysis for preconditioning remains valid since it merely assumes the columnwise stability of the RRQR factorization.

The analysis of [17] is based on the fact that applying the one-sided Jacobi SVD algorithm without preconditioning (i.e., DGESVJ/ZGESVJ) to $X$ produces a rowwise stable solution; see [17, Proposition 4.1]. The major difference between our algorithm and that in [17] is that we apply DGESVJ/ZGESVJ (assuming the working precision is double precision) to the matrix $XQ$ instead of $X$. Notice that the multiplication of $X$ and any unitary matrix can be computed in a rowwise stable manner. Naturally we can expect that applying the one-sided Jacobi SVD algorithm without preconditioning to the computed result $XQ$ is also rowwise stable, where $Q$ can be any unitary matrix. To show the stability of Algorithm 4, it suffices to establish the following Proposition 1, which is a revised version of [17, Proposition 4.1] tailored to our algorithm.

**Proposition 1.** Let $\hat{U}_X$ and $\hat{\Sigma}$, respectively, consist of the computed left singular vectors and singular values of the matrix $\Pi(XQ)$. Then there exists a unitary matrix $\hat{V}_X$ and a backward perturbation $F$ such that

\[ X + F = \hat{U}_X\hat{\Sigma}\hat{V}_X^*, \]

\(^8\) The constant $\varepsilon_{\text{qr}}$ in (2) needs to be chosen slightly larger than its tightest estimate so that (2) holds even when an extra QR factorization is performed.
where
\[
\|F(i,:)\|_2 \leq (\varepsilon_J(1 + \varepsilon_{\text{req}}) + \varepsilon_{\text{req}})\|X(i,:)\|_2 \quad (3)
\]
for all \(i\). In addition, if \(\hat{V}_X\) consists of the computed right singular vectors, then \(\hat{U}_X\hat{\Sigma}\hat{V}_X^\ast = (X + F)(I + E_0^\ast)\), where \(\|E_0\|_2 \leq \sqrt{n}\varepsilon_1\).

Proof. We only prove (3) since the rest is easy to verify.

There exists a unitary matrix \(\tilde{Q}\) and a small perturbation \(\Delta(X^\ast U_{\text{low}})\) such that
\[
X^\ast \text{working}(U_{\text{low}}) + \Delta(X^\ast U_{\text{low}}) = \tilde{Q}\hat{R}_1.
\]
Then the computed product satisfies \(\text{fl}(X\tilde{Q}) = (X + \Delta X_0)\tilde{Q}\), where
\[
\|\Delta X_0(i,:)\|_2 \leq \varepsilon_{\text{req}}\|X(i,:)\|_2. \quad (4)
\]
By [17, Proposition 4.1], there exists a unitary matrix \(\hat{V}_{XQ}\) and a perturbation \(F_{XQ}\) such that
\[
\text{fl}(X\tilde{Q}) + F_{XQ} = (X + \Delta X_0)\tilde{Q} + F_{XQ} = \hat{U}_X\hat{\Sigma}\hat{V}_{XQ}^\ast
\]
and \(\|F_{XQ}(i,:)\|_2 \leq \varepsilon_J\|\text{fl}(X\tilde{Q})(i,:)\|_2\). The unitary invariance of the 2-norm implies
\[
\|(F_{XQ}\hat{Q}^\ast)(i,:)\|_2 = \|F_{XQ}(i,:)\|_2 \\
\leq \varepsilon_J\|\text{fl}(X\tilde{Q})(i,:)\|_2 \\
\leq \varepsilon_J(\|X(i,:)\|_2 + \varepsilon_{\text{req}}\|X(i,:)\|_2) \\
\leq \varepsilon_J(1 + \varepsilon_{\text{req}})\|X(i,:)\|_2
\]
for all \(i\). Moreover, we have
\[
X + \Delta X_0 + F_{XQ}\hat{Q}^\ast = \hat{U}_X\hat{\Sigma}\hat{V}_X^\ast,
\]
where \(\hat{V}_X = \hat{Q}\hat{V}_{XQ}\). Let \(F = \Delta X_0 + F_{XQ}\hat{Q}^\ast\). We conclude that (3) holds because (4) and (5) imply that
\[
\|F(i,:)\|_2 \leq \|\Delta X_0(i,:)\|_2 + \|(F_{XQ}\hat{Q}^\ast)(i,:)\|_2 \leq (\varepsilon_{\text{req}} + \varepsilon_J(1 + \varepsilon_{\text{req}}))\|X(i,:)\|_2.
\]

By replacing [17, Proposition 4.1] with Proposition 1, Algorithm 4 fits into the framework of [17]—the rest of the analysis in [17, Section 5] remains valid. Therefore, Algorithm 4 also possesses nice high accuracy properties in working precision, though a lot of computations are performed in lower precision.

However, note that this analysis can be valid for any unitary matrix \(Q\) and cannot illustrate why the one-sided Jacobi SVD algorithm without preconditioning can converge such quickly when using SVD in lower precision as the preconditioner. Thus, in the next section, we analyze the efficiency of our new preconditioning strategy and show the advantage of using our special \(Q\) computed by 9–25 in Algorithm 4.

5 Efficiency of the preconditioning

In Algorithm 4, after Step 8, we obtain the matrix \(X\). Our new preconditioning strategy is as the following procedure:

\[
\begin{align*}
U\Sigma V^\ast & \leftarrow X, \\
B & \leftarrow X^\ast U, \\
QR & \leftarrow B, \\
Y & \leftarrow XQ,
\end{align*}
\]
where $U$, $V$, $Q \in \mathbb{C}^{n \times n}$ are unitary matrices, and the diagonal matrix $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ satisfies $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. Note that only the first step is computed in lower precision.

