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Spectral condition-number estimation of large sparse matrices

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Summary

We describe a randomized Krylov-subspace method for estimating the spectral condition number of a real matrix A or indicating that it is numerically rank deficient. The main difficulty in estimating the condition number is the estimation of the smallest singular value σ_{\min} of A . Our method estimates this value by solving a consistent linear least squares problem with a known solution using a specific Krylov-subspace method called LSQR. In this method, the forward error tends to concentrate in the direction of a right singular vector corresponding to σ_{\min} . Extensive experiments show that the method is able to estimate well the condition number of a wide array of matrices. It can sometimes estimate the condition number when running dense singular value decomposition would be impractical due to the computational cost or the memory requirements. The method uses very little memory (it inherits this property from LSQR), and it works equally well on square and rectangular matrices.

KEYWORDS

condition-number estimation, Krylov methods, randomized numerical linear algebra

1 | INTRODUCTION

This paper discusses the problem of estimating the spectral condition number of a large and sparse matrix $A \in \mathbb{R}^{m \times n}$. Without loss of generality, we assume that $m \geq n$ (we can estimate the condition number of A^T if $n > m$). The main difficulty is in estimating the smallest singular value σ_{\min} of A . Dense singular value decomposition (SVD) algorithms can approximate σ_{\min} well, and their running time is predictable; however, they are slow (their running time depends on the dimensions of the matrix and not on the number of nonzero entries in the matrix). More importantly, dense SVD algorithms require space that is proportional to mn when the matrix is $m \times n$, which is impractical for large sparse matrices. Likewise, if A is square and an LU factorization of A can be computed, then σ_{\min} can be estimated efficiently from the factorization¹; however, for some large sparse matrices, space requirements due to fill-in make this method impractical.

Symmetrization is not always an effective way to address the problem. If we compute the Gram matrix $A^T A$, we cannot estimate condition numbers $\kappa(A) = \sigma_{\max}/\sigma_{\min}$ greater than $1/\sqrt{\epsilon_m}$, where ϵ_m is the unit roundoff (machine precision), unless the minimum singular value is well separated.² The underlying reason is the use of $A^T A$ as an explicit matrix, which fails to take advantage of its structure. If we work with the augmented matrix

$$\begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix},$$

σ_{\min} is transformed into a pair of eigenvalues $\pm\sigma_{\min}$ in the middle of the spectrum. Such eigenvalues are difficult to compute accurately with the Lanczos algorithm and its variants,* and it is essentially impossible for such algorithms to determine whether there is an eigenvalue closer to zero than the one that has already been computed.

If one is interested in the smallest singular value of a large sparse matrix, then avoiding the impractical space requirements of dense SVD requires the use of a low-memory iterative method. Some Krylov-subspace methods estimate the condition number as the iteration progresses (e.g., LSQR). However, LSQR's condition-number estimator has some shortcomings that make it unreliable. We explain these in the next section.

The starting point of this paper is the following observation, which we explain in more detail in Section 3. Suppose b is a vector in the column space of A , and let $Ax^* = b$. Let $x^{(0)}, x^{(1)}, \dots$ be the iterates of a Krylov-subspace method applied to the problem $\arg \min \|Ax - b\|$ (all norms in this paper denote the 2-norm unless stated otherwise). If we knew the forward error $d^{(k)} = x^* - x^{(k)}$, we could use the Rayleigh quotients $\|Ad^{(k)}\|/\|d^{(k)}\|$ as an upper estimate on σ_{\min} . Now, if b is also a random vector, then the iterates $x^{(k)}$ tend to generate, at some point, forward errors $d^{(k)}$ such that the Rayleigh quotient $\|Ad^{(k)}\|/\|d^{(k)}\|$ estimates σ_{\min} well. The underlying reason is the tendency of Krylov-subspace methods to concentrate the forward error in the direction of a singular vector associated with σ_{\min} . This tendency is essentially the same as the tendency of the Lanczos algorithm to converge to outer eigenvalues first (see, e.g., section 7.3 in the work of Demmel⁴). Both tendencies reflect the uneven convergence of Krylov subspaces to singular- or eigenspaces: one in the singular unsymmetric case (LSQR) and the other in the symmetric case (Lanczos or conjugate gradients). This is often seen as a flaw in LSQR and in conjugate gradients (LSQR is mathematically equivalent to conjugate gradients applied to $A^T Ax = A^T b$). These solvers converge slowly when the coefficient matrix A is ill conditioned because it is difficult for them to get rid of the error in the right singular subspaces of A that correspond to its smallest singular values. However, one can also exploit this flaw, which acts as a sieve that captures a vector from this subspace.

In this paper, we use this observation to design a Krylov-subspace method that can estimate σ_{\min} (hence the spectral condition number $\sigma_{\max}/\sigma_{\min}$) accurately. To have access to the forward error, our algorithm generates a random x^* and computes $b = Ax^*$. The algorithm then proceeds with using LSQR on the problem $\arg \min \|Ax - b\|$, meanwhile monitoring the value of $\|Ad^{(k)}\|/\|d^{(k)}\|$ and keeping the vector $d^{(e)}$ for which it is minimized. Very little memory is needed, as the algorithm's memory usage is close to LSQR's. As the iteration progresses, the estimate of σ_{\min} does not deteriorate; we always keep the best $d^{(k)}$ found. However, it is undesirable to continue to run the algorithm when the estimate of σ_{\min} is unlikely to improve. To that end, we design a set of stopping criteria that are tuned toward the algorithm's goal of computing the condition number, as opposed to solving least squares equations, which is what LSQR's regular stopping criteria are tuned for. Some of our stopping criteria are the same as LSQR's, but others are based on the algorithm's knowledge of the forward error.

Our algorithm will never report an underestimate of σ_{\min} . Furthermore, in most cases, it also produces a certificate vector that proves that the estimate of σ_{\min} is indeed an upper bound. While we are unable to prove rigorous bounds on the quality of approximation nor a bound on the number of iterations until convergence, extensive experiments indicate that our method does not incorrectly report significant overestimates of σ_{\min} , at least when A is not close to being numerically rank deficient. When A is close to numerical rank deficiency, the algorithm reports a condition number near ϵ_m^{-1} , but the accuracy of the estimate is sometimes poor.

Our method also has some flaws. The main one is that it sometimes converges very slowly, making it essentially impossible to compute σ_{\min} . Our experience shows that the method always converges eventually, but that convergence might be too slow to be of practical use. There is no good way to determine how close the method is to termination, although it tends to behave consistently on related matrices (e.g., from the same application area). When $\kappa(A)$ is close to ϵ_m^{-1} , the method sometimes overestimates σ_{\min} by several orders of magnitude. The method sometimes converges very rapidly and sometimes very slowly. This is not related to the size of the problem and to how ill conditioned it is but to the distribution of singular values.

Even with these flaws, to the best of our knowledge, this method is the only practical way to compute σ_{\min} with reasonable accuracy (to within a factor of 2 or better) on many large matrices. Our implementation of the method in MATLAB is freely available,[†] and a C++ implementation is available inside the libSkylark library.[‡]

*For example, the ARPACK Users' Guide states that a shift-invert iteration is usually required to compute eigenvalues in the interior of the spectrum (see section 3.4 in the work of Lehoucq et al.³). Experiments with ARPACK on some of the matrices presented later in the paper, whose condition numbers our method was able to estimate, showed that ARPACK does not converge on them when it tries to compute the smallest-magnitude eigenvalues of the augmented matrix without inversion.

[†]See <https://github.com/sparse-condest/condest>.

[‡]See <https://xdata-skylark.github.io/libskylark/>.

The rest of this paper is organized as follows. Section 2 surveys related work on condition-number estimation. Section 3 presents a mathematical analysis of the quantity that we use to estimate σ_{\min} , to motivate the algorithm that we present in Section 4. Section 5 analyzes unique stopping criteria that our method relies upon. Section 6 illustrates and explores the behavior of our algorithm using numerical experiments.

2 | RELATED WORK

The largest singular value σ_{\max} of A can be computed accurately using a bounded number of matrix–vector products involving A and A^T . This can be done using the power method, for example, whose analysis for this application we explain in Section 4. The Lanczos method can reduce the number of matrix–vector products even further.⁵ Random projection methods can also estimate σ_{\max} .⁶

Estimating σ_{\min} is computationally more challenging, because applying the pseudoinverse is usually much harder than applying A itself. In general, existing random projection methods cannot efficiently estimate σ_{\min} unless a decomposition of A is computed or A is of low rank (or numerically low rank). If A is of low rank, random projection methods can be used to estimate the k th largest singular value, where k is the (numerical) rank.⁶ Another approach is to use iterative methods for computing singular triplets. Recently, variants of Lanczos that use implicit restarting, harmonic Ritz values, and other advanced techniques to further accelerate the convergence to the smallest singular triplets have been proposed.^{7,8} Another approach for computing singular triplets (including the smallest singular triplets) is the JDSVD method,⁹ which extends the Jacobi–Davidson method for singular value problems. The PRIMME_SVDS¹⁰ library implements a hybrid algorithm called PHSVDS,¹¹ which is based on carefully selecting an appropriate algorithm at each point of the computation. Moreover, worth mentioning is the inverse-free preconditioned Krylov subspace method.^{12,13}

The LINPACK condition-number estimator requires a triangular factorization of A (see chapter 15 in Higham's monograph¹⁴ for details on this and related estimators). The Gotsman–Toledo¹⁵ and Bischof et al.¹⁶ condition-number estimators, which are specialized to sparse matrices, also require triangular factorization. Estimators that require triangular factorization are less expensive than SVD, but they still cannot be applied to huge matrices.

