A unified framework for model-based clustering, linear regression and multiple cluster structure detection

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Abstract

A general framework for dealing with both linear regression and clustering problems is described. It includes Gaussian clusterwise linear regression analysis with random covariates and cluster analysis via Gaussian mixture models with variable selection. It also admits a novel approach for detecting multiple clusterings from possibly correlated sub-vectors of variables, based on a model defined as the product of conditionally independent Gaussian mixture models. A necessary condition for the identifiability of such a model is provided. The usefulness and effectiveness of the described methodology are illustrated using simulated and real datasets.

Keywords: Bayesian information criterion, Clusterwise linear regression, EM algorithm, Gaussian mixture model, Genetic algorithm, Variable selection

1. Introduction

Cluster analysis and regression are two fields of statistics useful for unsupervised and supervised statistical learning, respectively [Hastie et al. 2009]. Although their goals are quite different, there may be situations in which relevant information contained in a given dataset can be obtained using both types of analysis.

Consider, for example, a dataset characterised by the presence of an unknown cluster structure (a grouping of the given set of observations into
clusters), but suppose that this structure is confined in a sub-space of the variable space. Since the effect of the presence of uninformative variables is a masking of the cluster structure (see, e.g., Gordon [1999], the use of methods able to select the informative variables in a cluster analysis, such as those proposed by Fowlkes et al. (1988), Gnanadesikan et al. (1995), Brusco and Cradit (2001), Montanari and Lizzani (2001), Fraiman et al. (2008), Steinley and Brusco (2008a) and Witten and Tibshirani (2010), is crucial for a proper recovery of the unknown cluster structure from the observed data. If the variables are continuous, Gaussian mixture models can be employed. In these models it is assumed that the joint probability density function (p.d.f.) of the variables is a mixture of $K$ ($K \geq 1$) Gaussian components (one component for each cluster) (see, e.g., McLachlan and Peel 2000; Melnykov and Maitra 2010). The number of components is generally chosen through model selection criteria, such as the Bayesian information criterion (BIC) (Schwarz, 1978). Methods that simultaneously select the informative variables and find the cluster structure, based on Gaussian mixture models, have been proposed by Dy and Brodley (2004), Law et al. (2004), Tadesse et al. (2005), Raftery and Dean (2006), Pan and Shen (2007), Xie et al. (2008), Wang and Zhu (2008), Galimberti et al. (2009), Maugis et al. (2009a), Maugis et al. (2009b), Zeng and Cheung (2009), Zhou et al. (2009), Guo et al. (2010) and Andrews and McNicholas (2014). Comparisons among some of these methods, based on analyses of simulated and real datasets, can be found in Steinley and Brusco (2008b), Witten and Tibshirani (2010), Celeux et al. (2011), Celeux et al. (2014) and Andrews and McNicholas (2014). In particular, the variable selection methods proposed by Raftery and Dean (2006) are based on a model in which the vector of the examined variables is assumed to be partitioned into two sub-vectors: one is composed of the informative variables and the other contains the uninformative ones. Furthermore, it is assumed that the joint p.d.f. is the product of a Gaussian mixture model (with $K \geq 2$ components) for the distribution of the informative variables and a Gaussian linear regression model for the conditional distribution of the uninformative variables given the informative ones. The selection of the informative variables is then recast as a model comparison problem, based on the BIC. A local optimum in model space is found through a greedy search algorithm. In the model selected using these methods, the uninformative variables are assumed to linearly depend on all the informative ones. In some situations this assumption may be restrictive and could lead to erroneous model selections and, consequently, to erroneous results. To avoid this drawback,
two more versatile models have been proposed: one allows the uninformative variables to be explained by only a subset of the informative ones (Maugis et al., 2009a); the other also allows that some uninformative variables are independent of all the informative ones (Maugis et al., 2009b). The three methods just described make use of Gaussian linear regression models for performing variable selection in model-based cluster analysis. Thus, they embed a supervised learning process into an unsupervised one.

Consider another example in which the dataset provides information about responses and predictors for a regression problem. Furthermore, suppose that the sample observations come from a population composed of several sub-populations, each of which is characterised by a different regression equation, but the information about which sub-population each observation comes from is unknown. An approach able to deal with such an unobserved heterogeneity in a regression problem is represented by clusterwise regression. In this approach the dependence of the responses on the predictors is described by means of a finite mixture (see, e.g., Quandt and Ramsey, 1978; De Sarbo and Cron, 1988; De Veaux, 1989). With continuous responses Gaussian mixture models are generally employed, resulting in mixtures of Gaussian linear regression models. In an analysis based on these models, an unsupervised learning process is embedded into a supervised one.

In addition to the variable selection, another problem to be tackled when performing a cluster analysis is that datasets may also be characterised by the presence of several unknown cluster structures, that is different groupings of the same set of observations defined in different subspaces of the variable space. Since a classical assumption in most clustering methods is that one single cluster structure is contained in the data, some relevant information about the ways observations are clustered could be missed. Methods to deal with this problem are due, for example, to Soffritti (2003), Friedman and Meulman (2004), Belitskaya-Levy (2006), Galimberti and Soffritti (2007), Poon et al. (2013), Dang and Bailey (2015) and Liu et al. (2015). In the latter four papers, model-based methods are described. In particular, the solution proposed by Galimberti and Soffritti (2007) relies on a model in which the vector of the observed variables is assumed to be partitioned into independent sub-vectors, and a Gaussian mixture model is specified for each variable sub-vector.

In this paper a general framework is developed by exploiting the idea of combining the above mentioned unsupervised and supervised methods. More specifically, it incorporates Gaussian model-based clustering with variable
selection, Gaussian clusterwise linear regression (with a constraint on the regression coefficients) and a novel approach for detecting multiple cluster structures from possibly correlated variable sub-vectors. These three fields of statistics are brought together through the specification of a general and flexible model. The basic idea of the proposed framework is introduced in Section 2 while the theory is illustrated in Section 3. Namely, the general model is presented in Section 3.1. A theorem providing necessary conditions for its identifiability is proved in Section 3.2. Details about the maximum likelihood (ML) estimation of the model parameters and the issue of model selection are given in Sections 3.3 and 3.4 respectively. Section 4 contains experimental results obtained by exploring the model space in some simulated and real datasets through genetic algorithms. Concluding notes are reported in Section 5.

2. An introductory example

The basic idea of the framework developed in this paper is illustrated through an example referring to a dataset containing information about 17 male and 16 female students in an introductory statistics class at a US college. The dataset is available at http://economics-files.pomona.edu/GarySmith/StatSite/eclectic.html. The example focuses on three variables: student’s height, mother’s height and father’s height. Figure 1 shows the scatterplot matrix, where male and female students are represented using squares and circles, respectively.

From an unsupervised point of view, one may be interested in detecting whether the dataset is characterised by the presence of a cluster structure in the joint distribution of the three examined variables. Using the package mclust (Fraley and Raftery 2002; Fraley et al. 2012) for the R software environment (R Core Team 2015), Gaussian mixture models with $K = 1, 2, 3, 4$ components are fitted to the dataset, and the best model is selected according to the BIC. Since such a model results to be a Gaussian model with only one component, no evidence of any cluster structure emerges from this unsupervised analysis. This model is denoted as $M_1$ in Section 4.1.

As described in Section 1, the presence of a cluster structure may be masked by uninformative variables. Thus, a further analysis is carried out through the R package clustvarsel that implements the variable selection methods proposed by Raftery and Dean (2006). This analysis suggests that parents’ heights are informative variables while the students’ height can
Figure 1: Scatterplot matrix of the heights (in inches) in the students’ dataset.
be discarded. Furthermore, the best Gaussian mixture model for parents’ heights identifies $K = 2$ clusters. Figure 2 shows the two 85% ellipses obtained from the mean vectors and covariance matrices of this model. White and black colours are used to highlight observations assigned to different clusters. According to this analysis students with short parents can be separated from students with tall parents.

In order to measure the association between the detected cluster structure and the gender of the students, the joint classification of the students based on their gender and the segmentation obtained from the parents’ heights is examined, and the adjusted Rand index ($aRI$) (Hubert and Arabie, 1985) is computed. From the obtained results (see Table 1, left part) it emerges that such an association is very low. The joint model for the three examined
Table 1: Comparison between the classification of the students based on their
gender and the segmentations obtained from models $M_2$ (Structure 1) and
$M_5$ (Structure 2).

|     | Structure 1 | Structure 2 |
|-----|-------------|-------------|
|     | Cluster     | Cluster     |
| Gender | 1  | 2  | 1  | 2  |
| F     | 8  | 8  | 1  | 15 |
| M     | 13 | 4  | 16 | 1  |
| aRi   | 0.047       | 0.765       |

variables resulting from this analysis is denoted as $M_2$ in Section 4.1.

