LU-Cholesky QR algorithms for thin QR decomposition in an oblique inner product

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Abstract. This paper concerns thin QR decomposition in an oblique inner product. Cholesky QR is known as a fast algorithm for thin QR decomposition. On the other hand, this algorithm is not applicable for ill-conditioned matrices. The preconditioned Cholesky QR algorithms named LU-Cholesky QR for thin QR decomposition are recently proposed. We apply these preconditioning techniques to thin QR decomposition in an oblique inner product.

1. Introduction

We consider thin QR decomposition in an oblique inner product for full rank matrices $A \in \mathbb{R}^{m \times n}, m \geq n$ and $B \in \mathbb{R}^{m \times m}$ with $B$ being positive definite. This decomposition produces $B$-orthogonal columns $Q \in \mathbb{R}^{m \times n}$ and an upper triangular matrix $R \in \mathbb{R}^{n \times n}$ such that

$$A = QR, \quad Q^T B Q = I,$$

where $I$ is the identity matrix. Such a problem has applications in, for example, the solution of a generalized eigenvalue problem $Ax = \lambda Bx$ \cite{1}. For the $QR$-factors computed by numerical computations, $B$-orthogonality as $\|Q^T B - I\|$ and residual as $\|QR - A\|$ are important. Although CholeskyQR has weak numerical stability, Cholesky QR is known as a fast algorithm employed for thin QR decomposition \cite{2}. Besides, when CholeskyQR runs to compulsion, we can refine $B$-orthogonality using CholeskyQR2 \cite{3}. In this paper, we propose the fast and accurate numerical algorithms for this QR decomposition in an oblique inner product using Doolittle’s LU decomposition. There are advantages in terms of $B$-orthogonality, residual, and computation times, that is shown in numerical examples.

2. Preliminaries

We first define notation in this paper. Let $F$ be a set of binary floating-point numbers, and $u$ be the unit roundoff (binary64: $u = 2^{-53}$). The 2-norms for a vector $x = (x_i) \in \mathbb{R}^n$ and a matrix $A = (a_{ij}) \in \mathbb{R}^{m \times n}$ indicate that

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}, \quad \|A\|_2 = \max_{\|x\|_2 = 1} \|Ax\|_2.$$
A matrix $A^+$ denotes the Moore-Penrose pseudoinverse matrix of $A$, i.e., $A^+ = (A^T A)^{-1} A^T$. $\kappa_2(A)$ is the condition number such that $\kappa_2(A) = \|A\|_2 \|A^+\|_2$.

2.1. Cholesky QR algorithm

In this section, we first introduce Cholesky QR algorithms in an oblique inner product for $A \in \mathbb{F}^{m \times n}$, $B \in \mathbb{F}^{m \times m}$ using MATLAB-like notations.

```matlab
function [Q1, R1] = CholQR(A, B)
C = A' * B * A; % C \approx A^T BA
R1 = chol(C); % C \approx R_1^T R_1
Q1 = A / R1; % Q_1 \approx A R_1^{-1}
end
```

Since this algorithm is implementable using Level-3 routines in basic linear algebra subprograms (BLAS) and linear algebra package (LAPACK), CholeskyQR achieves high performance on speed. However, the paper [?] reports numerical instability of CholeskyQR. For a matrix $C$ as $\kappa_2(C) \gtrsim u_1$, Cholesky decomposition for $C$ breaks down in many cases. Here, we have

$$\kappa_2(A^T BA) \leq \kappa_2(A)^2 \kappa_2(B).$$  \hspace{1cm} (2)

Therefore, even if matrices $A$ and $B$ are well-conditioned, there is possibility that $C$ is ill-conditioned. This indicates that CholeskyQR has weak numerical stability.

2.2. Refinement of a Q-factor

Next, we consider the refinement after applying CholeskyQR for $A$ and $B$. The following algorithm named CholeskyQR2 [?] refines $B$-orthogonality $\|Q^T BQ - I\|_2$.

```matlab
function [Q2, R2] = CholQR2(A, B)
[Q1, R1] = CholQR(A, B);
[Q2, R] = CholQR(Q1, B);
R2 = R * R1;
end
```

For $m \gg n$, the cost of CholeskyQR2 is almost twice as much as that of CholeskyQR.

2.3. Shifted Cholesky QR algorithm

We introduce the shifted Cholesky QR algorithms [?] whose numerical stability is stronger than that of the standard Cholesky QR algorithms.

```matlab
function [Q1, R1] = sCholQR(A, B, s)
C = A' * B * A;
R1 = chol(C + s * I); % s is a positive constant
Q1 = A / R1;
end
```

Even if $\kappa_2(C) > u_1^{-1}$, $\kappa_2(C + s I) \leq u_1^{-1}$ is satisfied by the diagonal shift. In [?], the amount of shift is calculated as

$$s \approx 11(2m \sqrt{mn} + n(n + 1))u\|A\|_2^2 \|B\|_2.$$  \hspace{1cm} (3)
Similarly, the shifted CholeskyQR2 and shifted CholeskyQR3 are introduced as follows [7]:

function \([Q_2, R_2] = \text{sCholQR2}(A, B, s)\)
\([Q_1, R_1] = \text{sCholQR}(A, B, s);\)
\([Q_2, R] = \text{CholQR}(Q_1, B);\)
\(R_2 = R \ast R_1;\)
end

function \([Q_3, R_3] = \text{sCholQR3}(A, B)\)
\([Q_1, R_1] = \text{sCholQR}(A, B, s);\)
\([Q_3, R] = \text{CholQR2}(Q_1, B);\)
\(R_3 = R \ast R_1;\)
end

3. LU-Cholesky QR algorithms in an oblique inner product

In this section, we propose the LU-Cholesky QR algorithm employed for thin QR decomposition in an oblique inner product. We focus on the preconditioning using numerical computations of Doolittle’s LU decomposition of a given matrix \(A\) such that

\[ PA \approx \hat{L}\hat{U}, \]

where \(\hat{L}\) is a unit lower triangular matrix, \(\hat{U}\) is an upper triangular matrix, and \(P\) is a permutation matrix. It is well known that \(\hat{L}\) tends to be fairly well-conditioned even if \(A\) is ill-conditioned.

