Convergence analysis of an algorithm
for accurate inverse Cholesky factorization

高精度逆コレスキー分解アルゴリズムの
収束解析に関する研究

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CHAPTER 1

INTRODUCTION

Let $\mathbb{R}$ be the set of real numbers, and $\mathbb{F}$ be a set of floating-point numbers conforming to IEEE standard 754. The relative rounding error unit of floating-point arithmetic is denoted by $\mathbf{u}$. In binary64 (double precision) arithmetic, $\mathbf{u} = 2^{-53} \approx 1.1 \times 10^{-16}$. Throughout this paper, we assume that neither overflow nor underflow occurs. For $A \in \mathbb{R}^{n \times n}$ define $\kappa(A) := \|A\| \cdot \|A^{-1}\|$ as the condition number of A , where $\|\cdot\|$ stands for spectral norm for matrices and Euclidean norm for vectors.

In this thesis, we consider to treat the case where A is symmetric, positive definite and extremely ill-conditioned such that

$$\kappa(A) > \mathbf{u}^{-1}. \quad (1)$$

This means no correct digit can be expected in an approximate solution $\tilde{x}$ when solving a linear system $Ax = b$ in working precision $\mathbf{u}$. There are several applications in which the case (1) appears, for example, ill-conditioned Gramian matrices deriving from discretization of partial differential equations, Cholesky QR method [20] and so forth.

In about 1990, Rump [12] showed that a approximate inverse of extremely ill-conditioned matrix may still be useful as a preconditioner. He derived a method for inverting an extremely ill-conditioned matrix which requires the possibility to calculate a dot product in higher precision. Fortunately, Ogita et al. [8] developed a method for calculating a dot product in k -fold precision in 2005. In the same year, Ohta et al. [9] redeveloped Rump's method using the accurate dot product algorithm [8]. However, why Rump's method is so efficient for ill-conditioned matrices had not yet been known. In 2007, Oishi et al. [10] presented a proof why a modified version of the Rump's method works so well. In 2009, Rump [16] showed the mechanism of his method by himself. In 2010, Ogita [6] proposed a framework with the same spirit of Rump's method for an accurate and efficient computation of matrix factorizations such as inverse LU and inverse QR factorizations. He analyzed these algorithms in

detail and confirmed that it coincides with numerical results. Nevertheless, it is not possible to adapt his proposed framework directly to Cholesky factorization of A . Because a floating-point Cholesky factorization of an ill-conditioned matrix such that (1) may break down by the presence of an imaginary root due to the accumulation of rounding errors, even if the matrix is symmetric and positive definite. In 2012, Ogita and Oishi [7] derived an iterative algorithm to calculate a good approximate inverse of the exact Cholesky factor. To avoid the break-down, a diagonal shift is applied to A in the Ogita-Oishi's algorithm. As is the case with [6, 9], the Ogita-Oishi's algorithm is needed an algorithm for accurately computing a dot product as if computed in k -fold working precision and rounded into the sum of l pieces of working precision floating-point numbers for $k \geq 2$ and $1 \leq l \leq k$. Fortunately, such accurate dot product algorithms have been proposed in [8, 11, 16, 18, 19], and they are very fast. By numerical results in [7], the performance of this algorithm was evaluated. However, the Ogita-Oishi's algorithm has not been analyzed in detail and explained reasons for convergency.

This thesis has two purposes. The first is to analyze the behavior of the algorithm in detail and explain its convergency by the use of numerical error analysis. Main analysis to be explained is that each iteration of the Ogita-Oishi's algorithm reduces the condition number of a preconditioned matrix by a factor around $n^2\mathbf{u}$ until convergence, which is consistent with the numerical results. As is the case with [16], we do not give a completely rigorous proof but arguments how and why the algorithm works. The key of the analysis is in multiplicative corrections of a sum of m matrices $X = \sum_{i=1}^m X_i$, $X_i \in \mathbb{F}^{n \times n}$, which is an accurate inverse of $\hat{R}$ such that $A = \hat{R}^\top \hat{R}$ satisfying $\kappa(X^\top A X) = 1$. Note that $\hat{R}$ is upper triangular. The Ogita-Oishi's algorithm requires an algorithm for accurate dot product, which helps to treat extremely ill-conditioned matrices. We show that it is important to choose adequate computational precision for calculating dot products in the algorithm, which is sufficient for

convergence and almost optimal in terms of computational effort. As we will see this does influence the analysis. We justify the optimality of high precision arithmetic for dot product used in the Ogita-Oishi's algorithm by our numerical error analysis. This analysis is a vastly extended version of [22].

The second is to propose a modified version of the Ogita-Oishi's algorithm for calculating a more accurate inverse X of $\hat{R}$ than the original one. Namely, the proposed algorithm provides X satisfying

$$\|I - X^\top AX\| \approx \mathbf{u}.$$

In this thesis, we use the “ $\approx$ ” notation to indicate that two quantities are approximately equal. For example, for $x, y \in \mathbb{R}$, $x \approx y$ means that $|x| = \varphi \cdot |y|$ for reasonably small constant φ . As mentioned before, for the case (1), a floating-point Cholesky factorization may break down due to the accumulation of rounding errors. To avoid the break-down, a diagonal shift is applied to A in the Ogita-Oishi's algorithm. As we will see from some numerical results in Chapter 3, the Ogita-Oishi's algorithm gives an approximate inverse X satisfying

$$n^2 \mathbf{u} \approx \|I - X^\top AX\| < 1.$$

The diagonal shift is the reason why $n^2 \mathbf{u}$ is the lower bound. To overcome it, we find the condition such that Cholesky factorization of a preconditioned matrix never breaks down without the diagonal shift.

The rest of the thesis is organized as follows: in the following chapter, we explain some basic definitions, and we introduce an algorithm for accurately computing a dot product. Moreover, we state the algorithm [7] for an accurate inverse Cholesky factorization. In Chapter 3, we present detailed analysis of the algorithm. Furthermore, we present some numerical results for confirming our analysis and comparing the algorithm with a standard Cholesky factorization by using long precision arithmetic

[2, 5], in terms of measured computing time for verifying the positive definiteness of an input matrix. In Chapter 4, we propose a modified algorithm for an accurate inverse Cholesky factorization. Moreover, we present some numerical results for comparing the proposed algorithm with the original one in terms of both the accuracy on X and measured computing time for convergence. Finally, we conclude our results in Chapter 5. In addition, we give the complete Matlab-code for our algorithms.

CHAPTER 2

PRELIMINARIES

This section is structured as follows. In Section 2.1, we prepare some notations, definitions and error estimations of floating point arithmetic. In Section 2.2, we describe an algorithm of accurate matrix multiplication [11, 16]. In Section 2.3, we introduce the Ogita-Oishi algorithm [7] for an accurate inverse Cholesky factorization.

2.1. NOTATION AND DEFINITIONS

For $A = (a_{ij})$, $B = (b_{ij}) \in \mathbb{R}^{n \times n}$, $|A| = (|a_{ij}|) \in \mathbb{R}^{n \times n}$ denotes a nonnegative matrix consisting of entrywise absolute values, and an inequality $A \leq B$ is understood entrywise, i.e., $a_{ij} \leq b_{ij}$ for all (i, j) . The notation $A \geq O$ means that all elements of A are nonnegative. Similar notation applies to real vectors. Let I denote the identity matrix. For readability $\varphi(\gamma)$ denotes a constant such as $\varphi(\gamma) = c \cdot \gamma$ for factor c near 1.

The eigenvalues of A is denoted by $\lambda_i(A)$ with $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_n(A)$. The trace of $A = (a_{ij}) \in \mathbb{R}^{n \times n}$ is defined by

$$\text{tr}(A) := \sum_{i=1}^n a_{ii} = \sum_{i=1}^n \lambda_i(A).$$

Computing an approximate inverse of an upper triangular matrix $R \in \mathbb{F}^{n \times n}$ is denoted by

$$T := \text{triinv}(R),$$

which solves a matrix equation $RT = I$ for T using a standard numerical algorithm (e.g., `xTRSV` in BLAS and `xTRTRI` in LAPACK) in working precision such as binary64.

The sum of the absolute values of off-diagonal elements in the i -th row of A is denoted by

$$r_i(A) = \sum_{i \neq j} |a_{ij}|.$$

We assume that the following three types of rounding modes are defined in IEEE standard 754: Let $c \in \mathbb{R}$.

- (1) **Rounding to nearest even (default):** Round c to the nearest floating point number $\tilde{f} \in \mathbb{F}$ satisfying $|\tilde{f} - c| = \min_{f \in \mathbb{F}} |f - c|$.
- (2) **Rounding upwards:** Round c to the smallest floating point number $\overline{f} \in \mathbb{F}$ satisfying $\overline{f} \geq c$.
- (3) **Rounding downwards:** Round c to the largest floating point number $\underline{f} \in \mathbb{F}$ satisfying $\underline{f} \leq c$.

Let $fl(\cdot)$, $fl_{\Delta}(\cdot)$ and $fl_{\nabla}(\cdot)$ denote that an expression inside the parentheses is evaluated by floating-point arithmetic in rounding to nearest, rounding upwards and rounding downwards, respectively. We assume the use of the following standard model: For $a, b \in \mathbb{F}$ and $\circ \in \{+, -, *, /\}$ it holds that

$$fl(a \circ b) = (1 + \varepsilon)(a \circ b), \quad |\varepsilon| \leq \mathbf{u}. \quad (2)$$

For $0 \leq a \in \mathbb{F}$,

$$fl(a^{\frac{1}{2}}) = a^{\frac{1}{2}}(1 + \varepsilon_1), \quad |\varepsilon_1| \leq \mathbf{u}. \quad (3)$$

Let $\mathbb{F}_{[l]}$ be a set of sum of floating-point numbers such that

$$\mathbb{F}_{[l]} := \left\{ x \in \mathbb{R} : x = \sum_{i=1}^l x_i, x_i \in \mathbb{F}, l \in \mathbb{N} \right\}.$$

Note that $\mathbb{F} = \mathbb{F}_{[1]} \subseteq \mathbb{F}_{[l]} \subset \mathbb{R}$.

2.2. ACCURATE MATRIX MULTIPLICATION

The Ogita-Oishi's algorithm [7] requires an algorithm for accurate dot product as if calculated in k -fold precision, where the result is stored in l terms. In this paper we need only these two cases $l = 1$ and $l = k$. Fortunately we have a function of calculating $C_{1:l} \in \mathbb{F}_{[l]}^{n \times n}$ for any $k, l \in \mathbb{N}$, $l \leq k$ satisfying

$$|AB - C_{1:l}| \leq \varphi(\mathbf{u}^l)|AB| + \varphi(\mathbf{u}^k)|A||B|. \quad (4)$$

Note that

$$C_{1:l} = \sum_{i=1}^l C_i \quad \text{with } C_i \in \mathbb{F}^{n \times n}, i = 1, 2, \dots, l.$$

Namely, $C_{1:l}$ is an approximation of AB as if computed in k -fold working precision and rounded into l pieces of working precision floating-point numbers. We write such a function as

$$C_{1:l} := \{AB\}_k^l, \quad (5)$$

which provides $C_{1:l}$ satisfying (4).

Let $\langle A_M, A_R \rangle$ denote an interval matrix of the midpoint-radius representation such that

$$\langle A_M, A_R \rangle := \{X \in \mathbb{R}^{n \times n} : |X - A_M| \leq A_R\}$$

with a midpoint $A_M \in \mathbb{F}^{n \times n}$ and a radius $A_R \in \mathbb{F}^{n \times n}$, $A_R \geq O$. Similar notation in (5) applies to $B^\top AB$, i.e.,

$$\langle G, E \rangle := \{B^\top AB\}_k^1$$

which provides $G = G^\top, E \in \mathbb{F}^{n \times n}$ satisfying $B^\top AB \in \langle G, E \rangle$. Then we require

$$|B^\top AB - G| \approx \varphi(\mathbf{u})|B^\top AB| + \varphi(\mathbf{u}^k)|B^\top||A||B| =: E. \quad (6)$$

REMARK 1. *For (6), in practice, it can be realized by*

$$\langle C_{1:k}, E_1 \rangle := \{AB\}_k^k \quad \text{and} \quad \langle D, E_2 \rangle := \{B^\top C_{1:k}\}_k^1,$$

which satisfy

$$|AB - C_{1:k}| \leq \varphi(\mathbf{u}^k)|AB| + \varphi(\mathbf{u}^k)|A||B| =: E_1, \quad (7)$$

$$|B^\top C_{1:k} - D| \leq \varphi(\mathbf{u})|B^\top C_{1:k}| + \varphi(\mathbf{u}^k)|B^\top||C_{1:k}| =: E_2 \quad (8)$$

where $C_{1:k} \in \mathbb{F}_{[k]}^{n \times n}$, $D, E_1, E_2 \in \mathbb{F}^{n \times n}$. From (7) and (8), it holds that

$$\begin{aligned}
|B^\top AB - D| &\leq |B^\top AB - B^\top C_{1:k}| + |B^\top C_{1:k} - D| \\
&\leq |B^\top| |AB - C_{1:k}| + |B^\top C_{1:k} - D| \\
&\leq |B^\top| E_1 + E_2
\end{aligned} \tag{9}$$

and

$$\begin{aligned}
E_2 &= \varphi(\mathbf{u})(|B^\top AB| + |B^\top| E_1) + \varphi(\mathbf{u}^k) |B^\top| (|AB| + E_1) \\
&\approx \varphi(\mathbf{u}) |B^\top AB| + \varphi(\mathbf{u}^{k+1}) |B^\top| |A| |B| \\
&\quad + \varphi(\mathbf{u}^k) |B^\top| |AB| + \varphi(\mathbf{u}^{2k}) |B^\top| |A| |B| \\
&\approx \varphi(\mathbf{u}) |B^\top AB| + \varphi(\mathbf{u}^k) |B^\top| |A| |B|.
\end{aligned} \tag{10}$$

Inserting (7) and (10) into (9) implies

$$|B^\top AB - D| \approx \varphi(\mathbf{u}) |B^\top AB| + \varphi(\mathbf{u}^k) |B^\top| |A| |B|. \tag{11}$$

Such accurate dot product algorithms satisfying (4) have been proposed in [8, 18, 19]. In this thesis, we use error-free transformation algorithm of matrix multiplication by fast routines of matrix multiplication which have been developed in [11]. After this transformation, we apply an accurate summation algorithm [8, 16] for floating-point numbers.

We describe an algorithm for error-free transformation of the matrix $A \in \mathbb{F}^{m \times n}$ without rounding errors.

ALGORITHM 2.1 (Ozaki [11]). *This algorithm transforms A into $\sum_{i=1}^{h_A} D_i$ without rounding errors.*

```

function  $D_{1:h_A} = \text{Ozaki\_Split}(A)$ 

 $n = \text{size}(A, 2);$ 

 $\mu = \max(\text{abs}(A), [\ ], 2);$       %  $\mu \in \mathbb{F}^{m \times 1}$  with  $\mu(i) = \max_{1 \leq j \leq q} |a_{ij}|;$ 

 $\alpha = \text{fl}\left(\left\lfloor -\frac{\log_2(\mathbf{u}) + \lceil \log_2(n) \rceil}{2} \right\rfloor\right);$ 

 $\beta = \text{fl}\left(\left\lceil \frac{-\log_2(\mathbf{u}) + \log_2(n)}{2} \right\rceil\right);$ 

 $\omega = \text{fl}(2^{\lceil (\log_2(\mu) + \beta) \rceil});$ 

 $S = \text{repmat}(\omega, n);$       %  $S = \omega \cdot e^\top$  for  $e = (1, 1 \dots 1)^\top \in \mathbb{F}^n$ 

 $h_A = 1;$ 

While any(any( $A$ ))      % Determine if any array elements are nonzero

     $D_{h_A} = \text{fl}((A + S) - S);$ 

     $A = \text{fl}(A - D_{h_A});$ 

     $S = \alpha A;$ 

     $h_A = h_A + 1;$ 

```

Similarly, the matrix B is split into $\sum_{i=1}^{h_B} E_i$ by $E = \text{Ozaki\_Split}(B^\top)^\top$. After such matrix splitting, we can expand an accurate matrix multiplication by using floating-point matrix multiplications, which are performed fast by BLAS routines.

