Finding the Smallest Eigenvalue by Properties of Semidefinite Matrices*

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Abstract

We consider the smallest eigenvalue problem for symmetric or Hermitian matrices by properties of semidefinite matrices. The work is based on a floating-point Cholesky decomposition and takes into account all possible computational and rounding errors. A computational test is given to verify that a given symmetric or Hermitian matrix is not positive semidefinite, so it has at least one negative eigenvalue. This criterion helps us to find the smallest eigenvalue and singular value. Computational examples show that these results can be quite accurate.

Keywords: Positive semidefinite, Eigenvalue, Singular value, Cholesky decomposition
AMS subject classifications: 65G20

1 Introduction

If A is symmetric or Hermitian and positive semidefinite ($x^tAx \geq 0 \;\; for \;\; all \;\; x$) then a Cholesky factorization exists, but the theory and computation are more subtle than for positive definite A. In this paper we use a standard Cholesky decomposition to verify that a symmetric (Hermitian) matrix is not positive semidefinite, i.e. has at least one negative eigenvalue. For this work we make small changes in an algorithm that professor Rump applied in his paper "Verification of Positive Definiteness" [6] and also added to INTLAB [5]. Our method is based on standard IEEE 754 floating point arithmetic with rounding to nearest.

Denote by $\mathbb{F}$ ($\mathbb{F}+i\mathbb{F}$) the set of real (complex) floating-point numbers with relative rounding error unit epsand underflow unit eta. In case of IEEE 754 double precision,

$$\mathrm{eps} = 2^{-53}, \;\; \mathrm{eta} = 2^{-1074} \;\; and \;\; \gamma_k = \frac{k\mathrm{eps}}{1-k\mathrm{eps}} \;\; for \;\; k \geq 0$$

most of the properties are proved in [4, 7].
The main computational effort is one floating-point Cholesky decomposition. Using

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standard rounding error analysis, we find a rigorous bound on the smallest eigenvalue of a symmetric or Hermitian matrix. Also we obtain the smallest singular value for a lower triangular matrix L with $\operatorname{diag}(L) \equiv 1$.

2 Notation

Let $A^T = A \in M_n(\mathbb{F})$ or $A^\star = A \in M_n(\mathbb{F} + i\mathbb{F})$. The following algorithm computes the Cholesky factorization ($A = R^T R$).

$$for \quad j = 1 : n$$

$$for \quad i = 1 : j-1$$

$$r_{ij} = \left(a_{ij} - \sum_{k=1}^{i-1} r_{ki}^\star r_{kj} \right) \Big/ r_{ii}$$

$$end$$

$$r_{jj} = \left(a_{jj} - \sum_{k=1}^{j-1} r_{kj}^\star r_{kj} \right)^{1/2}$$

$$end$$

Note that R is upper triangular. In [6] is said the decomposition "runs to completion" if all square roots are real; for analysis see [2, 4]. Now let real $A^T = A \in M_n(\mathbb{F})$ or complex $A^\star = A \in M_n(\mathbb{F} + i\mathbb{F})$ be given, and suppose the Cholesky decomposition executed in floating-point arithmetic runs to completion. This implies $a_{jj} \geq 0$ and $\tilde{r}_{jj} \geq 0$. Note that we do not assume A to be positive semidefinite – underflow may occur. Then we can derive the following improved lower bound for the smallest eigenvalue of A. Rump [6] has proved:

Theorem 2.1 *Let $A^T = A \in M_n(\mathbb{F})$ or $A^\star = A \in M_n(\mathbb{F} + i\mathbb{F})$ be given. Denote the symbolic Cholesky factor of A by $\hat{R}$. For $1 \leq i, j \leq n$ define*

$$s(i,j) := |\{k \in N : 1 \leq k < \min(i,j) \quad and \quad \hat{r}_{ki}\hat{r}_{kj} \neq 0\}|, \tag{1}$$

and denote

$$\alpha_{ij} := \begin{cases} \gamma_{s(i,j)+2} & s(i,j) \neq 0 \\ 0 & otherwise \end{cases}$$