The LAPACK condition-number estimator estimates the 1-norm condition number.¹⁷ Higham and Tisseur derive a block version of the LAPACK 1-norm condition-number estimator.¹⁸ Both methods are blackbox in the sense that they require only matrix–vector products with the pseudoinverses of A and A^T . One way to compute these products is using factorization, but they can also be computed using an iterative solver. With an effective preconditioner, repeated applications of the pseudoinverse may be less expensive than the method that we propose, but without one, our method is less expensive. Kenney et al.¹⁹ describe a way to estimate the condition number of a square matrix using a single application of the inverse to one or several vectors. Vecharynski proposes a Rayleigh quotient–type iteration that uses a single iteration of a preconditioned iterative solver to compute an approximate singular vector given an approximate singular value (which is estimated from the previous singular-vector estimate).²⁰ Gaaf and Hochstenbach¹ propose to estimate the condition number of square matrices using the *extended Krylov subspace*. Computing a basis for the extended Krylov subspace requires applying the inverse of the matrix; hence, the method uses an LU factorization of the matrix.

The spectral condition number measures the normwise sensitivity of matrix–vector products and linear systems to small perturbations in the inputs. There are methods that estimate more focused metrics, such as the sensitivity of individual components of the inputs or output.¹⁹ Our method does not address this problem.

LSQR itself also estimates a condition number of A , the Frobenius condition number $\|A\|_F\|A^+\|_F$, where A^+ is the pseudoinverse of A . LSQR estimates the two norms by computing explicitly the Frobenius norm of two bidiagonal matrices that it computes as part of the algorithm, $B^{(l)}$ and $D^{(l)}$. The estimates rely on inequalities $\|B^{(l)}\|_F \leq \|A\|_F$ and $\|D^{(l)}\|_F \leq \|A^+\|_F$. However, this method has several serious shortcomings. First, the LSQR paper does not provide any evidence that the gap in the inequalities is small by the time the algorithm terminates. In particular, it appears difficult to come up with stopping criteria that will ensure that these estimates are accurate. Second, the inequalities depend on the theoretical (exact arithmetic) orthogonality of the Lanczos vectors, which are far from orthogonal when the algorithm is implemented in floating-point arithmetic.

As noted by Paige and Saunders,²¹ the spectral condition number can also be bounded using $\|B^{(l)}\|_2\|D^{(l)}\|_2$, but this is not done in practice (nor is it suggested by Paige and Saunders) since computing this quantity in each iteration is expensive.

Our method improves upon the condition-number estimates of LSQR in several ways. First, we devise a way to approximate the spectral condition number cheaply in each iteration; hence, our algorithm estimates the spectral condition number instead of the Frobenius condition number, as is done by LSQR. The spectral condition number is more relevant

for estimating the accuracy of linear solvers. Second, we use two estimators for σ_{\min} , one of which is similar in spirit to LSQR's use of $\|D^{(t)}\|_F$ and the other completely novel, which only relies on *properties that do hold in floating point*. In particular, in addition to the novel estimator, we use $R^{(t)}$ (another bidiagonal matrix formed by LSQR) instead of $D^{(t)}$ (as is done in LSQR), which is more robust to inexact arithmetic. Using $R^{(t)}$ is somewhat expensive, and this is why it is not used in LSQR; however, because of the other estimator, our algorithm needs to use this estimator only once. Third, the other estimate that our algorithm computes comes with a vector that proves that our estimate is an upper bound on σ_{\min} (the approximate singular vector). LSQR's estimate also provides an upper bound, but it does not provide a certificate vector that materializes the bound. Fourth, the stopping criteria of our algorithm are designed specifically to discover that the estimate of σ_{\min} is accurate; these criteria cannot be used in general in LSQR because they require knowledge of the forward error.

3 | THE FORWARD ERROR OF ITERATES ON A RANDOM RIGHT-HAND SIDE

In this section, we introduce the idea that underlies our algorithm, namely, that when applying LSQR to a random right-hand side, the forward error in the iterates is rich in the direction of the smallest singular vector.

Let x^* be a random vector, and let $b = Ax^*$. Paige and Saunders explain in section 7.1 of the LSQR paper²¹ that, in exact arithmetic, the LSQR iterates are identical to the iterates of conjugate gradients (see section 11.3 in the work of Golub and Van Loan²²) when applied to the normal equations, that is,

$$A^T A x^* = A^T b .$$

Therefore, the k th iterate $x^{(k)}$ satisfies

$$x^{(k)} = \arg \min_{x \in \mathcal{K}_k(A^T A, A^T b)} \|x^* - x\|_{A^T A},$$

where $\mathcal{K}_k(A^T A, A^T b)$ is the k -dimensional Krylov subspace and $\|\cdot\|_{A^T A}$ denotes the norm $\|v\|_{A^T A}^2 = v^T A^T A v$. We can therefore express $x^{(k)}$ as

$$x^{(k)} = p_0(A^T A) A^T b$$

for some degree- $(k - 1)$ polynomial p_0 and the error as

$$\begin{aligned} x^* - x^{(k)} &= x^* - p_0(A^T A) A^T b \\ &= x^* - p_0(A^T A) A^T A x^* \\ &= p(A^T A) x^* \end{aligned}$$

for a degree- k polynomial $p(z) = 1 - zp_0(z)$.

Let us denote the thin SVD of A and the eigendecomposition of its Gram matrix by

$$\begin{aligned} A &= U \Sigma V^T \\ A^T A &= V \Sigma^2 V^T , \end{aligned}$$

where $\Sigma^2 = \text{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_n^2)$ for some $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n = \sigma_{\min} \geq 0$. Then, we have

$$\begin{aligned} \min_{x^{(k)}} \|x^* - x^{(k)}\|_{A^T A}^2 &= \min_p \|p(A^T A) x^*\|_{A^T A}^2 \\ &= \min_p \|p(V \Sigma^2 V^T) x^*\|_{A^T A}^2 \\ &= \min_p \|V p(\Sigma^2) V^T x^*\|_{A^T A}^2 \\ &= \min_p \sum_{i=1}^n \alpha_i^2 \sigma_i^2 p^2(\sigma_i^2) , \end{aligned}$$

where $\alpha_i = (V^T x^*)_i$ and the minimization is over all polynomials $p(z)$ of degree k such that $p(0) = 1$.

Now, consider the $x^{(k)}$'s, the forward errors $d^{(k)} = x^* - x^{(k)}$, and the Rayleigh quotients

$$\frac{\|Ad^{(k)}\|}{\|d^{(k)}\|}.$$

In subsequent sections, we experimentally show that these quantities tend to σ_{\min} (and then diverge). To understand why this happens, let us express these quotients as

$$\begin{aligned} \frac{\|Ad^{(k)}\|^2}{\|d^{(k)}\|^2} &= \frac{\|A(x^* - x^{(k)})\|^2}{\|x^* - x^{(k)}\|_2^2} \\ &= \frac{\|AVp(\Sigma^2)V^Tx^*\|^2}{\|Vp(\Sigma^2)V^Tx^*\|^2} \\ &= \frac{\|U\Sigma p(\Sigma^2)V^Tx^*\|^2}{\|Vp(\Sigma^2)V^Tx^*\|^2} \\ &= \frac{\sum_{i=1}^n \alpha_i^2 \sigma_i^2 p^2(\sigma_i^2)}{\sum_{j=1}^n \alpha_j^2 p^2(\sigma_j^2)} \\ &= \sum_{i=1}^n \sigma_i^2 \frac{\alpha_i^2 p^2(\sigma_i^2)}{\sum_{j=1}^n \alpha_j^2 p^2(\sigma_j^2)}. \end{aligned} \quad (1)$$

LSQR chooses p among all degree- k polynomials with $p(0) = 1$ so as to minimize the numerator $\sum_{i=1}^n \alpha_i^2 \sigma_i^2 p^2(\sigma_i^2)$ in (1), which is equal to the square of the $A^T A$ norm of the forward error $d^{(k)}$. If x^* is a random vector with independent standard independent elements, then the α_i 's are also normal and independent; thus, we expect all the α_i 's to be roughly similar in magnitude. We do not expect very large or very small α_i 's. The term in the numerator involving $p^2(\sigma_i^2)$ is multiplied by $\alpha_i^2 \sigma_i^2$. If $\sigma_n < \sigma_{n-1}$, we expect the value of p^2 at $\sigma_1^2, \dots, \sigma_{n-1}^2$ to be small relative to $p^2(\sigma_n^2)$, because the term involving $p^2(\sigma_n^2)$ in the numerator of (1) is scaled by σ_n^2 ($\sigma_n = \sigma_{\min}$ is the smallest singular value), and the α_i 's are all similar in magnitude. In other words, to make the numerator of (1) small, the LSQR polynomial p must assume small values at large σ_i 's but can assume relatively large values at small σ_i 's.

If p^2 indeed assumes a small value at $\sigma_1^2, \dots, \sigma_{n-1}^2$ but a relatively large value at σ_n^2 and if the α_i 's are all similar, then the expressions

$$\frac{\alpha_i^2 p^2(\sigma_i^2)}{\sum_{j=1}^n \alpha_j^2 p^2(\sigma_j^2)}$$

are much smaller than 1 for $i = 1, \dots, n-1$ but close to 1 for $i = n$ (these expressions sum up to 1). If this is the case, our Rayleigh quotient approximates σ_n . The analysis generalizes easily to multiple singular values at σ_{\min} .

We have not analyzed rigorously the quality of this approximation as a function of the spectral gap (between σ_{\min} and the second smallest singular value) and of the random choice of x^* . Nevertheless, this mathematical analysis motivates our algorithm, which we describe in the next section.

4 | THE ALGORITHM

This section describes our algorithm for estimating the condition number of A . A detailed pseudocode description appears in Algorithm 1.

