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High-Dimensional Data Clustering

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Abstract

Clustering in high-dimensional spaces is a difficult problem which is recurrent in many domains, for example in image analysis. The difficulty is due to the fact that high-dimensional data usually live in different low-dimensional subspaces hidden in the original space. This paper presents a family of Gaussian mixture models designed for high-dimensional data which combine the ideas of subspace clustering and parsimonious modeling. These models give rise to a clustering method based on the Expectation-Maximization algorithm which is called High-Dimensional Data Clustering (HDDC). In order to correctly fit the data, HDDC estimates the specific subspace and the intrinsic dimension of each group. Our experiments on artificial and real datasets show that HDDC outperforms existing methods for clustering high-dimensional data.

Key words: Model-based clustering, subspace clustering, high-dimensional data, Gaussian mixture models, parsimonious models.

1 Introduction

Clustering in high-dimensional spaces is a recurrent problem in many fields of science, for example in image analysis. Indeed, the data used in image analysis are often high-dimensional and this penalizes clustering methods. In this paper, we focus on model based approaches, see [10] for a review on this topic. Popular clustering methods are based on the Gaussian Mixture Model (GMM) [32] and show a disappointing behavior when the size of the dataset is too small compared to the number of parameters to estimate. This well-known phenomenon is called

curse of dimensionality and was introduced by Bellman [3]. We refer to [35, 36] for a theoretical study of the effect of dimension in the supervised framework.

To avoid over fitting, it is necessary to find a balance between the number of parameters to estimate and the generality of the model. We propose a Gaussian mixture model which takes into account the specific subspace around which each cluster is located and therefore limits the number of parameters to estimate. The Expectation-Maximization (EM) algorithm [16] is used for parameter estimation and the intrinsic dimension of each group is determined automatically thanks to the BIC criterion and the scree-test of Cattell. This allows to derive a robust clustering method in high-dimensional spaces, called High Dimensional Data Clustering (HDDC). In order to further limit the number of parameters, it is possible to make additional assumptions on the model. For example, it can be assumed that classes are spherical in their subspaces or fix some parameters to be common between classes. The nature of the proposed parametrization allows HDDC to be robust with respect to the ill-conditioning or the singularity of empirical covariance matrices and to be efficient in terms of computing time. Finally, HDDC is evaluated and compared to standard clustering methods on artificial and real datasets.

This paper is organized as follows. Section 2 presents the state of the art on clustering of high-dimensional data. Section 3 introduces our parameterization of the Gaussian mixture model. Section 4 presents the clustering method HDDC, *i.e.* the estimation of the parameters of the models and of the hyper-parameters. Experimental results on simulated and real datasets are reported in Section 5.

2 Related work on high-dimensional clustering

Standard methods to overcome the *curse of dimensionality* consist in reducing the dimension of the data and/or to use a parsimonious Gaussian mixture model. More recently, methods which find clusters in different subspaces have been proposed. In this section, a brief survey of these works in clustering of high-dimensional data is presented.

2.1 Dimension reduction

Many methods use global dimension reduction techniques to overcome problems due to high dimensionality. A widely used solution is to reduce the dimension of data before using a classical clustering method. Dimension reduction techniques can be divided into techniques for *feature extraction* and *feature selection*. Feature extraction techniques build new variables carrying a large part of the global information. Among these techniques, the most popular one is Principal Component Analysis (PCA) [27] which is often used in data mining and image analysis. However, PCA is a linear technique, *i.e.* it only takes into account linear dependences between variables. Recently, many non-linear techniques have been proposed such as Kernel PCA [40], non-linear PCA [23, 25] and neural networks based techniques [15, 28, 39, 44]. In [41], the dimension reduction problem was considered in the Quadratic Discriminant Analysis framework. In contrast, feature selection techniques find an appropriate subset of the original variables to represent the data. A survey on feature selection can be found in [24]. A recent approach [38] proposes to combine global feature selection and model-based clustering. These global dimension reduction techniques are often advantageous in terms of performance, but suffer from the drawback of losing information which could be discriminant. Indeed, the clusters are usually hidden in different subspaces of the original feature space and a global approach cannot capture this.

2.2 Parsimonious models

Another solution is to use models which require the estimation of fewer parameters. For example, the eigenvalue decomposition of the covariance matrices [2, 13] allows to re-parameterize the covariance matrix of the classes in their eigenspaces. By fixing some parameters to be common between classes, this parameterization yields parsimonious models which generate clustering methods based on the EM algorithm. A review on parsimonious models can be found in [22]. These approaches are based on various Gaussian models from the most complex one (a full covariance matrix for each group) to the simplest one (a spherical covariance matrix for all groups) which yields a method similar to the k-means approach. However, these methods cannot efficiently solve the problem of the high-dimensionality when clusters live in low-dimensional subspaces.

2.3 Subspace clustering

Subspace clustering methods involve two kinds of approaches. On the one hand, projection pursuit clustering assumes that the class centers are located on a same unknown subspace [9, 14]. On the other hand, principal component clustering assumes that each class is located on a unknown specific subspace, see [8], Chapter 17, and [4] for an extension to fuzzy subspaces. For instance, the *Analyse factorielle typologique* [18] is based on an iterative algorithm similar to the k-means approach. Some subspace clustering methods use heuristic search techniques to find the subspaces, see for instance [1]. A review on this type of methods can be found in [34]. Most of them rely on geometric considerations and are not model-based. Regression clustering methods (sometimes called switching regression methods) offer an alternative based on probabilistic models. Some examples are [17, 37] while the original idea is due to [7]. However, it has been observed that discarding some dimensions may yield instabilities in presence of outliers or on small datasets. For this reason, the method proposed in this paper does not assume that there exist irrelevant dimensions and therefore does not discard any dimensions, but it models the smallest variances by a single parameter. Methods based on mixtures of factor analyzers [33, 45] rely on a latent variables model and on an EM based procedure to cluster high-dimensional data. More recently, Bocci *et al.* [6] proposed a similar approach to cluster dissimilarity data. The model of these methods is a mixture of Gaussian densities where the number of parameters is controlled through the dimension of the latent factor space. The advantage of such a model is to capture correlations without estimating full covariance matrices and without dimension truncation. In this paper, we propose an unified approach for subspace clustering in the Gaussian mixture model framework which encompasses these approaches and involves additional regularizations as in parsimonious models. A precise comparison between our approach and the mixtures of factor analyzers is achieved in paragraph 3.2.

3 A Gaussian model for high-dimensional data

Clustering divides a given dataset $\{x_1, \dots, x_n\}$ of n data points in \mathbb{R}^p into k homogeneous groups (see [26] for a review). A popular clustering technique uses

Gaussian mixture models, which assume that each class is represented by a Gaussian probability density. Data are therefore modeled by a density:

$$f(x, \theta) = \sum_{i=1}^k \pi_i \phi(x, \theta_i), \quad (1)$$

where ϕ is a p -variate normal density with parameter $\theta_i = \{\mu_i, \Sigma_i\}$ and π_i are the mixing proportions. This model requires to estimate full covariance matrices and therefore the number of parameters increases with the square of the dimension. However, due to the *empty space* phenomenon [43] it can be assumed that high-dimensional data live around subspaces with a dimension lower than the one of the original space. We therefore introduce low-dimensional class-specific subspaces in order to limit the number of parameters to estimate.

3.1 The Gaussian model $[a_{ij} b_i Q_i d_i]$

As in the classical Gaussian mixture model framework, we assume that class conditional densities are Gaussian $\mathcal{N}_p(\mu_i, \Sigma_i)$ with means μ_i and covariance matrices Σ_i , for $i = 1, \dots, k$. Let Q_i be the orthogonal matrix with the eigenvectors of Σ_i as columns. The class conditional covariance matrix Δ_i is therefore defined in the eigenspace of Σ_i by:

$$\Delta_i = Q_i^t \Sigma_i Q_i. \quad (2)$$

The matrix Δ_i is thus a diagonal matrix which contains the eigenvalues of Σ_i . It is further assumed that Δ_i is divided into two blocks:

$$\Delta_i = \left(\begin{array}{cc|cc} \boxed{\begin{array}{cc} a_{i1} & 0 \\ & \ddots \\ 0 & a_{id_i} \end{array}} & & & \mathbf{0} \\ & & & \\ \hline & & \boxed{\begin{array}{cc} b_i & 0 \\ & \ddots \\ 0 & b_i \end{array}} & \\ \mathbf{0} & & & \end{array} \right) \left. \begin{array}{l} \left. \vphantom{\Delta_i} \right\} d_i \\ \left. \vphantom{\Delta_i} \right\} (p - d_i) \end{array} \right) \quad (3)$$

with $a_{ij} > b_i$, $j = 1, \dots, d_i$, and where $d_i \in \{1, \dots, p - 1\}$ is unknown. The class specific subspace \mathbb{E}_i is defined as the affine space spanned by the d_i eigenvectors associated to the eigenvalues a_{ij} and such that $\mu_i \in \mathbb{E}_i$. Similarly, the affine

