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Verified bounds for singular values, in particular for the spectral norm of a matrix and its inverse

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Abstract The singular value decomposition and spectral norm of a matrix are ubiquitous in numerical analysis. They are extensively used in proofs, but usually it is not necessary to compute them. However, there are some important applications in the realm of verified error bounds for the solution of ordinary and partial differential equations where reasonably tight error bounds for the spectral norm of a matrix are mandatory. We present various approaches to this together with some auxiliary useful estimates.

Keywords Spectral norm · Verification · Error bounds · Condition number · INTLAB

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1 Introduction

The spectral norm of a matrix is ubiquitous in numerical analysis. In particular the singular value decomposition $A = U\Sigma V^T$ reveals most important properties of A,

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from the condition number over the distance to singularity to the solution of a linear or, in case of a rectangular matrix, underdetermined or least squares problem.

The singular value decomposition is indispensable for theoretical considerations, however, it is hardly computed in practice. The same applies, *mutatis mutandis* to the largest or smallest singular value, i.e. the spectral norm of a matrix or its inverse, respectively.

But there are some important applications where rigorous bounds for the extreme singular values are necessary. The apparently only known method [15] for computing rigorous error bounds for the solution of a large linear system $Ax = b$ with sparse matrix requires a rigorous lower bound for the smallest singular value of A. This was also used in the computation of verified error bounds for elliptic problems, see [9, 10]. Moreover, in the course of rigorous error bounds for the solution of other ordinary and partial differential equations [11, 19, 21, 22, 25, 27] a rigorous upper bound for the spectral norm is needed.

The better the accuracy of the bound for the singular values in both cases, the narrower the computed error bounds for the solution of the linear system or the partial differential equation. The first problem is addressed in [15] and [18]; in the following we derive some methods to compute rigorous and tight upper bounds for $\|A\|_2$.

This paper elaborates the details on an idea mentioned in the author's overview article to be published in Acta Numerica [19] on verification methods.

If not denoted otherwise, throughout the paper a norm $\|\cdot\|$ will denote the spectral norm $\|\cdot\|_2$. Singular values of a matrix $A \in \mathbb{K}^{m\times n}$ are denoted by $\sigma_1(A) \geq \cdots \geq \sigma_k(A)$, where $k := \min(m,n)$ and $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, and the Moore-Penrose inverse of A is denoted by A^+. Furthermore, $I_{m,n}$ denotes the left upper $m \times n$ submatrix of the identity matrix of dimension $\max(m,n)$. Mostly the dimension is clear from the context and we just use I without indices. We write $A \succ 0$ ($A \succeq 0$) to denote that a square symmetric (Hermitian) matrix A is positive (semi-)definite.

2 Some useful estimates

Let square $E \in \mathbb{K}^{n\times n}$ be given, and suppose $\|E\| \leq \alpha < 1$. A standard estimate to be found in every textbook on numerical computations [13] or matrix algorithms [5, 20] is

$$\|(I+E)^{-1}\| \leq \frac{1}{1-\alpha}. \tag{2.1}$$

The standard proof uses $(I+E)^{-1} = I - E + E^2 - \cdots$, so that $\|(I+E)^{-1}\| \leq 1 + \alpha + \alpha^2 \cdots = (1-\alpha)^{-1}$.

Following we extend this to a result with a simple proof which is surely known but, in our opinion, gives more insight into the matter. The only we need is the well-known fact (Theorem 3.3.16 in [7]) that

$$A, E \in \mathbb{K}^{m\times n} \quad \Rightarrow \quad |\sigma_i(A+E) - \sigma_i(A)| \leq \|E\| \quad \text{for } 1 \leq i \leq \min(m,n). \tag{2.2}$$

Note that the i-th singular values of $A+E$ and A match up to $\|E\|$, no reordering is necessary. Setting $A := I$ it follows for not necessarily square $E \in \mathbb{K}^{m\times n}$ and

$\|E\| \le \alpha$ that for all $1 \le i \le \min(m, n)$

$$1 - \alpha \le \sigma_i(I + E) \le 1 + \alpha. \tag{2.3}$$

If, in addition, $\alpha < 1$, then $I + E$ has full rank and the singular values of the pseudoinverse $(I + E)^+$ are the reciprocals of the singular values of $I + E$, so that

$$\frac{1}{1+\alpha} \le \sigma_i((I + E)^+) \le \frac{1}{1-\alpha}. \tag{2.4}$$

In other words, for small α, the unit ball is mapped, as expected, by $I + E$ or $(I + E)^+$ into an ellipsoid with half-axes not far from 1, and this idea is quantified in (2.3) and (2.4).

In particular it follows for square E that

$$\frac{1}{1+\alpha} \le \|(I + E)^{-1}\| \le \frac{1}{1-\alpha}. \tag{2.5}$$

Along the same lines we provide more details for another standard estimate, where in numerical textbooks [13] only the second inequality of (2.7) is given.

Lemma 2.1 *Let $A, R \in \mathbb{K}^{n\times n}$ be given, and suppose $\|I - RA\| \le \alpha < 1$. Then A and R are nonsingular, and*

$$\frac{\sigma_i(R)}{1+\alpha} \le \sigma_i(A^{-1}) \le \frac{\sigma_i(R)}{1-\alpha} \tag{2.6}$$

for all $1 \le i \le n$. In particular,

$$\frac{\|R\|}{1+\alpha} \le \|A^{-1}\| \le \frac{\|R\|}{1-\alpha}. \tag{2.7}$$

Proof We use the following multiplicative bound for singular values, see (Theorem 3.3.16 in [7]):

$$A, B \in \mathbb{K}^{m\times n} \quad \Rightarrow \quad \sigma_i(AB) \le \sigma_i(A)\|B\| \quad \text{for } 1 \le i \le \min(m, n). \tag{2.8}$$

Since the singular values and the spectral norm do not change under transposition, it follows

$$\sigma_i(AB) \le \|A\|\sigma_i(B)$$

as well. Applying this to $R = (I - (I - RA)) \cdot A^{-1}$ and using the right inequality in (2.3) gives the left inequality in (2.6), and applying (2.8) to $A^{-1} = (I - (I - RA))^{-1} \cdot R$ and using the right inequality in (2.5) proves the right inequality in (2.6). □

Again, we gain the insight that all singular values of A^{-1} and R cannot be too far apart, quantified by two-sided inequalities.

