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A modified algorithm for accurate inverse Cholesky factorization

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1 Introduction

Let $\mathbb{R}$ be the set of real numbers, and $\mathbb{F}$ a set of floating-point numbers conforming to IEEE standard 754. The relative rounding error unit of floating-point arithmetic is denoted by u. In binary64 (double precision) arithmetic, $u = 2^{-53} \approx 1.1 \times 10^{-16}$. 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. It is well-know that $\kappa(A)$ indicates the difficulty of the problem.

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

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

This means no correct digit can be expected in an approximate solution $\tilde{x}$ when solving a linear system $Ax = b$ in working precision u. However, in [1], Ogita and Oishi presented an iterative algorithm to calculate a good approximate inverse of the exact Cholesky factor. In the previous works, in about 1984, Rump [2] derived a method for inverting an extremely ill-conditioned matrix, which is based on the accurate dot product algorithms. In 2007, Oishi et al. [3] presented a proof why a modified version of the Rump's method works so well. In 2009, Rump [4] has shown the mechanism of his method by himself. In 2010, Ogita [5] presented algorithms for accurately calculating inverse LU and inverse QR factorizations. As mentioned before, in 2012, Ogita and Oishi [1] derived an algorithm for accurately calculating inverse of the exact Cholesky factor. However, why the Ogita-Oishi's algorithm is so efficient for ill-conditioned matrices has not yet been known.

Recently, in [6, 7], we analyzed the behavior of the algorithm in detail and explained its convergency by the use of numerical error analysis. We presented a detailed analysis showing 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^2u in each iteration until convergence, which is consistent with the numerical results.

For the case (1), Cholesky factorization sometimes breaks down by the presence of an imaginary root due to the accumulation of rounding errors, even if the matrix is symmetric and positive definite. To avoid the break-down, a diagonal shift is applied to A in the Ogita-Oishi's algorithm. The Ogita-Oishi's algorithm gives 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 $A = \hat{R}^T\hat{R}$ satisfying

$$n^2u \lesssim \|I - X^TAX\| < 1. \tag{2}$$

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The reason why n^2u is the lower bound is due to the diagonal shift. To overcome it, we find the condition such that Cholesky factorization of a preconditioned matrix never breaks down without the diagonal shift. In this paper, we 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

$$\|I - X^T AX\| \approx u.$$

The rest of the paper is organized as follows: in the following section, we explain the notation and state the definitions used in this paper. In Section 3, we introduce the algorithm for an accurate inverse Cholesky factorization and propose a modified algorithm. In Section 4, we present some numerical results for comparing the proposed algorithm with the original one in terms of both the accuracy on X.

2 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.

Let $A = A^T \in \mathbb{R}^{n\times n}$. The trace of A is defined by

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

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

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

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

$$T := triinv(R),$$

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.

For readability $\varphi(\gamma)$ denotes a constant such as $\varphi(\gamma) = c \cdot \gamma$ where $c := \mathcal{O}(1)$ with $0 < c \ll u^{-1}$.

Let $fl(\cdot)$ denote that an expression inside the parentheses is evaluated by floating-point arithmetic in rounding to nearest. 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 $\mathbb{F} = \mathbb{F}_{[1]} \subseteq \mathbb{F}_{[l]} \subset \mathbb{R}$.

Let $A \in \mathbb{F}_{[p]}^{n\times n}$ and $B \in \mathbb{F}_{[q]}^{n\times n}$ for $p, q \in \mathbb{N}$. Assume that we have a function of calculating $C \in \mathbb{F}_{[l]}^{n\times n}$ for any $k, l \in \mathbb{N}$, $l \leq k$ satisfying

$$|AB - C| \leq \varphi(u^l)|AB| + \varphi(u^k)|A||B|.$$

Note that $C = \sum_{i=1}^{l} C_i$ with $C_i \in \mathbb{F}^{n\times n}$, $i = 1, 2, \ldots, l$. Namely, C 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

$$C_{1:l} := \{AB\}_k^l, \tag{3}$$

which provides $C = C_{1:l}$ satisfying (2). Such accurate dot product algorithms satisfying (2) have been proposed in [8, 9, 10]. Moreover, algorithms for accurate matrix multiplication have been developed in [11].

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 (3) applies to $B^T AB$, i.e.,

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

which provides $G = G^T, E \in \mathbb{F}^{n\times n}$ satisfying $B^T AB \in \langle G, E \rangle$ with

$$|B^T AB - G| \leq \varphi(u)|B^T AB| + \varphi(u^k)|B^T||A||B| =: E. \tag{4}$$

3 Modified algorithm for accurate inverse Cholesky factorization

In this section, we first introduce the Ogita-Oishi algorithm for an accurate inverse Cholesky factorization. After that, we propose a modified version of the Ogita-Oishi's algorithm for calculating a better approximate inverse X of the exact Cholesky factor of A.