Given the drawbacks of the variable selection methods proposed by Raftery
and Dean (2006), further analyses are carried out by using two C++ soft-
wares (SelvarClust and SelvarClustIndep) that incorporate algorithms
for fitting and selecting models described in Maugis et al. (2009a, b). Par-
ents’ heights result to be informative variables also using these techniques
(with the same Gaussian mixture model with two components selected by clustvarsel). As far as the Gaussian linear regression model for the con-
ditional distribution of the students’ heights is concerned, only the father’s
height is selected as a predictor. The resulting model for the joint distribution
of the three heights is $M_3$ in Section 4.1.

The examined dataset can be analysed also from a supervised point of
view. Namely, the interest could be in predicting the height of a student from
his/her parents’ heights. In particular, this supervised analysis is performed
using two different models for the conditional distribution of the students’
heights: a Gaussian linear regression model and a mixture of two Gaussian
linear regression models with the same regression coefficients. Both models
are intentionally specified and estimated by ignoring the information about
gender. The fictitiously unobserved heterogeneity obtained in this way could
be captured by using a mixture of two Gaussian linear regression models. For
both types of models the fathers’ height results to be the only relevant pre-
dictor for the students’ height. Figure 3 shows the regression lines estimated
using the two models obtained after performing regression variable selection.
Models $M_4$ and $M_5$ in Section 4.1 denote the models for the joint distribution
of the three variables obtained by multiplying each of these regression mod-
els by the best Gaussian model for the marginal distribution of the parents’
Figure 3: Scatterplot of the student’s and father’s heights and fitted regression lines using a Gaussian linear model (left panel) and a clusterwise Gaussian linear model with two components having the same regression coefficients (right panel).

heights. In particular, using a mixture of two Gaussian regressions allows to produce a segmentation of the observations into two clusters. In the right panel of Figure 3 white and black colours are used to distinguish between such clusters. Differently from the cluster structure obtained from the unsupervised analysis of the parents’ heights, the cluster structure detected in this supervised analysis of the conditional distribution of the students’ heights is highly associated with their gender (see Table 1, right part).

The examined dataset is characterised by the presence of two different cluster structures that have been detected by combining methods for unsupervised and supervised statistical learning. In particular, the identification of such structures has required the specification of a model for the joint p.d.f. of the three examined variables obtained as the product of a mixture of two bivariate Gaussian distributions (for the marginal p.d.f. of the parents’ heights) and a mixture of two univariate Gaussian linear regression models with the same regression coefficients (for the conditional p.d.f. of the students’ height). This model is denoted as $M_6$ in Section 4.1, where further results obtained from the analysis of this dataset are presented. The basic idea of analysing the same dataset using different types of models in order
to extract relevant information from different perspectives is presented in a formal and more general way in Section 3.

3. A general framework for clustering and regression

3.1. Models for clustering and regression

For the ease of exposition assume initially that the examined dataset may be characterised by up to two unknown cluster structures, \( S_1 \) and \( S_2 \). Let \( X = (X_1, \ldots, X_L) \) be the random vector of \( L \) observed continuous variables and \( X^{S_1}, X^{S_2}, X^U \) be a splitting of \( X \) into three non-overlapping sub-vectors, where \( X^{S_2} \) and \( X^U \) can be empty. In particular, the sub-vector \( X^{S_g} \) is composed of \( L_g \) variables that provide information about the cluster structure \( S_g \) \((g = 1, 2)\), while the sub-vector \( X^U \) is composed of \( L_U \) uninformative variables, with \( L_1 + L_2 + L_U = L \).

The following set of assumptions is specified.

A1) The marginal distribution of \( X^{S_1} \) is given by a Gaussian mixture model. Namely:

\[
f \left( x^{S_1}; \theta_1 \right) = \sum_{k=1}^{K_1} \pi_k \phi_{L_1} \left( x^{S_1}; \mu_k, \Sigma_k \right),
\]

where \( K_1 \geq 1, \theta_1 = (\pi_1, \mu_1, \sigma_1), \pi_1 = (\pi^{(1)}_1, \ldots, \pi^{(K_1)}_1), \mu_1 = (\mu^{(1)}_1, \ldots, \mu^{(K_1)}_1), \sigma_1 = (\Sigma^{(1)}_1, \ldots, \Sigma^{(K_1)}_1), \) and \( \phi_{L_1} (\cdot; \mu^{(1)}_k, \Sigma^{(1)}_k) \) denotes the p.d.f. of the \( L_1 \)-dimensional normal distribution with mean vector \( \mu^{(1)}_k \) and covariance matrix \( \Sigma^{(1)}_k \).

A2) The conditional p.d.f. of \( X^{S_2} \) given \( X^{S_1} \) is equal to

\[
f \left( x^{S_2} | x^{S_1}; \theta_2 \right) = \sum_{k=1}^{K_2} \pi_k^{(2)} \phi_{L_2} \left( x^{S_2}; \mu^{(2)}_k, \Sigma^{(2)}_k \right),
\]

where \( K_2 \geq 1, \mu^{(2)}_k = \beta_0 + \lambda^{(2)}_k + B_{21}x^{S_1}, k = 1, \ldots, K_2, \)

with \( \beta_0 \) and \( \lambda^{(2)}_k \) denoting \( L_2 \)-dimensional vectors, and \( B_{21} \) representing a \( L_2 \times L_1 \) matrix. The condition defined by equation (3) is equivalent to assuming that the dependence of \( X^{S_2} \) on \( X^{S_1} \) is defined by a multivariate
linear regression model whose error terms follow a mixture of $K_2$ Gaussian components. Specifically,

$$X^{S_2} = \beta_0 + B_{21}X^{S_1} + \epsilon_2, \; \epsilon_2 \sim \sum_{k=1}^{K_2} \pi_k^{(2)} N_{L_2} \left( \lambda_k^{(2)}, \Sigma_k^{(2)} \right),$$

(4)

where $N_{L_2} \left( \lambda_k^{(2)}, \Sigma_k^{(2)} \right)$ denotes the $L_2$-dimensional normal distribution with mean vector $\lambda_k^{(2)}$ and covariance matrix $\Sigma_k^{(2)}$. Thus, the conditional distribution of $X^{S_2}$ given $X^{S_1}$ is described by a mixture of $K_2$ Gaussian linear regression models with the constraint that the effect of $X^{S_1}$ on the expected value of $X^{S_2}$ is the same for all the $K_2$ components of the mixture (2). In order to guarantee identifiability of model (4), it is necessary to require some constraints on $\beta_0$ or the $\lambda_k^{(2)}$’s. Namely, $\beta_0 = 0$ or $\sum_k \pi_k^{(2)} \lambda_k^{(2)} = 0$. This problem does not arise if model (3) is directly parameterized as follows:

$$\mu_k^{(2)} = \gamma_k^{(2)} + B_{21}x^{S_1}, \; k = 1, \ldots, K_2,$$

(5)

where $\gamma_k^{(2)} = \beta_0 + \lambda_k^{(2)}$. Then, $\theta_2 = (\pi_2, \gamma_2, B_{21}, \sigma_2)$, $\pi_2 = (\pi_1^{(2)}, \ldots, \pi_{K_2}^{(2)})$, $\gamma_2 = (\gamma_1^{(2)}, \ldots, \gamma_{K_2}^{(2)})$, $\sigma_2 = (\Sigma_1^{(2)}, \ldots, \Sigma_{K_2}^{(2)})$ (for further details see Soffritti and Galimberti [2011]).

A.3) The conditional distribution of $X^U$ given $(X^{S_1}, X^{S_2})$ follows a Gaussian linear regression model. Specifically:

$$X^U = \alpha_0 + A_1x^{S_1} + A_2x^{S_2} + \epsilon_U, \; \epsilon_U \sim N_{L_U} (0, \Sigma_U),$$

(6)

whose parameters are $\theta_U = (\alpha_0, A_1, A_2, \Sigma_U)$, where $\alpha_0$ is a $L_U$-dimensional vector, $A_1$ and $A_2$ represent matrices of dimension $L_U \times L_1$ and $L_U \times L_2$, respectively.

Thus, the joint p.d.f. of $X$ can be obtained as follows:

$$f(x; \theta) = \sum_{k=1}^{K_1} \phi_{L_1} \left( x^{S_1}; \mu_k^{(1)}, \Sigma_k^{(1)} \right) \times \sum_{k=1}^{K_2} \pi_k^{(2)} \phi_{L_2} \left( x^{S_2}; \gamma_k^{(2)} + B_{21}x^{S_1}, \Sigma_k^{(2)} \right) \times \phi_{L_U} \left( x^U; \alpha_0 + A_1x^{S_1} + A_2x^{S_2}, \Sigma_U \right),$$

(7)
where \( \theta = (\theta_1, \theta_2, \theta_U) \).

Some approaches for unsupervised and/or supervised analysis illustrated in Sections 1 and 2 can be obtained from model (7).

- When \( X^{S_2} = X^U = \emptyset \), the Gaussian mixture model used to detect the presence of a cluster structure in the joint distribution of \( X \) is obtained. The graphical representation of such a model is depicted in Figure 4(a), where \( Z \) denotes a nominal latent variable affecting the probability distribution of \( X \). If the number of categories of such a variable is greater than 1, then the joint distribution of \( X \) provides information about a latent cluster structure. Thus, \( Z \) can be considered as an indicator of cluster membership. This is the approach to cluster analysis based on Gaussian mixture models.

