Computing the Singular Value Decomposition with High Relative Accuracy

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Abstract

We analyze when it is possible to compute the singular values and singular vectors of a matrix with high relative accuracy. This means that each computed singular value is guaranteed to have some correct digits, even if the singular values have widely varying magnitudes. This is in contrast to the absolute accuracy provided by conventional backward stable algorithms, which in general only guarantee correct digits in the singular values with large enough magnitudes. It is of interest to compute the tiniest singular values with several correct digits, because in some cases, such as finite element problems and quantum mechanics, it is the smallest singular values that have physical meaning, and should be determined accurately by the data. Many recent papers have identified special classes of matrices where high relative accuracy is possible, since it is not possible in general. The perturbation theory and algorithms for these matrix classes have been quite different, motivating us to seek a common perturbation theory and common algorithm. We provide these in this paper, and show that high relative accuracy is possible in many new cases as well. The briefest way to describe our results is that we can compute the SVD of G to high relative accuracy provided we can accurately factor $G = XDY^T$ where D is

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diagonal and X and Y are any well-conditioned matrices; furthermore, the LDU factorization frequently does the job. We provide many examples of matrix classes permitting such an LDU decomposition.

1 Introduction

The *singular value decomposition (SVD)* of a real matrix G is the factorization $G = U\Sigma V^T$ where U and V are orthogonal matrices and Σ is nonnegative and diagonal. If G is m-by-n, with $m \geq n$ (otherwise transpose G), then U is m-by-n, $\Sigma = \mathrm{diag}(\sigma_1, ..., \sigma_n)$ with $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$, and V is n-by-n. We call the columns u_i of $U = [u_1, ..., u_n]$ the *left singular vectors*, the columns v_i of $V = [v_1, ..., v_n]$ the *right singular vectors*, and the σ_i the *singular values*.

Our goal is to compute the SVD (i.e. the u_i, v_i and σ_i) as accurately as the data deserves, using conventional floating point arithmetic. The phrase "as the data deserves" means that we assume that there is an unknown but bounded perturbation δG, and that we are given $\hat{G} = G + \delta G$ as input, not G itself. Thus a properly posed problem includes an input matrix $\hat{G}$, and some information about how δG is bounded. The inherent uncertainty in the data represented by the bound on δG will limit the accuracy with which we can compute the SVD of G, independent of any additional errors introduced by the algorithms.

To explain the higher accuracy to which we aspire to compute the SVD, we will contrast it with the accuracy provided by conventional SVD algorithms, such as QR iteration, bisection and inverse iteration, or divide-and-conquer [15, 35, 39]. Their model of uncertainty asserts that δG is bounded in norm, and that $\|\delta G\|/\|G\| \ll 1$ ($\|\cdot\|$ is the two-norm). This model of uncertainty is appropriate because roundoff error in these algorithms means that δG typically satisfies $\|\delta G\|/\|G\| = \Omega(\varepsilon)$ (i.e. at least order ε) where ε is the *machine precision*, or maximum relative error in any floating point operation (barring over/underflow, which we ignore). Indeed, just rounding the entries of G to store them in the machine usually makes $\|\delta G\|/\|G\| = \Omega(\varepsilon)$. Thus, including both input and roundoff error, these conventional algorithms only compute the SVD of $\hat{G} = G + \delta G$, where

$$\|\delta G\| \leq \eta \|G\| \text{ where } 0 \leq \eta \ll 1 \ . \tag{1}$$

This bound may be combined with *perturbation theorems* [54, 79, 45, 46] to derive the following conventional error bounds:

Let $\hat{U} = [\hat{u}_1, ..., \hat{u}_n]$, $\hat{\Sigma} = \mathrm{diag}(\hat{\sigma}_1, ..., \hat{\sigma}_n)$, and $\hat{V} = [\hat{v}_1, ..., \hat{v}_n]$ be the SVD of

$$\hat{G} = G + \delta G \quad \text{where } \|\delta G\| \leq \eta \|G\| \ . \tag{2}$$

Then the difference between the true and perturbed singular values is bounded by

$$|\sigma_i - \hat{\sigma}_i| \leq \eta \cdot \|G\| = \eta \cdot \sigma_1 \ . \tag{3}$$

Furthermore, the acute angle θ between the true and computed left singular vectors u_i and $\hat{u}_i$ (or between right singular vectors v_i and $\hat{v}_i$) is bounded by

$$\sin\theta \leq \frac{\eta}{\mathrm{abs_gap}(i, G, \hat{G})} \tag{4}$$

provided the *absolute gap*

$$\text{abs_gap}(i, G, \hat{G}) \equiv \min_{j \neq i} |\sigma_i - \hat{\sigma}_j| / \sigma_1 \tag{5}$$

between σ_i and the nearest other singular value is positive. (This is true when $m = n$; when $m > n$ then $\text{abs_gap}(i, G, \hat{G})$ for the left singular vectors is the minimum of the above expression and σ_i/σ_1.)

We call this accuracy provided by conventional algorithms *absolute accuracy*, to contrast it with the more stringent *relative accuracy* described in the next paragraph:

Let $\hat{U} = [\hat{u}_1, ..., \hat{u}_n]$, $\hat{\Sigma} = \text{diag}(\hat{\sigma}_1, ..., \hat{\sigma}_n)$, and $\hat{V} = [\hat{v}_1, ..., \hat{v}_n]$ be the SVD of

$$\hat{G} = (I + E)G \quad \text{where } \|E\| \leq \eta \; . \tag{6}$$

We call $\hat{G}$ in (6) a *multiplicative perturbation* of G, to contrast it with the *additive perturbation* of G in (2). Then we say the SVD of $\hat{G}$ approximates the SVD of G *with relative accuracy* η since [32, Thm. 3.1] [34, Lemma 6.4.]

$$|\sigma_i - \hat{\sigma}_i| \leq \eta \cdot \sigma_i \tag{7}$$

and the acute angle θ between u_i and $\hat{u}_i$ (or between v_i and $\hat{v}_i$) satisfies [32, Thm 3.3]

$$\sin\theta \leq \frac{O(\eta)}{\text{rel_gap}(i, G)} \tag{8}$$

provided that the *relative gap*

$$\text{rel_gap}(i, G) \equiv \min\left(\min_{j \neq i} \frac{|\sigma_i - \hat{\sigma}_j|}{\sigma_i} \; , \; 2 \right) \tag{9}$$

between σ_i and the nearest other singular value is at least about η (bound (8) is restated in more detail in Theorem 2.3 below).

Note that the both absolute upper bounds (3) and (4) are proportional to the largest singular value σ_1, whereas the relative bounds (7) and (8) are both proportional to the desired singular value σ_i, i.e. σ_1/σ_i times smaller. To make this difference between absolute and relative accuracy concrete, we consider bidiagonal matrices, which arise from computing the vibrational frequencies of a linear mass-spring system, as described in section 11.1. In particular, consider the 3-by-3 bidiagonal matrix

$$G = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 10^{-20} & 10^{-20} \\ 0 & 0 & 10^{-40} \end{bmatrix}$$

which has singular values $\sigma_1 \approx \sqrt{2}$, $\sigma_2 \approx 10^{-20}/\sqrt{2}$ and $\sigma_3 \approx 10^{-40}$. If we perturb G by multiplying each entry $g_{i,j}$ by a factor $1 + \epsilon_{i,j}$ with $|\epsilon_{i,j}| \leq 10^{-6}$, then absolute bounds (3) and (4) apply with $\eta = 10^{-6}$, which means that σ_2 and σ_3 could possibly be changed utterly, along with their associated singular vectors. In contrast, Theorem 10.1 below (as well as theorems in [6, 24, 20]) assert that relative bounds (7) and (8) apply with $\eta = 2.5 \cdot 10^{-6}$, so that all singular values and vectors

are perturbed in their fifth decimal places or less. Algorithms capable of computing the SVD of bidiagonal matrices with such high relative accuracy were published in [24, 20, 33].

Our interest in the notion of relative accuracy defined by bounds (7) and (8) arises for two reasons. First, there are a number of physical problems where the smallest singular values (or eigenvalues) are well-determined by the physical problem being modeled, and we need to compute them with some relative accuracy. For example, modes of vibration of finite element problems, and energy levels in quantum mechanical systems fall in this class. The second reason is that a large number of recent papers describe apparently unrelated classes of matrices G, and classes of perturbations δG, such that the SVDs of G and $\hat{G} = G + \delta G$ agree to high relative accuracy, as described by bounds (7) and (8). Many of these papers also provide quite different algorithms that compute the SVD with these bounds, where η is proportional to machine epsilon ε. These matrix classes include bidiagonal matrices as above [24, 20, 33], acyclic matrices [23] (see below for a definition), scaled diagonally dominant matrices [6], well-scalable symmetric positive definite matrices [25], and certain well-scalable symmetric indefinite matrices [78, 64, 63]. Some of these results depended on the multiplicative perturbation theory stated above, and others did not. In other words, special techniques were used in each case.

In this paper we present a single perturbation theory that includes all the cases in the above list, as well as several new ones. We also provide an algorithm, which with some variations computes the SVD to high relative accuracy in all known cases.

Here is an outline of our results.

In section 2 we define a *rank-revealing decomposition (RRD)* of a matrix G to be *any* representation of the form $G = XDY^T$, where D is diagonal, X and Y have at least as many rows as columns, and X and Y are "well-conditioned". The SVD is such a representation itself (with X and Y orthogonal), but there are many other such decompositions in numerical analysis, including the one provided by Gaussian elimination with complete pivoting (GECP), and QR with complete pivoting [57, 18, 41, 29].

Our overall SVD algorithm has two steps:

1. Compute any RRD $G = XDY^T$.
2. Compute the SVD of XDY^T using an algorithm from section 3.

The algorithms in section 3 are all based on Jacobi [25]. In section 3, we show that Step (2) computes the SVD with relative accuracy $O(\varepsilon \max(\kappa(X), \kappa(Y))$, where ε is machine precision and $\kappa(.)$ is the condition number. In other words, any RRD is "as good as" the SVD.

Thus, the challenge is to compute the RRD in Step (1) accurately enough, so that the SVD of the product of computed factors XDY^T is an accurate SVD of the input G. For example, it suffices to compute X and Y with errors that are small in norm, and D with small relative errors in the diagonal entries. Such an accurate decomposition is not possible for general matrices, so we must necessarily exploit the structure in certain classes of problems. We list the classes we have analyzed below:

- In section 4 we consider **graded matrices** of the form $G = D_1 B D_2$, where B is well-conditioned and D_1 and D_2 are diagonal and "contain" any ill-conditioning of G. We give a necessary and sufficient condition on B for the SVD of G to be determined to high relative accuracy by small normwise perturbations in B, independent of the scaling matrices D_1 and

D_2. Unfortunately, this condition requires that *all* submatrices of B have smallest singular values near $\|B\|$; since an n-by-n matrix has $O(4^n)$ submatrices, this condition is expensive to confirm and is often not satisfied. Therefore, we also give an an inexpensive posteriori relative error bound for the RRD of G provided by GECP and confirm its utility with numerical experiments.

- After some technical preliminaries in section 5, section 6 gives a necessary and sufficient condition on the **sparsity pattern** of G to guarantee that the SVD is determined to high relative accuracy when small relative changes are made in G's entries; this work generalizes [23]. In other words, we identify those sparsity patterns (a combinatorial property) such that *all* matrices with those patterns determine their SVDs accurately. The condition is simply that the bipartite graph representing the sparsity structure be *acyclic*. Furthermore, a one-line change is required to make GECP accurate enough to compute an accurate RRD; this change exploits the acyclic structure to recognize *exact cancellation* and so set certain matrix entries to zero exactly, that would otherwise consist entirely of roundoff error.

- Section 7 assumes that we know both the **sparsity and sign patterns** of a matrix, and again gives a necessary and sufficient condition that all matrices with a specific sparsity and sign pattern have SVD determined to high relative accuracy when small relative perturbations are made in their entries. The condition is that the sparsity and sign pattern be *total signed compound (TSC)* [14]. TSC matrices include acyclic matrices, tridiagonal matrices with positive off-diagonals and diagonals with alternating signs, and many others. Furthermore, a rather complicated modification of GECP is needed so that it computes an RRD with any guaranteed accuracy; this modified GECP costs as much as $O(n^4)$ instead of $O(n^3)$.

- Section 8 discusses **Cauchy matrices**, i.e. matrices whose entries are $C_{ij} = 1/(x_i+y_j)$, where $x_1, ..., x_n$ and $y_1, ..., y_n$ are given data. There is a classical formula for any minor of C that can be evaluated to high relative accuracy, which implies that every entry of the LDU factorization is determined to high relative accuracy. Using this classical formula straightforwardly to perform GECP would cost $O(n^5)$; details of an efficient $O(n^3)$ algorithm, and extensions to Vandermonde and other matrices with unit displacement rank, may be found in [22].

- Section 9 discusses **totally positive (TP)** matrices, i.e. matrices all of whose minors are nonnegative. The Hilbert matrix is an example (it is also Cauchy), and TP matrices arise elsewhere frequently in applied mathematics [44]. There are many ways to parameterize TP matrices; the parameters x_i and y_j above for a Cauchy matrix is one example of many. The existence of high relative accuracy formulas for minors, and so LDU factors, depends on choosing the right parameterization. There turns out to be a systematic way to develop good parameterizations, and corresponding high accuracy formulas for minors and LDU factors, for all TP matrices. Unfortunately, the costs of these formulas are sometimes exponential in n, and we do not know if we can do better. Still, the existence of these formulas amounts to a perturbation theory showing that the SVDs of TP matrices are determined to high relative accuracy.

- Section 10 considers **diagonally scaled totally unimodular (DSTU) matrices**. These include acyclic matrices as special cases, as well as the finite element problems considered in section 11. A *totally unimodular (TU) matrix* is an integer matrix Z each of whose minors is

-1, 0 or $+1$, and a DSTU matrix is of the form $D_1 Z D_2$, where D_1 and D_2 are diagonal and Z is TU. GECP must be again be modified to guarantee that it computes an accurate RRD.

- Section 11 discusses matrices arising in certain simple **finite element problems**. Usually the lowest frequencies (eigenvalues) are of physical interest, so we want to compute them accurately. The most natural formulation leads to the generalized eigenvalue problem $Kx = \lambda Mx$, where M is the *mass matrix*, and K is the *stiffness matrix*. In the simplest cases $K = Z^T D_K Z$ where D_K is a diagonal matrix of element stiffnesses, Z is a rectangular *incident matrix* or *assembly matrix*, and $M = D_M$ is diagonal too. In this case we can show that the eigenvalues of $Kx = \lambda Mx$ are the squares of the singular values of $G = D_K^{1/2} Z D_M^{-1/2}$. For a number of simple finite element problems, we will see that G is DSTU, and so can be solved by the algorithm in section 10. For more general finite element problems, we conjecture that the relative accuracy depends only on Z, i.e. the *geometry* of the problem, and not on D_K or D_M, i.e. not on the *material properties*. A similar analysis of linear systems arising in finite element problems appears in [58, 74, 75].

- Section 12 discusses which other linear algebra problems besides the SVD can be solved to high accuracy, given the combinatorial and algebraic conditions described in earlier sections.

The last section, section 13, lists open problems. Finally, we note that the sequence of initials of the last names of the authors, DGESVD, is the name of the most accurate LAPACK [2] routine currently available for the dense SVD (which only provides high absolute accuracy).

2 Rank Revealing Decompositions (RRDs)

We repeat the following informal definition from the introduction:

Let G be m-by-n with $m \geq n$. Let X be m-by-r, D be r-by-r, and Y be n-by-r, where $r \leq \min(m,n)$. Then $G = XDY^T$ is a rank-revealing decomposition (RRD) *of G if X and Y are well-conditioned, and D is diagonal and nonsingular.*

What "well-conditioned" means will depend on the problem at hand, and how much error the user is willing to tolerate.

The SVD itself is such a decomposition, with X and Y optimally conditioned, i.e. orthogonal. But there are many other RRDs as well, most importantly the decompositions (usually) provided by Gaussian elimination with complete pivoting (GECP), and by QR with complete pivoting (QRCP) [57, 18, 41]. The goal of this section and the next is to show that any RRD is as good as the SVD, in the sense that small changes in the factors of the RRD determine the SVD to high relative accuracy, and that there are efficient algorithms for computing the SVD this accurately, given any RRD.

Theorem 2.1 *Let $G = XDY^T$ be an RRD with SVD $G = U\Sigma V^T$, and let $\hat{G} = \hat{X}\hat{D}\hat{Y}^T$ with SVD $\hat{G} = \hat{U}\hat{\Sigma}\hat{V}^T$, where $\hat{X}$, $\hat{D}$ and $\hat{Y}$ are defined as follows:*

$$\hat{X} = X + \delta X \quad \text{where} \quad \frac{\|\delta X\|}{\|X\|} \leq \epsilon$$

$$\hat{D} = D + \delta D \quad \text{where} \quad \delta D \text{ is diagonal and } \frac{|\delta D_{ii}|}{|D_{ii}|} \leq \epsilon$$

$$\hat{Y} \quad = \quad Y + \delta Y \quad \text{where} \quad \frac{\|\delta Y\|}{\|Y\|} \leq \epsilon$$

where $0 \leq \epsilon < 1$. *Let* $\eta = \epsilon(2+\epsilon)\max(\kappa(X), \kappa(Y))$ *and* $\eta' = 2\eta + \eta^2$, *where* $\kappa(Z) = \sigma_{\max}(Z)/\sigma_{\min}(Z)$ *is the condition number of* Z. *Then the difference between the singular values of* G *and* $\hat{G}$ *is bounded as follows*

$$\frac{|\sigma_i - \hat{\sigma}_i|}{\sigma_i} \leq \eta' \ . \tag{10}$$

Furthermore, the angle θ *between* u_i *and* $\hat{u}_i$ *(or between* v_i *and* $\hat{v}_i$*) is bounded by*

$$\sin\theta \leq \sqrt{2}\left(\frac{1+\eta'}{1-\eta'} \cdot \frac{\eta'}{\text{rel_gap}(i,G) - \eta'} + \eta\right) \tag{11}$$

provided that the relative gap

$$\text{rel_gap}(i,G) \equiv \min\left(\min_{j \neq i} \frac{|\sigma_i - \hat{\sigma}_j|}{\sigma_i} \ , \ 2\right)$$

is at least η'.

The proof is simple. We use the *multiplicative perturbation theorems* stated in the introduction, which we repeat here.

