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Additional Information

Full rank Cholesky factorization for rank deficient matrices ☆

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Abstract

Let A be a rank deficient square matrix. We characterize the unique full rank Cholesky factorization $L_A L_A^T$ of A where the factor L_A is a lower echelon matrix with positive leading entries. We compute an extended decomposition for the normal matrix $B^T B$ where B is a rectangular rank deficient matrix. This decomposition is obtained without interchange of rows and without computing all entries of the normal matrix. Algorithms to compute both factorizations are given.

Keywords: Rank deficient matrices, Cholesky factorization.
AMS classification: 15A03, 15A23, 65F10, 65F35

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1. Introduction

A well-known factorization for a symmetric positive definite matrix $A \in \mathbb{R}^{m\times m}$ is the Cholesky factorization [5]. If A is symmetric positive semidefinite, this factorization can not be computed because there are null pivots. Nevertheless, if $\text{rank}(A) = r$, then there exists at least one lower triangular matrix L with nonnegative diagonal entries, such that, $A = LL^T$, and there is a permutation matrix Π, such that, $\Pi^T A \Pi$ has a unique Cholesky factorization, which takes the form

$$\Pi^T A \Pi = LL^T, \qquad L = \begin{bmatrix} L_{11} & \mathrm{O} \\ L_{21} & \mathrm{O} \end{bmatrix},$$

where L_{11} is an $r \times r$ lower triangular matrix with positive diagonal entries [7].

In this work we compute, without interchange of rows and columns, the unique Cholesky factorization of $A = L_A L_A^T$ where $L_A \in \mathbb{R}^{m\times r}$ is a lower echelon matrix with positive leading entries. We call this factorization the *full rank Cholesky factorization* of A.

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We can use this factorization for the normal equations of a rectangular matrix. Direct and iterative solution methods for linear least-squares problems have been studied in Numerical Linear Algebra, see [1, 2, 3, 5, 6] and references therein. Part of the difficulty is the fact that many methods solve the system by implicitly solving the normal equations

$$A^T Ax = A^T b, \tag{1}$$

with $A \in \mathbb{R}^{n\times m}$ and $b \in \mathbb{R}^m$.

The standard methods for solving (1) are based on the Cholesky factorization when A has full column rank [2]. In this case, $A^T A$ is a positive definite matrix and the Cholesky factorization is unique [5]. We consider the problem when A is a rank deficient matrix, i.e., $\operatorname{rank}(A) = r < \min\{n, m\}$ and we compute the full rank Cholesky factorization of the normal matrix $A^T A$ without doing the complete product of $A^T A$. This means that when the matrix A is rank deficient then not all of the entries of $A^T A$ are computed and $A^T A$ is never stored. We give a bound of the elements that must be computed of the product matrix $A^T A$.

Recall that a matrix is an upper echelon matrix if it satisfies that the first nonzero entry in each row is called *leading entry for that row*, each leading entry is to the right of the leading entry in the row above it and all zero rows are at the bottom. If, in addition, the matrix satisfies that each leading entry is the only nonzero entry in its column it is called upper reduced echelon matrix. A matrix is a lower (reduced) echelon matrix if its transpose is an upper (reduced) echelon matrix. Moreover, if each leading entry is equal to 1, we add the adjective *unit* to these definitions.

The paper is organized as follows, in Section 2 we define the full rank Cholesky factorization for square symmetric positive semidefinite matrices and we prove the existence and the uniqueness of this decomposition and in Section 3, given a rectangular matrix A, we obtain the full rank Cholesky factorization of $A^T A$ without doing the complete product of both matrices. The algorithms for computing these factorizations are presented with their computational cost.

2. The full rank Cholesky factorization for rank deficient matrices

In this section we prove the existence of the full rank Cholesky factorization for square symmetric positive semidefinite matrices that we define in the following definition.

Definition 1. *Let $A \in \mathbb{R}^{m\times m}$ be a symmetric positive semidefinite matrix with* $\operatorname{rank}(A) = r < m$. *We call $A = L_A L_A^T$ the full rank Cholesky factorization of A where $L_A = (l_{ij}) \in \mathbb{R}^{m\times r}$ is a lower echelon matrix with all the leading entries for each column positive. The matrix L_A is called the lower echelon Cholesky factor of A.*

Theorem 1 proves the existence of the full rank Cholesky factorization of $A \in \mathbb{R}^{m\times m}$ using the quasi-Gauss elimination process with no pivoting [4].