- When \( X^{S_2} = \emptyset, K_1 \geq 2, X^U \neq \emptyset \), a cluster structure is assumed to be hidden in the variable sub-space \( X^{S_1} \). Specifically, \( X^{S_1} \) and \( X^U \) represent the vectors of the informative and uninformative variables, respectively. The model associated with this situation can be graphically represented as in Figure 4(b). It represents the tool for model-based cluster analysis with variable selection according to the approach proposed by Raftery and Dean (2006).

- When \( K_1 = 1, X^{S_2} \neq \emptyset, X^U = \emptyset \), model (7) reduces to either a Gaussian linear regression model (if \( K_2 = 1 \)) or a mixture of Gaussian linear regression models (if \( K_2 > 1 \)) with the same regression coefficients (Soffritti and Galimberti, 2011) and Gaussian random covariates.

- When \( K_1 > 1, X^{S_2} \neq \emptyset, K_2 > 1 \), a novel model with two latent cluster structures is obtained. The marginal distribution of the variable sub-vector \( X^{S_1} \) provides information about the first structure while the second structure is hidden in the conditional distribution of \( X^{S_2} \) given \( X^{S_1} \). Thus, a novel approach for detecting two cluster structures from two possibly dependent sub-vectors of random variables is obtained. By setting \( B_{21} = 0 \) in equation (5), the second latent structure is, in fact, defined in the marginal distribution of \( X^{S_2} \), thus leading to the model proposed by Galimberti and Soffritti (2007). In both cases \( X^{S_1} \) and \( X^{S_2} \) represent vectors of informative variables. If, in addition, \( X^U \neq \emptyset \), then \( X^U \) is the vector of uninformative variables. In this latter case model (7) also allows to perform variable selection. The graphical
representation of model (7) when \((X^{S_1}, X^{S_2}, X^U)\) is a partition of \(X\) and both \(K_1\) and \(K_2\) are greater than 1 is given in Figure 4(c), where \(Z_1\) denotes the nominal latent variable (with \(K_1\) categories) that affects the probability distribution of \(X^{S_1}\), and \(Z_2\) denotes the nominal latent variable (with \(K_2\) categories) affecting the probability distribution of \(X^{S_2}\mid X^{S_1}\). Thus, in model (7), the sub-vector \(X^{S_2}\) is assumed to be conditionally independent of \(Z_1\) given \(X^{S_1}\). Furthermore, \(Z_1\) and \(Z_2\) are assumed to be independent.

![Graphical representations of three models obtained from equation (7).](image_url)

The model defined in equation (7) places two main restrictions. First, it forces the uninformative variables to linearly depend on all the remaining variables (see equation (6)). Furthermore, it prevents the possible presence of uninformative variables that are independent of any other variable. Models that do not impose these restrictions can be obtained as follows. Whenever \(X^U \neq \emptyset\), let \(X^{S_1}_U \subseteq X^{S_1}\) and, if \(X^{S_2} \neq \emptyset\), \(X^{S_2}_U \subseteq X^{S_2}\) denote the sub-vectors of \(X^{S_1}\) and \(X^{S_2}\), respectively, useful to predict the uninformative variables \(X^U\) according to a Gaussian linear regression model. Thus, equation (6) is modified as follows:

\[
X^U = \alpha_0 + A_{1U}X^{S_1}_U + A_{2U}X^{S_2}_U + \epsilon_U, \quad \epsilon_U \sim N_{L_U}(0, \Sigma_U),
\]

where \(A_{1U}\) and \(A_{2U}\) are matrices of dimensions \(L_U \times L_{1U}\) and \(L_U \times L_{2U}\), respectively, with \(L_{1U}\) and \(L_{2U}\) denoting the lengths of sub-vectors \(X^{S_1}_U\) and
Furthermore, let \((X^{S_1}, X^{S_2}, X^U, X^I)\) be a splitting of \(X\) into four non-overlapping sub-vectors, where the additional sub-vector \(X^I\) can be empty. Specifically, \(X^I\) contains \(L_I\) uninformative variables that are also independent of all the remaining variables. Thus, the resulting p.d.f. of \(X\) is defined as follows:

\[
f(x; \theta) = \sum_{k=1}^{K_1} \pi_k^{(1)} \phi_{L_1} \left( x^{S_1}; \mu_k^{(1)}, \Sigma_k^{(1)} \right) \times \sum_{k=1}^{K_2} \pi_k^{(2)} \phi_{L_2} \left( x^{S_2}; \gamma_k^{(2)} + B_{21} x^{S_1}, \Sigma_k^{(2)} \right) \times \phi_{L_U} \left( x^U; \alpha_0 + A_{1U} x^{S_1} + A_{2U} x^{S_2}, \Sigma_U \right) \times \phi_{L_I} \left( x^I; \mu_I, \Sigma_I \right),
\]

where \(\theta = (\theta_1, \theta_2, \theta_U, \theta_I)\), with \(\theta_I = (\mu_I, \Sigma_I)\).

The graphical representation of the models obtained from equation (9) by removing the second restriction is given in Figure 5(a); Figure 5(b) represents models resulting from the removal of both restrictions. When \(X^{S_2} = \emptyset\), \(X^U \neq \emptyset\) and \(X^I = \emptyset\), equation (9) gives the model proposed by Maugis et al. (2009a); if \(X^I \neq \emptyset\), the model introduced in Maugis et al. (2009b) is obtained.

![Graphical representations of two models](image)

Figure 5: Graphical representations of two models obtained from equation (9), where \(\bar{X}^{S_1} = X^{S_1} \setminus X^{S_1}_U\), \(\bar{X}^{S_2} = X^{S_2} \setminus X^{S_2}_U\).

Whenever \(X^{S_2} \neq \emptyset\), further more general models can be defined. For example, in equation (4) the variables in the sub-vector \(X^{S_2}\) are forced to
linearly depend on all the variables belonging to $X^{S_1}$. This restriction can be removed as follows. Let $X^{S_2} \subseteq X^{S_1}$ denote the sub-vector of $X^{S_1}$ composed of the predictors of $X^{S_2}$. Then, $\mu^{(2)}_k$ in equation (5) becomes

$$\mu^{(2)}_k = \gamma^{(2)}_k + B^{S_2}_{21} x^{S_1}, \quad k = 1, \ldots, K_2,$$

where the number of columns of matrix $B^{S_2}_{21}$ coincides with the length of $X^{S_2}$. If, in addition, $L_2 \geq 2$, it is possible to define a model in which a different sub-vector of the variables belonging to $X^{S_1}$ can be employed for predicting each variable in $X^{S_2}$. Such a model can be specified as follows. Let $X^{S_2}[l]$ be the $l$-th variable of $X^{S_2}$ and $X^{S_1}_l$ be the sub-vector of $X^{S_1}$ containing the predictors of $X^{S_2}[l]$. Then, $\mu^{(2)}_k$ can be obtained as follows:

$$\mu^{(2)}_k[l] = \gamma^{(2)}_k[l] + x^{S_1}_l \beta_l, \quad l = 1, \ldots, L_2,$$

where the notation $a[l]$ is used to denote the $l$-th element of vector $a$. The joint model for the vector $X^{S_2}$ resulting from equation (11) represents a seemingly unrelated linear regression model with a Gaussian mixture for the errors (for further details see Galimberti et al., 2015).

Models (7) and (9) can be easily modified so as to admit that the examined dataset may be characterised by up to, say, $G$ unknown cluster structures, where $G$ can be greater than 2. Let $(X^{S_1}, X^{S_2}, \ldots, X^{S_G}, X^U)$ be a splitting of $X$ into $G+1$ non-overlapping sub-vectors, where $X^{S_g}, g = 2, \ldots, G$, can be empty, and $L_g$ denotes the length of $X^{S_g}$ ($0 \leq L_g \leq L - \sum_{h=1}^{g-1} L_h$). For the marginal distribution of $X^{S_1}$ the same assumption $A1)$ is used for the previous models still holds. The remaining assumptions are modified as follows.

$A2*)$ For $g = 2, \ldots, G$, the conditional p.d.f. of $X^{S_g}$ given $(X^{S_1}, \ldots, X^{S_{g-1}})$ is equal to

$$f \left( x^{S_g} | (x^{S_1}, \ldots, x^{S_{g-1}}); \theta_g \right) = \sum_{k=1}^{K_g} \pi_k^{(g)} \phi_{L_g} \left( x^{S_g}; \mu_k^{(g)}, \Sigma_k^{(g)} \right),$$

where $K_g \geq 1$,

$$\mu_k^{(g)} = \gamma_k^{(g)} + \sum_{h=1}^{g-1} B_{gh} x^{S_h},$$

$B_{gh}$ is a $L_g \times L_h$ matrix, and $\theta_g = (\pi_g, \gamma_g, B_{g1}, \ldots, B_{g,g-1}, \sigma_g), \quad \pi_g = (\pi_1^{(g)}, \ldots, \pi_{K_g}^{(g)}), \quad \gamma_g = (\gamma_1^{(g)}, \ldots, \gamma_{K_g}^{(g)}), \quad \sigma_g = (\Sigma_1^{(g)}, \ldots, \Sigma_{K_g}^{(g)}).$ Thus, the
dependence of $X^S$ on $(X^{S_1}, \ldots, X^{S_{g-1}})$ is described by a multivariate linear regression model whose error terms follow a mixture of $K_g$ Gaussian components, with the constraint that the effect of $X^{S_h}$, $h = 1, \ldots, g - 1$, on $X^S$ is the same for all the $K_g$ components of the mixture (12).