Theorem 2.2 *[32, Thm. 3.1] Suppose* $\hat{G} = (I+E)G(I+F)$, *with* $\|E\| = \eta_E$ *and* $\|F\| = \eta_F$. *Let* $\eta = \max(\eta_E, \eta_F)$ *and* $\eta' = 2\eta + \eta^2$. *Then*

$$\frac{|\sigma_i - \hat{\sigma}_i|}{\sigma_i} \leq \eta_E + \eta_F + \eta_E\eta_F \leq \eta' \ . \tag{12}$$

Theorem 2.3 *[46, Thm. 3.5] Suppose* $\hat{G} = (I+E)G(I+F)$, *where* $\|E\| \leq \eta_E$ *and* $\|F\| \leq \eta_F$. *Let* $\eta = \max(\eta_E, \eta_F)$ *and* $\eta' = 2\eta + \eta^2$. *Then the acute angle* θ *between* u_i *and* $\hat{u}_i$ *(or between* v_i *and* $\hat{v}_i$*) is bounded by*

$$\sin\theta \leq \sqrt{2}\left(\frac{1+\eta'}{1-\eta'} \cdot \frac{\eta'}{\text{rel_gap}(i,G) - \eta'} + \eta\right) \tag{13}$$

provided that the relative gap

$$\text{rel_gap}(i,G) \equiv \min\left(\min_{j \neq i} \frac{|\sigma_i - \hat{\sigma}_j|}{\sigma_i} \ , \ 2\right)$$

between σ_i *and the nearest other singular value is at least* η'.

The paper [46] includes similar perturbation theorems for singular subspaces, not just singular vectors. These are useful when several singular values form a tight cluster, and bounds are desired for the space spanned by their corresponding singular vectors. It is also possible to reformulate the definition of relative gap to depend only on the σ_is rather than the $\hat{\sigma}_i$s too, at the cost of complicating the bounds somewhat.

Proof of Theorem 2.1: We write $\hat{G}$ in the form $(I+E)G(I+F)$: First write

$$\begin{aligned}
\hat{G} &= \hat{X}\hat{D}\hat{Y}^T \\
&= (X+\delta X)\hat{D}\hat{Y}^T \\
&= (I+\delta X X^+)X\hat{D}\hat{Y}^T \\
&\quad \text{where } X^+ \text{ is the Moore} - \text{Penrose pseudoinverse of } X \\
&= (I+E)X\hat{D}\hat{Y}^T \\
&\quad \text{where } E = \delta X X^+ .
\end{aligned}$$

Note that $\|E\| \le \|\delta X\| \cdot \|X^+\| \le \epsilon \|X\| \cdot \|X^+\| = \epsilon\kappa(X)$. Now we apply the same technique to the other two factors $\hat{D}$ and $\hat{Y}$. Note that $\hat{D} = D(I+D^{-1}\delta D) \equiv D(I+W)$, where W is diagonal with norm bounded by ϵ. Then

$$\begin{aligned}
\hat{G} &= (I+E)X\hat{D}\hat{Y}^T \\
&= (I+E)XD(I+W)(Y+\delta Y)^T \\
&= (I+E)XD(Y+YW+\delta Y(I+W))^T \\
&= (I+E)XD((I+[YW+\delta Y(I+W)]Y^+)Y)^T \\
&= (I+E)XDY^T(I+\{[YW+\delta Y(I+W)]Y^+\}^T) \\
&\equiv (I+E)XDY^T(I+F) \\
&= (I+E)G(I+F)
\end{aligned}$$

where $\|F\| \le \kappa(Y)(2\epsilon+\epsilon^2)$. Applying Theorems 2.2 and 2.3 to $\hat{G} = (I+E)G(I+F)$ yields the result. □

We note that we could have had different values of ϵ associated with δX, δY and δD in Theorem 2.1, rather than just one. That way, if $\kappa(X) \gg \kappa(Y)$, but $\frac{\|\delta X\|}{\|X\|} \equiv \epsilon_X \ll \epsilon_Y \equiv \frac{\|\delta Y\|}{\|Y\|}$ and $\epsilon_Y = \epsilon_D \equiv \max_i |\delta Dii|/|D_{ii}|$, then the final error will be proportional to $\kappa(X)\epsilon_X + \kappa(Y)\epsilon_Y$, rather than the larger $\max(\kappa(X),\kappa(Y)) \cdot \max(\epsilon_X,\epsilon_Y)$.

3 Computing the SVD from a Rank Revealing Decomposition

We present several algorithms for computing the SVD to high relative accuracy from an RRD $G = XDY^T$. These algorithms tradeoff speed and reliability in different ways, but (nearly) attain the minimum possible relative error bound $O(\varepsilon \max(\kappa(X),\kappa(Y))$ stated in Theorem 2.1 (recall that ε is machine epsilon). All the algorithms are slower than competing algorithms based on QR iteration or divide-and-conquer, but will not be much slower, thanks to recent work on accelerating Jacobi's method to nearly the speed of QR iteration [30].

Three of the algorithms are quite short, so we present them in their entirety, but only analyze the first one in detail, Algorithm 3.1, since it is always faster than the second algorithm, and very unlikely to be less accurate. The third algorithm is for the special case where X (or Y) is orthogonal, a special case that can be exploited to go faster.

Section 3.1 presents the algorithms and states the error analysis of Algorithm 3.1 without proofs. Section 3.2 presents the proofs, and section 3.3 presents numerical experiments.

3.1 Algorithms for Computing an Accurate SVD of a Rank Revealing Decomposition

Algorithm 3.1 *Computing the SVD $G = U\Sigma V^T$ given an RRD $G = XDY^T$. (Only the nonzero singular values and their corresponding singular vectors are computed).*

(1) Perform QR factorization with pivoting on XD to get $XD = QRP$, where P is a permutation. Thus $G = QRPY^T$.
(2) Multiply to get $W = RPY^T$. This must be conventional *matrix multiplication, e.g. Strassen's method [40] may not be used. Thus $G = QW$.*
(3) Compute the SVD of $W = \bar{U}\Sigma V^T$ using one-sided Jacobi [25]. Thus $G = Q\bar{U}\Sigma V^T$.
(4) Multiply $U = Q\bar{U}$. Strassen's method may be used. Thus $G = U\Sigma V^T$ is the desired SVD.

Thus, the total cost of the algorithm is one QR factorization with pivoting, two matrix-multiplications (one triangular), and one application of one-sided Jacobi, the most expensive step.

Theorem 3.1 *Let D' be a diagonal matrix, chosen so that $R' = D'^{-1}R$ is as well conditioned as possible. Then in floating point arithmetic with machine precision ε, Algorithm 3.1 computes the SVD of G with relative accuracy $\eta = O(\varepsilon\kappa(R') \cdot \max(\kappa(X), \kappa(Y)))$.*

In practice $\kappa(R')$ is usually close to 1 so that the error bound is close to the minimum given by the perturbation bound in Theorem 2.1. But the best we can prove is the following:

Theorem 3.2 *In the notation of Theorem 3.1, D' can be chosen so that $\kappa(R') = O(\min(n2^n, n^{3/2}\kappa(X))$.*

Algorithm 3.2 eliminates the factor $\kappa(R')$ from the error bound at the cost of two applications of one-sided Jacobi:

Algorithm 3.2 *Computing the SVD $G = U\Sigma V^T$ given an RRD $G = XDY^T$. (Only the nonzero singular values and their corresponding singular vectors are computed).*

(1) Compute the SVD of $XD = \bar{U}\bar{\Sigma}\bar{V}^T$ using one-sided Jacobi. Thus $G = \bar{U}\bar{\Sigma}\bar{V}^TY^T$.
(2) Multiply $W = \bar{\Sigma}(\bar{V}^TY^T)$, respecting parentheses. Strassen may be used inside the parentheses. Thus $G = \bar{U}W$.
(3) Compute the SVD $W = \bar{\bar{U}}\Sigma V^T$ using one-sided Jacobi. Thus $G = \bar{U}\bar{\bar{U}}\Sigma V^T$.
(4) Multiply $U = \bar{U}\bar{\bar{U}}$. Strassen may be used. Thus $G = U\Sigma V^T$ is the desired SVD.

Algorithm 3.3 applies in the special case where X is orthogonal. This would be the case if $G = XDY^T = P_1QRP_2$ were computed by QR with complete pivoting [57, 18, 41]. In this case P_1 and P_2 are permutation matrices, $D_{ii} = R_{ii}$, $X = P_1Q$, and $Y = D^{-1}RP_2$.

Algorithm 3.3 *Computing the SVD $G = U\Sigma V^T$ given an RRD $G = XDY^T$. X is assumed to be orthogonal. (Only the nonzero singular values and their corresponding singular vectors are computed).*

(1) Compute the SVD of $DY = \bar{U}\Sigma V^T$ using one-sided Jacobi. Thus $G = X\bar{U}\Sigma V^T$.
(2) Multiply $U = X\bar{U}$. Strassen may be used. Thus $G = U\Sigma V^T$ is the desired SVD.

Three other algorithms deserve mention, though we believe that Algorithms 3.1 through 3.3 are the only ones of interest in practice.

The first algorithm we discovered for this problem was based on an algorithm of Veselić and Slapničar. Assuming without loss of generality that $D_{ii} > 0$, we can write

$$\begin{aligned}
\begin{bmatrix} 0 & G \\ G^T & 0 \end{bmatrix} &= \begin{bmatrix} 0 & XDY^T \\ YDX^T & 0 \end{bmatrix} \\
&= \left\{ \frac{1}{\sqrt{2}} \cdot \begin{bmatrix} X & X \\ Y & -Y \end{bmatrix} \cdot \begin{bmatrix} D^{1/2} & 0 \\ 0 & D^{1/2} \end{bmatrix} \right\} \times \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \times \\
&\quad \left\{ \frac{1}{\sqrt{2}} \cdot \begin{bmatrix} X & X \\ Y & -Y \end{bmatrix} \cdot \begin{bmatrix} D^{1/2} & 0 \\ 0 & D^{1/2} \end{bmatrix} \right\}^T \\
&\equiv Z \times J \times Z^T
\end{aligned}$$

By construction, the columns of Z can be scaled so that its resulting condition number $\kappa(Z\tilde{D})$ is no larger than $\max(\kappa(X), \kappa(Y))$. Thus, we can apply Veselić's implicit J-orthogonal Jacobi algorithm [76] [63, Alg. 3.3.1] to compute the positive eigenvalues of ZJZ^T (and their eigenvectors), which are the singular values of G (and their singular vectors). The relative error in this algorithm is $O(\varepsilon\kappa(Z\tilde{D}))$ as desired, see Slapničar [63, Thm. 3.3.3]. Unlike Algorithm 3.1, this algorithm has no $\kappa(R')$ factor in the error bound, but it is likely to be slower.

A very similar algorithm appeared in [56], which essentially applied a Jacobi-like iteration to the pencil

$$F^TF - \lambda \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \text{ where } F = \begin{bmatrix} 0 & XD^{1/2} \\ YD^{1/2} & 0 \end{bmatrix}.$$

Finally, a similar algorithm appeared in [27, 28], in the context of computing the product SVD, which has essentially the same error bound as our Algorithm 3.1.

3.2 Error Analysis

3.2.1 Proof of Theorem 3.1

We proceed through the algorithm line by line, showing that the backward error introduced by every step but (3) is of the form $(I+E)G(I+F)$. The one-sided Jacobi algorithm in step (3) is described in [25, Alg. 4.1], and was shown to possess high relative accuracy when applied to matrices like W, which we will see is the product of a diagonal matrix D' and a well-conditioned matrix $R'PY^T$ (modulo roundoff). The algorithm in step (3) is essentially the version of the one-sided Jacobi algorithm of Rutishauser in [80], but with a more stringent stopping criterion. (Later, more elegant proofs by Drmač [28] and Mathias [50] also use the fact that errors during one-sided Jacobi are of the form $(I + E)G(I + F)$, so that the entire error analysis propagates errors "multiplicatively" rather than "additively".)

Step (1) of Algorithm 3.1 may be written

$$\begin{aligned}
G &= XDY^T \\
&= (QRP + E')Y^T
\end{aligned}$$

where Q, R and P are the computed results from step (1), and E' is the backward error. Since QR operates on columns of the matrix, it is easy to see that we can write

$$QRP = XD - E' = (X + \delta X)D$$

where for all i, column i of δX has norm bounded by $O(\varepsilon)$ times the norm of column i of X. Thus

$$QRP = (I + \delta X X^{+})XD = (I + E)XD$$

where $\|E\| \leq O(\varepsilon)\kappa(X)$. In other words, we may write

$$G = (I + E)^{-1}QRPY^{T} \quad .$$

Continuing with the algorithm, in Step (2) we multiply RPY^T to get the computed product W, which satisfies $W + \delta W = RPY^T$, where δW is the roundoff error. Since P is a permutation, the order in which we perform the two multiplications to form W does not matter. Since $R = D'R'$ where D' is diagonal, and we use conventional matrix multiplication, we can bound δW rowwise as follows (e_i^T denotes the i-th row of the identity matrix):

$$\begin{aligned} \|e_i^T \delta W\| &\leq O(\varepsilon)\|e_i^T R\| \cdot \|Y^T\| \\ &= O(\varepsilon)|D'_{ii}| \cdot \|e_i^T R'\| \cdot \|Y^T\| \quad . \end{aligned}$$

Defining $Z = D'^{-1}W$, $\delta Z = D'^{-1}\delta W$, and letting Z^+ be the pseudoinverse of Z we get

$$\|(Z + \delta Z)^{+}\| \leq \|R'^{-1}\| \cdot \|Y^{+}\| \quad ,$$

$$\|\delta Z\| = O(\varepsilon)\|R'\| \cdot \|Y^T\|$$

and

$$\begin{aligned} W + \delta W &= D'(Z + \delta Z) \\ &= D'Z(I + Z^{+}\delta Z) \\ &= W(I + F') \end{aligned}$$

where

$$\begin{aligned} \|F'\| &\leq \|Z^{+}\| \cdot \|\delta Z\| \\ &\approx \|(Z + \delta Z)^{+}\| \cdot \|\delta Z\| \\ &\leq O(\varepsilon) \cdot \kappa(R') \cdot \kappa(Y) \quad . \end{aligned}$$

Altogether then, after Step (2), we have

$$G = (I + E)^{-1}QW(I + F') \quad .$$

Next, in Step (3), we use one-sided Jacobi to compute the SVD of $W = D'Z$. We let $D'Z = \bar{U}'\Sigma'V'^T$ be the exact SVD, and let $\bar{U} = \bar{U}' - \delta\bar{U}$, $\Sigma = \Sigma' - \delta\Sigma$ and $V = V' - \delta V$ be the computed quantities returned by one-sided Jacobi. In [25] it is shown that to high relative accuracy $O(\varepsilon\kappa(Z)) = O(\varepsilon\kappa(R')\kappa(Y))$, $\bar{U}\Sigma V^T$ is the SVD of $D'Z$.

Continuing with the algorithm, we write

$$\begin{aligned} G &= (I+E)^{-1}Q(\bar{U}'\Sigma' V'^T)(I+F') \\ &= (I+E)^{-1}Q(\bar{U}+\delta\bar{U})(\Sigma+\delta\Sigma)(V+\delta V)^T(I+F') \\ &\quad \text{where } \bar{U},\ \Sigma, \text{ and } V \text{ are computed in Step (3) with errors } \delta\bar{U},\ \delta\Sigma, \text{ and } \delta V \\ &= (I+E)^{-1}(Q\bar{U}+Q\delta\bar{U})(\Sigma+\delta\Sigma)(V+\delta V)^T(I+F') \\ &= (I+E)^{-1}(U+\delta U+Q\delta\bar{U})(\Sigma+\delta\Sigma)(V+\delta V)^T(I+F') \\ &\quad \text{where } U \text{ is the computed product in Step (4) and } \delta U \text{ is the roundoff error.} \end{aligned}$$

Altogether, we get

$$(I+E)G(I+F) = (Q\bar{U}')\Sigma' V'^T = (U+Q\delta\bar{U}+\delta U)(\Sigma+\delta\Sigma)(V+\delta V)^T$$

where $I+F = (I+F')^{-1}$, so $\|E\| = O(\varepsilon\kappa(X))$ and $\|F\| \approx \|F'\| = O(\varepsilon\kappa(R')\kappa(Y))$. In other words, $(Q\bar{U}')\Sigma' V'^T$ is the true SVD of almost the right matrix $((I+E)G(I+F))$, and the computed SVD $U\Sigma V^T$ is almost the right SVD of almost the right matrix. (The fact that Q is not quite orthogonal does not matter here, since its nonorthogonality could be absorbed in the $I+E$ factor.)

Now apply multiplicative perturbation Theorem 2.2 to see that the relative error in the singular values $\Sigma+\delta\Sigma$ is bounded by $O(\varepsilon\max(\kappa(X),\kappa(R')\kappa(Y)))$. From the analysis in [25], the relative difference between $\Sigma+\delta\Sigma$ and the actual computed output Σ is also $O(\varepsilon\kappa(Z)) = O(\varepsilon\kappa(R')\kappa(Y))$. This proves that the relative error in the computed singular values is bounded by $O(\varepsilon\max(\kappa(X),\kappa(R')\kappa(Y)))$ as desired.

Finally, we consider the singular vectors. Multiplicative perturbation Theorem 2.3 bounds the difference between the singular vectors of G and those of $(I+E)G(I+F)$, namely the columns of $Q\bar{U}'$ and $V' = V+\delta V$, by $O(\varepsilon\max(\kappa(X),\kappa(R')\kappa(Y)))$ over the relative gaps. The analysis in [25] further bounds the the difference between the columns of $V+\delta V$ and the actual computed output V by $O(\varepsilon\kappa(Z)) = O(\varepsilon\kappa(R')\kappa(Y))$ over the relative gaps, yielding the desired error bound for the right singular vectors.

For the left singular vectors, we introduced errors in steps (4) and (5), which we express as

$$U = Q\bar{U}' - Q\delta\bar{U} - \delta U$$

where $Q\bar{U}'$ are the true singular vectors of $(I+E)G(I+F)$. As with the left singular vectors, the analysis in [25] shows that each column of $\delta\bar{U}$ is bounded in norm by $O(\varepsilon\kappa(R')\kappa(Y))$ over the appropriate relative gap. Multiplying by Q and adding δU (which is bounded in norm by $O(\varepsilon)$) does not change this norm bound. Therefore, the errors in the columns of U are bounded the same way. This yields the final desired error bound.