We can suppose, without lost of generality, that A has no zero rows or columns. Otherwise, if the zero rows of A, and the zero columns by symmetry, are indexed by $\{i_1, i_2, \ldots, i_s\} \subseteq \{1, 2, \ldots, m\}$, using the matrix denoted by $I^{\{i_1,i_2,\ldots,i_s\}} \in \mathbb{R}^{(m-s)\times m}$ and obtained from the $m \times m$ identity matrix without the rows indexed by $i_1, i_2, \ldots, i_s$, we construct the matrix $\bar{A}$ with no zero rows and columns, $\bar{A} = I^{\{i_1,i_2,\ldots,i_s\}} A \left(I^{\{i_1,i_2,\ldots,i_s\}}\right)^T \in \mathbb{R}^{(m-s)\times(m-s)}$. Now, if $\bar{A} = L_{\bar{A}} L_{\bar{A}}^T$ is full rank Cholesky factorization of $\bar{A}$, then the full rank Cholesky factorization of A is given by $A = L_A L_A^T$ with $L_A = \left(I^{\{i_1,i_2,\ldots,i_s\}}\right)^T L_{\bar{A}}$.

Theorem 1. *Let $A \in \mathbb{R}^{m\times m}$ be a symmetric positive semidefinite matrix, without zero rows and columns and with* $\operatorname{rank}(A) = r < m$. *Then, there is a unique lower echelon matrix $L_A = (l_{ij}) \in \mathbb{R}^{m\times r}$ with all the leading entries for each column positive and such that $A = L_A L_A^T$.*

Proof. Since A is symmetric positive semidefinite, the Gaussian elimination pivots p_i are nonnegative, $i = 1, 2, \ldots, m$. Since $\operatorname{rank}(A) = r$, then there are r positive pivots. Suppose that we can apply the Gaussian elimination process with no pivoting until the k-iteration and the $(k+1)$-pivot is zero, then we have

$$M_k \ldots M_1 A = A^{(k)} =$$
$$\left[\begin{array}{cccc|cccc}
p_1 & a_{1,2}^{(k)} & \cdots & a_{1,k}^{(k)} & a_{1,k+1}^{(k)} & a_{1,k+2}^{(k)} & \cdots & a_{1,m}^{(k)} \\
 & p_2 & \cdots & a_{2,k}^{(k)} & a_{2,k+1}^{(k)} & a_{2,k+2}^{(k)} & \cdots & a_{2,m}^{(k)} \\
 & & \ddots & \vdots & \vdots & \vdots & & \vdots \\
 & & & p_k & a_{k,k+1}^{(k)} & a_{k,k+2}^{(k)} & \cdots & a_{k,m}^{(k)} \\
\hline
 & & & & 0 & a_{k+1,k+2}^{(k)} & \cdots & a_{k+1,m}^{(k)} \\
 & & & & a_{k+1,k+2}^{(k)} & a_{k+2,k+2}^{(k)} & \cdots & a_{k+2,m}^{(k)} \\
 & & & & \vdots & \vdots & & \vdots \\
 & & & & a_{k+1,m}^{(k)} & a_{k+2,m}^{(k)} & \cdots & a_{m,m}^{(k)}
\end{array}\right],$$

where M_j is the Gauss transformation, for $j \in \{1, \ldots, k\}$ [5]. Since the element $a_{k+1,k+1}^{(k)} = 0$, by [5, Theorem 4.2.6] the entries $a_{k+1,j}^{(k)} = 0$ for $j = k+2, k+3, \ldots, m$. Then, we construct the matrix $A^{(k+1)} = I^{\{k+1\}} A^{(k)} \in \mathbb{R}^{(m-1)\times m}$, that is,