3.2. Model identifiability

Some results concerning parameter identifiability are developed for a class of models obtained from equation (15). Namely, models characterised by different values of $G$, different partitions of $X$ into $G$ (or $G + 1$) sub-vectors and different values of $K_1, \ldots, K_G$ are examined. Such models can be described from the partitions $(S_1, \ldots, S_G, U)$ of the variable index set $\mathcal{I} = \{1, \ldots, L\}$ (with $U$ possibly equal to $\emptyset$). In particular, the model class is obtained by admitting that $G \in \mathcal{I}$, $K_g \in \{2, \ldots, K_{g_{\text{max}}}\}$ for $g = 1, \ldots, G$, and $(S_1, \ldots, S_G, U) \in \mathcal{V}_G$, where $K_{g_{\text{max}}}$ denotes the maximum number of components specified by the researcher for the mixture model defined in equation (12), and $\mathcal{V}_G$ is the family of the partitions of the variable index set $\mathcal{I}$ into $G$ or $G + 1$ elements (as $U$ can be equal to the empty set). That is,
\( \mathcal{V}_G = \{(S_1, \ldots, S_G, U); (S_1, \ldots, S_G, U) \in \mathcal{F}^{G+1}, \forall g, S_g \cap S_h = \emptyset \} \), where \( \mathcal{F} \) denotes the family of subsets of \( \mathcal{I} \). The resulting model class is denoted as \( \mathcal{M} \), and the generic element of \( \mathcal{M} \) is denoted as \( M = (G, S_1, \ldots, S_G, U, K_1, \ldots, K_G) \). For each model \( M \in \mathcal{M} \) the parameterized densities are denoted by \( f(\cdot | \theta_M) \), with \( \theta_M = (\theta_1, \ldots, \theta_G, \theta_U) \). The corresponding parameter space is denoted by \( \mathcal{Q}_M \).

Let \( M = (G, S_1, \ldots, S_g, S_{g+1}, \ldots, S_G, U, K_1, \ldots, K_g, K_{g+1}, \ldots, K_G) \in \mathcal{M} \) be a given model under consideration. Then,

\[
\begin{align*}
\begin{multlined}[10em][l]
f \left( x_{S_g}^{g-1} x_{g+1}^{h-1} | x_h^{-1} x_k \right) = \sum_{k=1}^{K_g} \pi_k^{(g)} \phi_{L_g} \left( x_{S_g}^{g-1} \gamma_k^{(g)} + \sum_{h=1}^{g-1} B_{gh} x_h, \Sigma_k^{(g)} \right) \\
\times \sum_{k'=1}^{K_g} \pi_{k'}^{(g+1)} \phi_{L_{g+1}} \left( x_{S_{g+1}}^{g+1} \gamma_{k'}^{(g+1)} + \sum_{h=1}^{g} B_{(g+1)h} x_h, \Sigma_{k'}^{(g+1)} \right).
\end{multlined}
\end{align*}
\]

(16)

Then, consider the Cartesian product \( \{1, \ldots, K_g\} \times \{1, \ldots, K_{g+1}\} \) and let the \( t \)-th element of such a set be denoted as \( c_t = (k, k') \), where \( t = 1, \ldots, K_g \cdot K_{g+1} \). Using this notation it is possible to rewrite equation (16) as follows:

\[
\begin{align*}
f \left( x_{S_t}^{g-1} x_{t+1}^{h-1} | x_h^{-1} x_k \right) = \sum_{t=1}^{K_t} \pi_t \phi_{L_t} \left( x_{S_t}^{g-1} \gamma_t + \sum_{h=1}^{g-1} B_{th} x_h, \Sigma_t \right),
\end{align*}
\]

(17)

where \( S_t = S_g \cup S_{g+1}, K_t = K_g \cdot K_{g+1}, L_t = L_g + L_{g+1}, \)

\[
\begin{align*}
\pi_t &= \pi_k^{(g)} \pi_{k'}^{(g+1)}, \\
\gamma_t &= \left( \gamma_k^{(g)} + B_{(g+1)g} \gamma_k^{(g)} \right), \\
\Sigma_t &= \begin{bmatrix} \Sigma_k^{(g)} & \Sigma_{k'}^{(g), (g+1)} \\ B_{(g+1)g} \Sigma_k^{(g)} & \Sigma_{k'}^{(g), (g+1)} + B_{(g+1)g} \Sigma_{k'}^{(g), (g+1)} \end{bmatrix},
\end{align*}
\]

(18)

(19)

(20)

and \( B_{th} = \begin{bmatrix} B_{gh} \\ B_{(g+1)h} + B_{(g+1)g} B_{gh} \end{bmatrix} \).

In this case, for each \( \theta_M \in \mathcal{Q}_M \) there is a \( \theta^*_M \in \mathcal{Q}_M \), such that \( f(\cdot | \theta^*_M) = f(\cdot | \theta^*_M), \) where \( M^* = (G-1, S_1, \ldots, S_t, \ldots, S_G, U, K_1, \ldots, K_t, \ldots, K_G) \in \mathcal{M} \); thus, the identifiability cannot be ensured. This remark makes it possible to introduce a set of necessary conditions for identifiability. This set is defined in the following theorem.
Theorem 1. Let $\mathcal{M}'$ be the sub-class of $\mathcal{M}$ composed of the identifiable models. Then, $\forall M = (G, S_1, \ldots, S_g, \ldots, S_G, U, K_1, \ldots, K_g, \ldots, K_G) \in \mathcal{M}'$, $\forall g \ (1 \leq g \leq G)$, it is not possible to find any partition $(s_a, s_b)$ of $S_g$ such that $\forall t \ (1 \leq t \leq K_g)$ and $\forall h < g$ the following equalities hold:

\[
\pi_t^{(g)} = \pi_k^{(a)} \pi_{k'}^{(b)}, \quad (21)
\]

\[
\gamma_t^{(g)} = \begin{pmatrix} \gamma_k^{(a)} \\ \gamma_{k'}^{(b)} + B_{ba} \gamma_k^{(a)} \end{pmatrix}, \quad (22)
\]

\[
\Sigma_t^{(g)} = \begin{bmatrix} \Sigma_k^{(a)} & \Sigma_k^{(b)} B_{ba}' \\ B_{ba} \Sigma_k^{(a)} & \Sigma_{k'}^{(b)} + B_{ba} \Sigma_k^{(a)} B_{ba}' \end{bmatrix}, \quad (23)
\]

\[
B_{gh} = \begin{bmatrix} B_{ah} \\ B_{bh} + B_{ba} B_{ah} \end{bmatrix}, \quad (24)
\]

with $1 \leq k \leq K_a$, $1 \leq k' \leq K_b$, and $K_a \cdot K_b = K_g$.

Proof. Equalities (21)-(24) are sufficient conditions for the model $M$ to be unidentifiable. As remarked above, if these equalities hold for a given $g$, $f \left( x^{S_h} | x^{i_{h-1}^{g-1} S_h} \right)$ can be written as follows:

\[
f \left( x^{S_h} | x^{i_{h-1}^{g-1} S_h} \right) = f \left( x^{S_h} | x^{i_{h-1}^{g-1} S_h} \right) \times f \left( x^{S_h} | x^{i_{h-1}^{g-1} S_h}, x^{S_a} \right) = \sum_{k=1}^{K_g} \pi_k^{(a)} \phi_{L_a} \left( x^{S_h} ; \gamma_k^{(a)} + \sum_{h=1}^{g-1} B_{ah} x^{S_h}, \Sigma_k^{(a)} \right) \times \sum_{k'=1}^{K_g} \pi_k^{(b)} \phi_{L_b} \left( x^{S_h} ; \gamma_k^{(b)} + \sum_{h=1}^{g-1} B_{bh} x^{S_h} + B_{ba} x^{S_a}, \Sigma_k^{(b)} \right) \quad (25)
\]

where $L_a + L_b = L_g$. Thus, model $M$ is not identified. \hfill \Box

3.3. Parameter estimation

For a given model $M = (G, S_1, \ldots, S_G, U, K_1, \ldots, K_G) \in \mathcal{M}$, whose parameters are $\theta_M = (\theta_1, \ldots, \theta_G, \theta_U) \in Q_M$, the estimation can be performed using the ML method. Given a random sample $x = (x_1, \ldots, x_i, \ldots, x_n)$
drawn from model $M$, the log-likelihood is

$$l(\theta_M) = \sum_{i=1}^{n} \ln \left[ \sum_{k=1}^{K_1} \pi_k^{(1)} \phi_{L_1} \left( x_i^{S_1}; \mu_k^{(1)}, \Sigma_k^{(1)} \right) \right]$$

$$+ \sum_{g=2}^{G} \sum_{i=1}^{n} \ln \left[ \sum_{k=1}^{K_g} \pi_k^{(g)} \phi_{L_g} \left( x_i^{S_g}; \gamma_k^{(g)} + \sum_{h=1}^{g-1} B_{gh} x_i^{S_h}, \Sigma_k^{(g)} \right) \right]$$

$$+ \sum_{i=1}^{n} \ln \left[ \phi_{LU} \left( x_i^U; \alpha_0 + A_1 x_i^{S_1} + A_2 x_i^{S_2}, \Sigma_U \right) \right].$$