Lemma 2.1 suggests a generalization to rectangular matrices: the inequalities in (2.6) should remain true for the pseudoinverse A^+ of $A \in \mathbb{K}^{m\times n}$ with $R \in \mathbb{K}^{n\times m}$ with $m \le n$ and $\|I - RA\| \le \alpha < 1$. However, this is not true since there may be matrices R so that RA is of full rank and equal to the identity matrix and thus $\|I - RA\| = 0$, but R (and its singular values) are different from A^+ (and its singular values). An example is

$$A = \begin{pmatrix} 2 & -1 \\ -1 & 1 \\ 1 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \quad \text{with } I - RA = 0 \quad \text{but}$$

$$A^+ = \frac{1}{3}\begin{pmatrix} 1 & 1 & 2 \\ 0 & 3 & 3 \end{pmatrix}.$$

The above observations can be applied to matrices not too far from orthogonality, in this case also for rectangular matrices. More precisely, we quantify that the singular values of X cannot be far from 1, and those of X^H and X^{-1} cannot be too far apart provided $\|I - X^H X\|$ is small enough.

Lemma 2.2 *Let $X \in \mathbb{K}^{m \times n}$ be given, and suppose $\|I - X^H X\| \le \alpha < 1$. Then $m \ge n$, X has full rank, and*

$$\sqrt{1-\alpha} \le \sigma_i(X) \le \sqrt{1+\alpha} \quad \textit{and} \quad \frac{1}{\sqrt{1+\alpha}} \le \sigma_i(X^+) \le \frac{1}{\sqrt{1-\alpha}} \tag{2.9}$$

for all $1 \le i \le n$. In particular,

$$\sqrt{1-\alpha} \le \|X\| \le \sqrt{1+\alpha} \quad \textit{and} \quad \frac{1}{\sqrt{1+\alpha}} \le \|X^+\| \le \frac{1}{\sqrt{1-\alpha}}. \tag{2.10}$$

Proof The assertions $m \ge n$ and that X has full rank are obvious from the singular value decomposition of X, and observing

$$\sigma_i(X)^2 = \sigma_i(X^H X) = \sigma_i\big(I - (I - X^H X)\big)$$

and applying (2.3) and (2.4) proves the result. □

3 Bounds for the spectral norm

In the following we will describe four methods to compute bounds for the spectral norm of a matrix. The first three methods deliver very accurate bounds, often to the last bit; however, they rely on a singular or eigendecomposition of the matrix and are thus only suited for full matrices. Also all three methods require quite an amount of computing time.

In contrast, the fourth method is very fast and suited for (large and) sparse matrices, however, the bounds are less accurate. All methods simplify if the matrix is symmetric or Hermitian.

We concentrate on upper bounds because any nontrivial vector x implies a lower bound $\|Ax\|/\|x\|$ for $\|A\|$. Few power set iterations on $A^H A$ usually suffice for this. More precisely, for any $0 \neq x \in \mathbb{R}^n$ and $0 < \lambda \in \mathbb{R}$, the interval

$$X := \{\ell \in \mathbb{R} : |\ell - \lambda| \leq \|A^H(Ax) - \lambda^2 x\|^{1/2}\} \tag{3.1}$$

contains a singular value of A. Although it may be likely that power iterations on $A^H A$ yield an approximation λ^2 for the square of the largest singular value of A, so that X contains $\|A\|$, there is no proof for that. This is the task of this paper.

Immediate upper bounds for $\|A\|_2$ are the Frobenius norm $\|A\|_F = \sqrt{\sum_{ij} a_{ij}^2}$ and $\sqrt{\|A\|_1 \|A\|_\infty}$. However, both can be weak up to a factor $\sqrt{n}$. A less used bound is

$$\|A\| \leq \| \, |A| \, \| \tag{3.2}$$

for real or complex A, which follows by $\|Ax\| \leq \| \, |A||x| \, \|$ and $\| \, |x| \, \| = \|x\|$. A tight bound of $\|B\|$ for nonnegative B is obtained as follows. We have

$$\|B\|^2 = \|B^T B\| = \varrho(B^T B)$$

for ϱ denoting the spectral radius. But with B, also $B^T B$ is nonnegative, so Collatz' Theorem [1] in Perron-Frobenius Theory yields

$$\|B\|^2 \leq \max_i \frac{(B^T(Bx))_i}{x_i} \quad \text{for every positive vector } x. \tag{3.3}$$

Few power set iterations starting with $(1) \in \mathbb{R}^n$, the vector of 1's, gives an accurate upper bound on $\|B\|$. As is known [24], the bound improves monotonically in each step. Note that for nonnegative B and $x = (1)$, the bound in (3.3) is $\|B^T B\|_\infty$.

