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13th Scientific Meeting of the Classification and Data Analysis Group
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Giovanni C. Porzio
Carla Rampichini
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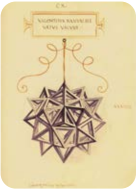

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MODEL-BASED CLUSTERING WITH SPARSE MATRIX MIXTURE MODELS

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ABSTRACT: In recent years we are witnessing to an increased attention towards methods for clustering matrix-valued data. In this framework, matrix Gaussian mixture models constitute a natural extension of the model-based clustering strategies. Regrettably, the overparametrization issues, already affecting the vector-valued framework in high-dimensional scenarios, are even more troublesome for matrix mixtures. In this work we introduce a sparse model-based clustering procedure conceived for the matrix-variate context. We introduce a penalized estimation scheme which, by shrinking some of the parameters towards zero, produces parsimonious solutions when the dimensions increase. Moreover it allows cluster-wise sparsity, possibly easing the interpretation and providing richer insights on the analyzed dataset.

KEYWORDS: model-based clustering, penalized likelihood, sparse matrix estimation, EM-algorithm

1 Introduction

Model-based clustering represents a well established framework to cluster multivariate data. When dealing with continuous data, the generative mechanism is routinely described by means of Gaussian Mixture Models (GMMs). Partitions are obtained by exploiting the one-to-one correspondence between the groups and the components of the mixture. This approach has been used in many different applications; nonetheless GMMs tend to be over-parameterized in high-dimensional settings where their usefulness might be jeopardized.

This problem complicates even further in three-way data scenarios, where multiple variables are measured on different occasions for the considered units. Here matrix-variate distributions have often been used and embedded in the mixtures framework, thus providing a valid solution when partitions of matrices are required (Viroli, 2011). In spite of its strenght points, this approach is dramatically over-parameterized even in moderate dimensions. Therefore, we propose a penalized model-based clustering strategy in the matrix-variate framework. Our approach reduces the number of parameters to be estimated, by shrinking some of them towards zero, and possibly leads to a gain in terms of interpretability. The rest of the paper is organized as follows. In Section 2 we introduce matrix Gaussian mixture models (MGMMs) and we outline our proposal. An application to real world data is reported in Section 3 alongside with some concluding remarks and possible future research directions.

2 Penalized matrix-variate mixture model

Let $\mathbf{X} = \{\mathbf{X}_1, \dots, \mathbf{X}_n\}$ be a set of n matrices with $\mathbf{X}_i \in \mathbb{R}^{p \times q}$. MGMM provides an extension of the GMM when clustering of matrices are needed. The density of $\mathbf{X}_i$ is then expressed as follows

$$f(\mathbf{X}_i;\Theta) = \sum_{k=1}^{K} \tau_k \phi_{(p\times q)}(\mathbf{X}_i; M_k, \Omega_k, \Gamma_k) \tag{1}$$

where $\Theta = \{\tau_k, M_k, \Omega_k, \Gamma_k\}_{k=1}^{K}$, τ_k's are the mixing proportions, with $\tau_k > 0$ and $\sum_k \tau_k = 1$. On the other hand $\phi_{(p\times q)}(\mathbf{X}_i; M_k, \Omega_k, \Gamma_k)$ denotes the density of a $p \times q$ matrix normal distribution where $M_k \in \mathbb{R}^{p\times q}$ is the mean of the *k-th* component while $\Omega_k \in \mathbb{R}^{p\times p}$ and $\Gamma_k \in \mathbb{R}^{q\times q}$ represent respectively the rows and the columns component precision matrices.

In (1) the number of parameters to estimate scales quadratically with both p and q, endangering the pratical usefulness of the model. Recently some solutions have been proposed, trying to overcome this issue (see Wang & Melnykov, 2020 and Sarkar *et al.* , 2020). These approaches present some drawbacks as they are computationally intensive and as they implement a rigid way to induce parsimony. Therefore in this work we take a different path, adopting a penalized estimation approach which implicitly assumes that M_k, Ω_k, Γ_k, for $k = 1, \dots, K$, possess some degree of sparsity.