(26)

Thus, since $l(\theta_M)$ is composed of $G+1$ parts, each of which only depends on a sub-vector of $\theta_M$, the maximization of $l(\theta_M)$ can be obtained by a separate maximization of the $G+1$ parts. More specifically, the ML estimation of $\theta_1$ can be computed using the EM algorithm for a Gaussian mixture model (see, e.g., Dempster et al. 1977; McLachlan and Peel 2000). As far as the ML estimation of $\theta_g$ ($g = 2, \ldots, G$) is concerned, it can be carried out by resorting to the EM algorithms developed by Soffritti and Galimberti (2011) and Galimberti et al. (2015). The EM algorithm described in the latter paper is also suitable to deal with models resulting from equation (11). Finally, $\hat{\theta}_U$ can be computed using the ML solution for a multivariate linear regression model with Gaussian error terms (see, e.g., Srivastava 2002).

All models for the random vector $X$ described in Section 3.1 are based on the use of Gaussian mixture models whose components are assumed to have unconstrained covariance matrices. Models with a reduced number of variance-covariance parameters can be obtained by reparameterising the component-covariance matrices of any mixture in model (15) according to their spectral decomposition and by imposing constraints on the resulting eigenvalues and/or eigenvectors over the mixture components (Banfield and Raftery 1993; Celeux and Govaert 1995). Namely, $\Sigma_k^{(g)} = \lambda_k^{(g)} D_k^{(g)} A_k^{(g)} D_k^{(g)\prime}$, where $\lambda_k^{(g)} = |\Sigma_k^{(g)}|^{1/L_g}$, $D_k^{(g)}$ is the matrix of eigenvectors of $\Sigma_k^{(g)}$ and $A_k^{(g)}$ is the diagonal matrix containing the eigenvalues of $\Sigma_k^{(g)}$ (normalized in such a way that $|A_k^{(g)}| = 1$). In this parameterisation, the volume, shape and orientation of the $k$th component in the mixture model (12) are determined by the parameters $\lambda_k^{(g)}$, $A_k^{(g)}$ and $D_k^{(g)}$, respectively. Thus, by constraining one or more of these parameters to be the same for all components, for $g = 1, \ldots, G$, parsimonious and interpretable models can be obtained. Thus, the model class $\mathcal{M}$ defined in Section 3.2 can be widened so as to include
such parsimonious models. Namely, a model of this widened class can be denoted as $M^* = (G, S_1, \ldots, S_G, U, K_1, \ldots, K_G, P_1, \ldots, P_G, P_U)$, where $P_g$ ($g = 1, \ldots, G$) denotes the parameterisation of the component-covariance matrices of the mixture model (12) and $P_U$ denotes the form (spherical, diagonal, unconstrained) of the covariance matrix $\Sigma_U$ in model (6). The parsimonious Gaussian mixture models (and their ML estimators) resulting from imposing (up to) fourteen different constraints on such parameters are illustrated in Celeux and Govaert (1995). They can be estimated using, for example, the package mclust. Details on the estimation of parsimonious Gaussian cluster-wise linear regression models can be found in Dang and McNicholas (2015). Models from this latter class are estimated and compared in Section 4.4.

3.4. Model selection

The selection of an appropriate model in the model space for a given dataset can be performed through the same methods usually employed to select the number of components or the parameterizations of the component-covariance matrices in model-based cluster analysis (see, e.g., McLachlan and Peel, 2000). A widely employed information-based criterion is the $BIC$:

$$BIC_M = 2l(\hat{\theta}_M) - npar_M \ln(n), \tag{27}$$

where $l(\hat{\theta}_M)$ and $npar_M$ denote the maximum value of the log-likelihood and number of estimated parameters in model $M$, respectively. Note that for models $M$ with a log-likelihood equal to the one defined in equation (26), $BIC_M$ can be obtained by summing the $BIC$ values associated with the $G + 1$ parts of $l(\theta_M)$.

In a Bayesian framework, $BIC$ provides an asymptotic approximation of the log-posterior probability of a model (Kass and Raftery, 1995). The use of this criterion can be motivated on the basis of both theoretical and practical results. Keribin (2000) proves that using the $BIC$ allows to consistently estimate the number of mixture components. The criteria for performing variable selection in Gaussian model-based cluster analysis proposed by Maugis et al. (2009a) and Maugis et al. (2009b), based on the $BIC$, are proved to be consistent under regularity conditions. A similar result is proved in Galimberti and Soffritti (2013) for selecting the partition of the variables in a parsimonious approach to model-based cluster analysis. From an applied point of view, good performances of the $BIC$ as a model selection criterion for Gaussian mixture models are reported in several papers, such as Biernacki
Table 2: Maximised log-likelihood and BIC value of seven models fitted to the heights dataset.

| Models | X^{S_1} | X^{S_2} | X^U | K_1 | K_2 | X^{S_i}_{U} | X^{S_i}_{S_2} | l(\hat{\theta}_M) | npar_M | BIC_M |
|--------|---------|---------|-----|-----|-----|-------------|-------------|----------------|--------|-------|
| M_1    | X       | \emptyset | \emptyset | 1  | -   | -           | -           | -235.51        | 9      | -502.48 |
| M_2    | X_1, X_2 | \emptyset | X_3  | 2  | -   | X_1, X_2   | -           | -231.82        | 11     | -502.10 |
| M_3    | X_1, X_2 | \emptyset | X_3  | 2  | -   | X_2        | -           | -232.68        | 10     | -500.33 |
| M_4    | X_1, X_2 | X_3  | \emptyset | 1  | 1   | -           | X_2        | -238.00        | 6      | -496.98 |
| M_5    | X_1, X_2 | X_3  | \emptyset | 1  | 2   | -           | X_2        | -235.15        | 8      | -498.27 |
| M_6    | X_1, X_2 | X_3  | \emptyset | 2  | 2   | -           | X_1, X_2   | -228.46        | 13     | -502.38 |
| M_7    | X_1, X_2 | X_3  | \emptyset | 2  | 2   | -           | X_2        | -229.83        | 12     | -501.63 |

and Govaert (1999) and Fraley and Raftery (2002). All results illustrated in Section 4 are obtained by using this criterion.

4. Experimental results

4.1. Further results from the introductory example

All models illustrated in Section 2 can be seen as a special case of the models described in Section 3.1. They are listed in Table 2 where X = (X_1, X_2, X_3) and X_1, X_2 and X_3 represent mother’s height, father’s height and student’s height, respectively. Model M_7 is an improvement of model M_6 resulting from the elimination of X_1 from the regressors in the model for X^{S_2}.

According to the BIC, the best model is M_4. It describes the marginal distribution of the parents’ heights with a Gaussian model in which the two heights are treated as independent and with the same variance; furthermore, the fathers’ height is used as a regressor in a Gaussian linear regression model for describing the conditional distribution of the students’ height. Thus, no evidence of cluster structure seems to be found in the dataset, neither in the distribution of the parents’ heights nor in the conditional distribution of the students’ height. However, the difference between the BIC of model M_4 and the one of other fitted models is low (Kass and Raftery 1995). Thus, models supporting the presence of a cluster structure in the marginal distribution of the parents’ heights (M_3), in the conditional distribution of the students’ height (M_5) and in both distributions (M_7) may be employed for this dataset.
4.2. Exploring the model space using genetic algorithms

In order to find the optimal model in the model space for a given dataset, all possible models have to be considered and compared. However, an approach based on such an exhaustive search is computationally expensive and time-consuming, especially when the number of observed variables is high. Thus, non-exhaustive strategies are needed. A solution is represented by genetic algorithms. They constitute stochastic optimisation techniques that exploit principles and operators of the biological evolution of a species for solving complex problems with a vast number of possible solutions (Goldberg, 1989). These algorithms are widely used in many fields of statistics (see, e.g., Chatterjee et al., 1996). Applications in subset selection problems can be found, for example, in Bozdogan (2004).