Let $\hat{U}$ and $\hat{\Sigma}$ denote the computed result using floating-point arithmetic by SVD of $X$; $\hat{Q}$ and $\hat{R}$ denote the computed results using floating-point arithmetic by the QR factorization of $\text{fl}(X\hat{U})$. Taking rounding errors into account, the computed quantities satisfy

\[ X = \hat{U}\hat{\Sigma}\hat{V}^* + \Delta X \quad \text{with} \quad \|\Delta X\|_F \leq \varepsilon_{\text{SVD}}\|X\|_F \quad \text{and} \quad \|\hat{U}^*\hat{U} - I\|_F \leq \varepsilon_U, \tag{6} \]

\[ \hat{B} := \text{fl}(X^*\hat{U}) = X^*\hat{U} + \Delta(X^*U) \quad \text{with} \quad \|\Delta(X^*U)\|_F \leq \sqrt{n} \gamma_n \|\hat{U}\|_2\|X\|_F, \tag{7} \]

\[ \hat{B} + \Delta \hat{B} = \hat{Q}\hat{R} \quad \text{with} \quad \|\Delta B\|_F \leq \varepsilon_{qr}\|\hat{B}\|_F \quad \text{and} \quad \|\hat{Q} - \hat{Q}\|_F \leq \varepsilon_Q, \tag{8} \]

\[ \hat{Y} := \text{fl}(X\hat{Q}) = X\hat{Q} + \Delta(X\hat{Q}) \quad \text{with} \quad \|\Delta(X\hat{Q})\|_F \leq \sqrt{n} \gamma_n \|\hat{Q}\|_2\|X\|_F, \tag{9} \]

where $\hat{V}$ and $\hat{Q}$ are unitary matrices. Moreover, if we use the one-sided Jacobi algorithm to compute SVD of $X$ in lower precision, (6) can be improved as, from [17, Proposition 4.1],

\[ X = \hat{U}\hat{\Sigma}\hat{V}^* + \Delta X \quad \text{with} \quad \|\Delta X(i,:)\|_2 \leq \varepsilon_{\text{SVD}}\|X(i,:)\|_2 \quad \text{and} \quad \|\hat{U}^*\hat{U} - I\|_F \leq \varepsilon_U. \tag{10} \]

In the above equations (6)–(10), $\varepsilon_{\text{SVD}}$ and $\varepsilon_U$ are functions of $n$ and $u_{\text{low}}$; $\gamma_n := n u/(1-n u)$, $\varepsilon_{qr}$ and $\varepsilon_Q$ are functions of $n$ and $u$. Equations (7) and (9) follow from [21, Equation 3.13] because

\[ \|\Delta(X^*U)\|_F \leq \gamma_n \|\hat{U}\|_F\|X\|_F \leq \sqrt{n} \gamma_n \|\hat{U}\|_2\|X\|_F \tag{11} \]

and it holds for $\|\Delta(X\hat{Q})\|_F$ similarly. Equation (8) is from [21, Theorem 19.4 and Equation (19.13)]. From (6), we easily obtain

\[ \|\hat{U}\|_2 \leq 1 + \varepsilon_U, \quad \|\hat{U}^*\hat{U}\|_2 \leq 1 + \varepsilon_U. \tag{12} \]

In the refinement stage of our algorithm, we apply the one-sided Jacobi algorithm to the matrix $\hat{Y}$. Thus, the speed of convergence of refinement depends on the orthogonality of $\hat{Y}$, i.e., when the columns of $\hat{Y}$ are closer to orthogonal, the convergence of the Jacobi algorithm is faster. Thus, we establish Theorem 1 to clarify how close $\hat{Y}$ is to orthogonality and to show the efficiency of our preconditioning.

**Theorem 1.** Assume that (6)–(10) hold together with

\[ \varepsilon_U\|\hat{\Sigma}\|_2\|\hat{\Sigma}^{-1}\|_2 + \sqrt{n} (\varepsilon_{\text{SVD}} + \sqrt{n} \gamma_n + \varepsilon_{qr} + \sqrt{n} \gamma_n \varepsilon_{qr})(1 + \varepsilon_U)\|X\|_2\|\hat{\Sigma}^{-1}\|_2 < \frac{\sqrt{2}}{2} - 1. \tag{13} \]

Then the matrix $\hat{Y}$ obtained by (6)–(9) satisfies the following inequality:

\[ \text{off}(\hat{\Sigma}^{-1}\hat{Y}^*\hat{Y}\hat{\Sigma}^{-1}) := \left( \sum_{i=1}^{n} \sum_{j=1,j\neq i}^{n} (\hat{\Sigma}^{-1}\hat{Y}^*\hat{Y}\hat{\Sigma}^{-1})_{ij} \right)^{1/2} \leq \frac{2(\sqrt{2} + \sqrt{3}) + 3}{1 - \varepsilon_U} \varepsilon_U + \frac{2(\sqrt{2} + \sqrt{3})(1 + \varepsilon_U)}{1 - \varepsilon_U} \sqrt{n} \varepsilon_{\text{SVD}}\|X\|_2\|\hat{\Sigma}^{-1}\|_2 \]

\[ + O(u + u^2_{\text{low}})\|X\|_2\|\hat{\Sigma}^{-1}\|_2. \tag{14} \]

Moreover, if (10) holds, then

\[ \text{off}(\hat{\Sigma}^{-1}\hat{Y}^*\hat{Y}\hat{\Sigma}^{-1}) \leq \frac{2(\sqrt{2} + \sqrt{3}) + 3}{1 - \varepsilon_U} \varepsilon_U + \frac{2(\sqrt{2} + \sqrt{3})(1 + \varepsilon_U)}{1 - \varepsilon_U} \sqrt{n} \varepsilon_{\text{SVD}}\|Z_{qr}^{-1}\|_2 \]

\[ + O(u + u^2_{\text{low}})\|X\|_2\|\hat{\Sigma}^{-1}\|_2. \tag{15} \]
with \( X = D_rZ_r \), where \( D_r \) is a diagonal matrix and each row of \( Z_r \) is a unit vector, i.e., \( Z_r \) consists of normalized rows of \( X \).

**Remark 1.** As shown in [17, Proposition 4.1], the computed SVD result of the Jacobi algorithm has rowwise backward stability. This implies that its accuracy depends primarily on the relative condition number of \( Z_r \) and maintains the validity of (10). Conversely, for the divide and conquer algorithm, compliance with (10) is typically not achieved. Note that (15) necessitates (10) in Theorem 1. Thus, the upper bound of \( \text{off}(\Sigma^{-1}Y^*Y\Sigma^{-1}) \) is primarily influenced by the condition number of \( X \) if we use the divide and conquer algorithm. If we use the Jacobi algorithm, it mainly depends on the relative condition number of \( Z_r \), which is usually much smaller than the condition number of \( X \). Thus, the matrix \( Q \) computed by the Jacobi algorithm is more accurate. This is the reason why we do not use the divide and conquer algorithm in our mixed precision algorithm.

To prove Theorem 1, we first establish Lemma 1 to reformulate (9). We use \( \text{up}(\cdot) \) and \( \text{low}(\cdot) \), respectively, to denote the strict upper and lower triangular parts plus half of the diagonal part of the matrix.