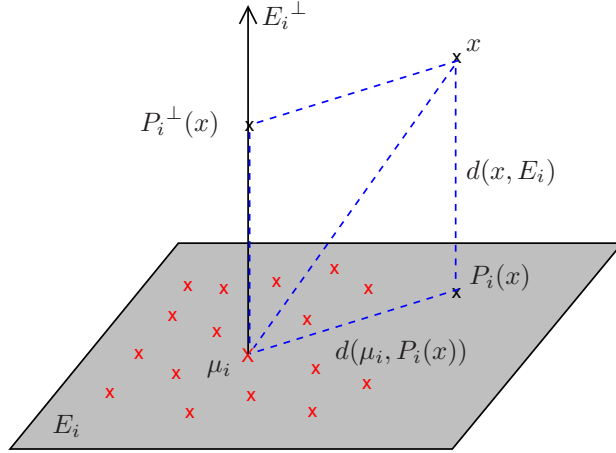


Figure 1: The subspaces \mathbb{E}_i and \mathbb{E}_i^\perp of the i th mixture component.

subspace \mathbb{E}_i^\perp is such that $\mathbb{E}_i \oplus \mathbb{E}_i^\perp = \mathbb{R}^p$ and $\mu_i \in \mathbb{E}_i^\perp$. In this subspace \mathbb{E}_i^\perp , the variance is modeled by the single parameter b_i . Let $P_i(x) = \tilde{Q}_i \tilde{Q}_i^t (x - \mu_i) + \mu_i$ and $P_i^\perp(x) = \bar{Q}_i \bar{Q}_i^t (x - \mu_i) + \mu_i$ be the projection of x on \mathbb{E}_i and \mathbb{E}_i^\perp respectively, where \tilde{Q}_i is made of the d_i first columns of Q_i supplemented by $(p - d_i)$ zero columns and $\bar{Q}_i = (Q_i - \tilde{Q}_i)$. Thus, \mathbb{E}_i is called the specific subspace of the i th group since most of the data live on or near this subspace. In addition, the dimension d_i of the subspace \mathbb{E}_i can be considered as the intrinsic dimension of the i th group, *i.e.* the number of dimensions required to describe the main features of this group. Figure 1 summarizes these notations. Following the notation system of [13], our mixture model is denoted by $[a_{ij} b_i Q_i d_i]$ in the sequel.

3.2 The sub-models of $[a_{ij} b_i Q_i d_i]$

By fixing some parameters to be common within or between classes, we obtain particular models which correspond to different regularizations. In the following, “free Q_i ” means that Q_i is specific for each class C_i and “common Q_i ” means that for each $i = 1, \dots, k$, $Q_i = Q$ and consequently the class orientations are the same. The family $[a_{ij} b_i Q_i d_i]$ is divided into three categories: models with free orientations, common orientations and common covariance matrices.

Models with common orientations It is also possible to assume that the class orientations are common, *i.e.* $Q_i = Q$ for each $i = 1, \dots, k$. However, this assumption does not necessarily imply that the class-specific subspaces are the same. Indeed, if the dimensions d_i are free, the intersection of the k class-specific subspaces is the one of the class with the smallest intrinsic dimension. This assumption can be interesting to model groups with some common properties and with additional specific characteristics. Several models of this category require a complex iterative estimation based on the FG algorithm [20] and therefore they will be not considered here. Consequently, only the models $[a_i b_i Q d]$, $[ab_i Q d]$ and $[a_i b Q d]$ will be considered in this paper since their parameters can be estimated using a simple iterative procedure. Note that a model similar to $[a_{ij} b Q d]$ was considered by Flury *et al.* in [21] in the supervised framework with an additional assumption on the means.

Models with common covariance matrices This branch of the family only includes two models $[a_j b Q d]$ and $[ab Q d]$. Both models indeed assume that the classes have the same covariance matrix $\Sigma = Q \Delta Q^t$. Particularly, fixing $d = (p - 1)$, the model $[a_j b Q d]$ reduces to a Gaussian mixture model (denoted by “Com-GMM” in the following) which yields in the supervised framework the well known Linear Discriminant Analysis (LDA). Remark that if $d < (p - 1)$, the model $[a_j b Q d]$ can be viewed as the a combination of a dimension reduction technique with a GMM with common covariance matrices, but without losing information since the information carried by the smallest eigenvalues is not discarded.

3.3 Characteristics of the models

Our family of models presented above only requires the estimation of d_i -dimensional subspaces and therefore the different models are significantly more parsimonious than the general Gaussian model if $d_i \ll p$. Table 1 summarizes some properties of the models considered here. The second column of this table gives the number of parameters to estimate. The third column provides the asymptotic order of the number of parameters (*i.e.* with the assumption that $k \ll d \ll p$). The fourth column gives the number of parameters for the particular case $k = 4, p = 100$ and $\forall i, d_i = 10$. The last column indicates whether the Maximum Likelihood (ML)

Model	Number of parameters	Asymptotic order	Nb of prms $k = 4, d = 10, p = 100$	ML estimation
$[a_{ij}b_iQ_id_i]$	$\rho + \bar{\tau} + 2k + D$	kpd	4231	CF
$[a_{ij}bQ_id_i]$	$\rho + \bar{\tau} + k + D + 1$	kpd	4228	CF
$[a_ib_iQ_id_i]$	$\rho + \bar{\tau} + 3k$	kpd	4195	CF
$[ab_iQ_id_i]$	$\rho + \bar{\tau} + 2k + 1$	kpd	4192	CF
$[a_ibQ_id_i]$	$\rho + \bar{\tau} + 2k + 1$	kpd	4192	CF
$[abQ_id_i]$	$\rho + \bar{\tau} + k + 2$	kpd	4189	CF
$[a_{ij}b_iQ_id]$	$\rho + k(\tau + d + 1) + 1$	kpd	4228	CF
$[a_jb_iQ_id]$	$\rho + k(\tau + 1) + d + 1$	kpd	4198	CF
$[a_{ij}bQ_id]$	$\rho + k(\tau + d) + 2$	kpd	4225	CF
$[a_jbQ_id]$	$\rho + k\tau + d + 2$	kpd	4195	CF
$[a_ib_iQ_id]$	$\rho + k(\tau + 2) + 1$	kpd	4192	CF
$[ab_iQ_id]$	$\rho + k(\tau + 1) + 2$	kpd	4189	CF
$[a_ibQ_id]$	$\rho + k(\tau + 1) + 2$	kpd	4189	CF
$[abQ_id]$	$\rho + k\tau + 3$	kpd	4186	CF
$[a_{ij}b_iQd_i]$	$\rho + \tau + D + 2k$	pd	1396	FG
$[a_{ij}bQd_i]$	$\rho + \tau + D + k + 1$	pd	1393	FG
$[a_ib_iQd_i]$	$\rho + \tau + 3k$	pd	1360	FG
$[a_ibQd_i]$	$\rho + \tau + 2k + 1$	pd	1357	FG
$[ab_iQd_i]$	$\rho + \tau + 2k + 1$	pd	1357	FG
$[abQd_i]$	$\rho + \tau + k + 2$	pd	1354	FG
$[a_{ij}b_iQd]$	$\rho + \tau + kd + k + 1$	pd	1393	FG
$[a_jb_iQd]$	$\rho + \tau + k + d + 1$	pd	1363	FG
$[a_{ij}bQd]$	$\rho + \tau + kd + 2$	pd	1390	FG
$[a_ib_iQd]$	$\rho + \tau + 2k + 1$	pd	1357	IP
$[ab_iQd]$	$\rho + \tau + k + 2$	pd	1354	IP
$[a_ibQd]$	$\rho + \tau + k + 2$	pd	1354	IP
$[a_jbQd]$	$\rho + \tau + d + 2$	pd	1360	CF
$[abQd]$	$\rho + \tau + 3$	pd	1351	CF
Full-GMM	$\rho + kp(p + 1)/2$	$kp^2/2$	20603	CF
Com-GMM	$\rho + p(p + 1)/2$	$p^2/2$	5453	CF
Diag-GMM	$\rho + kp$	$2kp$	803	CF
Sphe-GMM	$\rho + k$	kp	407	CF

Table 1: Properties of the HDDC models: $\rho = kp + k - 1$ is the number of parameters required for the estimation of means and proportions, $\bar{\tau} = \sum_{i=1}^k d_i [p - (d_i + 1)/2]$ and $\tau = d[p - (d + 1)/2]$ are the number of parameters required for the estimation of \tilde{Q}_i and \tilde{Q} , and $D = \sum_{i=1}^k d_i$. For asymptotic orders, we assume that $k \ll d \ll p$. CF means that the ML estimates are closed form. IP means that the ML estimation needs an iterative procedure. FG means that the ML estimation requires the iterative FG algorithm.

updates are in closed form or not. These characteristics are also given for five Gaussian mixture models: GMM with full covariance matrices for each class (Full-GMM), with common covariance matrices between classes (Com-GMM), with diagonal covariance matrices (Diag-GMM), with spherical covariance matrices (Sphe-GMM). Note that Celeux and Govaert recommend in [13] to make use of the models Diag-GMM and Sphe-GMM in clustering problems. We can observe that all models of our family require the estimation of fewer parameters than both Full-GMM and Com-GMM. In the particular case of 100-dimensional data, made of 4 classes and with common intrinsic dimensions d_i equal to 10, the model $[a_{ij}b_iQ_id_i]$ only requires the estimation of 4 231 parameters whereas Full-GMM and Com-GMM requires respectively the estimation of 20 603 and 5 453 parameters. Remark that the model $[a_{ij}b_iQ_id_i]$, which gives rise to quadratic separation between the groups, requires the estimation of fewer parameters than Com-GMM, which gives rise to linear separation between the groups.