ALGORITHM 2.2 (Ozaki [11]). *For $A \in \mathbb{F}^{m \times n}$ and $B \in \mathbb{F}^{n \times p}$, this algorithm product AB into unevaluated sum of floating-point matrices without rounding errors*

such that $AB = \sum_{i=1}^{h_A h_B} C_i$, $C_i \in \mathbb{F}^{m \times n}$.

$$\begin{aligned}
& \text{function } C_{h_A h_B} = \text{EFT\_mm}(A, B); \\
& [m, n] = \text{size}(A); [n, p] = \text{size}(B); \\
& D_{1:h_A} = \text{Ozaki\_Split}(A); h_A := \text{length}(D); \\
& E_{1:h_B} = \text{Ozaki\_Split}(B^\top); h_B := \text{length}(E); \\
& \text{for } i = 1 : h_B, \quad E_i = E_i^\top; \\
& \text{for } i = 1 : h_A \\
& \quad \text{for } j = 1 : h_B \\
& \quad \quad C_t = \text{fl}(D_i \cdot E_j);
\end{aligned} \tag{12}$$

After this transformation, we can guarantee a result with k -hold accuracy of the matrix product. Note that we need only these two cases $l = 1$ and $l = k$ in (4). We use an accurate summation algorithm **SumKK** and **SumK1** for $\sum_{i=1}^{h_A h_B} C_i$.

Let $x, y \in \mathbb{F}^n$. The following Knuth's algorithm transforms any pair of floating-point numbers (a, b) into a new pair (x, y) with

$$x + y = a + b \quad \text{and} \quad x = \text{fl}(a + b). \tag{13}$$

ALGORITHM 2.3 (Knuth [4]). *Error-free transformation for the sum of two floating-point numbers.*

$$\begin{aligned}
& \text{function } [x, y] = \text{Twosum}(a, b) \\
& \quad x = \text{fl}(a + b) \\
& \quad z = \text{fl}(x - a) \\
& \quad y = \text{fl}(a - (x - z) + (b - z))
\end{aligned}$$

Let $p_i, q_i \in \mathbb{F}$ for $1 \leq i \leq n$. The vector $p_1 \dots, p_n$ is transformed into the vector $\pi, q_2, \dots, q_n$, where the element π is the ordinary floating point summation $\text{fl}(\sum_{i=1}^n p_i)$ and the value of the sum does not change as $\sum_{i=1}^n p_i = \pi + \sum_{i=2}^n q_i$. This transformation is the following:

ALGORITHM 2.4 (Ogita et al. [8]). *Error-free vector transformation for summation.*

```
function  $q = \text{VecSum}(p)$ 

 $q_n = p_n$ 

for  $i = n - 1 : -1 : 1$ 

     $[q_i, q_{i+1}] = \text{TwoSum}(p_i, p_{i+1})$ 
```

We introduce an algorithm of the summation in k -fold precision and rounding into k results. Assume $n \geq k$.

ALGORITHM 2.5. *Summation as if computed in k -fold precision and rounded into k results $res_{1:k}$*

```
function  $res_{1:k} = \text{SumKK}(p, k)$ 

for  $i = 1 : k - 1$ 

     $p = \text{VecSum}(p)$ 

for  $i = 1 : k - 1$ 

     $res_i = p_i$ 

 $res_k = \text{fl}\left(\sum_{i=k}^n p_i\right)$ 
```

ALGORITHM 2.6 (Ogita [8]). *Summation as if computed in k -fold precision and rounded into one result res .*

function $res = \text{SumK1}(p, k)$

for $i = 1 : k - 1$

$p = \text{VecSum}(p)$

$res = \text{fl} \left(\sum_{i=1}^n p_i \right)$

As mentioned before there is the fast error-free transformation of a product of two floating-point matrices A, B into a sum of floating-point matrices. If this sum is calculated by **SumKK** and **SumK1** [8, 16], we can have the result of the dot product satisfying (4).

2.3. ACCURATE AND ROBUST INVERSE CHOLESKY FACTORIZATION

The following scheme compute the Cholesky factorization:

ALGORITHM 2.7 (Algorithm 10.2 [3]). *Give a symmetric positive definite $A = (a_{ij}) \in \mathbb{R}^{n \times n}$. This algorithm computes the Cholesky factrization $A = R^\top R$.*

for $j = 1 : n$

for $i = 1 : j - 1$

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

end

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

Let $A \in \mathbb{F}^{n \times n}$ be symmetric and positive definite. The Matlab-style notation

$$R := \text{chol}(A)$$

means a floating-point Cholesky factorization of A using a standard numerical algorithm (e.g., `xPOTRF` in LAPACK) such that $A \approx R^\top R$ where $R \in \mathbb{F}^{n \times n}$ is an upper triangular matrix. We say “run to completion” if no imaginary root appears in the factorization process. It is well known [3] that the computed Cholesky factor R always satisfies

$$\frac{\|A - R^\top R\|}{\|A\|} \leq \varphi(\mathbf{u}) \quad (14)$$

if the floating-point Cholesky factorization runs to completion. From the residual norm $\|A - R^\top R\|$ or its relative norm, only limited information on the accuracy of the Cholesky factorization can be obtained. Suppose the exact Cholesky factorization of A runs to completion such that $A = \hat{R}^\top \hat{R}$. Instead of (14), we use the following criterion:

$$\|I - X^\top A X\| < \varepsilon_{tol},$$

where X is an approximate inverse of $\hat{R}$ and ε_{tol} is a given tolerance, as the accuracy of the Cholesky factors.

As mentioned before, a floating-point Cholesky factorization of an ill-conditioned matrix A may break down due to the accumulation of the rounding errors. To avoid the break-down, a diagonal shift can be applied to A such as $\tilde{A} = fl(A + \delta I)$ for some suitable $\delta > 0$. It is advisable to obtain an optimal δ before executing `chol`($\tilde{A}$). Fortunately, it is possible. Rump [15] presented the following backward error bound of a floating-point Cholesky factorization based on the Demmel’s result [1]: if $2(n+1)\mathbf{u} < 1$, then

$$\Delta := A - R^\top R, \quad \|\Delta\| \leq c'_n \mathbf{u} \cdot \text{tr}(A), \quad c'_n := \frac{n+1}{1 - 2(n+1)\mathbf{u}}. \quad (15)$$

LEMMA 2.1 (cf. Theorem 2.3 in [17]). *Let $A = A^T \in \mathbb{F}^{n \times n}$. If $\lambda_n(A) \geq c'_n \mathbf{u} \cdot \text{tr}(A)$, then $\text{chol}(A)$ runs to completion barring overflow and underflow.*

In [7, 22], a diagonal shift is applied. In this thesis, we modified the diagonal shift of A for the sake of completeness using Lemma 2.1. Assume A is positive definite. Then $a_{ii} > 0$ for all i and $\lambda_n(A) > 0$. From (2), it holds for a diagonal matrix $D = (d_{ij}) \in \mathbb{R}^{n \times n}$ that

$$\tilde{A} = A + \delta I + D, \quad |d_{ii}| \leq \mathbf{u}(a_{ii} + \delta).$$

From Lemma 2.1, if $\lambda_n(\tilde{A}) \geq c'_n \mathbf{u} \cdot \text{tr}(\tilde{A})$, then $\text{chol}(\tilde{A})$ never breaks down. Here

$$\begin{aligned} c'_n \mathbf{u} \cdot \text{tr}(\tilde{A}) &= c'_n \mathbf{u} \cdot \text{tr}(A + \delta I + D) \leq c'_n \mathbf{u} \cdot \text{tr}(A + \delta I + |D|) \\ &\leq c'_n \mathbf{u}(1 + \mathbf{u})(\text{tr}(A) + n\delta). \end{aligned} \tag{16}$$

On the other hand, by a Weyl's theorem (e.g. Corollary 4.9 in [21]) it holds

$$\lambda_n(\tilde{A}) \geq \lambda_n(A + \delta I) - \|D\| > \delta - \max_{1 \leq i \leq n} |d_{ii}|,$$

and

$$\max_{1 \leq i \leq n} |d_{ii}| \leq \max_{1 \leq i \leq n} \mathbf{u}(a_{ii} + \delta) = \mathbf{u} \max_{1 \leq i \leq n} a_{ii} + \delta \mathbf{u} \leq \mathbf{u} \cdot \text{tr}(A) + \delta \mathbf{u},$$

so that

$$\lambda_n(\tilde{A}) \geq \delta - (\mathbf{u} \cdot \text{tr}(A) + \delta \mathbf{u}) = (1 - \mathbf{u})\delta - \mathbf{u} \cdot \text{tr}(A). \tag{17}$$

From (16) and (17), a sufficient condition such that $\text{chol}(\tilde{A})$ runs to completion is

$$(1 - \mathbf{u})\delta - \mathbf{u} \cdot \text{tr}(A) \geq c'_n \mathbf{u}(1 + \mathbf{u})(\text{tr}(A) + n\delta)$$

and

$$\delta \geq \frac{(1 + \mathbf{u})c'_n + 1}{1 - ((1 + \mathbf{u})nc'_n + 1)\mathbf{u}} \mathbf{u} \cdot \text{tr}(A). \tag{18}$$

If $(n+1)(n+3)\mathbf{u} < 1$, then a little computation yields

$$\frac{(1+\mathbf{u})c'_n + 1}{1 - ((1+\mathbf{u})nc'_n + 1)\mathbf{u}} \leq \frac{n+2}{1 - (n+1)(n+3)\mathbf{u}} =: c_n.$$

Thus, if we determine δ satisfying $\delta \geq c_n \mathbf{u} \cdot \text{tr}(A)$, then $\text{chol}(\tilde{A})$ runs to completion.

If $(n+1)(n+3)\mathbf{u} < 1$, then we define a diagonal shift of $A \in \mathbb{F}^{n \times n}$ by

$$\text{shift}(A) := c_n \mathbf{u} \cdot \text{tr}(A) \quad \text{with} \quad c_n = \frac{n+2}{1 - (n+1)(n+3)\mathbf{u}}. \quad (19)$$

THEOREM 2.1. *Let $A = A^T \in \mathbb{F}^{n \times n}$. Assume $(n+1)(n+3)\mathbf{u} < 1$. Let $\text{shift}(A)$ be defined as in (19). For any positive $\delta \in \mathbb{F}$ satisfying $\delta \geq \text{shift}(A)$, put $\tilde{A} := \text{fl}(A + \delta I)$. If A is positive definite, then $\text{chol}(\tilde{A})$ runs to completion barring overflow and underflow.*

Let $\tilde{R} := \text{chol}(\tilde{A})$. Define

$$\tilde{\Delta} := \tilde{A} - \tilde{R}^\top \tilde{R},$$

then it holds that $\|\tilde{\Delta}\| \leq \delta$. For $n\mathbf{u} < 1$, we have $c_n \approx n$ and

$$\|\tilde{\Delta}\| \leq c_n \mathbf{u} \cdot \text{tr}(A) \leq c_n \mathbf{u} \cdot n \|A\| \approx n^2 \mathbf{u} \|A\|. \quad (20)$$

The following algorithm calculates an upper triangular matrix $X_{1:m_k}^{(k)} \in \mathbb{F}_{[m_k]}^{n \times n}$ for some $k \in \mathbb{N}$ such that $\|X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)} - I\| < \varepsilon_{tol}$ for a symmetric matrix $A = (a_{ij}) \in \mathbb{F}^{n \times n}$ with $a_{ii} > 0$ for all i and a specified tolerance ε_{tol} satisfying $n^2 \mathbf{u} \leq \varepsilon_{tol} \leq 1$.

ALGORITHM 2.8 (Ogita-Oishi [7]). *Accurate inverse Cholesky factorization.*

function $[X_{1:m_k}^{(k)}] = \text{acc\_chol}(A, \varepsilon_{tol})$

$k = 0, \quad G^{(0)} := A, \quad E^{(0)} := O, \quad X_{1:1}^{(0)} := I$

repeat

$k = k + 1$

Compute $S^{(k)} \in \mathbb{F}^{n \times n}$ with

$$\begin{cases} S_{ii}^{(k)} = fl_{\Delta}(G_{ii}^{(k-1)} + \|E^{(k-1)}\|_{\infty}) \\ S_{ij}^{(k)} = G_{ij}^{(k-1)} \text{ for } i \neq j. \end{cases} \quad (21)$$

$$\delta_k := shift(S^{(k)}) \quad (22)$$

$$\tilde{S}^{(k)} := fl(S^{(k)} + \delta_k I) \quad (23)$$

$$R^{(k)} := \text{chol}(\tilde{S}^{(k)}) \quad (24)$$

$$T^{(k)} := \text{triinv}(R^{(k)}) \quad (25)$$

$$m_k := \lceil \frac{k}{2} \rceil + 1 \quad (26)$$

$$X_{1:m_k}^{(k)} := \{X_{1:m_{k-1}}^{(k-1)} T^{(k)}\}_{m_k}^{m_k} \quad (27)$$

$$\langle G^{(k)}, E^{(k)} \rangle := \{(X_{1:m_k}^{(k)})^{\top} A X_{1:m_k}^{(k)}\}_{k+1}^1 \quad (28)$$

$$\text{until } fl_{\Delta}(\|G^{(k)} - I\|_{\infty} + \|E^{(k)}\|_{\infty}) < \varepsilon_{tol} \quad (29)$$

REMARK 2. *Note that high precision computations of dot product are necessary only in (27) and (28). In [7], to determine how much precision is used for calculating $X^{(k-1)}T^{(k)}$ and $(X^{(k)})^{\top}AX^{(k)}$, we needed to compute $\lceil -\log(\|X^{(k-1)}\| \|T\|) / \log \mathbf{u} \rceil + 1$ and $\lceil -\log(\|A\| \|X^{(k)}\|^2) / \log \mathbf{u} \rceil + 2$, respectively. In Chapter 3, we will make sure that the computational precision in (27) and (28) are appropriate.*

REMARK 3. In (21) and (22), we slightly shift the diagonal part of $G^{(k-1)}$ to ensure the positive definiteness of $\tilde{S}^{(k)}$ with taking care of the rounding errors. For (21), in practice, $S^{(k)}$ can be obtained by calculating $G_{ii}^{(k-1)} + \|E^{(k-1)}\|_\infty$ in rounding upwards.

Moreover, we introduce the following theorem for later use.

THEOREM 2.2 (Theorem 1 in [7]). *Let A be a symmetric $n \times n$ matrix. If Algorithm 2.8 successfully stops at (29) for any $\varepsilon_{tol} \leq 1$, then A is positive definite.*

CHAPTER 3

CONVERGENCE ANALYSIS OF AN ALGORITHM FOR ACCURATE INVERSE CHOLESKY FACTORIZATION

This section is structured as follows. In Section 3.1, we analyze Algorithm 2.8 in detail and explain its convergency. In Section 3.2, we present some numerical results for confirming our analysis and comparing the algorithm with a standard Cholesky factorization by using long precision arithmetic [2, 5], in terms of measured computing time for verifying the positive definiteness of an input matrix.