Suppose $\alpha_{jj} < 1$ for all j. With

$$d_j := ((1-\alpha_{jj})^{-1} a_{jj})^{1/2} \quad and \quad M := 3(2n + \max \quad a_{\nu\nu}),$$

define

$$0 \leq \Delta(A) \in M_n(\vec{R}) \quad by \quad \Delta(A)_{ij} := \alpha_{ij} d_i d_j + M eta,$$

Then if the floating-point Cholesky decomposition of A runs to completion, the smallest eigenvalue $\lambda_{min}(A)$ of A satisfies

$$\lambda_{min}(A) > -\|\Delta(A)\|_2.$$

3 Arithmetical Issues

In Theorem 2.1, if the floating-point Cholesky decomposition of A is assumed to run to completion then a lower bound for λ_{min} is obtained. In [6], with this theorem and Corollary (2.4), an algorithm for testing positive definiteness is developed.

In this section, an upper bound for $\lambda_{\min}$ and Theorem 3.1 (floating-point Cholesky decomposition ends prematurely) are used to present an algorithm for testing not positive semidefiniteness. This algorithm is then used to find the smallest singular value of a matrix.

Theorem 3.1 *Let $A^T = A \in M_n(\mathbb{F})$ or $A^\star = A \in M_n(\mathbb{F} + i\mathbb{F})$ be given. Assume that the floating-point Cholesky decomposition of A ends prematurely. Then with the notation of Theorem 2.1,*

$$\lambda_{min} < \|\Delta(A)\|_2. \tag{2}$$

For a proof see [6].

With this result, we can establish the following test in pure floating-point arithmetic. In [6], floating-point subtraction with rounding downwards is used, but rounding upwards can also be used.

We use standard notation for rounding error analysis [4, 6].

Lemma 3.1 *Let $a, b \in \mathbb{F}$ and $c = fl(a \circ b)$ for $\circ \in \{+, -\}$, and define $\varphi = eps(1 + 2eps) \in \mathbb{F}$. Then*

$$fl(c - \varphi|c|) \le a \circ b \le fl(c + \varphi|c|),$$

We know that $\frac{1}{2}eps^{-1}eta$ is the smallest positive normalized floating-point number.
Proof: We use the fact that $fl(a \pm b) = a \pm b$ for $|a \pm b| < \frac{1}{2}eps^{-1}eta$ and

$$fl(a \pm b) = a \pm b(1 + \epsilon_1) \qquad |\epsilon_1| \le eps$$

otherwise.
If directed rounding is available, we can define $\tilde{A} = fl_\Delta(A + cI)$. Otherwise we can avoid directed rounding by using Lemma 3.1 and defining $\tilde{A} \in \mathbb{F}^{n\times n}$ by

$$\tilde{a}_{ij} := \begin{cases} fl(d + \varphi|d|) \quad \text{with} \quad d := fl(a_{ii} + c) & \text{if } i = j \\ a_{ij} & \text{otherwise} \end{cases}$$

where again $\varphi := eps(1 + 2eps) \in \mathbb{F}$. □

Theorem 3.2 *With the notation of Theorem 2.1, assume that $c \in \mathbb{F}$ is given with $\|\Delta(\tilde{A})\|_2 \le c$, where $\tilde{A} \in \mathbb{F}^{n\times n}$ satisfies $\tilde{a}_{ij} = a_{ij}$ for $i \ne j$ and $\tilde{a}_{ii} \ge a_{ii} + c$ for all i. If the floating-point Cholesky decomposition applied to $\tilde{A}$ ends prematurely, then A is not positive semidefinite, i.e. has at least one negative eigenvalue.*

See [6] for a proof of Theorem 3.2.