4 High-dimensional data clustering

In this section, we derive the EM-based clustering framework for the model $[a_{ij}b_iQ_id_i]$ and its sub-models. The related clustering method is denoted by High-Dimensional Data Clustering (HDDC). Let us recall that unsupervised classification organizes data in homogeneous groups using only the observed values of the p explanatory variables. Usually, in model-based clustering, the parameters $\theta = \{\pi_1, \dots, \pi_k, \theta_1, \dots, \theta_k\}$ with $\theta_i = \{\mu_i, \Sigma_i\}$ are estimated by the EM algorithm which repeats iteratively E and M steps. The reader could refer to [31] for further informations on the EM algorithm and its extensions. In particular, the models presented in this paper can be also used in the Classification EM and Stochastic EM algorithms [12]. Using our parameterization, the EM algorithm for estimating $\theta = \{\pi_i, \mu_i, \Sigma_i, a_{ij}, b_i, Q_i, d_i\}$ is detailed in the following.

4.1 The E step

This step computes, at iteration q and for each $i = 1, \dots, k$ and $j = 1, \dots, n$, the conditional probability $t_{ij}^{(q)} = \mathbb{P}(x_j \in C_i^{(q-1)} | x_j)$ which can be written from (1)

and using the Bayes formula as follows:

$$t_{ij}^{(q)} = \pi_i^{(q-1)} \phi(x_j, \theta_i^{(q-1)}) \bigg/ \sum_{\ell=1}^k \pi_\ell^{(q-1)} \phi(x_j, \theta_\ell^{(q-1)}).$$

Note that this conditional probability is mainly based on $\pi_i^{(q-1)} \phi(x_j, \theta_i^{(q-1)})$. and thus can be rewritten using the parameters of the model $[a_{ij} b_i Q_i d_i]$. In order not to overload the equations, the index of the current iteration q is omitted in the remainder of this paragraph. Writing $\phi(x, \theta_i)$ with the new class conditional covariance matrix Δ_i , we obtain:

$$-2 \log(\phi(x, \theta_i)) = (x - \mu_i)^t (Q_i \Delta_i Q_i^t)^{-1} (x - \mu_i) + \log(\det \Delta_i) + p \log(2\pi).$$

Since $Q_i^t Q_i = I_p$ and $Q_i = \tilde{Q}_i + \bar{Q}_i$, the above matrix inverse can be expanded as $(Q_i \Delta_i Q_i^t)^{-1} = \tilde{Q}_i \Delta_i^{-1} \tilde{Q}_i^t + \bar{Q}_i \Delta_i^{-1} \bar{Q}_i^t$ and thus:

$$\begin{aligned} -2 \log(\phi(x, \theta_i)) &= (x - \mu_i)^t \tilde{Q}_i \Delta_i^{-1} \tilde{Q}_i^t (x - \mu_i) + (x - \mu_i)^t \bar{Q}_i \Delta_i^{-1} \bar{Q}_i^t (x - \mu_i) \\ &\quad + \log(\det \Delta_i) + p \log(2\pi). \end{aligned}$$

Taking into account the structure of Δ_i and using the relations $\tilde{Q}_i (\tilde{Q}_i^t \tilde{Q}_i) = \tilde{Q}_i$ and $\bar{Q}_i (\bar{Q}_i^t \bar{Q}_i) = \bar{Q}_i$, it yields:

$$-2 \log(\phi(x, \theta_i)) = \|\tilde{Q}_i \tilde{Q}_i^t (x - \mu_i)\|_{\mathcal{A}_i}^2 + \frac{1}{b_i} \|\bar{Q}_i \bar{Q}_i^t (x - \mu_i)\|^2 + \log(\det \Delta_i) + p \log(2\pi),$$

where $\|\cdot\|_{\mathcal{A}_i}^2$ is the norm on \mathbb{E}_i such as $\|x\|_{\mathcal{A}_i}^2 = x^t \mathcal{A}_i x$ with $\mathcal{A}_i = \tilde{Q}_i \Delta_i^{-1} \tilde{Q}_i^t$. From the definitions of P_i and P_i^\perp (Paragraph 3.1) and in view of Figure 1, we have:

$$-2 \log(\phi(x, \theta_i)) = \|\mu_i - P_i(x)\|_{\mathcal{A}_i}^2 + \frac{1}{b_i} \|x - P_i(x)\|^2 + \log(\det \Delta_i) + p \log(2\pi).$$

The relation $\log(\det \Delta_i) = \sum_{j=1}^{d_i} \log(a_{ij}) + (p - d_i) \log(b_i)$ allows to conclude that:

$$t_{ij} = 1 \bigg/ \sum_{\ell=1}^k \exp \left(\frac{1}{2} (K_i(x_j) - K_\ell(x_j)) \right),$$

where $K_i(x) = -2 \log(\pi_i \phi(x, \theta_i))$ is called the cost function and is defined by:

$$K_i(x) = \|\mu_i - P_i(x)\|_{\mathcal{A}_i}^2 + \frac{1}{b_i} \|x - P_i(x)\|^2 + \sum_{j=1}^{d_i} \log(a_{ij}) + (p - d_i) \log(b_i) - 2 \log(\pi_i).$$

Let us note that $K_i(x)$ is mainly based on two distances: the distance between the projection of x on \mathbb{E}_i and the mean of the class and the distance between the observation and the subspace \mathbb{E}_i . This cost function favors the assignment of a new observation to the class for which it is close to the subspace and for which its projection on the class subspace is close to the mean of the class. The variance terms a_{ij} and b_i balance the importance of both distances. For example, if the data are very noisy, *i.e.* b_i is large, it is natural to balance the distance $\|x - P_i(x)\|^2$ by $1/b_i$ in order to take into account the large variance in \mathbb{E}_i^\perp .

4.2 The M step

This step maximizes at iteration q the conditional likelihood and uses the following update formulas. Mixture proportions and means are estimated by:

$$\hat{\pi}_i^{(q)} = \frac{n_i^{(q)}}{n}, \quad \hat{\mu}_i^{(q)} = \frac{1}{n_i^{(q)}} \sum_{j=1}^n t_{ij}^{(q)} x_j,$$

where $n_i^{(q)} = \sum_{j=1}^n t_{ij}^{(q)}$. Moreover, the update formula for the empirical covariance matrix of the fuzzy class C_i is:

$$W_i^{(q)} = \frac{1}{n_i^{(q)}} \sum_{j=1}^n t_{ij}^{(q)} (x_j - \hat{\mu}_i^{(q)})(x_j - \hat{\mu}_i^{(q)})^t.$$

The estimation of the specific parameters of HDDC is detailed below. Proofs of the following results are given in the Appendix.

Models with free orientations The ML estimators of model parameters are closed form for this category of models.

– Subspace \mathbb{E}_i : the d_i first columns of Q_i are estimated by the eigenvectors associated with the d_i largest eigenvalues λ_{ij} of W_i .

– Model $[a_{ij}b_iQ_id_i]$: the estimator of a_{ij} is $\hat{a}_{ij} = \lambda_{ij}$ and the estimator of b_i is the mean of the $(p - d_i)$ smallest eigenvalues of W_i and can be written as follows:

$$\hat{b}_i = \frac{1}{(p - d_i)} \left(\text{Tr}(W_i) - \sum_{j=1}^{d_i} \lambda_{ij} \right). \quad (4)$$

– Model $[a_{ij}bQ_id_i]$: the estimator of a_{ij} is $\hat{a}_{ij} = \lambda_{ij}$ and the estimator of b is:

$$\hat{b} = \frac{1}{(p - \xi)} \left(\text{Tr}(W) - \sum_{i=1}^k \hat{\pi}_i \sum_{j=1}^{d_i} \lambda_{ij} \right), \quad (5)$$

where $\xi = \sum_{i=1}^k \hat{\pi}_i d_i$ and $W = \sum_{i=1}^k \hat{\pi}_i W_i$ is the within-covariance matrix.

– Model $[a_i b_i Q_i d_i]$: the estimator of b_i is given by (4) and the estimator of a_i is:

$$\hat{a}_i = \frac{1}{d_i} \sum_{j=1}^{d_i} \lambda_{ij}. \quad (6)$$

– Model $[a b_i Q_i d_i]$: the estimator of b_i is given by (4) and the estimator of a is:

$$\hat{a} = \frac{1}{\xi} \sum_{i=1}^k \hat{\pi}_i \sum_{j=1}^{d_i} \lambda_{ij}. \quad (7)$$

– Model $[a_i b Q_i d_i]$: estimators of a_i and b are respectively given by (6) and (5).

– Model $[a b Q_i d_i]$: estimators of a and b are respectively given by (7) and (5).

– Models with common dimensions: the estimators of the models with common dimensions d_i can be obtained from the previous ones by replacing the values d_i by d for each $i = 1, \dots, k$. In this case, equations (5) and (7) can be simplified as:

$$\hat{a} = \frac{1}{d} \sum_{j=1}^d \lambda_j, \quad (8)$$

$$\hat{b} = \frac{1}{(p - d)} \left(\text{Tr}(W) - \sum_{j=1}^d \lambda_j \right), \quad (9)$$

where λ_j is the j th largest eigenvalue of W .

– Model $[a_j b_i Q_i d]$: the estimator of a_j is $\hat{a}_j = \lambda_j$ and the estimator of b_i is (4).

– Model $[a_j b Q_i d]$: the estimator of a_j is $\hat{a}_j = \lambda_j$ and the estimator of b is (9).

Models with common orientations Here, we assume in addition that the dimensions d_i are common between classes. The following ML estimators require an iterative procedure.