$$A^{(k+1)} = I^{\{k+1\}} A^{(k)} = I^{\{k+1\}} M_k \ldots M_1 A =$$
$$\left[\begin{array}{cccc|cccc}
p_1 & a_{1,2}^{(k+1)} & \cdots & a_{1,k}^{(k+1)} & a_{1,k+1}^{(k+1)} & a_{1,k+2}^{(k+1)} & \cdots & a_{1,m}^{(k+1)} \\
 & p_2 & \cdots & a_{2,k}^{(k+1)} & a_{2,k+1}^{(k+1)} & a_{2,k+2}^{(k+1)} & \cdots & a_{2,m}^{(k+1)} \\
 & & \ddots & \vdots & \vdots & \vdots & & \vdots \\
 & & & p_k & a_{k,k+1}^{(k+1)} & a_{k,k+2}^{(k+1)} & \cdots & a_{k,m}^{(k+1)} \\
\hline
 & & & & 0 & a_{k+2,k+2}^{(k+1)} & \cdots & a_{k+2,m}^{(k+1)} \\
 & & & & \vdots & \vdots & & \vdots \\
 & & & & 0 & a_{k+2,m}^{(k+1)} & \cdots & a_{m,m}^{(k+1)}
\end{array}\right] \in \mathbb{R}^{(m-1)\times m}$$

Now, we continue with this process to obtain the upper echelon matrix $A^{(m)} \in \mathbb{R}^{r\times m}$ such that

$$A = (A^{(m)})^T A^{(m)} = L_A L_A^T$$

Uniqueness follows from the quasi-Gauss elimination process with no pivoting (see [4]). $\square$

This result allow us to present an algorithm for computing the lower echelon Cholesky factor L_A of a symmetric positive semidefinite matrix A. If A has full rank, this algorithm computes the Cholesky factorization associated with a symmetric definite positive matrix.

Algorithm 1. *(Full rank Cholesky factorization for a symmetric positive semidefinite square matrix (by rows)). Let $A = (a_{ij}) \in \mathbb{R}^{m\times m}$ be a symmetric positive semidefinite matrix. This algorithm computes the full rank Cholesky factorization of $A = L_A L_A^T$ with $L_A = (l_{ij})$, the rank of A and the row vector $c = (c_j)$ with the indices of the linearly independent columns of A.*

Input: $A \in \mathbb{R}^{m\times m}$

(LINE 1) $l_{1,1} := \sqrt{a_{1,1}};\ r := 1;\ counter := 0;\ c := [1];$
(LINE 2)   *for* $i = 2, 3, \ldots, m$
(LINE 3)   *for* $j = 1, 2, \ldots, i - counter - 1$
(LINE 4) $l_{i,j} := \frac{a_{i,c_j} - \sum_{t=1}^{j-1} l_{c_j,t} l_{i,t}}{l_{c_j,j}};$
(LINE 5)   *endfor*
(LINE 6) $var := \sqrt{a_{i,i} - \sum_{t=1}^{i-counter-1} l_{i,t}^2};$
(LINE 7)   *if* $var = 0$ *then*
(LINE 8) $counter := counter + 1$
(LINE 9)   *elseif*
(LINE 10) $l_{i,i-counter} := var;$
(LINE 11) $c := [c\ \ i];$
(LINE 12) $r := r + 1;$
(LINE 13)   *endif*
(LINE 14)   *endfor*

Output: $L_A \in \mathbb{R}^{m\times r}$**,** $r = \text{rank}(A)$ **and** c

We put attention to line 7 of this algorithm because if it is worked with finite precision the comparative with zero will produce instability in the process. Therefore, the comparative in this line should be made with a certain tolerance in order to define an stopping criterion.

The computational cost of Algorithm 1 is given in the following proposition, where we use the notation O of Landau; the notation $O(n)$ denotes a quantity γ such that $|\gamma| \leq Cn$ for some constant $C > 0$.

