Non-Gaussian Mixtures for Dimension Reduction, Clustering, Classification, and Discriminant Analysis

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Abstract

We introduce a method for dimension reduction with clustering, classification, or discriminant analysis. This mixture model-based approach is based on fitting generalized hyperbolic mixtures on a reduced subspace within the paradigm of model-based clustering, classification, or discriminant analysis. A reduced subspace of the data is derived by considering the extent to which group means and group covariances vary. The members of the subspace arise through linear combinations of the original data, and are ordered by importance via the associated eigenvalues. The observations can be projected onto the subspace, resulting in a set of variables that captures most of the clustering information available. The use of generalized hyperbolic mixtures gives a robust framework capable of dealing with skewed clusters. Although dimension reduction is increasingly in demand across many application areas, the authors are most familiar with biological applications and so two of the three real data examples are within that sphere. Simulated data are also used for illustration. The approach introduced herein can be considered the most general such approach available, and so we compare results to three special and limiting cases. We also compare with well several established techniques. Across all comparisons, our approach performs remarkably well.

Keywords: Dimension reduction, generalized hyperbolic, mixture models, model-based clustering, model-based classification, model-based discriminant analysis

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1 Introduction

In this paper, we introduce a method for fitting generalized hyperbolic mixtures on a reduced subspace within the paradigms of model-based clustering, classification, and discriminant analysis. This is the most general case of work in this direction over the last few years, starting with an analogous approach based on Gaussian mixtures (Scrucca, 2010).

Many dimension reduction methods summarize the information available through a reduced subset of the original variables; however, they provide little information on the potential structure of the data at hand. The method proposed herein addresses this issue by revealing the underlying data clusters. At the same time, using heavy-tailed distributions, such as the generalized hyperbolic, to model data can be advantageous because they assign correct weights to extreme events (McNeil et al., 2005). The goal is to estimate a subspace that captures most of the clustering structure contained in the data. At the core of the method lies the sliced inverse regression (SIR) work of Li (1991, 2000), which reduces data dimensionality by considering the variation in both group means and covariances. The members of the subspace arise through linear combinations of the original data, and are ordered by importance via their associated eigenvalues. The original observations in the data can be projected onto the subspace, resulting in a set of variables that captures most of the clustering information available.

The remainder of the paper is outlined as follows. Section 2 presents the background material. We then outline our dimension reduction method for selecting a subset of the variables while retaining most of the clustering information contained within the data (Section 3). In Section 4, the algorithm is applied to simulated and real data sets and the performance of our method is compared with its Gaussian and non-Gaussian analogues as well as with other subspace clustering techniques. Section 5 provides the conclusions and suggestions for future work. Note that all computational work herein was carried out using R (R Core Team, 2013).
2 Background

2.1 Finite Mixture Models

Modern data sets used in many practical applications have grown in size and complexity, compelling the use of clustering and classification algorithms based on probability models. The model-based approach assumes that data are generated by a finite mixture of probability distributions. A $p$-dimensional random vector $X$ is said to arise from a parametric finite mixture distribution if its density is a convex set of probability densities, i.e.,

$$f(x|\vartheta) = \sum_{g=1}^{G} \pi_g f_g(x|\theta_g),$$

where $G$ is the number of components, $\pi_g$ are mixing proportions, so that $\sum_{g=1}^{G} \pi_g = 1$ and $\pi_g > 0$, and $\vartheta = (\pi_1, \ldots, \pi_G, \theta_1, \ldots, \theta_G)$ is the parameter vector. The $f_g(x|\theta_g)$ are called component densities and $f(x|\vartheta)$ is formally referred to as a $G$-component parametric finite mixture distribution. The use of mixture models in clustering applications can be traced back a half-century to an application of Gaussian mixture models (Wolfe, 1963). Gaussian mixture model-based approaches have been very popular due to their mathematical tractability, and until recently, they dominated literature in the field. Extensive details on finite mixture models are given by Everitt and Hand (1981), McLachlan and Basford (1988), and McLachlan and Peel (2000).

In the past several years, non-Gaussian approaches to model-based clustering, classification, and discriminant analysis have flourished. This includes work on the multivariate $t$-distribution (Peel and McLachlan, 2000; Greselin and Ingrassia, 2010; Andrews et al., 2011; Steane et al., 2012; Andrews and McNicholas, 2012a; McNicholas, 2013), shifted asymmetric Laplace distributions (Franczak et al., 2012), skew normal distributions (Lin, 2010), and skew $t$-distributions (Vrbik and McNicholas, 2012; Lee and McLachlan, 2013). Mixtures of generalized hyperbolic distributions (Browne and McNicholas, 2013) are particularly relevant to work described herein. While it is not feasible to provide an exhaustive listing here, suffice it to say that the breadth of research on non-Gaussian model-based clustering and classification is becoming as rich as that of its Gaussian precursor.
Generalized hyperbolic distributions were introduced by Barndorff-Nielsen (1977) and used to model eolian sand deposits, i.e., sand deposits arising from the action of wind. The name of the distribution was derived from the fact that its log-density has the shape of a hyperbola. Properties of generalized hyperbolic densities were discussed in Barndorff-Nielsen and Halgreen (1977) and Blæsild (1978) and, more recently, mixtures of these distributions appear in McNeil et al. (2005) and Härdle and Simar (2011). Generalized hyperbolic distributions can effectively model extreme values, making them very useful in the context of financial and risk management applications, where the normal distribution does not offer a good description of reality. The multivariate generalized hyperbolic family is extremely flexible and contains many special and limiting cases, such as the inverse Gaussian, Laplace, and skew-$t$ distributions.

### 2.2 Generalized Hyperbolic Mixtures

Recently, Browne and McNicholas (2013) proposed a multivariate generalized hyperbolic mixture model (HMM),

$$ f(x | \vartheta) = \sum_{g=1}^{G} \pi_g f_h(x | \lambda_g, \omega_g, \mu_g, \Sigma_g, \alpha_g), $$

where $\pi_g$ are the mixing proportions and the $g$th component density is

$$ f_h(x | \lambda_g, \omega_g, \mu_g, \Sigma_g, \alpha_g) = \frac{[\omega_g + \delta(x, \mu_g | \Sigma_g)]^{(\lambda_g - p/2)/2}}{\omega_g + \alpha_g^\top \Sigma_g^{-1} \alpha_g} \times \frac{K_{\lambda_g - p/2} \left( \sqrt{\omega_g + \alpha_g^\top \Sigma_g^{-1} \alpha_g} (\omega_g + \delta(x, \mu_g | \Sigma_g)) \right)}{(2\pi)^{p/2} |\Sigma_g|^{1/2} K_{\lambda_g}(\omega_g) \exp(- (x - \mu_g)^\top \Sigma_g^{-1} \alpha_g)}, $$

with index parameter $\lambda_g$, concentration parameter $\omega_g$, skewness parameter $\alpha_g$, location $\mu_g$, and scale matrix $\Sigma_g$. Here, $\delta(x, \mu_g | \Sigma_g) = (x - \mu_g)^\top \Sigma_g^{-1} (x - \mu_g)$ is the squared Mahalanobis distance between $x$ and $\mu_g$, with $K_{\lambda_g}$ and $K_{\lambda_g - p/2}$ denoting modified Bessel functions of the third kind.

The evaluation of modified Bessel functions in the density sometimes leads to numerical overflow or underflow. To avoid these issues, we use asymptotic expansions from Abramowitz
and Stegun (1972), i.e., for large $x$ or $\lambda$,

$$
K_\lambda(\lambda x) = \sqrt{\frac{\pi}{2\lambda}} \frac{\exp{-\lambda \rho}}{(1 + x^2)^{1/4}} \left[ 1 + \sum_{k=1}^{\infty} (-1)^k \frac{u_k(\tau)}{\lambda^k} \right],
$$

where

$$
\rho = \sqrt{1 + x^2 + \ln \left( \frac{x}{1 + \sqrt{1 + x^2}} \right)}.
$$

Here, $u_k(\tau)$ is the Debye polynomial represented by $u_0(\tau) = 1$ and

$$
u_{k+1}(\tau) = \frac{1}{2} \tau^2 (1 - \tau^2) u'_k(\tau) + \frac{1}{8} \int_{0}^{\tau} (1 - 5s^2) u_k(s) ds,
$$

for $k = 1, 2, \ldots$ and $\tau = 1/\sqrt{1 + x^2}$.