– Subspace \mathbb{E}_i : Given a_i and b_i , the d first columns of Q are estimated by the eigenvectors associated to the d largest eigenvalues of the matrix M defined by:

$$M(a_1, \dots, a_k, b_1, \dots, b_k) = \sum_{i=1}^k n_i \left(\frac{1}{b_i} - \frac{1}{a_i} \right) W_i.$$

– Model $[a_i b_i Q d]$: given Q , estimators of a_i and b_i are:

$$\hat{a}_i(Q) = \frac{1}{d} \sum_{j=1}^d q_j^t W_i q_j, \quad (10)$$

$$\hat{b}_i(Q) = \frac{1}{(p-d)} \left(\text{Tr}(W_i) - \sum_{j=1}^d q_j^t W_i q_j \right). \quad (11)$$

– Model $[a_i b Q_i d_i]$: given Q , the estimator of a_i is (10) and the estimator of b is:

$$\hat{b}(Q) = \frac{1}{(p-d)} \left(\text{Tr}(W) - \sum_{j=1}^d q_j^t W q_j \right). \quad (12)$$

– Model $[a b_i Q d]$: given Q , the estimator of b_i is (11) and the estimator of a is:

$$\hat{a}(Q) = \frac{1}{d} \sum_{j=1}^d q_j^t W q_j. \quad (13)$$

– Model $[a_i b Q d]$: given Q , estimators of a_i and b are respectively (10) and (12).

For example, it is possible to use the following iterative procedure to estimate the parameters associated to the model $[a_i b_i Q d]$:

– Initialization: the d first columns of $Q^{(0)}$ are the eigenvectors associated with the d largest eigenvalues of W .

– Until convergence: $a_i^{(\ell)} = \hat{a}_i(Q^{(\ell-1)})$, $b_i^{(\ell)} = \hat{b}_i(Q^{(\ell-1)})$ and the d first columns of $Q^{(\ell)}$ are the eigenvectors associated to the d largest eigenvalues of the matrix

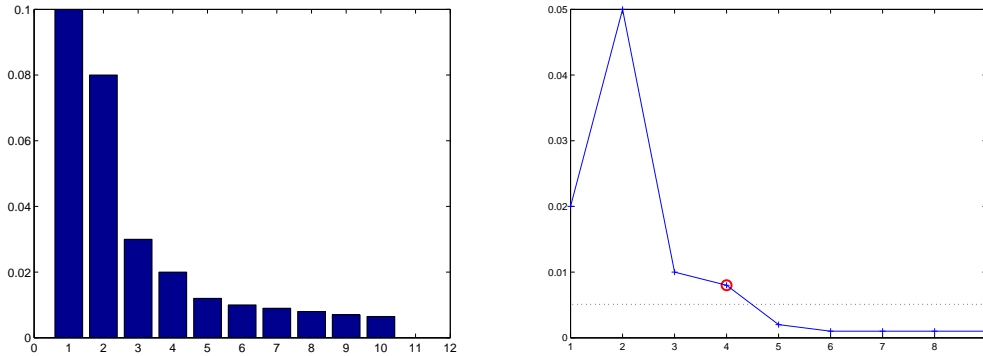


Figure 2: Estimation of the intrinsic dimension d_i using the scree-test of Cattell: plot of ordered eigenvalues of Σ_i (left) and differences between consecutive eigenvalues (right).

$$M(a_1^{(\ell)}, \dots, a_k^{(\ell)}, b_1^{(\ell)}, \dots, b_k^{(\ell)}).$$

Models with common covariance matrices In this category of models, the parameters can be updated in closed form.

– Subspace \mathbb{E}_i : the d first columns of the matrix Q are the eigenvectors associated to the d largest eigenvalues of W .

– Model $[a_j b Q d]$: the estimator of a_j is $\hat{a}_j = \lambda_j$ and the estimator of b is (9).

– Model $[ab Q d]$: estimators of a and b are respectively given by (8) and (9).

4.3 Hyper-parameters estimation

Within the M step, the intrinsic dimensions of each subclass have to be estimated. This is a difficult problem with no unique technique to use. Our approach is based on the eigenvalues of the class conditional covariance matrix Σ_i of the class C_i . The j th eigenvalue of Σ_i corresponds to the fraction of the full variance carried by the j th eigenvector of Σ_i . The class specific dimension d_i , $i = 1, \dots, k$ is estimated through the scree-test of Cattell [11] which looks for a break in the eigenvalues scree. The selected dimension is the one for which the subsequent eigenvalues differences are smaller than a threshold. Figure 2 illustrates this method: the graph on the right shows that the differences between eigenvalues after the fourth one are smaller than the threshold (dashed line). Thus, in this case, four dimensions

will be chosen and this corresponds indeed to a break in the scree (left graph). In our experiments, the threshold is chosen using the probabilistic criterion BIC [42] which consists in minimizing $\text{BIC}(m) = -2 \log(L) + \nu(m) \log(n)$, where $\nu(m)$ is the number of parameters of the model m given in Table 1 for HDDC, L is the likelihood and n is the number of observations. In addition, this approach allows to estimate k parameters by choosing only the value of the threshold t . In the case of common intrinsic dimensions between the groups, the dimension d is directly determined using BIC. The second hyper-parameter to estimate in any clustering method is the number of groups k . This parameter is also selected thanks to the BIC criterion, see the experiments presented in Section 5.

4.4 Numerical considerations

First, it is important to remark that the parametrization of the Gaussian model proposed here provides an explicit expression of Σ_i^{-1} whereas other classical methods, like Full-GMM and Com-GMM, need to numerically invert empirical covariance matrices which usually fails for singularity reasons. Some solutions however exist to overcome this problem for the models Full-GMM and Com-GMM, see for instance [29]. In contrast, this problem does not arise with HDDC since the cost function K_i does not require to invert Σ_i . Moreover, it appears in (4.1) that the cost function K_i does not use the projection on the subspace \mathbb{E}_i^\perp and consequently does not require the computation of the $(p - d_i)$ latest columns of the orientation matrix Q_i . In Section 4.2, it is shown that the ML estimators of these columns are the eigenvectors associated to the $(p - d_i)$ smallest eigenvalues of the empirical covariance matrix W_i . Therefore, HDDC does not depend on these eigenvectors whose determination is numerically unstable. Thus, HDDC is robust with respect to ill-conditioning and singularity problems. In addition, it is also possible to use this feature to reduce computing time by using the Arnoldi method [30] which only provides the largest eigenvalues and the associated eigenvectors of an ill-conditioned matrix. During our experiments, we noticed a reduction by a factor 60 of the computing time on a 1024-dimensional dataset compared to the classical approach. Furthermore, in the special case where the number of observations of a group n_i is smaller than the dimension p , our parametrization allows to use a linear algebra trick. Indeed, in this case, it is better from a nu-

Simulated data model	HDDC model					
	$[a_{ij}b_iQ_id_i]$	$[a_{ij}bQ_id_i]$	$[a_ib_iQ_id_i]$	$[a_ibQ_id_i]$	$[ab_iQ_id_i]$	$[abQ_id_i]$
$[a_{ij}b_iQ_id_i]$	357	373	349	359	349	360
$[a_{ij}bQ_id_i]$	403	404	397	396	397	397
$[a_ib_iQ_id_i]$	389	419	377	391	377	394
$[a_ibQ_id_i]$	438	440	419	419	420	420
$[ab_iQ_id_i]$	399	433	380	402	384	403
$[abQ_id_i]$	456	451	428	427	434	433

Table 2: BIC value for the HDDC models on different simulated datasets (the best ones are in bold).

merical point of view to compute the eigenvectors of the $n_i \times n_i$ matrix $\Upsilon_i \Upsilon_i^t$ than those of the $p \times p$ matrix $\Upsilon_i^t \Upsilon_i$, where Υ_i is the $n_i \times p$ matrix containing the mean-centered observations. In the case of data containing 13 observations in a 1024-dimensional space, it has been noticed a reduction by a factor 500 of the computing time compared to the classical approach.

5 Experimental results

In this section, we present results for artificial and real datasets illustrating the main features of HDDC. In the following experiments, HDDC will be compared to 3 classical Gaussian mixture models: GMM with full covariance matrices for each class (Full-GMM), with diagonal covariance matrices (Diag-GMM), with spherical covariance matrices (Sphe-GMM). A numerical regularization was necessary to invert the covariance matrices in the clustering method associated to the model Full-GMM, so that it is able to work with data of dimension larger than 50.