3.1. ANALYSIS

Following we analyze Algorithm 2.8 for input matrix $A \in \mathbb{F}^{n \times n}$ which is symmetric, positive definite and extremely ill-conditioned such that (1). The target of this section is to explain that the condition number of a preconditioned matrix $(X_{1:m_k}^{(k)})^\top A X_{1:m_k}^{(k)}$ eventually converges to 1 after some iterations. As is the case with [13], we do not give a totally rigorous proof, so we frequent use the notation “ $\approx$ ” to mean that two quantities are the same order of magnitude. We also use the the notation “ $\lesssim$ ”. For example, for $x, y \in \mathbb{R}$, $x \approx y$ means that $|x| \leq \varphi \cdot |y|$ for reasonably small constant φ . By the numerical results in [7], we observe the condition number of a preconditioned matrix is reduced by a factor around $n^2 \mathbf{u}$ until convergence. Hence we expect

$$\kappa((X_{1:m_k}^{(k)})^\top A X_{1:m_k}^{(k)}) \approx 1 + \prod_{i=1}^k \alpha_i \cdot \kappa(A), \quad \alpha_i := \frac{\delta_i}{\|(X_{1:m_{i-1}}^{(i-1)})^\top A X_{1:m_{i-1}}^{(i-1)}\|} \quad (30)$$

Assume $\|E^{(k-1)}\| \approx \mathbf{u}\|G^{(k-1)}\|$. Then

$$\delta_k = c_n \mathbf{u} \cdot \text{tr}(S^{(k)}) \approx n \mathbf{u} \cdot \text{tr}(G^{(k-1)}). \quad (31)$$

For this, it holds that $n \mathbf{u} \cdot \text{tr}(G^{(k-1)}) \geq n \mathbf{u} \|G^{(k-1)}\|$ and $n \mathbf{u} \cdot \text{tr}(G^{(k-1)}) \leq n^2 \mathbf{u} \|G^{(k-1)}\|$.

Therefore, δ_k can be understood as

$$n \mathbf{u} \|G^{(k-1)}\| \lesssim \delta_k \lesssim n^2 \mathbf{u} \|G^{(k-1)}\|.$$

Define $\alpha_k := \delta_k / \|(X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}\|$. Then $\|(X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}\| \approx \|G^{(k-1)}\|$ and

$$n\mathbf{u} \lesssim \alpha_k \lesssim n^2\mathbf{u}. \quad (32)$$

Consequently, (30) can be understood as

$$\kappa(X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}) \approx 1 + (n^2\mathbf{u})^k \cdot \kappa(A). \quad (33)$$

3.1.1. Preparation for analysis. In the same way as [7], the conditioned number of a computed Cholesky factor of ill-conditioned symmetric positive matrix is limited to not much more than around $\mathbf{u}^{-\frac{1}{2}}$.

OBSERVATION 3.1. *Let $A = A^\top \in \mathbb{F}^{n \times n}$ be positive definite. For $\delta := \text{shift}(A)$, put $\tilde{A} := fl(A + \delta I)$. Let $R := \text{chol}(\tilde{A})$. Define $\alpha := \delta / \|A\|$. Then*

$$\kappa(R) \approx \sqrt{\min\{\kappa(A), \alpha^{-1}\}}.$$

Argument If $\kappa(A) > u^{-1}$, then

$$\kappa(\tilde{A}) \approx \kappa(A + \delta I) \approx \frac{\|A\|}{\delta} \approx \alpha^{-1}$$

and $\kappa(R) \approx \alpha^{-\frac{1}{2}}$. Otherwise, $\kappa(\tilde{A}) \approx \kappa(A)$. Therefore, $\tilde{A}$ is not too ill-conditioned in any case and

$$\kappa(R) \approx \kappa(\tilde{A})^{\frac{1}{2}} \approx \kappa(A)^{\frac{1}{2}}.$$

Thus, we have

$$\kappa(R) \approx \sqrt{\min\{\kappa(A), \alpha^{-1}\}}.$$

□

We introduce the following lemmas for bounds on an inversion of a matrix.

LEMMA 3.1 (Lemma 14.1 in Higham [3]). Let $R \in \mathbb{F}^{n \times n}$ be a triangular matrix. Let $X := \text{triinv}(R)$. Then

$$|I - RX| \leq \gamma_n |R| |X| \quad \text{where} \quad \gamma_n = \frac{n\mathbf{u}}{1 - n\mathbf{u}}.$$

LEMMA 3.2. Let R and X be defined as in Lemma Table 3.1. Then

$$\|I - X^\top R^\top R X\| \leq 2\beta + \beta^2$$

where $\beta := \gamma_n \| |R| |X| \|$.

PROOF. From Lemma 3.1, we have

$$\|I - RX\| \leq \beta$$

and

$$\begin{aligned} \|I - X^\top R^\top R X\| &= \|I - (I - (I - X^\top R^\top))(I - (I - RX))\| \\ &\leq 2\|I - RX\| + \|I - RX\|^2 \\ &\leq 2\beta + \beta^2. \end{aligned}$$

□

If $\beta \leq 1$ satisfies, then $\beta^2 \leq 1$ and

$$\|I - X^\top R^\top R X\| \approx nu \|R\| \|X\|. \quad (34)$$

In the same way as Assumption 3.3 in [6], we present the following observation on the relationship between R and T .

OBSERVATION 3.2. Let A , R and δ be defined as in Observation 3.1. Let $T := \text{triinv}(R)$. Then

$$\|RT\| \approx 1 \quad \text{and} \quad \|(RT)^{-1}\| \approx 1. \quad (35)$$

Argument Define $\alpha := \delta/\|A\|$. From (32), we have $n\mathbf{u} \lesssim \alpha \lesssim n^2\mathbf{u}$. Observation 3.1 implies $\kappa(R) \approx \sqrt{\min(\kappa(A), \alpha^{-1})}$. Therefore, $\|R\|T\| \leq \kappa(R) \approx \alpha^{-\frac{1}{2}}$. From Lemma Table 3.1, we can expect in any case (35) holds. $\square$

In the same way as Observation 3.6 in [16], we present the following observation for the estimations of a norm of T and T^{-1} , respectively.

OBSERVATION 3.3. *Let A , R , T and δ be defined as in Observation 3.2. Define $\mu := \min(\kappa(A), \alpha^{-1})$ with $\alpha := \delta/\|A\|$. Then*

$$\|T\| \approx \frac{\mu^{\frac{1}{2}}}{\|R\|} \quad \text{and} \quad \|T^{-1}\| \approx \|R\|.$$

Argument By Observation 3.1, $\kappa(R)$ can be expected to be not much larger than $\alpha^{-\frac{1}{2}}$. Thus, we can expect in any case $\|T\| \approx \mu^{\frac{1}{2}}/\|R\|$. Since $T^{-1} = (RT)^{-1}R$, we have

$$\frac{\|R\|}{\|RT\|} \leq \|T^{-1}\| \leq \|(RT)^{-1}\| \|R\|.$$

From Observation 3.2, $\|RT\| \approx 1$ and $\|(RT)^{-1}\| \approx 1$. Hence, $\|T^{-1}\| \approx \|R\|$.

Next, we introduce the Rump's lemma in [16] for an estimation of a norm of a matrix.

LEMMA 3.3 (Lemma 3.7 in [16]). *Let a matrix $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$ be given which are not correlated. Suppose $n \geq 4$. Then*

$$\|A\| \geq E\left(\frac{\|Ax\|}{\|x\|}\right) \geq \frac{0.61}{\sqrt{n-1}}\|A\|,$$

where $E(\cdot)$ denotes an expectation value.

This means $\|A\|\|x\| \approx \|Ax\|$ in general.

3.1.2. Convergence. To explain (30), we first consider the case of $k = 1$ in Algorithm 2.8.

ANALYSIS 1. We utilize (22)–(28) at the first iteration in Algorithm 2.8. For readability, $R^{(1)}$, $T^{(1)}$ and $X_{1:m_1}^{(1)}$ are abbreviated to R_1 , T_1 and X_1 , respectively. Define

$$\mu_1 := \min(\kappa(A), \alpha_1^{-1}) \quad \text{with} \quad \alpha_1 := \frac{\delta_1}{\|A\|}.$$

If $A \in \mathbb{F}^{n \times n}$ is positive definite, $(n+1)(n+3)\mathbf{u} < 1$ and we can use high precision computations for dot product which satisfies (4), we analyze to show

$$\|X_1\| \approx \left(\frac{\mu_1}{\|A\|} \right)^{\frac{1}{2}}, \quad (36)$$

$$\|X_1^{-1}\| \approx \|A\|^{\frac{1}{2}}, \quad (37)$$

$$\|X_1^\top A X_1\| \approx 1 \quad \text{and} \quad (38)$$

$$\kappa(X_1^\top A X_1) \approx 1 + \alpha_1 \kappa(A). \quad (39)$$

REMARK 4. Note that for ill-conditioned A , i.e. $\kappa(A) > \alpha_1^{-1}$, we have $\mu_1 = \alpha_1^{-1}$, and the estimations (36) and (39) can be understood as

$$\|X_1\| \approx (\alpha_1 \|A\|)^{-\frac{1}{2}}.$$

REMARK 5. From (32), it holds that

$$n\mathbf{u} \lesssim \alpha_1 \lesssim n^2\mathbf{u}. \quad (40)$$

Argument Define

$$\Delta_1 := A - R_1^\top R_1.$$

From (15) and (20), it holds

$$\|\Delta_1\| \leq \|A - \tilde{A}\| + \|\tilde{A} - R_1^\top R_1\| \approx \alpha_1 \|A\| + \alpha_1 \|A\| \approx \alpha_1 \|A\|. \quad (41)$$

and

$$\|R_1\| \approx \|A\|^{\frac{1}{2}}. \quad (42)$$

By Observation 3.3 and (42), we have

$$\|X_1\| = \|T_1\| \approx \frac{\mu_1^{\frac{1}{2}}}{\|R_1\|} \approx \left(\frac{\mu_1}{\|A\|} \right)^{\frac{1}{2}}$$

and

$$\|X_1^{-1}\| \approx \|A\|^{\frac{1}{2}},$$

which explain (36) and (37), respectively.

Next we estimate $\|I - X_1^\top A X_1\|$ to show (38). It holds

$$\begin{aligned} \|I - X_1^\top A X_1\| &= \|I - X_1^\top (A - R_1^\top R_1 + R_1^\top R_1) X_1\| \\ &\leq \|I - X_1^\top R_1^\top R_1\| + \|X_1^\top (A - R_1^\top R_1) X_1\| \\ &\leq \|I - X_1^\top R_1^\top R_1 X_1\| + \|X_1^\top \Delta_1 X_1\|. \end{aligned} \quad (43)$$

From (36) and (42), we have

$$\|R_1\| \|X_1\| \approx \mu_1^{\frac{1}{2}}. \quad (44)$$

If A is ill-conditioned, i.e., $\kappa(A) \geq \alpha_1^{-1}$, then

$$\gamma_n \|R_1\| \|X_1\| \approx n\mathbf{u} \cdot \alpha_1^{-\frac{1}{2}} \lesssim (n\mathbf{u})^{\frac{1}{2}} < 1 \quad (45)$$

under the assumption $(n+1)(n+3)\mathbf{u} < 1$ and from (40). Otherwise,

$$\gamma_n \|R_1\| \|X_1\| \approx n\mathbf{u} \cdot \kappa(A)^{\frac{1}{2}} < 1. \quad (46)$$

Then, applying (34) yields

$$\|I - X_1^\top R_1^\top R_1 X_1\| \approx n\mathbf{u} \|R_1\| \|X_1\| \approx n\mathbf{u} \mu_1^{\frac{1}{2}}. \quad (47)$$

Moreover, using (41), (42) and (44), we have

$$\begin{aligned}\|X_1^\top \Delta_1 X_1\| &\leq \|X_1^\top\| \|\Delta_1\| \|X_1\| \approx \alpha_1 \|A\| \|X_1\|^2 \approx \alpha_1 (\|R_1\| \|X_1\|)^2 \\ &\approx \alpha_1 \mu_1.\end{aligned}\tag{48}$$

Inserting (47) and (48) into (43) implies

$$\|I - X_1^\top A X_1\| \approx n \mathbf{u} \mu_1^{\frac{1}{2}} + \alpha_1 \mu_1 \approx \alpha_1 \mu_1.$$

which explain (38). If A is ill-conditioned, i.e., $\kappa(A) \geq \alpha_1^{-1}$, then $\alpha_1 \mu_1 = \alpha_1 \alpha_1^{-1} \approx 1$.

Otherwise, $\alpha_1 \mu_1 = \alpha_1 \kappa(A) < 1$. Then, we have

$$\|X_1^\top A X_1\| \approx 1.\tag{49}$$

Finally, we estimate $\|(X_1^\top A X_1)^{-1}\|$ to show (39). It holds that

$$\begin{aligned}\|(X_1^\top A X_1)^{-1}\| &= \|(R_1 X_1)^{-1} (R_1 A^{-1} R_1^\top) ((R_1 X_1)^\top)^{-1}\| \\ &\leq \|(R_1 X_1)^{-1}\|^2 \|R_1 A^{-1} R_1^\top\|.\end{aligned}\tag{50}$$

Here, applying Observation 3.2 yields

$$\|(R_1 X_1)^{-1}\| \approx 1.\tag{51}$$

Let $\hat{R}_1$ denote the exact Cholesky factor of A such that $A = \hat{R}_1^\top \hat{R}_1$. Then

$$\begin{aligned}\|R_1 A^{-1} R_1^\top\| &= \|(R_1 \hat{R}_1^{-1}) ((\hat{R}_1^\top)^{-1} R_1^\top)\| = \|(R_1 \hat{R}_1^{-1})^\top (R_1 \hat{R}_1^{-1})\| \\ &= \|(\hat{R}_1^\top)^{-1} R_1^\top R_1 \hat{R}_1^{-1}\| = \|(\hat{R}_1^\top)^{-1} (A + \Delta_1) \hat{R}_1^{-1}\| \\ &\leq 1 + \|(\hat{R}_1^\top)^{-1} \Delta_1 \hat{R}_1^{-1}\| \leq 1 + \|\Delta_1\| \|\hat{R}_1^{-1}\|^2 \\ &= 1 + \|\Delta_1\| \|A^{-1}\|.\end{aligned}\tag{52}$$

From (41) and (52), we have

$$\|R_1 A^{-1} R_1^\top\| \approx 1 + \alpha_1 \kappa(A). \quad (53)$$

Inserting (51) and (53) into (50) implies

$$\|(X_1^\top A X_1)^{-1}\| \approx 1 + \alpha_1 \kappa(A).$$

This and (49) explain (39). □

Next, suppose we are at the $(k+1)$ -st iteration in Algorithm 2.8.