Proposition 1. *Let $A \in \mathbb{R}^{m\times m}$ with rank$(A) = r < m$. Algorithm 1 computes the elements of the lower echelon matrix $L_A \in \mathbb{R}^{m\times r}$ such that r is equal to the rank of A and the computational cost is $O(mr^2 - \frac{2}{3}r^3)$.*

Proof. The computational cost of Algorithm 1 is analyzed to compute the maximum floating point operations that could been made in the worst case, that is, when the first r columns of A are linearly independent. In this case, the pivots are in positions (i,i), for $i = 1, 2, \dots, r$, and the factor L_A can be written as follows:

$$L_A = \begin{bmatrix} l_{1,1} & 0 & \cdots & 0 & 0 \\ l_{2,1} & l_{2,2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ l_{r-1,1} & l_{r-1,2} & \cdots & l_{r-1,r-1} & 0 \\ l_{r,1} & l_{r,2} & \cdots & l_{r,r-1} & l_{r,r} \\ \vdots & \vdots & & \vdots & \vdots \\ l_{m,1} & l_{m,2} & \cdots & l_{m,r-1} & l_{m,r} \end{bmatrix}.$$

The following table gives all the floating point operations,

Elements	$+$	$\times$	$\div$	$\sqrt{}$	Total
$l_{1,1}$	0	0	0	1	1
$l_{i,1}$ for $i = \{2, \dots, m\}$	0	0	1	0	$m-1$
$l_{i,j}$ for $i = \{3, 4, \dots, r\}$ and $j = \{2, \dots, i-1\}$	$j-1$	$j-1$	1	0	$\frac{r^3}{3} - \frac{r^2}{2} - \frac{5r}{6} + 1$
$l_{i,j}$ for $i = \{r+1, \dots, m\}$ and $j = \{2, \dots, r\}$	$j-1$	$j-1$	1	0	$(m-r)(r^2-1)$
$l_{i,i}$ for $i = \{2, 3, \dots, r\}$	$i-1$	$i-1$	0	1	r^2-1
$l_{i,i}$ for $i = \{r+1, \dots, m\}$	r	r	0	1	$(m-r)(2r+1)$
Comparations					$m-1$

Table 1: Maximum floating point operations for computing L_A by Algorithm 1

Then, the total computational cost $T(m,r)$ can be described as follows,

$$T(m,r) = mr^2 + 2mr + 2m - \frac{2}{3}r^3 - \frac{3}{2}r^2 - \frac{5}{6}r - 1.$$

Hence, the Algorithm 1 has order $O(mr^2 - \frac{2}{3}r^3)$. □

Remark 1. *The order of Algorithm 1 is equal to the classic Cholesky factorization for a symmetric positive definite matrix $A \in \mathbb{R}^{m \times m}$. Nevertheless, if $r \ll m$, that is, if r is much smaller than m, then the total computational cost is significantly reduced.*

3. The full rank Cholesky factorization for the normal matrix

Now we consider the rectangular case, that is, let $A \in \mathbb{R}^{n\times m}$ be a rank deficient matrix without zero rows and columns with $\text{rank}(A) = r < \min\{n, m\}$. In this case, $A^T A \in \mathbb{R}^{m\times m}$ is a symmetric positive semidefinite matrix and by Theorem 1 we can obtain the full rank Cholesky factorization of $A^T A$ with no pivoting, that is, $A^T A = L_{A^T A} L_{A^T A}^T$ with $L_{A^T A} \in \mathbb{R}^{m\times r}$ lower echelon matrix with all the leading entries for each column positive. Frow now on and for simplicity we denote by $L = L_{A^T A}$.

The main problem to construct the full rank Cholesky factorization of $A^T A$ consists of doing the product of both matrices. Therefore, our main goal is to obtain the full rank Cholesky factorization of $A^T A$ without the need to compute all elements of the matrix $A^T A$ explicitly. First, we consider that A has full column rank and then we extend this result to rank deficient matrices.

Theorem 2. *Let $A \in \mathbb{R}^{n\times m}$ be a full column rank matrix, then the elements of the lower triangular Cholesky factor $L = (l_{i,j}) \in \mathbb{R}^{m\times m}$ of $A^T A$ can be obtained as follows:*

- $l_{1,1}^2 = \|A_1\|^2$
- *For* $i = 2, \ldots, m$

$$\begin{aligned} l_{i,j} &= \frac{\langle A_i, A_j\rangle - \sum_{k=1}^{j-1} l_{j,k} l_{i,k}}{l_{j,j}} \qquad \textit{for } j = 1, 2, \ldots, i-1 \\ l_{i,i}^2 &= \|A_i\|^2 - \sum_{k=1}^{i-1} l_{i,k}^2 \end{aligned}$$

where A_i denotes the i-th column of A, $i = 1, 2, \ldots, m$, and the norm $\|\cdot\|$ is the Euclidean norm associated with the inner product $\langle \cdot, \cdot \rangle$.