However, the amount of overestimation by (3.2) may also be a factor of $\sqrt{n}$ as by

$$\begin{aligned} \|A\|_2^2 &= \varrho(A^H A) \leq \varrho(|A^H A|) \leq \varrho(|A^H| \cdot |A|) = \| \, |A| \, \|_2^2 \\ &\leq \| \, |A|^H \|_1 \cdot \| \, |A| \, \|_\infty = \|A\|_\infty^2 \leq n \cdot \|A\|_2^2, \end{aligned} \tag{3.4}$$

and, as noted by Ludwig Elsner [4], the upper bound is sharp for Hadamard or Fourier matrices.[1] The proof in (3.4) uses $\varrho(A) \leq \varrho(B)$ if $A \leq |B|$ as by Perron-Frobenius Theory, and $\|A\|_\infty \leq \sqrt{n}\|A\|_2$. Numerical evidence suggests that for all bounds the overestimation is, in general, not far from $\sqrt{n}/2$.

To compute tight bounds of $\|A\|$ for general matrix A we start, for didactical reasons, with the weakest, but most obvious approach.

The singular value decomposition is a stable algorithm (in the backward sense), thus $A \approx U \Sigma V^H$ computed in floating-point gives accurate approximations Σ_{ii} (relative to $\sigma_1(A)$) for the singular values $\sigma_i(A)$. Rigorous error bounds and our first method to bound the spectral norm are obtained by Lemma 2.2 as follows. We state the result for square matrices and note that it is immediately extended to rectangular matrices.

[1] Thanks to Ludwig Elsner for pointing to these examples. We do not know whether the upper bound is also sharp for real matrices of those dimensions, for which no Hadamard matrix exists.

Theorem 3.1 *Let $A, U, V \in \mathbb{K}^{n\times n}$ be given, and define $\Sigma := U^H AV$. Assume*

$$\|I - U^H U\| \le \alpha < 1 \quad \text{and} \quad \|I - V^H V\| \le \beta < 1. \tag{3.5}$$

Furthermore, define $D, E \in \mathbb{K}^{n\times n}$ so that $\Sigma = D + E$ and D is diagonal. Then there is a numbering $\nu : \{1, \dots, n\} \to \{1, \dots, n\}$ with

$$\frac{|D_{ii}| - \|E\|}{\sqrt{(1+\alpha)(1+\beta)}} \le \sigma_{\nu(i)}(A) \le \frac{|D_{ii}| + \|E\|}{\sqrt{(1-\alpha)(1-\beta)}} \tag{3.6}$$

for all $1 \le i \le n$. In particular,

$$\|A\| \le \frac{\max_i |D_{ii}| + \|E\|}{\sqrt{(1-\alpha)(1-\beta)}}. \tag{3.7}$$

Remark It looks like a vicious circle that estimates of the spectral norms of $I - U^H U$, $I - V^H V$ and E are needed to estimate the norm of A. However, the former norms can be expected to be rather small, so a crude estimate suffices to obtain an accurate result.

Proof of Theorem 3.1 For $A, B \in \mathbb{K}^{n\times n}$ with nonsingular B apply (2.8) to $AB \cdot B^{-1}$ to obtain

$$\frac{\sigma_i(A)}{\|B^{-1}\|} \le \sigma_i(AB) \le \sigma_i(A)\|B\| \tag{3.8}$$

for $1 \le i \le n$. Applying (3.8) to $\Sigma \cdot V^{-1}$ and $U^{-H} \cdot (\Sigma V^{-1}) = A$ and using (2.10) implies

$$\frac{\sigma_i(\Sigma)}{\sqrt{(1+\alpha)(1+\beta)}} \le \sigma_i(A) \le \frac{\sigma_i(\Sigma)}{\sqrt{(1-\alpha)(1-\beta)}}, \tag{3.9}$$

and (2.2) proves the result. □

If A is symmetric or Hermitian, we can directly compute an eigen-decomposition and obtain the following

Corollary 3.1 *Let $A, V \in \mathbb{K}^{n\times n}$ be given, assume $A^H = A$, and define $\Sigma := V^H AV$. Assume*

$$\|I - V^H V\| \le \alpha < 1. \tag{3.10}$$

Furthermore, define $D, E \in \mathbb{K}^{n\times n}$ so that $\Sigma = D + E$ and D is diagonal. Then there is a numbering $\nu : \{1, \dots, n\} \to \{1, \dots, n\}$ with

$$\frac{|D_{ii}| - \|E\|}{1+\alpha} \le \sigma_{\nu(i)}(A) \le \frac{|D_{ii}| + \|E\|}{1-\alpha} \tag{3.11}$$

for all $1 \le i \le n$. In particular,

$$\|A\| \le \frac{\max_i |D_{ii}| + \|E\|}{1-\alpha}. \tag{3.12}$$

Theorem 3.1 and Corollary 3.1 establish our first method to bound the spectral norm. For the practical application we need several observations. In particular we have to discuss the inevitable presence of rounding errors. A very simple way to deal with this is using interval arithmetic, particularly by INTLAB [16], the Matlab toolbox for reliable computing. Most of our results are given in executable INTLAB code. For details on interval arithmetic, see [12].

First, an inclusion of $U^H AV$ is computed by

```
[U,S,V] = svd(A);
Sigma = U'*(A*intval(V));
```

The type concept forces `A*intval(V)` to be computed in interval arithmetic with interval matrix result, so that `Sigma` is an inclusion of the matrix $U^H AV$. To proceed we have to deal with all (real or complex) matrices included in the interval matrix `Sigma`$\in \mathbb{IK}^{n\times n}$. This is done as follows. The statements

```
M = mid(Sigma);
R = rad(Sigma);
```

compute matrices with floating-point entries such that, using entrywise comparison, for all $S \in$ `Sigma`,

$$\mathtt{M} - \mathtt{R} \leq S \leq \mathtt{M} + \mathtt{R},$$

so that

$$|\sigma_i(S) - \sigma_i(\mathtt{M})| \leq \|\mathtt{R}\|.$$

Note that `M` is real or complex, whereas `R` is real and nonnegative. The spectral norm of `R` is estimated by (3.3).