ANALYSIS 2. *We utilize (21)–(28) at the $(k+1)$ -st iteration in Algorithm 2.8 and the estimates in Analysis 1. For readability, $G^{(k)}$, $X_{1:m_k}^{(k)}$, $S^{(k+1)}$, $\tilde{S}^{(k+1)}$, $R^{(k+1)}$ and $X_{1:m_{k+1}}^{(k+1)}$, are abbreviated to G , X , S , $\tilde{S}$, R and X' , respectively. Define*

$$\mu := \min(\kappa(X^\top A X), \alpha_{k+1}^{-1}) \quad \text{with} \quad \alpha_{k+1} := \frac{\delta_{k+1}}{\|X^\top A X\|}. \quad (54)$$

Assume that $A \in \mathbb{F}^{n \times n}$ is positive definite, $(n+1)(n+3)\mathbf{u} < 1$ and we can use high precision computations for dot product which satisfies (4). Moreover, assume that

$$\|X\| \approx \left(\prod_{i=1}^k \alpha_i \cdot \|A\| \right)^{-\frac{1}{2}}, \quad (55)$$

$$\|X^{-1}\| \approx \|A\|^{\frac{1}{2}}, \quad (56)$$

$$\|X^\top A X\| \approx 1 \quad \text{and} \quad (57)$$

$$\kappa(X^\top A X) \approx 1 + \prod_{i=1}^k \alpha_i \cdot \kappa(A). \quad (58)$$

Then we analyze

$$\|X'\| \approx \mu^{\frac{1}{2}} \|X\|, \quad (59)$$

$$\|X'^{-1}\| \approx \|A\|^{\frac{1}{2}}, \quad (60)$$

$$\|X'^{\top} A X'\| \approx 1 \quad \text{and} \quad (61)$$

$$\kappa(X'^{\top} A X') \approx 1 + \alpha_{k+1} \cdot \kappa(X^{\top} A X). \quad (62)$$

REMARK 6. Note that for ill-conditioned $X^{\top} A X$, i.e. $\kappa(X^{\top} A X) \geq \alpha_{k+1}^{-1}$, we have $\mu = \alpha_{k+1}^{-1}$, and the estimations (59) and (62) can be understood as

$$\|X'\| \approx \left(\prod_{i=1}^{k+1} \alpha_i \cdot \|A\| \right)^{-\frac{1}{2}}$$

and

$$\kappa(X'^{\top} A X') \approx 1 + \prod_{i=1}^{k+1} \alpha_i \kappa(A) \lesssim 1 + (n^2 \mathbf{u})^{k+1} \kappa(A).$$

REMARK 7. From (32), we have

$$n\mathbf{u} \lesssim \alpha_{k+1} \lesssim n^2 \mathbf{u}. \quad (63)$$

Argument   Define

$$\Delta_2 := X^{\top} A X - R^{\top} R, \quad (64)$$

$$\Delta_3 := X' - X T. \quad (65)$$

From (21), (98), (23) and (28) in Algorithm 2.8, we have

$$\|X^{\top} A X - G\| \leq \|E\|, \quad (66)$$

$$\|G - S\| = \|E\|, \quad (67)$$

$$\|S - \tilde{S}\| \approx \delta_{k+1} = \alpha_{k+1} \|X^{\top} A X\|. \quad (68)$$

The computation of $X^\top AX$ by $\{X^\top AX\}_{k+1}^1$, (4), (55), (57) and (63) imply

$$\begin{aligned}\|E\| &\leq \varphi(\mathbf{u})\|X^\top AX\| + \varphi(\mathbf{u}^{k+1})\|X^\top\|\|A\|\|X\| \\ &\lesssim \mathbf{u} \cdot 1 + \mathbf{u}^{k+1} \cdot ((n\mathbf{u})^{\mathbf{k}})^{-1} \approx \mathbf{u}.\end{aligned}\tag{69}$$

From (57), (63), (66)–(69), it holds

$$\begin{aligned}\|X^\top AX - \tilde{S}\| &\leq \|X^\top AX - G\| + \|G - S\| + \|S - \tilde{S}\| \\ &\leq \|E\| + \|E\| + \alpha_{k+1}\|X^\top AX\| \\ &\approx \mathbf{u} + \mathbf{u} + \alpha_{k+1} \approx \alpha_{k+1}.\end{aligned}\tag{70}$$

This and (57) yield

$$\|\tilde{S}\| \approx 1 + \alpha_{k+1} \approx 1.\tag{71}$$

From (20) and (71), it holds

$$\|\tilde{S} - R^\top R\| \approx \alpha_{k+1}\|\tilde{S}\| \approx \alpha_{k+1}.\tag{72}$$

On (64), from (70) and (72), we have

$$\|\Delta_2\| \leq \|X^\top AX - \tilde{S}\| + \|\tilde{S} - R^\top R\| \approx \alpha_{k+1} + \alpha_{k+1} \approx \alpha_{k+1},\tag{73}$$

and

$$\|R\| \approx \|\tilde{S}\|^{\frac{1}{2}} \approx 1.\tag{74}$$

Hence Observation 3.3 and (74) yield

$$\|T\| \approx \frac{\mu^{\frac{1}{2}}}{\|R\|} \approx \mu^{\frac{1}{2}}, \quad \|T^{-1}\| \approx \|R\| \approx 1.\tag{75}$$

On (65), the computation of XT by $\{XT\}_{m_{k+1}}^{m_{k+1}}$ with $m_{k+1} = \lceil \frac{k+1}{2} \rceil + 1$ gives

$$\begin{aligned}\|\Delta_3\| &\leq \varphi(\mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1})\|XT\| + \varphi(\mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1})\|X\|\|T\| \\ &\approx \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1}\|X\|\|T\|.\end{aligned}\tag{76}$$

under the assumption (4). Combining (55), (63), (75) and (76) yields

$$\|\Delta_3\| \approx \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} \left(\prod_{i=1}^k \alpha_i \cdot \mu^{-1} \|A\| \right)^{-\frac{1}{2}} \lesssim \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} (n\mathbf{u})^{-\frac{k}{2}} \mu^{\frac{1}{2}} \|A\|^{-\frac{1}{2}} \tag{77}$$

In the similar way to (45) and (46), we have

$$\|\Delta_3\| \lesssim \mathbf{u} \|A\|^{-\frac{1}{2}}. \tag{78}$$

Now we estimate $\|X'\|$ in (59). Here we consider the relation between X' and XT .

Define $F := \Delta_3 T^{-1} X^{-1}$. Then

$$X' = (I + F)XT. \tag{79}$$

Combining (56), (75) and (78) yields

$$\|F\| \leq \|\Delta_3\| \|T^{-1}\| \|X^{-1}\| \approx \mathbf{u}, \tag{80}$$

and

$$\|I + F\| \approx 1 \quad \text{and} \quad \|(I + F)^{-1}\| \approx 1. \tag{81}$$

From (79), it follows

$$\frac{\|XT\|}{\|(I + F)^{-1}\|} \leq \|X'\| \leq \|I + F\| \|XT\|. \tag{82}$$

Therefore, by Lemma 3.3, (75) and (82), it follows

$$\|X'\| \approx \|XT\| \approx \|X\| \|T\| \approx \mu^{\frac{1}{2}} \|X\|,$$

which explains (59).

Next we estimate $\|X'^{-1}\|$ in (60). In a similar way to (82), we have $\|X'^{-1}\| \approx \|(XT)^{-1}\|$. Hence, from Lemma 3.3, (56) and (75), it follows

$$\|X'^{-1}\| \approx \|(XT)^{-1}\| \approx \|T^{-1}\| \|X^{-1}\| \approx \|A\|^{\frac{1}{2}},$$

which explains (60).

Next we estimate $\|I - X'^{\top}AX'\|$ to show (61). Then

$$\begin{aligned} \|I - X'^{\top}AX'\| &= \|I - (XT + \Delta_3)^{\top}A(XT + \Delta_3)\| \\ &\leq \|I - T^{\top}X^{\top}AXT\| + 2\|T^{\top}X^{\top}A\Delta_3\| + \|\Delta_3^{\top}A\Delta_3\|. \end{aligned} \quad (83)$$

Here

$$\begin{aligned} \|I - T^{\top}X^{\top}AXT\| &= \|I - T^{\top}(R^{\top}R + \Delta_2)T\| \\ &\leq \|I - T^{\top}R^{\top}RT\| + \|T^{\top}\Delta_2T\|. \end{aligned} \quad (84)$$

In a similar way to (47), applying (34) yields

$$\|I - T^{\top}R^{\top}RT\| \approx n\mathbf{u}\|T\|\|R\| \approx n\mathbf{u}\mu^{\frac{1}{2}}. \quad (85)$$

Moreover, by (73) and (75), we have

$$\|T^{\top}\Delta_2T\| \leq \|\Delta_2\|\|T\|^2 \approx \alpha_{k+1}\mu. \quad (86)$$

Inserting (85) and (86) into (84) implies

$$\|I - T^{\top}X^{\top}AXT\| \approx n\mathbf{u}\mu^{\frac{1}{2}} + \alpha_{k+1}\mu \approx \alpha_{k+1}\mu. \quad (87)$$

We estimate $\|T^\top X^\top A \Delta_3\|$ and $\|\Delta_3^\top A \Delta_3\|$ in (83). Using (57), (60), (63), (75) and (78), we have

$$\begin{aligned}\|T^\top X^\top A \Delta_3\| &= \|T^\top (X^\top A X) X^{-1} \Delta_3\| \leq \|T\| \|X^\top A X\| \|X^{-1}\| \|\Delta_3\| \\ &\lesssim \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} (n\mathbf{u})^{-\frac{k}{2}} \mu^{\frac{1}{2}}.\end{aligned}$$

In a similar way to (45) and (46), we have

$$\|T^\top X^\top A \Delta_3\| \lesssim \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} (n\mathbf{u})^{-\frac{k}{2}} (n\mathbf{u})^{-\frac{1}{2}} \approx \mathbf{u}. \quad (88)$$

Moreover, by (78), it holds

$$\|\Delta_3^\top A \Delta_3\| \leq \|\Delta_3\|^2 \|A\| \lesssim \mathbf{u}^2 \|A\|^{-1} \|A\| = \mathbf{u}^2. \quad (89)$$

Inserting (87)–(89) into (83) implies

$$\|I - X'^\top A X'\| \leq \alpha_{k+1} \mu + \mathbf{u} + \mathbf{u}^2 \approx \alpha_{k+1} \mu, \quad (90)$$

which explains (61).

To see (62), suppose first that $X^\top A X$ is not so ill-conditioned, i.e. $\kappa(X^\top A X) \leq \alpha_{k+1}^{-1}$. Then the definition (54) implies $\mu = \kappa(X^\top A X)$. Thus we have

$$\kappa(X'^\top A X') \approx 1 \approx \mu^{-1} \kappa(X^\top A X).$$

Second, suppose $X^\top A X$ is extremely ill-conditioned, i.e. $\kappa(X^\top A X) > \alpha_{k+1}^{-1}$. Then the definition (54) implies $\mu = \alpha_{k+1}^{-1}$. From (79), it holds that

$$\begin{aligned}\|(X'^\top A X')^{-1}\| &= \|((X T(I + F))^\top A X T(I + F))^{-1}\| \\ &\leq \|(T^\top X^\top A X T)^{-1}\| \|(I + F)^{-1}\|^2.\end{aligned} \quad (91)$$

On (91), it holds that

$$\begin{aligned}\|(T^\top X^\top AXT)^{-1}\| &= \|(RT)^{-1}R(X^\top AX)^{-1}R^\top((RT)^\top)^{-1}\| \\ &\leq \|(RT)^{-1}\|^2\|R(X^\top AX)^{-1}R^\top\|.\end{aligned}\tag{92}$$

Here, applying Observation 3.2 yields

$$\|(RT)^{-1}\| \approx 1.\tag{93}$$

Let $\hat{R}$ denote the exact Cholesky factor of $X^\top AX$ such that $X^\top AX = \hat{R}^\top \hat{R}$. Then

$$\begin{aligned}\|R(X^\top AX)^{-1}R^\top\| &= \|R\hat{R}^{-1}(\hat{R}^\top)^{-1}R^\top\| = \|(R\hat{R}^{-1})^\top(R\hat{R}^{-1})\| \\ &= \|(\hat{R}^\top)^{-1}R^\top R\hat{R}^{-1}\| = \|(\hat{R}^\top)^{-1}(X^\top AX + \Delta_2)\hat{R}^{-1}\| \\ &\leq 1 + \|(\hat{R}^\top)^{-1}\Delta_2\hat{R}^{-1}\|.\end{aligned}$$

Here, from (73) we have

$$\|(\hat{R}^\top)^{-1}\Delta_2\hat{R}^{-1}\| \leq \|\Delta_2\| \|(X^\top AX)^{-1}\| \approx \alpha_{k+1} \|(X^\top AX)^{-1}\|,$$

and

$$\|R(X^\top AX)^{-1}R^\top\| \approx 1 + \alpha_{k+1} \|(X^\top AX)^{-1}\|.$$

The assumption $\kappa(X^\top AX) > \alpha_{k+1}^{-1}$ with $\|X^\top AX\| \approx 1$ implies

$$\|R(X^\top AX)^{-1}R^\top\| \approx 1 + \alpha_{k+1} \|(X^\top AX)^{-1}\|.\tag{94}$$

Inserting (93) and (94) into (92) yields

$$\|(T^\top X^\top AXT)^{-1}\| \approx 1 + \alpha_{k+1} \|(X^\top AX)^{-1}\|.\tag{95}$$

Combining (81), (91) and (95), it follows that

$$\|(X'^\top AX')^{-1}\| \approx 1 \cdot (1 + \alpha_{k+1} \|(X^\top AX)^{-1}\|) \approx 1 + \alpha_{k+1} \|(X^\top AX)^{-1}\|.$$

From this, (57), (58) and (61), we have

$$\kappa(X'^\top AX') = \|X'^\top AX'\| \cdot \|(X'^\top AX')^{-1}\| \approx 1 + \alpha_{k+1} \kappa(X^\top AX)$$

which explains (62). $\square$

3.1.3. Computational complexity. The computational complexity in terms of time and space complexity of Algorithm 2.8 strongly depends on that of accurate matrix multiplication. We assume that an algorithm for accurate dot product based on the algorithms in [8, 11, 16] is used. For example, A and $X_{1:m_k}^{(k)}$ are split into $\sum_{i=1}^{h_A} D_i$ and $\sum_{i=1}^{h_X} E_i$ without rounding errors, respectively. After such matrix splitting, we have $AX_{1:m_k}^{(k)} = \sum_{i=1}^{h_A h_X} C_i$, $C_i \in \mathbb{F}^{n \times n}$ which requires $\mathcal{O}(h_A h_X n^3)$ flops. In practice, we can observe $h_A h_X \approx k^2$ at the k -th iteration. Therefore, it requires $\mathcal{O}(k^2 n^3)$ flops to compute the matrix multiplication $\{X_{1:m_{k-1}}^{(k-1)} T^{(k)}\}_{m_k}$ and $\{X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\}_{k+1}^1$ and $\mathcal{O}(n^3)$ flops to compute the rest of the algorithm at the k -th iteration. If the algorithm stops at $k = m$, then the total time complexity of Algorithm 2.8 becomes $\mathcal{O}(m^3 n^3)$ flops since $\sum_{k=1}^m k^2 n^3 = \mathcal{O}(m^3 n^3)$. By our analysis, we can see that the number of iterations m in Algorithm 2.8 as

$$m_1 = \left\lceil \frac{\log \varepsilon_{tol} - \log \kappa(A)}{\log(n^2 \mathbf{u})} \right\rceil \quad (96)$$

suffices to achieve (29).

3.2. NUMERICAL EXPERIMENTS

In this section we present some numerical results. All computations are done on Matlab 2011b and IEEE standard 754 binary64 (double precision) on a PC with 2 GHz Intel Core i7-3667U Processor, so that $\mathbf{u} = 2^{-53} \approx 1.11 \times 10^{-16}$.

For Algorithm 2.8, we adopt accurate matrix multiplication algorithms in [8, 11, 16]. From [11], the computations are automatically parallelized in BLAS and

LAPACK. We implement an algorithm for accurate matrix multiplication satisfying (4), which is based on Algorithm 2.1–2.6.

3.2.1. Results for extremely ill-conditioned matrices. We confirm our analysis of Algorithm 2.8 by some numerical experiments. As a stopping criterion for Algorithm 2.8, we set $\varepsilon_{tol} = 10^{-6}$. Define

$$\widehat{G}^{(k)} := (X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}.$$

From our analysis, we can expect $\kappa(\widehat{G}^{(k)})$ is reduced by a factor around $\alpha_k = \delta_k / \|\widehat{G}^{(k-1)}\|$ from (32) in each iteration until $\|I - \widehat{G}^{(k-1)}\| < \varepsilon_{tol}$. Then $n\mathbf{u} \lesssim \alpha_k \lesssim n^2\mathbf{u}$. From Section 3.1, we regard $\kappa(\widehat{G}^{(k)})$ as $\kappa(\widehat{G}^{(k)}) \approx (n^2\mathbf{u})^k \kappa(A)$. However, from (31), δ_k indeed depends on the trace of $\widehat{G}^{(k-1)}$, i.e., $\delta_k \approx n\mathbf{u} \cdot \text{tr}(\widehat{G}^{(k-1)})$. In some cases, $\text{tr}(\widehat{G}^{(k-1)}) \ll n\|\widehat{G}^{(k-1)}\|$ may occur. In this section, we define β_k as

$$\beta_k := \frac{\text{tr}(\widehat{G}^{(k-1)})}{\|\widehat{G}^{(k-1)}\|}.$$

Then

$$\delta_k \approx n\mathbf{u} \cdot \beta_k \|\widehat{G}^{(k-1)}\|.$$

Moreover, we define c_k as

$$\begin{aligned} c_1 &:= \beta_1 \\ c_k &:= c_{k-1} \cdot \beta_k \quad \text{for } k \geq 2. \end{aligned}$$

We observe how $\kappa(\widehat{G}^{(k)})$ reduces in each iteration by a factor $n\mathbf{u}\beta_k$, as compared with $n^2\mathbf{u}$.