The parametrization in (2) is one of several available for generalized hyperbolic distributions (cf. McNeil et al., 2005). In this case, the $p$-dimensional random vector $X$ is generated by combining a generalized inverse Gaussian (GIG) random variable $Y$ with a latent multivariate Gaussian random variable $U \sim \mathcal{N}(0, \Sigma)$. Note that the density of $Y \sim \text{GIG}(\omega, \eta, \lambda)$ is

$$
h(y|\omega, \eta, \lambda) = \frac{(y/\eta)^{\lambda-1}}{2\eta K_\lambda(\omega)} \exp \left\{ -\frac{\omega}{2} \left( \frac{y}{\eta} + \frac{\eta}{y} \right) \right\}.
$$

We fix $\eta = 1$ and use the relationship $X = \mu + Y\alpha + \sqrt{Y}U$. Full details on the derivation of this parametrization and its use in parameter estimation are given by Browne and McNicholas (2013).

### 2.3 Model-based clustering

Consider a clustering scenario in which none of the observations have known component membership. The generalized hyperbolic model-based clustering likelihood is

$$
\mathcal{L}(\vartheta | x) = \prod_{i=1}^{n} \sum_{g=1}^{G} \pi_g f_h(x_i | \lambda_g, \omega_g, \mu_g, \Sigma_g, \alpha_g).
$$
To facilitate discussion of parameter estimation, introduce $Z_{ig}$ to denote component membership, so that $z_{ig} = 1$ if observation $x_i$ belongs to component $g$ and $z_{ig} = 0$ otherwise.

Parameter estimation for generalized hyperbolic mixtures is carried out using the expectation-maximization (EM) algorithm (Baum et al., 1970; Orchard and Woodbury, 1972; Sundberg, 1974; Dempster et al., 1977). The EM algorithm is an iterative procedure for finding maximum likelihood estimates when data are incomplete or are treated as being incomplete. The EM algorithm is based on the complete-data log-likelihood (4), where the complete-data comprise the observed $x_i$, the missing $z_{ig}$, and the latent $y_{ig}$. Our complete-data log-likelihood is given by

$$\ell(\vartheta) = \sum_{i=1}^{n} \sum_{g=1}^{G} z_{ig} \left[ \log(\pi_g) + \sum_{j=1}^{p} \log[\phi(x_i|\mu_g + y_{ig}\alpha_g, y_{ig}\Sigma_g)] + \log[h(y_{ig}|\omega_g, \lambda_g)] \right], \tag{4}$$

where $X_i \sim \mathcal{N}(\mu_g + y_i\alpha_g, y_i\Sigma_g)$, $Y_{ig} \sim \text{GIG}(\omega_g, 1, \lambda_g)$. Two steps are iterated until convergence is reached. In the expectation step (E-step), the expected value of the complete-data log-likelihood is computed. Then in the maximization step (M-step), the expected value of the complete-data log-likelihood is maximized with respect to the model parameters. Extensive details of the EM algorithm for generalized hyperbolic mixtures are given by Browne and McNicholas (2013).

Convergence is determined via an asymptotic estimate of the log-likelihood (4) at iteration $k + 1$, namely

$$l_{\infty} = l_k + \frac{l_{k+1} - l_k}{1 - a^k},$$

where $a^k = (l_{k+1} - l_k)/(l_k - l_{k-1})$ denotes the Aitken acceleration (Aitken, 1926). After convergence, component memberships are usually estimated based on the maximum a posteriori (MAP) classification given by $\text{MAP}\{\hat{z}_{ig}\} = 1$ if $\arg\max_h\{\hat{z}_{ih}\} = g$ and $\text{MAP}\{\hat{z}_{ig}\} = 0$ otherwise, for $i = 1, \ldots, n$.

In our applications (Section 4), we assume that the number of components $G$ is unknown. This is not unusual in real model-based clustering applications, where a criterion is often used to determine $G$. The Bayesian information criterion (BIC; Schwarz, 1978) is the most popular choice and is given by $\text{BIC} = 2l(x, \hat{\vartheta}) - r \log n$, where $l(x, \hat{\vartheta})$ is the maximized log-likelihood, $\hat{\vartheta}$ denotes the maximum likelihood estimate of $\vartheta$, $r$ represents the estimated number of free parameters, and $n$ is the number of observations.


2.4 Model-based classification and discriminant analysis

Model-based classification, or partial classification (cf. McLachlan, 1982), is a semi-supervised analogue of model-based clustering that has historically received much less attention within the literature. However, model-based classification has garnered increased attention over the past few years and some authors (e.g., Dean et al., 2006; McNicholas, 2010) have demonstrated that model-based classification can give excellent performance in real applications. Model-based discriminant analysis (Hastie and Tibshirani, 1996) is a supervised analogue of model-based clustering that has similarly received much less attention until recently (e.g., Andrews and McNicholas, 2011, 2012a). Model-based classification and discriminant analysis are best explained through the associated likelihoods.

Consider the classification scenario where there are $n$ observations, $k$ of which have known group memberships. Under a model-based classification framework, all $n$ observations are used to estimate the group memberships for the $n-k$ observations with unknown group memberships. Following McNicholas (2010), we arrange the data so that the first $k$ observations have known group memberships; therefore, the likelihood is given by

$$L(\vartheta|x) = \prod_{i=1}^{k} \prod_{g=1}^{G} \left[ \pi_g f_h(x_i|\lambda_g, \omega_g, \mu_g, \Sigma_g, \alpha_g) \right] z_{ig} \prod_{j=k+1}^{n} \sum_{s=1}^{G} \pi_s f_h(x_j|\lambda_s, \omega_s, \mu_s, \Sigma_s, \alpha_s). \quad (5)$$

As in the case of model-based clustering, parameter estimation is carried out using the EM algorithm. From (3) and (5), we see that model-based clustering can be viewed as a special case of model-based classification that arises by considering (5) with $k = 0$.

For model-based discriminant analysis, we again have $n$ observations, $k$ of which have known group memberships. Again, we arrange the data so that the first $k$ observations have known group memberships; however, instead of using all $n$ observations to estimate the unknown group memberships, we only use the first $k$ observations (i.e., the labelled observations). First, we form the likelihood

$$L(\vartheta|x) = \prod_{i=1}^{k} \prod_{g=1}^{G} \left[ \pi_g f_h(x_i|\lambda_g, \omega_g, \mu_g, \Sigma_g, \alpha_g) \right] z_{ig}. \quad (6)$$

Then, the parameter estimates are computed via the EM algorithm and the a posteriori
expected values of the $Z_{ig}$ are used to estimate the group memberships of the remaining $n - k$ observations.

Fraley and Raftery (2002) discuss MCLUST DA, where they allow for multiple components per known group by using the BIC to choose the number of components as well as the best MCLUST model (i.e., covariance structure) for each group. However, for the discriminant analyses herein, we restrict HMMDR to one component per known group. In part, this is done because of the large number of parameters to be estimated and the relatively small number of observations in the real data sets we consider (cf. Section 4.3). However, it is also done because we believe that the flexibility inherent in generalized hyperbolic components makes it far less likely, relative to Gaussian components, that multiple components would be needed to model a class. This latter point will be investigated as part of future work (cf. Section 5).

2.5 Dimension reduction and model-based clustering (GMMMDR)

Scrucca (2010) proposed a method of dimension reduction for model-based clustering within the Gaussian mixtures framework, called GMMMDR. Given a $G$-component Gaussian mixture model (GMM), i.e.,

$$f(x|\vartheta) = \sum_{g=1}^{G} \pi_g f_g(x | \mu_g, \Sigma_g) = \sum_{g=1}^{G} \pi_g \left[ \frac{\exp \left\{ -\frac{1}{2} (x - \mu_g)^\top \Sigma_g^{-1} (x - \mu_g) \right\}}{(2\pi)^{\frac{p}{2}} |\Sigma_g|^{\frac{1}{2}}} \right],$$

the procedure finds the smallest subspace that captures the clustering information contained within the data. The core of the method is to identify those directions where the cluster means $\mu_g$ and the cluster covariances $\Sigma_g$ vary as much as possible, provided that each direction is $\Sigma$-orthogonal to the others.