Algorithm 1 The condition number estimation algorithm. Lines marked with * are inherited from LSQR. Some quantities, such as $\|\hat{x}\|$, $\|Ad^{(t)}\|$, $\|d^{(t)}\|$, and $\|b\|$, should be computed once and reused; the full expressions are shown multiple times for clarity

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1: Input:  $A \in \mathbb{R}^{m \times n}$ 
2: Parameters (defaults in parentheses):  $c_1$  ( $8\epsilon_m$ ),  $c_2$  ( $10^{-3}$ ),  $c_3$  ( $1/(64 \cdot \epsilon_m)$ ),  $c_4$  ( $\sqrt{\epsilon_m}$ ),  $c'_1$  ( $4\epsilon_m$ ), and maxit.
3:
4: Estimate  $\hat{\sigma}_{\max} = \sigma_{\max}$ , along with a certificate  $\hat{v}_{\max}$ , using power iteration.
5:  $\hat{\sigma}_{\min} = \hat{\sigma}_{\max}$ ,  $\hat{v}_{\min} = \hat{v}_{\max}$ 
6: Draw a random vector  $\hat{x} \in \mathbb{R}^n$  with independent normal entries
7:  $\tau \leftarrow \sqrt{2} \cdot \text{erf}^{-1}(c_2)/\|\hat{x}\|$ 
8:  $x^* \leftarrow \hat{x}/\|\hat{x}\|$ 
9:  $b \leftarrow Ax^*$ 
10: *  $\beta^{(0)} \leftarrow \|b\|$ ,  $u^{(0)} \leftarrow b/\beta^{(0)}$ 
11: *  $v^{(0)} \leftarrow Au^{(0)}$ ,  $\alpha^{(0)} \leftarrow \|v^{(0)}\|$ ,  $v^{(0)} \leftarrow v^{(0)}/\alpha^{(0)}$ 
12: *  $w^{(0)} \leftarrow v^{(0)}$ 
13: *  $x^{(0)} \leftarrow 0_{n \times 1}$ 
14: *  $\bar{\phi}^{(0)} \leftarrow \beta^{(0)}$ ,  $\bar{\rho}^{(0)} \leftarrow \alpha$ 
15:  $T \leftarrow \text{maxit}$  ▷ limit for  $T$ ; usually reduced later
16: for  $t = 1, \dots, T$  do
17:   *  $u^{(t)} \leftarrow Av^{(t-1)} - \alpha u^{(t-1)}$ 
18:   *  $\beta^{(t)} \leftarrow \|u^{(t)}\|$ 
19:   *  $u^{(t)} \leftarrow u^{(t)}/\beta^{(t)}$ 
20:   *  $v^{(t)} \leftarrow A^T u^{(t)} - \beta^{(t)} v^{(t)}$ 
21:   *  $\alpha^{(t)} \leftarrow \|v^{(t)}\|$ 
22:   *  $v^{(t)} \leftarrow v^{(t)}/\alpha^{(t)}$ 
23:   *  $\rho^{(t)} \leftarrow \|(\bar{\rho}^{(t-1)} \beta^{(t)})\|$ 
24:   *  $c^{(t)} \leftarrow \bar{\rho}^{(t-1)}/\rho^{(t)}$ ,  $s^{(t)} \leftarrow \beta^{(t)}/\rho^{(t)}$ 
25:   *  $\theta^{(t)} \leftarrow s^{(t)}\alpha^{(t)}$ ,  $\bar{\rho}^{(t)} \leftarrow -c^{(t)}\alpha^{(t)}$ 
26:   *  $\phi^{(t)} \leftarrow c^{(t)}\bar{\phi}^{(t-1)}$ ,  $\bar{\phi}^{(t)} \leftarrow s\bar{\phi}^{(t-1)}$ 
27:   *  $x^{(t)} \leftarrow x^{(t-1)} + (\phi^{(t)}/\rho^{(t)})w^{(t-1)}$ 
28:   *  $w^{(t)} \leftarrow v^{(t)} - (\theta^{(t)}/\rho^{(t)})w^{(t-1)}$ 
29:    $R_{tt}^{(t)} \leftarrow \rho^{(t)}$  ▷ Only diagonal and superdiagonal of  $R$  are kept in memory
30:   if  $t > 1$  set  $R_{t-1,t}^{(t)} \leftarrow \theta^{(t-1)}$ 
31:    $d^{(t)} \leftarrow x^* - x^{(t)}$ 
32:   if  $d^{(t)} = 0$  set  $\hat{\sigma}_{\min} \leftarrow \hat{\sigma}_{\max}$ ,  $\hat{v}_{\min} \leftarrow \hat{v}_{\max}$  and break for
33:   ▷ Due to finite precision arithmetic, when  $\kappa \neq 1$  getting  $d^{(t)} = 0$  is extremely unlikely.
34:   if  $\|Ad^{(t)}\| \leq \hat{\sigma}_{\min}\|d^{(t)}\|$  then
35:      $\hat{\sigma}_{\min} \leftarrow \|Ad^{(t)}\|/\|d^{(t)}\|$ ,  $\hat{v}_{\min} \leftarrow d^{(t)}$ 
36:   end if
37:   if  $\hat{\sigma}_{\min}/\hat{\sigma}_{\max} \leq c_4$  then  $c_1 \leftarrow c'_1$ 
38:   if  $T = \text{maxit}$  and  $(\frac{\|Ad^{(t)}\|}{\hat{\sigma}_{\max}\|x^{(t)}\| + \|b\|} \leq c_1$  or  $\|d^{(t)}\| \leq \tau$  or  $\hat{\sigma}_{\max}/\hat{\sigma}_{\min} \geq c_3)$  then
39:      $T \leftarrow \lceil 1.25t \rceil$ 
40:   end if
41: end for
42: Estimate  $\tilde{\sigma}_{\min} = \sigma_{\min}(R^{(T)})$ , using inverse power iteration
43:  $\tilde{\sigma}_{\min} \leftarrow \min(\tilde{\sigma}_{\min}, \hat{\sigma}_{\min})$ 
44: return  $\hat{\sigma}_{\max}/\hat{\sigma}_{\min}$ ,  $\hat{\sigma}_{\max}$ ,  $\hat{\sigma}_{\min}$ ,  $\hat{v}_{\max}$  and  $\hat{v}_{\min}$ ,  $\tilde{\sigma}_{\min}$ 

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The algorithm starts by estimating σ_{\max} and a corresponding certificate vector using power iteration on $A^T A$. By a *certificate vector* for an estimate $\hat{\sigma}_{\max}$, we mean a vector v such that $\|Av\|/\|v\| = \hat{\sigma}_{\max}$ (and similarly for estimates of σ_{\min}). We perform enough iterations to estimate σ_{\max} to within 10% of accuracy with a probability of at least $1 - 10^{-12}$. Using a

bound due to the work of Klein and Lu²³ (see section 4.4 thereof),[§] we find that given a relative error parameter ϵ and a failure probability parameter δ , if we perform

$$\left\lceil \frac{1}{\epsilon} \left(\ln(2n)^2 + \ln\left(\frac{1}{\epsilon\delta^2}\right) \right) \right\rceil$$

iterations, the relative error in our approximation is less than ϵ with a probability of at least $1 - \delta$. For the parameters $\epsilon = 10^{-1}$ and $\delta = 10^{-12}$, 1,004 iterations suffice even for matrices with up to 10^9 columns. For $\epsilon = 1/3$ and $\delta = 10^{-12}$, only 298 iterations suffice for matrices with up to 10^9 columns. (The accuracy of the σ_{\max} estimate in the power method is typically much higher than predicted by this bound, but the additional accuracy depends on the gap between the largest and second-largest singular values; the bound that we use makes no assumption on the gap.) It is possible to use other methods to find $\hat{\sigma}_{\max}$ and v (e.g., Lanczos). We chose power iteration because when we developed the algorithm, existing theoretical results allow us to write an expression for the number of iterations as a function of ϵ and δ , independent of the gap. Such strong bounds that guarantee high accuracy of σ_{\max} are desirable since the stopping criteria we use for the estimation of σ_{\min} depend on $\hat{\sigma}_{\max}$. Furthermore, for one singular pair, we empirically observed that the power method is typically faster than Lanczos and other iterative methods.

The main phase of the algorithm uses a modified LSQR iteration (see pages 50 and 51 in the works of Paige and Saunders^{21,24}) designed to estimate σ_{\min} and to produce a corresponding certificate vector. LSQR is a method for solving least squares problems $\min \|Ax - b\|_2$. At its core, LSQR uses the bidiagonalization procedure of Golub and Kahan to form iterates $u^{(0)}, u^{(1)}, \dots \in \mathbb{R}^m$, $v^{(0)}, v^{(1)}, \dots \in \mathbb{R}^n$, $\alpha^{(0)}, \alpha^{(1)}, \dots \in \mathbb{R}$, and $\beta^{(0)}, \beta^{(1)}, \dots \in \mathbb{R}$ such that

$$\begin{aligned} U^{(t+1)} (\beta^{(1)} e_1) &= b \\ AV^{(t)} &= U^{(t+1)} B^{(t)} \\ A^T U^{(t+1)} &= V^{(t)} (B^{(t)})^T + \alpha^{(t+1)} v^{(t+1)} e_{t+1}^T, \end{aligned}$$

where $U^{(t)} = [u^{(0)}, u^{(1)}, \dots, u^{(t)}]$ and $V_k = [v^{(0)}, v^{(1)}, \dots, v^{(k)}]$. LSQR uses these to find at iteration t the optimal minimizer inside the Krylov subspace $\mathcal{K}_t(A^T A, A^T b) = \text{span}\{A^T b, (A^T A)A^T b, \dots, (A^T A)^{t-1}A^T b\}$. In addition, LSQR forms additional bidiagonal matrices $R^{(0)}, R^{(1)}, \dots$ and estimates $\bar{\phi}^{(0)}, \bar{\phi}^{(1)}, \dots$ of the norm of the residual $r^{(t)} = b - Ax^{(t)}$ (see the work of Paige and Saunders²¹ for details). We also remark that the Golub and Kahan bidiagonalization is closely related to the Lanczos tridiagonalization of the augmented matrix and of the Gram matrix and that this connection is exploited by our algorithm.