3.1 Preliminaries

Let $A \in \mathbb{F}^{n\times n}$ be symmetric and positive definite. We say "run to completion" if no imaginary root appears in the factorization process. Throughout the paper, the Matlab-style notation

$$R = \mathrm{chol}(A)$$

means a floating-point Cholesky factorization of A using a standard numerical algorithm (e.g., `xPOTRF` in LAPACK) such that

$$A \approx R^T R$$

where $R \in \mathbb{F}^{n\times n}$ is an upper triangular matrix. Then it is known [12] that the computed Cholesky factor R always satisfies

$$\frac{\|A - R^\top R\|}{\|A\|} \leq \varphi(u) \tag{5}$$

if the floating-point Cholesky factorization runs to completion. However, it holds only limited information on the accuracy of the Cholesky factorization can be obtained from the residual norm $\|A - R^{\top}R\|$ or its relative norm. Thus we need another criterion. Instead of (5), we use the following criterion:

$$\|I - X^T AX\| < \varepsilon_{tol},$$

where ε_{tol} is a given tolerance, as the accuracy of the Cholesky factors.

As mentioned before, the floating-point Cholesky factorization of an ill-conditioned matrix A sometimes breaks down due to an accumulation of the rounding errors. To avoid the break-down, a diagonal shift can be applied to A. To obtain an optimal diagonal shift of A, we utilize the backward error analysis of floating-point Cholesky factorization in [13, 14] based on the Demmel's result [15]: if $2(n+1)u < 1$, then

$$\Delta := A - R^T R, \quad \|\Delta\| \le c'_n u \cdot \mathrm{tr}(A), \quad c'_n := \frac{n+1}{1-2(n+1)u}. \tag{6}$$

If $(n+1)(n+3)u < 1$, then we define a diagonal shift of A by

$$shift(A) := c_n u \cdot \mathrm{tr}(A) \quad \text{with} \quad c_n = \frac{n+2}{1-(n+1)(n+3)u}. \tag{7}$$

Let $\tilde{A} := fl(A+\delta I)$ where $\delta := shift(A)$. Let $\tilde{R} = chol(\tilde{A})$. From [13, 14, 15] and Theorem 1 in [16], if A is positive definite, then $chol(\tilde{A})$ runs to completion.

The following is an algorithm for an accurate inverse Cholesky factorization:

Algorithm 1 (Ogita-Oishi [1]) *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 $n^2u \lesssim \varepsilon_{tol} \le 1$, the following algorithm calculates an upper triangular matrix $X^{(k)}_{1:m_k} \in \mathbb{F}^{n\times n}_{[m_k]}$ for some $k \in \mathbb{N}$ such that $\|X^{(k)T}_{1:m_k} A X^{(k)}_{1:m_k} - I\| < \varepsilon_{tol}$.*

1: $k = 0, \quad G^{(0)} := A, \quad E^{(0)} := O, \quad X^{(0)}_{1:1} := I$
2: ***repeat***
3: $\quad k = k + 1$
4: $\quad$ *Compute* $S^{(k)} \in \mathbb{F}^{n\times n}$ *with* $S^{(k)}_{ii} \ge G^{(k-1)}_{ii} + \|E^{(k-1)}\|$, $S^{(k)}_{ij} = G^{(k-1)}_{ij}$ *for* $i \ne j$
5: $\quad \delta_k := shift(S^{(k)})$
6: $\quad \tilde{S}^{(k)} := fl(S^{(k)} + \delta_k I)$
7: $\quad R^{(k)} := chol(\tilde{S}^{(k)})$
8: $\quad T^{(k)} := triinv(R^{(k)})$
9: $\quad X^{(k)}_{1:m_k} := \{X^{(k-1)}_{1:m_{k-1}} T^{(k)}\}^{m_k}_{m_k}$ $\qquad$ // $m_k := \lceil \frac{k}{2} \rceil + 1$
10: $\quad \langle G^{(k)}, E^{(k)} \rangle := \{(X^{(k)}_{1:m_k})^T A X^{(k)}_{1:m_k}\}^{1}_{k+1}$
11: ***until*** $\|G^{(k)} - I\| + \|E^{(k)}\| < \varepsilon_{tol}$

Remark 1 *In Step 4 and 5, 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 [16]. For Step 4, in practice, $S^{(k)}$ can be obtained by calculating $G^{(k-1)}_{ii} + \|E^{(k-1)}\|$ in rounding upwards.*