Finding these directions is achieved through the generalized eigen-decomposition of the kernel matrix $M$, defined by Scrucca (2010) as $Mv_i = l_i \Sigma v_i$, where $l_1 \geq l_2 \geq \cdots \geq l_d > 0$ and $v_i^\top \Sigma v_j = 1$ if $i = j$ and $v_i^\top \Sigma v_j = 0$ otherwise. Note that there are $d = \min\{p, G - 1\}$ directions that span the subspace. This kernel contains the variations in cluster means $M_1 = \sum_{g=1}^{G} \pi_g (\mu_g - \mu)(\mu_g - \mu)^\top$ and variations in cluster covariances $M_{II} = \sum_{g=1}^{G} \pi_g (\Sigma_g - \Sigma)\Sigma^{-1}(\Sigma_g - \Sigma)^\top$, such that $M = M_1 \Sigma^{-1} M_1 + M_{II}$.
Here, $\mu = \sum_{g=1}^{G} \pi_g \mu_g$ is the global mean, $\Sigma = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)(x_i - \mu)^\top$ is the covariance matrix, and $\Sigma = \sum_{g=1}^{G} \pi_g \Sigma_g$ is the pooled within-cluster covariance matrix. Fitting of the Gaussian mixtures within GMMDR is done using the MCLUST family (Fraley and Raftery, 1999). The MCLUST family is a subset of ten of the 14 Gaussian parsimonious clustering models (GPCMs) introduced by Celeux and Govaert (1995). The GPCMs arise from the imposition of various constraints on eigen-decomposed component covariance matrices (cf. Banfield and Raftery, 1993; Fraley and Raftery, 2002).

### 2.6 Non-Gaussian extensions to GMMDR

The work of Scrucca (2010) has already been extended to two non-Gaussian mixture settings. In the context of model-based clustering, Morris and McNicholas (2013a) proposed a $t$-distribution analogue of GMMDR, called $t$MMDR. This approach uses the $t$EIGEN family of models (Andrews and McNicholas, 2012a), which is a $t$-analogue of the GPCM family of models. The most general, i.e., unconstrained, member of the $t$EIGEN family is a mixture model with component density

$$f_t(x|\mu_g, \Sigma_g, \nu_g) = \frac{\Gamma(\nu_g+p/2)|\Sigma_g|^{-1/2}}{(\nu_g/2)\Gamma(\nu_g/2)(1 + \delta(x, \mu_g|\Sigma_g)/\nu_g)^{-\nu_g+p/2}},$$  

(7)

where $\mu_g$ is the mean, $\Sigma_g$ is a scale matrix, $\nu_g$ is the number of degrees of freedom, and $\delta(x, \mu_g|\Sigma_g)$ is defined as before. Of course, a mixture model with component density (7) is just a mixture of multivariate $t$-distributions, which has been applied for robust clustering for some time (McLachlan and Peel, 1998; Peel and McLachlan, 2000).

Morris and McNicholas (2013b) developed an analogue of GMMDR for shifted asymmetric Laplace (SAL) mixtures (Franczak et al., 2012), named SALMMDR. For SAL mixtures, the component density is

$$f_s(x|\alpha_g, \mu_g, \Sigma_g) = \frac{2 \exp\left\{(x - \mu_g)^\top \Sigma_g^{-1} \alpha_g\right\}}{(2\pi)^{p/2}|\Sigma_g|^{1/2}} \left\{\frac{\delta(x, \mu_g|\Sigma_g)}{2 + \alpha_g^\top \Sigma_g^{-1} \alpha_g}\right\}^{\nu/2} K_\nu(u),$$

with mean $\mu_g$, scale matrix $\Sigma_g$, and skewness $\alpha_g$. Here, $u = \sqrt{(2 + \alpha_g^\top \Sigma_g^{-1} \alpha_g)\delta(x, \mu_g|\Sigma_g)}$, $K_\nu$ is the modified Bessel function of the third kind with index $\nu = (2-p)/2$, and $\delta(x, \mu_g|\Sigma_g)$
is as defined previously. The use of SAL mixtures is effective for clustering data with asymmetric components, and they can perform better than Gaussian mixtures in these cases.

The approach introduced herein (Section [3]) aims to combine the robustness offered by the tMMDR approach with the elegance and asymmetry afforded by SALMMDR.

3 Methodology

The dimension reduction approach of Scrucca (2010) is extended through development of a generalized hyperbolic analogue. While Scrucca (2010) only considered model-based clustering, we need to emphasize that we will also develop methods for model-based classification and discriminant analysis for GMMDR and all of its non-Gaussian analogues considered herein. This is the first time that any of these approaches will have been used for classification and discriminant analysis.

Given a generalized hyperbolic mixture (2), we wish to find a subspace $S(\beta)$ where the cluster means and cluster covariances vary the most. Although $\mu_g$ is a mean and $\Sigma_g$ is a covariance matrix in (2), note that they are not the mean and covariance matrix of the random variable $X$ with the density in (2), except for the special case where $\alpha_g = 0$. The true mean of $X$ in (2) is $\tilde{\mu}_g := \mu_g + \alpha_g$, and the true covariance of $X$ in (2) is $\tilde{\Sigma}_g := \Sigma_g + \alpha_g \alpha_g^\top$. Thus, we define the kernel matrix $M_{\text{HMM}}$ for generalized hyperbolic mixtures to be

$$M_{\text{HMM}} = \sum_{g=1}^G \pi_g (\tilde{\mu}_g - \mu)(\tilde{\mu}_g - \mu)^\top \Sigma^{-1} \sum_{g=1}^G \pi_g (\tilde{\mu}_g - \mu)(\tilde{\mu}_g - \mu)^\top + \sum_{g=1}^G \pi_g (\tilde{\Sigma}_g - \bar{\Sigma}) \Sigma^{-1}(\tilde{\Sigma}_g - \bar{\Sigma})^\top,$$

where $\Sigma = \frac{1}{n} \sum_{i=1}^n (x_i - \mu)(x_i - \mu)^\top$ denotes the overall covariance matrix and $\bar{\Sigma} = \sum_{g=1}^G \pi_g \tilde{\Sigma}_g$ is the pooled within-cluster covariance matrix.

**Proposition 3.1** The directions where the cluster means $\tilde{\mu}_g$ and the cluster covariances $\tilde{\Sigma}_g$ vary the most are obtained from the eigen-decomposition

$$M_{\text{HMM}}v_i = l_i \Sigma v_i,$$

10
where \( l_1 \geq l_2 \geq \cdots \geq l_d > 0 \) and \( v_i^\top \Sigma v_j = 1 \) if \( i = j \) and \( v_i^\top \Sigma v_j = 0 \) otherwise.

The eigenvectors \([v_1, \ldots, v_d] \equiv \beta\), with \( d = \min\{p, G - 1\}\), form the basis of the dimension reduction subspace \( S(\beta) \). These eigenvectors are defined as the HMMDR directions.

**Proposition 3.2** Let \( S(\beta) \) be the subspace spanned by the HMMDR directions obtained from the eigen-decomposition of \( M_{\text{HMM}}(9) \).

i. The projections of the parameters onto \( S(\beta) \) are given by \( \beta^\top \hat{\mu}_g \) and \( \beta^\top \hat{\Sigma}_g \beta \), respectively.

ii. The projections of the \( n \times p \) data matrix \( X \) onto the subspace \( S(\beta) \) are computed from \( X\beta \). These projections are defined as the HMMDR variables.

For an \( n \times p \) data matrix \( X \), the kernel \( M_{\text{HMM}}(8) \) is obtained using the estimates from the fit of an HMM on \( X \), via the EM algorithm. Then the HMMDR directions are calculated from the generalized eigen-decomposition of \( M_{\text{HMM}}(8) \) with respect to the overall covariance matrix \( \Sigma \). The HMMDR directions are ordered based on eigenvalues, which means that directions associated with eigenvalues close to zero can be disregarded in practical applications because clusters will superimpose greatly along these directions.