First, we deal with the Higham's test matrices [3] on Matlab:

`randsvd` — Random matrix with pre-assigned singular values.

`A = gallery('randsvd',n,kappa,mode,kl,ku)`

returns a banded (multidiagonal) random matrix of order `n` with

TABLE 3.1. Results for Higham's test matrix with $n = 2000$ and $\kappa(A) \approx 2.89 \cdot 10^{16}$.

k	$\kappa(X^{(k)})$	I		β_k
		$\sqrt{(n^2 \mathbf{u})^k}$	$\sqrt{(n \mathbf{u})^k c_k}$	
1	$4.74 \cdot 10^4$	$4.74 \cdot 10^4$	$4.74 \cdot 10^4$	1999
2	$1.70 \cdot 10^8$	$2.25 \cdot 10^9$	$2.25 \cdot 10^9$	2000
3	$1.70 \cdot 10^8$	$1.07 \cdot 10^{14}$	$1.07 \cdot 10^{14}$	2000

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	$(n \mathbf{u})^k c_k \kappa(A)$	$\ I - \widehat{G}^{(k)}\ $
1	$1.29 \cdot 10^7$	$1.29 \cdot 10^7$	$1.29 \cdot 10^7$	$1.00 \cdot 10^0$
2	$1.00 \cdot 10^0$	$5.72 \cdot 10^{-3}$	$5.72 \cdot 10^{-3}$	$5.68 \cdot 10^{-3}$
3	$1.00 \cdot 10^0$	$2.54 \cdot 10^{-12}$	$2.54 \cdot 10^{-12}$	$4.47 \cdot 10^{-10}$

`cond(A) = kappa` and singular values from the distribution mode.

If `n` is a two-element vector, `A` is `n(1)`-by-`n(2)`.

Mode may be one of the following values:

- 1: One large singular value.
- 2: One small singular value.
- 3: Geometrically distributed singular values (default).
- 4: Arithmetically distributed singular values.
- 5: Random singular values with uniformly distributed logarithm.

We generate matrices A by $A = \text{gallery}('randsvd', n, cnd, 3)$. We set $n = 2000$ and $cnd = 10^{16}$. Then $A \in \mathbb{F}^{2000 \times 2000}$ with $\kappa(A) \approx 2.89 \cdot 10^{16}$ is generated whose results are shown in Table 3.1.

Next, we deal with the Hilbert matrix. Due to rounding errors the condition number of floating-point Hilbert matrix is limited not far from $\mathbf{u}^{-1}$. Therefore we use the Hilbert matrix scaled by the least common multiple of the denominators as follows:

$$H_n = (h_{ij}) \in \mathbb{F}^{n \times n} \quad \text{with} \quad h_{ij} := \text{lcm}(1, 2, \dots, 2n-1)/(i+j-1).$$

TABLE 3.2. Results for scaled Hilbert matrix with $n = 21$ and $\kappa(A) \approx 8.16 \cdot 10^{29}$.

k	$\kappa(X^{(k)})$	I		β_k
		$\sqrt{(n^2 \mathbf{u})^k}$	$\sqrt{(n \mathbf{u})^k c_k}$	
1	$1.77 \cdot 10^7$	$4.42 \cdot 10^6$	$1.77 \cdot 10^7$	1.3062
2	$9.85 \cdot 10^{13}$	$1.95 \cdot 10^{13}$	$9.95 \cdot 10^{13}$	12.8547
3	$9.03 \cdot 10^{14}$	$8.61 \cdot 10^{19}$	$4.52 \cdot 10^{20}$	17.9578

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	$(n \mathbf{u})^k c_k \kappa(A)$	$\ I - \widehat{G}^{(k)}\ $
1	$2.61 \cdot 10^{15}$	$4.19 \cdot 10^{16}$	$2.60 \cdot 10^{15}$	$1.00 \cdot 10^0$
2	$8.41 \cdot 10^1$	$2.15 \cdot 10^3$	$8.24 \cdot 10^1$	$9.88 \cdot 10^{-1}$
3	$1.00 \cdot 10^0$	$1.10 \cdot 10^{-10}$	$4.00 \cdot 10^{-12}$	$4.09 \cdot 10^{-12}$

Here H_n is an integer matrix whose elements are exactly representable in binary64 floating-point numbers for $n \leq 21$ with $\kappa(H_{21}) = 8.16 \cdot 10^{29}$. The results of Algorithm 2.8 for $A = H_{21}$ are shown in Table 3.2.

Moreover, we generate a test matrix with a specified condition number by $A := Q\Sigma Q^\top \in \mathbb{F}_{[\lceil \log_{10}(cnd)/\mathbf{u} \rceil]}^{n \times n}$, where $Q \in \mathbb{F}^{n \times n}$ is a random orthogonal matrix, $\Sigma := \text{logspace}(1, \log_{10}(cnd), n)$ and cnd is the condition number of A . We name this function *testmatrix*(n, cnd). We also give the complete Matlab-code in Appendix. We set $n = 100$, $cnd = 10^{100}$. Then $A \in \mathbb{F}_{[7]}^{100 \times 100}$ with $\kappa(A) \approx 1.00 \cdot 10^{100}$ is generated, whose results are shown in Table 3.3. Finally, we deal with the random matrix, which is based on the function *randmat* in INTLAB [14], and surely generates symmetric and positive definite matrices. We name the function *randmatsym*(n, cnd). This function use unit lower triangular L and compute $A = L^\top A$, $A = A^\top A$ until $\kappa(A) \geq cnd$. We set $n = 500$ and $cnd = 10^{50}$. Then $A \in \mathbb{F}^{500 \times 500}$ with $\kappa(A) \approx 4.756 \cdot 10^{53}$ is generated, whose results are shown in Table 3.4. And, we set $n = 1000$ with $cnd = 10^{100}$. Then $A \in \mathbb{F}^{1000 \times 1000}$ with $\kappa(A) \approx 8.297 \cdot 10^{102}$ is generated, whose results are shown in Table 3.5.

In all of the numerical experiments, it can be seen that the convergence speed of $\kappa(\widehat{G}^{(k)})$ for $k \geq 2$ is about $(n^2 \mathbf{u})^k \kappa(A)$ during $\kappa(\widehat{G}^{(k)}) > \mathbf{u}^{-1}$, which is consistent with (62) in Analysis 2 as expected. However, for $k = 1$, we can observe $\kappa(\widehat{G}^{(1)})$ is relatively

TABLE 3.3. Result for the test matrix with $n = 100$ and $\kappa(A) \approx 1.00 \times 10^{100}$.

k	$\kappa(X^{(k)})$	1		β_k
		$\frac{1}{\sqrt{(n^2\mathbf{u})^k}}$	$\frac{1}{\sqrt{(n\mathbf{u})^k c_k}}$	
1	$8.93 \cdot 10^{06}$	$9.40 \cdot 10^{05}$	$8.93 \cdot 10^{06}$	1.1083
2	$2.22 \cdot 10^{13}$	$8.83 \cdot 10^{11}$	$2.22 \cdot 10^{13}$	14.261
3	$4.02 \cdot 10^{19}$	$8.30 \cdot 10^{17}$	$4.02 \cdot 10^{19}$	26.927
4	$6.03 \cdot 10^{25}$	$7.80 \cdot 10^{23}$	$6.03 \cdot 10^{25}$	39.316
5	$7.89 \cdot 10^{31}$	$7.33 \cdot 10^{29}$	$7.89 \cdot 10^{31}$	51.545
6	$9.30 \cdot 10^{37}$	$6.89 \cdot 10^{35}$	$9.29 \cdot 10^{37}$	63.657
7	$1.00 \cdot 10^{44}$	$6.47 \cdot 10^{41}$	$1.00 \cdot 10^{44}$	75.678
8	$7.10 \cdot 10^{49}$	$6.08 \cdot 10^{47}$	$1.01 \cdot 10^{50}$	87.624
9	$1.00 \cdot 10^{50}$	$5.71 \cdot 10^{53}$	$9.50 \cdot 10^{55}$	99.406

k	$\kappa(\widehat{G}^{(k)})$	$(n^2\mathbf{u})^k \kappa(A)$	$(n\mathbf{u})^k c_k \kappa(A)$	$\ I - \widehat{G}^{(k)}\ $
1	$1.25 \cdot 10^{86}$	$1.13 \cdot 10^{88}$	$1.26 \cdot 10^{86}$	$1.00 \cdot 10^{00}$
2	$2.02 \cdot 10^{73}$	$1.28 \cdot 10^{76}$	$2.03 \cdot 10^{73}$	$1.00 \cdot 10^{00}$
3	$6.18 \cdot 10^{60}$	$1.45 \cdot 10^{64}$	$6.18 \cdot 10^{60}$	$1.00 \cdot 10^{00}$
4	$2.75 \cdot 10^{48}$	$1.64 \cdot 10^{52}$	$2.75 \cdot 10^{48}$	$1.00 \cdot 10^{00}$
5	$1.61 \cdot 10^{36}$	$1.86 \cdot 10^{40}$	$1.61 \cdot 10^{36}$	$1.00 \cdot 10^{00}$
6	$1.16 \cdot 10^{24}$	$2.11 \cdot 10^{28}$	$1.16 \cdot 10^{24}$	$1.00 \cdot 10^{00}$
7	$9.92 \cdot 10^{11}$	$2.39 \cdot 10^{16}$	$9.92 \cdot 10^{11}$	$1.00 \cdot 10^{00}$
8	$1.98 \cdot 10^{00}$	$2.70 \cdot 10^{04}$	$9.85 \cdot 10^{-1}$	$4.96 \cdot 10^{-1}$
9	$1.00 \cdot 10^{00}$	$3.06 \cdot 10^{-8}$	$1.11 \cdot 10^{-12}$	$2.23 \cdot 10^{-12}$

much less than $(n^2\mathbf{u})\kappa(A)$. This difference is caused by regarding $\delta_1 \approx n^2\mathbf{u}\|A\|$ instead of $\delta_1 \approx n\mathbf{u} \cdot \text{tr}(A)$. In fact, we observe $\beta_1 \approx 1$ in Table 3.2 and Table 3.3. This means $\delta_1 \approx n\mathbf{u}\|A\|$. In the same way in Table 3.4 and Table 3.5, we can observe $\beta_1 \approx 20$, which is much less than n . In Table 3.1, we can observe $\beta_1 \approx n$. This means $\delta_1 \approx n^2\mathbf{u}\|A\|$. In our analysis, the perturbation $\delta_k \approx \alpha_k \|\widehat{G}^{(k-1)}\|$ causes an improvement of $X^{(k)}$ as a preconditioner by a factor $1/\sqrt{\alpha_k}$. Therefore, $\kappa(\widehat{G}^{(k)})$ is reduced by a factor around α_k in each iteration until $\kappa(\widehat{G}^{(k)}) \approx 1$. In Table 3.2, Table 3.4 and Table 3.5, for $k = 1$, $\delta_1 \approx n\mathbf{u}\beta_1\|A\|$ causes an improvement of $X^{(1)}$ as a preconditioner by a factor $1/\sqrt{n\mathbf{u}\beta_1}$ rather than $1/\sqrt{n^2\mathbf{u}}$ in practice. Therefore, $\kappa(\widehat{G}^{(1)})$ reduces by a factor $n\mathbf{u}\beta_1$ from $\kappa(A)$. For $k \geq 2$, we can observe $\beta_k \approx n$, so that $\delta_k \approx n^2\mathbf{u}\|\widehat{G}^{(k-1)}\|$. It means $n\mathbf{u}\beta_k \approx n^2\mathbf{u}$ as shown in the tables.

TABLE 3.4. Result for Rump's random matrix with $n = 500$ and $\kappa(A) \approx 4.756 \times 10^{53}$.

k	$\kappa(X^{(k)})$	1		β_k
		$\frac{1}{\sqrt{(n^2 \mathbf{u})^k}}$	$\frac{1}{\sqrt{(n \mathbf{u})^k c_k}}$	
1	$8.94 \cdot 10^5$	$1.90 \cdot 10^5$	$8.94 \cdot 10^5$	22.48
2	$1.86 \cdot 10^{11}$	$3.60 \cdot 10^{10}$	$1.86 \cdot 10^{11}$	417.24
3	$3.64 \cdot 10^{16}$	$6.82 \cdot 10^{15}$	$3.64 \cdot 10^{16}$	462.86
4	$7.00 \cdot 10^{21}$	$1.29 \cdot 10^{21}$	$7.00 \cdot 10^{21}$	483.46
5	$6.13 \cdot 10^{26}$	$2.45 \cdot 10^{26}$	$1.33 \cdot 10^{27}$	494.23
6	$6.90 \cdot 10^{26}$	$4.65 \cdot 10^{31}$	$2.53 \cdot 10^{32}$	499.07

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	$(n \mathbf{u})^k c_k \kappa(A)$	$\ I - \widehat{G}^{(k)}\ $
1	$5.95 \cdot 10^{41}$	$1.32 \cdot 10^{43}$	$5.95 \cdot 10^{41}$	$1.00 \cdot 10^0$
2	$1.38 \cdot 10^{31}$	$3.68 \cdot 10^{32}$	$1.38 \cdot 10^{31}$	$1.00 \cdot 10^0$
3	$3.59 \cdot 10^{20}$	$1.02 \cdot 10^{22}$	$3.59 \cdot 10^{20}$	$1.00 \cdot 10^0$
4	$9.71 \cdot 10^9$	$2.85 \cdot 10^{11}$	$9.71 \cdot 10^9$	$1.00 \cdot 10^0$
5	$1.27 \cdot 10^0$	$7.91 \cdot 10^0$	$2.67 \cdot 10^{-01}$	$2.11 \cdot 10^{-1}$
6	$1.00 \cdot 10^0$	$2.20 \cdot 10^{-10}$	$7.43 \cdot 10^{-12}$	$3.52 \cdot 10^{-11}$

TABLE 3.5. Result for Rump's random matrix with $n = 1000$ and $\kappa(A) \approx 8.297 \times 10^{102}$.

k	$\kappa(X^{(k)})$	I		β_k
		$\sqrt{(n^2 \mathbf{u})^k}$	$\sqrt{(n \mathbf{u})^k c_k}$	
1	$6.96 \cdot 10^{05}$	$9.49 \cdot 10^{04}$	$6.96 \cdot 10^{05}$	18.5542
2	$8.25 \cdot 10^{10}$	$9.00 \cdot 10^{09}$	$8.25 \cdot 10^{10}$	641.5675
3	$8.64 \cdot 10^{15}$	$8.54 \cdot 10^{14}$	$8.64 \cdot 10^{15}$	808.4217
4	$8.68 \cdot 10^{20}$	$8.10 \cdot 10^{19}$	$8.68 \cdot 10^{20}$	886.8454
5	$8.52 \cdot 10^{25}$	$7.68 \cdot 10^{24}$	$8.52 \cdot 10^{25}$	929.4879
6	$8.27 \cdot 10^{30}$	$7.29 \cdot 10^{29}$	$8.27 \cdot 10^{30}$	954.4152
7	$7.96 \cdot 10^{35}$	$6.91 \cdot 10^{34}$	$7.96 \cdot 10^{35}$	969.8176
8	$7.61 \cdot 10^{40}$	$6.56 \cdot 10^{39}$	$7.61 \cdot 10^{40}$	981.9896
9	$7.25 \cdot 10^{45}$	$6.22 \cdot 10^{44}$	$7.25 \cdot 10^{45}$	989.9882
10	$6.71 \cdot 10^{50}$	$5.90 \cdot 10^{49}$	$6.90 \cdot 10^{50}$	995.4252
11	$2.88 \cdot 10^{51}$	$5.60 \cdot 10^{54}$	$6.54 \cdot 10^{55}$	998.9877

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	$(n \mathbf{u})^k c_k \kappa(A)$	$\ I - \widehat{G}^{(k)}\ $
1	$1.71 \cdot 10^{91}$	$9.22 \cdot 10^{92}$	$1.71 \cdot 10^{91}$	$1.00 \cdot 10^{00}$
2	$1.22 \cdot 10^{81}$	$1.02 \cdot 10^{83}$	$1.22 \cdot 10^{81}$	$1.00 \cdot 10^{00}$
3	$1.11 \cdot 10^{71}$	$1.14 \cdot 10^{73}$	$1.11 \cdot 10^{71}$	$1.00 \cdot 10^{00}$
4	$1.10 \cdot 10^{61}$	$1.27 \cdot 10^{63}$	$1.10 \cdot 10^{61}$	$1.00 \cdot 10^{00}$
5	$1.14 \cdot 10^{51}$	$1.41 \cdot 10^{53}$	$1.14 \cdot 10^{51}$	$1.00 \cdot 10^{00}$
6	$1.21 \cdot 10^{41}$	$1.56 \cdot 10^{43}$	$1.21 \cdot 10^{41}$	$1.00 \cdot 10^{00}$
7	$1.31 \cdot 10^{31}$	$1.74 \cdot 10^{33}$	$1.31 \cdot 10^{31}$	$1.00 \cdot 10^{00}$
8	$1.43 \cdot 10^{21}$	$1.93 \cdot 10^{23}$	$1.43 \cdot 10^{21}$	$1.00 \cdot 10^{00}$
9	$1.58 \cdot 10^{11}$	$2.15 \cdot 10^{13}$	$1.58 \cdot 10^{11}$	$1.00 \cdot 10^{00}$
10	$1.84 \cdot 10^{01}$	$2.38 \cdot 10^{03}$	$1.74 \cdot 10^{01}$	$9.46 \cdot 10^{-01}$
11	$1.00 \cdot 10^{00}$	$2.65 \cdot 10^{-7}$	$1.94 \cdot 10^{-09}$	$2.05 \cdot 10^{-09}$

3.2.2. Comparison with long precision arithmetic. We present some numerical results comparing Algorithm 2.8 with a standard Cholesky factorization applying a diagonal shift by using long precision arithmetic such as GMP [2] and MPFR [5]. We measure computing time for verifying the positive definiteness of an input matrix. For this purpose, we use the Rump’s corollary in [15].