5.1 Simulation study: model selection

Given that HDDC is a model-based clustering method, the well-known criterion BIC can be used for selecting the best adapted model to the data. Here, we used BIC and the cluster recognition rate to compare the different models of HDDC. The cluster recognition rate can be computed since true partitions are known and is defined as the maximum rate over the correct matchings between the true

Simulated data model	HDDC model					
	$[a_{ij}b_iQ_id_i]$	$[a_{ij}bQ_id_i]$	$[a_ib_iQ_id_i]$	$[a_ibQ_id_i]$	$[ab_iQ_id_i]$	$[abQ_id_i]$
$[a_{ij}b_iQ_id_i]$	0.967	0.828	0.973	0.919	0.975	0.903
$[a_{ij}bQ_id_i]$	0.730	0.727	0.779	0.782	0.758	0.751
$[a_ib_iQ_id_i]$	0.979	0.871	0.983	0.929	0.986	0.917
$[a_ibQ_id_i]$	0.826	0.800	0.882	0.863	0.875	0.865
$[ab_iQ_id_i]$	0.965	0.825	0.980	0.844	0.952	0.822
$[abQ_id_i]$	0.712	0.752	0.797	0.793	0.711	0.707

Table 3: Cluster recognition rate for the HDDC models on different simulated datasets (the best ones are in bold).

groups and the found clusters. It is impossible to report in this section numerical experiments for all the discussed models. Therefore, we limit ourselves to models with free orientations since we believe that these models are able to tackle different situations. We performed extensive simulations (50 replications for each of the 6 data models) and then used the 6 different models with free orientations in HDDC to cluster the simulated data. For each dataset, 3 Gaussian densities are simulated in \mathbb{R}^{100} according to one of the 6 models with free orientations, *i.e.* free matrices Q_i , and with the following parameters: $\{d_1, d_2, d_3\} = \{2, 5, 10\}$, $\{\pi_1, \pi_2, \pi_3\} = \{0.4, 0.3, 0.3\}$ and close means and random matrices Q_i . Each one of the 6 datasets was made of 1000 points. Tables 2 and 3 present respectively the BIC value and the cluster recognition rate on average for the 6 considered HDDC models on the different simulated datasets. First of all, it appears that BIC and the cluster recognition rate select in general the same models and this confirm that BIC is a useful tool in model-based clustering. Unsurprisingly, the models used to simulate the data obtain small BIC values and satisfying cluster recognition rates. However, it appears that the model $[a_ib_iQ_id_i]$ is usually selected by BIC as the best model and its cluster recognition rates are very good for each type of simulated data. Thus, the model $[a_ib_iQ_id_i]$ seems to have the right number of degrees of freedom and the assumption that Δ_i has only 2 different eigenvalues is an efficient way to regularize the estimation. Note that models $[a_ibQ_id_i]$ and $[ab_iQ_id_i]$ are also often selected by BIC and provide good cluster recognition rates.

Nb of groups k	Dimensions d_i	BIC value
2	2,16	414
3	2,5,10	407
4	2,2,5,10	414
5	2,5,5,10,12	416
6	2,5,6,10,10,12	424

Table 4: Selection of the number of groups using BIC with the model $[a_i b_i Q_i d_i]$ of HDDC: data are made of 3 groups with intrinsic dimensions $d_i = \{2, 5, 10\}$.

5.2 Simulation study: hyper-parameters selection

Here, we are interested in the selection of the number of groups and of the intrinsic dimension of the clusters. In this experiment, 3 Gaussian densities are simulated in \mathbb{R}^{100} according to the model $[a_i b_i Q_i d_i]$ with the following parameters: $\{d_1, d_2, d_3\} = \{2, 5, 10\}$, $\{\pi_1, \pi_2, \pi_3\} = \{0.4, 0.3, 0.3\}$, $\{a_1, a_2, a_3\} = \{150, 100, 75\}$, $\{b_1, b_2, b_3\} = \{15, 15, 15\}$, close means and random matrices Q_i . The dataset was made of 1000 points. Table 4 presents the choices of group intrinsic dimensions for the different values of k and the corresponding BIC values. First of all, it appears that the criterion BIC can be successfully used for choosing the number of clusters as in standard Gaussian mixture models. Indeed, the BIC value associated to the model $[a_i b_i Q_i d_i]$ are computed for different values of k , the number of groups, and BIC indicates that the most likely value is $k = 3$ which is correct. In addition, the intrinsic dimensions d_i , estimated by HDDC for $k = 3$, are indeed the ones of the simulated data. It is also interesting to observe the evolution of the estimation of dimensions d_i according to the number of clusters. For instance, if we consider the case of a mixture of 2 Gaussian densities, HDDC seems to correctly fit the first 2-dimensional cluster and create a second cluster made of the two other real groups. In addition, the estimated dimension of this second cluster is approximately the sum of the intrinsic dimensions of the two real groups. Similarly, for $k = 4$, HDDC divides the first real group into two new clusters with intrinsic dimensions equal to 2. As a conclusion, our approach for dimension estimation allows to correctly identify the cluster subspaces.

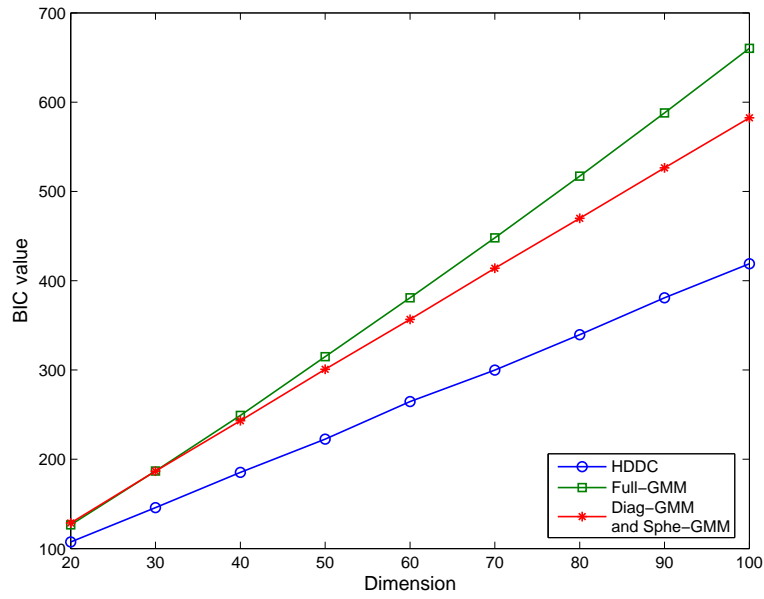


Figure 3: Influence of the dimensionality on the BIC value for different Gaussian mixture models.

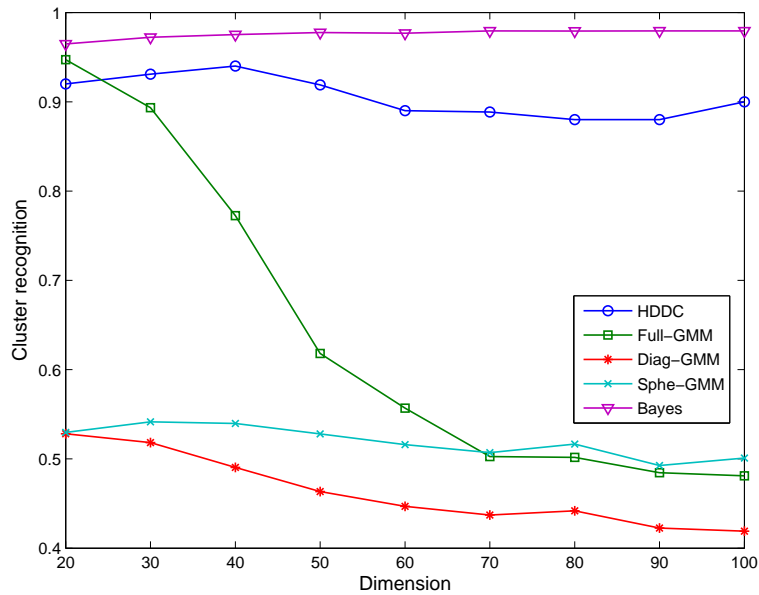


Figure 4: Influence of the dimensionality on cluster recognition rate for different Gaussian mixture models.

5.3 Simulation study: influence of the dimensionality

In this paragraph, we highlight the dimensionality effect on the different clustering methods. Three Gaussian densities are simulated in \mathbb{R}^p , $p = 20, \dots, 100$, according to the model $[a_i b_i Q_i d_i]$ with the same parameters as in the previous experiment. The performance of methods is measured by the average cluster recognition rate computed on 50 replications. The studied clustering methods were initialized using the same random partition. Figures 3 and 4 respectively show the influence of the dimensionality on the BIC value and the cluster recognition rate for different Gaussian mixture models: model $[a_i b_i Q_i d_i]$ of HDDC, Full-GMM, Diag-GMM and Sphe-GMM. It is not surprising to observe on Figure 3 that BIC selects the model $[a_i b_i Q_i d_i]$ as the best model since the data are simulated according to this model. However, it is interesting to remark that, the more the dimension increases, the larger the difference between the BIC values of the different models is, and that in favor of the model $[a_i b_i Q_i d_i]$. Figure 4 shows that data dimension does not influence the performance of HDDC which is very close to the performance of the Bayes decision rule (computed with the true densities). In addition, HDDC provides a cluster recognition rate similar to Full-GMM in low dimensions. Full-GMM is known to be very sensitive to the data dimension and, indeed, gives bad results as soon as the dimension increases. The models Diag-GMM and Sphe-GMM cannot correctly fit the data since they are too parsimonious for this complex dataset. However, one can observe that Sphe-GMM is not sensitive to the data dimension whereas Diag-GMM is. To summarize, HDDC is not sensitive to the dimension and works very well both in low and in high-dimensional spaces. In addition, the model $[a_i b_i Q_i d_i]$ outperforms models requiring a higher number of parameters (Full-GMM) and models requiring a smaller number of parameters (Diag-GMM and Sphe-GMM).