Similar to GMMDR, the estimation of the HMMDR variables can be interpreted as feature selection, where the members are reduced through a set of linear combinations of the original variables. It is possible that this set of features contains estimated HMMDR variables that do not offer any clustering information but require parameter estimation. [Scrucca (2010)] uses the selection method of [Raftery and Dean (2006)] to prune the subset of GMMDR features. We follow this approach to select the most appropriate HMMDR variables. Two subsets of features, \( s \) and \( s' = \{s \setminus i\} \subset s \), for example, can be compared using the BIC difference

\[
\text{BIC}_{\text{diff}}(Z_i \in s) = \text{BIC}_{\text{clust}}(Z_s) - \text{BIC}_{\text{not clust}}(Z_s) = \frac{\text{BIC}_{\text{clust}}(Z_s) - \text{BIC}_{\text{clust}}(Z_{s'}) + \text{BIC}_{\text{reg}}(Z_i|Z_{s'})}{1} - \frac{\text{BIC}_{\text{clust}}(Z_s')}{2} + \frac{\text{BIC}_{\text{reg}}(Z_i|Z_{s'})}{3}, \tag{10}
\]

where term 1 in (10) denotes the BIC value for the best clustering model fitted using features in \( s \), term 2 denotes the BIC value for the best clustering model fitted using features in \( s' \), and term 3 denotes the BIC value for the regression of the \( i \)th feature on the remaining features in \( s' \).
Because the space of all possible subsets contains $2^d - 1$ elements, where $d = \min\{p, G - 1\}$, a full feature search is not usually feasible. To this end, we employ the forward greedy search algorithm of [Scrucca (2010)] to find a local optimum in the model space. The procedure is based on the forward-backward search algorithm of [Raftery and Dean (2006)]; however, a backward step is not necessary here because the HMMDR variables are $\Sigma$-orthogonal.

The method can be summarized into three main stages. The initial step selects the first feature that maximizes the BIC difference in (10) between the best clustering model and the model that assumes no clustering, i.e., a single component. The following step selects the next feature amongst those not previously included to be the one that maximizes the BIC difference in (10). This process is iterated until all of the BIC differences for the inclusion of a variable become negative.

At each stage, the search over the model space is performed with respect to the model parameterization and the number of clusters. This algorithm can be applied to the three frameworks under consideration: model-based clustering, classification, and discriminant analysis, by modifying the likelihood functions (3), (5), and (6) in the EM procedure accordingly. We can now summarize our new method, which we call HMMDR:

1. Fit an HMM (1) to the data using the EM algorithm.

2. Estimate the HMMDR directions: identify directions where the cluster means and cluster variances vary the most, provided each direction is $\Sigma$-orthogonal to the others. This is done through the eigen-decomposition of the kernel matrix $M_{HMM}$ in (8).

3. Select the HMMDR variables: compute the set of features by projecting the data onto the estimated subspace and use the greedy search algorithm to discard the ones that provide no clustering information.

4. Fit an HMM (1) on the selected HMMDR variables and return to step 2.

5. Repeat steps 2–4 until none of the features can be discarded.
4 Applications

4.1 Performance assessment

Although the data analyses herein are treated as regular clustering and classification examples, we know the true class labels in all cases. Therefore, we can compare our predicted classifications to the true class labels in each case. To do this, we use the adjusted Rand index (ARI; Hubert and Arabie, 1985), which is the Rand index (Rand, 1971) corrected for chance agreement. The Rand index is based on pairwise agreement and takes a value between 0 and 1, where 1 indicates perfect agreement between two partitions. The correction that leads to the ARI accounts for the fact that random classification is expected to result in some correct agreements; accordingly, the ARI has an expected value of 0 under random classification and, as with the Rand index, perfect classification corresponds to a value of 1. Negative ARI values are possible and indicate classification results worse than would be expected by random classification.

4.2 Simulated data

First, we employ a data simulation scheme based on two scenarios to test the HMMDR algorithm. In Scenario I, we generate three variables from a multivariate normal distribution with means $\mu_1 = (0, -2, 0)$, $\mu_2 = (2, 4, 0)$, $\mu_3 = (-2, -4, 2)$ and common covariance matrix $\Sigma = \text{diag}(0.5)$. Also, we use three different sample sizes, $n \in \{100, 500, 1000\}$. In Scenario II, we modify Scenario I by adding five noise variables generated from standard normal distributions. Figure 1 illustrates a typical example of the three components.

We run each scenario 25 times for each possible combination of data dimension and model framework. The results are given in Table 1. HMMDR generally exhibits high ARI values across both scenarios and all sample sizes for model-based clustering, classification, and discriminant analysis. We notice a slight drop in classification performance for Scenario II with 100 observations; however, performance on noisy data improves for larger $n$. One feature is selected throughout Scenario I, and as expected, the addition of noise tends to lead to a slight increase in the number of features for Scenario II.
Figure 1: Scatterplot illustrating a typical example of the simulated multivariate Gaussian components in Scenarios I and II.

Table 1: Summary of results for the best HMMDR models fitted to the simulated data, based on 25 runs. Computing time in seconds represents the average time for a single run.

| Method            | Scenario I (no noise)          | Scenario II (with noise)          |
|-------------------|--------------------------------|----------------------------------|
|                   | $n = 100$ | $n = 500$ | $n = 1000$ | $n = 100$ | $n = 500$ | $n = 1000$ |
| Clustering        | Avg. ARI | 1          | 0.9703         | 0.9646         | 0.9218        | 0.9839        | 0.9763        |
|                   | Std. dev. | 0          | 0.0192         | 0.0201         | 0.2056        | 0.0228        | 0.0256        |
|                   | Features  | 2          | 1–2            | 1              | 3–4         | 2–3          | 2             |
|                   | Avg. time | 14.4       | 16.7           | 18.5           | 24.7        | 25          | 37.7          |
| Classification    | Avg. ARI | 1          | 0.9939         | 0.9817         | 0.9488        | 0.9940        | 0.9801        |
|                   | Std. dev. | 0          | 0.0103         | 0.0177         | 0.1870        | 0.0243        | 0.0366        |
|                   | Features  | 1          | 1–2            | 1–2            | 3–4         | 2–3          | 2             |
|                   | Avg. time | 12.7       | 13.4           | 15.4           | 21.5        | 22.7          | 26.1          |
| Discriminant anal.| Avg. ARI | 0.9701      | 0.9821         | 0.9704         | 0.9110        | 0.9821        | 0.9750        |
|                   | Std. dev. | 0.0671      | 0.0283         | 0.0562         | 0.2122        | 0.0191        | 0.0381        |
|                   | Features  | 1–2        | 1–2            | 1–2            | 1–3         | 2–3          | 2             |
|                   | Avg. time | 12.5       | 13.23          | 15             | 20          | 21.8         | 31.3          |

Next, we simulate data with higher dimensions using the R package clusterGeneration (Qiu and Joe, 2006). Four-component data sets, each with $n_g = 60$ observations per component, are generated by setting the degree of separation between them to 0.6 (with 1 denoting most separation) and choosing arbitrary positive definite covariance matrices. In total, 75 data sets were generated in this way, i.e., 25 data sets for each of three values for data dimension.
\( p \in \{10, 30, 50\} \). Figure 2 depicts a typical example of the four components.

![Figure 2: Scatterplot of simulated higher dimensional data indicating the four clusters.](image)

The results (Table 2) indicate that our HMMDR method consistently achieves excellent classification and dimension reduction performance for model-based clustering, classification, and discriminant analysis.

Table 2: Summary of results for the best HMMDR models for the simulated data, based on 25 runs. Computing time in seconds represents the average time for a single run.

| Method    | Dim. | ARI   | Std. dev. | Feat. | Comp. | Avg. time |
|-----------|------|-------|-----------|-------|-------|-----------|
| Clustering| 10   | 1     | 0         | 2     | 4     | 1069      |
|           | 30   | 1     | 0         | 4–5   | 4     | 3662      |
|           | 50   | 0.94  | 0.2018    | 6–8   | 4     | 5137      |
| Classification| 10  | 1     | 0         | 2     | 4     | 625       |
|            | 30   | 1     | 0         | 3–4   | 4     | 1500      |
|            | 50   | 0.97  | 0.0620    | 5–7   | 4     | 2612      |
| Disc. analysis| 10 | 1     | 0         | 2–3   | 4     | 616       |
|             | 30   | 0.96  | 0.0785    | 4–6   | 4     | 1628      |
|             | 50   | 0.95  | 0.1676    | 5–7   | 4     | 2710      |
4.3 Real data

To gauge the performance of our algorithm on real data, we compare results with the eight methods outlined below. Except for $k$-means, we choose these particular comparator methods because they provide model-based analyses while implicitly reducing the dimension space.