Better upper bounds for $\|\Delta(A)\|_2$ are obtained by the fact that the nonzero elements of R must be inside the envelope of A. In [6], various bounds with different properties are computed.
For a matrix A with nonzero diagonal, define

$$t_j = j - \min\{i | a_{ij} \ne 0\}. \tag{3}$$

This is the number of nonzero elements above the diagonal in the j-*th* column of A. We have $0 \le t_j \le n-1$ for all j, and the Cholesky decomposition implies

$$s(i,j) \le \min(t_i, t_j) \quad \text{for all } i,\ j.$$

Defining

$$\delta_i = ((1-\beta_i)^{-1}\beta_i a_{ii})^{1/2} \ \ \text{with} \ \ \beta_i := \gamma_{t_i+2},$$

we have $\alpha_{ij} d_i d_j \le \delta_i \delta_j$, and $\delta = (\delta_1, \ldots, \delta_n) \in R^n$, and using Theorem 2.1 yields

$$\|\Delta(A)\|_2 \le \delta^T \delta + nM\text{eta}.$$

This bound requires only $o(n)$ operations. The quality of the bound can be improved by reordering and scaling according to the Van der Sluis Theorem in [4]. With this bound and the theorem in next section, we can computationally verify a symmetric (Hermitian) is not positive semidefinite.

4 Applied Results

In this section we use the next theorem to change algorithm in [6] to another algorithm that returns either "matrix is proved to be not positive semidefinite", or no conclusion. In summary, the algorithm is:

1. $A \leftarrow A + c * \text{speye}(n)$, where speye is the sparse identity matrix, and the computations are done with upward rounding.
2. $[R, p] = \text{chol}(A)$, floating-point Cholesky Decomposition, with appropriate rounding mode.
3. $p \neq 0$, Matrix A is not proved to be positive semidefinite.
4. $p = 0$, positive semidefiniteness could not be verified.

This process helps us to find the smallest eigenvalue of a symmetric(Hermitian) matrix and the smallest singular value of a lower triangular matrix L with $\text{diag}(L) \equiv 1$.

Theorem 4.1 *Let symmetric $A \in M_n(\mathbb{F})$ or Hermitian $A \in M_n(\mathbb{F} + i\mathbb{F})$ be given. With t_j as in (3), define*

$$\beta_i := \gamma_{t_i+2}, \quad \beta_i^{'} := \beta_i(1-\beta_i)^{-1} \ \ \textit{and} \ \ \beta_i^{''} := \beta_i^{'}(1+eps),$$

for $i \in \{1, \ldots, n\}$, assume $\sum_{i=1}^{n} \beta_i^{''} < 1$, and let $c \in \mathbb{F}$ be such that

$$c \ge \left(1 - \sum_{i=1}^{n} \beta_i^{''}\right)^{-1} \left(\sum_{i=1}^{n} \beta_i^{''} a_{ii} + nM\,eta\right). \tag{4}$$

Let $\tilde{A} := fl_{\Delta}(A + cI)$ be the floating-point computation of $A + cI$ with rounding upwards. If the floating-point Cholesky decomposition of $\tilde{A}$ ends prematurely, then the matrix A has at least one negative eigenvalue.

Proof:

$$\delta_i = ((1-\beta_i)^{-1}\beta_i a_{ii})^{1/2} \ \ \text{with} \ \ \beta_i := \gamma_{t_i+2},$$
$$\beta_i^{'} = \beta_i(1-\beta_i)^{-1}$$

Then

$$\|\Delta(A)\|_2 \le \delta^T \delta + nM\text{eta}$$

$$= \sum_{i=1}^{n}[((1-\beta_i)^{-1}\beta_i a_{ii})^{1/2}]^2 + nM\text{eta} = \sum_{i=1}^{n}\beta_i^{'} a_{ii} + nM\text{eta}. \tag{5}$$