Proof. Since $A \in \mathbb{R}^{n\times m}$ has full column rank, then $A^T A \in \mathbb{R}^{m\times m}$ is a symmetric positive definite matrix and it admits a unique Cholesky factorization:

$$A^T A = LL^T, \quad L \in \mathbb{R}^{m\times m},$$

where L is a lower triangular matrix with positive diagonal entries. Then,

$$\|Ae_i\|^2 = e_i^T A^T A e_i = e_i^T L L^T e_i = \|L^T e_i\|^2$$

with e_i the i-th canonical vector of $\mathbb{R}^m$, $i = 1, 2, \ldots, m$. That is,

$$\|A_i\|^2 = \sum_{t=1}^{i} l_{i,t}^2$$

and therefore

$$l_{i,i}^2 = \|A_i\|^2 - \sum_{t=1}^{i-1} l_{i,t}^2.$$

Using the fact that $\langle A_i, A_j\rangle = \langle L^t e_i, L^t e_j\rangle = \sum_{k=1}^{j-1} l_{j,k} l_{i,k} + l_{j,j} l_{i,j}$ for $i = 2, \ldots, m$, $j = 1, 2, \ldots, i-1$, then the elements $l_{i,j}$ can be written as follows,

$$l_{i,j} = \frac{\|A_i + A_j\|^2 - \|A_i\|^2 - 2\sum_{k=1}^{j-1} l_{j,k} l_{i,k} - \|A_j\|^2}{2 l_{j,j}} = \frac{\langle A_i, A_j\rangle - \sum_{k=1}^{j-1} l_{j,k} l_{i,k}}{l_{j,j}}.$$

□

Proposition 2. *Let $A \in \mathbb{R}^{n\times m}$ with rank$(A) = r < \min\{n, m\}$. Then, the unique lower echelon matrix with positive leading entries and full column rank $L \in \mathbb{R}^{m\times r}$, such that, $A^T A = LL^T$ can be obtained without directly computing the complete product of $A^T A$, i.e., only in the worst case $\frac{(2m-r)(r+1)}{2}$ elements of the matrix $A^T A$ are computed.*

Proof. Since $A \in \mathbb{R}^{n\times m}$ does not have full column rank, then $A^T A \in \mathbb{R}^{m\times m}$ is a symmetric positive semidefinite matrix and by Theorem 1 admits a unique lower echelon matrix $L = (l_{i,j}) \in \mathbb{R}^{m\times r}$ with all the leading entries for each column positive, such that, $A^T A = LL^T$.

Now, we apply Theorem 2 to obtain the elements of L. Since A does not have full column rank, there exists k, $1 < k \leq m$, such that, $l_{k,k} = 0$. By Proposition 1, the entries $l_{j,k} = 0$, for $j = k+1, \ldots, m$ and this column will not belong to L. In fact, there are $m - r$ indices $\{k_1, \ldots, k_{m-r}\} \subset \{1, \ldots, m\}$ such that $l_{k_i,k_i} = 0$ given the echelon form of L. When the first r columns of the matrix A are linear independent, it is the case when it is necessary to compute more elements of the matrix $A^T A$. In this case, the quantity of inner products $\langle A_i, A_j\rangle$ is $m + (m-1) + \cdots + (m-r+1) = \frac{(2m-r)(r+1)}{2}$. □

The last results allow us to describe an algorithm for computing the full rank Cholesky factorization for the normal matrix $A^T A$, without doing the complete product of the two matrices, for any rectangular matrix A with no zero rows and columns.