1. Robust principal component analysis (ROBPCA) (Hubert et al., 2005) paired with $t$-mixtures via the $t$EIGEN family: principal components analysis resistant to outliers, with robust loadings computed by using projection-pursuit techniques and the minimum covariance determinant method. We use the R package rrcov (Todorov and Filzmoser, 2009) for the ROBPCA computations as well as the teigen package (Andrews and McNicholas, 2012b).

2. Parsimonious Gaussian mixture models (McNicholas and Murphy, 2008): Gaussian mixtures of factor analyzers are used to parameterize the covariance structure. The R package pgmm (McNicholas et al., 2011) is used to derive the results.

3. Mixtures of common factor analyzers (?): model-based density estimation, where common component-factor loadings are used to reduce the number of parameters. The R package mcfa (Baek et al., 2009) is used herein.

4. FisherEM (Bouveyron and Brunet, 2012): a subspace clustering method based on Gaussian mixtures, where an EM-like algorithm estimates both the discriminative subspace and the parameters of the model. The R package FisherEM (Bouveyron and Brunet, 2012) is employed to carry out the computations.

5. Clustvarsel (Raftery and Dean, 2006) paired with Gaussian mixtures via the MCLUST family: a greedy procedure to find the (locally) optimal subset of variables in a data set. The R package clustvarsel (Dean and Raftery, 2009) is used to derive the results.

6. $k$-means: partitions $n$ observations into $k$ clusters, where each observation belongs to the cluster with the nearest mean. The R function kmeans is used herein.

7. GMMDR: the approach of Scrucca (2010) based on Gaussian mixtures.

8. $t$MMDR: the $t$-analogue of GMMDR. Fitting of the $t$-mixtures was carried out with the R package teigen.
9. SALMMDR: the SAL analogue of GMMMDR.

For the analyses in this section, we fit HMMDR and comparator methods to the scaled version of each data set. Where appropriate, we use the MCLUST hierarchical agglomerative procedure for initialization (cf. Fraley and Raftery, 1999). In the case of HMMDR and its analogues, we allow the number of components to vary between \( G = 1 \) and \( G = 6 \). Note that we use the term ‘analogue’ somewhat loosely here, because we do not consider decomposed covariance structures for either generalized hyperbolic mixtures or shifted asymmetric Laplace mixtures (Table 3).

Table 3: Details about the component covariance structures for each of the four MMDR methods used.

| Method | Covariance | Eigen-decomposed | Model family |
|--------|------------|------------------|--------------|
| HMMDR  | \( \Sigma_g + \alpha_g \alpha_g^\top \) | No               | –            |
| SALMMDR| \( \Sigma_g + \alpha_g \alpha_g^\top \) | No               | –            |
| tMMDR  | \( \nu_g^{-2} \Sigma_g, \nu_g > 2 \) | Yes             | tEIGEN       |
| GMMDR  | \( \Sigma_g \) | Yes             | MCLUST       |

In the context of model-based classification and discriminant analysis, we use the approach of McNicholas (2010) to simulate a situation in which some of the group memberships are unknown. For each observation \( x_i \), a random number is generated from a uniform distribution on \([0, 1]\). If the random number is less than 0.5, then \( x_i \) is taken as known; otherwise, \( x_i \) is taken as unknown.

We utilize the functionality of teigen to fit both Gaussian mixtures and t-mixtures for model-based classification (cf. Andrews and McNicholas, 2012a). Similarly, teigen and mclust (Fraley et al., 2012) were employed for model-based discriminant analysis. For each data set, the procedures were run 25 times, using hierarchical agglomerative starting values of the unknown \( \hat{z}_{ig} \). Note that the number of unknown observations varied from run to run, and so each method was applied to data sets with different numbers of observations. This is evidenced by the results of the model-based classification and discriminant analysis (Tables 10, 14, and 17).

Although some computing times for HMMDR are shown (Tables 1 and 2), we did not provide comparisons with its analogues for two reasons. First, GMMDR employs the R package mclust, which is built on a Fortran backend; however, the other approaches do not have this
advantage and so comparison would be meaningless. Second, as outlined in Table 3, only two methods use a decomposed covariance structure, and so comparing computing times for all four algorithms would again be misleading.

Note that we choose each real data set on the basis that it has previously been used to illustrate the performance of some of the comparator methods. We consider that this approach facilitates a very fair comparison. In all cases, we illustrate model-based clustering, classification, and discriminant analysis. For model-based classification and discriminant analysis, the ARI is computed based only on unlabelled observations.

4.3.1 Swiss bank notes data and female voles data

Flury and Riedwyl (1988) present six measurements taken from Swiss bank notes (length, diagonal, left, right, top, and bottom) and available through the R package gclus (Hurley 2010). Each bank note is either genuine or counterfeit. In terms of model-based clustering, HMMDR and its comparators were fitted to these data and the resulting MAP classifications show very high ARI values for most methods (Table 5), with HMMDR and k-means being the only methods to cluster the bank notes data perfectly. For model-based classification, HMMDR, SALMMDR, and tMMDR produce perfect classifications of the unknown observations (Table 7). However, only HMMDR provides perfect model-based discriminant analysis results on the bank notes. We note that HMMDR selected the minimum number of features in all three scenarios, i.e., one feature.

Flury (1997, Table 5.3.7) discuss seven measurements of female voles from two species (Mi- crotus californicus and Microtus ochrogaster, Table 4) originally studied by Airoldi and Hoffmann (1984). The data are available within the R package flury (Flury 2010).

Table 4: Measurements taken for the female vole data.

| Age in days | Incisive foramen length | Zygomatic width |
|-------------|-------------------------|-----------------|
| Condyle incisive length | Skull height | Interorbital width |
| Alveolar length of upper molar tooth row |

Tables 6 and 8 indicate that, out of all of the procedures fitted to the voles data, HMMDR is the only one giving perfect classification results in all three paradigms.
4.3.2 Wine data

Forina et al. (1986) recorded several chemical and physical properties for three types of Italian wines: Barolo, Grignolino, and Barbera. As shown in Table 9, thirteen properties for 178 wines are available from the R package gclus (Hurley, 2004).

Within the model-based clustering framework, HMMDR is the best performer (ARI = 0.97, Table 11), with only two misclassified observations (Table 10). The model-based classification scenario (Table 12) reveals that HMMDR, SALMMDR, and tMMDR produce perfect
Table 9: Chemical and physical properties available for the wine data in gclus.

| Property                  | Feature                          |
|---------------------------|----------------------------------|
| Alcohol                   | Proline                          |
| Malic acid                | Ash                              |
| Hue                       | Total phenols                    |
| Color intensity           | Nonflavonoid phenols             |
| Flavonoids                | Proanthocyanins                  |
| OD280/OD315 of diluted wines | Alkalinity of ash                |

classification results. With an ARI of 0.92, HMMDR gives the best performance within the model-based discriminant analysis paradigm.

Table 10: Model-based clustering, classification, and discriminant analysis results for our HMMDR approach fitted to the wine data. Model-based classification and discriminant analysis results are based on 25 runs.

| Wine     | HMMDR clust. | HMMDR class. | HMMDR disc. |
|----------|--------------|---------------|-------------|
| Wine     | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 |
| Barolo   | 59 | 0 | 0 | 875 | 0 | 0 | 625 | 50 | 0 |
| Grignolino | 0 | 68 | 2 | 0 | 925 | 0 | 0 | 825 | 0 |
| Barbera  | 0 | 0 | 48 | 0 | 0 | 500 | 0 | 0 | 550 |
| ARI; Features | 0.97; 7 | 1; 5 | 0.92; 8 |

Table 11: Summary of model-based clustering results for the wine data.

| Method       | ARI | Feat. | Comp. |
|--------------|-----|-------|-------|
| HMMDR        | 0.97| 7     | 3     |
| SALMMDR      | 0.92| 10    | 3     |
| tMMDR        | 0.93| 4     | 3     |
| GMMMDR       | 0.85| 5     | 3     |
| ROBPCA       | 0.83| 4     | 3     |
| FisherEM     | 0.91| 2     | 3     |
| clustvarsel  | 0.78| 5     | 3     |
| mcfa         | 0.90| 3     | 3     |
| pgmm         | 0.79| 2     | 3     |
| kmeans       | 0.90| -     | 3     |

Table 12: Summary of model-based classification and discriminant analysis results for the wine data, based on 25 runs.

| Method       | ARI | Feat. | Comp. |
|--------------|-----|-------|-------|
| HMMDR class. | 1   | 5     | 3     |
| SALMMDR class.| 1  | 10    | 3     |
| tMMDR class. | 1   | 5     | 3     |
| GMMMDR class.| 0.93| 3–8   | 3     |
| HMMDR disc.  | 0.92| 8     | 3     |
| SALMMDR disc.| 0.88| 8     | 3     |
| tMMDR disc.  | 0.85| 1–8   | 3     |
| GMMMDR disc. | 0.85| 2–8   | 3     |

Figure 3 illustrates three of the estimated HMMDR directions obtained from our model-based clustering of the wine data (Table 10). The edge histograms depict the distribution of
the observations from the estimated directions, coloured by estimated cluster allocation. The plot on the left-hand side reveals quite clearly the underlying cluster structure in the data. Although there is some overlap in these two directions, only two wines were misclassified by the HMMDR method and so some of the other dimensions must give additional clarity.