In general, a genetic algorithm starts from the examination of the chromosomes (ordered sequences of genes) that compose an initial population. Each of these chromosomes is randomly generated; it is assigned a value summarising its fitness. Then, an iterative evolution process is performed, based on three main genetic operators (selection, crossover, mutation), with the goal of generating novel populations composed of chromosomes characterised by improved fitness values. The selection operator consists in a weighted random sampling from the initial population with weights that are generally proportional to the chromosomes’ fitness. The chromosomes selected in this way reproduce and their offspring will compose a novel generation. Such a generation is obtained after crossover and mutation. Namely, crossover is a random process of genome recombination that applies to pairs of chromosomes; mutation is a random alteration of a gene in a chromosome. The chromosomes of the resulting novel generation are assigned their fitness and the evolution process repeats. Usually, the algorithm stops when either a maximum number of populations has been generated or a satisfactory value of the fitness has been reached for the population.

A first genetic algorithm is developed for finding the model \( \hat{M} \) such that

\[
\hat{M} = \arg\max_{M \in \mathcal{M}} BIC_M, \tag{28}
\]

where \( \mathcal{M} \) is the class of models illustrated in Section 3.2 having up to two cluster structures \((G = 2)\). In this algorithm each model \( M \) is represented as a chromosome whose fitness is given by \( BIC_M \). The evolution process is composed of two parts:

a) information extraction for the specification of model \([1]\);
In part a) the examined chromosomes have a binary gene for each variable in \( X \) (with 1/0 denoting a variable selected/not selected for \( X^{S_1} \), respectively); they also have two genes associated with the number of components to be used in models (1) and (2). The possible values of these two latter genes are the integer numbers between 1 and a maximum value chosen by the researcher (\( K_{1\text{max}} \) for model (1), \( K_{2\text{max}} \) for model (2)). Thus, chromosomes of length \( L + 2 \) are examined in the first part of the algorithm. Let \( M_a \) be the best model detected at the end of part a) and let \( \hat{S}_1, \hat{K}_1 \) be the solution for \( S_1, K_1 \) obtained from \( M_a \).

If \( \hat{L}_1 < L \), where \( \hat{L}_1 \) denotes the length of \( X^{\hat{S}_1} \), in the second part of the genetic algorithm a solution for \( S_2, K_2 \) and \( U \) is searched by keeping fixed the solution for \( S_1, K_1 \) obtained from the model \( M_a \). Specifically, the chromosomes are composed of \( L - \hat{L}_1 + 1 \) genes, with a binary gene for each variable in \( X \setminus X^{\hat{S}_1} \) (where 1 and 0 denote a variable selected and not selected for \( X^{S_2} \), respectively), and an additional gene (with positive integer values) associated with the number of components for model (2). The model \( M_b \) obtained at the end of this second part provides \( \hat{S}_2, \hat{K}_2, \hat{U} \), where \( \hat{U} = \mathcal{I} \setminus \hat{S}_1 \setminus \hat{S}_2 \). Thus, \( \hat{U} \) will not be empty when \( \hat{L}_1 + \hat{L}_2 < L \), with \( \hat{L}_2 \) denoting the length of \( X^{\hat{S}_2} \). The final solution of the algorithm is \( \hat{M} = (\hat{S}_1, \hat{S}_2, \hat{U}, \hat{K}_1, \hat{K}_2) \). All models examined and estimated with this genetic algorithm have unconstrained covariance matrices. The results of an evaluation of its effectiveness, based on simulated datasets generated by models with unconstrained covariance matrices, are provided in Section 4.3.

A second genetic algorithm is developed for carrying out the model search in the wider class of parsimonious models illustrated in Section 3.3 with \( G = 2 \). The search is still decomposed in two parts that are similar to those described above; the only difference is in the structure of the chromosomes. Namely, in part a) the examined chromosomes have two additional genes (with positive integer values up to 14) for distinguishing the parsimonious parameterisations to be used in models (1) and (2). In part b) an additional gene is necessary to denote the parsimonious parameterisation in model (2); another gene (with three possible values) is added for indicating the form of the covariance matrix \( \Sigma_U \) in model (6). Section 4.4 shows the results obtained from the analysis of two real datasets based on this second algorithm.

These genetic algorithms have been implemented in R by exploiting the package GA [Scrucca 2013]. Each execution requires the specification of
the following tuning parameters: $K_{1\text{max}}, K_{2\text{max}}, N_1$ and $N_2$ (dimension of the examined populations in parts $a$ and $b$), respectively, $d_{1\text{max}}$ and $d_{2\text{max}}$ (maximum number of generations to be examined in the two parts of the algorithm). The specific values of these tuning parameters employed in the analyses are detailed in the following Sections. In both algorithms linear-rank selection and single point crossover operators are used. The probability of crossover between pairs of chromosomes is set equal to 0.8 in all analyses. As far as the mutation is concerned, this genetic transformation is randomly carried out in a parent chromosome with a probability of 0.1.

4.3. A Monte Carlo study

The performance of the first genetic algorithm is evaluated through a Monte Carlo experiment in which artificial datasets are generated in the Euclidean space $\mathbb{R}^8$ using model (7), where $X^{S_1} = (X_1, X_2, X_3)$, $K_1 = 2$, $X^{S_2} = (X_4, X_5, X_6)$, $K_2 = 2$, and $X^U = (X_7, X_8)$.

Specifically, the parameters of the marginal p.d.f. of $X^{S_1}$ are: $\pi_1^{(1)} = 0.5$,

$$\mu_1^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mu_2^{(1)} = \begin{pmatrix} 5 \\ -5 \\ 5 \end{pmatrix}, \quad \Sigma_1^{(1)} = \begin{pmatrix} 1 & -0.6 & -0.3 \\ -0.6 & 1 & -0.4 \\ -0.3 & -0.4 & 1 \end{pmatrix},$$

$$\Sigma_2^{(1)} = \begin{pmatrix} 1 & 0.6 & 0.3 \\ 0.6 & 1 & 0.4 \\ 0.3 & 0.4 & 1 \end{pmatrix}.$$ 

The parameters of the conditional p.d.f. of $X^{S_2}$ given $X^{S_1}$ are: $\pi_1^{(2)} = 0.5$,

$$\gamma_1^{(2)} = \begin{pmatrix} -2 \\ -1 \\ 3.5 \end{pmatrix}, \quad \gamma_2^{(2)} = \begin{pmatrix} 4 \\ 5 \\ -2.5 \end{pmatrix}, \quad B_{21} = \begin{pmatrix} 1.5 & 2 & 1.5 \\ 1.5 & -2.5 & -2 \\ 1.5 & 2 & -2.5 \end{pmatrix},$$

$$\Sigma_1^{(2)} = \begin{pmatrix} 1 & 0.5 & 0.6 \\ 0.5 & 1 & 0.4 \\ 0.6 & 0.4 & 1 \end{pmatrix}, \quad \Sigma_2^{(2)} = \begin{pmatrix} 1 & -0.5 & -0.6 \\ -0.5 & 1 & -0.4 \\ -0.6 & -0.4 & 1 \end{pmatrix}.$$ 

Finally, the parameters of the conditional p.d.f. of $X^U$ given $(X^{S_1}, X^{S_2})$ are: $\alpha_0 = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$, $A_1 = \begin{pmatrix} 2 & 2 & 2 \\ -2 & -2 & -2 \end{pmatrix}$, $A_2 = -A_1$ and $\Sigma_U = \begin{pmatrix} 2.25 & 0 \\ 0 & 1 \end{pmatrix}$.

The main goal of this experiment is to evaluate the effectiveness of the genetic algorithm (with the BIC as a fitness measure) in selecting the model
the datasets come from. To this end, one hundred samples of \( n = 200 \) observations each are generated and analysed using the algorithm. Since the algorithm’s performance may depend on how large is the exploration of the model space, the algorithm is executed by changing the values of the tuning parameters \( N_1 \) and \( d_{1\text{max}} \) that control the information extraction for the specification of model (1). Namely, the examined values are 120, 160 and 200 for \( N_1 \); 30, 40 and 50 for \( d_{1\text{max}} \). The other tuning parameters are kept constant throughout the experiment; they are set as follows: \( K_{1\text{max}} = K_{2\text{max}} = 3 \), \( N_2 = 80 \) and \( d_{2\text{max}} = 20 \). Greater values of \( N_2 \) and \( d_{2\text{max}} \) are not examined because some preliminary analyses have highlighted that increasing them has a little impact on the results. This is mainly due to the fact that in part b) of the algorithm the exploration of the model space is carried out conditionally on the results obtained in part a). Thus, nine executions of the algorithm are performed. The same analysis is carried out with the sample size \( n = 400 \).

The effectiveness of the genetic algorithm is evaluated with respect to the ability to recover the correct variable partition. The percentage of datasets for which \( X^{S_1}, X^{S_2} \) and \( X^U \) are successfully identified is generally high, especially with \( n = 400 \) (see Tables 3 and 4, first row). The most common error is represented by a partition in which both uninformative variables are allocated to the variable sub-vector that defines the first cluster structure, and \( X_2 \) is wrongly inserted in the variable sub-vector that defines the second cluster structure. Whenever the exploration of the model space is widened, an improvement in the effectiveness of the algorithm is generally obtained. This improvement is almost exclusively associated with an increase in the tuning parameter \( N_1 \). Using a value greater than 30 for the maximum number of examined generations, in association with any examined value of \( N_1 \), is completely useless with \( n = 400 \).