The main idea in our algorithm is to use a random right-hand side so the forward error will tend to concentrate in the direction corresponding to σ_{\min} . To be able to access the forward error, we also generate the right-hand side in a way that gives us access to it. Specifically, our algorithm first generates a uniformly distributed random vector x^* on the unit sphere by first generating a vector \hat{x} with normally distributed independent random components and then setting $x^* = \hat{x}/\|\hat{x}\|$. The algorithm multiplies it by A to produce a nearly consistent right-hand side b . While in exact arithmetic we would have had a consistent right-hand side ($b = Ax^*$), due to finite precision, it is only nearly consistent: $\|b - Ax^*\| \leq O(\epsilon_m) \cdot \|A\|$.

Our algorithm modifies LSQR by adding a few steps to each iteration. At the end of each (standard) LSQR iteration, we have an updated approximate solution $x^{(t)}$ and an estimate of $\|r^{(t)}\| = \|Ax^{(t)} - b\|$, denoted by $\bar{\phi}^{(t)}$. The equality of $\bar{\phi}^{(t)}$ and $\|r^{(t)}\|$ depends on the orthogonality of the Lanczos vectors, which lose orthogonality in floating-point arithmetic as the algorithm progresses; hence, in practice, $\bar{\phi}^{(t)}$ and $\|r^{(t)}\|$ may differ significantly. Our algorithm also computes the forward error $d^{(t)} = x^* - x^{(t)}$ and $\|d^{(t)}\|$. We thus have

$$\begin{aligned} \|Ad^{(t)}\| &= \|A(x^* - x^{(t)})\| \\ &= \|b - Ax^{(t)}\| \\ &= \|r^{(t)}\|, \end{aligned}$$

which, in exact arithmetic, equals $\bar{\phi}^{(t)}$; however, to improve the robustness of the algorithm, we compute $\|Ad^{(t)}\|$ explicitly. (In our numerical experiments, we have found $\bar{\phi}^{(t)}$ to be an accurate estimate, but we prefer to avoid any reliance on the orthogonality of the Lanczos vectors in our algorithm.) We also compute $\|x^{(t)}\|$.

[§]Note that the statement of lemma 6 in the work of Klein and Lu²³ is incorrect; the proof shows the correct bound. Moreover, the discussion that follows the proof of the lemma repeats the error in the statement of the lemma.

Next, the algorithm computes the ratio $\|Ad^{(t)}\|/\|d^{(t)}\|$, which, like any Rayleigh quotient, is an upper bound on σ_{\min} . Note that this upper bound is not affected by the inconsistency of the linear system. If this ratio is the smallest we have seen so far, the algorithm treats it as an estimate of σ_{\min} and stores both the ratio and the certificate $d^{(t)}$. When the algorithm terminates, it outputs the best ratio it has found and the corresponding certificate.

We use three stopping criteria. The first criterion, which is the one used by the standard LSQR algorithm for consistent systems, stops the algorithm when the *normwise backward error* (see section 7.1 in the work of Higham¹⁴) drops below a threshold, that is,

$$\frac{\|r^{(t)}\|}{\hat{\sigma}_{\max} \|x^{(t)}\| + \|b\|} \leq c_1, \quad (2)$$

where $\hat{\sigma}_{\max}$ is our estimate of $\|A\|$ and c_1 is a parameter that is set by default to $8\epsilon_m$. It has been observed experimentally²⁵ that for consistent systems, as long as c_1 is of the order of magnitude ϵ_m or greater, this criterion will be eventually met in spite of the loss of orthogonality in the biorthogonalization process; however, the left-hand side of (2) does not seem to decrease much below the value required to satisfy the inequality.²⁵

In many cases, our second stopping criterion will stop the algorithm well before the residual is that small. This second condition is

$$\|d^{(t)}\| \leq \frac{\sqrt{2} \cdot \text{erf}^{-1}(c_2)}{\|\hat{x}\|}, \quad (3)$$

where erf^{-1} is the inverse error function, computed using a numerical approximation, and c_2 is a parameter that is set by default to 10^{-3} , which corresponds to $\text{erf}^{-1}(c_2) \approx 8.9 \times 10^{-4}$. This criterion is not used by LSQR; it requires knowledge of the error, which LSQR does not have in general. We explain this stopping criterion and how the choice of c_2 affects the algorithm in the next section.

The third stopping criterion is

$$\frac{\hat{\sigma}_{\max}}{\hat{\sigma}_{\min}} \geq c_3, \quad (4)$$

where c_3 is a parameter that is set by default to $1/(64 \cdot \epsilon_m)$. In other words, at this threshold, we consider the matrix to be numerically rank deficient, and we do not attempt to estimate the exact condition number. Standard LSQR uses a different condition-number estimate in a similar stopping criterion, for regularization.²¹

To achieve good accuracy even for matrices that are terribly ill conditioned (condition number close to $1/\epsilon_m$), the stopping criteria are refined in two additional ways.

1. If, at some point, we have

$$\frac{\hat{\sigma}_{\max}}{\hat{\sigma}_{\min}} \geq c_4,$$

where c_4 is a parameter that is set by default to $\sqrt{\epsilon_m}$, we set c_1 (residual-based stopping threshold) to c'_1 , which is set by default to $4\epsilon_m$. The rationale is that when the matrix is ill conditioned, the residual-based test is less accurate; hence, we lower the threshold to compensate.

2. Even when the method detects convergence using one of its three criteria (small residual, small error, and numerical rank deficiency), it keeps iterating. The number of extra iterations is one quarter of the number performed until convergence was detected. This rule is a heuristic that tries to improve the accuracy of the condition-number estimate. The cost of this heuristic is obviously limited, and it can be turned off by the user.

In addition, our algorithm also stores the matrix $R^{(t)}$, one of two bidiagonal matrices that LSQR incrementally constructs but normally discards. In exact arithmetic, the singular values of $R^{(t)}$ converge to the singular values of A .^{26,27} Once the algorithm terminates, we compute $\tilde{\sigma}_{\min} \approx \sigma_{\min}(R^{(t)})$; if it is smaller than the best $\|Ad^{(t)}\|/\|d^{(t)}\|$ estimate, we output both estimates. One estimate ($\tilde{\sigma}_{\min}$) is tighter, but it comes with no certificate vector; the other is more loose, but it comes with a certificate. Generating the certificate for the Lanczos estimate requires storing the Lanczos vectors or repeating the iterations. The former is obviously too expensive, whereas the latter might be redundant if the user is satisfied with the certificate already computed. We note that the singular values of $R^{(t)}$ tend to converge first to large singular values of A ; thus, this estimate is not very likely to be better than $\|Ad^{(t)}\|/\|d^{(t)}\|$.

Storing $R^{(t)}$ and estimating $\sigma_{\min}(R^{(t)})$ are relatively inexpensive since $R^{(t)}$ is bidiagonal. We estimate it by running inverse iteration on $R^{(t)}$, again performing enough iterations to get to within 10% of accuracy with very high probability ($1 - 10^{-12}$; this is a parameter in the code). The cost of a single inverse power iteration is only $O(t)$. Since we use power iteration, the error in $\tilde{\sigma}_{\min}$ is one sided: It is always the case that $\tilde{\sigma}_{\min} \geq \sigma_{\min}(R^{(t)})$ (because it is generated by a Rayleigh quotient). In addition, $\sigma_{\min}(R^{(t)}) \geq \sigma_{\min}$. Therefore, $\tilde{\sigma}_{\min}$ is also an upper bound on σ_{\min} , not just an estimate. We remark that $\tilde{\sigma}_{\min}$ is guaranteed to be an upper bound on σ_{\min} only in exact arithmetic. In floating point, it is possible for $\tilde{\sigma}_{\min}$ to drop below σ_{\min} .

5 | ANALYSIS OF THE SMALL-ERROR STOPPING CRITERION

We now explain the second stopping criterion (3). Suppose that the smallest singular value of A is simple and that it is well separated from the next smallest singular values. Let $x^* = \sum_{i=1}^n \alpha_i v_i$ be the initial vector represented in the basis of the right singular vectors of A . As LSQR progresses toward finding x^* , it will tend initially to resolve components in the direction of the largest singular vectors. Since the v_n direction is not present in $x^{(0)} = 0$, we expect it to be not present during the initial iterations, that is, $(v_n)^T x^{(t)} \approx 0$. This implies that we expect for the initial iterations to have $|(v_n)^T (x^* - x^{(t)})| \approx |\alpha_n|$; thus, $\|x^* - x^{(t)}\| \geq |\alpha_n|$. Now, at some point in the iteration, the solution $x^{(t)}$ will be roughly $x^{(t)} \approx \sum_{i=1}^{n-1} \alpha_i v_i$, that is, the error remains mostly in the direction of the smallest singular subspace, but the v_n direction is not present at all. At that point, $\|x^* - x^{(t)}\| \approx |\alpha_n|$. LSQR will now start to resolve that error at least partially, and the norm of the error will decrease below $|\alpha_n|$. If we stop the iteration when $\|x^* - x^{(t)}\| \gg |\alpha_n|$, the error is unlikely to be a good estimate of a small singular vector. If we stop when $\|x^* - x^{(t)}\| \leq |\alpha_n|$, we will likely have a good estimate of a small singular value. Ideally, we want to stop immediately when $\|x^* - x^{(t)}\|$ drops below $|\alpha_n|$. Stopping later (when the error is much smaller than $|\alpha_n|$) does not do any harm, since we report the best Rayleigh quotient seen, but it does not improve the estimate by much.

The second stopping criterion is designed so that the test passes only if the condition $\|x^* - x^{(t)}\| \leq |\alpha_n|$ holds with high probability. It is based on the following proposition.