**Lemma 1.** Assume that (6)–(9) hold. Let \( E_1 = \Delta(X^*U) + \Delta B \) and \( E_Y = -\hat{U}^*E_1^*\hat{Q} + X(Q - \hat{Q}) + \Delta(X\hat{Q}) \). Then

\[
\hat{Y} = \hat{U}^*\hat{R}^* + E_Y
\]  

with

\[
\|E_1\|_F \leq \sqrt{n} (\gamma_1 + \epsilon_u) \|X\|_2 \quad \text{and} \quad \|E_Y\|_F \leq O(u)\|X\|_2,
\]

where \( \hat{R} \) satisfies

\[
\hat{Q}\hat{R} = \hat{V}\hat{\Sigma} + \hat{V}\hat{\Sigma}E_U + \Delta X^*\hat{U} + E_1
\]

where \( \hat{R} \) satisfies

\[
\hat{Q}\hat{R} = \hat{V}\hat{\Sigma} + \hat{V}\hat{\Sigma}E_U + \Delta X^*\hat{U} + E_1
\]

and \( E_1 \) satisfies

\[
\|E_1\|_F \leq \|\Delta(X^*U)\|_F + \|\Delta B\|_F
\]

\[
\leq \|\Delta(X^*U)\|_F + \epsilon_u (\|X^*\hat{U}\|_F + \|\Delta(X^*U)\|_F)
\]

\[
\leq \sqrt{n} (\gamma_1 + \epsilon_u) \|X\|_2.
\]

Furthermore, by (20), we have

\[
X\hat{Q} = \hat{U}^*\hat{R}^* - \hat{U}^*E_1^*\hat{Q}.
\]

Combined with (19), we obtain (16) and (17) because

\[
\|E_Y\|_F \leq (1 + \epsilon_u)\|E_1\|_F + \epsilon_Q\|X\|_2 + \sqrt{n} \gamma_1 \|X\|_2 \|\hat{Q}\|_F \leq O(u)\|X\|_2.
\]

Note that \( \hat{R} \) is the computed \( R \)-factor in the QR factorization of \( X^*\hat{U} + E_1 \) by (20). Then

\[
\hat{Q}\hat{R} = X^*\hat{U} + E_1
\]

\[
= V\hat{\Sigma} + \hat{V}\hat{\Sigma}E_U + \Delta X^*\hat{U} + E_1
\]

\[
= V\hat{\Sigma}(I + \text{up}(E_U)) + \hat{V}\hat{\Sigma}\text{low}(E_U) + \Delta X^*\hat{U} + E_1.
\]

\[
\hat{Q}\hat{R} = X^*\hat{U} + E_1
\]

\[
= V\hat{\Sigma} + \hat{V}\hat{\Sigma}E_U + \Delta X^*\hat{U} + E_1
\]

\[
= V\hat{\Sigma}(I + \text{up}(E_U)) + \hat{V}\hat{\Sigma}\text{low}(E_U) + \Delta X^*\hat{U} + E_1.
\]
From the proof of Lemma 1, the matrix \( \hat{R} \) is also the \( R \)-factor in the QR factorization of \( \hat{V}^* (X^* \hat{U} + E_1) \). Then, according to (18a), we have

\[
\hat{V}^* \hat{Q} \hat{R} = \hat{\Sigma} + F_1
\]

with \( F_1 = \hat{\Sigma} E_U + \hat{V}^* \Delta X^* \hat{U} + \hat{V}^* E_1 \). Equation (23) can be viewed as a perturbed QR factorization. The following Lemma 2, which is derived from [10, Theorem 6.1], provides a useful tool to handle the QR factorization of a perturbed matrix.

**Lemma 2.** Let \( X \in \mathbb{R}^{n \times n} \) be of full column rank. The QR factorization of \( X \) is \( X = QR \). Suppose that \( F \in \mathbb{R}^{n \times n} \) satisfies \( \|X| \cdot |F\|_2 < 1 \) and \( \|FR^{-1}\| < \sqrt{3/2} - 1 \). Then \( X + F \) has the unique QR factorization \( X + F = (Q + \Delta Q)(R + \Delta R) \)

with
\[
\|\Delta RR^{-1}\|_F \leq (\sqrt{2} + \sqrt{3}) \|FR^{-1}\|_F.
\]

Moreover, if \( Q = I \) and \( RR^{-1}_D \) is diagonal, then
\[
\|\Delta R\|_F \leq 8\|F\|_F\|RR^{-1}_D\|_2\|R_D\|_2.
\]

**Proof.** The first statement is a direct consequence of [10, Theorem 6.1]. Thus, we only need to prove the second one.

Let \( D = RR^{-1}_D \). According to [10, Section 6], we have
\[
\Delta RR^{-1}_D = \text{up}(FR^{-1}_D + D^{-1}R^{-1}_D F^* D + D^{-1}R^{-1}_D (F^* F - \Delta R^* \Delta R) R^{-1}_D).
\]

Combined with the first statement, it holds that
\[
\|\Delta RR^{-1}_D\|_F \\
\leq \|FR^{-1}_D\|_F + \|D^{-1}\text{up}(R^{-1}_D F^* D)\|_F + \|FR^{-1}_D D^{-1}\|_F\|FR^{-1}_D\|_F + \|\Delta RR^{-1}_D D^{-1}\|_F\|\Delta RR^{-1}_D\|_F \\
\leq 2\|FR^{-1}_D\|_F + \|FR^{-1}_D D^{-1}\|_F\|FR^{-1}_D\|_F + (\sqrt{2} + \sqrt{3})\|FR^{-1}_D D^{-1}\|_F\|\Delta RR^{-1}_D\|_F.
\]

Under the assumption \( \|FR^{-1}\|_F \leq \sqrt{3/2} - 1 \), \( \|\Delta RR^{-1}_D\|_F \) can be bounded by
\[
\|\Delta RR^{-1}_D\|_F \leq \frac{2 + \|FR^{-1}\|_F}{\sqrt{2} + \sqrt{3}}\|FR^{-1}_D\|_F < 8\|FR^{-1}_D\|_F \leq 8\|F\|_F\|RR^{-1}_D\|_2
\]
and \( \|\Delta R\|_F \leq \|\Delta RR^{-1}_D\|_F\|R_D\|_2 \). This completes the proof.

With the aid of Lemmas 1 and 2, we are ready to prove Theorem 1.

