A non-asymptotic penalization criterion for model selection in mixture of experts models

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Abstract

Mixture of experts (MoE) is a popular class of models in statistics and machine learning that has sustained attention over the years, due to its flexibility and effectiveness. We consider the Gaussian-gated localized MoE (GLoME) regression model for modeling heterogeneous data. This model poses challenging questions with respect to the statistical estimation and model selection problems, including feature selection, both from the computational and theoretical points of view. We study the problem of estimating the number of components of the GLoME model, in a penalized maximum likelihood estimation framework. We provide a lower bound on the penalty that ensures a weak oracle inequality is satisfied by our estimator. To support our theoretical result, we perform numerical experiments on simulated and real data, which illustrate the performance of our finite-sample oracle inequality.

Keywords. Oracle inequality, mixture of experts, mixture of regressions, model selection, penalized maximum likelihood.

Contents

1 Introduction 2
2 Notation and framework 3
  2.1 GLoME models ........................................... 3
  2.1.1 Gaussian gating functions .......................... 4
  2.1.2 Gaussian experts .................................... 4
  2.2 High-dimensional regression via GLLiM models .......... 5
  2.3 Collection of GLoME models ........................... 6
  2.4 Penalized maximum likelihood estimator and losses ........ 7

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1 Introduction

Mixture of experts (MoE) models, originally introduced in Jacobs et al. (1991) and Jordan & Jacobs (1994), are flexible models that generalize the classical finite mixture models as well as finite mixtures of regression models (McLachlan & Peel, 2000, Sec. 5.13). Their flexibility comes from allowing the mixture weights (or the gating functions) to depend on the explanatory variables, along with the component densities (or experts). In the context of regression, MoE models with Gaussian experts and soft-max or Gaussian gating functions are the most popular choices and are powerful tools for modeling more complex non-linear relationships between responses and predictors that arise from different subpopulations. This is largely because of their universal approximation properties, which have been extensively studied for not only finite mixture models (Genovese et al., 2000, Rakhlin et al., 2005, Nguyen et al., 2013, Ho et al., 2016a,b, Nguyen et al., 2020d,b) but also conditional densities of MoE models (Jiang & Tanner, 1999, Norets et al., 2010, Nguyen et al., 2016, Ho et al., 2019, Nguyen et al., 2019, 2020a). Detailed reviews on practical and theoretical aspects of MoE models can be found in Yuksel et al. (2012), Masoudnia & Ebrahimpour (2014) and Nguyen & Chamroukhi (2018).

In this paper, we examine MoE models with Gaussian gating functions, first introduced by Xu et al. (1995), for clustering and regression. From hereon in, we refer to these models as the Gaussian-gated localized MoE (GLoME) and we refer to MoE models with soft-max gating functions as soft-max-gated MoE (SGaME). It is worth mentioning that GLoME have been thoroughly studied in the statistics and machine learning literatures under several contexts: localized MoE (Ramamurti & Ghosh, 1996, 1998, Moerland, 1999, Bouchard, 2003), normalized Gaussian networks (Sato & Ishii, 2000), MoE modeling of priors in Bayesian nonparametric regression (Norets & Pelenis, 2014, Norets & Pati, 2017), cluster-weighted modeling (Ingrassia et al., 2012), supervised Gaussian locally-linear mapping (GLLiM) in inverse regression (Deleforge et al., 2015), deep mixture of linear inverse regressions (Lathuilière et al., 2017) and multiple-output Gaussian gated mixture of linear experts (Nguyen et al., 2019). It is also interesting to point out that supervised GLLiM in Deleforge et al. (2015) is an affine instance of a GLoME model, where linear combination of bounded functions are considered instead of affine for mean functions of Gaussian experts.

One of the main disadvantages of SGaME models is the difficulty of applying an EM algorithm, which requires an internal iterative numerical optimization procedure (e.g., iteratively-reweighted least squares, Newton-Raphson algorithm) to update the soft-max parameters. To overcome this problem, we instead use the Gaussian gating network that enables us to link GLoME with finite mixtures of...
Gaussian models. Then, the maximization with respect to the parameters of the gating network can be solved analytically with the EM algorithm framework, which decreases the computational complexity of the estimation routine. Furthermore, we then can also make use of well established theoretical results for finite mixture models.