Claim 1. Suppose that $x^* = \hat{x}/\|\hat{x}\|$, where \hat{x} is a vector with normally distributed independent random components, and assume $x^* = \sum_{i=1}^n \alpha_i v_i$ to be x^* represented in the basis of the right singular vectors of A . If

$$\|x^* - y\| \leq \frac{\sqrt{2} \cdot \text{erf}^{-1}(\delta)}{\|\hat{x}\|},$$

then $\|x^* - y\| \leq |\alpha_n|$ holds with probability of at least $1 - \delta$ for $0 < \delta < 1$.

Proof. Let $\hat{y} = \|\hat{x}\|y$ and $\hat{\alpha}_n = \|\hat{x}\|\alpha_n$. Obviously, $\|x^* - y\| \leq |\alpha_n|$ if and only if $\|\hat{x} - \hat{y}\| \leq |\hat{\alpha}_n|$. Therefore, if we find a value τ such that $\Pr(|\hat{\alpha}_n| \geq \tau) \geq 1 - \delta$, then the condition $\|\hat{x} - \hat{y}\| \leq \tau$ implies that $\|\hat{x} - \hat{y}\| \leq |\hat{\alpha}_n|$, and hence, $\|x^* - y\| \leq |\alpha_n|$, with a probability of at least $1 - \delta$. Since $\|v_n\| = 1$, we have $\hat{\alpha}_n \sim N(0, 1)$. Therefore,

$$\Pr(|\hat{\alpha}_n| \geq \sqrt{2} \cdot \text{erf}^{-1}(\delta)) = 1 - \delta;$$

hence, $\tau = \sqrt{2} \cdot \text{erf}^{-1}(\delta)$ can be used. The condition $\|\hat{x} - \hat{y}\| \leq \tau$ is now equivalent to $\|x^* - y\| \leq \tau/\|\hat{x}\|$, which is exactly the criteria in the proposition statement. \square

The choice of c_2 in the algorithm determines our confidence that $\|x^* - x^{(t)}\|$ dropped below $|\alpha_n|$. We use a default value of 10^{-3} , which implies a small probability of failure, but not a tiny one. The user can, of course, change the value if he or she needs higher confidence (in either case, the error is one sided). Another approach is to use a much larger c_2 and to repeat the algorithm ℓ times (possibly in a single run, exploiting matrix–matrix multiplications), for instance, $\ell = 3$. The probability that we succeed in at least one run is at least $1 - c_2^\ell$. For $c_2 = 10^{-2}$, setting $\ell = 3$ or so should suffice. In our experience, it is better to make c_2 smaller than to set $\ell > 1$, but we did not do a formal analysis of this issue.

If the smallest singular value is multiple (associated with a singular subspace of dimension $k > 1$), our situation is even better, because we can stop when $x^* - x \approx \sum_{i=n-k+1}^n \alpha_i v_i$, when $\|x^* - x\| \approx \sqrt{\alpha_{n-k+1}^2 + \dots + \alpha_n^2}$, which is even more likely to be larger than our stopping criterion.

When the smallest singular value is not well separated, the stopping criterion is still sound, but the Rayleigh quotient estimate we obtain is not as accurate, because in such cases, $x^* - x$ tends to be a linear combination of singular vectors

corresponding to several singular values. These singular values are all small, but they are not exactly the same, thereby pulling the Rayleigh quotient up a bit.

6 | NUMERICAL INVESTIGATIONS

This section illustrates and explores the behavior of our algorithm using numerical experiments.

6.1 | Experiments on synthetic matrices

We begin by exploring the behavior of our method on synthetic $1,000 \times 400$ full-rank real matrices with prescribed singular values and random singular vectors.

The first matrix has 10 singular values at 10^{-8} , 300 that are distributed logarithmically between 10^{-3} and 10^{-2} , and 90 at 1. The large gap between the smallest singular value and the next larger one makes the problem relatively easy for our algorithm. Figure 1 shows the behavior of our method on one matrix generated with this spectrum. In the first 90 iterations or so, the backward error (left-hand side in (2)) diminishes logarithmically; the norm of $x^{(t)} - x^*$ drops a bit but then stops dropping much. These two effects cause our estimate $\hat{\sigma}_{\min}$ to also diminish roughly logarithmically. The Lanczos estimate $\sigma_{\min}(R^{(t)})$ drops a bit initially but stagnates from iteration 30 or so. What is happening up to iteration 90 or so is that the Golub–Kahan bidiagonalization resolves the singular values in the 10^{-3} -to- 10^{-2} cluster, whereas LSQR removes much of the projection of the corresponding singular vectors from the residual and from the error. Around iteration 160, Lanczos has resolved enough of the spectrum in the 10^{-3} -to- 10^{-2} cluster, and the smallest singular value of $R^{(t)}$ starts moving toward 10^{-8} . At that point, most of the remaining errors consist of singular vectors corresponding to the singular value 10^{-8} , which causes our estimate to be accurate (to within nine decimal digits). The norm of $x^{(t)} - x^*$ is still large, because the error contains a significant component in the subspace associated with the 10^{-8} singular values. At this point, around iteration 225, when the topmost black curve starts dropping again, LSQR starts to resolve the error in this subspace, the backward error starts decreasing again, and the norm of $x^{(t)} - x^*$ starts decreasing, which causes stopping criterion (3) to be met about 30 iterations later.

Figure 2 visualizes the behavior described in the previous paragraph by plotting the projection of the forward error on the right singular vectors. We see that up to around iteration 50, the error associated with singular spaces associated with singular values other than 1 remains very large. From that point on to about iteration 150, the error in subspaces corresponding to values between 10^{-3} and 10^{-2} is resolved, but the error associated with the singular value 10^{-8} is still very large. This is a point where our method finds the smallest singular value and its certificate (the error). As LSQR starts

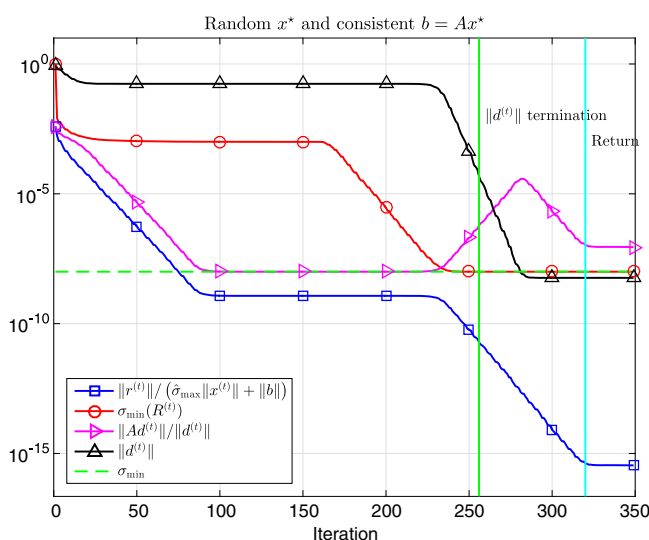


FIGURE 1 The behavior of the method on one matrix described in the text. The vertical lines indicate the iterations at which the stopping criterion was triggered (green) and the iteration at which the algorithm would have returned (after performing 25% extra iterations; we ran the algorithm longer in this case)

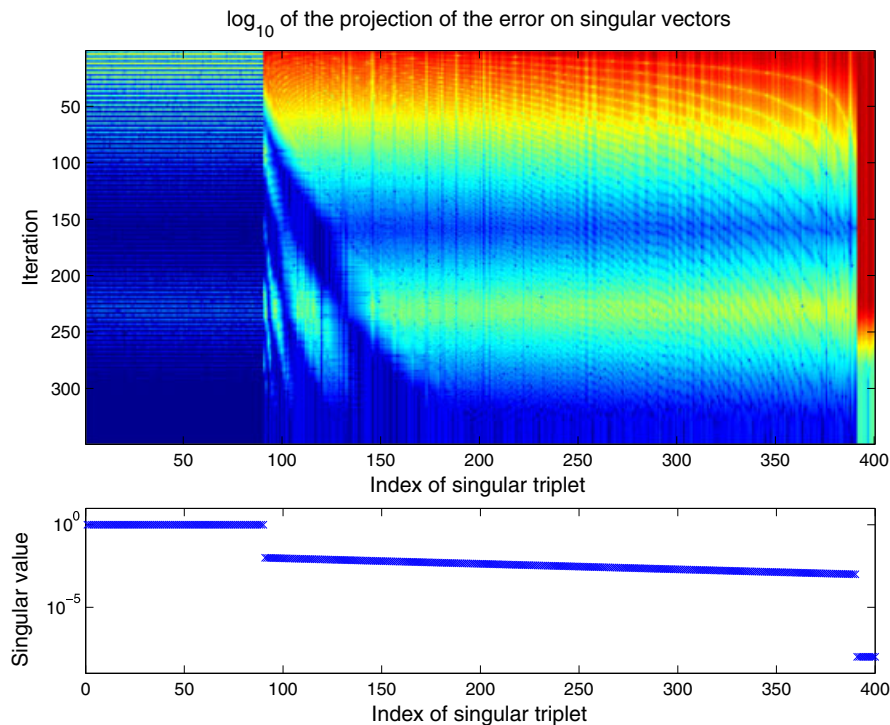


FIGURE 2 The projection of the forward error on the right singular vectors in the experiment shown in Figure 1. The bottom plot shows the singular values of A , and the top image shows the projections. Blue represents values near ϵ_m , green represents values near $\sqrt{\epsilon_m}$, and red represents values near 1

to resolve the error in the 10^{-8} singular subspace, the errors in the 10^{-3} to 10^{-2} subspaces grow (perhaps due to loss of orthogonality), but they are reduced again later.

The method yielded similar results when the smallest singular value was moved down to 10^{-13} , with convergence after about 440 iterations and an estimate that is correct to within five decimal digits. The value $\sigma_{\min} = 10^{-13}$ is about the lower limit for which the $\|d^{(t)}\|$ stopping criterion is useful.