**Proof of Theorem 1.** By (18b), we have
\[
\hat{\Sigma} (I + \text{up}(E_U)) + \hat{\Sigma} \text{low}(E_U) + \hat{V}^* \Delta X^* \hat{U} + \hat{V}^* E_1 = \hat{V}^* \hat{Q} \hat{R} = (Q + \Delta Q)(R + \Delta R)
\]

with \( Q = I \) and \( R = \hat{\Sigma} (I + \text{up}(E_U)) \). Similarly to (31), we conclude by (16) and (24) that
\[
\text{off}(\hat{\Sigma}^{-1} \hat{V}^* \hat{\Sigma}^{-1}) \leq \frac{1}{1 - \varepsilon_U} \left( \|\hat{\Sigma}^{-1} \Delta R\|_F^2 + 2(1 + \varepsilon_U)\|\hat{\Sigma}^{-1} \Delta R\|_F + 2\varepsilon_U + \frac{\varepsilon_U}{1 - \varepsilon_U} + O(u^2_{\text{low}}) + 2(1 + \varepsilon_U)(1 + \varepsilon_U + \|\hat{\Sigma}^{-1} \Delta R\|_F)\|E_Y\|_F \|\hat{\Sigma}^{-1}\|_2 + \|E_Y\|_F \|\hat{\Sigma}^{-1}\|_2 \right).
\]

(25)
Then we only need to estimate $\|\hat{\Sigma}^{-1} \Delta R\|_F$.

Since the diagonal elements of $\hat{\Sigma}$ are in descending order and $\Delta R$ is an upper triangular matrix, we have

$$\|\hat{\Sigma}^{-1} \Delta R\|_F \leq \|\hat{\Sigma}^{-1} \Delta R \hat{\Sigma} \|_F \leq \|\Delta R \hat{\Sigma}^{-1}\|_F. \tag{26}$$

The relationship between $\Delta R \hat{\Sigma}^{-1}$ and $\Delta R \hat{\Sigma}^{-1}$ is

$$\Delta R \hat{\Sigma}^{-1} = \Delta R(I + \text{up}(E_U))^{-1} - 1) \hat{\Sigma}^{-1}.$$ 

Combined with (26), it follows that

$$\|\hat{\Sigma}^{-1} \Delta R\|_F \leq \|\Delta R \hat{\Sigma}^{-1}\|_F + \frac{\epsilon_U}{1 - \epsilon_U} \|\Delta R\|_F \|\hat{\Sigma}^{-1}\|_2 \tag{27}$$

Note that (24) and the assumption (13) allow us to apply Lemma 2 to bound $\|\Delta R\|_F$ and $\|\Delta R \hat{\Sigma}^{-1}\|_F$, i.e.,

$$\|\Delta R\|_F \leq 8 \frac{1 + \epsilon_U}{1 - \epsilon_U} \|\hat{\Sigma} \text{low}(E_U) + \bar{V}^* X^* \bar{U} + \bar{V}^* E_1\|_F$$

$$\leq 8 \frac{1 + \epsilon_U}{1 - \epsilon_U} (\|\hat{\Sigma} \text{low}(E_U)\|_F + \|\Delta X^* \bar{U}\|_F + \|E_1\|_F)$$

$$\leq 8 \frac{1 + \epsilon_U}{1 - \epsilon_U} (\epsilon_U \|\hat{\Sigma}\|_F + \sqrt{n}(1 + \epsilon_U)(\epsilon_{SVD} + \sqrt{n} \gamma_n + \epsilon_{qr} + \sqrt{n} \gamma_n \epsilon_{qr})\|X\|_2 + \Delta R \hat{\Sigma}^{-1} \|_F \|\hat{\Sigma}^{-1}\|_2)$$

and

$$\|\Delta R \hat{\Sigma}^{-1}\|_F \leq (\sqrt{2} + \sqrt{3}) (\|\hat{\Sigma} \text{low}(E_U) + \bar{V}^* X^* \bar{U} + \bar{V}^* E_1\|_F$$

$$\leq (\sqrt{2} + \sqrt{3}) (\|\hat{\Sigma} \text{low}(E_U)\|_F + \|\Delta X^* \bar{U}\|_F + \|E_1\|_F)$$

$$\leq (\sqrt{2} + \sqrt{3}) (\epsilon_U + \|\Delta X^* \bar{U}\|_F + O(\|X\|_2) \|\hat{\Sigma}^{-1}\|_2) \|\hat{\Sigma}^{-1}\|_2.$$ 

It remains to estimate $\|\Delta X^* \bar{U} \hat{\Sigma}^{-1}\|_F$. By (6), we obtain

$$\|\Delta X^* \bar{U} \hat{\Sigma}^{-1}\|_F \leq \sqrt{n} \epsilon_{SVD}(1 + \epsilon_U)\|X\|_2 \|\hat{\Sigma}^{-1}\|_2.$$

Combined with (25), we conclude (14).

Further, if (10) holds, we can obtain

$$\|\Delta X^* \bar{U} \hat{\Sigma}^{-1}\|_F = \|\hat{\Sigma}^{-1} \bar{U}^* \Delta X\|_F$$

$$= \|\hat{\Sigma}^{-1} (\bar{U}^* \Delta X)\|_F$$

$$\leq \|\bar{V} \hat{\Sigma}^{-1} \bar{U} \Delta X\|_F + \|\hat{\Sigma}^{-1} \bar{U} \Delta X\|_F$$

$$\leq \|\bar{V} \hat{\Sigma}^{-1} \bar{U} \Delta X\|_F + \|\Delta X^* \bar{U}\|_F + O(\|X\|_2) \|\hat{\Sigma}^{-1}\|_2$$

Together with

$$\|X^{-1} \Delta X\|_F \leq \sqrt{n} \epsilon_{SVD} \|Z_r^{-1}\|_2,$$

we have

$$\|\Delta X^* \bar{U} \hat{\Sigma}^{-1}\|_F \leq \sqrt{n} \epsilon_{SVD} \|Z_r^{-1}\|_2 + O(\|u_{low} + u\|_2) \|\hat{\Sigma}^{-1}\|_2.$$ 

Combined with (25), we arrive at (15) because

$$\|\hat{\Sigma}^{-1} \Delta R\|_F \leq (\sqrt{2} + \sqrt{3}) \epsilon_U + \sqrt{n} \epsilon_{SVD} \|Z_r^{-1}\|_2 + O(\|u_{low} + u\|_2) \|\hat{\Sigma}^{-1}\|_2. \tag{28}$$
The effectiveness of our mixed precision Jacobi SVD algorithm is largely based on the quadratic convergence of the Jacobi algorithm. Our mixed precision Jacobi SVD algorithm also inherits this property under mild assumptions. In order to show this, we first derive the following theorem.