Figure 3: Plots of some of the estimated HMMDR directions for the wine data obtained from model-based clustering (direction 2 vs. 4 on the left-hand side, and direction 4 vs. 5 on the right-hand side). Symbols indicate true cluster membership and colours indicate the estimated HMMDR cluster allocation. The edge histograms depict the estimated distributions of the observations in each cluster.

4.3.3 Wisconsin breast cancer data

Mangasarian et al. (1995) presented a study of breast cancer from Wisconsin, undertaken to establish whether fine needle aspiration of breast tissue samples could classify tumour status. Several attributes are recorded (Table 13) for 681 cases of potentially cancerous tumours, of which 238 were actually malignant. These data are available in the R package faraway (Faraway 2011).

Within the model-based clustering framework, HMMDR selected three features and gave the best classification performance (ARI = 0.89, Table 14). The tMMDR (ARI = 0.86) and
Table 13: Tissue sample properties of the Wisconsin breast cancer data.

| Marginal adhesion | Epithelial cell size | Clump thickness |
|-------------------|----------------------|-----------------|
| Bare nuclei       | Mitoses              | Cell shape uniformity |
| Bland chromatin   | Normal nucleoli      | Cell size uniformity |

*k*-means (ARI = 0.84) approaches are close behind; however, the rest of the comparators did not produce particularly good results on these data (Table 13). For the model-based classification and discriminant analysis scenarios, HMMDR gave classification performance similar to clustering and was again the best performer over the 25 runs (Table 16).

Table 14: Model-based clustering, classification, and discriminant analysis results for our HMMDR approach on the breast cancer data. Model-based classification and discriminant analysis results are based on 25 runs.

| Status     | HMMDR clust. 1 | HMMDR clust. 2 | HMMDR class. 1 | HMMDR class. 2 | HMMDR disc. 1 | HMMDR disc. 2 |
|------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Malignant  | 236            | 2              | 2925           | 125            | 2575           | 200            |
| Benign     | 17             | 426            | 100            | 4925           | 50             | 4675           |
| ARI; Features | 0.89; 3    |                 | 0.89; 2        |                 | 0.87; 6        |                 |

Table 15: Summary of model-based clustering results for the breast cancer data.

| Method     | ARI | Feat. | Comp. |
|------------|-----|-------|-------|
| HMMMDR     | 0.89| 3     | 2     |
| SALMMDR    | 0.80| 5     | 2     |
| tMMDR      | 0.86| 3     | 2     |
| GMMDR      | 0.58| 5     | 2     |
| ROBPCA     | 0.55| 5     | 3     |
| FisherEM   | 0.79| 1     | 2     |
| clustvarsel| 0.78| 2     | 2     |
| mcfa       | 0.65| 3     | 2     |
| pgmm       | 0.31| 1     | 2     |
| kmeans     | 0.84| -     | 2     |

Table 16: Summary of model-based classification and discriminant analysis results for the breast tissue data, based on 25 runs.

| Method     | ARI | Feat. | Comp. |
|------------|-----|-------|-------|
| HMMMDR     | 0.89| 2     | 2     |
| SALMMDR    | 0.85| 4     | 2     |
| tMMDR      | 0.86| 1-2   | 2     |
| GMMDR      | 0.86| 1     | 2     |
| HMMMDR     | 0.87| 6     | 2     |
| SALMMDR    | 0.84| 7     | 2     |
| tMMDR      | 0.85| 2     | 2     |
| GMMDR      | 0.84| 1-7   | 2     |

Figure 4 illustrates three of the estimated HMMMDR directions obtained from the model-based clustering output shown in Table 14. The plots depict quite clearly the inherent
cluster structure in the data, and we notice that the malignant breast tissues are quite tightly packed in their cluster. The red histogram on the top edge of the left-hand side of Figure 4 is a nice illustration of the need to model skewness.

Figure 4: Plots of some of the estimated HMMDR directions for the breast cancer data obtained from model-based clustering (direction 1 vs. 3 on the left-hand side, and direction 2 vs. 3 on the right-hand side). Symbols indicate true cluster membership and colours indicate the estimated HMMDR cluster allocation. The edge histograms depict the estimated distributions of the observations in each cluster.

4.3.4 Colon data

Alon et al. (1999) analyzed gene expression data from microarray experiments of colon tissue, probed by oligonucleotide arrays. These data contain 62 tissue samples with 2000 genes: 40 tumour tissues and 22 normal tissues. The data are available in the R package plsgenomics (Boulesteix et al., 2011). The challenge here is dealing with the large number of gene expression levels compared with the small number of tissue samples. As is the case with microarray data in general, there are many non-informative genes that can obstruct the clustering of the samples. Thus, gene filtering was carried out prior to further analysis. While McLachlan et al. (2002) and McNicholas and Murphy (2010) used the EMMIX-
GENE procedure (McLachlan et al., 2002) to reduce the dimensionality of the colon data, we considered a different method.

Our gene filtering approach is to find differentially expressed genes based on modified t-tests, using the R Bioconductor package siggenes (Schwender, 2012). This package contains the function `sam`, which implements the Significance Analysis of Microarrays (SAM) method proposed by Tusher et al. (2001). SAM computes a statistic $d_i$ for each gene $i$, measuring the strength of the relationship between gene expression and the response variable (which is the class variable in our case). It uses repeated permutations of the data to determine if the expression of any gene is significantly related to the response. The cutoff for significance is determined by a tuning parameter $\Delta$, chosen by the user based on the false positive rate. We employed 100 permutations and chose $\Delta = 2.4$, which yielded 23 genes for analysis (Table 20, Appendix A).

Even with the dimensionality reduced to 23 genes, the analysis of the colon data was quite challenging. When HMMDR was fitted to these data within the model-based clustering paradigm, five observations were misclassified (Table 17), corresponding to an ARI of 0.70. This was the best result, with tMMDR (ARI = 0.64) being the next best performer (Table 18). For model-based classification and discriminant analysis, HMMDR gave better performance with ARI values of 0.86 and 0.83, respectively (Table 19). We note that SALMMDR, tMMDR, and GMMDR also gave improved performance within the model-based classification and discriminant analysis paradigms; however, HMMDR was the best approach across all paradigms.

Table 17: Model-based clustering, classification, and discriminant analysis results for the colon data. Model-based classification and discriminant analysis results are based on 25 runs.

|        | HMMDR clust. | HMMDR class. | HMMDR disc. |
|--------|--------------|---------------|--------------|
|        | 1  | 2  | 1  | 2  | 1  | 2  | 1  | 2  |
| Normal |    |    | 22  | 0  | 225  | 0  | 220  | 15  |
| Tumour | 5  | 35 | 25  | 425 | 15  | 420 |
| ARI; Features | 0.70; 3 | 0.86; 5 | 0.83; 6 |

It is interesting to note that McNicholas and Murphy (2010) obtained similar clustering results to HMMDR for the colon data. They considered a subset of 461 genes and the
Table 18: Summary of model-based clustering results for the best models fitted to the colon data.

| Method     | ARI  | Feat. | Comp. |
|------------|------|-------|-------|
| HMMDR      | 0.70 | 3     | 2     |
| SALMMDR    | 0.59 | 10    | 2     |
| tMMDR      | 0.64 | 1     | 2     |
| GMMDR      | 0.59 | 1     | 2     |
| ROBPCA     | 0.36 | 3     | 3     |
| FisherEM   | 0.59 | 1     | 2     |
| clustvarsel| 0.35 | 3     | 4     |
| mcfa       | 0.64 | 5     | 2     |
| pgmm       | 0.40 | 3     | 2     |
| kmeans     | 0.59 | -     | 2     |

Table 19: Summary of model-based classification and discriminant analysis results for the colon data, based on 25 runs.

| Method     | ARI  | Feat. | Comp. |
|------------|------|-------|-------|
| HMMDR class.| 0.86 | 5     | 2     |
| SALMMDR class.| 0.71 | 6     | 2     |
| tMMDR class.| 0.75 | 1     | 2     |
| GMMDR class.| 0.73 | 1     | 2     |
| HMMDR disc.       | 0.83 | 6     | 2     |
| SALMMDR disc.     | 0.70 | 7     | 2     |
| tMMDR disc.       | 0.74 | 1     | 2     |
| GMMDR disc.       | 0.70 | 1     | 2     |

The best model fitted to these data had six latent factors, with five misclassified tissues and an ARI of 0.70. Although equal to two significant figures, we point out for completeness that our HMMDR approach has a very slightly higher ARI value (0.699 vs. 0.697). McLachlan et al. (2002) also analyzed these data; they selected 446 genes and identified five types of clusterings on this subset. However, these clusterings did not correspond to the tissue type.