When A is rank deficient, there are infinitely many solutions to the system $Ax = b$. The solution x^* , which was generated randomly, has no special property that distinguishes it from other solutions (like minimum norm); hence, no least squares solver can recover x^* . Therefore, it is unlikely that $\|d^{(t)}\|$ will become small enough to cause our method to stop. In this case, the method stops because the residual eventually becomes very small (close to ϵ_m) or because the estimated condition number becomes too big (stopping condition (4)). In Figure 3, we illustrate the behavior of the algorithm on a rank-deficient matrix; the matrix has 10 singular values that are 10^{-16} (numerical zeros), 300 distributed logarithmically between 10^{-3} and 10^{-2} , and 90 at 1. The algorithm stopped because the condition number got too big; however, a few iterations later, it would have stopped because $\|r^{(t)}\|$ became too small (stopping condition (2)). Our estimate is not accurate (around 1.8×10^{-15} , a relative error of 18), but it still indicates to the user that the matrix is numerically rank deficient. Stopping criteria (2) and (4) and the relatively inaccurate estimates they yield are triggered only when the matrix is close to rank deficiency (condition number of about 10^{14} or larger).

Can

$$\|\arg \min_x \|Ax - b\|_2\|_2^{-1}$$

estimate σ_{\min} if we take b to be a random unit vector? If A has fewer columns than rows or is rank deficient, then with high probability, a random b is not in the column space of A . On some matrices, the minimizer has a norm that is larger than the norm of b by about a factor of σ_{\min}^{-1} . However, unless there is a large gap between the smallest singular values and the rest, the minimizer has a smaller norm, and the norms ratio fails to accurately estimate σ_{\min}^{-1} . Figure 4 shows the relative errors in this estimate for matrices whose singular values are distributed linearly between σ_{\min} and 1. The errors are huge, sometimes by more than three orders of magnitude. This is not a particularly useful method. This method amounts to one half of inverse iteration on $A^T A$; thus, it is not surprising that it is not accurate. Performing more iterations would make the method more reliable, but at the cost of applying the pseudoinverse many times.

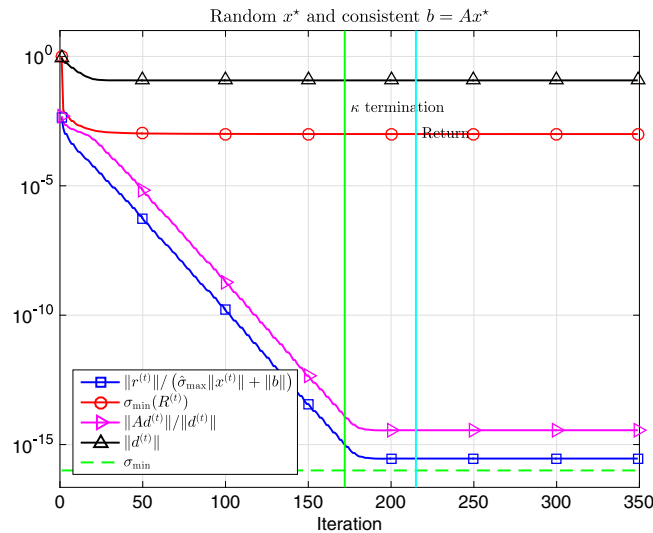


FIGURE 3 The behavior of the method on a numerically rank-deficient matrix described in the text. Termination here occurred due to criterion (4)

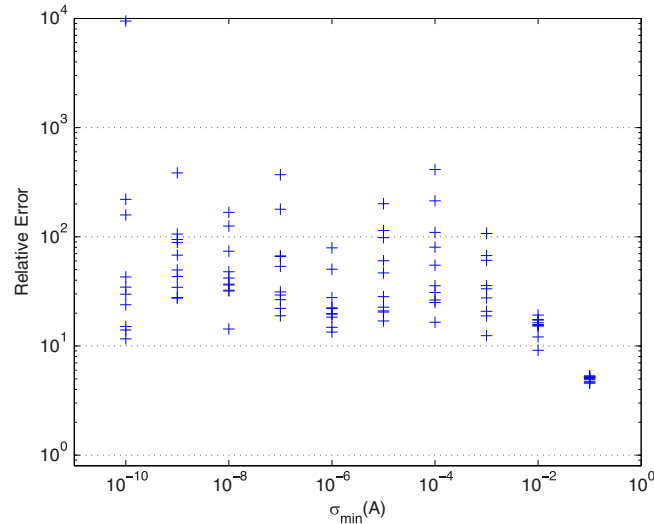


FIGURE 4 Estimating σ_{\min} by $\|A^+b\|^{-1}$ for a unit-length random b with normal independent components

This estimator is clearly biased (the estimate is always larger than σ_{\min}), so is any fixed number of steps of inverse iteration. Kenney et al.¹⁹ derive an unbiased estimator of this type for the Frobenius-norm condition number. To the best of our knowledge, this is not possible in the Euclidean norm.

Other distributions of the singular values lead to more accurate estimates in this method. However, will this method work with an approximate minimizer produced by an iterative method? The following experiment suggests that the answer is no, at least for LSQR. The matrix used in the experiment has 50 singular values distributed logarithmically between 10^{-10} and 10^{-9} , 50 more distributed logarithmically between 10^{-1} and 1, and the rest are all 1. The results, presented in Figure 5, indicate that there is no good way to decide when to terminate LSQR when used in this way to estimate σ_{\min} . We obviously cannot rely on the residual approaching ϵ_m , because the problem is inconsistent. The original LSQR paper²¹ suggests another stopping condition, that is,

$$\frac{\|A^T r^{(t)}\|}{\hat{\sigma}_{\max} \|r^{(t)}\|} \leq c,$$

but our experiment shows that this ratio may fail to get close to ϵ_m . In our experiment, the best local minimum is around 10^{-10} , six orders of magnitude larger than ϵ_m . Moreover, at that local minimum, around iteration 60, the estimate

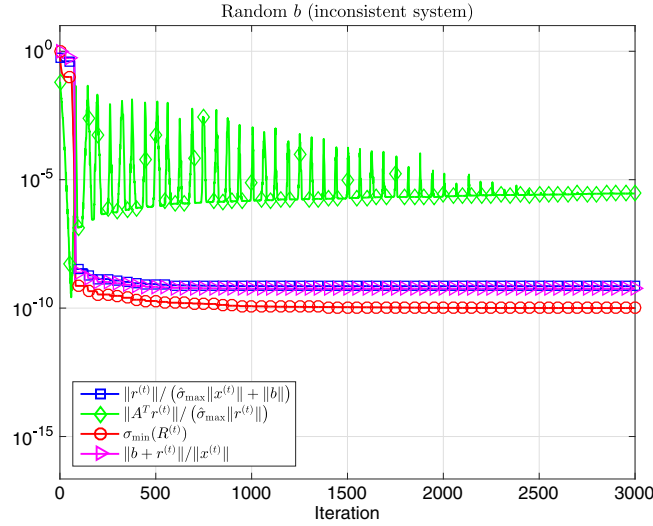


FIGURE 5 Running LSQR with an inconsistent right-hand side b

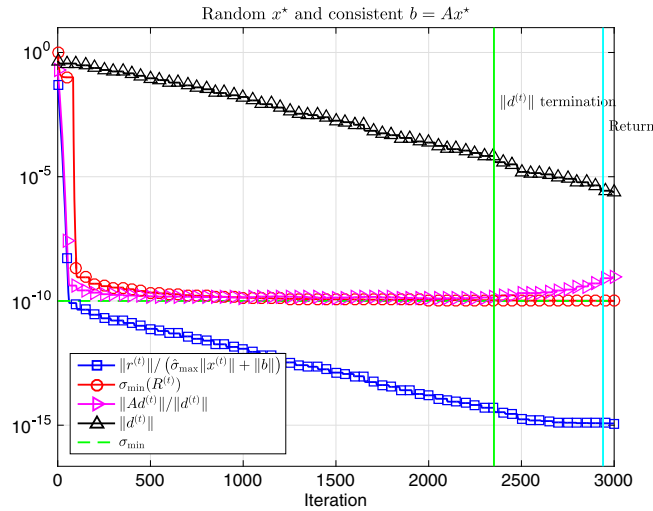


FIGURE 6 Running our method on the same matrix as in Figure 5

$\|b + r^{(t)}\|/\|x^{(t)}\|$ is still near 1, very far from σ_{\min} . The Lanczos estimate $\sigma_{\min}(R^{(t)})$ is also very inaccurate at that time. There does not appear to be a good way to decide when to stop the iterations and to report the best estimate seen so far.

On matrices with this singular value distribution, our method detects convergence after 2,400–2,500 iterations, returning a certified estimate of σ_{\min} that is accurate to within 15%–40% (the accuracy of the Lanczos estimate is better, with relative errors smaller than 10%). Figure 6 shows a typical run. The number of iterations is large, but the stopping criteria are robust.

In Figure 7, all the singular values are distributed linearly from 10^{-8} up to 1 (the dimensions of all matrices in this subsection are again $1,000 \times 400$). Convergence is fairly slow. The gap between $\sigma_{\min} = \sigma_{400} = 10^{-8}$ and σ_{399} is relatively large, around $\frac{1}{400}$; hence, σ_{\min} is computed accurately. When many singular values are distributed logarithmically or nearly so, convergence is very slow, and the small relative gap between σ_{\min} and the next-larger singular values causes the method to return a less accurate estimate. Figure 8 plots the convergence when 200 singular values are distributed logarithmically between 10^{-3} and 1 and the rest are at 1. We do not see a period of stagnation during which the error is a good estimate of ν_{\min} . The certified estimate is only accurate to within 31% and the Lanczos estimate to within 10% (much worse than when the smallest singular value is well separated from the rest).

