

Pivot Tightening for Direct Methods for Solving Symmetric Positive Definite Systems of Linear Interval Equations

On the occasion of the 100th anniversary of Cholesky's method on Dec. 2, 2010*

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Abstract The paper considers systems of linear interval equations, i.e., linear systems where the coefficients of the matrix and the right hand side vary between given bounds. We focus on symmetric matrices and consider direct methods for the enclosure of the solution set of such a system. One of these methods is the interval Cholesky method, which is obtained from the ordinary Cholesky decomposition by replacing the real numbers by the related intervals and the real operations by the respective interval operations. We present a method by which the diagonal entries of the interval Cholesky factor can be tightened for positive definite interval matrices, such that a breakdown of the algorithm can be prevented. In the case of positive definite symmetric Toeplitz matrices, a further tightening of the diagonal entries and also of other entries of the Cholesky factor is possible. Finally, we numerically compare the interval Cholesky method with interval variants of two methods which exploit the Toeplitz structure with respect to the computing time and the quality of the enclosure of the solution set.

Keywords Positive definite interval matrix · Interval Cholesky method · Toeplitz system

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1 Introduction

Systems of linear interval equations arise when the entries of the coefficient matrix and the right hand side of systems of linear equations vary between given bounds, cf. [1, Sect. 3.4]. The solution set of such a system

$$[A]x = [b], \quad (1)$$

where $[A] = [\underline{A}, \overline{A}]$ is a given n -by- n matrix interval and $[b] = [\underline{b}, \overline{b}]$ is a given vector interval with respect to the usual entry-wise partial order, is the set

$$\Sigma([A], [b]) := \{x \in \mathbf{R}^n \mid Ax = b, \quad A \in [A], \quad b \in [b]\}. \quad (2)$$

We will assume throughout that all $A \in [A]$ are non-singular. Then by continuity, the set (2) is compact and connected. It can be described explicitly only in very simple cases. Therefore one attempts to find a vector interval which encloses the set (2) as tightly as possible.

The best known method by which such an enclosure can be found is interval Gaussian elimination [1, Section 4.5], [2, Chap. 15], which is obtained from the usual (termed *ordinary* henceforth) Gaussian elimination by replacing the real numbers by the related intervals and the real operations by the respective interval operations; we assume that the reader is familiar with interval arithmetic, e.g. [1, Chap. 1], [2, Chaps. 1–4]. However, interval Gaussian elimination may fail due to division by an interval pivot containing zero, even if ordinary Gaussian elimination succeeds for all matrices $A \in [A]$. There are some classes of interval matrices for which interval Gaussian elimination cannot fail, e.g., the H -matrices, see [1, Theorem 4.5.7], [2, Chap. 17]. If ordinary Gaussian elimination is applied without pivoting, the pivots can be represented as the ratio of two successive leading principal minors. For some classes of matrices with an identical sign pattern of their inverses the ranges of the ordinary pivots over the matrix interval can be given explicitly and these ranges do not contain 0, see [3]. These classes include a subclass of the inverse nonnegative matrices, the nonsingular totally nonnegative matrices, and the inverse M -matrices. By replacing an interval pivot containing 0 by the range of the respective ordinary pivot the breakdown of the interval Gaussian elimination can be avoided. This tightening of the interval pivot has the additional advantage that the resulting enclosure of the solution set (2) is not larger than the one obtained by the usual interval Gaussian elimination, and may be smaller. Moreover, the range of the pivots can be obtained by running a few instances of ordinary Gaussian elimination procedures in parallel.

In this paper we consider the case of symmetric matrices and consequently restrict the discussion to the set

$$[A]_{sym} := \{A \in [A] \mid A^T = A\}. \quad (3)$$

and to the *symmetric solution set*

$$\Sigma_{sym}([A], [b]) := \{x \in \mathbf{R}^n \mid Ax = b, \quad A \in [A]_{sym}, \quad b \in [b]\}. \quad (4)$$

A method to compute an enclosure of the symmetric solution set is the interval variant of the ordinary Cholesky decomposition [4,5]. As for interval Gaussian elimination, the interval Cholesky method may fail due to an interval containing 0 for which the square root has to be taken to obtain the next interval pivot, even if all matrices $A \in [A]$ are positive definite and therefore possess a Cholesky decomposition. Presently, we are not able to give the range of a pivot, so we use a positive lower bound for it in order to tighten the respective interval pivot. Of special interest are symmetric Toeplitz matrices for which we present additional techniques for tightening.