**Theorem 2.** Assume that (6)–(9) hold together with
\[ \varepsilon_U \| \hat{\Sigma} \|_2 \| \hat{\Sigma}^{-1} \|_2 + \sqrt{n} (\varepsilon_{\text{SVD}} + \sqrt{n} \gamma_n + \varepsilon_{\text{qr}} + \sqrt{n} \gamma_n \varepsilon_{\text{qr}}) (1 + \varepsilon_U) \| X \|_2 \| \hat{\Sigma}^{-1} \|_2 < \sqrt{\frac{3}{2}} - 1. \] (29)

Then the matrix \( \hat{Y} \) obtained by (9) satisfies
\[ \text{off}(\hat{Y}^* \hat{Y}) := \left( \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} |(\hat{Y}^* \hat{Y})_{ij}|^2 \right)^{1/2} \leq \delta, \]
where
\[ \delta = \frac{17 \varepsilon_U}{1 - \varepsilon_U} \| \hat{\Sigma} \|_2^2 + \frac{16(1 + \varepsilon_U)}{1 - \varepsilon_U} \sqrt{n} \varepsilon_{\text{SVD}} \| X \|_2 \| \hat{\Sigma} \|_2 + O(u + u_{\text{low}}^2) \| X \|_2 \| \hat{\Sigma} \|_2. \] (30)

**Proof.** By (16) and (23), we have
\[ \text{off}(\hat{Y}^* \hat{Y}) \leq \text{off}(\hat{R}^* \hat{U}^* \hat{U}^{-1} \hat{R}^*) + 2(1 + \varepsilon_U) \| \hat{R} \|_2 \| E_Y \|_F + \| E_Y \|_F^2 \]
\[ \leq \text{off}((\Delta R + \hat{\Sigma})(I + E_U)^{-1}(\Delta R^* + \hat{\Sigma}^*)) + 2(1 + \varepsilon_U) \| \hat{R} \|_2 \| E_Y \|_F + \| E_Y \|_F^2 \]
\[ \leq \frac{1}{1 - \varepsilon_U} \| \Delta R \|_F^2 + 2 \| \Delta R \|_F \| \hat{\Sigma} \|_2 + \frac{\varepsilon_U}{1 - \varepsilon_U} \| \hat{\Sigma} \|_2^2 \]
\[ + 2(1 + \varepsilon_U) (\| \hat{\Sigma} \|_2 + \| \Delta R \|_F) \| E_Y \|_F + \| E_Y \|_F^2. \] (31)

Then we only need to estimate \( \| \Delta R \|_F \). By (21), it follows that
\[ \| \Delta R \|_F \leq 8 \| F_1 \|_F \]
\[ \leq 8 \varepsilon_U \| \hat{\Sigma} \|_2 + (1 + \varepsilon_U) \varepsilon_{\text{SVD}} \| X \|_2 + \| E_1 \|_F \]
\[ \leq 8 \varepsilon_U \| \hat{\Sigma} \|_2 + 8(1 + \varepsilon_U) \varepsilon_{\text{SVD}} \| X \|_2 + O(u) \| X \|_2. \]

Substituting this estimate into (31) yields the conclusion. \( \square \)

Using Theorem 2 and the theory developed in [31], we obtain Theorem 3 on quadratic convergence. Although rounding error is not taken into account, Theorem 3 still provides an explanation for the rapid convergence of our mixed precision Jacobi SVD algorithm after switch from lower precision back to working precision.

**Theorem 3.** Let \( Y^{(k)} \) be the matrix \( \hat{Y} \) after \( k \) Jacobi sweeps. If
\[ 4\sqrt{2} \delta < d \leq \min_{\sigma_i(Y^{(k)}) \neq \sigma_j(Y^{(k)})} \left| \sigma_i^2(Y^{(k)}) - \sigma_j^2(Y^{(k)}) \right|, \]
where \( \delta \) is defined in (30), then
\[ \text{off}((Y^{(k+1)})^* Y^{(k+1)}) \leq \frac{\sqrt{34}}{3d} \left( \text{off}((Y^{(k)})^* Y^{(k)}) \right)^2. \]

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6 Efficiency of the method to switch precisions

In the discussion of Section 3.3, we have mentioned two methods to switch precisions: one is

\[ B \leftarrow X^*U, \quad Q_1R_1 \leftarrow B, \quad Y_1 \leftarrow XQ_1, \]

the other is

\[ Q_2R_2 \leftarrow V, \quad Y_2 \leftarrow XQ_2, \]

where \( U \) and \( V \) satisfy \( X = USV^* \). Although mathematically we have \( Q_1 = Q_2 \) and \( Y_1 = Y_2 \) in exact arithmetic, the computed results are different if rounding errors are taken into account. We use subscripts to represent computed results by different methods.

In practice the second method is more costly because \( V \) needs to be accumulated. Hence the first method is preferred from a performance viewpoint. In the following we show that \( Y_1 \) is better than \( Y_2 \) in finite precision arithmetic, in the sense that the columns of \( Y_1 \) are more orthogonal.

Let us regard the result computed in working precision as the accurate one. Suppose the computed quantities computed by these two methods satisfy

\[ X^*\hat{U} = Q_1R_1, \quad Y_1 = XQ_1, \tag{32} \]

and

\[ Y_2 = XV, \tag{33} \]

respectively, where \( \hat{U} \) and \( \tilde{V} \) satisfy (10). Theorem 4 characterizes the orthogonality of \( Y_1 \) and \( Y_2 \) after normalizing the columns.

**Theorem 4.** Under the assumptions that (10), (13), (32) and (33), it holds that

\[ \| Y_1\hat{\Sigma}^{-1} - \hat{U}\|_2 \leq \varepsilon_U (1 + \varepsilon_U) (\sqrt{2} + \sqrt{3}) (\varepsilon_U + \sqrt{n} \varepsilon_{\text{SVD}} \| Z^{-1}_r \|_2) \]

and

\[ \| Y_2\tilde{\Sigma}^{-1} - \hat{U}\|_2 \leq n \varepsilon_{\text{SVD}} \| X \|_2 \| \hat{\Sigma}^{-1} \|_2. \]

**Proof.** First we analyze \( Y_1 \) computed by the first method. By Lemma 1 and the assumptions, we easily obtain

\[ Y_1 = \hat{U}^{-*} \hat{R}^* = \hat{U}^{-*} (I + \text{up}(E_U)^*) \hat{\Sigma} + \hat{U}^{-*} \Delta R^* = \hat{U}^{-*} (I + \text{up}(E_U)^* + \Delta R^* \hat{\Sigma}^{-1}) \hat{\Sigma} \]

with \( \Delta R = \hat{R} - \hat{\Sigma}(I + \text{up}(E_U)) \). Similarly to (28), we draw the first conclusion because

\[ \| Y_1(:,i)\|_2 \leq \| \hat{U}^{-*}\|_2 \| I + \text{up}(E_U)^* + \Delta R^* \hat{\Sigma}^{-1}\|_2 \| \hat{\Sigma}(;i)\|_2 \]

\[ \leq (1 + \varepsilon_U) (1 + \varepsilon_U + (\sqrt{2} + \sqrt{3}) (\varepsilon_U + \sqrt{n} \varepsilon_{\text{SVD}} \| Z^{-1}_r \|_2)) \| \hat{\Sigma}(;i)\|_2. \]