COROLLARY 3.1 (Corollary 2.4 in [15]). *Let $\tilde{A} \in \mathbb{F}^{n \times n}$ be given with $\tilde{A} = A$ for $i \neq j$ and $\tilde{A} \leq A - cI$ where $c := c'_n \mathbf{u} \cdot \text{tr}(A) \in \mathbb{F}$ for $i = j$. If the floating-point Cholesky factorization applied to $\tilde{A}$ runs to completion, then A is positive definite.*

We adopt the following Matlab routine `mpfr_chol_spd`, in which computational precision 2^{-d} is doubled per iteration with starting at $d = 53$:

```
function [info] = mpfr_chol_spd(A)
n = size(A);
d = 53;                                % d=106, 212, 424,...
kmax = 20;
for k = 1:kmax
    Eps = 2^(-d);
    feature('setround',inf);           % rounding upwards
    c_n = (n+1)/(1 - 2*(n+1)*Eps);
    alpha = c_n*Eps*trace(A);         % shift for A
    if k == 1
        feature('setround',-inf);     % rounding downwards
        B = A - alpha*eye(n);
    end
    feature('setround',0.5);           % rounding to nearest
    if k == 1
        [R,info] = chol(B);           % Matlab's chol for d=53
    else
end
```

```

        info = mpfr_vchol(A,alpha,d);
    end
    if info == 0
        return
    end
    d = 2*d;
end

```

In this function, we use GMP [2] and MPFR [5], which are widely used as fast and standard long precision libraries. We implement Cholesky factorization using MPFR as Matlab's MEX function `mpfr_vchol` without any parallelization. In `mpfr_vchol`, the double precision input A and the shift `alpha` is converted to d -bit precision numbers. Then d -bit precision arithmetic is internally used. If Cholesky factorization runs to completion, then `info` = 0 as the result of `mpfr_vchol` is obtained. We give the complete C-code `mpfr_vchol` in Appendix. Note that only one core is used for `mpfr_chol_spd`, so that its computing time may be halved in an ideal case.

As mentioned before, Algorithm 2.8 uses for accurate matrix multiplication, which is based on the algorithms for accurate sum and dot product proposed in [8, 18, 19]. Note that the resultant m_1 where the number of iterations for Algorithm 2.8 coincides with (96). From Theorem 3.2 in Chpter 2, we set $\varepsilon_{tol} = 1$.

Now we observe the computing time for two examples. We again use Rump matrix [13]. Here, t_1 and t_2 denote the computing time for Algorithm 2.8 and that for `mpfr_chol_spd`, respectively.

First, we fix $n = 2000$ and vary anticipated condition numbers cnd from 10^{20} to 10^{100} . The results are displayed in Table 3.6. As can be seen, t_1 gradually increases according to the condition numbers. For more than $cnd = 10^{60}$, t_1 is from 2 to 3 times larger than t_2 . This is because the computational cost of the Algorithm 2.8 is strongly dependent on that of an algorithm for accurate matrix multiplication which

TABLE 3.6. Result for Rump matrix $randmatsym(n, cnd)$ with $n = 2000$ and several anticipated condition numbers cnd (t_i : elapsed time [sec], m_1 : number of iterations for Algorithm 2.8, d : computational precision for MPFR as 2^{-d}).

cnd	$\kappa(A)$	Algorithm 2.8		mpfr_chol_spd	
		t_1	m_1	t_2	$\frac{d}{53}$
10^{20}	$8.4424 \cdot 10^{21}$	70.731	3	126.214	2
10^{40}	$8.0047 \cdot 10^{42}$	199.59	5	290.470	4
10^{60}	$1.4189 \cdot 10^{65}$	436.04	7	294.928	4
10^{80}	$5.2528 \cdot 10^{83}$	749.46	9	520.633	8
10^{100}	$5.9425 \cdot 10^{107}$	1431.87	12	530.825	8

TABLE 3.7. Result for Rump matrix $randmatsym(n, cnd)$ with several n and $\kappa(A) \approx 10^{19}$ (t_i : elapsed time [sec], m : number of iterations for Algorithm 2.8, d : computational precision for MPFR as 2^{-d}).

n	Algorithm 2.8		mpfr_chol_spd	
	t_1	m_1	t_2	$\frac{d}{53}$
500	1.02	2	2.096	2
1000	4.60	2	16.219	2
2000	28.08	2	126.525	2
3000	224.44	3	424.724	2
4000	496.18	3	975.986	2
5000	1015.08	3	2003.862	2

requires $\mathcal{O}(m^3n^3)$ flops, while that of `mpfr_vchol` requires $\mathcal{O}(n^3)$ with large constant per iteration. Namely, in case of A being extremely ill-conditioned, i.e. $\kappa(A) \geq 10^{60}$, `mpfr_chol_spd` has an advantage over Algorithm 2.8 in terms of computational cost.

Next, we fix $cnd = 10^{19}$ and vary n from 500 to 5000. The results are displayed in Table 3.7. As expected, t_1 is much smaller than t_2 . We observe that t_2 increases in $\mathcal{O}(n^3)$ according to the dimension n , while t_1 does not in $\mathcal{O}(m^3n^3)$ for smaller n . Note that the BLAS and the LAPACK routines adopted in Matlab are provided by Intel Math Kernel Library are highly optimized. In particular, in the case of $n \geq 4000$, we expect that they achieve near-peak performance. It turns out that Algorithm 2.8 brings out the computer performance to the maximum rather than `mpfr_chol_spd`.

CHAPTER 4

A MODIFIED ALGORITHM FOR ACCURATE INVERSE CHOLESKY FACTORIZATION

In this chapter, we consider the accuracy on $X_{1:m_k}^{(k)} \in \mathbb{F}_{[m_k]}^{n \times n}$ provided by Algorithm 2.8. In Section 4.1, a modified version of the algorithm is proposed. It is explained that the proposed algorithm gives more accurate results than the original one by a numerical analysis in Section 4.2. In Section 4.3, Numerical evidence is also shown.

4.1. PROPOSED ALGORITHM

From (90) in Analysis 2 in Section 3.1, it holds that

$$\|I - X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\| \approx \alpha_k \mu$$

where $\mu := \min(\kappa((X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}), \alpha_k^{-1})$. From (32), we have $n\mathbf{u} \lesssim \alpha_k \lesssim n^2\mathbf{u}$. If $\kappa((X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}) > \alpha_k^{-1}$, then the definition of μ implies $\mu = \alpha_k^{-1}$ and

$$\|I - X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\| \approx 1.$$

Otherwise, $\mu = \kappa((X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)})$ and

$$\|I - X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\| < 1.$$

Furthermore, in the best case as $\kappa((X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}) = 1$, we have $\mu = 1$ and

$$\|I - X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\| \approx \alpha_k.$$

Therefore, it holds that

$$\alpha_k \approx \|I - X_{1:m_k}^{(k)\top} A X_{1:m_k}^{(k)}\| < 1. \quad (97)$$

The reason why α_k is the lower bound is due to the diagonal shift (98) in Algorithm 2.8. To overcome (97), we add a condition such that Cholesky factorization never breaks down without a diagonal shift.

For a symmetric matrix $A = (a_{ij}) \in \mathbb{F}^{n \times n}$ with $a_{ii} > 0$ for all i , the following algorithm calculates an upper triangular matrix $X_{1:m_M}^{(M)} \mathbb{F}_{[m_k]}^{n \times n}$ where $M := k + 1$ for some $k \in \mathbb{N}$ such that $\|X_{1:m_M}^{(M)T} A X_{1:m_M}^{(M)} - I\| \approx \mathbf{u}$.

ALGORITHM 4.1. *Accurate inverse Cholesky factorization, modified version.*

$$\begin{aligned}
& \text{function } [X_{1:m_M}^{(M)}] = \text{accchol\_mod}(A) \\
& k = 0, \quad G^{(0)} := A_{1:1}, \quad E^{(0)} := O, \quad X_{1:1}^{(0)} := I \\
& \text{repeat} \\
& \quad k = k + 1 \\
& \quad \text{Compute } S^{(k)} \in \mathbb{F}^{n \times n} \text{ with} \\
& \quad \quad \begin{cases} S_{ii}^{(k)} = \text{fl}_\Delta(G_{ii}^{(k-1)} + \|E^{(k-1)}\|_\infty) \\ S_{ij}^{(k)} = G_{ij}^{(k-1)} \text{ for } i \neq j. \end{cases} \\
& \quad \delta_k := \text{shift}(S^{(k)}) \\
& \quad R^{(k)} := \text{chol}(\text{fl}(S^{(k)} + \delta_k I)) \tag{98} \\
& \quad T^{(k)} := \text{triinv}(R^{(k)}) \\
& \quad m_k := \lceil \frac{k}{2} \rceil + 1 \\
& \quad X_{1:m_k}^{(k)} := \{X_{1:m_{k-1}}^{(k-1)} T^{(k)}\}_{m_k} \\
& \quad \langle G^{(k)}, E^{(k)} \rangle := \{X_{1:m_k}^{(k)T} A X_{1:m_k}^{(k)}\}_{k+1}^1 \tag{99} \\
& \quad \beta := \text{fl}_\nabla(\min(G_{ii}^{(k)} - r_i(G^{(k)}))) \\
& \quad \mu := \text{fl}_\Delta(c'_n \mathbf{u} \cdot \text{tr}(G^{(k)})) \quad \% c'_n := \frac{n+1}{1-2(n+1)\mathbf{u}} \\
& \text{until } \beta > \max(\mu, \|E^{(k)}\|_\infty) \tag{100} \\
& \quad R^{(M)} := \text{chol}(G^{(M-1)}) \quad \% M := k + 1 \\
& \quad T^{(M)} := \text{triinv}(R^{(M)}) \\
& \quad m_M := \lceil \frac{k+1}{2} \rceil + 1 \\
& \quad X_{1:m_M}^{(M)} := \{X_{1:m_k}^{(M-1)} T^{(M)}\}_{m_M}
\end{aligned}$$

In the following, we explain how to determine (100). For readability, $G^{(k)}$, $X_{1:m_k}^{(k)}$ and $X_{1:m_M}^{(M)}$ where $M := k + 1$ are abbreviated to G , X and X' , respectively. Let R' be a computed Cholesky factor of G , i.e., $R' = \text{chol}(G)$. Define

$$\Delta_1 := G - X^\top AX, \quad (101)$$

$$\Delta_2 := G - R'^\top R', \quad (102)$$

$$T := \text{triinv}(R'), \quad (103)$$

$$\Delta_3 := X' - XT, \quad (104)$$

By the definition (102), it is necessary to satisfy

$$\lambda_n(G - \Delta_2) > 0.$$

By (15) and a Weyl's theorem (e.g. Corollary 4.9 in [21]) for (102), it holds that

$$\lambda_n(G - \Delta_2) \geq \lambda_n(G) - \|\Delta_2\|, \quad \|\Delta_2\| \leq c'_n \mathbf{u} \cdot \text{tr}(G). \quad (105)$$

The Gerschgorin's circle theorem implies

$$\lambda_k(G) \in \bigcup_{i=1}^n \{x \in \mathbb{R} : |x - G_{ii}| \leq r_i(G)\}, \quad k = 1, 2, \dots, n$$

and

$$\lambda_n(G) \geq \beta \quad \text{where} \quad \beta := \min(G_{ii} - r_i(G)). \quad (106)$$

From (105) and (106), we have

$$\lambda_n(G - \Delta_2) \geq \beta - \|\Delta_2\|. \quad (107)$$

Moreover, to ensure the positive definiteness of A with taking care of the rounding errors, it is necessary to satisfy

$$\lambda_n(X^\top AX) > 0.$$

By a Weyl's theorem (e.g. Corollary 4.9 in [21]) for (101), it holds that

$$\lambda_n(X^\top AX) \geq \lambda_n(G) - \|\Delta_1\|.$$

From (106), we have

$$\lambda_n(X^\top AX) \geq \beta - \|\Delta_1\|. \quad (108)$$

Therefore, combining (107) and (108), the sufficient condition to make $chol(G)$ run to completion and to ensure the positive definiteness of A is

$$\beta > \max(\|\Delta_1\|, \|\Delta_2\|). \quad (109)$$

4.2. ANALYSIS OF ACCURACY ON X

The target of this subsection is to explain that $\|X'^\top AX' - I\| \approx \mathbf{u}$ if $G^{(k)}$ satisfy (109) at the k -th iteration. For later use, we present the following observation.

OBSERVATION 4.1. *Let $A = (a_{ij}) \in \mathbb{F}^{n \times n}$ be symmetric and positive definite. Split $A = I + E$. Let E_U be the strictly upper triangular part of E . Suppose $\|E\| \leq \alpha \ll 1$. Let a triangular matrix $R = (r_{ij}) \in \mathbb{F}^{n \times n}$ be a computed Cholesky factor of A , i.e., $R = chol(A)$. We use Algorithm 2.7. Then*

$$R \approx I + E_U, \quad \|E_U\| \leq \alpha \quad \text{and} \quad \|A - R^\top R\| \lesssim \mathbf{u} + n\alpha^2.$$

Argument First, we estimate diagonal and off-diagonal elements of R , respectively. Here $\text{fl}(\cdot)$ means that arithmetic inside the parenthesis is done in binary64

floating point arithmetic. It follows that

$$\begin{aligned} r_{jj} &= \text{fl} \left((a_{jj} - \sum_{k=1}^{j-1} r_{kj}^2)^{\frac{1}{2}} \right) = (1 + \epsilon)(a_{jj} - \epsilon_1)^{\frac{1}{2}} \\ &= (1 + \epsilon)(1 + \epsilon')^{\frac{1}{2}} \approx 1 + \frac{1}{2}\epsilon' \end{aligned} \quad (110)$$

$$|\epsilon| \leq \mathbf{u}, \quad |\epsilon_1| \leq (n-1)\alpha^2, \quad |\epsilon'| \approx \alpha,$$

and

$$r_{ij} = \text{fl} \left((a_{ij} - \sum_{k=1}^{i-1} r_{ki}r_{kj})/r_{ii} \right) = a_{ij} + \epsilon_2 \quad \text{for } i < j, \quad |\epsilon_2| \approx \alpha^2. \quad (111)$$

Thus, we have $r_{jj} \lesssim 1 + \frac{1}{2}\alpha$ and $|r_{ij}| \lesssim \alpha$. Then $R \approx I + E_U$.