The organisation of the paper is as follows: In the next section we introduce our notation. We present pivot tightening for the interval Cholesky method and the interval variants of two algorithms for solving systems of linear interval equations with a Toeplitz structure in Sections 3 and 4, respectively, and conclude with some remarks in Section 5.

2 Notation

Denote by \mathbf{IR} the set of the compact and nonempty real intervals. We equip \mathbf{R}^n and $\mathbf{R}^{n \times n}$, the sets of real n -vectors and of real n -by- n matrices, respectively, with the usual entry-wise order \leq . Vector and matrix intervals with respect to this partial order can be regarded as \mathbf{IR}^n , the set of vectors with n components taken from \mathbf{IR} , and $\mathbf{IR}^{n \times n}$, the set of n -by- n matrices over \mathbf{IR} , respectively. Consequently we write

$$[b] = [\underline{b}, \bar{b}] = ([b_i])_{i=1}^n = ([\underline{b}_i, \bar{b}_i])_{i=1}^n$$

and

$$[A] = [\underline{A}, \bar{A}] = ([a_{ij}])_{i,j=1}^n = ([\underline{a}_{ij}, \bar{a}_{ij}])_{i,j=1}^n.$$

As usual, we identify a degenerate interval (vector, matrix) with the (only) real number (vector, matrix) it contains. In order to distinguish an interval quantity from a real quantity we call the latter a *point* quantity.

For $[A] \in \mathbf{IR}^{n \times n}$ we define its *midpoint matrix* by $A_c := \frac{1}{2}(\underline{A} + \bar{A})$ and its *radius matrix* by $\Delta A := \frac{1}{2}(\bar{A} - \underline{A})$. Then $[A]$ can be represented as $[A_c - \Delta A, A_c + \Delta A]$. A matrix $A = (a_{ij})$ is a *vertex matrix* of $[A]$ if $a_{ij} \in \{\underline{a}_{ij}, \bar{a}_{ij}\}$, $i, j = 1, \dots, n$. Of special interest are the vertex matrices which can be represented in the form

$$A_{yz} := A_c - \text{diag}(y_1, \dots, y_n) \cdot \Delta A \cdot \text{diag}(z_1, \dots, z_n),$$

where $y, z \in Y_n := \{-1, 1\}^n$. The cardinality of the set of these matrices is at most 2^{2n-1} ; in the case that we allow only $y = z$ we have at most 2^{n-1} matrices, see [6].

3 Interval Cholesky Method

3.1 Positive definite interval matrices

Here we are concerned with *symmetric* interval matrices, i.e., $[A]^T = [A]$. We call $[A]$ *positive definite* if all matrices in $[A]_{sym}$ are positive definite. The following theorem shows that this property can be inferred from at most 2^{n-1} (symmetric) vertex matrices.

Theorem 1 ([6, 7]) *Let $[A] = [A]^T \in \mathbf{IR}^{n \times n}$. The interval matrix $[A]$ is positive definite if and only if the matrices A_{zz} are positive definite for all $z \in Y_n$.*

We consider now the symmetric solution set (4). A method for its enclosure is the interval Cholesky method, which is obtained from the ordinary Cholesky algorithm by replacing the real numbers by the related intervals and the real operations by the corresponding interval operations [4, 5]. The square root of an interval $a = [\underline{a}, \bar{a}]$ is defined by $[a]^{\frac{1}{2}} := \{a^{\frac{1}{2}} \mid a \in [a]\}$, provided that $0 \leq \underline{a}$.