We apply Doolittle’s LU decomposition to preconditioning of CholeskyQR.

function \([Q_1, R_1] = \text{LU-CholQR}(A, B)\)
\([\hat{L}, \hat{U}, p] = \text{lu}(A); \ % PA \approx \hat{L}\hat{U}\]
\(C = \hat{L}' \ast B(p, p) \ast \hat{L}; \ % B(p, p) = PBPT\]
\(R = \text{chol}(C);\)
\(R_1 = R \ast U;\)
\(Q_1 = A/R_1;\)
end

If a given matrix \(A\) is ill-conditioned, \(\kappa_2(A) \geq \kappa_2(L)\), so that the point of this algorithm is that \(\kappa_2(\hat{L}^T PBPT\hat{L}) \preceq \kappa_2(A^T BA)\) is expected. Hence, even if a matrix \(A\) is ill-conditioned, the proposed algorithm for \(A\) and \(B\) being \(\kappa_2(B) < u^{-1}\) can run to completion.

Next, LU-CholeskyQR2 algorithm is explained.

function \([Q_2, R_2] = \text{LU-CholQR2}(A, B)\)
\([Q_1, R_1] = \text{LU-CholQR}(A, B);\)
\([Q_2, R] = \text{CholQR}(Q_1, B);\)
\(R_2 = R \ast R_1;\)
end

LU-CholeskyQR2 aims to refine \(B\)-orthogonality such as the original CholeskyQR2 algorithm introduced in Section 2.2.
4. Numerical results
We show the numerical results. The matrices $A$ and $B$ are generated by MATLAB as follows:

$$A = \text{gallery}('randsvd', [m, n], \text{cnd}A, 3, m, n, 1),$$
$$B = \text{gallery}('randsvd', m, \text{cnd}B, 3, m, 1).$$

These matrices $A$ and $B$ satisfy $\kappa_2(A) \approx \text{cnd}A$, $\kappa_2(B) \approx \text{cnd}B$ and $\|A\|_2, \|B\|_2 \approx 1$. Hence, for simplicity, we obtain the shift amount $s$ in (3) as $s \approx 11(2m\sqrt{mn} + n(n + 1))u$ for sCholQR, sCholQR2, and sCholQR3. Figure 1 compares $B$-orthogonality of the shifted Cholesky QR and the LU-Cholesky QR algorithms for various $\kappa_2(B)$ for $\text{cnd}A = 10^9$ and $\text{cnd}A = 10^{14}$. The figure indicates that the $B$-orthogonality of the $Q$-factor computed by the proposed algorithms is comparable to that computed by the shifted Cholesky QR. From right side in Fig. 1, although the standard Cholesky QR algorithms break down when $\kappa_2(B) \gtrsim 10^{10}$ and $\text{cnd}A = 10^{14}$, LU-Cholesky QR algorithms can be applied to ill-conditioned matrices.

![Figure 1. Comparison of $B$-orthogonality ($m = 1024$, $n = 256$, $\text{cnd}A = 10^9$ (left) and $\text{cnd}A = 10^{14}$ (right)).](image)

Figure 2 compares residual of shifted Cholesky QR and LU-Cholesky QR algorithms for various $\kappa_2(B)$ for $\text{cnd}A = 10^9$ and $\text{cnd}A = 10^{14}$. The residual of the $QR$-factors computed by the proposed algorithms is comparable to that computed by the shifted Cholesky QR.

Finally, we compare the computation times for random matrices generated by MATLAB function such as $A = \text{randn}(m, n)$ and $B = \text{randn}(m)$. The computation environment of the computer and MATLAB are as follows:

CPU: Intel Core i7-8550U, Memory: 16 GB, MATLAB R2019a

From Fig. 3, computation times of the sCholQR, the sCholQR2, and the sCholQR3 are 1, 2, and 3 times as same as that of the standard CholeskyQR algorithm, respectively. On the other hand, the cost of LU decomposition is much lower than that of CholeskyQR algorithm. Hence, computation times of CholeskyQR and LU-CholeskyQR algorithms are comparable.

Conclusion
We proposed the preconditioned Cholesky QR algorithms for thin QR decomposition in an oblique inner product. The cost of preconditioning is much smaller than that of the standard CholeskyQR algorithm. The numerical stability of the proposed algorithms is better than that of the shifted Cholesky QR algorithms. Therefore, the proposed algorithms are practical in terms of computation performance on speed, accuracy, and stability.
Figure 2. Comparison of residual. \( m = 1024, n = 256 \) (\( m = 1024, n = 256, \text{cnd}A = 10^9 \) (left) and \( \text{cnd}A = 10^{14} \) (right)).

Figure 3. Comparison of computation times [sec] for various \( n \). \( (m = 10,000) \)

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