3.2.2 Proof of Theorem 3.2

The factor $\kappa(R')$ in the error bound depends on how well the pivoting during the QR decomposition of XD "reveals the rank" of XD. By choosing $D'_{ii} = R_{ii}$, the standard column-pivoting bound [35] shows that $\kappa(R')$ is at most $O(n2^n)$. It is usually smaller, but the upper triangular "Kahan matrix" $XD = R$, where $R_{ii} = 10^{1-i}$, $R_{ij} = -\sqrt{.99}\cdot 10^{1-i}$ for $j > i$, which is left invariant by QR with column pivoting (and/or row pivoting [57, 18]), shows that this bound is attainable. Yet better

pivoting schemes are available [67, 7, 16, 17, 38, 42, 53]. For example, Eisenstat and Gu have a pivoting scheme that reduces $O(2^n)$ to $O(n^{1+(1/4)\log_2 n})$, analogous to the pivot growth bound for GECP [36]. See also [52].

We argue that $\kappa(R') = O(n^{3/2}\kappa(X))$ as follows [1]. Write $R = D'R' = R_cD$, where we assume w.l.o.g that the permutation from the QR decomposition is I. Choose $D'_{ii} = \|R_{i,\cdot}\|$, the 2-norm of the i-th row of R. Thus $\|R'_{i,\cdot}\| = 1$ and $\|R'\| \le \sqrt{n}$. Since $XD = QR = QR_cD$, we see that R_c and X have the same singular values, and so the same condition number. Now $D'R' = R_cD$ implies $R'^{-1} = D^{-1}R_c^{-1}D'$, so

$$\begin{aligned}
|R'^{-1}|_{ij} &= \frac{D'_{jj}}{D_{ii}}|R_c^{-1}|_{ij} \quad \text{for } i \le j \\
&= \frac{\|R_{j,\cdot}\|}{\|R_{\cdot,i}\|}\|X_{\cdot,i}\| \cdot |R_c^{-1}|_{ij} \\
&\quad \text{where } R_{\cdot,i} \text{ is the } i-\text{th column of } R \\
&\le \frac{\|R_{j,\cdot}\|}{|R_{i,i}|}\|X_{\cdot,i}\| \cdot |R_c^{-1}|_{ij} \\
&\le \frac{\sqrt{n-j+1}|R_{i,i}|}{|R_{i,i}|}\|X_{\cdot,i}\| \cdot |R_c^{-1}|_{ij} \\
&= \sqrt{n-j+1}\|X_{\cdot,i}\| \cdot |R_c^{-1}|_{ij}
\end{aligned}$$

so that $\|R'^{-1}\| \le n\|X\| \cdot \|X^+\| = n\kappa(X)$. Thus $\kappa(R') \le n^{3/2}\kappa(X)$ as desired, completing the proof.

One can also argue that if $D_{i,i} \gg D_{i+1,i+1}$, then R' will be close to the identity, and in any event at least as well conditioned as X: Since D_{ii} is sorted and strongly graded, it is likely that QR with pivoting applied to XD will not actually permute any columns. Indeed, it would only permute columns if the smallest singular value of the i leading columns of X were of order $D_{i+1,i+1}/D_{i,i} \ll 1$, contradicting the assumption that X is well conditioned. Then as above we can write $XD = QR \equiv QR_cD$, so $\kappa(R_c) = \kappa(X)$. Now choose $D' = D$, so $R' = D^{-1}R_cD$. Since R_c is upper triangular and D is graded from large to small on the diagonal, it is easy to see that each superdiagonal entry $R_{c,ij}$ is multiplied by $D_{jj}/D_{ii} \ll 1$. The same is true of $R'^{-1} = D^{-1}R_c^{-1}D$, so R' becomes even more nearly diagonal than R_c, and even better conditioned. (It is obvious that the condition number with respect to the Frobenius norm decreases, but one can also prove that the condition number with respect to many operator norms decreases [47].)

3.3 Numerical Experiments

In this section, we present results of numerical experiments with Algorithm 3.1, assuming we that are given an RRD $G = XDY^T$. We used Sun FORTRAN on a Sun SPARC 20 Workstation, with IEEE arithmetic. Our single precision procedure, `SGEPSV`, is implemented as follows. In step (1) we compute the QR factorization using LAPACK's [2] `SGEQPF` procedure, which does QR decomposition with column pivoting. Steps (2) and (4) are implemented using calls to the BLAS 3 [26] procedures `STRMM` and `SGEMM`, where we are careful to use an `STRMM` based on conventional matrix multiplication rather than Strassen's method, as required by the error analysis in Theorem 3.1. Step (3) has several possible implementations; we use the right-handed Jacobi scheme, i.e. the matrix

[1] We thank the editor, Pete Stewart, for pointing this out to us.

V is the accumulated product of Jacobi rotations. Since the dimension r of D is less than the number of columns n of G, we save time by first computing the LQ factorization of W and apply one-sided Jacobi to L. (We note that Algorithm 3.1 has a dual formulation that interchanges the roles of X and Y. An optimized version would choose between versions depending on the sizes of the dimensions m, r and n, but we will not pursue this here.)

We also use double precision versions of our routines, which have names beginning with `D` instead of `S`.

This set of experiments was designed to confirm the error analysis of Algorithm 3.1. We did this by constructing a set of X, D and Y with known condition numbers, computing the SVD of XDY^T using both single precision and double precision (note that $G = XDY^T$ is never formed explicitly), and seeing whether the differences between the single precision and double precision singular values satisfied the error bound in Theorem 3.1 (they did). We also monitored the size of the $\kappa(R')$ term in the error analysis, and confirmed that it never grew larger than about 100.

More precisely, here is what we did. We generated test triples (X, D, Y) with dimensions $m = 200$, $r = 100$ and $n = 150$, and with specified values of $\kappa(X)$, $\kappa(D)$ and $\kappa(Y)$. In addition, X and Y had columns with unit 2-norm. The specified condition numbers were chosen to be $\kappa(X) = 10^i$ for $i = 2, 3, ..., 6$, $\kappa(D) = 10^j$ for $j = 2, 4, ..., 16$, and $\kappa(Y) = 10^k$ for $k = 2, 3, ..., 6$. X, D and Y were computed by the LAPACK [2] test matrix generator `DLATM1`, with their actual singular value distribution controlled by the parameter `MODE` [2]. Two sets of modes where used, $(5, 4, -5)$ and $(3, -4, 5)$ for (X, D, Y), respectively. Finally, for each of the $5 \cdot 8 \cdot 5 = 200$ values of (i, j, k), and each of the 2 `MODE` settings, 4 random triplets (X, D, Y) were generated, for $200 \cdot 2 \cdot 4 = 1600$ tests in all.

For each test triplet, we computed the singular values in single (yielding $\sigma_{S,i}$) and in double (yielding $\sigma_{D,i}$), and computed the error measure

$$\epsilon(G) = \frac{\max_i \frac{|\sigma_{S,i} - \sigma_{D,i}|}{\sigma_{D,i}}}{\max\{\kappa(X), \kappa(Y)\}} \quad . \tag{14}$$

By Theorem 3.1, this ratio can be as large $O(\varepsilon_S \cdot \kappa(R'))$, where $\varepsilon_S = 2^{-24} \approx 6 \cdot 10^{-8}$, and $\kappa(R')$ should be $O(1)$. In fact, $\epsilon(G)$ never exceeded $6.1 \cdot 10^{-8}$ in all 1600 test cases. Furthermore, by choosing the D' in Theorem 3.1 so that each row of R' had unit 1-norm, $\|(R')^{-1}\|_1$ never exceeded 111. One can also show that $O(\varepsilon)\|(R')^{-1}\|_1$ bounds the overall backward error $\frac{\|\delta X\|}{\|X\|} + \frac{\|\delta Y\|}{\|Y\|}$ in the computed SVD $U\Sigma V^T = (X + \delta X)D(Y + \delta Y)$, another way to confirm the accuracy.

As a further accuracy test we computed

$$\epsilon(i, k) = \max_{\kappa_2(X)=10^i, \kappa_2(Y)=10^k} \max_j \frac{|\sigma_{S,j} - \sigma_{D,j}|}{\sigma_{D,j}} \tag{15}$$

which should behave like $\varepsilon_S \cdot 10^{\max(i,k)} \approx 10^{\max(i,k)-7}$. This behavior is confirmed by the plot of $\epsilon(i, k)$ versus i and k in Figure 1.

[2] |`MODE`|=3 makes the singular values geometrically distributed from $1/\kappa$ to 1, |`MODE`|=4 makes the singular values arithmetically distributed from $1/\kappa$ to 1, and |`MODE`|=5 sets the singular values to random numbers in the range from $1/\kappa$ to 1, such that their logarithms are uniformly distributed.

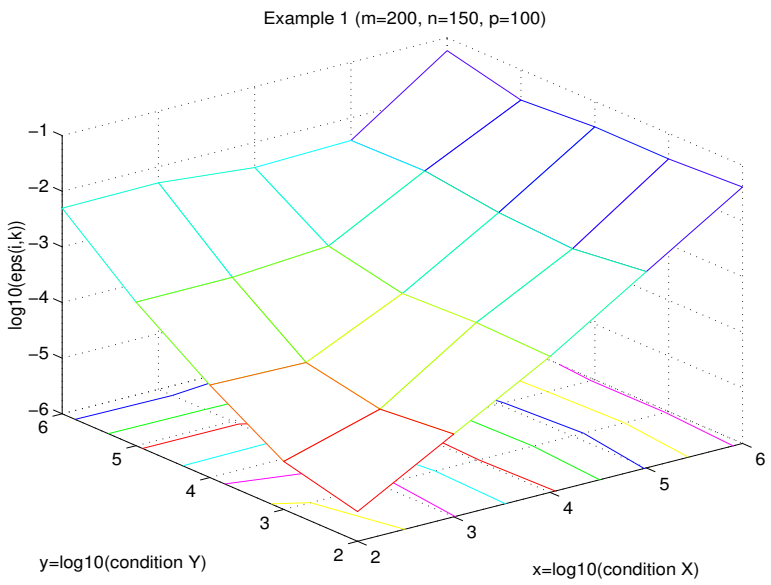


Figure 1: The values of of $\log_{10} \epsilon(i,k)$ for $2 \leq i,k \leq 6$.

4 Computing an Accurate RRD of a Graded Matrix

If G is the of the form $G = D_1 B D_2$ where D_1 and D_2 are diagonal with entries of widely varying magnitudes, and B is "well-behaved" in some sense, then G is called a graded matrix. There is a large literature on conditions under which graded matrices permit significantly more accurate eigensolutions [6, 25, 49, 68], or solutions of linear systems [60, 61, 62], or of least squares problems [57, 18, 1, 4, 66, 73, 72]). Here, we give necessary and sufficient conditions for the SVD of a graded matrix to be determined to high relative accuracy, and provide a corresponding algorithm.

Our algorithm uses GECP to get a RRD, and we provide a condition estimator for the relative error as well (see Theorem 4.2). It seems that QR with complete pivoting could be used as well [57, 18, 41, 29], since it does as well in our numerical tests, but this has not been completely proven. We briefly discuss alternatives based on bidiagonalization (or tridiagonalization) and show their flaws [77, 5].

We also discuss the relationship of this with previous work on graded symmetric eigenproblems (section 4.3) and weighted least squares (section 4.4).

We begin with the case of one-sided grading, i.e. $D_1 = I$ or $D_2 = I$, which requires just diagonal scaling to get an RRD. Then we discuss the two-sided case, which has a combinatorial set of conditions on B to guarantee high relative accuracy of the SVD of $D_1 B D_2$ for *any* D_1 and D_2.

So first suppose that B has full column rank, and we only scale its columns to get $G = BD_2$. Then if B is well-conditioned, the factorization $G = BD_2 \equiv XDY^T$ with $X = B$, $D = D_2$ and $Y = I$ is rank revealing. Thus we see that if B is well-conditioned and of full-column rank, and we consider perturbations $G + \delta G = (B + \delta B)D_2$ where $\|\delta B\| \ll \|B\|$, then G's SVD is determined to high relative accuracy independent of column scaling D_2. If we are given G but not its factors B and D_2, then we can recover nearly the best conditioned B by simply dividing each column of G by its 2-norm [71]. This discussion also applies to $G = D_1 B$, where B is well-conditioned and has full row rank. Of course for this simple case it is unnecessary to compute an RRD in order to get an accurate SVD, but rather just apply one-sided Jacobi, a fact we exploited in step (3) of

Algorithm 3.1, and which is further discussed in [25, 50, 27]. (The first paper remarking on the high accuracy of Jacobi appears to be [58].)

Extensions of these results to $G = D_1 B D_2$ (or $G = D_1 B$ with B full column rank) are unavoidably combinatorial in nature, requiring conditions on *all* submatrices of B, not just B itself. The first result of this kind for the SVD appears in [37], although related results for least squares problems appear in [65, 51, 74] (see section 4.4). In [37], Gu and Eisenstat show that for the n-by-n matrices $G = D_1 B D_2$ and $G + \delta G = D_1(B + \delta B)D_2$ to have singular values agreeing to high relative accuracy, *independent* of D_1 and D_2, the smallest singular values of *all* square submatrices of B must be large enough. In fact, they show that the relative error bound on the singular values is essentially $\|\delta B\|/\chi_1$, where χ_1 is the smallest singular value of any square submatrix of B. There are exponentially many square submatrices, $\sum_{i=1}^{n} \left(\begin{array}{c} n \\ i \end{array} \right)^2 = O(4^n)$ of them. To see that this error bound is attainable, suppose without loss of generality that the submatrix $\hat{B}$ of B with the smallest singular value is the leading k-by-k submatrix of B. Then set the leading k diagonal entries of D_1 and D_2 to one, and let the rest be very small. Then the k largest singular values of B are essentially the singular values of $\hat{B}$, and the k-th singular value is as sensitive as claimed. Note that even the *largest* singular value of G may be the worst conditioned; suppose $0 < \epsilon \ll 1$ in the following example:

$$
\begin{aligned}
G &= \begin{bmatrix} 0 & 1 \\ 1 & \epsilon \end{bmatrix} = \begin{bmatrix} \frac{1}{\epsilon} & 0 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & \epsilon \end{bmatrix} \\
G + \delta G &= \begin{bmatrix} 1 & 1 \\ 1 & \epsilon \end{bmatrix} = \begin{bmatrix} \frac{1}{\epsilon} & 0 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & \epsilon \end{bmatrix} \quad .
\end{aligned}
$$

Here, G is nearly orthogonal, and $\|\delta G\| \approx \|G\|$. Thus, even a single zero matrix entry means that with appropriately chosen D_1 and D_2, the largest singular value can be ill-determined. Note that D_1, D_2 and B are not uniquely determined by G; we could have chosen $D_1 = D_2 = I$ and $B = G$ in the above example, and concluded that all singular values of G were well-conditioned. In practice D_1 and D_2 may be extra information supplied by the user along with G, in which case they determine the allowable uncertainty in entries of G. But we may also just be given G without D_1 and D_2, in which case we would like an error bound corresponding to the "best" D_1 and D_2. These observations, and the exponential expense of computing χ_1, motivates us to find a simpler, easily computable error bound.

Our error bound below will have the three attractive properties of

1. being small when χ_1 is large,
2. costing just $O(n^3)$ or even $O(n^2)$ to compute, and
3. being small just when n particular submatrices of B are well-conditioned, i.e. those determining the accuracy of LU decomposition; the choice of submatrices will depend on D_1 and D_2.

To see the connection between well-conditioned submatrices of B and accurate LU decomposition, recall that all intermediate results in LU decomposition can be expressed as Schur complements

like $B_{22} - B_{21}B_{11}^{-1}B_{12}$ below:

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} I & 0 \\ B_{21}B_{11}^{-1} & I \end{bmatrix} \cdot \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} - B_{21}B_{11}^{-1}B_{12} \end{bmatrix}$$

Thus if all leading principal minors B_{11} are well-conditioned, each Schur complement will be determined accurately. If we permit arbitrary diagonal scaling

$$G = D_1 B D_2 = \begin{bmatrix} D_{11} & 0 \\ 0 & D_{12} \end{bmatrix} \cdot \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \cdot \begin{bmatrix} D_{21} & 0 \\ 0 & D_{22} \end{bmatrix}$$

then the diagonal matrices "factor through" the Schur complement in simple ways:

$$G = \begin{bmatrix} I & 0 \\ D_{12}(B_{12}B_{11}^{-1})D_{11}^{-1} & I \end{bmatrix} \cdot \begin{bmatrix} D_{11}B_{11}D_{21} & D_{11}B_{12}D_{22} \\ 0 & D_{12}(B_{22} - B_{21}B_{11}^{-1}B_{12})D_{22} \end{bmatrix} \quad .$$

On the other hand, allowing arbitrary D_1 and D_2 means that *any* submatrix of B is a candidate leading principal submatrix B_{11} after GECP reorders rows and columns. This is why Gu and Eisenstat ask that *every* principal submatrix of B be well-conditioned [37].

However, by assuming D_1 and D_2 are approximately sorted (with the diagonal entries more or less decreasing from top to bottom), which can always be achieved with row and/or column permutations of G, then we need only look at the conditioning of the n leading principal submatrices of B, rather than all submatrices. This is because the natural pivot order is a good approximation of the one GECP would choose. This gives us a much cheaper criterion for high relative accuracy than Gu and Eisenstat, at the cost of a somewhat weaker bound.

In particular, suppose we have already permuted the rows and columns of the m-by-n matrix G so that $G = D_1 B D_2$ has the diagonal entries of D_1 and D_2 in roughly decreasing order. Suppose w.l.o.g that $m \geq n$. Define

$$\tau = \max\left(\max_{1 \leq i < j \leq m} \frac{D_{1,j}}{D_{1,i}}, \max_{1 \leq i < j \leq n} \frac{D_{2,j}}{D_{2,i}} \right) \quad \text{and} \quad \bar{\tau} \equiv \max(\tau, 1) \quad . \tag{16}$$

Note that $\bar{\tau} = 1$ exactly when the diagonal entries of D_1 and D_2 are in nonincreasing order, and not much larger than 1 if they are more or less decreasing. When $\tau \ll 1$ then we say that G is *strongly graded* and we will see that this can be used to improve the error bound.

Let $B = LU$ be an LU decomposition of B without pivoting, where L and U are lower and upper triangular, respectively, but not necessarily unit diagonal. The next theorem shows that if L and U are well-conditioned, which will be true if the smallest singular values of all leading principal submatrices of B are large enough compared to $\|B\|$, and if τ is not much larger than 1, then the SVDs of G and $G + \delta G = D_1(B + \delta B)D_2$ will agree to high relative accuracy when $\|\delta B\|/\|B\|$ is small.

We will need the following notation. Since L is m-by-n with $m \geq n$, write it as $L = \begin{bmatrix} L_1 \\ L_2 \end{bmatrix}$ where L_1 is n-by-n. Now let $L^{\#} \equiv \begin{bmatrix} L_1^{-1} \\ -L_2 L_1^{-1} \end{bmatrix}$, $I^{\#} = \begin{bmatrix} I^{n \times n} \\ O^{(m-n) \times n} \end{bmatrix}$, $I_{\#} = \begin{bmatrix} O^{n \times (m-n)} \\ I^{(m-n) \times (m-n)} \end{bmatrix}$, and $\tilde{L} \equiv [L, I_{\#}]$. Note that $\tilde{L}^{-1} = [L^{\#}, I_{\#}]$. When $m = n$, $L = \tilde{L}$, $L^{-1} = \tilde{L}^{-1} = L^{\#}$, and $I^{\#} = I$.