Since $\tilde{A} = fl_{\Delta}(A + cI)$, we have $\tilde{a}_{ii} = (a_{ii} + c)(1 + \epsilon_i)$ with $0 \leq \epsilon_i \leq \text{eps}$ for all i, and

$$\sum_{i=1}^{n}\beta_i^{'}(a_{ii} + c)(1 + \epsilon_i) + nM\text{eta} = \sum_{i=1}^{n}\beta_i^{'}\tilde{a}_{ii} + nM\text{eta}.$$

Then, by a little computation and using (5), we have:

$$\beta_i^{''} := \beta_i^{'}(1 + \text{eps}), \qquad \sum_{i=1}^{n}\beta_i^{''} < 1,$$

so

$$\begin{aligned} c &\geq \frac{\sum_{i=1}^{n}\beta_i^{''}a_{ii} + nM\text{eta}}{1 - \sum_{i=1}^{n}\beta_i^{''}} \\ &= \frac{\sum_{i=1}^{n}\beta_i^{'}(1 + \text{eps})a_{ii} + nM\text{eta}}{1 - \sum_{i=1}^{n}\beta_i^{''}} \\ &= \frac{\sum_{i=1}^{n}\beta_i^{'}a_{ii} + nM\text{eta} + \text{eps}\sum_{i=1}^{n}\beta^{'}a_{ii}}{1 - \sum_{i=1}^{n}\beta_i^{''}} \geq \|\Delta(A)\|_2, \end{aligned}$$

and

$$\|\Delta(\tilde{A})\|_2 \leq \sum_{i=1}^{n}\beta_i^{'}(a_{ii} + c)(1 + \text{eps}) + nM\text{eta} \leq c. \tag{6}$$

Now suppose the floating-point Cholesky decomposition of $\tilde{A}$ ends prematurely. Then $\tilde{A} = A + cI + D$ with diagonal $D \geq 0$, and Theorems 3.1 and 3.2 imply

$$\lambda_{min}(A) = \lambda_{min}(\tilde{A} - D) - c \leq \lambda_{min}(\tilde{A}) - c < \|\Delta(\tilde{A})\|_2 - c \leq 0.$$

□

Now we want to find the smallest eigenvalue of a symmetric or Hermitian matrix based on Theorem 4.1. For $s = \|A\|_1$, the matrix $A - sI$ has only nonpositive eigenvalues and $A + sI$ is positive semidefinite. We bisect the interval $[-s, s]$ to find a narrow interval $[s_1, s_2]$ such that Theorem 4.1 verifies existence of at least one negative eigenvalue of $A - s_2I$.
We have $s_1 < \lambda_{min}(A) < s_2$ so $\lambda_{min} \approx \frac{1}{2}(s_1 + s_2)$ and

$$\tilde{a}_{ij} := \begin{cases} \dfrac{s_2 - s_1}{|s_1 + s_2|} & \text{if } s_1, s_2 \neq 0, \\ s_2 - s_1 & \text{otherwise.} \end{cases}$$

For the following, Table 1 shows results on various matrices out of the Harwell-Boeing matrix market. We display the name of the matrix, dimension (n), the total number of nonzero elements (nnz), the smallest eigenvalue $\lambda_{\min}(A)$ and accuracy.
All matrices are normed to $\|A\|_1 \approx 1$ by a suitable power of 2 to have comparable results for different matrices. For some matrices (like "bcsstk24" and "bcsstk25") the smallest eigenvalue is enclosed to almost maximum accuracy, and for some matrices (such as "bcsstk19", "s3rmq4m1" and "s3rmt3m1") the smallest eigenvalue is enclosed to almost minimum accuracy.