5.4 Simulation study: full rank Gaussian model

In this last simulation study, the capacity of HDDC models to deal with full rank Gaussian data is investigated. Three Gaussian densities in \mathbb{R}^p , $p = 50$, are simulated with full rank covariance matrices, *i.e.* according to the model Full-GMM. The covariance matrices of the groups were different (different orientations and eigenvalues) but with the same condition number fixed to 100. Recall that the

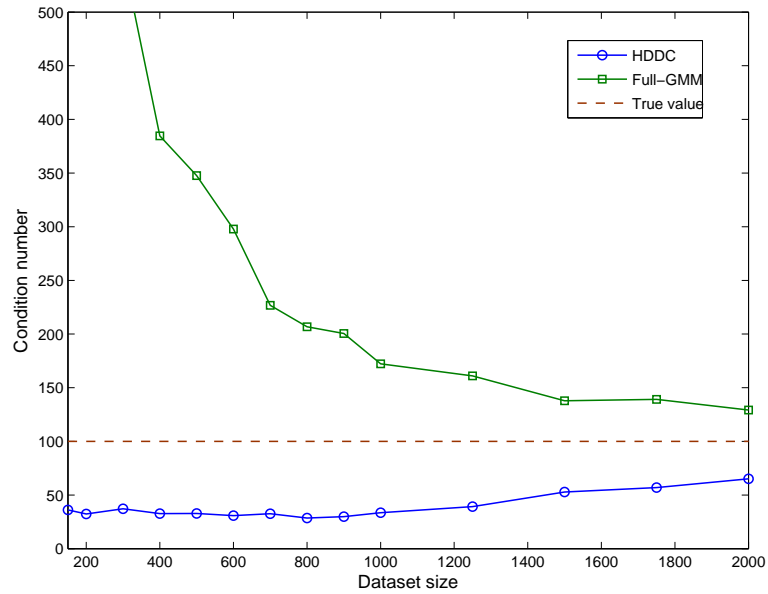


Figure 5: Influence of the dataset size on the condition number for the full rank data.

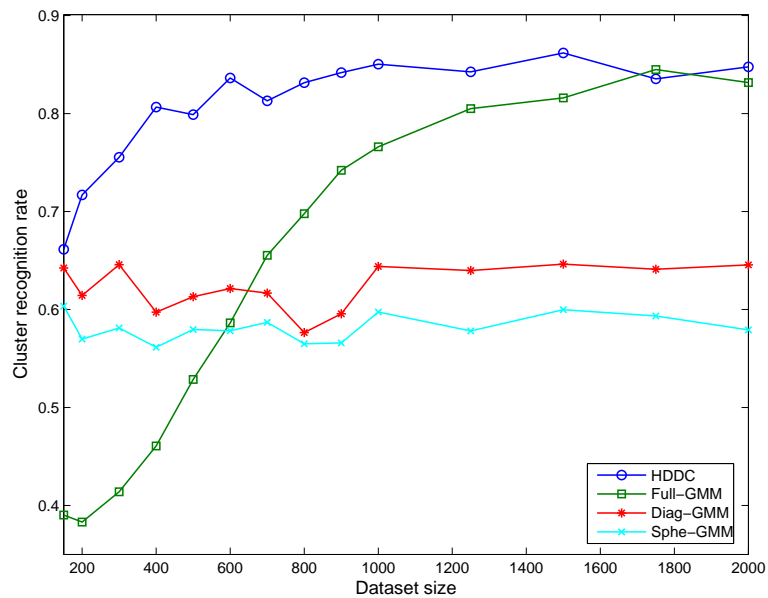


Figure 6: Influence of the dataset size on the cluster recognition rate for the full rank data.

condition number of a matrix is the ratio of its largest and smallest eigenvalues. For this experiment, we used HDDC with the model $[a_{ij}b_iQ_id_i]$ and the clustering methods associated to the classical Gaussian models Full-GMM, Diag-GMM and Sphe-GMM. In order to observe the behavior of the studied clustering methods with respect to the *curse of the dimensionality*, the cluster recognition rate is computed for different dataset sizes n since this phenomenon occurs when the size of the dataset becomes too small compared to the dimension. As an illustration, Figure 5 presents a comparison between the condition number of the estimated covariance matrix associated to the first group used by the Full-GMM method and the ratio \hat{a}_{11}/\hat{b}_1 , which is the corresponding condition number of the covariance matrix estimated by HDDC, for different sizes of the full rank dataset $n = 150, \dots, 2000$. It appears that, for small datasets (*i.e.* n smaller than 1000), the condition number of the empirical covariance matrix (associated to the model Full-GMM) explodes, whereas the condition number associated to the estimated covariance matrix in the model $[a_{ij}b_iQ_id_i]$ remains stable. Figure 6 shows the consequence on the behavior of the studied clustering methods. First, observe that both Diag-GMM and Sphe-GMM models do not obtain satisfying results for any dataset size. This is due to the fact that the assumptions made by those models are wrong for the simulated data and they are thus not able to correctly fit these data. Second, HDDC obtains a similar cluster recognition rate to the model Full-GMM, which is the model used to simulate the data, when the dataset size is large (*i.e.* n larger than 1500). Furthermore, HDDC appears to be more efficient to cluster these data than the model Full-GMM when the dataset size becomes small. Indeed, the cluster recognition rate of HDDC is almost constant for dataset sizes between 1500 and 500. However, when the dataset size is smaller than 500, the HDDC performance decreases to the results obtained by the parsimonious models Diag-GMM and Sphe-GMM. These experiments demonstrate that, even with data which are not favorable to our model, HDDC is more efficient than both complex and parsimonious models on small datasets.

5.5 Real data study: comparison with variable selection

In this experiment, HDDC is compared with the variable selection method for model-based clustering introduced in [38], and denoted by VS-GMM in the follow-

Model	Variables	Cluster recognition rate
Sphe-GMM	Original	0.605
VS-GMM	Original	0.925
Sphe-GMM	Princ. comp.	0.605
VS-GMM	Princ. comp.	0.935
HDDC $[a_i b_i Q_i d_i]$	Original	0.950

Table 5: Classification results for the Crabs data: comparison of different model-based clustering methods.

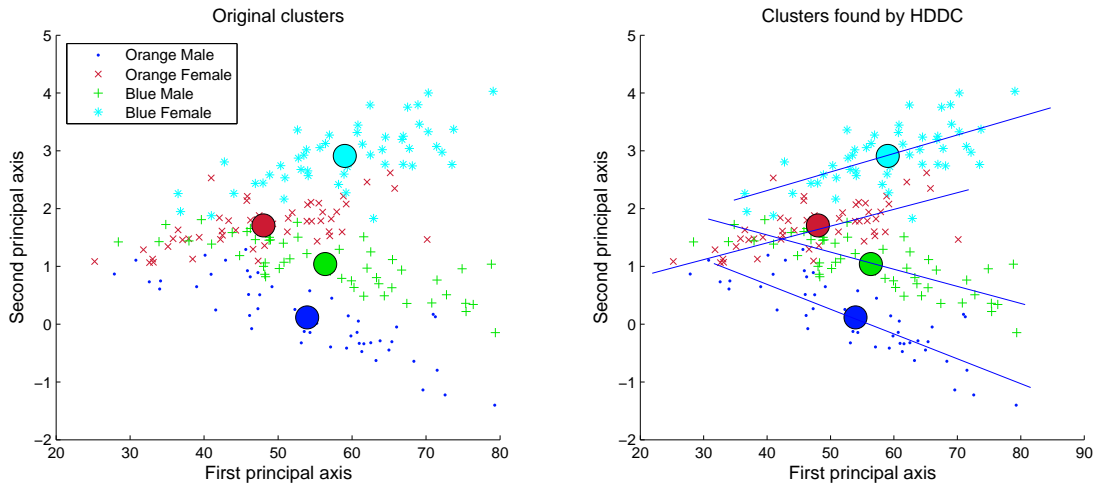


Figure 7: Clustering results using HDDC: on the left panel, crabs data projected on the two first principal axes and, on the right panel, clustering result obtained with the model $[a_i b_i Q_i d_i]$ of HDDC and the estimated specific subspaces of the mixture components (blue lines).

ing. The authors considered the variable selection problem as a model selection problem. Selection is made using approximate Bayes factors and combined with a greedy search algorithm. In addition, it is possible to perform this variable selection on the original variables, but also on the principal components using PCA as a pre-processing step. In order to compare HDDC to this variable selection technique, we used the same dataset as in [38]. The *Leptograpsus* crabs dataset consists of 200 subjects equally distributed into 4 classes: Orange Male, Orange Female, Blue Male and Blue Female. There are 5 variables for each subject: width of frontal lip (FL), rear width (RW), length along the mid-line of the carapace (CL), maximum of the width of the carapace (CW) and body depth (BD) in mm. The left panel of Figure 7 shows the Crabs data projected on the two first principal axes and the big circles represent the cluster means.

Table 5 gives the classification error rate for the classical model Sphe-GMM, the VS-GMM method and HDDC. The second column of this table indicates on which variables is performed the clustering. HDDC obtains a cluster recognition rate equal to 95% and the variable selection method of Raftery *et al.* obtains 93.5% whereas the classical model Sphe-GMM obtains a cluster recognition rate equal to 60.5%. HDDC found that each cluster lives in a 1-dimensional subspace embedded into the original 5-dimensional space. The right panel of Figure 7 shows the specific subspaces (blue lines) of the 4 mixture components obtained with the model $[a_i b_i Q_i d_i]$ of HDDC. For this illustration, the data is projected on the two first principal components since results obtained with VS-GMM on these variables are better than on the original ones. It can be observed that the specific axes of the different clusters are very correlated and this explains that HDDC provides a better clustering result than the variable selection method VS-GMM.