Theorem 4.1

$$\begin{aligned}\frac{|\sigma_i(G+\delta G)-\sigma_i(G)|}{\max(\sigma_i(G+\delta G),\sigma_i(G))} &\le \frac{\bar\tau\left\{\kappa(\tilde L)+\kappa(U)\right\}\cdot\max\left\{\|\bar L-I^{\#}\|,\|\bar U-I\|\right\}}{1-\bar\tau\left\{\kappa(\tilde L)+\kappa(U)\right\}\cdot\max\{\|\bar L-I^{\#}\|,\|\bar U-I\|\}}\\ &\le \bar\tau\left\{\kappa(\tilde L)+\kappa(U)\right\}\cdot\|L^{\#}\|\cdot\|U^{-1}\|\cdot\|\delta B\|+O(\|\delta B\|^2)\ ,\end{aligned}$$

where $G=D_1BD_2$, $B=LU$ (without pivoting), $\bar\tau$ is defined in equation (16), and $I^{\#}+\tilde L^{-1}\delta BU^{-1}\equiv\bar L\bar U$ is the LU decomposition without pivoting.

Proof: We want to write $G+\delta G=D_LGD_R$, where D_L and D_R are close to identity matrices, and then apply Theorem 2.2. To this end, write

$$G+\delta G=D_1(LU+\delta B)D_2=D_1(\tilde LI^{\#}U+\delta B)D_2=D_1\tilde L\left(I^{\#}+\tilde L^{-1}\delta BU^{-1}\right)UD_2=D_1\tilde L(\bar L\bar U)UD_2\ .$$

Hence

$$\begin{aligned}G+\delta G &= \left(D_1\tilde L\tilde{\bar L}\right)\cdot\left(I^{\#}\right)\cdot(\bar UUD_2)\\ &\quad \text{where } \tilde{\bar L}=[\bar L,I_{\#}]\\ &= \left(D_1\tilde L\tilde{\bar L}\right)\cdot\left(\tilde L^{-1}D_1^{-1}GD_2^{-1}U^{-1}\right)\cdot(\bar UUD_2)\\ &= \left(D_1\tilde L\tilde{\bar L}\tilde L^{-1}D_1^{-1}\right)\cdot G\cdot\left(D_2^{-1}U^{-1}\bar UUD_2\right)\\ &\equiv D_L\cdot G\cdot D_R.\end{aligned}$$

If L and U are well-conditioned, $\tilde L^{-1}\delta BU^{-1}$ will be small, so $\tilde{\bar L}$ and $\bar U$ are close to the identity. In fact, to first order in δB, we can write

$$\bar L=I^{\#}+\mathrm{tril}\left(\tilde L^{-1}\delta BU^{-1}\right)\quad\text{and}\quad\bar U=I+\mathrm{triu}\left(\tilde L^{-1}\delta BU^{-1}\right),\tag{17}$$

where $\mathrm{tril}(X)$ is the strictly lower triangular part of X, and $\mathrm{triu}(X)$ is the upper triangular part of X, including the diagonal (see also [69]). Thus

$$\|\tilde{\bar L}-I\|\le\|\tilde L^{-1}\|\cdot\|\delta B\|\cdot\|U^{-1}\|\quad\text{and}\quad\|\bar U-I\|\le\|\tilde L^{-1}\|\cdot\|\delta B\|\cdot\|U^{-1}\|,$$

and it follows that

$$\|D_L-I\|=\|D_1\tilde L(\tilde{\bar L}-I)\tilde L^{-1}D_1^{-1}\|\le\bar\tau\|\tilde L(\tilde{\bar L}-I)\tilde L^{-1}\|\le\bar\tau\kappa(\tilde L)\cdot\|\tilde{\bar L}-I\|,$$

which is true in any absolute norm, since the (i,j) entry of the lower triangular matrix $\tilde L(\tilde{\bar L}-I)\tilde L^{-1}$ is multiplied by $|D_{1,i}/D_{1,j}|\le\bar\tau$. Similarly,

$$\|D_R-I\|\le\bar\tau\kappa(U)\cdot\|\bar U-I\|\ .$$

Plugging these relations into Theorem 2.2 and simplifying, we obtain Theorem 4.1. □

When G is strongly graded ($\tau\ll1$) then the offdiagonals of D_L-I and D_R-I are both multiplied by $\tau\ll1$, which improves the error bound. In this case, only the diagonal of $\tilde L^{-1}\delta BU^{-1}$ matters.

One can also use Theorem 2.3 to prove a similar result about the singular vectors of G and $G + \delta G$, but we will omit this.

We note that the higher order terms we dropped in Theorem 4.1 remain small as long as τ is not much larger than 1.

In general we will be given G, but not D_1 and D_2, so we can not sort them. Instead, we seek an a posteriori bound, that can be evaluated after GECP on G, that bounds the relative error in the SVD of G introduced by roundoff during GECP; this bound will implicitly pick "good" D_1 and D_2. After stating this bound, we will show it is close to the perturbation bound in Theorem 4.1.

We use the same notation as before: if X is m-by-n, $\tilde{X} \equiv [X, I_{\#}]$ is m-by-m. Also, $\tilde{\text{tril}}(X) \equiv [\text{tril}(X), O^{m\times(m-n)}]$.

Theorem 4.2 *Let $P_1 G P_2 \approx \hat{L} \cdot \hat{U}$ be the factorization of the m-by-n ($m \geq n$) matrix G computed by GECP in floating point arithmetic with machine precision ε. $\hat{L}$ is unit lower triangular, and $\hat{U}$ is upper triangular. To first order in ε, the relative error introduced in the singular values by roundoff during GECP is bounded by*

$$3n\varepsilon\{\| \, |\tilde{\hat{L}}| \cdot \tilde{\text{tril}}(|\tilde{\hat{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\tilde{\hat{L}}^{-1}| \, \| + \| \, |\hat{U}^{-1}| \cdot \text{triu}(|\tilde{\hat{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\hat{U}| \, \|\}.$$

Proof: We write $G + \delta G = D_L G D_R$ as before. The first term in the error bound comes from bounding $\|D_L - I\|$ and plugging into Theorem 2.2, and the second term comes from bounding $\|D_R - I\|$.

Assume without loss of generality that the permutations involved in the factorization are identities. We use the fact that the backward error δG in the decomposition $G + \delta G = \hat{L} \cdot \hat{U}$ is bounded component-wise by $|\delta G| \leq 3n\epsilon |\hat{L}| \cdot |\hat{U}|$. Then we factor $G = D_L^{-1} (G + \delta G) D_R^{-1}$ as follows:

$$G = \hat{L} \cdot \hat{U} - \delta G = \tilde{\hat{L}} \cdot \left(I^{\#} - \tilde{\hat{L}}^{-1} \cdot \delta G \cdot \hat{U}^{-1} \right) \cdot \hat{U} = \tilde{\hat{L}} \cdot (\bar{L}\bar{U}) \cdot \hat{U},$$

where $I^{\#} - \tilde{\hat{L}}^{-1} \delta G \hat{U}^{-1} = \bar{L}\bar{U}$ is the LU decomposition without pivoting. It follows that

$$\begin{aligned} G &= \left(\tilde{\hat{L}} \cdot \tilde{\bar{L}} \right) \cdot \left(I^{\#} \right) \cdot \left(\bar{U} \cdot \hat{U} \right) \\ &= \left(\tilde{\hat{L}} \cdot \tilde{\bar{L}} \right) \cdot \left(\tilde{\hat{L}}^{-1} (G + \delta G) \hat{U}^{-1} \right) \cdot \left(\bar{U} \cdot \hat{U} \right) \\ &= \left(\tilde{\hat{L}} \cdot \tilde{\bar{L}} \cdot \tilde{\hat{L}}^{-1} \right) \cdot (G + \delta G) \cdot \left(\hat{U}^{-1} \cdot \bar{U} \cdot \hat{U} \right) \\ &\equiv D_L^{-1} (G + \delta G) D_R^{-1}. \end{aligned}$$

Taking absolute values, we see that

$$|D_L - I| = | \, \tilde{\hat{L}} \cdot \left(\tilde{\bar{L}}^{-1} - I \right) \cdot \tilde{\hat{L}}^{-1} \, |.$$

Similarly to (17), we can write to first order that

$$| \, \tilde{\bar{L}}^{-1} - I \, | \leq 3n\varepsilon \cdot \tilde{\text{tril}}(\, |\tilde{\hat{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}| \,),$$

and hence

$$|D_L - I| \leq 3n\epsilon|\hat{\tilde{L}}| \cdot \tilde{\text{tril}}(|\hat{\tilde{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\hat{\tilde{L}}^{-1}| \ .$$

Similarly,

$$|D_R - I| \leq 3n\epsilon|\hat{U}^{-1}| \cdot \text{triu}(|\hat{\tilde{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\hat{U}| \ .$$

The theorem is proved by plugging these relations into Theorem 2.2 and dropping the higher order terms. □

Theorem 4.2 provides a computable error bound which can be used in practice. The diagonal matrices D_1 and D_2 do not appear explicitly in the expression. The expression in Theorem 4.2 does not change if we replace $\hat{L}$ and $\hat{U}$ by $\hat{L} \cdot D$ and $D^{-1} \cdot \hat{U}$, respectively, for any non-singular diagonal matrix D. Hence there is no need to choose D_1, D_2, and D "optimally" to compute the error bound.

The obvious question is whether the bound in Theorem 4.2 is useful, i.e. whether it is close to the perturbation bound in Theorem 4.1. The next corollary shows that they are indeed close. We make the reasonable assumption that the permutations P_1 and P_2 computed by GECP nearly sort D_1 and D_2, so that $\bar{\tau}$ in equation (16) is not much bigger than 1. This sorting property is a natural consequence of complete pivoting: it moves the largest potential pivot into the upper left corner. This lets us write $P_1 G P_2 \approx \hat{L}\hat{U} = D_1 L U D_2$, where we can take

$$\hat{L} = D_1 L D_1'^{-1} \quad \text{and} \quad \hat{U} = D_1' U D_2 \ , \ \text{where} \ D_1' = D_1(1:n, 1:n) \ .$$

Hence $L \cdot U$ is the LU decomposition of the unscaled matrix $D_1^{-1} \cdot (P_1 G P_2) \cdot D_2^{-1}$.

Corollary 4.1 *To first order, the relative error introduced in the singular values by computing the decomposition $G = \hat{L} \cdot \hat{U}$ in floating point arithmetic with machine precision ϵ is bounded by*

$$3n\bar{\tau}\epsilon\{ \ \| \ |\tilde{L}| \cdot \tilde{\text{tril}}(|\tilde{L}^{-1}| \cdot |L| \cdot |U| \cdot |U^{-1}|) \cdot |\tilde{L}^{-1}| \ \| + \| \ |U^{-1}| \cdot \text{triu}(|\tilde{L}^{-1}| \cdot |L| \cdot |U| \cdot |U^{-1}|) \cdot |U| \ \| \ \},$$

where $\bar{\tau}$ is defined in (16).

Remark. In other words, the error bound is small if L and U are well-conditioned, and $\bar{\tau}$ is not much larger than 1, as in Theorem 4.1.

Proof: Similar to the proof of Theorem 4.1, it is easy to check that

$$\begin{aligned} \| \ |\hat{\tilde{L}}| \cdot \tilde{\text{tril}}(|\hat{\tilde{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\hat{\tilde{L}}^{-1}| \ \| &= \|D_1 \cdot |\tilde{L}| \cdot \tilde{\text{tril}}(|\tilde{L}^{-1}| \cdot |L| \cdot |U| \cdot |U^{-1}|) \cdot |\tilde{L}^{-1}| \cdot D_1^{-1}\| \\ &\leq \bar{\tau} \cdot \| \ |\tilde{L}| \cdot \text{tril}(|\tilde{L}^{-1}| \cdot |L| \cdot |U| \cdot |U^{-1}|) \cdot |\tilde{L}^{-1}| \ \| \ , \end{aligned}$$

and

$$\| \ |\hat{U}^{-1}| \cdot \text{triu}(|\hat{\tilde{L}}^{-1}| \cdot |\hat{L}| \cdot |\hat{U}| \cdot |\hat{U}^{-1}|) \cdot |\hat{U}| \ \| \leq \bar{\tau} \cdot \| \ |U^{-1}| \cdot \text{triu}(|\tilde{L}^{-1}| \cdot |L| \cdot |U| \cdot |U^{-1}|) \cdot |U| \ \|.$$

Combining these relations with Theorem 4.2, Corollary 4.1 immediately follows. □

Similar to Theorem 4.2, the expression in Corollary 4.1 does not change if we replace L and U by $L \cdot D$ and $D^{-1} \cdot U$, respectively, for any non-singular diagonal matrix D. Hence there is no need to choose D "optimally" to minimize the error bound.

As in Theorem 4.1, the higher order terms we dropped off in Theorem 4.2 and Corollary 4.1 remain higher order so long as $\bar{\tau}$ is not much larger than one.

One may also ask how Corollary 4.1 is quantitatively related to the results of Gu and Eisenstat [37]. Unfortunately, the relation is not so obvious, other than that the expression is not large if the smallest singular values of all the principal submatrices of B in $G = D_1 B D_2$ are large enough.

Given G, one can ask which D_1 and D_2 are "optimal", in the sense of giving a smallest error or perturbation bound. This can be reduced to linear programming, but since we see no use for it in practice, we will not present it here.

Finally, we briefly consider the case $G = D_1 B$, where B has full column rank; the interesting case is when B has more rows m than columns n. In this case, we can do arbitrary column pivoting in the pursuit of a good LU decomposition, so that we expect a good decomposition (following Gu and Eisenstat) when *all* k-by-n submatrices of B have singular values that are not too small, or (following Corollary 4.1) when the k-by-n submatrices of B corresponding to the largest n entries of D_1 are well-conditioned. We pursue this in section 4.4 below, when we discuss weighted least squares problems.

4.1 Numerical Experiments

In this section, we have four goals:

1. We want to assess the accuracy of GECP followed by Algorithm 3.1 in computing the SVD, and show that it attains the predicted error bounds. It does.

2. We want to assess the error bound in Theorem 4.2, to see how close it is to the actual error. It turns out to be pessimistic, but still gives useful information in double precision, if not single.

3. We want to see how well QRCP followed by lgorithm 3.3 Algorithm 3.3 works. Although a complete error analysis remain to be done, it seems that this method is as effective on graded matrices as GECP + Algorithm 3.1.

4. We want to show that complete pivoting plays an essential role, by showing that QR with column pivoting cannot be used in its place.

5. We want to show that the one-sided Jacobi algorithm from [25] is often as accurate as the more complicated algorithm proposed here (GECP plus Algorithm 3.1), but that it can fail.

We generate square random 200-by-200 matrices G in the form $G = D_1 B D_2$, where B is a random matrix with equilibrated column and row norms and with the spectral condition number 10^i, $i = 1, 2, \ldots, 7$, and D_1 and D_2 are random diagonal matrices with $\kappa(D_2) = 10^k$, $k = 2, 4, 8, 10, 12, 14, 16$ and $\kappa(D_1) = \sqrt{\kappa(D_2)}$. For each fixed pair of parameters (i, k) we use two different `MODE`s of singular value distributions for the triple B, D_1, D_2 (see section 3.3) where for each choice of the mode we generate 2 test matrices of the type $G = D_1 B D_2$. This makes a total of 196 test matrices, or 28 for each value of i.

Note that we do not directly control the condition numbers of the LU factors of the (permuted) B by this process, or the sorting of D_1 and D_2, which is what the error bounds ultimately depend on (see Theorem 4.1). Nonetheless, we argue that we roughly control $\|L^{-1}\|$ and $\|U^{-1}\|$, since $B = LU$ implies

$$\|B^{-1}\|^{1/2} \leq (\|U^{-1}\| \cdot \|L^{-1}\|)^{1/2}$$

$$
\begin{aligned}
&\leq \max(\|U^{-1}\|, \|L^{-1}\|) \\
&= \max(\|B^{-1}L\|, \|UB^{-1}\|) \\
&\leq \|B^{-1}\| \cdot \max(\|L\|, \|U\|) \quad .
\end{aligned}
$$

Therefore, we choose the following error measure

$$
\epsilon(i) = \max_{G=D_2AD_1, \kappa(A)=10^i} \max_k \frac{|\sigma_{S,k} - \sigma_{D,k}|}{\sigma_{D,k}} \quad . \tag{18}
$$

For GECP followed by Algorithm 3.1 we expect $\epsilon(i) \stackrel{<}{\approx} \varepsilon_S 10^i \approx 10^{7-i}$, for the reasons just discussed. Table 1 displays the computed results:

- Row 1, Column 2: The expected relative error 10^{i-7} for GECP and Algorithm 3.1 applied to the 28 test matrices with $\kappa(A) = 10^i$.
- Row 1, Column 3: The maximum measured relative error $\epsilon(i)$ for GECP and Algorithm 3.1 on the same set of matrices.
- Row 1, Column 4: The bound from Theorem 4.2 for $\epsilon(i)$ for GECP and Algorithm 3.1 for the same set of matrices *computed in double precision.*
- Row 2, Column 2: The maximum measured relative error $\epsilon(i)$ for the algorithm consisting of QR decomposition and Algorithm 3.3 for the same set of matrices.
- Row 2, Column 3: The maximum measured relative error for QRCP and Algorithm 3.3 for the same set of matrices.
- Row 2, Column 4: The maximum measured relative error $\epsilon(i)$ for the one-sided Jacobi algorithm alone for the same set of matrices.

Since columns 2 and 3 in row 1 of Table 1 roughly agree, GECP followed by Algorithm 3.1 is as accurate as predicted. Column 4 of row 1 shows that the error bound from Theorem 4.2 predicts that the *double precision* algorithm delivers at least about 5 to 8 digits of accuracy, which is pessimistic, but useful. The corresponding error bounds for the *single precision* algorithm are all about $\varepsilon_S/\varepsilon_D \approx 5 \cdot 10^8$ times larger, and so all about 1 or larger. In other words, the bound of Theorem 4.2 provides useful bounds in double precision, but is too pessimistic to be useful in single precision.