In this work, we are interested in controlling and accounting for model complexity when selecting the best number of mixture components of a model. In general, model selection is often performed using the AIC or the BIC criteria (Akaike, 1974, Schwarz et al., 1978). An important limitation of these criteria, however, is that they are only valid asymptotically. This implies that there are no finite sample guarantees when using AIC or BIC, for choosing between different levels of complexity. The slope heuristic of Birgé & Massart (2007), supported by a non-asymptotic oracle inequality, is a method that permits finite sample inference in place of AIC and BIC. Recent reviews and practical issues regarding the slope heuristic can be found in Baudry et al. (2012) and Arlot (2019). Theorem 7.11 from Massart (2007) provides a model selection result regarding the construction of a penalized criterion that leads to good model selection outcomes, where the penalty is defined by the model complexity. It provides support for the slope heuristic approach in a finite sample setting.

Following the concentration inequality-based methods for likelihood penalization of Massart (2007), Massart & Meynet (2011) and Cohen & Pennec (2011), a number of finite-sample oracle results have been established for the least absolute shrinkage and selection operator (LASSO) (Tibshirani, 1996) and general penalized maximum likelihood estimators (PMLE). These results include the works of Meynet (2013) and Devijver (2015a,b, 2017) for finite mixture regression models, and Montuelle & Pennec (2014) and Nguyen et al. (2020c) for SGaME models. However, to the best of our knowledge, we are the first to provide finite-sample oracle inequalities for PMLE of GLoME models, via Theorem 3.1.

Note that for the Gaussian gating parameters, the technique for handling the logistic weights in the SGaME models of Montuelle & Pennec (2014) is not directly applicable to the GLoME framework, due to the quadratic form of the canonical link. Therefore, we propose a reparameterization trick to bound the metric entropy of the Gaussian gating parameters space; see Equation (5.3) and Appendix A.2 for more details. Furthermore, it is worth noting that we can establish that Theorem 3.1 is a general version of Theorem 1 from Montuelle & Pennec (2014) when using linear functions, via Lemma 3.5.

The main contribution of our paper is a theoretical result: a non-asymptotic oracle bound on the risk that provides the lower bound on the regularization parameters that ensures non-asymptotic control of the estimator Kullback-Leibler loss for the GLoME model. The goal of this paper is to study the conditions on penalty functions that guarantee the weak oracle inequality for GLoME models. As such, the remainder of the article proceeds as follows. In Section 2, we introduce the notations and framework for GLoME models and their special cases, GLLiM models. In Section 3, we state the main result of the article: a weak oracle inequality satisfied by the PMLE. Our result is then illustrated via numerical experiments in Section 4. Section 5 is devoted to the proofs of the main results, based on a general model selection theorem. Some conclusions are provided in Section 6. The proofs of technical lemmas can be found in Appendix A.

2 Notation and framework

We consider a regression framework and aim at capturing the potential nonlinear relationship between the multivariate response $Y = (Y_j)_{j \in [L]} : [L] = \{1, \ldots, L\}$ and the set of covariates $X = (X_j)_{j \in [D]}$. Let $((X_i, Y_i))_{i \in [n]} \in (\mathcal{X} \times \mathcal{Y})^n \subset (\mathbb{R}^D \times \mathbb{R}^L)^n$ be a random sample, and let $x$ and $y$ denote the observed values of the random variables $X$ and $Y$, respectively.

2.1 GLoME models

We consider an extension of the MoE model of Xu et al. (1995), which extended the original MoE from Jacobs et al. (1991) to a regression setting. More specifically, we consider the following GLoME model, defined by (2.1), which is motivated by an inverse regression framework where the role of input and response variables should be exchanged such that $Y$ becomes the covariates and $X$ plays the role.
of a multivariate response. Then its corresponding conditional density is defined as follows:

\[ s_{\psi_K}(x|y) = \sum_{k=1}^{K} g_k(y; \omega) \Phi_D(x; \nu_k(y), \Sigma_k), \]  

\[ g_k(y; \omega) = \frac{\pi_k \Phi_L(y; c_k, \Gamma_k)}{\sum_{j=1}^{K} \pi_j \Phi_L(y; c_j, \Gamma_j)}. \]