Similarly, bounds α and β satisfying (3.5) are computable. The corresponding programs are included in INTLAB. The matrices D and E are computed by

```
D = diag(diag(M));
E = M - D;
```

Estimating $\|\mathtt{E}\|$ as before yields the desired bounds for $\|A\|$.

A matrix product costs $2n^3$ operations in general, however, $V^T V$ can be computed in n^3 floating-point operations using symmetry. In the following we refer to the number of operations by Matlab routines, which is $2n^3$ for $V^T V$ because the symmetry is not used.

Moreover we need to compute bounds for the product of two floating-point matrices (resulting in an interval matrix), and the product of a floating-point and an interval matrix. Both are implemented using midpoint-radius arithmetic [17] in INTLAB, where the conversion from infimum-supremum to midpoint-radius representation uses Oishi's trick [14].[2] Then the former product requires 2, and the latter product requires 3 (ordinary) matrix multiplications.

[2]Denote by $\nabla(\cdot)$ and $\Delta(\cdot)$ the result obtained by executing *all* operations within the parenthesis in rounding downwards and rounding upwards, respectively. Then $[\nabla(A\cdot B), \Delta(A\cdot B)]$ is an inclusion of the true (real) product $A\cdot B$ of two floating-point matrices A, B. For $A \in \mathbb{F}^{n\times n}$ and an interval matrix $\langle mB, rB\rangle = \{B \in \mathbb{R}^{n\times n} : mB - rB \leq B \leq mB + rB\}$ an inclusion of their product is $[\nabla(A\cdot mB - rC), \Delta(A\cdot mB + rC)]$ using $rC := \Delta(|A|\cdot rB)$. For details see [17] or [12].

Hence the total computational cost using Theorem 3.1 for general real matrix A is $39n^3 + \mathcal{O}(n^2)$ divided into

$$\begin{aligned}
21n^3 &\ \text{ full singular value decomposition,}\\
8n^3 &\ \text{ inclusions of } U^T U \text{ and } V^T V \text{ to bound } \alpha, \beta,\\
4n^3 &\ \text{ inclusion of } B := AV,\\
6n^3 &\ \text{ inclusion of } U^T B,
\end{aligned}$$

whereas for symmetric A using Corollary 3.1 the cost is $18n^3 + \mathcal{O}(n^2)$ divided into

$$\begin{aligned}
4n^3 &\ \text{ eigen-decomposition,}\\
4n^3 &\ \text{ inclusions of } V^T V \text{ to bound } \alpha,\\
4n^3 &\ \text{ inclusion of } B := AV,\\
6n^3 &\ \text{ inclusion of } V^T B.
\end{aligned}$$

We mention that $\|I - U^T U\|$ and $\|I - V^T V\|$ can be estimated by standard a priori estimates [5]. For general matrix A it is superior to use the following, which will be the basis for our second and third method.

Theorem 3.2 *Let $A, V \in \mathbb{K}^{n\times n}$ be given, and define $B := AV$. Assume*

$$\|I - V^H V\| \le \alpha < 1. \tag{3.13}$$

Furthermore, define $D, E \in \mathbb{K}^{n\times n}$ so that $B^H B = D + E$ and D is diagonal. Then there is a numbering $\nu : \{1, \dots, n\} \to \{1, \dots, n\}$ with

$$\sqrt{\frac{D_{ii} - \|E\|}{1+\alpha}} \le \sigma_{\nu(i)}(A) \le \sqrt{\frac{D_{ii} + \|E\|}{1-\alpha}} \tag{3.14}$$

for all $1 \le i \le n$. In particular,

$$\|A\| \le \sqrt{\frac{\max_i D_{ii} + \|E\|}{1-\alpha}}. \tag{3.15}$$

Proof For $1 \le i \le n$ we have $\sigma_i(AV) = \sqrt{\sigma_i(B^H B)}$ and $|D_{ii} - \big(\sigma_{\nu(i)}(AV)\big)^2| \le \|E\|$ for a suitable numbering ν. Applying (3.8) to AV and $AV \cdot V^{-1}$ and using (2.10) shows

$$\frac{\sigma_j(AV)}{\sqrt{1+\alpha}} \le \sigma_j(A) \le \frac{\sigma_j(AV)}{\sqrt{1-\alpha}}$$

for $1 \le j \le n$. Using (2.2) proves the result. □

In the practical application, V is an approximation to the matrix of right singular vectors of A. Note that this implies that $B = AV \approx U\Sigma$, so that $B^H B$ is close to a diagonal matrix.

There are two ways to obtain V. First, a simplified singular value decomposition can be used, and second by a symmetric (Hermitian) eigen-decomposition of $A^H A$. Then one proceeds as before to compute an upper bound for $\|A\|$. This establishes our second and third method.

The computational costs for real matrix A using the simplified singular value decomposition are $28n^3 + \mathcal{O}(n^2)$ divided into

$$\begin{aligned} 12n^3 &\ \text{ simplified singular value decomposition,} \\ 4n^3 &\ \text{ inclusion of } V^T V \text{ to bound } \alpha, \\ 4n^3 &\ \text{ inclusion of } B = AV, \\ 8n^3 &\ \text{ inclusion of } B^T B, \end{aligned}$$

whereas using the eigen-decomposition of $A^T A$ takes $18n^3 + \mathcal{O}(n^2)$ divided into

$$\begin{aligned} 2n^3 &\ \text{ approximate computation of } A^T A, \\ 4n^3 &\ \text{ eigen-decomposition of } A^T A, \\ 4n^3 &\ \text{ inclusion of } B = AV, \\ 8n^3 &\ \text{ inclusion of } B^T B. \end{aligned}$$

In all approaches up to now the matrix V of right singular vectors of A occurs. This means that neither approach is applicable to sparse matrices because V will, in general, be a full matrix. The following, fourth and final method works for sparse matrices as well.