To this aim, we introduce a penalized likelihood strategy to obtain $\hat{\Theta}$. The log-likelihood function to be maximized is defined as

$$\ell(\Theta;\mathbf{X}) = \sum_{i=1}^{n} \log\left\{\sum_{k=1}^{K} \tau_k \phi_{p\times q}(\mathbf{X}_i; M_k, \Omega_k, \Gamma_k)\right\} - p_{\lambda_1,\lambda_2,\lambda_3}(M_k, \Omega_k, \Gamma_k) \tag{2}$$

with the penalization term $p_{\lambda_1,\lambda_2,\lambda_3}(M_k, \Omega_k, \Gamma_k)$ equals to

$$p_{\lambda_1,\lambda_2,\lambda_3}(M_k, \Omega_k, \Gamma_k) = \sum_{k=1}^{K} \lambda_1 ||P_1 * M_k||_1 + \sum_{k=1}^{K} \lambda_2 ||P_2 * \Omega_k||_1 + \sum_{k=1}^{K} \lambda_3 ||P_3 * \Gamma_k||_1$$

Table 1. *Adjusted Rand Index (ARI) and number of free estimated parameters for three clustering procedures.*

	Sparsemixmat	Sarkar *et al.* , 2020	GMM
ARI	0.7883	0.7772	0.3841
# of parameters	218	275	850

P_1, P_2, P_3 are matrices with non-negative entries, $||A||_1 = \sum_{jh} |A_{jh}|$, $\lambda_1, \lambda_2, \lambda_3$ are the penalization parameters while $*$ denotes the element-wise product.
To estimate Θ, we devise an ad-hoc EM-algorithm which maximizes the *penalized complete data log-likelihood* associated with (2). The E-step computes class membership a posteriori probabilities via the standard updating formula. On the other hand the M-step consists of three partial optimization cycles. An estimate for M_k is obtained by means of a cell-wise coordinate ascent algorithm while, to estimate Ω_k and Γ_k, we propose a suitable modification of the graphical LASSO (Friedman *et al.* , 2008). The resulting model, inducing sparsity in the precision matrices, accounts for cluster-wise conditional independence patterns, which might ease the interpretation of the results, and possibly provides indications about irrelevant variables. Moreover the number of parameters is reduced without imposing rigid structures.

3 Application and concluding remarks

We employ the procedure outlined in Section 2 to obtain a partition of the Landsat satellite data, where $n = 845$ matrices, with dimensions 4×9, coming from three different classes are available (see Viroli, 2011 for a detailed description). In Table 1 we report the results obtained with the proposed procedure (Sparsemixmat) and with two plausible competitors being the approach by Sarkar *et al.* , 2020 and the standard GMM applied to the unfolded two-way representation of the data. Our model outperforms the competitors, when recovering the true clustering structure is the aim. Furthermore, we provide the most parsimonious solution, displaying the lowest number of non zero estimated parameters. The retrieved sparse matrix structures are graphically displayed, for the three classes, in Figure 1. While the clustering is mainly driven by the different patterns in M_k's, the Γ_k's are the ones showing the highest degree of sparsity, with different intensities for the three classes.

The promising results obtained in the application demonstrate how the penalized matrix-variate mixture model proposed in this work might alleviate the flaws of standard three-way data clustering in high-dimensional scenarios.

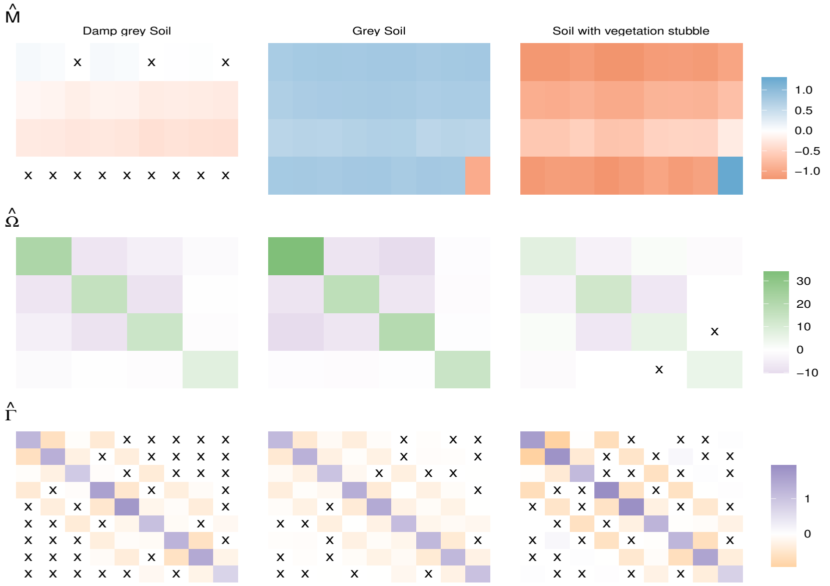

Figure 1. *Sparsely estimated M_k (upper plots), Ω_k (middle plots) and Γ_k (lower plots) for $k = 1,2,3$. Entries that are shrunk to 0 by the estimator are highlighted with an $\times$.*

Our proposal is able to effectively reduce the number of parameters to estimate while, at the same time, flexibly accounting for different relationships among the variables and for different level of sparsity across the groups. Future research directions would focus on the derivation of an appropriate model selection procedure, determining jointly reasonable values for the penalty coefficients as well as for the number of mixture components.

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