Algorithm 2. *(The full rank Cholesky factorization for the normal matrix (by rows)). Let $A = [A_1, \ldots, A_m] \in \mathbb{R}^{n\times m}$. This algorithm computes the full rank Cholesky factorization of $A^T A = LL^T$ with $L = (l_{i,j})$, the rank of A and the row vector $c = (c_j)$ with the indices of the linearly independent columns of A.*

Input: $A \in \mathbb{R}^{n\times m}$

$l_{1,1} := \sqrt{\langle A_1, A_1\rangle}$; $r := 1$; *counter* $:= 0$; $c := [1]$;
  for $i = 2, 3, \ldots, m$
    for $j = 1, 2, \ldots, i - \textit{counter} - 1$
      $l_{i,j} := \frac{\langle A_i, A_{c_j}\rangle - \sum_{t=1}^{j-1} l_{c_j,t} \cdot l_{i,t}}{l_{c_j,j}}$;
    endfor
    var $:= \sqrt{\langle A_i, A_i\rangle - \sum_{t=1}^{i-\textit{counter}-1} l_{i,t}^2}$;
    if var $= 0$ *then*
      counter $:=$ *counter* $+ 1$;

(LINE 9) *elseif*
(LINE 10) $l_{i,i-counter} := var;$
(LINE 11) $c := [c \;\; i];$
(LINE 12) $r := r+1;$
(LINE 13) *endif*
(LINE 14) *endfor*

Output: $L \in \mathbb{R}^{m\times r}$**,** $r = \mathrm{rank}(A)$ **and** c

Remark 2. *Analogously to the Algorithm 1 the comparative in line 7 should be made with a certain tolerance in order to define an stopping criterion.*
The Algorithm 2 computes the elements of L by rows, other algorithm could be proposed for computing the elements of L by columns, being the computational cost similar to the Algorithm 2. The two algorithms can be stopped after the computation of some rows (or columns) of the factor L and the algorithm by columns has the advantage that the entries can be obtained by parallel processing.

The following table shows the maximum number of floating point operations for computing the factor L by Algorithm 2,

Elements	$+$	$\times$	$\div$	$\surd$	Total
$l_{1,1}$	$n-1$	n	0	1	$2n$
$l_{i,1}$ for $i=\{2,\ldots,m\}$	$n-1$	n	1	0	$2n(m-1)$
$l_{i,j}$ for $i=\{3,4,\ldots,r\}$ and $j=\{2,\ldots,i-1\}$	$n+j-2$	$n+j-1$	1	0	$\frac{r^3}{3}-r^2-\frac{2r}{3}+$ $n(r^2-3r+2)$
$l_{i,j}$ for $i=\{r+1,\ldots,m\}$ and $j=\{2,\ldots,r\}$	$n+j-2$	$n+j-1$	1	0	$-r^3+(m+1-2n)r^2+$ $(2mn+2n-m)r-2mn$
$l_{i,i}$ for $i=\{2,3,\ldots,r\}$	$n+i-2$	$n+i-1$	0	1	$r^2+2nr-r-2n$
$l_{i,i}$ for $i=\{r+1,\ldots,m\}$	$n+r-1$	$n+r$	0	1	$-2r^2+(2m-2n)r+$ $2mn$
Comparations					$m-1$

Table 2: Maximum floating point operations for computing L by Algorithm 2

Using the Table 2 we obtain the computational cost $T(n,m,r)$ of Algorithm 2 in the worst case, that is, when the first r columns of A are the linearly independent columns of A, as follows,

$$T(n,m,r) = 2mnr + mr^2 - nr^2 - \frac{2}{3}r^3 + 2mn + mr - nr - r^2 - \frac{5}{3}r + m - 1$$

In this way, following a similar argument as in the proof of Proposition 1, we have the following result,

Proposition 3. *Let $A \in \mathbb{R}^{n\times m}$ with rank$(A) = r \leq \min\{n, m\}$. Algorithm 2 computes the elements of the lower echelon matrix $L \in \mathbb{R}^{m\times r}$ such that r is equal to the rank of A (equivalently, the rank of $A^T A$) and the computational cost is $O(2mnr + mr^2 - nr^2 - \frac{2r^3}{3})$.*

Remark 3. *If $m = n$, then the cost of the Algorithm 2 is $O(2m^2 r - \frac{2r^3}{3})$. In addition if $r \ll m$, the total computational cost is significantly reduced.*

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