Next, we estimate $\|A - R^\top R\|$. On the off-diagonal elements, it holds [3, p.197] that

$$|a_{ij} - \sum_{k=1}^i r_{ki}r_{kj}| \leq \gamma_i \sum_{k=1}^i |r_{ki}||r_{kj}| \quad \text{where} \quad \gamma_i = \frac{i\mathbf{u}}{1 - i\mathbf{u}}.$$

Here, from (110) and (111), we have

$$\begin{aligned} |a_{ij} - \sum_{k=1}^i r_{ki}r_{kj}| &\leq \gamma_i \left(\sum_{k=1}^{i-1} |r_{ki}||r_{kj}| + |r_{ii}||r_{ij}| \right) \\ &\approx (n-1)\mathbf{u}((n-2)\alpha^2 + (1 + \frac{1}{2}\alpha)\alpha) \approx n\mathbf{u}\alpha. \end{aligned}$$

From (110), $r_{jj}^2 = (1 + \epsilon)^2(a_{jj} - \epsilon_1) \approx (1 + 2\epsilon)a_{jj}$. Hence, it holds that

$$\begin{aligned} |a_{jj} - \sum_{k=1}^j r_{kj}^2| &\leq |a_{jj} - r_{jj}^2| + \sum_{k=1}^{j-1} r_{kj}^2 \approx |a_{jj} - (1 + 2\epsilon)a_{jj}| + (n-1)\alpha^2 \\ &\approx 2|\epsilon|a_{jj} + n\alpha^2 \approx \mathbf{u} + n\alpha^2. \end{aligned}$$

Therefore, we have $\|A - R^\top R\| \approx n\mathbf{u}\alpha + \mathbf{u} + n\alpha^2 \approx \mathbf{u} + n\alpha^2$.

REMARK 8. If $n\alpha^2 < \mathbf{u}$, then $\|A - R^\top R\| \approx \mathbf{u}$.

OBSERVATION 4.2. *Let R and E_U be defined as in Observation 4.1. Let $T := \text{trinv}(R)$. Then*

$$T \approx I - E_U \quad \text{and} \quad \|T\| \approx 1.$$

Argument From Observation 4.1, it follows that $R \approx I + E_U$ and $\|E_U\| \ll 1$. Then

$$T = (I + E_U)^{-1} = I - E_U + E_U^2 - E_U^3 + \dots \approx I - E_U$$

and

$$\|T\| \approx 1.$$

OBSERVATION 4.3. *Let R , T and E_U be defined as in Observations 4.1 and 4.2. Then*

$$\|I - T^\top R^\top R T\| \approx \alpha^2.$$

Argument From Observations 4.1 and 4.2, it follows that

$$RT \approx (I + E_U)(I - E_U) = I - E_U^2$$

and

$$\|I - T^\top R^\top R T\| \approx \|I - (I - E_U^2)^\top (I - E_U^2)\| \approx \|E_U^2\| \leq \alpha^2.$$

Next, we estimate $\|I - X'^\top A X'\|$ by the use of numerical error analysis.

ANALYSIS 3. *We utilize (101)–(104). Assume that $A \in \mathbb{F}^{n \times n}$ is positive definite, $(n+1)(n+3)\mathbf{u} < 1$ and we can use high precision computations for dot product which*

satisfies (4). Assume X is nearly the best case as

$$\kappa(X^\top AX) \approx 1 \quad \text{and} \quad \|I - X^\top AX\| \approx \alpha < 1.$$

We analyze to show

$$\|I - X'^\top AX'\| \approx \mathbf{u} + n\alpha^2. \quad (112)$$

Argument From Analysis 2 in Chapter 3, we have

$$\|X^\top AX\| \approx 1, \quad (113)$$

$$\|X\| \lesssim ((n\mathbf{u})^k \|A\|)^{-\frac{1}{2}} \quad \text{and} \quad (114)$$

$$\|X^{-1}\| \approx \|A\|^{\frac{1}{2}}. \quad (115)$$

The computation of X' in m_M -fold working precision gives

$$\|\Delta_3\| \leq \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} \|X\| \|T\| \lesssim \mathbf{u}^{\lceil \frac{k+1}{2} \rceil + 1} \left(\frac{(n\mathbf{u})^{-k}}{\|A\|} \right)^{\frac{1}{2}} \approx u \|A\|^{-\frac{1}{2}}. \quad (116)$$

Then

$$\begin{aligned} \|I - X'^\top AX'\| &= \|I - (XT + \Delta_3)^\top A(XT + \Delta_3)\| \\ &\leq \|I - T^\top X^\top AXT\| + 2\|T^\top X^\top A\Delta_3\| + \|\Delta_3^\top A\Delta_3\|. \end{aligned} \quad (117)$$

Here

$$\begin{aligned} \|I - T^\top X^\top AXT\| &= \|(I - T^\top GT) - T^\top \Delta_1 T\| \\ &= \|(I - T^\top (R'^\top R' + \Delta_2)T) - T^\top \Delta_1 T\| \\ &\leq \|I - T^\top R'^\top R'T\| + \|T^\top \Delta_2 T\| + \|T^\top \Delta_1 T\|. \end{aligned} \quad (118)$$

From Observation 4.3, we have

$$\|I - T^\top R'^\top R' T\| \approx \alpha^2. \quad (119)$$

The computation of $X^\top AX$ by $\{X^\top AX\}_{k+1}^1$, (4), (113) and (114) imply

$$\begin{aligned} \|\Delta_1\| &\leq \varphi(\mathbf{u})\|X^\top AX\| + \varphi(\mathbf{u}^{k+1})\|X^\top\|\|A\|\|X\| \\ &\lesssim \mathbf{u} \cdot 1 + \mathbf{u}^{k+1} \cdot ((n\mathbf{u})^k)^{-1} \approx \mathbf{u}. \end{aligned} \quad (120)$$

From Observation 4.1, we have

$$\|\Delta_2\| \approx \mathbf{u} + n\alpha^2. \quad (121)$$

From Observation 4.2, (120) and (121), it follows that

$$\|T^\top \Delta_2 T\| \leq \|T\|^2 \|\Delta_2\| \approx \mathbf{u} + n\alpha^2, \quad \|T^\top \Delta_1 T\| \leq \|T\|^2 \|\Delta_1\| \approx \mathbf{u}. \quad (122)$$

Inserting (119) and (122) into (118) yields

$$\|I - T^\top X^\top A X T\| \approx \alpha^2 + \mathbf{u} + n\alpha^2 + \mathbf{u} \approx n\alpha^2 + \mathbf{u}. \quad (123)$$

Moreover, we estimate $\|T^\top X^\top A \Delta_3\|$ and $\|\Delta_3^\top A \Delta_3\|$ in (117). By Observation 4.2, (115), (116) and (120), it holds

$$\begin{aligned} \|T^\top X^\top A \Delta_3\| &= \|T^\top X^\top A X X^{-1} \Delta_3\| = \|T^\top (G - \Delta_1) X^{-1} \Delta_3\| \\ &\leq \|T\|(\|G\| + \|\Delta_1\|)\|X^{-1}\|\|\Delta_3\| \approx \mathbf{u} \end{aligned} \quad (124)$$

and

$$\|\Delta_3^\top A \Delta_3\| \leq \|\Delta_3\|^2 \|A\| \approx \mathbf{u}^3. \quad (125)$$

Inserting (123)–(125) into (117) implies

$$\|I - X'^\top AX'\| \lesssim \mathbf{u} + n\alpha^2 + \mathbf{u} + \mathbf{u}^3 \approx \mathbf{u} + n\alpha^2. \quad (126)$$

which explains (112). $\square$

If $n\alpha^2 \approx n^5 \mathbf{u}^2 < \mathbf{u}$ satisfies, then

$$\|I - X'^\top AX'\| \approx \mathbf{u}. \quad (127)$$

REMARK 9. Here, $n\alpha^2$ in (126), is an upper bound of the rounding errors. As we will see in Subsection 4.3, Algorithm 4.1 gives $\|I - X'^\top AX'\| \approx \mathbf{u}$ for larger n such that $n\alpha^2 > \mathbf{u}$ in practice.

4.2.1. Computational complexity. We assume accurate dot product based on the algorithm in [8, 11, 16] is used in Algorithm 4.1. It requires $\mathcal{O}(k^2 n^3)$ flops to compute the matrix multiplication $X^{(k-1)}T^{(k)}$ and $X^{(k)T}AX^{(k)}$ and $\mathcal{O}(n^3)$ flops to compute the rest of the algorithm at the k -th iteration. If the iterations stop at $k = m_2 = M - 1$, then the computational cost of the part of Algorithm 4.1 becomes $\mathcal{O}(m_2^3 n^3)$ flops since $\sum_{k=1}^{m_2} k^2 n^3 = \mathcal{O}(m_2^3 n^3)$. After the iterations, it requires $\mathcal{O}(M^2 n^3)$ flops to compute the matrix multiplication $X^{(M-1)}T^{(M)}$ and $\mathcal{O}(n^3)$ flops to compute the rest of the algorithm. Then, the total cost of Algorithm 4.1 becomes $\mathcal{O}(M^3 n^3)$ flops. From (62), we can see that the number of iterations m_2 in Algorithm 4.1 is estimated as

$$m_2 = \left\lceil \frac{\log \kappa(A)}{\log \alpha} \right\rceil, \quad \text{and} \quad M = m_2 + 1. \quad (128)$$

We will confirm it in Section 4.3.

4.3. NUMERICAL EXPERIMENTS

In this section we present some numerical results. All computations are done on Matlab 2012b using IEEE standard 754 binary64 (double precision) on Mac OS X version 10.8 with Intel Core i7-3667U Processor, so that $\mathbf{u} = 2^{-53} \approx 1.11 \times 10^{-16}$.

We present some numerical results for comparing the proposed algorithm (Algorithm 4.1) with the original one (Algorithm 2.8), in terms of both the accuracy on X and measured computing time. For Algorithms 2.8 and 4.1, we adopt accurate matrix multiplication algorithms in [11]. Then the computations are automatically parallelized in BLAS and LAPACK. Define

$$\widehat{G}^{(k)} := (X_{1:m_{k-1}}^{(k-1)})^\top A X_{1:m_{k-1}}^{(k-1)}.$$

First, we observe some numerical results in terms of the accuracy on X . From (97), the lower bound of $\|I - X_{1:m_k}^\top A X_{1:m_k}\|$ in Algorithm 2.8 is about $n^2 \mathbf{u}$. Thus, we set $\varepsilon_{tol} = 10^{\lceil \log_{10} n^2 \mathbf{u} \rceil}$ as a stopping criterion for Algorithm 2.8. We deal with the Hilbert matrix as the first example. The results of Algorithm 2.8 for $A = H_{21}$ are shown in Table 4.1. As the second example, we deal with the Rump matrix [13] as an ill-conditioned matrix, which is based on the function *randmat* in INTLAB [14], and surely generates symmetric and positive definite matrices. We name the function *randmatsym*(n, cnd). We set $n = 500$ with $cnd = 10^{50}$. Then $A \in \mathbb{F}^{500 \times 500}$ with $\kappa(A) \approx 4.756 \times 10^{53}$ is generated, and the results are shown in Table 4.2. Moreover, we set $n = 1000$ with $cnd = 10^{100}$. Then $A \in \mathbb{F}^{1000 \times 1000}$ with $\kappa(A) \approx 8.297 \times 10^{102}$ is generated, and the results are shown in Table 4.3.

Let m_1 and m_2 denote the number of iterations for Algorithm 2.8 and that for Algorithm 4.1, respectively. Put $M = m_2 + 1$. On Algorithm 2.8, it can be seen from Table 4.1 – Table 3.5 that $\kappa(\widehat{G}^{(k)})$ is reduced by a factor around $n^2 \mathbf{u}$ in each iteration until $\|I - \widehat{G}^{(m_1)}\| \approx \alpha$, which is consistent with (97) as expected. Moreover, we can observe that $\|I - \widehat{G}^{(m_1)}\|$ in Algorithm 2.8 increases according to the dimension n ,

TABLE 4.1. Results for scaled Hilbert matrix $\kappa(A) \approx 8.16 \cdot 10^{29}$ and $\varepsilon_{tol} = 10^{-13}$.

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	Algorithm 2.8	Algorithm 4.1
			$\ I - \widehat{G}^{(k)}\ $	$\ I - \widehat{G}^{(k)}\ $
1	$2.61 \cdot 10^{15}$	$4.19 \cdot 10^{16}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
2	$8.35 \cdot 10^{01}$	$2.15 \cdot 10^{03}$	$9.88 \cdot 10^{-01}$	$9.88 \cdot 10^{-01}$
3	$1.00 \cdot 10^{00}$	$1.10 \cdot 10^{-10}$	$4.04 \cdot 10^{-12}$	$4.04 \cdot 10^{-12}$
4	$1.00 \cdot 10^{00}$	$5.65 \cdot 10^{-24}$	$5.13 \cdot 10^{-14}$	$3.79 \cdot 10^{-16}$

TABLE 4.2. Result for Rump matrix with $n = 500$, $\kappa(A) \approx 4.756 \times 10^{53}$ and $\varepsilon_{tol} = 10^{-10}$.

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	Algorithm 2.8	Algorithm 4.1
			$\ I - \widehat{G}^{(k)}\ $	$\ I - \widehat{G}^{(k)}\ $
1	$5.95 \cdot 10^{41}$	$1.32 \cdot 10^{43}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
2	$1.38 \cdot 10^{31}$	$3.68 \cdot 10^{32}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
3	$3.59 \cdot 10^{20}$	$1.02 \cdot 10^{22}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
4	$9.71 \cdot 10^{09}$	$2.85 \cdot 10^{11}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
5	$1.27 \cdot 10^{00}$	$7.91 \cdot 10^{00}$	$2.11 \cdot 10^{-01}$	$2.11 \cdot 10^{-01}$
6	$1.00 \cdot 10^{00}$	$2.20 \cdot 10^{-10}$	$3.52 \cdot 10^{-11}$	$3.88 \cdot 10^{-16}$

TABLE 4.3. Result for Rump matrix with $n = 1000$, $\kappa(A) \approx 8.297 \times 10^{102}$ and $\varepsilon_{tol} = 10^{-9}$.

k	$\kappa(\widehat{G}^{(k)})$	$(n^2 \mathbf{u})^k \kappa(A)$	Algorithm 2.8	Algorithm 4.1
			$\ I - \widehat{G}^{(k)}\ $	$\ I - \widehat{G}^{(k)}\ $
1	$1.71 \cdot 10^{91}$	$9.22 \cdot 10^{92}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
2	$1.22 \cdot 10^{81}$	$1.02 \cdot 10^{83}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
3	$1.11 \cdot 10^{71}$	$1.14 \cdot 10^{73}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
4	$1.10 \cdot 10^{61}$	$1.27 \cdot 10^{63}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
5	$1.14 \cdot 10^{51}$	$1.41 \cdot 10^{53}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
6	$1.21 \cdot 10^{41}$	$1.56 \cdot 10^{43}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
7	$1.31 \cdot 10^{31}$	$1.74 \cdot 10^{33}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
8	$1.43 \cdot 10^{21}$	$1.93 \cdot 10^{23}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
9	$1.58 \cdot 10^{11}$	$2.15 \cdot 10^{13}$	$1.00 \cdot 10^{00}$	$1.00 \cdot 10^{00}$
10	$1.84 \cdot 10^{01}$	$2.38 \cdot 10^{03}$	$9.46 \cdot 10^{-01}$	$9.46 \cdot 10^{-01}$
11	$1.00 \cdot 10^{00}$	$2.65 \cdot 10^{-07}$	$2.05 \cdot 10^{-09}$	$3.88 \cdot 10^{-16}$
12	$1.00 \cdot 10^{00}$	$2.94 \cdot 10^{-17}$	$1.11 \cdot 10^{-10}$	-

while $\|I - \widehat{G}^{(M)}\|$ from Algorithm 4.1 in Table 4.1 – Table 3.5 is always around $\mathbf{u}$, which is consistent with (127) as expected. Thus, Algorithm 4.1 gives more accurate results

TABLE 4.4. Result for Rump matrix $randmatsym(n, cnd)$ with $n = 500$, several anticipated condition numbers cnd and $\varepsilon_{tol} = 10^{-10}$. (t_i : elapsed time [sec], m_i : number of iterations.)

cnd	$\kappa(A)$	Algorithm 2.8			Algorithm 4.1		
		t_1	m_1	$\ I - G^{(m_1)}\ $	t_2	M	$\ I - G^{(M)}\ $
10^{20}	$5.76 \cdot 10^{21}$	1.83	3	$2.78 \cdot 10^{-11}$	0.96	3	$4.44 \cdot 10^{-16}$
10^{40}	$3.32 \cdot 10^{43}$	4.88	5	$2.78 \cdot 10^{-11}$	3.55	5	$4.44 \cdot 10^{-16}$
10^{60}	$3.26 \cdot 10^{63}$	10.52	7	$2.78 \cdot 10^{-11}$	8.39	7	$4.44 \cdot 10^{-16}$
10^{80}	$1.10 \cdot 10^{87}$	22.69	10	$2.78 \cdot 10^{-11}$	15.29	9	$4.44 \cdot 10^{-16}$
10^{100}	$3.18 \cdot 10^{99}$	28.27	11	$2.78 \cdot 10^{-11}$	24.55	11	$4.44 \cdot 10^{-16}$

than Algorithm 2.8. As can be seen, in Table 3.5, Algorithm 4.1 requires less iterations than Algorithm 2.8. The reason is that the stopping criterion (100) in Algorithm 4.1 is satisfied when $\kappa(\hat{G}^{(m_2)}) \approx 1$ and the iterations finish, while Algorithm 2.8 continues one more iteration until satisfying $\|I - \hat{G}^{(k)}\| \approx n^2 \mathbf{u}$ even though $\kappa(G^{(k)}) \approx 1$.