The effectiveness is also evaluated with respect to the ability of the genetic algorithm to recover the two latent cluster structures. This task is carried out by computing the adjusted Rand index between the true cluster structures and the structures estimated by the algorithm. Although in some datasets the true variable partition is not correctly detected, the first cluster structure identified by the genetic algorithm perfectly coincides with the first true one in all samples (aRi=1). Also the agreement between the second true cluster structure and the second estimated one is very high: the mean (over 100 datasets) of the aRi is greater that 0.996 in all executions of the algorithm for both sample sizes. These results are due to the fact that there is a clear-
Table 3: Distribution of 100 simulated datasets according to the partition of $X$ obtained with the genetic algorithm in the executions with $n = 200$.

| $N_1$ | 120 | 160 | 200 |
|-------|-----|-----|-----|
| $d_{1\text{max}}$ | 30 | 40 | 50 | 30 | 40 | 50 | 30 | 40 | 50 |
| Correct classification of all variables | 76 | 79 | 80 | 91 | 88 | 91 | 91 | 91 | 90 |
| Correct recovery of $X^{S_1}$ only | 4 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 4 |
| $\hat{S}_1 = (1, 3, 7, 8), \hat{S}_2 = (2, 4, 5, 6)$ | 14 | 14 | 13 | 5 | 8 | 5 | 6 | 6 | 5 |
| Other wrong partitions | 6 | 4 | 4 | 1 | 0 | 1 | 0 | 0 | 1 |

Table 4: Distribution of 100 simulated datasets according to the partition of $X$ obtained with the genetic algorithm in the executions with $n = 400$.

| $N_1$ | 120 | 160 | 200 |
|-------|-----|-----|-----|
| $d_{1\text{max}}$ | 30 | 40 | 50 | 30 | 40 | 50 | 30 | 40 | 50 |
| Correct classification of all variables | 87 | 87 | 87 | 92 | 92 | 92 | 95 | 95 | 95 |
| Correct recovery of $X^{S_1}$ only | 1 | 1 | 1 | 2 | 2 | 2 | 2 | 2 | 2 |
| $\hat{S}_1 = (1, 3, 7, 8), \hat{S}_2 = (2, 4, 5, 6)$ | 9 | 9 | 9 | 5 | 5 | 5 | 3 | 3 | 3 |
| Other wrong partitions | 3 | 3 | 3 | 1 | 1 | 1 | 0 | 0 | 0 |

cut separation between clusters in both $X^{S_1}$ and $X^{S_2}$; furthermore, in all datasets in which the genetic algorithm selects wrong variable partitions, two variables in both $X^{\hat{S}_1}$ and $X^{\hat{S}_2}$ are always correctly selected.

4.4. Results from real datasets

Examples are carried out using two benchmark real datasets: the crabs dataset and the AIS dataset. The crabs dataset is described in Venables and Ripley (2002) and is available in the R package MASS. It reports $L = 5$ morphological measurements (in mm) for $n = 200$ crabs of the species Leptograpsus variegatus: frontal lobe size (FL), rear width (RW), carapace length (CL), carapace width (CW) and body depth (BD). Namely, the sample is composed of 50 crabs each of two colours (blue and orange) and both sexes. The AIS dataset is described in Cook and Weisberg (1994) and is available in the R package sn (Azzalini, 2014). It contains information concerning
Table 5: Classification of the crabs according to their colour and gender (BF = blue female, BM = blue male, OF = orange female, OM = orange male) and the cluster membership estimated by the model selected using mclust.

| Cluster | Colour and gender |
|---------|-------------------|
|         | BF   | BM   | OF   | OF   |
| 1       | 49   | 11   | 0    | 0    |
| 2       | 0    | 0    | 5    | 50   |
| 3       | 0    | 39   | 0    | 0    |
| 4       | 1    | 0    | 45   | 0    |
| aRi     | 0.794|

$n = 202$ athletes (102 males and 100 females) at the Australian Institute of Sport. In particular, the analysis described in this Section focuses on $L = 9$ variables: red cell count (RCC), white cell count (WCC), hematocrit (Hc), hemoglobin (Hg), plasma ferritin concentration (Fe), body mass index (BMI), sum of skin folds (SSF), body fat percentage (Bfat) and lean body mass (LBM). Each dataset is analysed using the second genetic algorithm illustrated in Section 4.2. For comparison purposes, analyses are carried out also using the R packages mclust and clustvarsel and the softwares SelvarClust and SelvarClustIndep.

4.4.1. Crabs dataset

The best Gaussian mixture model fitted to the joint p.d.f. of the five morphological measurements using mclust (with a maximum number of components equal to five) is a mixture of four Gaussian ellipsoidal components with the same volume and shape. This result is obtained with an option for the initialisation of the EM algorithm that transforms the variables using a singular value decomposition. The value of BIC for such a mixture model is $-2842.3$. Table 5 reports the cross classification of the crabs based on the maximum estimated posterior probabilities and their gender and colour. The clustering obtained from this model reproduces quite well the four classes of crabs defined from gender and colour.

According to the variable selection methods implemented in clustvarsel only four morphological measurements are relevant for clustering the crabs. They are frontal lobe size, rear width, carapace width and body depth. The best Gaussian mixture model fitted to the p.d.f. of these measurements is a mixture of four Gaussian ellipsoidal components with the same volume
Table 6: Classification of the crabs according to their colour and gender and the cluster membership estimated by the model selected using \texttt{clustvarsel}.

| Cluster | Colour and gender |
|---------|------------------|
|         | BF   | BM   | OF   | OF   |
| 1       | 50   | 10   | 0    | 0    |
| 2       | 0    | 0    | 5    | 50   |
| 3       | 0    | 40   | 0    | 0    |
| 4       | 0    | 0    | 45   | 0    |
| aRi     | 0.815|

and shape. Using this model allows to obtain a partition of the crabs with an increased agreement with the partition based on gender and colour (see Table 6). The same result is also obtained using both \texttt{SelvarClust} and \texttt{SelvarClustIndep}. The \textit{BIC} value of the resulting joint model for the five measurements, obtained as described in Section 3.3, is equal to $-2811.2$, thus leading to an improved model with respect to the one obtained without variable selection.

The splitting of the five measurements produced by two independent executions of the genetic algorithm (using the tuning parameters $N_1 = N_2 = 400$, $d_{1\text{max}} = d_{2\text{max}} = 40$, $K_{1\text{max}} = K_{2\text{max}} = 5$ in the first execution and $N_1 = N_2 = 500$, $d_{1\text{max}} = d_{2\text{max}} = 50$, $K_{1\text{max}} = K_{2\text{max}} = 5$ in the second) is: $X_{S_1} = (\text{RW}, \text{CL})$, $X_{S_2} = (\text{FL}, \text{CW}, \text{BD})$, $X_{U} = \emptyset$. A mixture of two Gaussian components is selected for both the joint marginal p.d.f. of (RW, CL) and the conditional p.d.f. of (FL, CW, BD) $|$(RW, CL). Namely, the two components are ellipsoidal with the same volume and shape in the mixture model for (RW, CL), while they are spherical with the same volume in the model for (FL, CW, BD) $|$(RW, CL). The \textit{BIC} value of the resulting joint model is $-2812.7$. Thus, two cluster structures are detected. Tables 7 and 8 show some classifications of the crabs pertaining to the first and the second cluster structure, respectively. The clustering of crabs resulting from the analysis of rear width and carapace length reproduces quite well the classification of crabs based on their gender, while it is not associated with the classification based on colour. On the contrary, an almost perfect agreement arises from the comparison between this latter classification and the clustering obtained by modelling the dependence of frontal lobe size, carapace width and body depth on rear width and carapace length using a clusterwise
Table 7: Comparison between the first cluster structure detected by the genetic algorithm in the joint marginal distribution of RW and CL and the classifications of crabs based on their colour and/or gender.

| Cluster | Colour and gender | Colour | Gender |
|---------|-------------------|--------|--------|
|         | BF    | BM    | OF    | OF    | B     | O     | F     | M     |
| 1       | 50    | 7     | 50    | 3     | 57    | 53    | 100   | 10    |
| 2       | 0     | 43    | 0     | 47    | 47    | 43    | 0     | 90    |
| aRi     | 0.400 |       |       |       |       |       |       | 0.810 |

Table 8: Comparison between the second cluster structure detected by the genetic algorithm in the conditional distribution of \((FL, CW, BD) | (RW, CL)\) and the classifications of crabs based on their colour and/or gender.

| Cluster | Colour and gender | Colour | Gender |
|---------|-------------------|--------|--------|
|         | BF    | BM    | OF    | OF    | B     | O     | F     | M     |
| 1       | 50    | 50    | 1     | 0     | 100   | 1     | 51    | 50    |
| 2       | 0     | 0     | 49    | 50    | 0     | 99    | 49    | 50    |
| aRi     | 0.486 |       |       |       |       |       | 0.980 |       |

Gaussian linear regression model with two components. The second cluster structure detected in the dataset does not take into account differences in gender.