Column 2 of row 2 shows that QR combined with one-sided Jacobi is *not* nearly as accurate an SVD algorithm. Column 3 of row 2 shows that QRCP is as accurate an SVD algorithm, although existing error analyses are not as complete [41]. Existing theory [25] guarantees high relative accuracy for the algorithms in columns 2 and 4 of row 2 only when G is scaled from one side ($G = BD_1$). Therefore, it is something of a surprise that Column 4 of row 2 shows one-sided Jacobi to be about as accurate as our more sophisticated algorithm GECP with Algorithm 3.1. This leads us to ask whether there are examples where GECP with Algorithm 3.1 is significantly more accurate than simple one-sided Jacobi.

The following 3-by-3 example shows how one-sided Jacobi can fail when the new algorithm succeeds. Let γ and δ satisfy $1 \gg \gamma \gg \delta > 0$; $\gamma = 10^{-20}$ and $\delta = 10^{-40}$ will do in double precision.

i	Expected $\epsilon(i)$ for GECP + Algorithm 3.1 in single precision	Measured $\epsilon(i)$ for GECP + Algorithm 3.1 in single precision	Bound for $\epsilon(i)$ for GECP + Algorithm 3.1 from Theorem 4.2 in double precision
1	10^{-6}	$4 \cdot 10^{-6}$	$2 \cdot 10^{-8}$
2	10^{-5}	$9 \cdot 10^{-6}$	$3 \cdot 10^{-8}$
3	10^{-4}	$1 \cdot 10^{-4}$	$3 \cdot 10^{-8}$
4	10^{-3}	$1 \cdot 10^{-3}$	$4 \cdot 10^{-8}$
5	10^{-2}	$8 \cdot 10^{-3}$	$1 \cdot 10^{-7}$
6	10^{-1}	$1 \cdot 10^{-1}$	$1 \cdot 10^{-6}$
7	1	1	$1 \cdot 10^{-5}$

i	Measured $\epsilon(i)$ for QR + Algorithm 3.3 in single precision	Measured $\epsilon(i)$ for QRCP + Algorithm 3.3 in single precision	Measured $\epsilon(i)$ for Jacobi SVD in single precision
1	0.7	$2 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
2	0.9	$2 \cdot 10^{-5}$	$8 \cdot 10^{-6}$
3	> 2	$8 \cdot 10^{-5}$	$1 \cdot 10^{-4}$
4	> 50	$1 \cdot 10^{-3}$	$9 \cdot 10^{-4}$
5	> 300	$9 \cdot 10^{-3}$	$7 \cdot 10^{-3}$
6	> 1000	$1 \cdot 10^{-1}$	$2 \cdot 10^{-2}$
7	> 1000	$6 \cdot 10^{-1}$	1

Table 1: Accuracy of Overall SVD Algorithms

Let

$$
\begin{aligned}
G &= \begin{bmatrix} 1 & \gamma & \gamma \\ -\gamma & \gamma & \gamma^2 \\ 0 & \delta & 0 \end{bmatrix} \\
&= D_1 \cdot B \cdot D_2 \\
&\equiv \begin{bmatrix} 1 & & \\ & \gamma & \\ & & \delta \end{bmatrix} \cdot \begin{bmatrix} 1 & \gamma & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ & 1 & \\ & & \gamma \end{bmatrix} .
\end{aligned}
$$

Since D_1 and D_2 are sorted, and the leading principal minors of B are well-conditioned, the SVD of G is determined to high relative accuracy. GECP applied to G requires no pivot exchanges, and yields very accurate LDU factors, with L and U nearly identity matrices, so that Algorithm 3.1 computes a very accurate SVD with singular values nearly equal to 1, γ, and $2\gamma\delta$.

But if we apply one-sided Jacobi to the right of G so that it rotates columns 2 and 3 first, then we lose all accuracy in the smallest singular value $2\gamma\delta$. (In a Matlab experiment with $\gamma = 10^{-20}$ and $\delta = 10^{-40}$, we get $5 \cdot 10^{-57}$ instead of $2 \cdot 10^{-60}$.) This occurs because the first Jacobi rotation angle is $O(1)$ rather than $O(\gamma)$, which does not respect the column scaling, and so causes a large backward error in B.

4.2 Comments on Tridiagonalization and Bidiagonalization

Suppose that we have a symmetric matrix A whose eigenvalues we want to compute via tridiagonalization. It has long been observed that tridiagonal reduction tends to respect grading [49], yet we argue that tridiagonalization can fail to preserve high relative accuracy even in the limit as A converges to a diagonal matrix. This is because the first Householder transformation, the one that zeros out $A(3:n,1)$ and $A(1,3:n)$, will depend on the values of $A(2:n,1)$, which are approaching zero. Since they can approach zero in any way, the first (normalized) Householder vector can take on any value, so the first reflector can be arbitrary. In particular, all its entries can be $O(1)$ in magnitude, so it can easily destroy diagonal dominance in the trailing submatrix $A(2:n,2:n)$. This occurs no matter how the diagonal of A is sorted. This is easy to observe in simple numerical experiments with $A(i,i) = 10^{-20i}$. A similar example appears in [77], example (4.2).

In [21] an example is given of a symmetric tridiagonal matrix that determines its tiniest eigenvalue accurately, but where QR iteration with any choice of shift destroys the accuracy of this eigenvalue.

In the case of bidiagonalization one can find graded examples where the rows and columns must be ordered very carefully for bidiagonalization to preserve high relative accuracy. In particular, in $G = D_1 B D_2$ D_1 and D_2 are not sorted, nor are the leading principal submatrices of B well-conditioned. In other words, there appears to be no simple rule to choose a successful ordering of rows and columns to preserve high relative accuracy. We refer to [5] for a more comprehensive study of the accuracy of bidiagonalization, and how to improve it.

4.3 Graded Symmetric Eigenvalue Problems

The cases studied in [6] and [25], where the SVD is determined to high relative accuracy, are essentially subsumed by this analysis. In [6], *scaled diagonally dominant (s.d.d.)* matrices were

studied, i.e. symmetric matrices of the form $G = D(E+N)D$, where D was an arbitrary diagonal matrix, E was diagonal with diagonal entries ± 1, and N satisfied $\|N\|_2 \equiv \gamma < 1$. It is easy to see that a symmetric permutation that sorts D leaves all principal submatrices of $E+N$ with singular values between $1-\gamma$ and $1+\gamma$, i.e. well conditioned if γ is small. In [25], symmetric positive definite matrices of the form DAD were studied, where D is any diagonal matrix and A is symmetric positive definite and well-conditioned. Again, a symmetric permutation to sort D leaves the leading principal submatrices of A no worse conditioned than A itself, by the Cauchy Interlace Theorem.

4.4 Relationship to Weighted Least Squares Problems

In [65, 51, 74, 75, 43], the weighted least squares problem $\min_x \|D^{1/2}(Ax-b)\|_2$ is considered, with the goal of deriving algorithms and error bounds that hold independent of the diagonal scaling matrix D. In these papers it is shown that the condition number essentially depends on the following combinatorial object: Suppose A is full rank and m-by-n, and let x_{WLS} be the unique solution of the weighted least squares problem. Let Q be any m-by-n unitary matrix with the same column space as A; the Q from the QR decomposition of A will do. Let ρ be the smallest nonzero singular value of any k-by-n submatrix of Q, for $1 \le k \le m$. Then the norm of the "weighted projector" $P_D \equiv A(A^TDA)^{-1}A^TD$ that maps b to its best approximation $Ax_{WLS} = P_Db$ is at most $\|P_D\| \le \rho^{-1}$, independent of D. It is easy to confirm that P_D does not change if A is postmultiplied by any nonsingular n-by-n matrix, which is why we can replace A by Q. To see why the combinatorial definition of ρ is natural, we can let D have k diagonal entries equal to 1 and the rest very small; this essentially selects a k-by-n submatrix $\hat{Q}$ of Q, with the large columns of P_D approximately given by $Q(\hat{Q}^T\hat{Q})^{-1}\hat{Q}$, whose norm is the reciprocal of smallest singular value of $\hat{Q}$.

Since we are interested in the whole SVD, not just the pseudoinverse, we cannot replace A by Q. But suppose that A were unitary (or just well-conditioned). Then the conditions imposed in [65, 51, 74, 43] are essentially the same as the conditions in the last paragraph of the first part of section 4.

5 Computing an Accurate RRD: Combinatorial and Algebraic Conditions

In this section we will discuss *combinatorial and algebraic conditions* on G i.e. conditions on G's sparsity pattern and sign pattern, or on algebraic relationships among the entries of G, that guarantee that the LDU factors from Gaussian elimination with complete pivoting (GECP) are determined accurately enough to yield a good RRD of G. In later sections we will show how to modify the GECP algorithm to compute the LDU factors as accurately as we need. Then we will use Algorithm 3.1 to compute the SVD of G. In this section we just motivate and outline these conditions, and leave the details to subsequent sections.

We begin with the fact that every final or intermediate value computed by Gaussian elimination, with any legal pivot order (i.e. not leading to divide-by-zero), is either *a minor or quotient of minors of* G. The conditions we impose on G will guarantee that *all* minors of G can be computed accurately. Since the quotient of two values known to high relative accuracy is also known to high relative accuracy, this implies that L, D and U can be computed accurately, for any legal pivot order.

More specifically, we will use the following classical result:

Lemma 5.1 *Let $G = P_r L D U P_c$ be any factorization of G computed by Gaussian elimination with any pivot order not leading to division by zero. Here P_r and P_c are permutations, L and U are unit triangular, and D is diagonal. We also write this as $G = P_r \bar{L} \bar{U} P_c$, where either $\bar{L} = L$ and $\bar{U} = DU$, or $\bar{U} = U$ and $\bar{L} = LD$. Let G_s be any Schur complement of G, i.e.*

$$G_s = G_{22} - G_{21} G_{11}^{-1} G_{12} \quad \text{where} \quad G = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} .$$

Then

1. *Every minor of G_s is a quotient of minors (or just a minor) of G.*
2. *Every minor of G^{-1} is plus or minus a quotient of minors of G.*
3. *Every entry of L, D, U, $\bar{L}$ and $\bar{U}$ is either zero or a quotient of minors (or just a minor) of G.*
4. *Every minor of L, D, U, $\bar{L}$ and $\bar{U}$ consisting of consecutive rows is either zero or a quotient of minors (or just a minor) of G.*
5. *Every entry of L^{-1}, D^{-1}, U^{-1}, $\bar{L}^{-1}$ and $\bar{U}^{-1}$ is either zero or a quotient of minors (or just a minor) of G.*

These facts follow from Sylvester's determinant identity [70, p. 87], or more specifically from observations like

$$D_{n,n} = \frac{D_{1,1} \cdots D_{n-1,n-1} \cdot D_{n,n}}{D_{1,1} \cdots D_{n-1,n-1}} = \frac{\det(G)}{\det(G(1:n-1, 1:n-1))}$$

(assuming $P_r = P_c = I$).

To see what conditions we must impose on G to compute its minors accurately, let us consider a general algebraic expression $e(\zeta_1, \zeta_2, ..., \zeta_k)$, where $e(\cdot)$ is defined by a fixed sequence of additions, subtractions, multiplications and divisions. We assume that each real datum ζ_i is known to high relative accuracy, and we may also know its sign. For e to be determined to high relative accuracy by the data ζ_i, *independent of the magnitudes of the* ζ_i, it is clearly necessary and sufficient for e to be defined by

(1) multiplications and divisions, and

(2) addition of quantities with the same sign.

For example, $(\zeta_1^2 + \zeta_2^2) \cdot \zeta_3^3 / \zeta_4$ is accurately determined, but $\zeta_1 + \zeta_2$ is not unless it is also known that $\zeta_1 \zeta_2 > 0$. In other words, the only forbidden operation is true subtraction, because cancellation in leading digits can leave the sum $s = \zeta_1 + \zeta_2$ with arbitrarily less relative accuracy than in ζ_1 or in ζ_2, if ζ_1 and $-\zeta_2$ are close.

Here is a more formal way to describe this property of e: Let $\hat{e}(\cdot)$ be another expression which differs from $e(\cdot)$ only by having the result of each operation multiplied by a different $1 + \delta$, where $|\delta| \leq \varepsilon \ll 1$; in other words $\hat{e}()$ is the value of e computed in floating point with machine precision

ε. (Here and elsewhere we ignore the possibility of over/underflow.) Also let $|\hat{\zeta}_i - \zeta_i| \leq \eta|\zeta_i|$ for all i, where $0 < \eta \ll 1$. Then

$$\frac{|\hat{e}(\hat{\zeta}_1, ..., \hat{\zeta}_k) - e(\zeta_1, ..., \zeta_k)|}{|e(\zeta_1, ..., \zeta_k)|} = O(\max(\eta, \varepsilon)) \quad . \tag{19}$$

Requirements (1) and (2) leave us enough freedom to find accurate expressions e for the minors of a variety of interesting matrix classes, as we outline below. But we can solve still more problems if we permit ourselves one more operation, which is only justified in (well-implemented) floating point arithmetic:
(3) addition or subtraction if the operands are original data, i.e. ζ_i and ζ_j.

Here is the justification. Consider an expression $e(\zeta_1, ..., \zeta_k)$ consisting of operations (1), (2) and (3), and where the ζ_i are floating point numbers, and let $\hat{e}(\cdot)$ be the floating point version of e as above. Then

$$\frac{|\hat{e}(\zeta_1, ..., \zeta_k) - e(\zeta_1, ..., \zeta_k)|}{|e(\zeta_1, ..., \zeta_k)|} = O(\varepsilon) \quad . \tag{20}$$

Equation (20) holds because if there is cancellation in computing the sum or difference $\zeta_i - \zeta_j$ of two floating point numbers, then the sum or difference is *exact* [3]. Comparing with equation (19), we see that we compute an approximation $\hat{e}(\zeta_i)$ of the true value $e(\zeta_i)$ to high relative accuracy, but if the ζ_i themselves are uncertain, there is no bound on the difference $\hat{e}(\hat{\zeta}_i) - e(\zeta_i)$. Put another way, an algorithm based on property (3) will compute accurate minors (and eventually an accurate SVD) of the problem *as stored in the machine*, whether or not the minors and SVD of the problem in the machine are very sensitive to changes in ζ_i[4]. But if we do not need to use (3), then we have the further information that small relative changes in the ζ_i would not have significantly changed the minors or SVD.

In the case of complex data ζ_i, we cannot allow operation (2), addition of quantities of like sign, because taking powers of a complex number in the first quadrant (the natural generalization of positive reals) can lead to numbers in any quadrant, depending on magnitudes of the real and imaginary parts.

Armed with this understanding of which expressions e can be evaluated accurately, consider just the determinant of G itself, which we assume to be n-by-n. Its Laplace expansion is

$$\det(G) = \sum_p [\mathrm{sign}(p) \cdot g_{1,p_1} \cdot g_{2,p_2} \cdots g_{n,p_n}] \tag{21}$$

where the sum is over all permutations $p = (p_1, ..., p_n)$ of $(1, ..., n)$, and $\mathrm{sign}(p) = \pm 1$ is the sign of the permutation p. This is a sum and difference of monomials $\prod_i g_{i,p_i}$. We want to know when an expression $e = \det(G)$ exists satisfying requirements (1), (2) and possibly (3). We begin by assuming that the entries $g_{i,j}$ are themselves the initial data (ζ_is), and each nonzero $g_{i,j}$ is only known to high relative accuracy. Later we will consider the case when the $g_{i,j}$ are given as algebraic expression in the initial data.

Think of G as having a fixed sparsity pattern, so some $g_{i,j}$ are known to be zero. Any monomials containing such a zero factor are identically zero. Any monomial that is a product of n nonzero

[3] This assumes addition and subtraction are implemented with guard digits, and so excludes the Cray C90 and its predecessors and emulators.

[4] This will be the case for Cauchy matrices, for example.

terms is determined to high relative accuracy. If we further fix the signs of each $g_{i,j}$, then each nonzero monomial will have a fixed sign as well.

So when is the expansion (21) of $\det(G)$ determined to high relative accuracy by the initial data $g_{i,j}$? There are only 3 cases:

1. If all monomials are exactly 0, because each contains a zero $g_{i,j}$, then $\det(G)$ is exactly 0 (to high relative accuracy!).

2. If exactly one monomial is nonzero, then $\det(G)$ is determined to high relative accuracy, since the monomial is.

3. If two or more monomials are nonzero, and the $g_{i,j}$ have independent small relative errors and independent signs, then cancellation can destroy relative accuracy in the sum. We can avoid cancellation and guarantee high relative accuracy if the signs of the $g_{i,j}$ are restricted so that all nonzero monomials have the same sign.

We claim that those matrices, *all* of whose minors have 0 or 1 nonzero monomials in their Laplace expansions, are precisely the matrices whose graphs are acyclic [23]; we define this further in section 6 below. In other words, there is a simple necessary and sufficient condition for a sparse matrix to have each minor either zero or equal to a single monomial, and so determined to high relative accuracy. For these matrices, which have been extensively studied before, there are several available high accuracy SVD algorithms.

If all the minors of a matrix have Laplace expansions where each nonzero monomial has the same sign, as described in case 3 above, then the matrix is called *total signed compound (TSC)* as defined in [14]. We discuss this in detail in section 7 below. In other words, we can completely characterize which sparsity patterns (the acyclic ones), or which sparsity and sign patterns (the TSC ones) guarantee accurate minors, and so accurate LDU factors and an accurate SVD.

In both these cases, acyclic matrices and TSC matrices, straightforward GECP will *not* determine the entries of L, D and U to high relative accuracy. This is because cancellation may occur. In other words, we need to modify GECP, based on the special structure of these matrices, that compute the same LDU factorization but without cancellation. We discuss these algorithms below. Unfortunately, their complexities can be larger than for GECP ($O(n^4)$ instead of $O(n^3)$ for TSC matrices); it is an open problem to find faster algorithms.

Now we consider the case where the matrix entries $g_{i,j}$ are not the initial data, but rather algebraic expressions in the initial data. This means that there are alternate expressions for the minors that are potentially evaluatable to high relative accuracy. In subsequent sections we discuss 3 examples in detail: Cauchy matrices (section 8), totally positive matrices (section 9), and diagonally scaled totally unimodular matrices (section 10).

6 Acyclic Matrices

Some of this material originally appeared in [23]; we summarize it here for completeness. Let $\mathcal{G}$ be the class of matrices with a given sparsity pattern, i.e. the locations of the nonzero entries are given. We let $\mathrm{Gr}(\mathcal{G})$ denote the *graph of* $\mathcal{G}$, i.e. the bipartite graph with one node for each row, one node for each column, and an edge (i, j) if and only if entry (i, j) is allowed to be nonzero.