Figure 5 illustrates three of the estimated HMMDR directions obtained from the model-based clustering output from Table 17. The plots depict the inherent cluster structure in the colon tissues and, as we would expect, the misclassified tissues are generally close to the cluster boundaries.
Figure 5: Plots of some of the estimated HMMDR directions for the colon data obtained from model-based clustering (direction 2 vs. 3 on the left-hand side, and direction 1 vs. 2 on the right-hand side). Symbols indicate true cluster membership and colours indicate the estimated HMMDR cluster allocation. The edge histograms depict the estimated distributions of the observations in each cluster.

5 Conclusions

This paper introduced an effective dimension reduction technique for model-based clustering, classification, and discriminant analysis using multivariate mixtures of generalized hyperbolic distributions. Our method, known as HMMDR, focused on identifying the smallest subspace of the data that captured the inherent cluster structure. The HMMDR approach was illustrated using simulated and real data, where it performed favourably compared to its existing special cases, i.e., GMMDR, tMMDR, and SALMMDR. This is the first time that these special cases have been applied to model-based classification and discriminant analysis. In clustering applications, HMMDR consistently outperformed several other model-based dimension reduction methods (ROBPCA, pgmm, FisherEM, clustvarsel, and mcfa).

The real data sets used for our illustrations were selected because they were previously illustrated the performance of some of the comparator methods. Therefore, it is quite remarkable that HMMDR consistently outperformed all comparator methods on all data sets. We be-
lieve that HMMDR has the potential to become a gold-standard for dimension reduction and clustering, classification, and discriminant analysis; to this end, an R package is currently in development so that our approach will be available to the wider community. As part of the development of this R package, we will study whether incorporating generalized hyperbolic analogues of the GPCM models into our approach is beneficial. While such an approach is taken within GMMDR and tMMDR, we believe that careful study is needed before determining whether adding these analogues is desirable. This also ties in with whether multiple components should be available to represent a class in HMMDR discriminant analysis, another topic deserving of further work. Finally, the application of our approach within the fractionally-supervised classification framework [Vrbik and McNicholas 2013] will also be a subject of future work.

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References

Abramowitz, M. and Stegun, I. (1972). *Handbook of Mathematical Functions*. Dover, New York, 9th edition.

Airoldi, J.-P. and Hoffmann, R. S. (1984). Age variation in volves (Microtus californicus, M. ochrogaster) and its significance for systematic studies. *Occasional papers of the Museum of Natural History, University of Kansas, Lawrence KS*, 111:1–45.

Aitken, A. C. (1926). On Bernoulli’s numerical solution of algebraic equations. *Proceedings of the Royal Society of Edinburgh*, 46:289–305.
Alon, U., Barkai, N., Notterman, D., Gish, K., Ybarra, S., Mack, D., and Levine, A. (1999). Broad patterns of gene expression revealed by clustering analysis of tumor and normal colon tissues probed by oligonucleotide arrays. Proceedings of the National Academy of Sciences, 96(12):6745–6750.

Andrews, J. L. and McNicholas, P. (2012a). Model-based clustering, classification, and discriminant analysis via mixtures of multivariate $t$-distributions: The tEIGEN family. Statistics and Computing, 22(5):1021–1029.

Andrews, J. L. and McNicholas, P. D. (2011). Mixtures of modified $t$-factor analyzers for model-based clustering, classification, and discriminant analysis. Journal of Statistical Planning and Inference, 141(4):1479–1486.

Andrews, J. L. and McNicholas, P. D. (2012b). teigen: Model-based clustering and classification with the multivariate $t$-distribution. R package version 1.0.

Andrews, J. L., McNicholas, P. D., and Subedi, S. (2011). Model-based classification via mixtures of multivariate $t$-distributions. Computational Statistics and Data Analysis, 55(1):520–529.

Baek, J., McLachlan, G. J., and Flack, L. K. (2009). mcfa: Fits mixtures of common factor analyzers to a given data set. R package version 1.0.2.

Banfield, J. D. and Raftery, A. E. (1993). Model-based Gaussian and non-Gaussian clustering. Biometrics, 49(3):803–821.

Barndorff-Nielsen, O. (1977). Exponentially decreasing distributions for the logarithm of particle size. Proceedings of the Royal Society A, 353:401–419.

Barndorff-Nielsen, O. and Halgreen, C. (1977). Infinite divisibility of the hyperbolic and generalized inverse Gaussian distributions. Z. Wahrscheinlichkeitstheorie verw. Gebiete, 38:309–311.

Baum, L. E., Petrie, T., Soules, G., and Weiss, N. (1970). A maximization technique occurring in the statistical analysis of probabilistic functions of Markov chains. Annals of Mathematical Statistics, 41:164–171.
Blæsild, P. (1978). The shape of the generalized inverse Gaussian and hyperbolic distributions. Research Report 37, Aarhus University, Denmark, Department of Theoretical Statistics.

Boulesteix, A.-L., Lambert-Lacroix, S., Peyre, J., and Strimmer, K. (2011). *plsgenomics: PLS analyses for genomics*. R package version 1.2-6.

Bouveyron, C. and Brunet, C. (2012). Simultaneous model-based clustering and visualization in the Fisher discriminative subspace. *Statistics and Computing*, 22(1):301–324.

Browne, R. P. and McNicholas, P. D. (2013). A mixture of generalized hyperbolic distributions. arXiv: 1305.1036.

Celeux, G. and Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition*, 28:781–793.

Dean, N., Murphy, T. B., and Downey, G. (2006). Using unlabelled data to update classification rules with applications in food authenticity studies. *Journal of the Royal Statistical Society: Series C*, 55(1):1–14.

Dean, N. and Raftery, A. E. (2009). *clustvarsel: Variable Selection for Model-Based Clustering*. R package version 1.3.

Dempster, A. P., Laird, N. M., and Rubin, D. B. (1977). Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society: Series B*, 39(1):1–38.

Everitt, B. S. and Hand, D. J. (1981). *Finite Mixture Distributions*. Chapman and Hall, London.

Faraway, J. (2011). *faraway: Functions and datasets for books by Julian Faraway*. R package version 1.0.5.

Flury, B. (2010). *Flury: Data Sets from Flury, 1997*. R package version 0.1-3.

Flury, B. and Riedwyl, H. (1988). *Multivariate Statistics: A Practical Approach*. Cambridge University Press.

Flury, B. D. (1997). *A First Course in Multivariate Statistics*. Springer, New York.
Forina, M., Armanino, C., Castino, M., and Ubigli, M. (1986). Multivariate data analysis as a discriminating method of the origin of wines. *Vitis*, 25:189–201.

Fraley, C. and Raftery, A. E. (1999). MCLUST: Software for model-based cluster analysis. *Journal of Classification*, 16:297–306.

Fraley, C. and Raftery, A. E. (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*, 97(458):611–631.

Fraley, C., Raftery, A. E., and Scrucca, L. (2012). *mclust*: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. R package version 4.0.

Franczak, B., Browne, R. P., and McNicholas, P. D. (2012). Mixtures of shifted asymmetric Laplace distributions. arXiv: 1207.1727v3.