Table 1: Accuracy of determination of $\lambda_{min}(A)$

Matrix	n	nnz(A)	$\lambda_{\min}(A)$	accuracy
nos1	237	1017	7.179912×10^{-9}	4.131036×10^{-5}
nos2	957	4137	1.374003×10^{-11}	2.125679×10^{-2}
nos3	960	15844	1.116235×10^{-6}	4.474995×10^{-7}
nos6	675	3255	1.490150×10^{-8}	1.804826×10^{-5}
nos7	729	4617	6.218675×10^{-11}	5.847953×10^{-3}
494bus	494	1666	1.895505×10^{-7}	1.542731×10^{-6}
685bus	685	3249	9.443388×10^{-7}	3.786334×10^{-7}
1138bus	1138	4054	2.683175×10^{-8}	1.185381×10^{-5}
bcsstk08	1074	12960	2.143812×10^{-8}	1.974372×10^{-5}
bcsstk09	1083	18437	3.307233×10^{-6}	1.245038×10^{-7}
bcsstk10	1086	22070	1.589878×10^{-7}	1.870267×10^{-6}
bcsstk11	1473	34241	3.450428×10^{-10}	9.970089×10^{-4}
bcsstk12	1473	34241	3.450428×10^{-10}	9.970089×10^{-4}
bcsstk13	2003	83883	1.631271×10^{-11}	1.639344×10^{-2}
bcsstk14	1806	63454	7.532640×10^{-11}	4.347826×10^{-2}
bcsstk15	3948	117816	1.479874×10^{-11}	1.960784×10^{-2}
bcsstk16	4884	290378	7.101325×10^{-12}	4.347826×10^{-2}
bcsstk17	10974	428650	7.137364×10^{-12}	6.666666×10^{-2}
bcsstk18	11948	149090	2.651683×10^{-13}	5.303367×10^{-13}
bcsstk19	817	6853	1.422774×10^{-12}	2.000000×10^{-1}
bcsstk20	485	3135	4.906076×10^{-13}	9.812153×10^{-13}
bcsstk21	3600	26600	1.679812×10^{-9}	1.886436×10^{-4}
bcsstk22	138	696	1.574716×10^{-6}	2.632306×10^{-7}
bcsstk23	3134	45178	4.129391×10^{-13}	8.258782×10^{-13}
bcsstk24	3562	159910	4.505463×10^{-13}	9.010926×10^{-13}
bcsstk25	15439	252241	4.965233×10^{-13}	9.930466×10^{-13}
bcsstk26	1922	30336	1.734873×10^{-9}	1.840603×10^{-4}
bcsstk27	1224	56126	2.139279×10^{-6}	1.596163×10^{-7}
bcsstk28	4410	219024	3.793892×10^{-10}	7.390983×10^{-4}
bcsstk29	13992	619488	-4.456757×10^{-3}	6.918194×10^{-11}
bcsstk30	28924	2043492	-1.621731×10^{-3}	2.254227×10^{-10}
bcsstk31	35588	1181416	-2.489720×10^{-3}	1.535309×10^{-10}
bcsstk32	44609	2014701	-3.938285×10^{-3}	7.106851×10^{-11}
bcsstm10	1086	22092	-3.930151×10^{-3}	7.484557×10^{-11}
bcsstm12	1473	19659	1.655245×10^{-7}	2.860420×10^{-6}
bcsstm27	1224	56126	-9.092098×10^{-5}	2.896654×10^{-9}
s1rmq4m1	5489	262411	1.131622×10^{-8}	3.356943×10^{-5}
s1rmt3m1	5489	217651	1.131880×10^{-8}	2.633866×10^{-5}
s2rmq4m1	5489	263351	1.849629×10^{-10}	1.605136×10^{-3}
s2rmt3m1	5489	217681	9.233019×10^{-11}	5.128210×10^{-3}
s3dkt3m2	90449	3686223	3.735724×10^{-13}	7.471449×10^{-13}
s3rmq4m1	5489	262943	1.444858×10^{-12}	3.333333×10^{-1}
s3rmt3m1	5489	217669	1.141553×10^{-12}	3.333333×10^{-1}
s3rmt3m3	5357	207123	1.049923×10^{-12}	3.333333×10^{-1}
e40r0000	17281	553216	-1.525591×10^{-7}	2.571163×10^{-6}
fidapm11	22294	617874	-8.589980×10^{-3}	3.659472×10^{-11}
af23560	23560	460598	-1.900918×10^{-2}	2.227833×10^{-11}