3.2 The algorithm [4]

Let $[A] \in \mathbf{IR}^{n \times n}$ with $[A] = [A]^T$ and $[b] \in \mathbf{IR}^n$. Define the lower triangular matrix $[L] \in \mathbf{IR}^{n \times n}$ by
for $j = 1, \dots, n$:

$$[l_{jj}] := \left([a_{jj}] - \sum_{k=1}^{j-1} [l_{jk}]^2 \right)^{\frac{1}{2}},$$

$$[l_{ij}] := \left([a_{ij}] - \sum_{k=1}^{j-1} [l_{ik}] \cdot [l_{jk}] \right) / [l_{jj}], \quad i = j+1, \dots, n;$$

compute vectors $[y], [x^C] \in \mathbf{IR}^n$ by

$$[y_i] := \left([b_i] - \sum_{j=1}^{i-1} [l_{ij}] \cdot [y_j] \right) / [l_{ii}], \quad i = 1, \dots, n;$$

(forward substitution)

$$[x_i^C] := \left([y_i] - \sum_{j=i+1}^n [l_{ji}] \cdot [x_j^C] \right) / [l_{ii}], \quad i = n, n-1, \dots, 1.$$

(backward substitution)

The algorithm is feasible if and only if $0 < \underline{l}_{jj}^2$, $j = 1, \dots, n$. In this case the above algorithm yields the enclosure

$$\Sigma_{sym}([A], [b]) \subseteq [x^C].$$

It is known that the interval Cholesky method may break down even if $[A]$ is positive definite [4]¹. In the next subsection we present a method by which the breakdown of the algorithm can be avoided. In analogy to interval Gaussian elimination, we call the diagonal entries $[l_{ii}]$ *interval pivots*. For the ordinary Cholesky decomposition, l_{ii} can be represented as the square root of the ratio of two successive leading principal minors, cf. [8, formula (42) on p. 38], i.e.,

$$l_{jj} = \left(\frac{\det A[\{1, 2, \dots, j\}]}{\det A[\{1, 2, \dots, j-1\}]} \right)^{\frac{1}{2}}, \quad j = 1, \dots, n.$$

From this representation and Fisher's inequality [9, p. 478] follows the bound

$$l_{jj} \leq a_{jj}^{\frac{1}{2}}, \quad j = 1, \dots, n,$$

which may be employed to tighten the interval pivot.

Since any principal submatrix of a positive definite matrix is again positive definite, we may restrict the discussion to

$$p(A) := l_{nn}^2(A) = \det A / \det A',$$

where A' is the submatrix of A obtained by deletion of its last row and column.

Conjecture 1 Let $[A] = [A]^T \in \mathbf{IR}^{n \times n}$ be positive definite. Then the minimum value of p over $[A]_{sym}$ is attained at a matrix A_{zz} , $z \in Y_n$.

Remark: From [3, Proposition 3.1] it follows that the minimum value is attained at a matrix

$$A = (a_{ij})_{i,j=1}^n \in [A] \quad \text{with} \quad a_{jj} = \underline{a}_{jj}, \quad j = 1, \dots, n, \quad (5)$$

and that it is attained at a symmetric vertex matrix if all matrices from $[A]$ have identical sign patterns of their inverses. Evidence of the conjecture is provided by Theorem 1 and formula (6) below. By [10, Theorem 1.2], a lower bound for the minimum value is provided by the minimum value of p over all matrices A_{yz} , $y, z \in Y_n$ (note that $p(A)$ is the reciprocal value of the entry in the bottom right position of A^{-1}).

So long as this conjecture is not settled, we will use positive lower bounds for the interval pivots, which will be presented in the next subsection.

3.3 Interval pivot tightening

Since the eigenvalues of A and A' interlace, e.g., [9, p. 189], we obtain

$$\lambda_1(A) \leq p(A),$$

where $\lambda_1(A)$ denotes the smallest eigenvalue of A . By [11], it is known that

$$\min_{A \in [A]_{sym}} \lambda_1(A) = \min_{z \in Y_n} \lambda_1(A_{zz}). \quad (6)$$

¹ An example will be given in Subsection 3.3 (Example 1).

By solving two eigenvalue problems (instead of 2^{n-1}) we obtain a lower bound for the minimum eigenvalue in (6)

$$\lambda_1(A_c) - \rho(\Delta A) \leq \min_{A \in [A]_{sym}} \lambda_1(A) \quad (7)$$

[12], where $\rho(\Delta A)$ denotes the spectral radius of ΔA . It was pointed out in [13] that the minimum eigenvalue of $[A]$ is attained for matrices satisfying (5) such that on the left-hand side of (7) the diagonal of A_c can be restricted to the diagonal of \underline{A} and only zeros are on the diagonal of ΔA . However, even this improved bound may be nonpositive, in which case it is useless for pivot tightening.