Theorem 6.1 *The following three conditions are* equivalent*:*

1. $\mathrm{Gr}(\mathcal{G})$ *is acyclic.*

2. *For all matrices $G \in \mathcal{G}$, and for any pivot sequence that does not divide by zero, small relative changes in the entries of G cause only small relative changes in the entries of L, D and U computed by Gaussian elimination.*

3. *For all matrices $G \in \mathcal{G}$, small relative changes in G cause only small relative perturbations in the SVD, in the sense of bounds (7) and (8).*

Acyclic matrices include bidiagonal matrices, "broken arrow" matrices (which are nonzero only on the diagonal and in one row or one column), and exponentially many other permutation-inequivalent patterns. All acyclic matrices are very sparse, with at most $2n-1$ nonzeros in an n-by-n acyclic matrix.

We sketch the proof of Theorem 6.1; details are in [23]. Let $\mathrm{Gr}(G)$ be defined for a particular matrix G just as it was defined for a class $\mathcal{G}$ above: there is one node per row, one node per column, and an edge (i,j) if and only if $g_{i,j} \neq 0$. Recall that a *perfect matching* in a graph with $2n$ nodes is a set of n edges where each node is the endpoint of exactly one edge. We depend on the elementary fact that there is a one-to-one correspondence between the monomials in the determinant expansion of any matrix G, and perfect matchings in $\mathrm{Gr}(G)$: Each monomial corresponds to a unique choice of n nonzeros in G, one in each row and one in each column; each such set of n nonzeros corresponds to n edges forming a perfect matching between the n row nodes and n columns nodes. It is a simple graph theoretic lemma that a bipartite graph is acyclic if and only if each subgraph has at most one perfect matching (a cycle can be used to construct two perfect matchings, and vice versa). In other words $\mathrm{Gr}(G)$ is acyclic if the determinant expansion of each submatrix of G has at most one nonzero term, which is equivalent to each minor being determined to high relative accuracy, which is sufficient for an accurate LDU decomposition, and an accurate SVD. To see that $\mathrm{Gr}(\mathcal{G})$ being acyclic is necessary, note that if there are two or more terms in the determinant expansion of some k-by-k minor, then we can choose the matrix entries so that the minor is zero because of cancellation, and the matrix outside the k-by-k submatrix defining the minor is exactly zero. Then both D_{kk} and σ_k are exactly zero, but become nonzero with arbitrarily small perturbations of any matrix entry that makes the minor nonzero. In other words, if the graph is cyclic, neither the SVD nor LU decomposition may be determined to high relative accuracy, for certain values of the matrix entries.

See Theorem 10.2 below for quantitative bounds on the accuracy with which the SVD is determined.

We can sometimes take advantage of the acyclic structure to compute the SVD quickly. For example, if the matrix is bidiagonal, various algorithms based on QR [24, 20] and QD [33] are available. For singular values of general acyclic matrices, bisection [23] is available, but until now no relatively accurate algorithm for the singular vectors was available.

We defer discussion of the algorithm for high accuracy LDU factorization of an acyclic matrix to section 10, where we present it as a special case of a more general algorithm.

7 Total Signed Compound (TSC) Matrices

The following definitions are taken from [14]. Let $\mathcal{S}$ be the set of all matrices with a given sparsity and sign pattern, i.e. the locations and signs of the nonzero entries are given. For example $\mathcal{S}$ could

be the set of all square matrices with positive numbers on the main diagonal, negative numbers on the first superdiagonal, and zeros elsewhere. $\mathcal{S}$ is called *sign nonsingular (SNS)* if it contains only square matrices, and the Laplace expansion (21) of the determinant of each $G \in \mathcal{S}$ is the sum of monomials of like-sign, with at least one nonzero monomial. $\mathcal{S}$ is called *total signed compound (TSC)* if every square submatrix of any $G \in \mathcal{S}$ is either SNS, or structurally singular (i.e. no nonzero monomials appear in its determinant expansion).

Another, constructive definition of TSC matrices is as follows [14, 59]. We will need it later for our algorithm. Every TSC matrix can be obtained by starting with a 1-by-1 nonzero matrix and applying the following four construction rules repeatedly in some order:

1. If G is TSC then permuting the rows, permuting the columns, or multiplying a row or column by -1 leaves G TSC.
2. If G_1 and G_2 are TSC, so is the direct sum $G = \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \end{bmatrix}$.
3. If $G_1 = \begin{bmatrix} G_1' \\ x_1^T \end{bmatrix}$ and $G_2 = \begin{bmatrix} x_2^T \\ G_2' \end{bmatrix}$ are TSC, where x_1^T is the last row of G_1 and x_2^T is the first row of G_2, then then so is the *weak direct sum* $G = \begin{bmatrix} G_1' & 0 \\ x_1^T & x_2^T \\ 0 & G_2' \end{bmatrix}$. Weak direct sums can also be formed by having G_1 and G_2 overlap in one column.
4. If the m-by-n matrix G' is TSC, with $G'_{ij} \neq 0$, then so is the $m+1$-by-$n+1$ matrix G obtained as follows:

$$G = \left[\begin{array}{ccc|c} & & & 0 \\ & & & \vdots \\ & & & 0 \\ & G' & & G_{i,n+1} \\ & & & 0 \\ & & & \vdots \\ & & & 0 \\ \hline 0, \cdots 0, & G_{m+1,j}, & 0, \cdots 0 & G_{m+1,n+1} \end{array}\right] \tag{22}$$

   where we can also set $G'_{i,j}$ to zero. The new possibly nonzero entries $G_{m+1,n+1}$, $G_{m+1,j}$ and $G_{i,n+1}$ must be chosen so that the two monomials in the minor $G_{m+1,n+1} \cdot G'_{i,j} - G_{i,n+1} \cdot G_{m+1,j}$ have the same sign (or are zero).

It is easy to confirm that the examples below are obtained by repeated application of construction (4) above:

$$\begin{bmatrix} + & + & & & \\ + & - & + & & \\ & + & + & + & \\ & & + & - & + \\ & & & + & + \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} + & + & + & + & + \\ + & - & & & \\ + & & - & & \\ + & & & - & \\ + & & & & - \end{bmatrix} .$$

TSC matrices are quite sparse, as the following lemma shows:

Lemma 7.1 *An m-by-n TSC matrix has at most $1.5(m+n)-2$ nonzero entries.*

Proof: We use induction on $m+n$, and the fact that a large TSC matrix is built from smaller TSC matrices according to construction rules 2, 3 and 4 (rule 1 does not change the nonzero count). The formula is obviously true when $m = n = 1$. In rule 2, suppose G_i is m_i-by-n_i. By induction G_i has at most $1.5(m_i+n_i)-2$ nonzeros, and it is easy to confirm that G has at most $[1.5(m_1+n_1)-2]+[1.5(m_2+n_2)-2] = 1.5(m+n)-4 < 1.5(m+n)-2$ nonzeros, as desired. Rule 3 is similar. For rule 4 we use the fact that G has at most 3 more nonzeros than G'. □

Theorem 7.1 *The following three conditions are* equivalent*:*

1. *$\mathcal{S}$ is TSC.*
2. *For all matrices $G \in \mathcal{S}$, and for any pivot sequence that does not divide by zero, small relative changes in the entries of G cause only small relative changes in the entries of L, D and U computed by Gaussian elimination.*
3. *For all matrices $G \in \mathcal{S}$, small relative changes in G cause only small relative perturbations in the SVD, in the sense of bounds (7) and (8).*

Proof: The proof is entirely analogous to that of Theorem 6.1. We use the lack of cancellation in all minors to conclude that all entries of L, D and U are determined to high relative accuracy, and hence that the SVD is determined to high accuracy. Similarly, If G is not TSC, we can construct a matrix where a minor vanishes by cancellation, so that some entry of D, or some singular value, is "accidentally" zero. □

To show how to modify the standard Gaussian elimination algorithm to factor TSC matrices with high relative accuracy, we need the following lemma:

Lemma 7.2 *There is an algorithm for computing the determinant of an n-by-n TSC matrix to high relative accuracy, that requires at most $4n-1$ floating point operations.*

Proof: As in the last lemma, we will use induction on n, exploiting the constructibility of any TSC matrix using the 4 rules above. A practical algorithm would represent a TSC matrix as a tree whose nodes represent applications of the 4 rules, processing the tree in topological order, but we will omit these details. In particular, we will not discuss the complexity of building this tree (which could possibly exceed the cost of the floating point operations).

Rule 1 has a trivial effect on the determinant, either leaving it unchanged or negating it.

If G is constructed by Rule 2, then there are two cases, depending on whether G_1 and G_2 are both square or not. If they are not square, $\det(G)$ is clearly 0. Otherwise, $\det(G) = \det(G_1)\det(G_2)$, which computes $\det(G)$ to high relative accuracy from $\det(G_1)$ and $\det(G_2)$, at the cost of 1 flop plus the costs of $\det(G_1)$ and $\det(G_2)$.

Now suppose G is constructed by Rule 3, where G_i is m_i-by-n_i. Since G is square, $n_1+n_2 = m_1+m_2-1 \equiv n$. For $\det(G)$ to be nonzero, the two zero blocks in G can not be too big; in particular we need $m_1-1+n_2 \le n$ and $m_2-1+n_1 \le n$. There are only two solutions of these simultaneous inequalities and equations: $m_1 = n_1$ and $m_2-1 = n_2$, or $m_1-1 = n_1$ and $m_2 = n_2$. In the first case $\det(G) = \det(G_1)\det(G_2')$, and in the second case $\det(G) = \det(G_1')\det(G_2)$, either of which costs 1 flop plus the costs of $\det(G_1)$ and $\det(G_2')$ (or $\det(G_1')$ and $\det(G_2)$).

Finally, consider Rule 4. If $G_{m+1,n+1} \neq 0$, then we can do one step of Gaussian elimination starting from the bottom of the matrix in equation (22) to get

$$G = \left[\begin{array}{c|c} & \begin{matrix}0\\ \vdots \\ 0\end{matrix} \\ I & G_{i,n+1}/G_{m+1,n+1} \\ & \begin{matrix}0\\ \vdots \\ 0\end{matrix} \\ \hline 0 & 1 \end{array}\right] \cdot \left[\begin{array}{c|c} G'' & 0 \\ \hline 0, \cdots 0, G_{m+1,j}, 0, \cdots 0 & G_{m+1,n+1} \end{array}\right]$$

where $G'' = G'$ except that $G'_{i,j}$ has been changed to $G''_{i,j} = G'_{i,j} - G'_{i,n+1}G'_{m+1,j}/G'_{m+1,n+1}$; there is no cancellation in this formula because of the TSC property, so $G''_{i,j}$ is computed to high relative accuracy, and G'' is still TSC. Then $\det(G) = G_{m+1,n+1} \cdot \det(G'')$, which costs 4 flops plus the cost of $\det(G'')$. If $G_{m+1,n+1} = 0$, we expand by minors in the last column, so $\det(G) = \pm G_{i,n+1} \cdot G_{m+1,j} \cdot \det(G''')$, where G''' is the $n-2$-by-$n-2$ submatrix of G' lying outside row i and column j. This costs 2 flops plus the cost of $\det(G''')$.

If C_n is the maximum cost of $\det(G)$ when G is n-by-n, then combining the above 4 rules yields

$$C_n \leq \max(\max_{n_1+n_2=n}(1 + C_{n_1} + C_{n_2}), 3 + C_{n-1}, 2 + C_{n-2})$$

which has solution $C_n = 4n - 1$. $\square$

Here is a simple version of Gaussian elimination with pivoting for TSC matrices, that computes all entries of L, D and U to high relative accuracy:

Algorithm 7.1 *Performing Gaussian elimination with pivoting $G = P_r L D U P_c$ in a forward stable manner on an m-by-n TSC matrix G, where $m \geq n$.*

for $i = 1$ *to* $\min(m-1, n)$
  pivot so that G_{ii} *is nonzero*
  $D_{ii} = G_{ii}$
  for $j = i+1$ *to* m
    $L_{ji} = G_{ji}/D_{ii}$
  endfor
  for $j = i+1$ *to* m
    for $k = i+1$ *to* n
(*) $G_{jk} = G_{jk} - L_{ji} \cdot G_{ik}$
(**) *If the last subtraction has two nonzero operands with the same sign, then recompute G_{jk} as the quotient of two minors, each computed using Lemma 7.2*
    endfor
  endfor
  for $k = i+1$ *to* n
    $U_{ik} = G_{ik}/D_{ii}$
  endfor

The above algorithm is essentially identical to conventional Gaussian elimination, except for line (**).

Theorem 7.2 *Algorithm 7.1 computes all the entries of the L, D and U factors of a TSC matrix G to high relative accuracy, for any pivot sequence not dividing by zero. The cost of the algorithm is $O(mn^3)$.*

Proof: The only possible source of forward instability in Algorithm 7.1 is the subtraction in line (*), and line (**) is a "brute force" way to recompute the result of line (*) so as to guarantee high relative accuracy. The complexity bound follows since line (**) can cost as much as $O(n)$ by Lemma 7.2. □

If the pivot sequence is given in advance, the complexity drops from $O(n^4)$ to $O(n^3)$, because we do not need to compute all entries of all Schur complements in order to choose the maximum pivot at each step. For an example illustrating how the complexity can be as large as $O(n^4)$, consider

$$G = \begin{bmatrix} 1 & y^T \\ x & DP \end{bmatrix}$$

where x and y have positive entries just less than 1, D is a negative definite diagonal matrix with entries of tiny but widely varying magnitudes, and P is a permutation matrix. In this case L and U can be dense, with Lemma 7.2 *always* invoked in line (**). Note that we need to recompute the entries of intermediate Schur complements accurately enough to choose the correct pivot sequence. One could probably modify the test in line (**) to invoke Lemma 7.2 less frequently, for example, only when cancellation is severe enough.

We have not developed bounds on the condition numbers of the L and U factors, but we suspect that they can only grow polynomially, rather than exponentially, with dimension.

8 Cauchy Matrices

In this section and the next we consider matrices whose entries are rational functions of a number of parameters. These matrices will have the property that expressions for their minors exist, that can be evaluated to high relative accuracy when the parameters are given floating point numbers. This then determines their LDU factors to high relative accuracy, and so their SVDs to high relative accuracy.

Cauchy matrices are defined to have entries $C_{i,j} = 1/(x_i + y_j)$, where the x_i and y_j are the initial data. Every submatrix of a Cauchy matrix is Cauchy. The well-known formula for $\det(C)$ is

$$\det(C) = \frac{\prod_{1 \le i < j \le n} (x_j - x_i)(y_j - y_i)}{\prod_{1 \le i,j \le n} (x_i + y_j)} \tag{23}$$

Every factor $x_j - x_i$, $y_j - y_i$, or $x_i + y_j$ is computed to high relative accuracy, as are their products and quotients, for the reasons discussed in section 5.

For example, consider the Hilbert matrix, where $x_i = i$ and $y_j = j - 1$. When $n = 13$, the determinant as computed by Gaussian elimination with no pivoting, partial pivoting or complete pivoting has lost all relative accuracy compared to the true value of the above formula, of about

$1.44 \cdot 10^{-92}$. In contrast, using equation (23) to compute the determinant yields nearly all the digits correct.

Note that small relative changes in the x_i and y_j do *not* necessarily guarantee small relative changes in $\det(C)$, as the 1-by-1 example with $x_1 = -1$ and $y_1 = 1 + \epsilon$ shows. But since formulas like (23) can be evaluated to high relative accuracy, they simply give the right answer for the data stored in the machine, independent of conditioning. Thus, we will compute an accurate SVD of the Cauchy matrix defined by the floating point numbers x_i and y_j, independent of how sensitive the SVD is to small changes in those numbers.

The Hilbert matrix is an example of a very well-conditioned Cauchy matrix in the following sense: Small relative changes in the data $x_i = i$ and $y_j = j - 1$ will only cause small relative changes in all the factors $x_j - x_i$, $y_j - y_i$ and $x_i + y_j$ appearing in equation (23), and so small relative changes in the LDU factors and SVD. Only when there is significant cancellation in one of these factors are the LDU factorization and SVD sensitive. For further analysis, see [22].

The amount of work required to compute the LDU factorization with formula (23) is much larger than the work required for straightforward Gaussian elimination. Its most straightforward use would cost $O(n^5)$, by using it to compute all $O(n^3)$ entries of Schur complements encountered during GECP. An efficient $O(n^3)$ algorithm is presented in [22], which includes extensions to Vandermonde and other unit-displacement-rank matrices.

9 Totally Positive Matrices

A matrix is *totally positive (TP)* if all of its minors are nonnegative [44]. This suggests that there should be formulas for minors that somehow automatically guarantee nonnegativity, and so high relative accuracy. However, total nonnegativity alone is not enough to guarantee that GECP can be performed accurately. For example, the Hilbert matrix is TP, but unless we exploit further information about the matrix, such as it being Cauchy, straightforward GECP will not be accurate enough. Similarly, a symmetric tridiagonal matrix T with positive offdiagonal entries is strictly totally positive if and only if it is positive definite [44, Thm. 3.2]. Simply knowing the entries of T to high relative accuracy does not determine the SVD to high relative accuracy, but knowing the entries of T's bidiagonal Cholesky factor to high relative accuracy does [33, 55]. So achieving high relative accuracy requires not just total positivity but an appropriate parameterization that permits minors to be evaluated to high relative accuracy. We give many examples of this below.

The rest of this section is organized as follows. First, we give several examples of TP matrices and their parameterizations where high accuracy formulas for their minors exist [3, 12, 11, 44]. Indeed, it was recently shown [12] that there is a universal parameterization of all totally positive matrices with this property, although this parameterization is not always convenient to use. Second, we show that well known *composition laws* for producing new TP matrices from previous ones also produce new high accuracy formulas from previous ones. This can be used to generate many matrices for which high accuracy formulas exist. Unfortunately, the formulas we present are often combinatorially expensive, so they are not always practical for large problems. Still, they show that high relative accuracy is achievable, and motivate us to seek more economical formulas for problems of particular interest.

9.1 Examples of Totally Positive Matrices with High Accuracy Formulas for their Minors

1. *Cauchy matrices* are TP, provided the x_i and y_j in $C_{ij} = 1/(x_i + y_j)$ satisfy $0 < x_1 < x_2 < \cdots < x_n$ and $0 < y_1 < y_2 < \cdots < y_n$. Formula (23) can be used to compute minors to high relative accuracy. (Actually, we only need $0 < x_1 + y_1$ to guarantee total positivity, but insist on the stronger conditions $x_1 > 0$ and $y_1 > 0$ so that no cancellation can occur when adding $x_1 + y_1$. Such a parameterization can be obtained by using $x_i + c$ and $y_j - c$ for an appropriate c.)