Table 2: Accuracy of determination of $\lambda_{min}(H)$

Dimension	$\lambda_{min}(H)$	accuracy	$\lambda_{min}(H) Matlab$
100	4.5333×10^{-13}	9.0665×10^{-13}	-6.9998×10^{-17}
300	3.9548×10^{-13}	7.9096×10^{-13}	-8.2682×10^{-17}
500	2.5571×10^{-13}	5.1142×10^{-13}	-7.4669×10^{-17}
1000	3.6212×10^{-13}	7.2425×10^{-13}	-5.1042×10^{-17}
2000	2.5625×10^{-13}	5.1250×10^{-13}	-7.7758×10^{-17}
3000	3.1393×10^{-13}	6.2785×10^{-13}	-7.0075×10^{-17}

Table 3: Accuracy of determination of $\sigma_{min}(L)$

Dimension	$\sigma_{min}(L)$	accuracy
100	7.243781×10^{-3}	5.396916×10^{-9}
300	4.589570×10^{-3}	2.322655×10^{-8}
500	2.242722×10^{-3}	7.102137×10^{-8}
700	2.285277×10^{-3}	8.117293×10^{-8}
1000	2.007210×10^{-3}	6.279454×10^{-8}
1500	2.046545×10^{-3}	7.242206×10^{-8}
2000	1.310475×10^{-3}	2.069148×10^{-7}
3000	1.426971×10^{-3}	2.138952×10^{-7}
4000	1.379455×10^{-3}	1.325055×10^{-7}
5000	1.229878×10^{-3}	1.900621×10^{-7}

We also used this method to find the smallest eigenvalue of the Hilbert matrix. This matrix is symmetric positive definite and original elements are

$$\tilde{H}_{ij} = \frac{1}{i+j-1},$$

but rounding errors cause Matlab to give us $\lambda_{min}(H) < 0$; see Table 2.

Now we use this work to find the smallest singular value for lower triangular matrix L with $\mathrm{diag}(L) \equiv 1$.

$$L = \begin{pmatrix} 1 & 0 & \dots & & & 0 \\ \star & 1 & 0 & \dots & & 0 \\ \star & \dots & 1 & \dots & \dots & \\ \star & \star & \dots & \dots & 1 & 0 \\ \star & \star & \dots & & \star & 1 \end{pmatrix}, \tag{7}$$

One possibility is to use $A = L^T L$, which is positive semidefinite, and use Theorem 4.1 to calculate the smallest eigenvalue for the matrix A. Doing so, we have:

$$\sigma_{\min}(L) = \sqrt{\lambda_{\min}(A)}, \tag{8}$$

Table 3 shows the results for lower triangular matrices with different rank and prandom elements below the diagonal. For example we could calculate, the smallest singular value for the matrix A with “dimension(A)=5000” to about 7 decimal figures. Table 3 shows that, when the dimension increased, accuracy in the last column decreased.

The disadvantage is that this method is restricted to condition number [1, 3], about 10^8 or 10^{10}. The above matrices are well-conditioned, with smallcondition number; for example for matrix $L_{3000\times 3000}$ the condition number is 2.288663×10^3. Note that all matrices are scaled to $\|A\|_1 \approx 1$.

5 Summary

In this paper, we used the results of Sections 3, 4 and Theorem 4.1 to find the smallest eigenvalue of a symmetric (Hermitian) matrix and the smallest singular value of a lower triangular matrix L with $\operatorname{diag}(L) \equiv 1$. This is done by verifying positive semidefiniteness. The verification needs one floating-point Cholesky decomposition. The computation either verifies that a given symmetric (Hermitian) matrix is not positive semidefinite, so has one or more negative eigenvalue or else comes to no conclusions.

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