In [14] we employ the following lower bounds for the smallest eigenvalue of a positive definite symmetric matrix A , which do not require the computation of any eigenvalue. We use the following partition of a positive definite matrix A

$$A = \begin{pmatrix} A' & d \\ d^T & c \end{pmatrix}.$$

Let β_{n-1} be any lower bound for $\lambda_1(A')$. Then we have the lower bound [15] of complexity $O(n)$

$$\beta_n = \frac{1}{2} \left(c + \beta_{n-1} - \sqrt{(c - \beta_{n-1})^2 + 4d^T d} \right) \leq \lambda_1(A). \quad (8)$$

This bound may not be positive. If this case occurs we use the following bound [16]

$$\tilde{\beta}_n = \frac{1}{2} \left(c + \beta_{n-1} - \sqrt{(c - \beta_{n-1})^2 + 4\beta_{n-1}d^T(A')^{-1}d} \right) \leq \lambda_1(A). \quad (9)$$

which is always positive. Here, $(A')^{-1}d$ should be computed as the solution x of $A'x = d$. Then the computation of $\tilde{\beta}_n$ can be arranged recursively in such a way that, starting with $\beta_1 = a_{11}$, the j -th step needs $3j^2 + O(j)$ arithmetic operations (and one square root), $j = 2, \dots, n$. This can be seen as follows: If we have computed the Cholesky decomposition $L_{i-1}L_{i-1}^T = A_{i-1}$ of the leading principal submatrix of order $i-1$ of A then one square root and $j^2 + O(j)$ arithmetic operations are required to compute the Cholesky factor of A_i . Forward and backward substitution, cf. Subsection 3.2, each need j^2 operations to solve the respective linear system.

It should be noted that sharper positive bounds are given in [17], which require the additional computation of $(A')^{-2}$ (and $(A')^{-3}$).

If in the j th step the bound (9) is applied to the 2^{j-1} leading principal submatrices of order j of the vertex matrices A_{zz} , $j = 2, \dots, n$, the computation requires approximately 2^n square roots and $3n^22^n + O(n2^n)$ arithmetic operations. This can be seen as follows: In the j th step, 2^{j-1} matrices are

Table 1 Matrices $A_{zz}, z \in Y_3$, together with associated bounds

matrix	$\begin{pmatrix} 4 & 3 & 1 \\ 3 & 4 & 3 \\ 1 & 3 & 4 \end{pmatrix}$	$\begin{pmatrix} 4 & 3 & 1 \\ 3 & 4 & 2 \\ 1 & 2 & 4 \end{pmatrix}$	$\begin{pmatrix} 4 & 2 & 1 \\ 2 & 4 & 3 \\ 1 & 3 & 4 \end{pmatrix}$	$\begin{pmatrix} 4 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{pmatrix}$
bound (8)	-1	-0.192	-0.316	0.550
bound (9)	0.177	0.658	0.619	

involved. Therefore, $3j^22^{j-1} + O(j2^{j-1})$ arithmetic operations are required. Now use the identity, see [18, p. 199, Example 4],

$$\sum_{j=1}^n jx^{j-1} = \frac{1 - (n+1)x^n + nx^{n+1}}{(x-1)^2}, \quad x \neq 1. \quad (10)$$

Differentiating on both sides, putting $x = 2$, and multiplying both sides by 2 yields

$$\sum_{j=1}^n j^22^{j-1} = n^22^n + O(n2^n). \quad (11)$$

The lower bounds (7) and (8) are much easier to compute than (6) and (9) but only the latter are always positive. Obviously, the computation of (9) requires less effort than (6). Also, it is easier to compute (9) in a guaranteed way, i.e., such that all rounding errors are covered.

Example 1 We consider the following matrix interval. Let

$$[A] := \begin{pmatrix} [4, 6] & [2, 3] & 1 \\ [2, 3] & 4 & [2, 3] \\ 1 & [2, 3] & [4, 5] \end{pmatrix}.$$

By Theorem 1, it is easily checked that $[A]$ is positive definite. The interval Cholesky method breaks down due to $\underline{l}_{33}^2 = -79/252$.