Next, we observe the measured computing time for the algorithms. We again use $randmatsym(n, cnd)$. Here, t_1 and t_2 denote the computing time for Algorithm 2.8 and that for Algorithm 4.1, respectively. For reference, let t_0 and m_0 denote the computing time and the number of iterations for Algorithm 2.8 with setting $\varepsilon_{tol} = 10^{-6}$, respectively. First, we fix $n = 500$ and vary anticipated condition numbers cnd from 10^{20} to 10^{100} . The results are displayed in Table 4.4. As can be seen, t_1 and t_2 gradually increase according to the condition numbers, and t_2 is smaller than t_1 . This is because Algorithm 2.8 needs to calculate (28) which requires $\mathcal{O}(m_1^2 n^3)$ flops, while Algorithm 4.1 does not. Namely, in the case of $m_1 = M$, the computational cost of Algorithm 4.1 is less than that of Algorithm 2.8. Second, we fix $cnd = 10^{19}$ and vary n from 500 to 5000. The results are displayed in Table 4.5. As expected, t_2 is smaller than t_1 , which is a similar result to the previous example.

It turns out that Algorithm 4.1 is faster and gives more accurate results than Algorithm 2.8. All the numerical results shown in Table 4.1 – Table 4.5 are consistent with our analysis mentioned in Subsection 4.2.

TABLE 4.5. Result for Rump matrix $randmatsym(n, cnd)$ with several n and $\kappa(A) \approx 10^{19}$. (t_i : elapsed time [sec], m_i : number of iterations.)

n	ε_{tol}	Algorithm 2.8			Algorithm 4.1		
		$t_1 (t_0)$	$m_1(m_0)$	$\ I - G^{(m_1)}\ $	t_2	M	$\ I - G^{(M)}\ $
500	10^{-10}	1.74 (1.76)	3 (3)	$2.85 \cdot 10^{-11}$	1.28	3	$4.44 \cdot 10^{-16}$
1000	10^{-9}	12.03 (11.96)	3 (3)	$1.57 \cdot 10^{-10}$	6.53	3	$6.67 \cdot 10^{-16}$
2000	10^{-9}	70.61 (68.51)	3 (3)	$6.55 \cdot 10^{-10}$	38.10	3	$4.80 \cdot 10^{-16}$
3000	10^{-8}	225.03 (221.92)	3 (3)	$1.10 \cdot 10^{-09}$	118.14	3	$4.80 \cdot 10^{-16}$
4000	10^{-8}	849.85 (495.80)	4 (3)	$1.78 \cdot 10^{-09}$	613.04	4	$4.44 \cdot 10^{-16}$
5000	10^{-8}	1728.70 (1018.03)	4 (3)	$2.78 \cdot 10^{-09}$	1234.72	4	$9.77 \cdot 10^{-16}$

REMARK 10. One may be interested in comparing Algorithm 4.1 with a standard Cholesky factorization applying long precision arithmetic. Such numerical results for Algorithm 2.8 are presented in terms of measured computing time for verifying the positive definiteness of an input matrix in Section 3. For Algorithm 4.1, we expect that similar results to those in this section are provided.

CHAPTER 5

CONCLUSION

In Chapter 3, we presented detailed analysis of the algorithm for accurate and robust inverse Cholesky factorization for symmetric positive definite matrices which are extremely ill-conditioned. The presented analysis shows that if we can use high precision computations for dot product, then the condition number of a preconditioned matrix is reduced by a factor around $n^2\mathbf{u}$ in each iteration. Moreover, from our presented analysis, we can choose adequate computational precision for calculating dot products in the algorithm, which is sufficient for convergence and almost optimal in terms of computational effort. The numerical results are consistent with our analysis.

In Chapter 4, we propose a modified version of the Ogita-Oishi's algorithm [7] for calculating an accurate inverse of the exact Cholesky factor for ill-conditioned matrices. The presented analysis shows that the proposed algorithm (Algorithm 4.1) gives more accurate results than the original one (Algorithm 2.8). The numerical results are consistent with our analysis. Moreover, the computational cost of Algorithm 4.1 is less than that of Algorithm 2.8. Thus, Algorithm 4.1 is faster than Algorithm 2.8.

APPENDIX A

EXECUTABLE MATLAB CODE

The following is executable Matlab-code for Algorithm 2.8. The code for `Ozaki_Split`, `acc_trmm_LU`, `acc_trmm_LL1` and `acc_trmm_LL2` are provided by Associate Professor Katsuhisa Ozaki at Shibaura Institute of Technology.

```
function [X,flag] = accchol(A,tol)
% accchol: Accurate inverse Cholesky factorization
% satisfying norm(X'*A*X-I,inf) < tol (*)
% (input)
%   A: real square matrix
%   tol: tolerance for (*)
% (output)
%   X: upper triangular matrix, X=X_1...,X_{k}
%   flag  0: Positive definiteness of A could not be verified.
%          1: A is proved to be positive definite.
%          2: A is proved to be indefinite.
n = size(A,1);
I = speye(n); % identity matrix
% symmetry check
if ~isequal(A,A')
    error('Input matrix must be symmetric.')
end
% Initialization
flag = 0;
kmax = 20;
X = [];
Eps = 2^-53;
cn = (n+1)*(n+3)*Eps ;
if cn < 1
```



```

        setround(1) % set rounding upwards
        C_n = (n + 2)*Eps/(1 - cn);
    else
        error('n is too large.')
    end
    % rounding upwards remains.
    dA = diag(double(A));
    if any(dA <= 0), flag = 2; return, end % Check diagonal elements
    maxdiagA = max(dA);
    delta = C_n*sum(dA);
    B = double(A) + delta*I;
    setround(0) % set rounding to nearest
    [R,p] = chol(B); % Cholesky factorization: B ~ R'*R
    if p ~= 0, flag = 2; return, end
    T = triinv(R); % approximate inverse of upper triangular matrix
    for k=2:kmax
        [B,v] = triple_prod(A,X,k); % Inclusion of X'*A*X in k-fold precision
        dB = diag(B);
        if any(dB <= 0), flag = 2; return, end % Check diagonal elements
        % Diagonal shift of B
        setround(1) % set rounding upwards
        Enorm = norm(v,inf);
        maxdiagB = max(dB);
        delta = C_n*sum(dB);
        % rounding upwards remains.
        cc = mag(norm(intval(B) - I,inf)) + Enorm;
        setround(0) % set rounding to nearest
    end
end

```

```

    if cc < tol
        flag = 1;
        return
    end
    if k == kmax, error('accchol does not converge.'), end
    setround(1) % set rounding upwards
    B = B + delta*I;
    setround(0) % set rounding to nearest
    [R,p] = chol(B);
    if p ~= 0, flag = 2; return, end
    T = triinv(R); % approximate inverse of upper triangular matrix
    m = ceil((k-1)/2) + 1;
    % Accurate matrix multiplication
    % in approximately K-fold precision stored in K results (Point result)
    X = acc_trmm_LU(X,T,m,); % Algorithm 2.1--2.5
end
return

% Inclusion of the triple product  $X'A*X$  in  $k+1$ -fold precision
function [B,v] = triple_prod(A,X,k)
n = size(A,1);
e = ones(n,1);
X2 = X';
if isacc(X2), X2 = cell(X2); end
X3 = Ozaki_Split(X2,'L'); %Algorithm 2.1
% Accurate matrix multiplication
% in approximately K-fold precision stored in K-fold results (Interval result)

```

```

C = acc_trmm_LL1(X3,A,k); % Algorithm 2.1--2.5
C=transcell(C);
%  $A \cdot X$  in  $\langle C, \text{Crad} \rangle$ 
Crad = C{end};
C{end} = zeros(n,n);
% Accurate matrix multiplication
% in approximately K-fold precision stored in 1 results (Interval result)
B = acc_trmm_LL2(X3,C,k,1); % Algorithm 2.1--2.4, 2.6
B = 0.5*(B + B');
%  $X^T \cdot C$  in  $\langle B, \text{Brad} \rangle$ 
Brad = rad(B);
B = mid(B);
%  $X' \cdot A \cdot X$  in  $\langle B, \text{Brad} + \text{abs}(X') \cdot \text{Crad} \rangle$ 
setround(1)
t = Crad*e;
v = Brad*e;
if isacc(X)
    for i=length(X):-1:1
        v = v + abs(X{i}')*t;
    end
else
    v = v + abs(X')*t;
end
setround(0)
return
end

```

The following is executable Matlab-code for Algorithm 4.1.

```
function [X,flag] = accchol_mod(A)
% accchol_mod: Improved version of Accurate inverse Cholesky factorization
% (input)
%   A: real square matrix
% (output)
%   X: upper triangular matrix,  $X=X_{\{1\}} \dots X_{\{k\}}$ 
%   flag 0: Positive definiteness of A could not be verified.
%         1: A is proved to be positive definite.
%         2: A is proved to be indefinite.

% symmetry check
if ~isequal(A,A')
    error('Input matrix must be symmetric.')
end

n = size(A,1);
I = speye(n); % identity matrix
% Initialization
flag = 0;
kmax = 20;
X = [];
Eps = 2^-53;
cn = (n+1)*(n+3)*Eps ;
if cn < 1
    setround(1) % set rounding upwards
    C_n = (n + 2)*Eps/(1 - cn);
else
```

```

        error('n is too large.')
    end

    %rounding upwards remains.
    dA = diag(double(A));
    if any(dA <= 0), flag = 2; return, end % Check diagonal elements
    maxdiagA = max(dA);
    delta = C_n*sum(dA);
    B = double(A) + delta*I;
    setround(0)

    [R,p] = chol(B); % Cholesky factorization:  $B \sim R'R$ 
    if p ~= 0, flag = 2; return, end
    T = triinv(R);      % Solve  $R*X = I$ .
    for k=2:kmax
        % Inclusion of  $X'A*X$  in k-fold precision stored 1 result
        [B,v] = triple_prod(A,X,k);
        dB = diag(B);
        if any(dB <= 0), flag = 2; return, end % Check diagonal elements
        setround(1)
        Enorm = norm(v,inf);
        b = sum(abs(B-diag(dB)),2);
        C_n2 = (n + 1)*Eps/(1 - 2*(n + 1)*Eps);
        max_error = max(C_n2*sum(dB),Enorm);
        setround(-1)
        cc = min(dB-b);
        setround(0)
        if cc > max_error % Stopping criterion
            [R,p] = chol(B);

```

```

        if p == 0
            flag = 1;
            T = triinv(R);
            m = ceil(k/2) + 1;
            X = acc_trmm_LU(X,T,m); % Algorithm 2.1--2.5
            return
        else
            error('this should not occur!!!')
        end
    end

    if k == kmax, error('accchol_mod does not converge. '), end
    setround(1)
    dB_E = diag(B)+Enorm;
    delta = C_n*sum(dB_E) ;
    B = B + delta*I;
    setround(0)

    [R,p] = chol(B);
    if p ~= 0, flag = 2; return, end
    T = triinv(R);
    m = ceil(k/2) + 1;
    % Computed and stored in m-fold precision
    X = acc_trmm_LU(X,T,m); % % Algorithm 2.1--2.5
end
return

```

The following is executable Matlab-code for `testmatrix`.

```
function A = testmatrix(n,cnd)
    d = logspace(1,log10(cnd),n)
    D = diag((1).^[1:n].*d);
    B = rand(n);
    [Q,R] = qr(B);
    k = ceil(log(cnd)/log(2^53));
    % Accurate computation of  $Q*D*Q'$  with
    % k-fold working precision
    T = acc_mm(D,Q',k);
    A = acc_mm(Q,T,k);
    % Enforce symmetric and positive definite matrix
    if iscell(A)
        for i=1:length(A)
            L = tril(A{i},-1);
            A{i} = L + L' + diag(diag(A{i}));
        end
    else
        A = 0.5*(A + A');
    end
end
```

The following is executable C-code for `mpfr_vchol`.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <gmp.h>
#include <mpfr.h>

#define GMP_RNDN MPFR_RNDN
#define GMP_RNDZ MPFR_RNDZ
#define GMP_RNDU MPFR_RNDU
#define GMP_RNDD MPFR_RNDD

int vchol(mpfr_t *A, unsigned int n)
{
    unsigned int i, j, k;
    mpfr_t t;
    mp_prec_t prec;
    int info = 0;
    prec = mpfr_get_prec(*A);
    mpfr_init2(t, prec);
    for (k = 0; k < n; k++) {
        if (mpfr_sgn(A[k+k*n]) <= 0) {
            info = 1;
            break;
        } else {
            mpfr_sqrt(A[k+k*n], A[k+k*n], GMP_RNDN);
        }
    }
    for (i = k + 1; i < n; i++) {
```



```

mpfr_div(A[i+k*n], A[i+k*n], A[k+k*n], GMP_RNDN);
}
for (j = k + 1; j < n; j++) {
for (i = j; i < n; i++) {
mpfr_mul(t, A[i+k*n], A[j+k*n], GMP_RNDN);
mpfr_sub(A[i+j*n], A[i+j*n], t, GMP_RNDN);
}
}
}
mpfr_clear(t);
return info;
}

int mpfr_vchol(double *dA, double al, int ns, int ps)
{
unsigned int N;
mp_prec_t p;
mpfr_t *B;
mpfr_t alpha;
unsigned int i, j;
int info;
N = (unsigned int)ns;
p = (mp_prec_t)ps;
mpfr_set_default_prec(p);
mpfr_init_set_d(alpha, al, GMP_RNDN);
B = (mpfr_t *)malloc(N * N * sizeof(mpfr_t));
for (i = 0; i < N*N; i++) {
    mpfr_init_set_d(B[i], dA[i], GMP_RNDN);

```

```

    }

    for (i = 0; i < N*N; i+=N) {
        mpfr_sub(B[i], B[i], alpha, GMP_RNDD);
    }

/* Cholesky factorization */
info = vchol(B, N);
for (i = 0; i < N*N; i++) {
    mpfr_clear(B[i]);
}
free(B);
return info;
}

```

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