This approach is based on verifying positive definiteness of a given matrix. Such methods were originally developed to solve systems of sparse linear equations. In [15] we perform for given symmetric (Hermitian) A and for some positive s an (approximate) Cholesky decomposition of a shifted matrix

$$B := A - 2sI \approx G^H G \quad \text{and} \quad E := G^H G - B. \tag{3.16}$$

It follows that

$$|\lambda_i(B) - \lambda_i(G^H G)| \le \|E\|.$$

Since $G^H G$ is positive semidefinite we have $\lambda_n(B) \ge -\|E\|$, and, provided $s \ge \|E\|$, it follows

$$\lambda_n(A) = 2s + \lambda_n(B) \ge 2s - \|E\| \ge s > 0 \quad \text{implying} \quad \sigma_{\min}(A) = \lambda_n(A) \ge s.$$

For the residual $G^H G - B$ error bounds are computed by interval arithmetic.

In [2], see also [6], Demmel proved that if the Cholesky decomposition applied to a real symmetric matrix A runs to completion, and if during the execution no overflow and underflow occurs, then the computed Cholesky factor $\tilde{G}$ satisfies

$$\tilde{G}^T \tilde{G} = A + \Delta A \quad \text{with } |\Delta A| \le \frac{\gamma_{n+1}}{1 - \gamma_{n+1}} dd^T, \tag{3.17}$$

where $d_i = a_{ii}^{1/2}$ and $\gamma_k := k\mathrm{eps}/(1-k\mathrm{eps})$. Here eps denotes the relative rounding error unit which is about 10^{-16} in double precision IEEE 754 [8].

In [18] we use this idea to show that if the Cholesky decomposition of a symmetric or Hermitian matrix executed in pure floating-point runs to completion, then there is an a priori lower bound for the smallest eigenvalue, which is roughly $-p \cdot \mathrm{eps} \cdot \mathrm{trace}(A)$ for p denoting the average number of nonzero off-diagonal elements per row. Our estimate is also valid in the presence of underflow.

Applying this to a shifted matrix $A - sI$ yields algorithm `isspd` (see [18]), which is now included in INTLAB, to prove positive definiteness of a matrix: if `isspd(A)` yields the result 1, it is proved that A is positive definite, if the result is 0, nothing can be said. Algorithm `isspd` is particularly fast because it uses only floating-point arithmetic.

Let $A \in \mathbb{K}^{n\times n}$ be given. Obviously, $A^H A$ is positive semidefinite, and $\|A^H A\| = \|A\|^2$. Let $\tilde{\alpha}$ be an approximation of $\|A\|$, and define $\alpha := (1+e)\tilde{\alpha}$ for $e > 0$. Then

$$\alpha^2 I - A^H A \succeq 0 \quad \Rightarrow \quad \|A\| \le \alpha. \tag{3.18}$$

If A is symmetric or Hermitian, then the singular values coincide with the absolute values of the eigenvalues. This means

$$A^H = A\colon \quad \alpha I - A \succeq 0 \quad \text{and} \quad \alpha I + A \succeq 0 \quad \Rightarrow \quad \|A\| \le \alpha. \tag{3.19}$$

One may argue that often it is not advisable to use $A^H A$. For example, least squares problems are sometimes solved using normal equations; however, this squares the condition number and is sometimes much worse than to orthogonalize the system [23]. In our case this argument does not apply. The condition number of $\alpha^2 I - A^H A$ is the important quantity. Suppose $\tilde{\alpha} = \|A\|$ and $\alpha^2 I - A^H A$ is positive semidefinite for $\alpha := (1+e)\tilde{\alpha}$. Then, regardless how large the condition number of A is,

$$\mathrm{cond}(\alpha^2 I - A^H A) = \frac{\sigma_1(\alpha^2 I - A^H A)}{\sigma_n(\alpha^2 I - A^H A)} \le \frac{\alpha^2}{(1+e)^2\tilde{\alpha}^2 - \tilde{\alpha}^2} = \frac{(1+e)^2}{(1+e)^2 - 1} \approx \frac{1}{2e} \tag{3.20}$$

for small e. That means for anticipated 6 decimal digits accuracy of the norm bound, the condition number of $\alpha^2 I - A^H A$ is only about $5 \cdot 10^5$, and algorithm `isspd` will have no problem to verify positive definiteness.

This already defines an algorithm to verify an upper bound of the spectral norm of A. However, some care is necessary to obtain an efficient implementation. First, if the input matrix is an interval matrix $\mathbf{A}$, split it into midpoint-radius form $\mathbf{A} = \langle M, R\rangle := \{A : M - R \le A \le M + R\}$ using entrywise and, for complex matrices, partial ordering to obtain[3]

$$\forall A \in \mathbf{A}\colon \quad \|A\| \le \|M\| + \|R\|. \tag{3.21}$$

[3]In INTLAB complex matrices are stored in midpoint-radius format, and for real matrices, stored in infimum-supremum format, the commands `M = mid(A)` and `R = rad(A)` ensure $A \subseteq \langle M, R\rangle$.

Since the radius matrix R is nonnegative we can use (3.3). For the following we may assume $A \in \mathbb{K}^{n\times n}$.

The initial approximation $\tilde{\alpha} \approx \|A\|$ is computed by some power iterations on $A^H A$. A good starting vector is $x^{(0)} := A \cdot (1)$. We then set $\alpha := (1+e)\tilde{\alpha}$ for some positive e aiming to verify $\|A\| \le \alpha$. The value e determines the accuracy of the bound; a value like $e = 10^{-6}$ aims on 6 digits accuracy.