2. An n-by-n *generalized Vandermonde matrix* has entries $V_{i,j} = z_j^{e_i}$, where $0 \le e_1 < e_2 < \cdots < e_n$ are given integers. The usual Vandermonde matrix is given by $e_i = i - 1$. Every submatrix of a generalized Vandermonde matrix is also generalized Vandermonde. The formula for $\det(V)$ is [48, eqn. 3.1]

$$\det(V) = [\prod_{1 \le i < j \le n} (z_j - z_i)] \cdot s_\mu(z_1, ..., z_n) \tag{24}$$

   where s_μ is the so-called *Schur function*, and μ is the *partition* $\mu = (e_n - (n-1), e_{n-1} - (n-2), ..., e_2 - 1, e_1)$. A great deal is known about Schur functions [48], but for the purposes of showing that GECP can in principle be implemented very accurately, all we need to know is that if we write s_μ as a sum of monomials [48, p. 73]

$$s_\mu = \sum_i [\alpha_i z_1^{\beta_{i1}} z_2^{\beta_{i2}} \cdots z_n^{\beta_{in}}] \tag{25}$$

   then all its nonzero coefficients α_i are positive integers (see [48, p. 73] for a combinatorial formula for the α_i and $\beta_{i,j}$). Therefore, if the z_j satisfy $0 < z_1 < z_2 < \cdots < z_n$, equations (24) and (25) tell us that V is TP, and provide us a formula for $\det(V)$ that can be evaluated to high relative accuracy. Unfortunately, the number of monomials in the Schur function grows very quickly as a function of μ, so this is not a practical formulas for large matrices. There are alternate formulas for Schur functions, as *Jacobi-Trudi* determinants [48, I, eqn. (3.4)], but these appear to be no easier to evaluate to high relative accuracy than the original problem.

3. *Upper triangular Toeplitz matrices* T with certain special forms are TP. The most basic ones (from which we build others below) are bidiagonal matrices with 1 on the diagonal and first superdiagonal (each minor is 0 or 1), matrices with 1 on and everywhere above the diagonal (each minor is 0 or 1), and the Taylor matrix $T_{ij} = 1/(j-i)!$ (each minor is rational, and can in principle be evaluated exactly using rational Gaussian elimination).

4. Brenti [12, Thm. 3.1.] [11] has recently shown that there is a one-to-one correspondence between totally positive matrices T and planar, finite, nonnegatively edge-labeled directed graphs, with certain distinguished *row nodes* and *column nodes*. Given such a graph, T_{ij} is given as a sum, over all paths π from row node i to column node j, of the product of the edge weights along π. If the edge weights are known to high relative accuracy, this sum is determined to high relative accuracy. Furthermore, any r-by-r minor of T can also be defined as a sum over certain r-tuples of nonintersecting paths of products of edge weights, which again is determined to high relative accuracy.

The proof of Brenti's theorem involves the construction of an appropriate graph given a TP matrix T. This construction is nothing other than Gaussian elimination [19, Thm 1.1], with the restriction of eliminating using only adjacent rows or columns, thus expressing T as a product of (TP) Gauss transforms, which differ from a diagonal matrix by only one entry of the first super- or subdiagonal, and (TP) shifts. In other words, the problem of building the desired graph to high relative accuracy is equivalent to the problem we wanted to solve in the first place, Gaussian elimination to high relative accuracy[5].

Brenti [12, Thm. 3.3.] also showed that there is a "universal graph" for all n-by-n TP matrices, where the edge weights are arbitrary nonnegative reals. In other words, these nonnegative reals parameterize the set of all n-by-n TP matrices. And given these parameters to high relative accuracy, the graph provides a way to compute any minor to high relative accuracy. Again, computing these parameters from a TP matrix T is done with a variation of Gaussian elimination.

The paper [19, Thm 1.2] also shows that a strictly TP matrix may be reduced by a strictly TP similarity to a strictly TP tridiagonal matrix, which raises the possibility of efficient high accuracy eigendecompositions of nonsymmetric TP matrices, though we have not pursued this.

9.2 Composition Laws for Totally Positive Matrices

1. If A is TP with high accuracy formulas for all minors, then the same is true of A^T.

2. If A and B are m-by-r and r-by-n TP matrices, respectively, their m-by-n product AB is also TP. This follows from the Cauchy-Binet Theorem, which expresses each k-by-k minor of AB as a sum of $\begin{pmatrix} r \\ k \end{pmatrix}$ products of minors of A and of B. If we have high accuracy formulas for all minors of A and B, Cauchy-Binet also gives us a high accuracy formula for all minors of AB, as a sum of products of nonnegative minors, each of which is computable to high relative accuracy.

Example 9.1 Suppose X and Y are TP Vandermonde with entries $X_{ji} = x_j^{i-1}$ and $Y_{ji} = y_j^{i-1}$ respectively, and $D = \mathrm{diag}(d_1, ..., d_n)$ with $d_i > 0$, then $P = X^T D Y$ is TP, with entries $P_{ij} = \sum_{k=1}^{n} d_k x_i^{k-1} y_j^{k-1}$. In particular, suppose $0 < x_0 < x_1, 0 < y_0 < y_1$, and $d_k = 1/(k-1)!$; then

$$\begin{aligned}
\det(P) &\equiv \det \begin{bmatrix} e^{x_0 y_0} & e^{x_0 y_1} \\ e^{x_1 y_0} & e^{x_1 y_1} \end{bmatrix} \\
&= \det \left(\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots \\ 1 & x_1 & x_1^2 & \cdots \end{bmatrix} \cdot \mathrm{diag}\left(\frac{1}{0!}, \frac{1}{1!}, \frac{1}{2!}, \cdots \right) \cdot \begin{bmatrix} 1 & y_0 & y_0^2 & \cdots \\ 1 & y_1 & y_1^2 & \cdots \end{bmatrix}^T \right) \\
&= \sum_{0 \le i < j} \det \left(\begin{bmatrix} x_0^i & x_0^j \\ x_1^i & x_1^j \end{bmatrix} \cdot \mathrm{diag}\left(\frac{1}{i!}, \frac{1}{j!} \right) \cdot \begin{bmatrix} y_0^i & y_0^j \\ y_1^i & y_1^j \end{bmatrix}^T \right)
\end{aligned}$$

[5] This is yet another example of the "no free lunch" principle in getting error bounds.

$$= (x_1 - x_0) \cdot (y_1 - y_0) \cdot \sum_{0 \le i < j} \left(\frac{(x_0 x_1 y_0 y_1)^i}{i! \cdot j!} \cdot \sum_{k=0}^{j-i-1} x_0^k x_1^{j-i-1-k} \cdot \sum_{k=0}^{j-i-1} y_0^k y_1^{j-i-1-k} \right) ,$$

all of whose factors are evaluatable to high relative accuracy, for the reasons discussed in section 5.

Example 9.2 As another example, consider $D_1 A D_2$, where A is TP and Toeplitz, and D_1 and D_2 are positive definite diagonal with $D_{1,ii} = \alpha^{1-i}$, and $D_{2,ii} = \alpha^{i-1}$. Then $D_1 A D_2$ is also a TP Toeplitz matrix, with the i-th diagonal multiplied by α^i. Any minor of $D_1 A D_2$ is equal to the corresponding minor of A times an appropriate power of α.

3. Let A be TP and $S = \mathrm{diag}(+1, -1, +1, -1, ...)$. Then $SA^{-1}S$ is also TP, and every minor of $SA^{-1}S$ is a quotient of minors of A. In other words, A^{-1} has a checkerboard sign pattern. For example, if A is upper bidiagonal Toeplitz with 1 on the diagonal and first superdiagonal, then $SA^{-1}S$ is upper triangular Toeplitz with all ones on and above the diagonal.

4. Theorems of Aissen, Schoenberg, Whitney; Whitney; and Erdrei [3, p. 215] show that *all* totally positive Toeplitz matrices can be assembled from the above operations applied to the basic TP Toeplitz matrices mentioned earlier. A row of an upper triangular totally positive Toeplitz matrix is called a *Pólya frequency sequence* [44, 3].

5. If A is TP, so is any Schur complement of A. Since any minor of the Schur complement is a quotient of minors of A, high accuracy formulas for minors of A yield high accuracy formulas for minors of the Schur complement.

6. Let $A(x_1, x_2, ...x_p)$ be a TP matrix, when $0 < x_1 < x_2 < \cdots < x_p$. Then if $\phi(x)$ is a nonnegative strictly increasing function, $B = A(\phi(x_1), \phi(x_2), ..., \phi(x_p))$ is also TP. To get a high accuracy formula for minors of B from the corresponding formula for minors of A, we require (1) that $\phi(x)$ can be evaluated to high relative accuracy if x is given to high relative accuracy, and (2) that $\phi(x) - \phi(y)$ can be evaluated to high relative accuracy, if x and y are floating point numbers. For example, if $\phi(x)$ is a polynomial in x with nonnegative coefficients, it satisfies these conditions.

10 Diagonally Scaled Totally Unimodular (DSTU) matrices

The following definition is taken from [13]. A matrix Z with integer entries is called *totally unimodular (TU)* if all of its minors are -1, 0 or $+1$. In particular, the entries of Z must be -1, 0 or $+1$. We further define a matrix G to be *diagonally scaled totally unimodular (DSTU)* if it can be written $G = D_L Z D_R$, where Z is TU, and D_L and D_R are diagonal. In our applications Z will be known exactly, but the diagonal entries of D_L and D_R will only be known to high relative accuracy. The determinant $\det(G) = \det(D_L) \cdot \det(Z) \cdot \det(D_R)$ is determined to high relative accuracy since $\det(Z)$ is known exactly, and the other two determinants are products of numbers known to high relative accuracy. Since any submatrix of a DSTU matrix is DSTU, all minors are determined to high relative accuracy, so all entries of the L, D and U factors of G are determined to high relative accuracy.

A variety of characterizations of TU matrices are given in [13, sec. 2.3]. We limit ourselves to two examples: the acyclic matrices discussed in section 6, and the finite element matrices from linear mass-spring systems in section 11.1, which we discuss in that section. We also note that the *reduced note-arc incidence (RNAI) matrices* of [74] are a special case of TU matrices. In [23], we characterized acyclic sparsity patterns as follows:

Theorem 10.1 *Let $\mathcal{G}$ be the class of matrices with a given sparsity pattern. Let $Z \in \mathcal{G}$ be the unique matrix with all entries equal to 0 or 1. Then $\mathcal{G}$ is acyclic if and only if all matrices $G \in \mathcal{G}$ can be written $G = D_L Z D_R$ for some diagonal matrices D_L and D_R.*

Since Z is acyclic too, each minor of Z consists of at most one monomial, and so is -1, 0 or $+1$. Thus, Z is TU and $G = D_L Z D_R$ is DSTU.

It remains to give an algorithm for performing GECP on a DSTU matrix, and to show that the L and U factors it computes are well-conditioned.

Algorithm 10.1 *Performing Gaussian elimination with pivoting $G = P_r L D U P_c$ in a forward stable manner on an m-by-n DSTU matrix $G = D_L Z D_R$, where $m \geq n$.*

for $i = 1$ *to* $\min(m-1, n)$
  pivot so that G_{ii} *is nonzero*
  $D_{ii} = G_{ii}$
  for $j = i+1$ *to* m
    $L_{ji} = G_{ji}/D_{ii}$
  endfor
  for $j = i+1$ *to* m
    for $k = i+1$ *to* n
(*) $G_{jk} = G_{jk} - L_{ji} \cdot G_{ik}$
(***) *If the last subtraction has two nonzero operands, set* $G_{jk} = 0$
    endfor
  endfor
  for $k = i+1$ *to* n
    $U_{ik} = G_{ik}/D_{ii}$
  endfor

The above algorithm is essentially identical to conventional Gaussian elimination, except for line (***).

Theorem 10.2 *Algorithm 10.1 computes all the entries of the L, D and U factors of a DSTU matrix G to high relative accuracy, for any pivot sequence not dividing by zero. If we use complete pivoting, and $m = n$, then the entries of L^{-1} and U^{-1} are bounded by 1 in absolute value, so that $\kappa(L) = O(n^2)$ and $\kappa(U) = O(n^2)$. If $m > n$, so L is m-by-n, then $\kappa(L) = O(mn)$. These bounds are attainable. In other words, L and U have condition numbers that grow at most quadratically with dimension.*

Proof: First we show that Algorithm 10.1 is forward stable for any pivot sequence not dividing by zero. Since floating point multiplication and division are forward stable (i.e. they compute

the result to high relative accuracy if the operands are known to high relative accuracy), the only potential source of inaccuracy is the subtraction in line (*). We claim that the only situation in which G_{jk} and $L_{ji} \cdot G_{ik}$ are both nonzero is when they are equal (in exact arithmetic), so the result is exactly zero; this situation is accounted for in line (***).

To see that line (***) in Algorithm 10.1 computes G_{jk} exactly if the if-test is satisfied, we note that G_{ij} before executing (*), G_{jk} after executing (*), and $L_{ji} \cdot G_{ik}$ are all quotients of minors of G (or products of quotients of minors of G), i.e. quotients of monomials in the variables $D_{L,ii}$ and $D_{R,jj}$, with coefficients ± 1, or zero. (We call a monomial with coefficient ± 1 a ± 1-monomial for short.) Now think of (*) as a polynomial identity $m_1 = m_2 + m_3$ among ± 1-monomials (or zero) m_i in the variables $D_{L,ii}$, $D_{L,ii}^{-1}$, $D_{R,ii}$ and $D_{R,ii}^{-1}$. Then since all coefficients can only be 0 or ± 1, the only way both m_2 and m_3 can be nonzero is if their sum m_1 cancels exactly to zero. Thus m_1 must be zero if m_2 and m_3 are nonzero. This completes the proof that Algorithm 10.1 is forward stable.

Next we show that with complete pivoting, the entries of U^{-1} and L^{-1} are bounded by one in absolute value if $m = n$. It suffices to consider U. We use the fact that any entry U_{ij}^{-1} is both a quotient of minors of G, and a quotient of minors of U. Since G is DSTU, its minors are ± 1-monomials in the diagonal entries of D_L and D_R, so we can write $U_{ij}^{-1} = \mathrm{mono}_n(D_L, D_R)/\mathrm{mono}_d(D_L, D_R)$. Since U is a unit triangular matrix, its determinant is 1, so U_{ij}^{-1} is really just a minor of U, which in turn is a sum $\sum_k \mathrm{mono}_k(U)$, of ± 1-monomials in the entries of U. Since all $|U_{kl}| \leq 1$ by complete pivoting, $|\mathrm{mono}_k(U)| \leq 1$ too. We will show that at most one term $\mathrm{mono}_k(U)$ in the sum for $U_{ij}^{-1} = \sum_k \mathrm{mono}_k(U)$ is nonzero, implying that $|U_{ij}^{-1}| \leq 1$ as desired.

To this end, note that each $\mathrm{mono}_k(U) = \mathrm{mono}_{n,k,U}(D_L, D_R)/\mathrm{mono}_{d,k,U}(D_L, D_R)$ is the quotient of ± 1-monomials of diagonal entries of D_L and D_R, since each entry of U is the quotient of minors of G, each of which is a ± 1-monomial in D_L and D_R. This implies

$$\frac{\mathrm{mono}_n(D_L, D_R)}{\mathrm{mono}_d(D_L, D_R)} = U_{ij}^{-1} = \sum_k \frac{\mathrm{mono}_{n,k,U}(D_L, D_R)}{\mathrm{mono}_{d,k,U}(D_L, D_R)} \quad .$$

Now think of this as a polynomial identity in the variables $D_{L,ii}$, $D_{L,ii}^{-1}$, $D_{R,ii}$ and $D_{R,ii}^{-1}$. This algebraic identity can only hold if there is exact cancellation among the monomials in the sum on the right, so that at most one term remains after cancellation. This completes the proof that $|U_{ij}^{-1}| \leq 1$. Thus $\|U\| \leq n$ and $\|U^{-1}\| \leq n$ (in the 1, 2, or ∞ norm), and $\kappa(U) \leq n^2$.

The same argument applies to L when L is square, and may be modified easily when L is rectangular.

To see that the condition number $O(n^2)$ can be attained, consider the acyclic matrix G defined by the following Matlab program:

$G = \mathrm{eye}(4 \cdot n + 1);$
$G(1, 2 : n + 1) = \mathrm{ones}(1, n);$
$G(n + 2 : 2 \cdot n + 1, 1) = \mathrm{ones}(n, 1);$
$G(n + 2 : 3 \cdot n + 2, 4 \cdot n + 1) = \mathrm{ones}(1, n);$
$G(2 \cdot n + 2 : 3 \cdot n + 1, n + 2) = \mathrm{ones}(n, 1);$

Then L, U, L^{-1} and U^{-1} all contain n-by-n blocks of $+1$s (or -1s). $\square$

To illustrate the phenomenon of exact cancellation, consider the (singular) acyclic matrix

$$G = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad .$$

If we choose G_{11} as the pivot, then after one step the trailing 2-by-2 submatrix has each entry equal to -1. Choosing any of these entries as the next pivot causes exact cancellation in the third and final pivot, which is zero. This phenomenon can also occur with nonsingular acyclic matrices, such as

$$G = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \quad . \tag{26}$$

It is probably possible to implement Algorithm 10.1 in $o(n^3)$ time, but since the subsequent Algorithm 3.1 for computing the SVD itself takes $\Theta(n^3)$ operations, we have not pursued this. It remains to design a high accuracy algorithm for the singular vectors of an acyclic matrix taking $o(n^3)$ time.

We present numerical examples in section 11.3.

10.1 Accurate SVDs of other matrices of the form $G = D_L Z D_R$

In the last section we considered the case where Z was TU, i.e. each minor of the integer matrix Z was bounded by 1 in absolute value. It is natural to ask what happens when the bound on each minor is $\bar{k} > 1$. In this case one can still compute an accurate LDU decomposition of G, by performing GECP on Z in rational arithmetic, and using D_L and D_R only for pivot selection (diagonally scaling each Schur complement of Z just in order to choose the largest entry, but performing the actual elimination on Z itself). The bound $\bar{k}$ on minors of Z implies that any rational number s/r in lowest terms appearing during Gaussian elimination on Z has s and r bounded in magnitude by $\bar{k}$; this is why the TU case of $\bar{k} = 1$ was so easy. The argument that showed $|U_{ij}^{-1}| \leq 1$ may be extended to show that $|U_{ij}^{-1}| \leq \bar{k}^2$, whence $\kappa(U) \leq (\bar{k}n)^2$. We do not know if this is attainable for $\bar{k} > 1$.

