Matrix Inversion Using Cholesky Decomposition

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1 Introduction

Matrix inversion with the use of the Cholesky decomposition technique is used for inversion of the positive-definite and symmetric matrices. Once one has such type of a matrix, the numerical approach based on the Cholesky technique is more efficient than e.g. more general Gauss-Jordan elimination.

The classical matrix inversion algorithms that are based on the Cholesky decomposition require $\mathcal{O}(n^3)$ operations. Krishnamoorthy & Menon (2011) suggest a modified method of the matrix inversion based on the Cholesky decomposition. It has fewer operations comparing to the classical method. We will describe these methods below and implement in the code the idea of Krishnamoorthy & Menon (2011).

Cholesky decomposition technique may be applied to Hermitian matrices (i.e. complex square matrices that is equal to its own conjugate transpose). We will apply the method to the matrices with real elements.

2 Algorithm description

2.1 Classical method with Cholesky decomposition

If $A \in \mathcal{R}^{N\times N}$ is a square symmetric matrix with real positive elements then the Cholesky decomposition may transform it to

$$A = R^{\mathrm{T}} R$$

where R is the upper triangular matrix and R^{T} its transpose. The elements of $R = r_{ij}$, $i \leq j \leq N$ are given by the expressions

$$r_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} r_{ki}^2}$$

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

Table 1: Number of operations for the matrix inverse

Method	Number of operations
Classical	$\frac{5}{6}n^3$
Modified	$\frac{1}{2}n^3$

It is important to follow a certain order when calculating the elements r_{ij} because each next element uses values of the previous elements. The order is the following: from the element r_{11} on the left to the right and then down to the next row starting again from the diagonal element.

If $X \in \mathcal{R}^{N\times N}$ and $X = A^{-1}$ then

$$AX = I \tag{1}$$

where I is the identity matrix of order N. Then we can rewrite this as

$$R^{\mathrm{T}}RX = I. \tag{2}$$

By letting $B = RX$, we derive

$$R^{\mathrm{T}}B = I \tag{3}$$

and

$$RX = B. \tag{4}$$

By solving equations (3) and (4) we may derive the inverse matrix A^{-1}.

2.2 Modified method with Cholesky decomposition

The modification proposed by Krishnamoorthy & Menon (2011) allows us to skip the process of solving the equation (3).

Let $B = \left(R^{\mathrm{T}}\right)^{-1}$. The diagonal elements of R^{T} and R are the same. The diagonal elements of R^{-1} are inversions of the diagonal elements of R. Therefore, we construct matrix S with elements

$$s_{ij} = \begin{cases} 1/r_{ii} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

Krishnamoorthy & Menon (2011) state that the matrix S is the correct solution to the diagonal elements of the matrix B. Therefore, there is no need to compute B but just enough to use the backward substitution in order to solve for x_{ij} from the equation

$$Rx_i = s_i \tag{6}$$

where x_i and s_i are the i-th columns in the matrices X and S respectively.

3 Time complexity

Classical Cholesky decomposition requires $\frac{1}{6}n^3$ operations. Then there are two equations to be solved using the backward-substitution. They require $\frac{1}{3}n^2$ operations each. So, the total number of operations with the classical method is $\frac{5}{6}n^3$ (Table 1).

The modified method requires solution of one equation only and thus $\frac{1}{3}n^3$ operations. That, with the Cholesky decomposition ($\frac{1}{6}n^3$ operations) gives the total number of operations $\frac{1}{2}n^3$ (Table 1).

The modified Cholesky method for the matrix inverse is the main algorithm of our project.

Krishnamoorthy & Menon (2011) Matrix Inversion Using Cholesky Decomposition
`https://arxiv.org/abs/1111.4144`