The model selected by the genetic algorithm assumes that FL, CW and BD linearly depend on both RW and CL. Since this assumption could be restrictive, models are also estimated in which a different set of regressors is allowed for each of the three regression equations in the multivariate linear regression model of frontal lobe size, carapace width and body depth. According to the BIC, the best solution obtained after examining these further models is a mixture of two seemingly unrelated linear regression models in which frontal lobe size and carapace width are both regressed on carapace length and rear width, while body depth only depends on carapace length. The clustering of the crabs resulting from such a model coincides with the classification of crabs based on their colour (aRi=1). The joint model for the five morphological measurements given by the product of this seemingly unrelated linear regression model and the Gaussian mixture model for CL and RW described above has a BIC value \((-2808.3\) which is slightly higher than the best model obtained performing model-based variable selection.
Table 9: Classification of the athletes according to their gender and the cluster membership estimated by the models selected using mclust, clustvarsel, SelvarClust and SelvarClustIndep.

|       | mclust | clustvarsel | SelvarClust | SelvarClustIndep |
|-------|--------|-------------|-------------|------------------|
| Cluster | Cluster | Cluster | Cluster | Cluster |
| Gender | Cluster | Cluster | Cluster | Cluster |
| F      | 97  2  1 | 39  61  0 | 2  1  97 | 2  97  1 |
| M      | 2  40  60 | 13  1  88 | 25  75  2 | 23  2  77 |
| aRi    | 0.682 | 0.586 | 0.735 | 0.745 |

This model allows to detect the presence of two different cluster structures in the dataset, each of which is strongly or perfectly associated with one of the two known classifications that characterise this dataset. As a consequence of above, the two detected cluster structures are independent one another.

4.4.2. AIS dataset

The best Gaussian mixture model resulting from the analysis performed through mclust (with a maximum number of components equal to five and using the same initialisation of the EM algorithm employed in the analysis of the crabs dataset) is a mixture of three Gaussian ellipsoidal components with the same orientation. The value of BIC for such a mixture model is $-9028.2$. The clustering obtained from this model reproduces quite well the two classes of athletes based on their gender (see Table 9, left part).

The three examined variable selection methods lead to different decisions about the variables that provide relevant information on the clustering of the athletes (see Table 10). Using clustvarsel (with a maximum number of components for the p.d.f. of the informative variables equal to five), only the biometrical variables are selected. The best Gaussian mixture model fitted to the p.d.f. of these variables is a mixture of three Gaussian ellipsoidal components with the same shape. The BIC value of the resulting joint model for the nine variables is $-9008.1$. Thus, according to the BIC, this joint model is better than the best model detected without variable selection. However, the partition of the athletes resulting from the best mixture model for the biometrical variables shows a slightly lower agreement with the partition based on gender (see Table 9).

Softwares SelvarClust and SelvarClustIndep also select two blood
Table 10: Variables selected by the packages clustvarsel, SelvarClust and SelvarClustIndep from the AIS dataset.

| Package          | Selected variables |
|------------------|--------------------|
| clustvarsel      | BMI, SSF, Bfat, LBM |
| SelvarClust      | BMI, SSF, Bfat, LBM, Fe, Hg |
| SelvarClustIndep | BMI, SSF, Bfat, LBM, Fe, Hc |

Table 11: Cluster structures detected by the genetic algorithm and their association with the classification of the athletes based on gender.

|                   | Structure 1 | Structure 2 |
|-------------------|-------------|-------------|
| Gender            | 1 2 3       | 1 2 3       |
| F                 | 98 1 1      | 50 49 1     |
| M                 | 1 74 27     | 54 34 14    |
| aRi               | 0.754       | 0.015       |

composition variables: one is plasma ferritin concentration and the other is hemoglobin or hematocrit. Namely, the best joint model obtained after three independent executions of SelvarClust is given by the product of a Gaussian mixture model with three equally-oriented components for the joint marginal distribution of BMI, SSF, Bfat, LBM, Fe and Hg, and a Gaussian linear regression model for the conditional distribution of the remaining variables in which only Hg is used as a regressor and the covariance matrix is unconstrained. The BIC value of the joint model obtained in this way is $-8935.3$. Using SelvarClustIndep the best model is composed of a mixture of $K = 3$ Gaussian components with the same orientation for the joint marginal distribution of BMI, SSF, Bfat, LBM, Fe and Hc, and a Gaussian linear regression model for the conditional distribution of the remaining variables in which the selected regressors are Hc, BMI and Bfat and the covariance matrix is diagonal. None of the uninformative variables results to be independent of all the informative ones. Overall, this joint model registers a BIC of $-8934.5$. As far as the recovery of the classification based on gender is concerned, the partitions of the athletes resulting from the mixture models for the variables selected by SelvarClust and SelvarClustIndep reach a very similar performance, that is slightly better than the ones obtained using both mclust and clustvarsel (see Table[9]).
The results obtained from two independent executions of the genetic algorithm (using the tuning parameters $N_1 = N_2 = 300$, $d_{1\text{max}} = d_{2\text{max}} = 30$, $K_{1\text{max}} = K_{2\text{max}} = 4$ in the first execution and $N_1 = N_2 = 700$, $d_{1\text{max}} = d_{2\text{max}} = 70$, $K_{1\text{max}} = K_{2\text{max}} = 5$ in the second) highlight the existence of two cluster structures. Namely, the first structure is found in the sub-vector $X^S_1 = (\text{BMI}, \text{SSF}, \text{Bfat}, \text{LBM}, \text{Hg})$. The best model for the p.d.f. of this sub-vector is a mixture of three Gaussian ellipsoidal components with the same orientation. The recovery of males and females classes obtained using the segmentation of the athletes based on this model is slightly improved (see Table 11, left part). The second cluster structure is found in the conditional distribution of the sub-vector $X^S_2 = (\text{Hc}, \text{Fe})$ given $X^S_1$, resulting from a mixture of three Gaussian components with diagonal covariance matrices having the same volume. The partition of the athletes obtained from this second mixture model is not associated with the athletes’ gender (see Table 11, right part). Since in model (7) the latent variables $Z_1$ and $Z_2$ are assumed to be independent, this latter result is not surprising. Thus, the second structure is reasonably associated with other (unobserved) factors independent of the gender. Finally, red and white cell counts compose $X^U$ and, thus, result to be uninformative variables. Their conditional distribution is modelled using a Gaussian linear regression model with a diagonal regression covariance matrix. The $BIC$ value of the joint model for the nine variables is $-8933.2$.

An improvement of the clusterwise linear regression model with three components selected for $(\text{Hc}, \text{Fe})$ is obtained after performing regressors selection. This task is carried out by allowing each dependent variable to have its own specific set of regressors. Furthermore, all fourteen parsimonious parameterisations are estimated for each examined model. According to the $BIC$, the best solution is obtained using a model in which haematocrit is regressed on hemoglobin, sum of skin folds and body fat percentage, while the selected predictors for plasma ferritin concentration are hemoglobin, body mass index, body fat percentage and lean body mass. The component-covariance matrices of this model are unconstrained. In a similar way, the best Gaussian linear regression model for $(\text{RCC}, \text{WCC})$ is the one that has haematocrit as a predictor for both dependent variables and sum of skin folds only for WCC. The covariance matrix of this model is diagonal. Since the joint model for the nine variables obtained in this way has a $BIC$ value of $-8856.9$, it seems to provide a good description of the relevant information contained in the
AIS dataset.

5. Conclusions

The proposed framework relies on a very general model that makes it possible to compare the results of different (supervised and unsupervised) analyses carried out on a given dataset. Namely, this model allows to perform variable selection in model-based clustering according to the methods proposed by Raftery and Dean (2006), Maugis et al. (2009a) and Maugis et al. (2009b). It also allows to carry out model selection in multivariate linear regression analysis and seemingly unrelated linear regression analysis by assuming either a Gaussian model or a Gaussian mixture model for the distribution of the errors (Soffritti and Galimberti, 2011; Galimberti et al., 2015). Furthermore, using the proposed model enables the detection of the presence of multiple cluster structures from possibly correlated variable sub-vectors.

It should be noted that the process of selecting a model in this framework may be quite complex and may prevent the methodology illustrated in this paper from being used with high-dimensional datasets. Resorting to genetic algorithms can partly mitigate this drawback. This kind of algorithms is able to globally explore the model space, thus avoiding the main problems that typically characterise stepwise or greedy search strategies. Clearly, the effectiveness of a genetic algorithm greatly depends on how large is the performed exploration of the model space. However, no general rule about how to choose proper values of the population size and the number of generations in a genetic algorithm is known. The Monte Carlo study summarised in Section 4.3 suggests that an important role is played by the population size. A proper choice of the tuning parameters in a genetic algorithm as well as other aspects concerning model selection (e.g.: a comparison with other strategies for exploring the model space; how to deal with high-dimensional datasets) represent topics for future research. Nevertheless, the experimental results illustrated in Sections 4.1 and 4.4 show that for some datasets the joint use of supervised and unsupervised learning methods allows to extract unknown relevant information that otherwise would be missed, thus supporting the usefulness of the proposed framework.
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