For symmetric or Hermitian A we have to verify, following (3.19), that $\alpha I - A$ and $\alpha I + A$ are positive semidefinite. For a given floating-point number `alpha` the computation of `alpha*speye(n)`[4] causes no rounding error, but the computation of $\alpha I \pm A$ may. But rather than using interval operations (producing an interval matrix to be verified to be positive definite by `isspd`) we use directed rounding. The INTLAB code

```
setround(-1)
B = alpha*speye(n)-A;
setround(0)
```

uses the definition of floating-point arithmetic by IEEE 754 to switch the rounding mode to downwards (towards $-\infty$) to compute a matrix B satisfying $B \le \alpha I - A$, and switches the rounding mode back to nearest. But rounding errors may only occur for the diagonal elements of B, so that

$$B = \alpha I - A - D \quad \text{for nonnegative and diagonal } D.$$

This means that D is positive semidefinite and if `isspd(B)` returns 1 it follows that

$$\alpha I - A \succeq B \succ 0.$$

Proceeding similarly for $\alpha I + A$ defines an algorithm to bound $\|A\|$ for a symmetric (Hermitian) matrix. Note that, according to (3.21) and (2.2), for a given interval matrix $\mathbf{A}$ the norm of all $A \in \mathbf{A}$ is bounded including non-symmetric (-Hermitian) matrices provided the midpoint matrix of $\mathbf{A}$ is symmetric (Hermitian).

Now let non-symmetric (-Hermitian) $A \in \mathbb{K}^{n\times n}$ be given. In this case the product $A^H A$ is calculated in interval arithmetic, and (3.21), (3.3) and the method already described are used to bound $\|A^H A\|$ and thus $\|A\|$.

The computational cost for real symmetric matrices by (3.19) is $\frac{4}{3}n^3 + \mathcal{O}(n^2)$ for the two (floating-point) Cholesky decompositions in algorithm `isspd`, and for general real matrices by (3.18) it is $\frac{14}{3}n^3 + \mathcal{O}(n^2)$ divided into

$$\begin{aligned} 4n^3 &\ \text{ inclusion of } A^T A, \\ 2/3n^3 &\ \text{ Cholesky decomposition in } \texttt{isspd}. \end{aligned}$$

Note that in contrast to the previous methods this is the verification of a sufficient criterion. If the initial approximation is too weak and e too small, α has to be increased and tested again.

Summarizing the computational cost for the four presented methods for general real input matrix are given in Table 1, and for real symmetric matrix in Table 2.

[4] `speye(n)` is the Matlab notation for the sparsely stored $n \times n$ identity matrix.

Table 1 Number of floating-point operations to bound $\|A\|$ for general matrix A

Method	Flops
Theorem 3.1	$39n^3 + \mathcal{O}(n^2)$
Theorem 3.2 using singular values of A	$28n^3 + \mathcal{O}(n^2)$
Theorem 3.2 using eigenvectors of $A^T A$	$20n^3 + \mathcal{O}(n^2)$
the method in (3.18)	$\frac{14}{3}n^3 + \mathcal{O}(n^2)$

Table 2 Number of floating-point operations to bound $\|A\|$ for symmetric matrix A

Method	Flops
Corollary 3.1	$18n^3 + \mathcal{O}(n^2)$
the method in (3.19)	$\frac{4}{3}n^3 + \mathcal{O}(n^2)$

4 Computational results

Following we test the presented routines using Matlab. All tests are performed on a Laptop with Intel Core 2 Duo CPU with 1.6 GHz and 32-bit Windows. Concerning computing times, note that there is some interpretation overhead.

First, we generate general random matrices of different dimension. The accuracy of the four methods listed in Table 1 is of the order 10^{-13} for the first three methods, and about 10^{-6} for the fourth method. Accuracy means the relative error of the midpoint of the inclusion compared with the endpoints.

In Table 3 we list the computing times of the four methods, where the time for the built-in Matlab routine `norm(A)` is normed to 1. As expected by Table 1, the fourth method is the fastest. Note that the simplified version of the singular value decomposition (computing only the right singular vectors) is not available in Matlab, so the third method is slower than expected by the flop-count. For larger dimensions there is not much penalty for the computation of verified error bounds rather than an approximation.

The results for symmetric, Hermitian and for ill-conditioned matrices are very similar, so they are not displayed. Also for interval matrices the results are very similar because the additional effort using (3.21) and (3.3) is negligible.

Finally we tested sparse matrices in the Harwell-Boeing test case library [3]. Selected results for matrices of larger dimension are listed in Table 4, that is the name of the matrix, its dimension, and the ratio of computing time for the verified bound divided by the norm estimation by the Matlab routine `normest`. The tested matrices are real but not necessarily symmetric.

For most matrices there is a reasonable penalty for the verification. The matrix "psmigr2" is exceptional with a density of less than 6%, but with a density of more than 91% for $A^T A$. Occasionally, the verification is faster than the approximation.