The following results are rounded down to three decimal places. The minimal eigenvalue according to (6) is 0.228. Formula (7) with diagonal minimization gives the lower bound 0.222. The four matrices $A_{zz}, z \in Y_3$, together with the associated bounds according to (8) and (9) are given in Table 1. Thus, if the bounds (8) and (9) are used, \underline{l}_{33}^2 can be improved to 0.177.

Since $[A]$ contains only nonsingular totally nonnegative matrices, the minimum of p over $[A]$ is $6/7$, see [3, Example 4.4].

3.4 Positive definite Toeplitz matrices

In this subsection we consider symmetric Toeplitz matrices

$$T(a_1, \dots, a_n) = \begin{pmatrix} a_1 & a_2 & \cdots & a_n \\ a_2 & a_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_2 \\ a_n & \cdots & a_2 & a_1 \end{pmatrix}. \quad (12)$$

If such a matrix is positive definite then the pivots of the Cholesky decomposition are monotonically decreasing [19]

$$l_{nn} \leq \dots \leq l_{22} \leq l_{11} \leq a_1^{\frac{1}{2}}. \quad (13)$$

Now let $[A]$ be a symmetric Toeplitz interval matrix $[A] = T([a_1], \dots, [a_n])$. Denote by $[A]_{T, sym}$ the set of all symmetric Toeplitz matrices contained in $[A]$. We want to enclose the *symmetric Toeplitz solution set*

$$\Sigma_{T, sym}([A], [b]) := \{x \in \mathbf{R}^n \mid Ax = b, A \in [A]_{T, sym}, b \in [b]\}.$$

Assume now that $[A]_{T, sym}$ contains only positive definite matrices. Then (13) can be employed to tighten the interval pivots: Suppose that we have already computed $[l_{jj}]$ and $[l_{j+1, j+1}]$.

$$(i) \quad \text{If } \bar{l}_{j+1, j+1} > \bar{l}_{jj} \quad \text{then put } \bar{l}_{j+1, j+1} := \bar{l}_{jj}; \quad (14)$$

$$(ii) \quad \text{If } \underline{l}_{j+1, j+1} > \underline{l}_{jj} \quad \text{then put } \underline{l}_{jj} := \underline{l}_{j+1, j+1}. \quad (15)$$

In case (ii) the entries in the column below $[l_{jj}]$ should be recomputed; this may tighten $[l_{j+1, j+1}]$, too.

Of special interest are entry-wise nonnegative symmetric Toeplitz matrices with monotone and convex decay of their off-diagonal entries. In [20] it was shown that for these matrices nonnegativity and monotonicity are maintained throughout the Cholesky decomposition.

Theorem 2 ([20]) *Let T be given as in (12). Assume for simplicity that $a_1 = 1$. Suppose that the sequence a_2, \dots, a_n satisfies the relations*

$$(i) \quad 1 \geq a_2 \geq a_3 \geq \dots \geq a_n \geq 0,$$

$$(ii) \quad 1 - a_2 \geq a_2 - a_3 \geq \dots \geq a_{n-1} - a_n \geq 0.$$

Then the Cholesky factor L , $T = LL^T$ is entry-wise nonnegative and satisfies

$$l_{ij} \geq l_{i+1, j}, \quad i = 1, \dots, n-1, \quad j = 1, \dots, i; \quad (16)$$

$$l_{jj}l_{ij} \geq a_{i-j+1} - a_{i-j+2} + a_i \cdot (a_{j-1} - a_j), \quad j = 2, \dots, n, i = j, \dots, n. \quad (17)$$

In particular, setting $i = j$ in (17) we obtain a lower bound on the pivots

$$l_{jj}^2 \geq 1 - a_2 + a_j \cdot (a_{j-1} - a_j), \quad j = 2, \dots, n. \quad (18)$$

In the following example we apply (14), (15) as well as obvious extensions of formulae (16) and (18) to symmetric Toeplitz interval matrices. It should be noted that in contrast to the lower bounds presented in Subsection 3.3 the tightening approach tailored to these special Toeplitz matrices costs nearly nothing. Once the respective interval entries of the matrix $[L]$ are computed, formulae (14) – (16) do not require any arithmetic operations and each application of (18) costs 4 arithmetic operations.