Remark 2 *Assume* $\|E^{(k-1)}\| \approx u\|G^{(k-1)}\|$. *Then*

$$\delta_k \;=\; c_n u \cdot \mathrm{tr}(S^{(k)}) \approx nu \cdot \mathrm{tr}(G^{(k-1)}).$$

Therefore, it holds that

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

Define $\alpha_k := \delta_k / \|(X^{(k-1)})^T A X^{(k-1)}\|$. *Then* $\|(X^{(k-1)})^T A X^{(k-1)}\| \approx \|G^{(k-1)}\|$ *and*

$$nu \lesssim \alpha_k \lesssim n^2 u.$$

If $\kappa(S^{(k)}) \gtrsim u^{-1}$, *then*

$$\kappa(\tilde{S}^{(k)}) \approx \kappa(S^{(k)} + \delta_k I) \approx \frac{\|S^{(k)}\|}{\delta_k} \approx \frac{\|G^{(k-1)}\| + u\|G^{(k-1)}\|}{\alpha_k \|G^{(k-1)}\|} \approx \alpha_k^{-1}.$$

Otherwise, $\kappa(\tilde{S}^{(k)}) \approx \kappa(G^{(k-1)})$. *Therefore,* $\tilde{S}^{(k)}$ *is not too ill-conditioned in any case and*

$$\kappa(R^{(k)}) \approx \kappa(\tilde{S}^{(k)})^{\frac{1}{2}} \approx \kappa((X^{(k-1)})^T A X^{(k-1)})^{\frac{1}{2}}.$$

Thus, we have

$$\kappa(R^{(k)}) \approx \sqrt{\min(\kappa((X^{(k-1)})^T A X^{(k-1)}), \alpha_k^{-1})}.$$

In [7], we explained that

$$\kappa((X^{(k)})^T A X^{(k)}) \lesssim 1 + \prod_{i=1}^{k} \alpha_i \cdot \kappa(A) \lesssim (n^2 u)^k \kappa(A). \tag{8}$$

Namely, the condition number of a preconditioned matrix $(X^{(k)})^T A X^{(k)}$ is reduced by a factor around $n^2 u$ in each iteration and eventually converges to 1 after some iterations in Algorithm 1. Moreover, we show it is important to choose adequate computational precision for calculating dot products in Algorithm 1, which is sufficient for convergence and almost optimal in terms of computational effort.

3.2 Proposed algorithm

The following is a modified algorithm for an accurate inverse Cholesky factorization:

Algorithm 2 *For a symmetric matrix* $A = (a_{ij}) \in \mathbb{F}_{\Sigma}^{n \times n}$ *with* $a_{ii} > 0$ *for all* i, *the following algorithm calculates an upper triangular matrix* $X_{1:m_M}^{(M)} \in \mathbb{F}_{\Sigma}^{n \times n}$ *where* $M := k+1$ *for some* $k \in \mathbb{N}$ *such that* $\|X_{1:m_M}^{(M)T} A X_{1:m_M}^{(M)} - I\| \approx u$.

1: $k = 0, \quad G^{(0)} := A, \quad E^{(0)} := O, \quad X^{(0)}_{1:1} := I$
2: ***repeat***
3: $\quad k = k + 1$
4: $\quad$ *Compute* $S^{(k)} \in \mathbb{F}^{n\times n}$ *with* $S^{(k)}_{ii} \geq G^{(k-1)}_{ii} + \|E^{(k-1)}\|$, $S^{(k)}_{ij} = G^{(k-1)}_{ij}$ *for* $i \neq j$
5: $\quad \delta_k := shift(S^{(k)})$
6: $\quad \tilde{S}^{(k)} := fl(S^{(k)} + \delta_k I)$
7: $\quad R^{(k)} := chol(\tilde{S}^{(k)})$
8: $\quad T^{(k)} := triinv(R^{(k)})$
9: $\quad X^{(k)}_{1:m_k} := \{X^{(k-1)}_{1:m_{k-1}} T^{(k)}\}^{m_k}_{m_k}$ // $m_k := \lceil \frac{k}{2} \rceil + 1$
10: $\quad \langle G^{(k)}, E^{(k)} \rangle := \{(X^{(k)}_{1:m_k})^T A X^{(k)}_{1:m_k}\}^1_{k+1}$
11: $\quad \beta := \min(G^{(k)}_{ii} - r_i(G^{(k)}))$
12: $\quad \mu := c'_n u \cdot \mathrm{tr}(G^{(k)})$ // $c'_n := \frac{n+1}{1-2(n+1)u}$
13: ***until*** $\beta > \max(\mu, \|E^{(k)}\|)$
14: $R^{(M)} := chol(G^{(M-1)})$ // $M := k + 1$
15: $T^{(M)} := triinv(R^{(M)})$
16: $X^{(M)}_{1:m_M} := \{X^{(M-1)}_{1:m_k} T^{(M)}\}^{m_M}_{m_M}$ // $m_M := \lceil \frac{k+1}{2} \rceil + 1$