The accuracy of both the approximation and the computed bounds is of similar quality in almost all examples, namely about 10^{-6} corresponding to 6 correct decimal figures. In few cases, the verified bounds are a little more accurate than the approximation. For example, for the matrix "bcsstk21" the inclusion $1.273_{11}^{19} \cdot 10^8$ is computed in $\frac{1}{5}$ of the computing time for the approximation $1.272817 \cdot 10^8$. Note

Table 3 Computing times for full matrices, time t for the Matlab routine normed to 1

n	t_1/t	t_2/t	t_3/t	t_4/t
100	10.98	9.81	7.65	3.32
200	9.25	8.66	6.02	1.51
500	13.35	12.79	6.68	1.23
1000	11.16	10.84	5.19	1.14

Table 4 Ratio of computing times for sparse matrices

Matrix	n	$time(verification)/time(estimation)$
bcspwr10	5300	1.1
bcsstk15	3948	1.4
bcsstk16	4884	2.4
bcsstk17	10974	2.0
bcsstk18	11948	2.5
bcsstk21	3600	0.2
bcsstk23	3134	5.4
bcsstk24	3562	0.9
bcsstk25	15439	3.5
bcsstk28	4410	3.4
bcsstk29	13992	0.9
bcsstm21	3600	8.6
bcsstm23	3134	3.9
bcsstm24	3562	1.6
bcsstm25	15439	0.5
cegb3024	3024	0.9
cegb3306	3306	1.3
lshp3025	3025	1.9
lshp3466	3466	2.0
man5976	5976	0.8
psmigr1	3140	46.8
psmigr2	3140	366.7
saylr4	3564	9.1
sherman3	5005	1.7
sherman5	3312	14.8
sstmodel	3345	1.5

that the accuracy of the approximation can only be verified if verified error bounds are known.

5 Application to differential equations

As has been mentioned, bounds for the spectral norm of a matrix or its inverse are needed in the course of the computation of rigorous error bounds for the solution of certain ordinary and partial differential equations [9–11, 19, 21, 22]. More precisely, bounds for the extreme singular values are needed in the following two applications.

Let a two-point boundary value problem of the form

$$\begin{cases} -u'' = ru^N + f, & 0 < x < 1, \\ u(0) = u(1) = 0, \end{cases} \tag{5.1}$$

be given with $N \geq 2$ and $r \in L^\infty$, $f \in L^2$, or an elliptic problem

$$\begin{cases} -\nabla \cdot (a\nabla u) = g(u), & x \in \Omega, \\ u = 0, & x \in \partial\Omega \end{cases} \tag{5.2}$$

for a bounded convex polygonal domain $\Omega \subset \mathbb{R}^n$ for $n \in \{2, 3\}$, for smooth $a(x)$ with $a(x) \geq a_0 > 0$ and Fréchet differentiable $g : H_0^1(\Omega) \to L^2(\Omega)$.

After approximation with some spline functions or some finite element basis functions, a positive definite stiffness matrix D and some matrix G arise. Depending on the application, the matrix G may be symmetric (Hermitian) or not; in any case it has to be verified to be nonsingular.

In order to compute verified bounds for the infinite dimensional problem, in the first example (5.1) an upper bound for the largest (in absolute value) eigenvalue $\lambda_{\max}$ of the matrix eigenvalue problem

$$DG^{-1}DG^{-1}Dv = \lambda Dv \tag{5.3}$$

is necessary [19], where G is symmetric. First note that the eigenvalues of a generalized eigenvalue problem $Av = \lambda Bv$ are real for a Hermitian matrix A and positive definite B. This is because

$$v^H Av = \lambda v^H Bv, \tag{5.4}$$

where $v^H Bv > 0$ because B is positive definite, and the left hand side of (5.4) is real because A is Hermitian. So λ in (5.3) must be real and nonzero. Moreover, λ is an eigenvalue of $(G^{-1}D)^2$, and along the same lines as above one shows $\lambda > 0$. Moreover, because D is positive definite,

$$\lambda' D - DG^{-1}DG^{-1}D \succeq 0 \quad \Leftrightarrow \quad \lambda' \geq \lambda_{\max}. \tag{5.5}$$

So choosing λ' a little larger than an approximation of $\lambda_{\max}$ and verifying that $\lambda' D - DG^{-1}DG^{-1}D$ is positive semidefinite by algorithm `isspd` gives the desired estimate. Note that an inclusion of $G^{-1}D$ is computed by the INTLAB algorithm `verifylss(G,D)`. Note this also verifies the nonsingularity of G.

In the second example (5.2) two problems arise. First, G is symmetric and an upper bound for

$$\alpha := \|L^T G^{-1} L\| \tag{5.6}$$

is needed, where $LL^T = D$ denotes the Cholesky decomposition of D. Here the size of G may be too large to compute an inclusion of the full matrix G^{-1}. For $\Lambda(A)$

denoting the spectrum of A, set

$$\lambda_{\max}(A) := \max\{|\lambda| : \lambda \in \Lambda(A)\} \quad \text{and} \quad \lambda_{\min}(A) := \min\{|\lambda| : \lambda \in \Lambda(A)\}. \tag{5.7}$$

It is known that always

$$\sigma_{\min}(A) \le \lambda_{\min}(A) \quad \text{and} \quad \lambda_{\max}(A) \le \sigma_{\max}(A). \tag{5.8}$$

Then the symmetry of G and using $\Lambda(AB) = \Lambda(BA)$ implies

$$\alpha^2 = \lambda_{\max}(L^T G^{-1} L \cdot L^T G^{-1} L) = \lambda_{\max}((G^{-1}D)^2) = \lambda_{\max}(G^{-1}D)^2 \tag{5.9}$$

or

$$\alpha^{-1} = \lambda_{\min}(D^{-1}G). \tag{5.10}$$

We have

$$\alpha^{-1} = \min\{|\lambda| :\ Gv = \lambda Dv,\ 0 \ne v \in \mathbb{C}^n\}, \tag{5.11}$$

and by (5.4) it follows that $+\alpha^{-1}$ or $-\alpha^{-1}$ is a real eigenvalue of $D^{-1}G$. We show that

$$\beta > 0 \quad \text{and} \quad G - \beta D \succeq 0 \quad \Rightarrow \quad \alpha^{-1} \ge \beta. \tag{5.12}$$

Suppose $\beta > \alpha^{-1}$. Then

$$G + \alpha^{-1} D \succeq G - \alpha^{-1} D = G - \beta D + (\beta - \alpha^{-1}) D \succ 0 \tag{5.13}$$

because D is symmetric positive definite, so that $\pm\alpha^{-1}$ is no eigenvalue of $D^{-1}G$, a contradiction.

