Covariance Structure Approximation under High-Dimensionality with the use of improved Kullback–Leibler divergence

Monika Mokrzycka[1], **Jolanta Pielaszkiewicz**[2] **and Johan Alenlöv**[2]

[1] *Institute of Plant Genetics, Polish Academy of Sciences, Poznań, 60-479, Poland*
[2]*Department of Computer and Information Science, Linköping University, Linköping, 58-183, Sweden*

Abstract

Covariance approximation and structure identification become challenging in high-dimensional settings when the sample covariance matrix is singular. We propose to utilize an improved Kullback–Leibler divergence framework for comparing and approximating Kronecker structured covariance matrices for matrix-variate elliptically contoured distributions. The approach jointly estimates a regularization parameter and the underlying covariance matrix by positive-definite separable covariance structures. Method applies number of penalty functions representing different prior distributions on underlying parameter. Simulation studies show that the proposed method reliably identifies covariance structures as well as approximate structural parameters in high-dimensional settings. Applications to food-habit, barley, and gene-expression data illustrate its practical usefulness across longitudinal, repeated-measurement, and phylogenetic settings. The proposed framework provides a flexible approach to regularized covariance approximation and structure identification when conventional methods are hindered by high dimensionality and singularity problems.

Keywords

regularization, elliptical distribution, Kronecker product, covariance matrix, Kullback-Leibner divergence

Acknowledgements

This research was funded by the NAWA Bekker program under project no. BPN/BEK/2023/1/00142 (M. Mokrzycka).