Compared with Algorithm 1, we add the condition such that Cholesky factorization of $G^{(k-1)}$ never breaks down without a diagonal shift. In the following, we explain how to determine it. For readability, $G^{(k)}$, $X^{(k)}_{1:m_k}$ and $X^{(M)}_{1:m_M}$ where $M := k+1$ are abbreviated to G, X and X', respectively. Let R' be a computed Cholesky factor of G, i.e., $R' = chol(G)$. Define

$$\Delta_1 := G - X^T A X, \tag{9}$$
$$\Delta_2 := G - R'^T R', \tag{10}$$
$$T := triinv(R'), \tag{11}$$
$$\Delta_3 := X' - XT. \tag{12}$$

By the definition (10), it is necessary to satisfy

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

By (6) and a Weyl's theorem (e.g. Corollary 4.9 in [17]) for (10), it holds that

$$\lambda_n(G - \Delta_2) \geq \lambda_n(G) - \|\Delta_2\|, \quad \|\Delta_2\| \leq c'_n u \cdot \mathrm{tr}(G). \tag{13}$$

The Gerschgorin's circle theorem implies

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

and

$$\lambda_n(G) \geq \beta \quad \text{where} \quad \beta := \min(G_{ii} - r_i(G)). \tag{14}$$

From (13) and (14), we have

$$\lambda_n(G - \Delta_2) \geq \beta - \|\Delta_2\|. \tag{15}$$

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

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

By a Weyl's theorem (e.g. Corollary 4.9 in [17]) for (9), it holds that

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

From (14), we have

$$\lambda_n(X^T AX) \geq \beta - \|\Delta_1\|. \tag{16}$$

Therefore, combining (15) and (16), the sufficient condition to make $chol(G)$ run to completion and to ensure the positive definiteness of A is

$$\beta > \max(\|\Delta_1\|, \|\Delta_2\|). \tag{17}$$

In [16], we explained that if $n^5 u < 1$ satisfies, then

$$\|I - X'^T AX'\| \approx u. \tag{18}$$

4 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 2 GHz Intel Core i7 Duo processor, so that $u = 2^{-53} \approx 1.11 \times 10^{-16}$.

We present some numerical results for comparing the proposed algorithm (Algorithm 2) with the original one (Algorithm 1), in terms of the accuracy on X. For Algorithms 1 and 2, we adopt accurate matrix multiplication algorithms in [11]. Then the computations are automatically parallelized in BLAS and LAPACK. From (2), the lower bound of $\|I - X^T AX\|$ in Algorithm 1 is about $n^2 u$. Thus, we set $\varepsilon_{tol} = 10^{\lceil \log_{10} n^2 u \rceil}$ as a stopping criterion for Algorithm 1. We deal with the Rump matrix [18] as an ill-conditioned matrix, which is based on the function *randmat* in INTLAB [19], and surely generates symmetric and positive definite matrices. We name the function $randmatsym(n, cnd)$. 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 1. Let m_1 and m_2 denote the number of iterations for Algorithm 1 and that for Algorithm 2, respectively. Put $M = m_2 + 1$. On Algorithm 1, it can be seen from Table 1 that $\kappa(G^{(k)})$ is reduced by a factor around $n^2 u$ in each iteration until $\|I - G^{(m_1)}\| \approx n^2 u$, which is consistent with (2) and (8) as expected. On the other hand, $\|I - G^{(M)}\|$ from Algorithm 2 in Tables 1 is around u, which is consistent with (18) as expected. Thus, Algorithm 2 gives more accurate results than Algorithm 1. As can be seen, in Table 1, Algorithm 2 requires less iterations than Algorithm 1. The reason is that the stopping criterion (17) in Algorithm 2 is satisfied when $\kappa(G^{(m_2)}) \approx 1$ and the iterations finish, while Algorithm 1 continues one more iteration until satisfying $\|I - G^{(k)}\| \approx n^2 u$ even if $\kappa(G^{(k)}) \approx 1$.

Table 1: Result for Rump matrix with $n = 1000$, $\kappa(A) \approx 8.297 \times 10^{102}$, $n^2u \approx 1.11 \cdot 10^{-10}$ and $\varepsilon_{tol} = 10^{-9}$.

			Algorithm 1	Algorithm 2
k	$\kappa(G^{(k)})$	$(n^2u)^k\kappa(A)$	$\|I - G^{(k)}\|$	$\|I - G^{(k)}\|$
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	$1.00 \cdot 10^{00}$	$2.94 \cdot 10^{-17}$	$1.11 \cdot 10^{-10}$	-

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