11 Finite Element Problems

As described earlier, the most natural finite element formulation leads to a generalized eigenproblem of the form $Kx = \lambda Mx$, where M is the *mass matrix*, and K is the *stiffness matrix*. Typically we write $K = Z_K^T D_K Z_K$ where Z_K is the *incidence matrix* or *assembly matrix*, and D_K is the (block) diagonal matrix of individual element stiffnesses. We may similarly write $M = Z_M^T D_M Z_M$. Assume first for simplicity that Z_M is square and invertible, and that D_M and D_K are positive definite diagonal. Then we can pre- and postmultiply the eigenproblem $K - \lambda M$ by $D_M^{-1/2} Z_M^{-T}$ and $Z_M^{-1} D_M^{-1/2}$, respectively, to get the eigenproblem $G^T G - \lambda I$, where

$$G = D_K^{1/2}(Z_K Z_M^{-1}) D_M^{-1/2} \equiv D_1 B D_2 \quad .$$

Thus, the problem reduces to finding the SVD of $G = D_1 B D_2$.

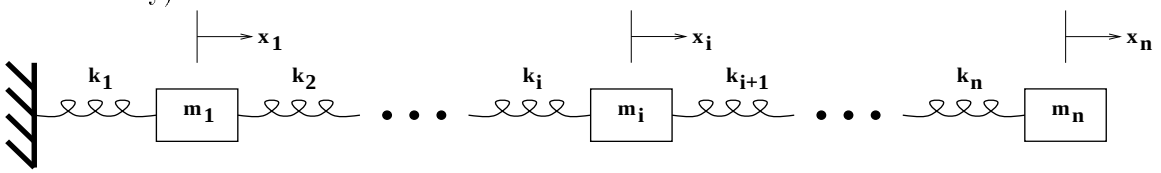
We can think of G as the "unassembled" finite element problem. The diagonal matrices $D_1 = D_K^{1/2}$ and $D_2 = D_M^{-1/2}$ depend only on the *material properties* of the finite element problem (such as masses and spring constants in the example below), whereas $B = Z_K Z_M^{-1}$ depends only on the *geometry and meshing*. In the examples we have studied, the (worst case) relative accuracy of the SVD of G depends *only* on B, i.e. the geometry and meshing, *not* on the material properties in D_1 and D_2. This is because D_1 and D_2 affect the pivot choice during GECP, but the accuracy depends only on the conditioning of submatrices of B. In contrast, we will show that the conventional assembled problem $K - \lambda M$ may unavoidably destroy high relative accuracy. A similar phenomenon in the case of linear systems was analyzed in [74, 75].

We will study simple one dimensional and two dimensional finite element element problems that reduce to the SVD of $G = D_1 B D_2$ (in sections 11.1 and 11.2 respectively). In both these simple cases the geometry is simple enough that full relative accuracy is always guaranteed. Still, the two dimensional example is general enough to cover some interesting elliptic problems. Section 11.3 includes numerical examples.

In the more general case where Z_M is not square and invertible, we would need to compute the generalized SVD (GSVD) of the pair $(D_K^{1/2} Z_K, D_M^{1/2} Z_M)$. Many of the perturbation theorems and algorithms of this paper may be extended to this case. For example, we can show that a conventional piecewise linear discretization of the Sturm-Liouville problem $-(a(x)y')' = \lambda \rho(x) y$ on $0 < x < 1$ with rather general boundary conditions leads to a GSVD formulation that determines its small modes of vibration to high relative accuracy [31], and for which we have an algorithm that depends on material in this paper and in [28]. We will report on these and other finite element problems in more detail in a future paper.

11.1 Linear Mass Spring Systems

A *linear mass spring system* consists of masses m_i that may move only horizontally, and springs with spring constants k_l connecting arbitrary pairs of masses m_i and m_j. Each mass may also be connected by a spring to an immovable wall, as shown below (in the simple case of nearest-neighbor connections only):



x_i = position of i-th mass (0 = equilibrium)
m_i = mass of i-th mass
k_i = spring constant of i-th spring

Newton's Law applied to the system in the figure yields $M\ddot{x}(t) = -Kx(t)$, where $x(t) =$

$[x_1(t), ..., x_n(t)]^T$, $M = \mathrm{diag}(m_1, ..., m_n)$, and

$$K = \begin{bmatrix} k_1 + k_2 & -k_2 & & & \\ -k_2 & k_2 + k_3 & -k_3 & & \\ & \ddots & \ddots & \ddots & \\ & & -k_{n-1} & k_{n-1} + k_n & -k_n \\ & & & -k_n & k_n \end{bmatrix} .$$

Seeking solutions of the form $x(t) = e^{\mu t} x$ leads to the usual generalized eigenproblem $Kx = -\mu^2 Mx \equiv \lambda Mx$. We will see below that this formulation does *not* preserve high relative accuracy in the eigenvalues.

To reformulate the problem so that high relative accuracy is preserved, we write $K = Z_K^T D_K Z_K$ where $D_K = \mathrm{diag}(k_1, ..., k_n)$ and Z_K is the bidiagonal *incidence matrix*

$$Z_K = \begin{bmatrix} 1 & & & \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix} \tag{27}$$

where the nonzero $z_{K,ij}$ indicates that spring i is connected to mass j. Furthermore, $M = Z_M^T D_M Z_M$ where $D_M = \mathrm{diag}(m_1, ..., m_n)$ and $Z_M = I$, so our problem reduces to finding the SVD of $G = D_K^{1/2} Z_K D_M^{-1/2}$, which is a bidiagonal matrix with entries $G_{i,i} = \sqrt{k_i/m_i}$ and $G_{i+1,i} = -\sqrt{k_{i+1}/m_i}$. The singular values of G are the square roots of the eigenvalues. Each entry of G is determined to about as many decimal places as the spring constants k_i and masses m_i. G is bidiagonal, and so acyclic, and so its singular values are determined to about as many decimal places as the data, which is as accurate an answer as the data deserves.

More generally, when there are springs between arbitrary pairs of masses, or arbitrary masses and the wall, Z_K will have the following structure. Row i will have -1 and $+1$ in columns j and k, respectively, if spring i connects masses j and k. Row i will have ± 1 in column j if spring i connects mass j to the wall. It was shown by Hoffman and Kruskal that Z_K is *totally unimodular (TU)* [13, Thm. 2.3.3.], although if no masses are connected to a wall then Z_K is called an *oriented incidence matrix* and the result goes back to Poincaré. Thus, $G = D_K^{1/2} Z_K D_M^{-1/2}$ is a *diagonally scaled unimodular matrix (DSTU)*, and its SVD can be computed to high relative accuracy as described in section 10.

Now we show that the conventional assembled formulation $Kx = \lambda Mx$ does *not* necessarily preserve high relative accuracy, when the k_i and m_i have widely varying magnitudes. First, accuracy can be lost by a conventional algorithm like divide-and-conquer that only guarantees high absolute accuracy in the computed eigenvalues. Second, and *independently* of the algorithm used to solve the eigenproblem, accuracy can be lost simply by forming *and rounding* K from the data k_i. For example, Suppose $n = 3$, $M = I$, $k_1 = k_3 = 1$, and $k_2 = \varepsilon/2$ (so $\mathrm{fl}(k_1 + k_2) = k_1$). Then the correctly rounded K is

$$\mathrm{fl}(K) = \begin{bmatrix} 1 & -\varepsilon/2 & 0 \\ -\varepsilon/2 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

This matrix is easily seen to have a tiny negative eigenvalue near $-\varepsilon^2/8$, whereas its true tiniest eigenvalue must be positive, in fact near $\varepsilon/4$ (Matlab returns 0 in place of $-\varepsilon^2/8$).

11.2 Two Dimensional Finite Element Problems

Consider a planar mass-spring system, with n masses connected by s springs to other masses and walls in an arbitrary way, but such that all masses and springs lie in a plane when in equilibrium. Now we consider small motions transverse to the plane, and ask for the frequencies of vibration. It will turn out that the resulting SVD problem is also DSTU, as in the last section, letting us compute all its singular value to high relative accuracy.

More specifically, consider mass i, with mass m_i and displacement x_i from the equilibrium plane. Let $k_{i,j}$ be the spring constant for the spring connecting masses i and j, and $k_{i,0}$ be the (total) spring constant for any springs connecting mass i to a wall. Either $k_{i,j}$ or $k_{i,0}$ is zero if no such spring exists. The equation of motion for mass i is

$$m_i \ddot{x}_i(t) = \sum_{\text{neighbors } j \text{ of } i} k_{i,j}(x_j(t) - x_i(t)) - k_{i,0}x_i(t) \quad .$$

The usual substitution $x_i(t) = e^{\mu t}x_i$ leads to $Kx = -\mu^2 Mx = \lambda x$ where $M = \mathrm{diag}(m_1, ..., m_n)$, $K = Z_K^T D_K Z_K$, $D_K = \mathrm{diag}(k_1, ..., k_s)$ and Z_K has the same structure as in the 1D case: Row i will have -1 and $+1$ in column j and k if spring i connects masses j and k, and row i will have ± 1 in column j if spring i connects mass j to a wall. Thus $G = D_K^{1/2} Z_K M^{-1/2}$ is DSTU, and we can compute all its singular values to high relative accuracy.

Consider the special cases where each spring constant is 1, and masses are laid out on a square grid with connections to the 4 nearest neighbors to the north, east, south and west, and boundary masses are connect to the wall. Then K is the familiar pentadiagonal matrix arising from the usual finite difference approximation of the Laplacian. Since the Laplacian in high dimensions can also be factored in the same way, we see that quite general elliptic eigenvalue problems can be dealt with.

11.3 Numerical Examples

In this example, we apply Algorithm 10.1, GECP for DSTU matrices, followed by Algorithm 3.1, to several linear mass-spring systems, and compare the results to several other algorithms. These examples will be rank deficient.

We generate 6-by-6 test matrices of the type $G = D_1 B D_2$, where

$$B = \begin{bmatrix} 1 & & & -1 & & \\ & 1 & & & -1 & \\ & & 1 & & -1 & \\ 1 & -1 & & & & \\ & 1 & -1 & & & \\ & & 1 & & & -1 \end{bmatrix}$$

and D_1 and D_2 are diagonal with $\kappa(D_1) = 10^i$, $\kappa(D_2) = 10^j$, $1 \le i, j \le 8$. For each fixed (i, j) we generate 90 test matrices, using 9 different types of distributions of the singular values of D_1 and D_2, for a total of $8 \cdot 8 \cdot 90 = 5760$ test matrices.

The algorithms tested are as follows:

- Algorithm 10.1 (GECP on DSTU matrices) followed by Algorithm 3.1. We call the combined algorithm `SLUSVD` in single precision and `DLUSVD` in double precision).

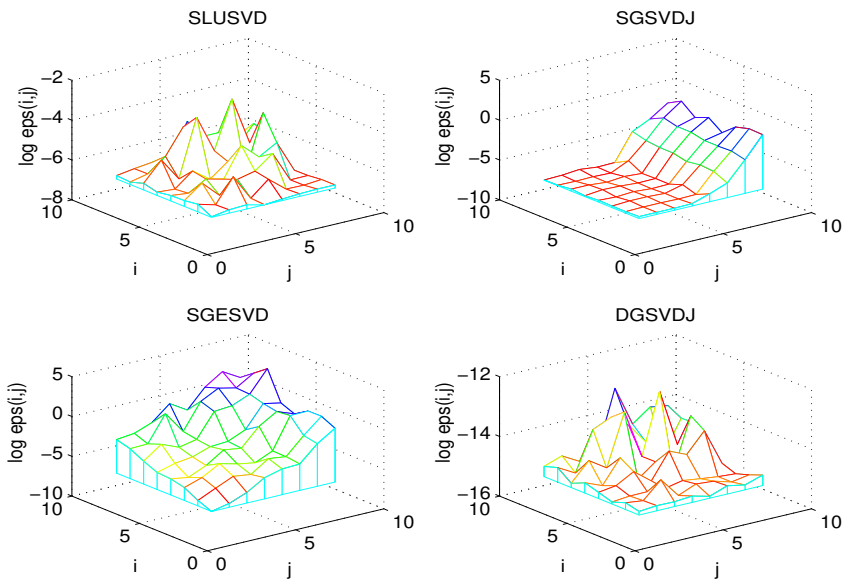


Figure 2: The values of of $\log_{10} \varepsilon(i,j)$ for $1 \le i,j \le 8$.

- One-sided Jacobi in single precision (`SGSVDJ`) and double precision (`DGSVDJ`).
- QR based SVD in single precision from LAPACK `SGESVD`.

Since in this case only the first, LU based method can determine the rank exactly, we measure the relative error only in the $\mathrm{rank}(G) = 5$ nonzero singular values. We use $\varepsilon(i,j)$ to denote the maximal relative error in nonzero singular values of all test matrices with fixed $\kappa(D_1) = 10^i$ and $\kappa(D_2) = 10^j$. As a reference, we use the singular values computed by `DLUSVD`.

The measured values of $\varepsilon(i,j)$ for various algorithms are given in Figure 2. This figure shows that the single precision algorithm `SLUSVD` delivers at least 5 correct digits in all cases, whereas one-sided Jacobi or QR in single precision can lose all relative accuracy. One-sided Jacobi in double precision always delivers at least 13 decimal digits, although theory does not guarantee this.

12 Solving other linear algebra problems with high relative accuracy

It is natural to ask when other linear algebra problems have solutions determined to high relative accuracy, given the combinatorial and algebraic properties of previous sections. We consider matrix inversion, computing the QR factorization, and (more generally) solving least squares problems.

First we consider computing G^{-1}. Since each entry of G^{-1} is ± 1 times a quotient of an $n-1$-by-$n-1$ minor of G and $\det(G)$, we only need these n^2+1 largest minors to be determined accurately. Then it is immediate that all our earlier conditions that imply that *all* minors are determined accurately also imply that all entries of the inverse are determined accurately.

For example, previous authors have noted that a linear system with a Vandermonde coefficient matrix V can be solved quite accurately precisely when it is TP, although only some authors used this language [40, 8, 10, 9]. This high accuracy phenomenon is now understandable, since linear

system solving can also be expressed in terms of minors, and should apply to all linear systems with TP coefficient matrices. It is worth noting that the standard fast algorithm for Vandermonde systems can be described as providing a factorization of a TP Vandermonde into a product of simpler TP matrices, each of which has simple high accuracy formulas for all its minors (this factorization, which applies to non-TP Vandermondes, appears in [35]), thus providing another high accuracy way to evaluate Schur functions [48]. But fast algorithms remain hard to design. Perhaps the successes in divide and conquer algorithms for TP linear system solving can be translated into similar algorithms for the pivoted LDU decomposition and so SVD.

Since accurate matrix inversion requires only that the n^2+1 largest minors be determined accurately, it is possible to compute an accurate inverse more often than an accurate SVD. If the Laplace expansions of the n^2+1 largest minors of G are sums of monomials of like sign, so that each entry of G^{-1} is determined to high relative accuracy, then Brualdi and Shader call G *strongly sign nonsingular*, or S^2NS [14]. To see that these matrices form a strictly larger class than either acyclic or TSC matrices, consider

$$G = \begin{bmatrix} D_1 & X \\ 0 & D_2 \end{bmatrix} \quad , \quad G^{-1} = \begin{bmatrix} D_1^{-1} & -D_1^{-1} X D_2^{-1} \\ 0 & D_2^{-1} \end{bmatrix}$$

where D_1 and D_2 are nonsingular diagonal matrices, and X is arbitrary. G^{-1} is determined to high relative accuracy, even though G may be neither acyclic nor TSC, depending on X. In other words, determining the inverse to high relative accuracy is strictly "easier" than computing either the LU decomposition or SVD to high relative accuracy. And since an accurate inverse determines the tiniest singular value accurately (by taking its 2-norm) we see that *computing the tiniest (and of course largest) singular values accurately is strictly easier than computing the interior singular values*. See [14] for further discussion of S^2NS and similar matrices.

Now we consider the QR factorization $G = QR$ and least squares problems $\min_x \|Gx - b\|_2$. It is natural to expect similar high accuracy results as before, because of the following well-known facts:

- R^TR is the Cholesky factorization of G^TG, so that each entry of R is a (quotient of) square root(s) of minor(s) of G^TG.
- $QQ^T = G(G^TG)^{-1}G^T$, so if G^TG is accurately invertible, we expect that Q might be determined accurately.
- The pseudoinverse $G^+ = (G^TG)^{-1}G^T$, so again we expect this might be accurate if G^TG is accurately invertible.

For example, it is natural to conjecture that a theorem like Theorem 6.1 is true for the QR decomposition. Indeed, we believe that the entries of R in $G = QR$ are determined to high relative accuracy for all $G \in \mathcal{G}$ if and only if $\mathrm{Gr}(\mathcal{G})$ is acyclic, but we have not been able to prove this. It also seems likely that the Householder vectors determining Q are determined to high accuracy. See also [14, sec 11.2].

On the other hand, being TSC is definitely not enough to guarantee an accurate QR decomposition. For example, consider $G = \begin{bmatrix} 1 & 1 \\ 1 & -1-\epsilon \end{bmatrix}$; there is unavoidable cancellation in computing R_{12}. However, the diagonal entries of R are determined to high relative accuracy if G is TSC. This

follows from thinking of R as the Cholesky factor of G^TG, and the diagonal entries of R as square roots of quotients of principal minors of G^TG. By the Cauchy-Binet theorem, a principal minor of G^TG can be written as a sum of squares of minors of G, each of which is determined to high relative accuracy. This also implies that G^TG is accurately invertible if G is TP, although there will be cancellation in the products defining QQ^T and G^+ above, since $(G^TG)^{-1}$ will have a checkerboard sign pattern.

It remains to characterize those matrices whose QR factorization, and associated least squares problems, can be solved to high relative accuracy.

13 Open Problems

We listed a number of open problems throughout the paper. We reiterate the most important ones here.

1. Several matrix classes we introduced required expensive variations on GECP to compute accurate LDU factorizations: TSC matrices cost $O(n^4)$ and totally positive matrices could be exponential in n. It is desirable to have faster algorithms in all these cases. A natural question is the "subtraction-free" complexity of computing a Schur function, as discussed in section 9.1.

2. We only discussed finite element problems that could be reduced to the SVD of a single matrix. But the most general case involves the generalized SVD of two matrices. We have studied this for two-dimensional trusses, Sturm-Liouville problems, and have made some progress with more general cases. But a complete analysis remains to be done. Such an analysis would start with any continuous problem that determined its smallest eigenvalues to high relative accuracy, and then describe the finite element discretizations preserving this accuracy, along with algorithms to compute them this accurately.

3. We have described mostly dense matrix algorithms in this paper, costing $O(n^3)$ and sometimes more. Large eigenproblems typically require iterative methods (such as Lanczos) to compute a few eigenvalues at a reasonable cost. It would be desirable to identify matrix classes and inexpensive iterative algorithms that preserve high relative accuracy, or just determine what relative accuracy can be expected from iterative methods.

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