Considering \( Y_2 \) computed by the second method, we have

\[ Y_2 = XV = \hat{U} \hat{\Sigma} + \Delta XV \]

and then

\[ Y_2\hat{\Sigma}^{-1} = \hat{U} + \Delta XV \hat{\Sigma}^{-1}. \]

Together with

\[ \| \Delta XV \hat{\Sigma}^{-1}\|_2 \leq n \varepsilon_{\text{SVD}} \| X \|_2 \| \hat{\Sigma}^{-1} \|_2, \]

we conclude the proof.

\[ \square \]
Theorem 4 shows that both $Y_1 \hat{\Sigma}^{-1}$ and $Y_2 \hat{\Sigma}^{-1}$ are close to have orthogonal columns. However, because $\|Z_r^{-1}\|_2$ is often much smaller than $\|X\|_2 \|\hat{\Sigma}^{-1}\|_2$, the columns of $Y_1$ are thus more orthogonal compared to those of $Y_2$. Therefore, the first method is preferred both computationally and numerically.

7 Numerical Experiments

In this section we present numerical experiments on the x86-64 architecture of our mixed precision algorithm described in Algorithm 4. We choose IEEE double precision as the working precision, and IEEE single precision as the lower precision. Our implementation is derived from XGEJSV and XGESVJ in LAPACK version 3.9.0, and makes use of XGEQRF, XGEQP3, xGESVJ, and xGESVD for the computations in single precision, where $X \in \{D, Z\}$ and $x \in \{S, C\}$. All experiments have been performed on a Linux cluster with two twelve-core Intel Xeon E5-2670 v3 2.30 GHz CPUs and 128 GB of main memory. Programs are compiled using the GNU Fortran compiler version 6.3.1 with optimization flag -O2, and are linked with the OpenBLAS library version 0.3.9.

7.1 Experiment settings

In the following, we compare Algorithm 4 with the double precision solver XGEJSV in LAPACK. XGEJSV is a good implementation of Algorithm 2, which mainly consists of two stages: QR preconditioning and the one-sided Jacobi SVD algorithm (i.e., Algorithm 1). In LAPACK, Algorithm 1 is implemented in XGESVJ.

All left and right singular vectors are explicitly requested in these solvers. We report the relative run time, which is the ratio of the wall clock time of a solver (or its components) over that consumed by XGEJSV. There are several tunable parameters required by Algorithm 4. In the following experiments, we choose these parameters as follows: $\text{tol}_\text{alg} = 10^{-2}$, $\text{tol}_\text{orth} = 10^{-5}$, $\text{tol}_\text{cond} = 1.5 \cdot n^{1/4}$.

In performance plots, the labels ‘QR pre’, ‘xGESVD/xGESVJ’, ‘switch’ and ‘XGESVJ’, respectively, represent the four components of Algorithm 4: QR preconditioning, the single precision SVD algorithm as a preconditioning, switching precisions, and the double precision one-sided Jacobi SVD algorithm as a refinement. Moreover, the numbers in the bar mean the number of sweeps performed by the one-sided Jacobi SVD algorithm (in the working precision).

Similar to [18], the test matrices are randomly generated matrices of the form $A = BD$, where $B$ is with unit column norms and $D$ is a diagonal matrix. We can prescribe the condition numbers of $D$ and $B$ as follows. We first use XLATM1 to generate two diagonal matrices $D$ and $\Sigma$ with given condition numbers $\kappa(D)$ and $\kappa(\Sigma)$, respectively. Then the matrix $B$ is constructed through $B = W_1 \Sigma W_2 W_3$, where $W_1$ and $W_2$ are unitary factors in the QR factorization of randomly generated matrices, and $W_3$ is carefully chosen so that $B$ has unit column norms [9, 11].

In our experiments, we test 16 combinations of $\kappa(D)$ and $\kappa(B)$ as shown in Table 1. The parameter MODE is used by XLATM1 to specify different types of test matrices; see Table 2 for details. Both square and rectangular matrices are tested. For square matrices, we choose two typical cases: $\kappa(D)$, $\kappa(B) = (10^2, 10^{12})$ and $\kappa(D)$, $\kappa(B) = (10^{20}, 10^{12})$; for rectangular matrices, we only test the case $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$.

7.2 Performance tests of the basic mixed precision Jacobi SVD algorithm

We first show the performance of the basic mixed precision algorithm (Algorithm 3) in Figure 1. It can be seen that Algorithm 3 only can achieve about $1.1 \times 1.4 \times$ speedup compared to DGEJSV.
Table 1: The description of different types of test matrices.

| ID of matrices | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|----------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| MODE of $D$   | 1  | 1  | 1  | 2  | 2  | 2  | 8  | 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| MODE of $\Sigma$ | 2  | 3  | 4  | 5  | 3  | 4  | 5  | 2  | 3  | 5  | 2  | 3  | 4  |   |   |   |

Table 2: Explanation of different modes of $\text{XLATM1}$ for generating $D = \text{diag}(d)$.

| MODE | Description |
|------|-------------|
| 1    | clustered at $1/\kappa$, where $d(1) = 1$, $d(2:n) = 1/\kappa$ |
| 2    | clustered at 1, where $d(1:n-1) = 1$, $d(n) = 1/\kappa$ |
| 3    | Geometric distribution, where $d(i) = 1/\kappa^{(i-1)/(n-1)}$ |
| 4    | Arithmetic distribution, where $d(i) = 1 - (i-1)/(n-1)(1 - 1/\kappa)$ |
| 5    | Log-random distribution, where $d(i) \in (1/\kappa, 1)$ so that their logarithms are random and uniformly distributed |

Figure 1: Relative run time of Algorithm 3 for $4096 \times 4096$ real matrices with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.

This is far below the ideal speedup on the x86-64 architecture, which is $2 \times$. In fact, we can see from Figure 1 that the computation in single precision does not effectively accelerate the convergence in double precision because the refinement stage (Line 4) still requires too many Jacobi iterations to converge. Therefore, Algorithm 3 is not very satisfactory.