5.6 Real data study: Martian surface characterization

Here, we propose to use HDDC to analyze and segment images of the Martian surface. Visible and near infrared imaging spectroscopy is a key remote sensing technique to study and monitor the system of the planets. Imaging spectrometers, which are inboard of an increasing number of satellites, provide high-dimensional hyper-spectral images. In March 2004, the OMEGA instrument (Mars Express, ESA) [5] has collected 310 Gbytes of raw images. The OMEGA imaging spec-

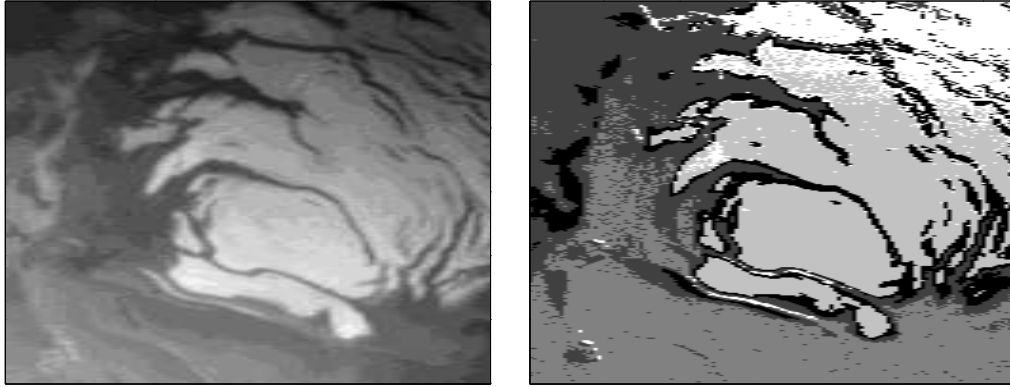


Figure 8: Characterization of the Martian surface composition using HDDC: on the left, image of the studied zone and, on the right, segmentation using HDDC on the 256-dimensional spectral data associated to the image.

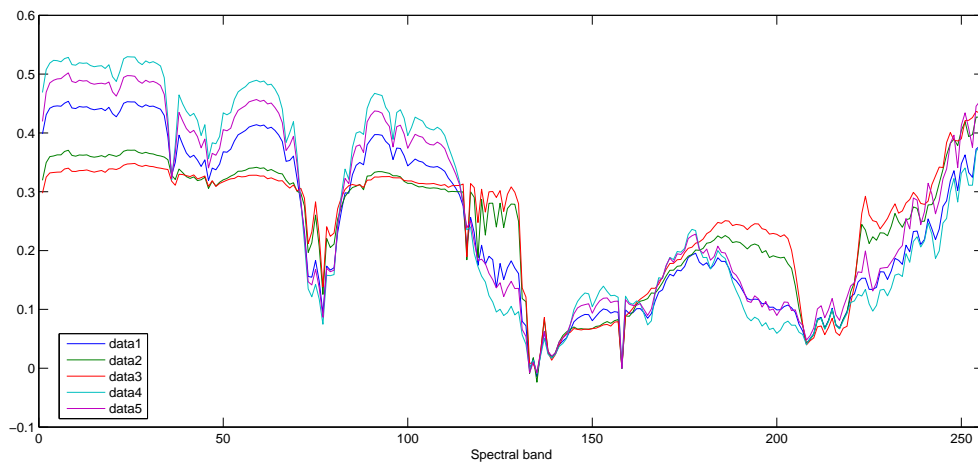


Figure 9: Spectral means of the 5 mineralogical classes found using HDDC.

trometer has mapped the Martian surface with a spatial resolution varying between 300 to 3000 meters depending on spacecraft altitude. It acquires for each resolved pixel the spectrum from 0.36 to 5.2 μm in 256 contiguous spectral channels. OMEGA is designed to characterize the composition of surface materials, discriminating between various classes of silicates, hydrated minerals, oxides and carbonates, organic frosts and ices. For this experiment, a 300×128 image of the Martian surface is considered and a 256-dimensional spectral observation is associated to each of the 38 400 pixels. The image of the studied zone is presented on the left panel of Figure 8. According to the experts, there are $k = 5$ mineralogical classes to identify.

The right image of Figure 8 shows the segmentation obtained with the model $[a_i b_i Q_i d_i]$ of HDDC. First of all, observe that the segmentation of HDDC is very precise on the main part of the image. The poor results of the top right part of the image are due to the planet curvature and could be corrected. In particular, the experts of the domain appreciated that our method is able to detect a mixture of ice and carbonate around the ice zones (clear zones of the image). Figure 9 shows the spectral means of the 5 classes and this allows the experts to determine the mineralogical and molecular composition of each class. Remind that this study is done without taking into account the spatial relations between the pixels of a image. A natural extension of this work is therefore to combine HDDC with the modeling of the spatial relations using, for example, hidden Markov random fields. This experiment demonstrates that HDDC can be efficiently used on real high-dimensional data and with large datasets. In addition, a main interest of HDDC for this application is to provide posterior probabilities that each pixel belongs to the classes.

6 Conclusion

In this paper, new Gaussian mixture models designed for high-dimensional data are introduced. It is assumed that the intrinsic dimension of each mixture component is much smaller than the one of the original space. In addition, outside the specific subspace of each group, the noise variance is modeled by a single parameter. Additional constraints can be imposed on the parameters within or between

the groups in order to obtain further regularized models. This parameterization in the eigenspaces of the mixture components gives rise to an EM-based clustering method, called High-Dimensional Data Clustering (HDDC). Experiments on artificial and real datasets demonstrated the effectiveness of the different models of HDDC compared to classical Gaussian mixture models. In particular, the model $[a_i b_i Q_i d_i]$ provides very satisfying results for many types of data.

Acknowledgments

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A Appendix: parameters estimation

First of all, we introduce the following useful formulation of the log-likelihood:

$$-2 \log(L) = \sum_{i=1}^k n_i \sum_{j=1}^p \left(\log(\delta_{ij}) + \frac{1}{\delta_{ij}} q_{ij}^t W_i q_{ij} \right) + c^{st}, \quad (14)$$

where δ_{ij} is the j th diagonal coefficient of Δ_i and q_{ij} is the j th column of Q_i . We refer to [19] for a demonstration of this result.

A.1 Models with free orientations

Subspace \mathbb{E}_i : The log-likelihood is to be maximized under the constraint $q_{ij}^t q_{ij} = 1$, which is equivalent to finding a saddle point of the Lagrange function:

$$\mathcal{L} = -2 \log(L) - \sum_{j=1}^p \theta_{ij} (q_{ij}^t q_{ij} - 1),$$

where θ_{ij} are the Lagrange multipliers. Using the expression (14) of the log-likelihood, the gradient of \mathcal{L} with respect to q_{ij} is:

$$\nabla_{q_{ij}} \mathcal{L} = 2 \frac{n_i}{\delta_{ij}} W_i q_{ij} - 2 \theta_{ij} q_{ij},$$

and by multiplying this quantity on the left by q_{ij}^t , we obtain:

$$q_{ij}^t \nabla_{q_{ij}} \mathcal{L} = 0 \Leftrightarrow \theta_{ij} = \frac{n_i}{\delta_{ij}} q_{ij}^t W_i q_{ij}.$$

Consequently, $W_i q_{ij} = \frac{\theta_{ij} \delta_{ij}}{n_i} q_{ij}$ and thus q_{ij} is the eigenvector of W_i associated with the eigenvalue $\lambda_{ij} = \frac{\theta_{ij} \delta_{ij}}{n_i} = q_{ij}^t W_i q_{ij}$. As the vectors q_{ij} are eigenvectors of the symmetric matrix W_i , this implies that $q_{ij}^t q_{i\ell} = 0$ if $j \neq \ell$. The log-likelihood can therefore be re-written as follows:

$$-2 \log(L) = \sum_{i=1}^k n_i \left(\sum_{j=1}^{d_i} \left(\log(a_{ij}) + \frac{\lambda_{ij}}{a_{ij}} \right) + \sum_{j=d_i+1}^p \left(\log(b_i) + \frac{\lambda_{ij}}{b_i} \right) \right) + c^{st},$$

and, using the relation $\sum_{j=d_i+1}^p \lambda_{ij} = \text{Tr}(W_i) - \sum_{j=1}^{d_i} \lambda_{ij}$, we obtain:

$$-2 \log(L) = \sum_{i=1}^k n_i \left(\sum_{j=1}^{d_i} \log(a_{ij}) + (p - d_i) \log(b_i) + \frac{\text{Tr}(W_i)}{b_i} + \sum_{j=1}^{d_i} \left(\frac{1}{a_{ij}} - \frac{1}{b_i} \right) \lambda_{ij} \right) + c^{st}. \quad (15)$$

Thus, minimizing $-2 \log(L)$ with respect to λ_{ij} is equivalent to minimizing the quantity $\sum_{i=1}^k n_i \sum_{j=1}^{d_i} \left(\frac{1}{a_{ij}} - \frac{1}{b_i} \right) \lambda_{ij}$. Since $\left(\frac{1}{a_{ij}} - \frac{1}{b_i} \right) < 0$, $\forall j = 1, \dots, d_i$, λ_{ij} must therefore be as larger as possible. Thus, the column vector q_{ij} , $\forall j = 1, \dots, d_i$, is estimated by the eigenvector associated to the j th largest eigenvalue of W_i .