Example 2 We consider

$$[A] = T(1, [.5625, .625], [.25, .3125], [.0625, .125], [0, .0625]).$$

Each symmetric Toeplitz matrix contained in $[A]$ satisfies the monotonicity and convexity assumptions (i), (ii) of Theorem 2 and is therefore positive definite by [20]. The following results are obtained by running the interval Cholesky method implemented in INTLAB [21] with different tightening techniques.

We obtain the following interval pivots, which can be improved according to (14) and (15) (rounded outwards to four decimal places)

$$\begin{aligned} [l_{22}] &= [.7806, .8268], \\ [l_{33}] &= [.7192, .8604], \quad \text{and by (14)} \quad \bar{l}_{33} := .8268, \\ [l_{44}] &= [.5842, .9048], \quad \text{and by (14)} \quad \bar{l}_{44} := .8268, \\ [l_{55}]^2 &\text{ becomes } [-.1254, .9167]; \quad \text{therefore we apply (18) to obtain} \\ [l_{55}]^2 &= [.3750, .9167], [l_{55}] = [.6123, .9575], \quad \text{and by (14)} \quad \bar{l}_{55} := .8268, \\ &\text{and by (15), } [l_{44}] = [.6123, .8268]. \end{aligned}$$

Since we have improved \underline{l}_{44} we recompute $[l_{54}]$ and improve \bar{l}_{54} from .9602 to .9162. On the other hand, formula (16) can be used to improve it to .8268. Now we recompute $[l_{55}]^2$ and obtain $[-.1129, .9167]$ which does not represent any improvement. By (18), $[l_{44}]$ can be tightened to $[-.6187, .8268]$.

4 Interval Bareiss and Trench Algorithms

The algorithms by Bareiss [22] and Trench [23] are well known direct algorithms of complexity $O(n^2)$ for solving (not necessarily symmetric) point Toeplitz systems. Both have symmetric variants [22, 24]. In [25] we present interval variants of both algorithms and investigate their feasibility. Both point algorithms require division by certain quantities which can be represented as the ratio of two successive leading principal minors [22, Cor. 1], [23, p. 276]. Therefore, all results for the diagonal pivots of the (point) Cholesky method carry over to the interval variants of the symmetric Bareiss and Trench algorithms. In particular, we can employ the useful tightening tools (14) and (15).

Symmetric strictly diagonally dominant (point) matrices with positive diagonal entries are instances of positive definite matrices, e.g., [9, Cor. 7.2.3]. In [25] we show that the interval variants of the Bareiss and the Trench algorithms are feasible for strictly diagonally dominant interval Toeplitz matrices. Recently, both interval algorithms were applied in [26] to a large number of systems of linear interval equations up to order $n = 100$ with randomly generated symmetric strictly diagonally dominant interval Toeplitz matrices with positive intervals on the diagonal and compared with respect to the quality of the enclosure and computing time. The outcome confirmed the results of the preliminary computations reported in [25]. For $n = 5$ it turned out that

in most cases (for $n = 50$ in all cases) the Bareiss² algorithm yields the tightest enclosure of the symmetric Toeplitz solution set. On the other hand, the Bareiss algorithm very often needs more computing time (over four times for $n = 5$, about nine times for $n = 50$, and about 18 times more for $n = 100$) and requires about twice the memory space. The interval Cholesky method, although computing an enclosure for the possibly larger symmetric solution set (4), behaves for larger n like the Bareiss algorithm with respect to tightness of the enclosure and computing time.

5 Conclusions

We have shown how for the interval Cholesky method the breakdown due to an interval containing zero for which the square root has to be taken can always be avoided. This can be accomplished by a tightening of the pivot. In the case of the interval Cholesky method applied to interval Toeplitz matrices, further entries in the resulting triangular form can be tightened. As a positive side effect, this tightening may lead to a smaller enclosure of the symmetric solution set.

If $[A]$ is a Toeplitz interval matrix, then the matrices A_{zz} which play a prominent role in the approaches of Subsection 3.3 are in general not Toeplitz. In a future paper we will adapt these approaches to the Toeplitz structure and apply them to the interval variants of the Bareiss and Trench algorithms.

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