7.3 Performance tests of the mixed precision RRQR algorithm

In this subsection, we show the relative run time of Algorithm 5 in Figures 2 and 3. It can be seen that the speedup of Algorithm 5 over LAPACK's $\text{DGEQP3}$ depends on the test matrices. For most matrices it achieves about $2 \times$ speedup in general. Therefore, it is worth developing a mixed precision algorithm for RRQR.
7.4 Performance tests of the mixed precision Jacobi SVD algorithm

Figures 4 and 5 show the relative run time of the SVD for 4096 × 4096 real matrices computed by Algorithm 4. It can be seen that when $\kappa(D)$ is moderate, Algorithm 4 achieves about 2× speedup in general compared to DGEJSV. There are several cases (ID ∈ {8, 11, 14}) that the speedup is only about 20%. These matrices are all generated with $\text{MODE}(\Sigma) = 2$. In these cases, the QR preconditioning stage is very effective so that after preconditioning the columns of $X$ are close to orthogonal with $X(:,i)^*X(:,j) \approx 10^{-2}$ for $i \neq j$. However, it still takes a lot of effort for the single precision Jacobi SVD algorithm to improve the orthogonality from $O(10^{-2})$ to $O(10^{-6})$. Thus, the performance gain for using a mixed precision algorithm is limited for these cases.
When \( \kappa(D) \) is extremely large, there are more cases that the run time of Algorithm 4 is almost the same as that of \textsc{dgejsv} as shown in Figure 5. In these cases, the QR preconditioning stage is sufficiently effective, so that the one-sided Jacobi algorithm in double precision can converge very rapidly after preconditioning, making the SVD in single precision useless. By the techniques mentioned in Section 3.5, we can detect these cases in an early stage and directly move on to the double precision Jacobi SVD algorithm. Algorithm 4 is still slightly faster than \textsc{dgejsv}, because the time spent on the RRQR algorithm is reduced by exploiting mixed precision techniques.
Similar results for 4096 × 4096 complex matrices are shown in Figures 6 and 7. The speedup of Algorithm 4 over ZGEJSV is about 2× for most matrices, while those generated by MODE(Σ) = 2 have much lower speedup. For a few test matrices the speedup is even higher than 3×, mainly because ZGEJSV ran into a conservative branch that requires accumulating V explicitly. Algorithm 4 safely avoids the accumulation of V in these cases.

Figure 8 shows the relative run time for rectangular matrices of size 12288 × 4096 with (κ(D), κ(B)) = (10^{20}, 10^{12}). The behavior is very similar to that for square matrices. A 2×
speedup is observed for most matrices, except for those generated by \texttt{MODE}(\Sigma) = 2.

In Figure 9, we use double–double\(^9\) and IEEE double precision as our working and lower precisions, respectively, to show the relative run time of Algorithm 4 for square matrices of size 1024 \(\times\) 1024 with \((\kappa(D), \kappa(B)) = (10^2, 10^{12})\). In this case, we use the subroutine of MPLAPACK (see [27]) to perform double–double operations. Since the level 3 BLAS in MPLAPACK is not well-optimized, the proportion of QR preconditioning and switching precision is very large. But it still can be seen that our mixed precision algorithm effectively accelerates the one-sided Jacobi SVD algorithm.

We have tested our mixed precision algorithms for a number of matrices with different sizes. These test results can be found in the Appendix.

7.5 Accuracy tests

In this subsection, we demonstrate that Algorithm 4 computes singular values to satisfactory relative accuracy.

We test 16 types of 1024 \(\times\) 1024 matrices as in Table 1 with \((\kappa(D), \kappa(B)) = (10^{20}, 10^9)\) and measure the accuracy of the computed singular values. Let \(\hat{\lambda}_i^{\text{Alg4}}\)’s and \(\hat{\lambda}_i^{\text{GEJSV}}\)’s, respectively, be the computed singular values by Algorithm 4 and \texttt{DGEJSV}. We measure the relative difference between \(\hat{\lambda}_i^{\text{Alg4}}\) and \(\hat{\lambda}_i^{\text{GEJSV}}\) by

\[
\left| \frac{\hat{\lambda}_i^{\text{Alg4}} - \hat{\lambda}_i^{\text{GEJSV}}}{\hat{\lambda}_i^{\text{GEJSV}}} \right|
\]

The maximum relative difference observed in our experiments is \(4.79 \times 10^{-14}\).

We also measure the backward error

\[
\max_i \left\{ \frac{\| (A - U\Sigma V^*)(:, i) \|_2}{\| A(:, i) \|_2} \right\}
\]

\(^9\)Double–double is a multiple-component format floating-point number, represented by two 64-bit floating-point numbers. See, e.g., [20].
and the orthogonality of $U$ and $V$ by
\[ \|U^*U - I\|_F, \quad \|V^*V - I\|_F. \]
the largest values of these quantities are $3.21 \times 10^{-14}$, $5.85 \times 10^{-12}$, and $9.07 \times 10^{-13}$, respectively. Therefore, Algorithm 4, as a mixed precision algorithm, achieves the same level of relative accuracy compared to DGEJSV.

### 7.6 Tests of different switching precisions methods

In this subsection, we test several methods for switching precisions using test matrices with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$. We compare three methods as follows.

1. Compute $X = U\Sigma V^*$ in single precision by the Jacobi SVD algorithm, and then obtain $Y \leftarrow XQ$, where $Q$ is $Q$-factor in the QR factorization of $X^*U$.

2. Compute $X = U\Sigma V^*$ in single precision by the Jacobi SVD algorithm, and then obtain $Y \leftarrow XQ$, where $Q$ is $Q$-factor in the QR factorization of $V$.

3. Compute $X = U\Sigma V^*$ in single precision by the divide and conquer algorithm, and then obtain $Y \leftarrow XQ$, where $Q$ is $Q$-factor in the QR factorization of $X^*U$.

In Figure 10, we see that the first method is the most accurate one. The first method is better than the second one, which is consistent with the prediction made by Theorem 4. The divide and conquer algorithm is not a good choice here since the columns of $Y$ are far from orthogonal.

### 8 Conclusions

In this paper we propose a mixed precision one-sided Jacobi SVD algorithm. Our algorithm uses QR preconditioning and SVD in a lower precision to produce an initial guess, and then use the
one-sided Jacobi SVD algorithm in working precision to refine the solution. Special care is taken in converting the solution from lower precision to working precision so that the transformed solution is reasonably accurate and enables fast convergence in the refinement process. On the x86-64 architecture our algorithm achieves about $2 \times$ speedup compared to DGEJSV/ZGEJSV in LAPACK for most test matrices. Though a large portion of computations is performed in single precision, the final solution is as accurate as that produced by double precision solvers DGEJSV/ZGEJSV. This is confirmed both theoretically and experimentally.

Our numerical experiments were performed on the x86-64 architecture, where single precision arithmetic is usually twice faster compared to double precision arithmetic. The situation becomes different on modern GPUs—the performance gap between lower and higher precision arithmetic is often far larger than $2 \times$, and more floating-point formats (fp64, fp32, fp16, etc.) are available. We expect that our algorithm will likely achieve higher speedup on GPUs. High performance implementations of the mixed precision Jacobi SVD algorithm on GPUs is planned as our future work.