Model $[a_{ij} b_i Q_i d_i]$: starting from equation (15), the partial derivative of $-2 \log(L)$ with respect to a_{ij} and b_i are:

$$-2 \frac{\partial \log(L)}{\partial a_{ij}} = n_i \left(\frac{1}{a_{ij}} - \frac{\lambda_{ij}}{a_{ij}^2} \right) \quad \text{and} \quad -2 \frac{\partial \log(L)}{\partial b_i} = \frac{n_i(p - d_i)}{b_i} - \frac{n_i}{b_i^2} \left(\text{Tr}(W_i) - \sum_{j=1}^{d_i} \lambda_{ij} \right).$$

The condition $\frac{\partial \log(L)}{\partial a_{ij}} = 0$ implies that $\hat{a}_{ij} = \lambda_{ij}$ and the condition $\frac{\partial \log(L)}{\partial b_i} = 0$ implies that:

$$\hat{b}_i = \frac{1}{(p - d_i)} \left(\text{Tr}(W_i) - \sum_{j=1}^{d_i} \lambda_{ij} \right).$$

Model $[a_{ij}bQ_id_i]$: the partial derivative of $-2\log(L)$ with respect to b is:

$$-2\frac{\partial \log(L)}{\partial b} = \frac{n(p-\xi)}{b} - \frac{1}{b^2} \sum_{i=1}^k n_i \left(\text{Tr}(W_i) - \sum_{j=1}^{d_i} \lambda_{ij} \right),$$

and the condition $\frac{\partial \log(L)}{\partial b} = 0$ proves that:

$$\hat{b} = \frac{1}{(p-\xi)} \left(\text{Tr}(W) - \sum_{i=1}^k \hat{\pi}_i \sum_{j=1}^{d_i} \lambda_{ij} \right).$$

Model $[a_ib_iQ_id_i]$: from (15), the partial derivative of $-2\log(L)$ with respect to a_i is:

$$-2\frac{\partial \log(L)}{\partial a_i} = \frac{n_id_i}{a_i} - \frac{n_i}{a_i^2} \sum_{j=1}^{d_i} \lambda_{ij},$$

and the condition $\frac{\partial \log(L)}{\partial a_i} = 0$ implies that:

$$\hat{a}_i = \frac{1}{d_i} \sum_{j=1}^{d_i} \lambda_{ij}.$$

Model $[ab_iQ_id_i]$: the partial derivative of $-2\log(L)$ with respect to a is:

$$-2\frac{\partial \log(L)}{\partial a} = \frac{n\xi}{a} - \frac{1}{a^2} \sum_{i=1}^k n_i \sum_{j=1}^{d_i} \lambda_{ij},$$

and the condition $\frac{\partial \log(L)}{\partial a} = 0$ gives:

$$\hat{a} = \frac{1}{\xi} \sum_{i=1}^k \hat{\pi}_i \sum_{j=1}^{d_i} \lambda_{ij}.$$

Model $[a_jb_iQ_id]$: the partial derivative of $-2\log(L)$ with respect to a_j is:

$$-2\frac{\partial \log(L)}{\partial a_j} = \frac{n}{a_j} - \frac{1}{a_j^2} \sum_{i=1}^k n_i \lambda_{ij}.$$

The condition $\frac{\partial \log(L)}{\partial a_j} = 0$ and the relation $\sum_{i=1}^k n_i \lambda_{ij} = n\lambda_j$ imply that $\hat{a}_j = \lambda_j$.

A.2 Models with common orientations

Subspace \mathbb{E}_i : Starting from the likelihood expression (14), we can write:

$$\begin{aligned} -2\log(L) &= \sum_{i=1}^k n_i \sum_{j=1}^d \left(\log(a_i) + \frac{1}{a_i} q_j^t W_i q_j \right) + \sum_{i=1}^k n_i \sum_{j=d+1}^p \left(\log(b_i) + \frac{1}{b_i} q_j^t W_i q_j \right) + c^{st}, \\ &= \sum_{i=1}^k n_i (d \log(a_i) + (p-d) \log(b_i)) + \sum_{j=1}^d q_j^t A q_j + \sum_{j=d+1}^p q_j^t B q_j + c^{st}, \end{aligned}$$

where $A = \sum_{i=1}^k \frac{n_i}{a_i} W_i$ and $B = \sum_{i=1}^k \frac{n_i}{b_i} W_i$. Note that $\sum_{j=d+1}^p q_j^t B q_j$ can be written using the trace of B : $\sum_{j=d+1}^p q_j^t B q_j = \text{Tr}(B) - \sum_{j=1}^d q_j^t B q_j$. This yields:

$$-2\log(L) = \sum_{i=1}^k n_i (d \log(a_i) + (p-d) \log(b_i)) - \sum_{j=1}^d q_j^t (B-A) q_j + \text{Tr}(B) + c^{st}$$

Consequently, the gradient of $\mathcal{L} = -2\log(L) - \sum_{j=1}^p \theta_j (q_j^t q_j - 1)$ with respect to q_j is:

$$\nabla_{q_j} \mathcal{L} = -2(B-A)q_j - 2\theta_j q_j,$$

where θ_j is the j th Lagrange multiplier. The relation $\nabla_{q_j} \mathcal{L} = 0$ is equivalent to $(B-A)q_j = -\theta_j q_j$ which means that q_j is eigenvector of the matrix $(B-A)$. In order to minimize the quantity $-2\log(L)$, the d first columns of Q must be the eigenvectors associated with the d largest eigenvalues of $(B-A)$.

Model $[a_i b_i Q d]$: Starting from equation (16), the partial derivatives of $-2\log(L)$ with respect to a_i and b_i are:

$$-2 \frac{\partial \log(L)}{\partial a_i} = \frac{n_i d}{a_i} - \frac{n_i}{a_i^2} \sum_{j=1}^d q_j^t W_i q_j \quad \text{and} \quad -2 \frac{\partial \log(L)}{\partial b_i} = \frac{n_i (p-d)}{b_i} - \frac{n_i}{b_i^2} \left(\text{Tr}(W_i) - \sum_{j=1}^d q_j^t W_i q_j \right).$$

The condition $\frac{\partial \log(L)}{\partial a_i} = 0$ and $\frac{\partial \log(L)}{\partial b_i} = 0$ give respectively:

$$\hat{a}_i(Q) = \frac{1}{d} \sum_{j=1}^d q_j^t W_i q_j \quad \text{and} \quad \hat{b}_i(Q) = \frac{1}{(p-d)} \left(\text{Tr}(W_i) - \sum_{j=1}^d q_j^t W_i q_j \right).$$

Model $[a_i b Q d]$: The partial derivative of $-2 \log(L)$ with respect to b is:

$$-2 \frac{\partial \log(L)}{\partial b} = \frac{n(p-d)}{b} - \frac{n}{b^2} \left(\text{Tr}(W) - \sum_{j=1}^d q_j^t W q_j \right),$$

and the condition $\frac{\partial \log(L)}{\partial b} = 0$ implies that:

$$\hat{b}(Q) = \frac{1}{(p-d)} \left(\text{Tr}(W) - \sum_{j=1}^d q_j^t W q_j \right).$$

Model $[ab_i Q d]$: The partial derivative of $-2 \log(L)$ with respect to a is:

$$-2 \frac{\partial \log(L)}{\partial a} = \frac{nd}{a} - \frac{n}{a^2} \sum_{j=1}^d q_j^t W q_j,$$

and the condition $\frac{\partial \log(L)}{\partial a} = 0$ proves that:

$$\hat{a}(Q) = \frac{1}{d} \sum_{j=1}^d q_j^t W q_j.$$

A.3 Models with common covariance matrices

Subspace \mathbb{E}_i : The log-likelihood can be written as follows:

$$-2 \log(L) = n \left(\sum_{j=1}^d \log(a_j) + (p-d) \log(b) + \frac{\text{Tr}(W)}{b} + \sum_{j=1}^d \left(\frac{1}{a_j} - \frac{1}{b} \right) q_j^t W q_j \right) + c^{st}.$$

The gradient of $\mathcal{L} = -2 \log(L) - \sum_{j=1}^p \theta_j (q_j^t q_j - 1)$ with respect to q_j is:

$$\nabla_{q_j} \mathcal{L} = 2n \left(\frac{1}{a_j} - \frac{1}{b} \right) W q_j - 2\theta_j q_j,$$

where θ_j is the j th Lagrange multiplier. The relation $\nabla_{q_j} \mathcal{L} = 0$ implies that q_j is eigenvector of W . In order to minimize $-2 \log(L)$, the first columns of Q must be the eigenvectors associated to the d largest eigenvalues of W .

Model $[a_j b Q d]$: The partial derivatives of $-2 \log(L)$ with respect to a_j and b are:

$$-2 \frac{\partial \log(L)}{\partial a_j} = \frac{n}{a_j} - \frac{n}{a_j^2} q_j^t W q_j \quad \text{and} \quad -2 \frac{\partial \log(L)}{\partial b} = \frac{n(p-d)}{b} - \frac{n}{b^2} \sum_{j=d+1}^p q_j^t W q_j.$$

The condition $\frac{\partial \log(L)}{\partial a_i} = 0$ implies that $\hat{a}_j = \lambda_j$. The combination of the condition $\frac{\partial \log(L)}{\partial b} = 0$ with the relation $\sum_{j=d+1}^p \lambda_j = \text{Tr}(W) - \sum_{j=1}^d \lambda_j$ gives the estimator of b :

$$\hat{b} = \frac{1}{(p-d)} \left(\text{Tr}(W) - \sum_{j=1}^d \lambda_j \right).$$

Model $[ab Q d]$: The partial derivatives of $-2 \log(L)$ with respect to a is:

$$-2 \frac{\partial \log(L)}{\partial a} = \frac{nd}{a} - \frac{n}{a^2} \sum_{j=1}^d q_j^t W q_j,$$

and the condition $\frac{\partial \log(L)}{\partial a} = 0$ implies that:

$$\hat{a} = \frac{1}{d} \sum_{j=1}^d \lambda_j.$$

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