It follows $\alpha \le \beta^{-1}$ if $G - \beta D \succeq 0$. The latter can be effectively verified by algorithm `isspd` in INTLAB, also for large and sparse matrices G and D. A suitable value for β is found by purely numerical means, for example some power set iteration.

This approach is applicable if the eigenvalues of $D^{-1}G$, which are real by (5.4), are positive (which is proved a posteriori by the verification). Fortunately, in many applications this is true. If this is not the case, then we use (5.10) to see

$$\alpha^{-2} = \lambda_{\min}(D^{-1}G)^2 \ge \sigma_{\min}(D^{-1}G)^2 = \sigma_{\min}(D^{-1}G^2D^{-1}) = \lambda_{\min}(D^{-2}G^2). \tag{5.14}$$

Now the eigenvalues of $D^{-2}G^2$ are positive, and we proceed as before to show

$$G^2 - \beta D^2 \succeq 0 \quad \Rightarrow \quad \alpha^{-2} \ge \beta. \tag{5.15}$$

It follows $\alpha \le \beta^{-1/2}$ if $G^2 - \beta D^2 \succeq 0$, and the method is again effectively applicable to large and sparse matrices G and D. There is a drawback in the estimation of the smallest eigenvalue by the smallest singular value in (5.14). Fortunately, the effect is small in the application to (5.2). The method can be applied to (5.1) as well. Here, however, the estimate is significantly weaker than (5.5).

Finally, to compute verified bounds for the infinite dimensional problem in the second example for (5.2), G is still symmetric, but an upper bound for

$$\alpha := \|L^T G^{-1} L_1\| \tag{5.16}$$

is necessary, where $L_1 L_1^T = D_1$ is the Cholesky factorization of some other positive definite matrix D_1. We proceed as in (5.9) and obtain

$$\alpha^2 = \lambda_{\max}(L_1^T G^{-1} L \cdot L^T G^{-1} L_1) = \lambda_{\max}(D_1 G^{-1} D G^{-1}) \tag{5.17}$$

and

$$\begin{aligned}\alpha^{-2} &= \lambda_{\min}(G D^{-1} G D_1^{-1}) \ge \sigma_{\min}(G D^{-1} G)\sigma_{\min}(D_1^{-1})\\ &= \frac{\lambda_{\min}(G D^{-1} G)}{\|D_1\|} = \frac{\lambda_{\min}(D^{-1} G^2)}{\|D_1\|}.\end{aligned} \tag{5.18}$$

As before we show

$$G^2 - \beta D \succeq 0 \quad \Rightarrow \quad \lambda_{\min}(D^{-1} G^2) \ge \beta, \tag{5.19}$$

so that $G^2 - \beta D \succeq 0$ proves

$$\alpha \le \sqrt{\frac{\|D_1\|}{\beta}}. \tag{5.20}$$

An upper bound for $\|D_1\|$ is computed by the methods discussed in Sect. 3, so that using algorithm `isspd` the method is effectively applicable for large and sparse matrices G, D and D_1. The only drawback is the underestimation in (5.18) by splitting the minimum singular values. Fortunately, the underestimation is almost negligible in practice.

Following are some computational results for problems arising in eigenvalue excluding methods for infinite dimensional operators [26]. Consider the two-dimensional self-adjoint eigenvalue problem

$$\begin{cases} -\Delta u + \nu(3u_h^2 - 2(a+1)u_h + a)u = \lambda u, & x \in \Omega,\\ u = 0, & x \in \partial\Omega,\end{cases} \tag{5.21}$$

where $\Omega = (0, 1) \times (0, 1)$, ν and a are positive constants, and u_h is an approximate solution of the Allen-Cahn equation

$$\begin{cases} -\Delta u = \nu u(u-a)(1-u), & x \in \Omega,\\ u = 0, & x \in \partial\Omega.\end{cases} \tag{5.22}$$

For parameter values $\nu = 150$ and $a = 0.01$, and u_h being lower and upper branch finite element solutions with linear element functions on a uniform triangular mesh on Ω, rigorous exclusion regions of eigenvalues for (5.21) are computed. Here both the problems (5.6) and (5.18) arise.

Table 5 Bounds for matrix norms in (5.6) and (5.18), time in seconds

Dimension	Bound for $\|L^T G^{-1} L\|$		Bound for $\|L^T G^{-1} L_1\|$	
	Using (5.12)/in [26]	$t_{(5.12)}/t_{[26]}$	Using (5.19)/in [26]	$t_{(5.19)}/t_{[26]}$
81	18.418/18.416	0.0046/0.17	2.656/2.594	0.0033/0.088
841	23.410/23.407	0.0096/5.9	3.268/3.258	0.024/5.9
9,801	24.516/–	0.16/–	3.5902/–	0.57/–
89,401	24.671/–	2.6/–	3.463/–	388/–
998,001	30.98/–	245/–	failed	

In Table 5 we summarize some computational results for our methods proposed in (5.12) and (5.19), and compare it to the method used in [26].

As can be seen, the norm estimate by the previous method in [26] is slightly better than our estimate, however, our methods are much faster. For dimensions 9801 and larger, the previous method was not applicable. Our method computes a verified upper bound of the matrix norm in (5.6) for dimension up to almost 1 million, however, for the matrix norm in (5.18) it fails because the problem is too ill-conditioned. For the large dimension, however, computing time increases significantly due to cache misses.

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