LSQR might have several periods of stagnation. This happens when the spectrum contains several well-separated clusters. Figure 9 plots the convergence when the matrix has a multiple singular value at 10^{-10} , a multiple singular value at

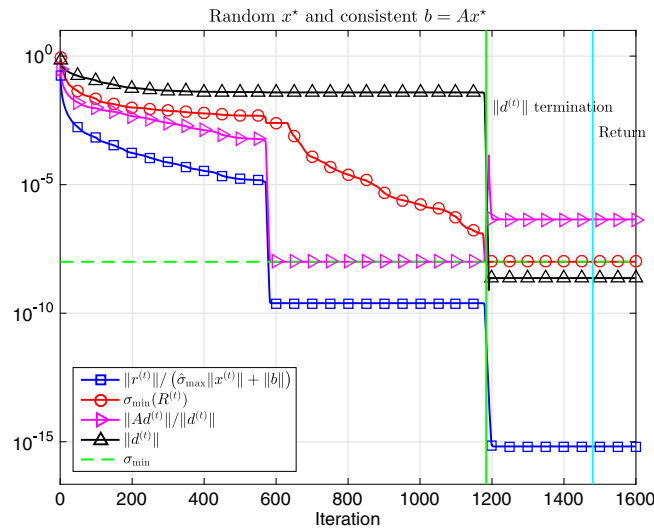


FIGURE 7 Singular values are distributed linearly from 10^{-8} up to 1

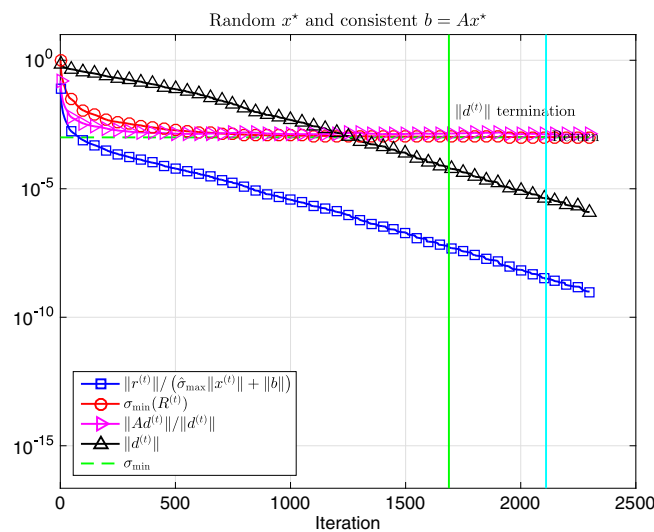


FIGURE 8 Two hundred singular values are distributed logarithmically from 10^{-3} up to 1, and the rest are equal to 1

10^{-7} (both with multiplicity 10), 300 singular values that are distributed logarithmically between 10^{-3} and 10^{-2} , and the rest are at 1. We see multiple stagnation periods of the residual, the error, the Lanczos estimate, and our certified estimate.

6.2 | Experiments on large structured random matrices

The next set of experiments was performed on sparse matrices that motivated this project. These matrices have exactly three nonzeros per column, where the location of the nonzeros is random and uniform and their values are $+1$ or -1 with equal independent probabilities. This type of matrices arises when simulating the evolution of random two-dimensional complexes in various stochastic models.²⁸ Such $m \times n$ matrices tend to be well conditioned when $n < 0.9m$ and rank deficient when $n > 0.95m$. Figure 10 shows that the method converges quite quickly even on large matrices in both the well-conditioned and rank-deficient cases. On smaller matrices of this type, we were able to assess the accuracy of the method. For $m = 1,000$, on $n = 900$, the algorithm yielded a relative error of 22% (the Lanczos estimate was off by 78%), and on $n = 450$, the algorithm yielded a relative error of 41% (the Lanczos estimate was off by 18%). Problems of this type of size $m = 1,000,000$ required a similar number of iterations and were easily solved on a laptop. It is worth noting that due to the random structure of the nonzero pattern, it is likely that factorization-based condition-number estimators will be very slow when applied to this type of matrices.

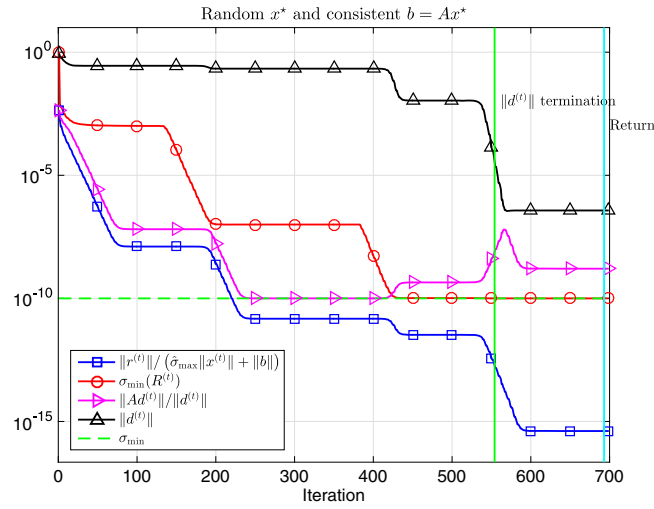


FIGURE 9 Two hundred singular values are distributed logarithmically from 10^{-3} up to 1, and the rest are equal to 1

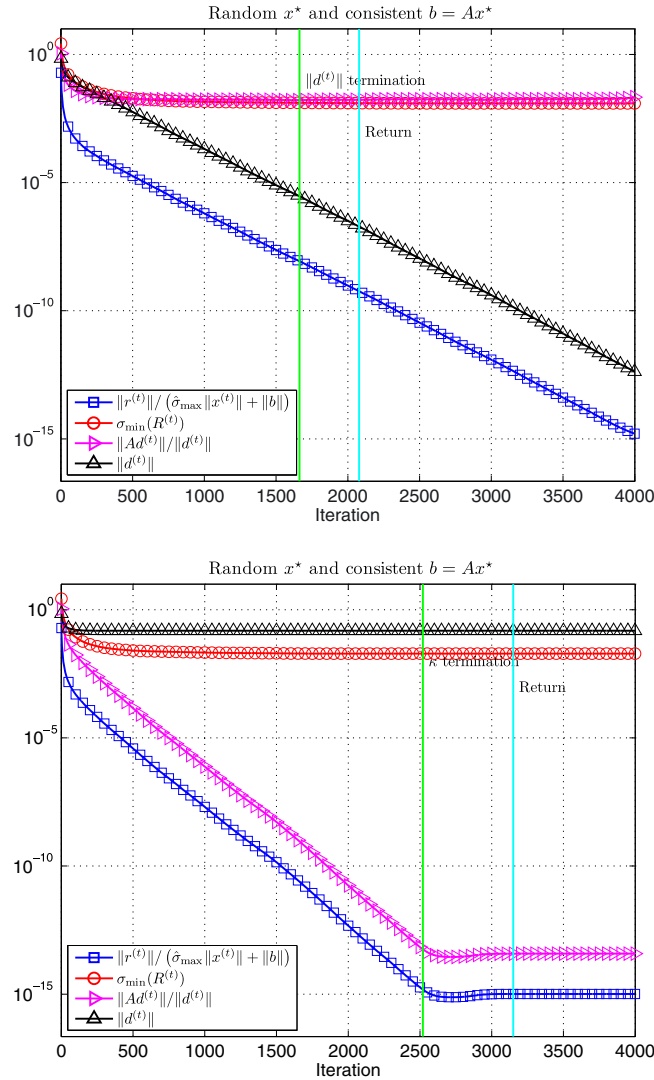


FIGURE 10 Random matrices with three nonzeros per row. On the top, we see the convergence on a $100,000 \times 90,000$ matrix and, on the bottom, the convergence on a $100,000 \times 95,000$ matrix

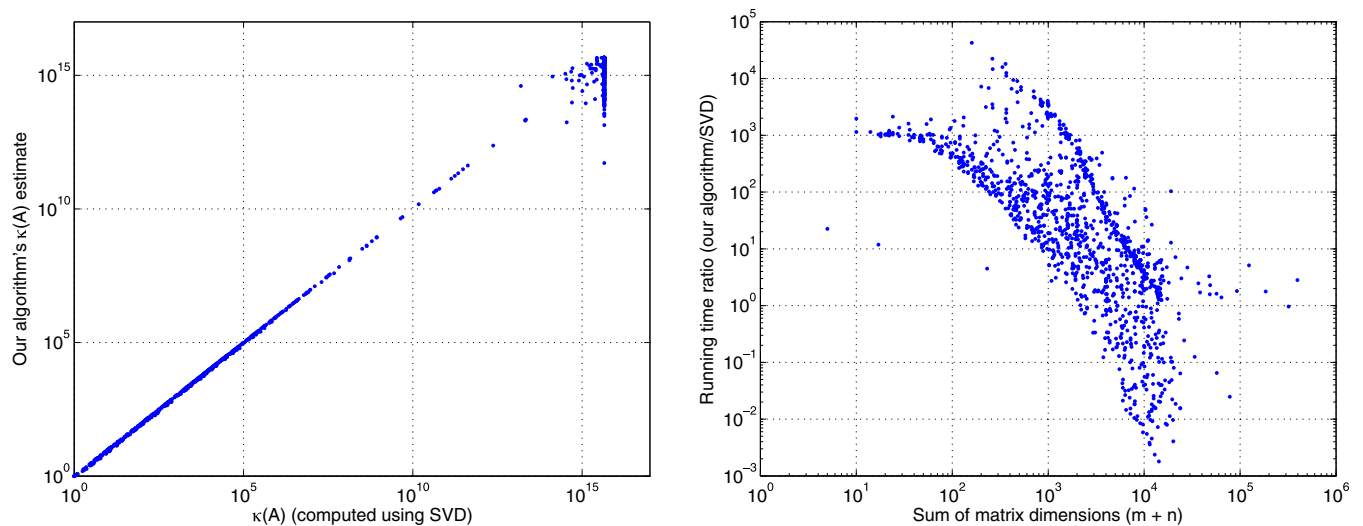


FIGURE 11 Correlation between the actual condition number and the one that we obtain from our algorithm when it converges (left) and the computational cost of our method (implemented in MATLAB), relative to the dense singular value decomposition (SVD), as a function of matrix size (right)

6.3 | Experiments on many real-world matrices

We ran both dense SVD and our method on all the matrices from Tim Davis's sparse matrix collection,²⁹ for which $mn^2 < 256 \times 10^9$. Our method converged in 100,000 iterations or less on 1,024 out of the 1,468 matrices in this category.

