Statistica Sinica **35** (2025), 1-22
doi:https://doi.org/10.5705/ss.202023.0065

ON BLOCK CHOLESKY DECOMPOSITION FOR SPARSE INVERSE COVARIANCE ESTIMATION

Xiaoning Kang[1], Jiayi Lian[2] and Xinwei Deng*[2]

[1]*Dongbei University of Finance and Economics and* [2]*Virginia Tech*

Abstract: The modified Cholesky decomposition is popular for inverse covariance estimation, but often needs pre-specification on the full information of variable ordering. In this work, we propose a block Cholesky decomposition (BCD) for estimating inverse covariance matrix under the partial information of variable ordering, in the sense that the variables can be divided into several groups with available ordering among groups, but variables within each group have no orderings. The proposed BCD model provides a unified framework for several existing methods including the modified Cholesky decomposition and the Graphical lasso. By utilizing the partial information on variable ordering, the proposed BCD model guarantees the positive definiteness of the estimated matrix with statistically meaningful interpretation. Theoretical results are established under regularity conditions. Simulation and case studies are conducted to evaluate the proposed BCD model.

Key words and phrases: Graphical model, modified Cholesky decomposition, regularization, sparsity, variable ordering.

1. Introduction

The estimation of covariance and inverse covariance matrices is of fundamental importance in the multivariate statistics with a broad spectrum of applications, such as linear discriminant analysis (Clemmensen et al., 2011), portfolio optimization (Deng and Tsui, 2013), and assimilation (Nino-Ruiz, Sandu and Deng, 2019). In high-dimensional data, sparse estimation of an inverse covariance matrix has specially attracted great attention, since it is closely related to a graphical model for inferring the conditional independence between variables of multivariate normal data. However, estimation of a large inverse covariance matrix often encounters two challenges. First, the estimated matrix needs to be positive definite for the valid statistical inferences. Second, the number of parameters in the model increases quickly in a quadratic order in terms of the matrix dimensionality.

Existing studies on the inverse covariance estimation in the literature generally fall into two categories. Denote the random variables of interest by $\boldsymbol{X} = (X_1, \ldots, X_p)'$ with mean $\mathbf{0}$ for simplicity and covariance matrix $\boldsymbol{\Sigma}$. The

*Corresponding author. E-mail: xdeng@vt.edu