Finally, we remark that it is possible to develop a mixed precision Jacobi algorithm that computes the spectral decomposition of a Hermitian matrix. A preliminary discussion can be found in Appendix B.

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A Supplementary experiments for SVD problem

In the following we provide more numerical experiments of the mixed precision Jacobi algorithm. In the figures of this section, the $x$-axis represents the size of test matrices and the $y$-axis represents the relative run time of Algorithm 4 comparing with XGEJSV in LAPACK.

Figures 11 and 12 show the relative run time for different sizes $\{2048, 4096, 6144, 8192\}$ real square matrices with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$ and $(\kappa(D), \kappa(B)) = (10^{20}, 10^2)$, respectively. Similarly, Figures 13 and 14 show the relative run time for different sizes $\{2048, 4096, 6144, 8192\}$ complex square matrices with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$ and $(\kappa(D), \kappa(B)) = (10^{20}, 10^2)$, respectively. Figure 15 shows the relative run time for different sizes $\{6144 \times 2048, 12288 \times 4096, 18432 \times 6144\}$ real rectangular matrices with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$.

B Jacobi SVD method for symmetric eigenvalue problem

We consider the symmetric eigenvalue problem

$$AX = X\Lambda,$$

where $A$ is a given Hermitian matrix and $\Lambda$ is a diagonal matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$. It is possible to use, for instance, the QR algorithm to compute an approximate spectral decomposition in lower precision, and then use the Jacobi algorithm to refine the solution in working precision. This mixed precision approach, which is essentially a Jacobi algorithm, is preferred when high relative accuracy of the spectrum is of interest. However, since two-sided Jacobi eigenvalue algorithm has very low efficiency, we consider applying the one-sided Jacobi SVD algorithm in the refinement stage.

Suppose that the SVD of $A$ is $A = U \Sigma V^\ast$. A simple case is that $A$ is either positive semidefinite or negative semidefinite. In this case $\Lambda = U^\ast AU$ is diagonal, so that the output from the one-sided Jacobi SVD algorithm can be directly used. Complication occurs when $A$ is indefinite. Let $\sigma_1 > \sigma_2 > \cdots > \sigma_m$ be the distinct singular values of $A$ without counting multiplicity. Then we have

$$\tilde{A} = U^\ast AU = \begin{bmatrix} \tilde{A}_1 & \tilde{A}_2 & \cdots & \tilde{A}_m \end{bmatrix},$$

where the size of each diagonal block $\tilde{A}_i$ is the multiplicity of the singular value $\sigma_i$, so that both $\sigma_i$ and $-\sigma_i$ can possibly be eigenvalues of $A$. We can identify the size of these diagonal blocks by computing the gap of consecutive singular values—if two singular values are really close, they are regarded as the same. Then each diagonal block is further diagonalized through a usual symmetric eigensolver in working precision. This step is expected to be modestly cheap unless $A^2$ has some eigenvalues with very high multiplicity. Finally, as a postprocessing step, the eigenvalues of $A$ are sorted in ascending order to match the output format of a usual symmetric eigensolver.
Figure 11: Relative run time of Algorithm 4 with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$ for real square matrices of different sizes $\{2048, 4096, 6144, 8192\}$. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.
Figure 12: Relative run time of Algorithm 4 with $(\kappa(D), \kappa(B)) = (10^{20}, 10^2)$ for real square matrices of different sizes \{2048, 4096, 6144, 8192\}. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.
Figure 13: Relative run time of Algorithm 4 with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$ for complex square matrices of different sizes \{2048, 4096, 6144, 8192\}. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.
Figure 14: Relative run time of Algorithm 4 with $(\kappa(D), \kappa(B)) = (10^{20}, 10^2)$ for complex square matrices of different sizes \{2048, 4096, 6144, 8192\}. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.
Figure 15: Relative run time of Algorithm 4 with $(\kappa(D), \kappa(B)) = (10^2, 10^{12})$ for real rectangular matrices of different sizes \{6144 × 2048, 12288 × 4096, 18432 × 6144\}. The numbers in the bars denote the numbers of iterations required by the Jacobi algorithm.
Algorithm 6 Mixed precision algorithm for symmetric eigenvalue problem

Input: An \( n \times n \) Hermitian matrix \( A \).
Output: The spectral decomposition of \( A \).

1. Compute the spectral decomposition of \( \text{lower}(A) \), i.e., \( \text{lower}(A) = X_{\text{low}} \Lambda_{\text{low}} X_{\text{low}}^* \).
2. Orthogonalize the columns of \( X_{\text{low}} \) in working precision, \( \text{working}(X_{\text{low}}) = QR \), where \( R \) is not explicitly formed.
3. Apply the one-sided Jacobi SVD algorithm to \( AQ \) to obtain \( AQ = U \Sigma V^* \), where \( V \) is not explicitly formed.
4. Identify the block structure (34).
5. Diagonalize each diagonal block \( \tilde{A}_i \), and accumulate the corresponding unitary transformation on \( U \).
6. Reorder the eigenvalues and eigenvectors of \( A \).

We implement the mixed precision one-sided Jacobi eigenvalue algorithm (i.e., Algorithm 6) based on LAPACK subroutines \texttt{xSYEVD} and \texttt{XGEJSV}. Then test matrices with parameters \( \text{MODE}_C = 4 \), \( \kappa(B) = 10^{16} \) and \( \kappa(D) = 1 \), i.e. \( A = B \), are used to compare Algorithm 6 with the QR algorithm in terms of accuracy.

From Figure 16, we can see that Algorithm 6 is more accurate than the QR algorithm, especially for eigenvalues with small magnitude. However, we remark that Algorithm 6 is slower than any popular dense symmetric eigensolver. We observe that, compared to \texttt{DSYEV} in LAPACK, Algorithm 6 is usually much slower on CPU; see Figure 17. Thus, Algorithm 6 is of interest only when eigenvalues need to be computed to high relative accuracy.

Figure 16: Relative error of computed eigenvalues of a \( 1024 \times 1024 \) real symmetric matrix. Left: Relative errors computed by Jacobi and QR algorithms. Right: ratio of the relative error of the mixed precision Jacobi algorithm to that of the QR algorithm for each individual eigenvalue.
Figure 17: Relative run time of Algorithm 6 with $\kappa(A) = 10^{15}$ for real symmetric matrices of the size 2048. Different MODEs represent different eigenvalue distributions; see Table 2. For MODE = 1 or 5, the relative run time exceeds 2, rendering it impractical, so the excess was disregarded.