Out of the 1,468 matrices, 404 had condition number $1/(64 \cdot \epsilon_m) \approx 7 \times 10^{13}$ or larger. Our method converged on 278 of them, delivering condition-number estimates of 5×10^{11} or larger. In other words, on all the matrices that were close to rank deficiency, our method detected that the condition number is large, but in some cases, it underestimated the actual condition number.

On matrices with condition number smaller than $64/\epsilon_m$, our method always estimated the condition number to within a relative error of 24% or less. Figure 11 shows a scatterplot of the condition number reported by our method when it converged versus the condition number reported by MATLAB's dense SVD.

We ran the method again on some of the matrices on which it failed to converge in 100,000 iterations, allowing the method to run longer. It converged in all cases. For example, on `nos1`, the method detected convergence after 169,791 iterations. The σ_{\min} estimate it returned was actually from iteration 90,173, which means that at iteration 100,000, it actually converged, but the algorithm was not yet able to detect convergence. We note that `nos1` is a square matrix of dimension 237; the method can be slow even on small matrices. Figure 12 presents histograms of the dense-SVD condition numbers of matrices on which our method converged or did not converge. The histograms show that our method can fail to converge (in 100,000 iterations) on both well-conditioned and ill-conditioned matrices. It also appears that full-rank ill-conditioned matrices are more likely to cause our method difficulties than either well-conditioned or rank-deficient matrices.

We remark that one clearly sees the effect of inexact arithmetic in these experiments. Since LSQR on an $m \times n$ matrix is equivalent to CG on an $n \times n$ matrix, with exact arithmetic, our method's iteration count should never exceed the dimension. In practice, we see that the number of iterations may well exceed the dimension (e.g., the `nos1` matrix). This is because of the loss of orthogonality due to floating-point rounding.

The running time of our method obviously varies a lot and is not easy to characterize. However, on large matrices, it is often much faster than dense SVD, as shown in Figure 11.

6.4 | Experiments on large real-world matrices

We ran the algorithm on a few very large matrices from the same matrix collection. As on the smaller matrices, the method sometimes converged, although, sometimes, it exceeded the maximal number of iterations (up to 1,000,000). Table 1 shows a sample of the statistics of successful runs; they indicate that when the singular spectrum is clustered, the method works well even on very large matrices.

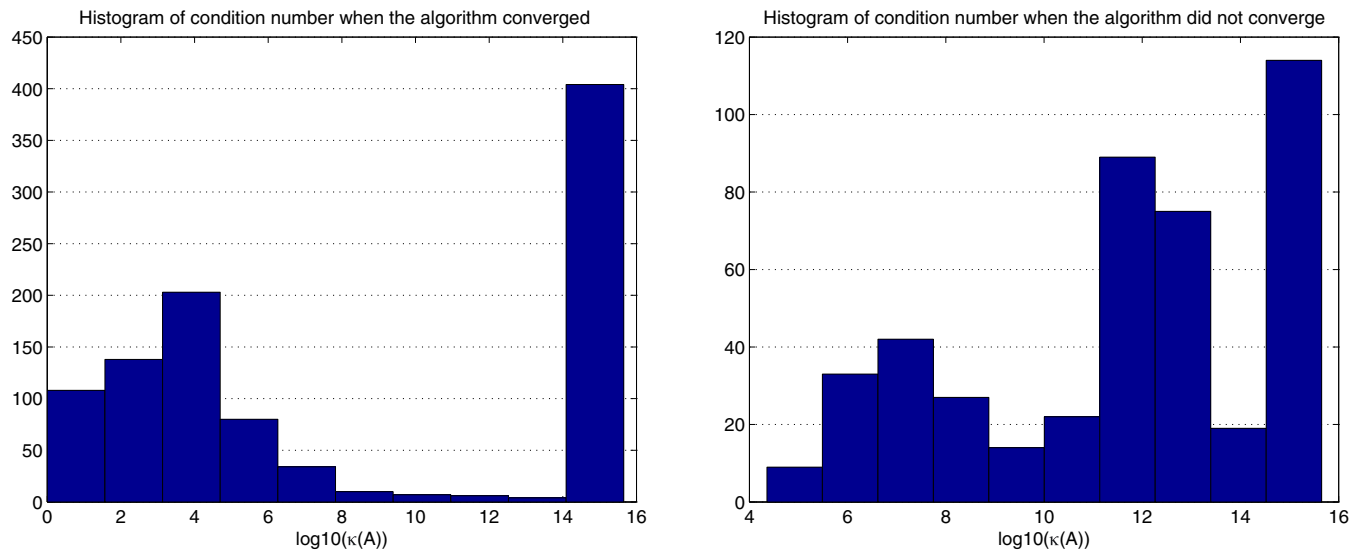


FIGURE 12 Histogram of the condition number of matrices on which our algorithm converged (left) and did not converge (right)

TABLE 1 Large real-world matrices whose condition number was successfully computed by our method. Matrices with an underline indicate a structurally rank-deficient matrix or a matrix indicated in the matrix collection as numerically rank deficient

	<i>m</i>	<i>n</i>	time (s)	condest it. (#mv)	κ (est.)	irlba		PRIMME	
						#mv	κ (est.)	#mv	κ (est.)
rajat10	30,202	30,202	3.7	3,017 (6,634)	1.1e+03	43,016	1.3e+03	5,248	1.3e+03
flower_7_4	67,593	27,693	0.6	129 (858)	1.5e+01	104	2.0e+01	402	1.9e+01
flower_8_4	125,361	55,081	3.2	648 (1,896)	2.8e+13	4,584	2.4e+16	3,556	3.7e+00
<u>wheel_601</u>	902,103	723,605	358	5,260	1.3e+14	FAIL		FAIL	
<u>Franz11</u>	47,104	30,144	0.3	73 (746)	∞	712	3.3e+16	528	4.9e+00
lp_ken_18	154,699	105,127	10	2,234 (5,068)	2.5e+14	169,096	5.7e+16	24,832	6.5e+02
lp_pds_20	108,175	33,874	3.3	848 (2,296)	1.4e+14	7,304	2.8e+16	6,178	6.8e+00
cage15	5,154,859	5,154,859	162	73 (746)	1.1e+01	72	1.2e+01	92	1.2e+01
atmosmodl	1,489,752	1,489,752	663	6,699 (13,998)	8.5e+02	662,536	1.1e+03	15,546	1.1e+03
Rucci1	1,977,885	109,900	2,194	20,576 (41,752)	6.5e+03	1,728,264	6.8e+03	28,604	6.8e+03
LargeRegFile	2,111,154	801,374	146	1,304 (3,208)	1.0e+04	21,032	1.1e+04	4,886	1.1e+04
sls	1,748,122	62,729	119	848 (2,296)	9.7e+02	8,296	1.3e+03	3,218	1.3e+03

We also attempted to approximate the condition number using two singular value solvers: irlba³⁰ and PRIMME.¹⁰ Both are general-purpose singular value solvers; thus, in order to make a fair comparison with our algorithm (which is designed for condition-number estimation), we judiciously chose the stopping criteria. From PRIMME, we use the library's option to supply special convergence criteria and stop the method once the residual has dropped below 10% the current estimate of σ_{\min} . For irlba, we set the code's convergence tolerance to 10^{-15} when our code detected rank deficiency, and to $1/\kappa_{\text{est}}$ otherwise, where κ_{est} is the condition-number estimate obtained using our method (of course, this stopping criterion cannot be used in practice, and we use it only for the sake of empirical evaluation). For both algorithms, we restrict the number of iterations to 100,000. Since the different libraries are implemented in different languages (irlba and our algorithm are implemented in MATLAB, whereas PRIMME does most of the work in C), we measure only the number of matrix–vector products. For the matrices reported in Table 1, unless the matrix is very well conditioned, our algorithm clearly outperforms irlba. As for PRIMME, when the condition number is not too large, PRIMME tends to require less matrix–vector products. However, PRIMME fails to detect very ill-conditioned matrices.

7 | SUMMARY

We have presented an adaptation of LSQR to the estimation of the condition number of matrices.

Our method is yet another tool in the spectral condition-number estimation toolbox. It relies almost solely on matrix–vector multiplications; thus, it can be applied to very large sparse matrices. It does not require much memory, and it is at least as fast as a single application of unpreconditioned LSQR to solve a least squares problem. The method never returns an overestimate of the condition number.

In many cases, the method is orders of magnitude faster than competing methods, especially if A is large and has no sparse triangular factorization.

However, the performance of the method depends on the distribution of the singular values of A , and some distributions lead to very slow convergence. When convergence is slow or nonexistent, the method still provides a lower bound on the condition number, but it may be loose. In such cases, methods that are based on orthogonal or triangular factorizations or on preconditioned iterative solvers may be faster.

Our method is primarily based on one known property: that the forward error in LSQR tends to converge to an approximate singular vector associated with σ_{\min} . This property of LSQR and related Krylov-subspace solvers is normally seen as a deficiency (because it slows down the convergence to the minimizer), but it turns out to be beneficial for condition-number estimation.

We have not explored whether a similar technique can be used in other least squares Krylov methods, such as LSMR,³¹ MINRES,³² and MINRES-QLP.³³

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