Greselin, F. and Ingrassia, S. (2010). Constrained monotone EM algorithms for mixtures of multivariate *t*-distributions. *Statistics and Computing*, 20(1):9–22.

Härdle, W. K. and Simar, L. (2011). *Applied Multivariate Statistical Analysis*. Springer.

Hastie, T. and Tibshirani, R. (1996). Discriminant analysis by Gaussian mixtures. *Journal of the Royal Statistical Society: Series B*, 58(1):155–176.

Hubert, L. and Arabie, P. (1985). Comparing partitions. *Journal of Classification*, 2:193–218.

Hubert, M., Rousseeuw, P. J., and Vanden Branden, K. (2005). ROBPCA: a new approach to robust principal components analysis. *Technometrics*, 47:64–79.

Hurley, C. (2004). Clustering visualizations of multivariate data. *Journal of Computational and Graphical Statistics*, 13(4):788–806.

Hurley, C. (2010). *gclus*: Clustering Graphics. R package version 1.3.

Lee, S. X. and McLachlan, G. J. (2013). On mixtures of skew normal and skew *t*-distributions. arXiv:1211.3602v2.

Li, K. C. (1991). Sliced inverse regression for dimension reduction (with discussion). *Journal of the American Statistical Association*, 86:316–342.
Li, K. C. (2000). High dimensional data analysis via the SIR/PHD approach. Unpublished manuscript.

Lin, T.-I. (2010). Robust mixture modeling using multivariate skew t-distributions. *Statistics and Computing*, 20:343–356.

Mangasarian, O. L., Street, W. N., and Wolberg, W. H. (1995). Breast cancer diagnosis and prognosis via linear programming. *Operations Research*, 43(4):570–577.

McLachlan, G. J. (1982). *The classification and mixture maximum likelihood approaches to cluster analysis*, volume 2 of *Handbook of Statistics*, pages 199–208. North-Holland, Amsterdam.

McLachlan, G. J. and Basford, K. E. (1988). *Mixture Models: Inference and applications to clustering*. Marcel Dekker Inc., New York.

McLachlan, G. J., Bean, R. W., and Peel, D. (2002). Mixture model-based approach to the clustering of microarray expression data. *Bioinformatics*, 18:413–422.

McLachlan, G. J. and Peel, D. (1998). Robust cluster analysis via mixtures of multivariate t-distributions. In *Lecture Notes in Computer Science*, volume 1451, pages 658–666. Springer-Verlag, Berlin.

McLachlan, G. J. and Peel, D. (2000). *Finite Mixture Models*. John Wiley & Sons, New York.

McNeil, A. J., Frey, R., and Embrechts, P. (2005). *Quantitative Risk Management: Concepts, Techniques and Tools*. Princeton University Press.

McNicholas, P. D. (2010). Model-based classification using latent Gaussian mixture models. *Journal of Statistical Planning and Inference*, 140:1175–1181.

McNicholas, P. D. (2013). Model-based clustering and classification via mixtures of multivariate t-distributions. In Guidici, P., Ingrassia, S., and Vichi, M., editors, *Statistical Models for Data Analysis*, Studies in Classification, Data Analysis, and Knowledge Organization, pages 233–240. Springer International Publishing Switzerland.

McNicholas, P. D., Jampani, K. R., McDaid, A. F., Murphy, T. B., and Banks, L. (2011). *pgmm: Parsimonious Gaussian Mixture Models*. R package version 1.0.
McNicholas, P. D. and Murphy, T. B. (2008). Parsimonious Gaussian mixture models. *Statistics and Computing*, 18:285–296.

McNicholas, P. D. and Murphy, T. B. (2010). Model-based clustering of microarray expression data via latent Gaussian mixture models. *Bioinformatics*, 26(21):2705–2712.

Morris, K. and McNicholas, P. D. (2013a). Dimension reduction for model-based clustering via mixtures of multivariate $t$-distributions. *Advances in Data Analysis and Classification*, 7(3):321–338.

Morris, K. and McNicholas, P. D. (2013b). Dimension reduction for model-based clustering via mixtures of shifted asymmetric Laplace distributions. *Statistics and Probability Letters*, 83(9):2088–2093.

Orchard, T. and Woodbury, M. A. (1972). A missing information principle: theory and applications. In Le Cam, L. M., Neyman, J., and Scott, E. L., editors, *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Theory of Statistics*, pages 697–715. University of California Press, Berkeley.

Peel, D. and McLachlan, G. J. (2000). Robust mixture modelling using the $t$-distribution. *Statistics & Computing*, 10:339–348.

Qiu, W.-L. and Joe, H. (2006). Generation of random clusters with specified degree of separation. *Journal of Classification*, 23(2):315–334.

R Core Team (2013). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Raftery, A. E. and Dean, N. (2006). Variable selection for model-based clustering. *Journal of the American Statistical Association*, 101(473):168–178.

Rand, W. M. (1971). Objective criteria for the evaluation of clustering methods. *Journal of the American Statistical Association*, 66:846–850.

Schwarz, G. (1978). Estimating the dimension of a model. *Annals of Statistics*, 6:461–464.

Schwender, H. (2012). *siggenes: Multiple testing using SAM and Efron's empirical Bayes approaches*. R package version 1.32.0.
Scrucca, L. (2010). Dimension reduction for model-based clustering. *Statistics & Computing, 20*(4):471–484.

Steane, M. A., McNicholas, P. D., and Yada, R. (2012). Model-based classification via mixtures of multivariate t-factor analyzers. *Communications in Statistics – Simulation and Computation, 41*(4):510–523.

Sundberg, R. (1974). Maximum likelihood theory for incomplete data from an exponential family. *Scandinavian Journal of Statistics, 1*:49–58.

Todorov, V. and Filzmoser, P. (2009). An object-oriented framework for robust multivariate analysis. *Journal of Statistical Software, 32*(3):1–47.

Tusher, V., Tibshirani, R., and Chu, G. (2001). Significance analysis of microarrays applied to the ionizing radiation response. *Proceedings of the National Academy of Sciences, 98*(9):5116–5121.

Vrbik, I. and McNicholas, P. D. (2012). Analytic calculations for the EM algorithm for multivariate skew-mixture models. *Statistics and Probability Letters, 82*(6):1169–1174.

Vrbik, I. and McNicholas, P. D. (2013). Fractionally-supervised classification. arXiv:1307.3598v2.

Wolfe, J. H. (1963). Object cluster analysis of social areas. Master’s thesis, University of California, Berkeley.
A Selected genes for the colon data.

Table 20: Genes selected with SAM for the colon data.

| Gene ID | Description |
|---------|-------------|
| Hsa.462 | Human serine kinase mRNA |
| Hsa.549 | Transcription factor IIIA |
| Hsa.601 | Human aspartyl-tRNA synthetase alpha-2 subunit mRNA |
| Hsa.627 | Human monocyte-derived neutrophil-activating protein (MONAP) mRNA |
| Hsa.773 | Macrophage migration inhibitory factor (Human) |
| Hsa.821 | Human hmgI mRNA for high mobility group protein Y |
| Hsa.831 | Mitochondrial matrix protein P1 precursor (Human) |
| Hsa.957 | Human nucleolar protein (B23) mRNA |
| Hsa.1832 | Myosin regulatory light chain 2, smooth muscle isoform (Human) |
| Hsa.2097 | Human vasoactive intestinal peptide (VIP) mRNA |
| Hsa.2645 | H.sapiens ckshs2 mRNA for Cks1 protein homologue |
| Hsa.2928 | H.sapiens mRNA for p cadherin |
| Hsa.3016 | S-100P protein (Human) |
| Hsa.3306 | Human gene for heterogeneous nuclear ribonucleoprotein (hnRNP) core protein A1 |
| Hsa.3331 | Nucleoside diphosphate kinase A (Human) |
| Hsa.5971 | Human splicing factor SRp30c mRNA |
| Hsa.6472 | Tubulin beta chain (Haliotis discus) |
| Hsa.6814 | Collagen alpha 2(XI) chain (Homo sapiens) |
| Hsa.8125 | Human |
| Hsa.8147 | Human desmin gene |
| Hsa.36689 | H.sapiens mRNA for GCAP-II/uroguanylin precursor |
| Hsa.36952 | Complement factor D precursor (Homo sapiens) |
| Hsa.37937 | Myosyn heavy chain, nonmuscle (Gallus gallus) |