Here, \( g_k(\cdot; \omega) \) and \( \Phi_D(\cdot; \nu_k(\cdot), \Sigma_k), k \in [K] \), are called Gaussian gating functions and Gaussian experts, respectively. Furthermore, we decompose the parameters of the model as follows: \( \psi_K = (\omega, \nu, \Sigma) \in \Omega_K \times Y_K \times V_K =: \Psi_K \), \( \omega = (\pi, c, \Gamma) \in (\Pi_{K-1} \times C_K \times V'_K) =: \Omega_K \), \( \pi = (\pi_k)_{k \in [K]} \), \( c = (c_k)_{k \in [K]} \), \( \Gamma = (\Gamma_k)_{k \in [K]} \), \( \nu = (\nu_k)_{k \in [K]} \in Y_K \), \( \Sigma = (\Sigma_k)_{k \in [K]} \in V_K \). Note that \( \Pi_{K-1} = \left\{ (\pi_k)_{k \in [K]} \in (\mathbb{R}^+)^K, \sum_{k=1}^{K} \pi_k = 1 \right\} \) is a \( K - 1 \) dimensional probability simplex, \( C_K \) is a set of \( K \)-tuples of mean vectors of size \( L \times 1 \), \( V'_K \) is a sets of \( K \)-tuples of elements in \( \mathcal{S}_L^{++} \), where \( \mathcal{S}_L^{++} \) denotes the collection of symmetric positive definite matrices on \( \mathbb{R}^L \), \( Y_K \) is a set of \( K \)-tuples of mean functions from \( \mathbb{R}^L \) to \( \mathbb{R}^D \), and \( V_K \) is a set containing \( K \)-tuples from \( \mathcal{S}_D^{++} \).

In order to establish our oracle inequality, Theorem 3.1, we need to assume that \( Y \) is a bounded set in \( \mathbb{R}^L \) and some classical boundedness conditions on the parameter space.

### 2.1.1 Gaussian gating functions

For a matrix \( A \), let \( m(A) \) and \( M(A) \) be, respectively, the modulus of the smallest and largest eigenvalues of \( A \). We shall restrict our study to bounded Gaussian gating parameter vectors \( \omega = (\pi, c, \Gamma) \in \Omega_K \). Specifically, we assume that there exist deterministic positive constants \( a_{\pi}, a_c, a_\Gamma, A_\Gamma, a_\pi \leq \pi_k \). We denote the space of gating functions as

\[ \mathcal{P}_K = \left\{ g = (g_k(\cdot; \omega))_{k \in [K]} : \forall k \in [K], g_k(y; \omega) = \frac{\pi_k \Phi_L(y; c_k, \Gamma_k)}{\sum_{j=1}^{K} \pi_j \Phi_L(y; c_j, \Gamma_j)}, \omega \in \tilde{\Omega}_K \right\}. \]

### 2.1.2 Gaussian experts

Following the same structure for the means of Gaussian experts from Montuelle & Pennec (2014), the set \( \mathcal{Y}_K \) will be chosen as a tensor product of a compact set of moderate dimension (e.g., a set of polynomials of degree smaller than \( d_Y \), whose coefficients are smaller in absolute values than \( T_Y \)). Then, \( \mathcal{Y}_K \) is defined as a linear combination of a finite set of bounded functions whose coefficients belong to a compact set. This general setting includes polynomial bases when the covariates are bounded, Fourier bases on an interval, as well as suitably renormalized wavelet dictionaries. More specifically, we define \( \mathcal{Y}_K = \mathcal{Y}_K^K \), with

\[ \mathcal{Y}_b = \left\{ y \mapsto (v_j(y))_{j \in [D]} : = \left( \sum_{i=1}^{d_Y} \alpha_i^{(j)} \varphi_{Y,i}(y) \right)_{j \in [D]} : \| \alpha \|_\infty \leq T_Y \right\}, \]

where \( d_Y \in \mathbb{N}^* \), \( T_Y \in \mathbb{R}^+ \), and \( \left( \varphi_{Y,i} \right)_{i \in [d_Y]} \) is a collection of bounded functions on \( Y \). In particular, we focus on the bounded \( Y \) case and assume that \( Y = [0,1]^L \) without loss of generality. In this case, \( \varphi_{Y,i} \) can be chosen as monomials with maximum (non-negative) degree \( d_Y \). Recall that a multi-index \( r = (r_l)_{l \in [L]} \), \( r_l \in \mathbb{N}^* \cup \{0\} \), \( \forall l \in [L] \), is an \( L \)-tuple of nonnegative integers. We define \( |r| = \sum_{l=1}^{L} r_l \) and the number \( |r| \) is called the order or degree of \( Y^r \). Then, \( \mathcal{Y}_K = \mathcal{Y}_p^K \), where

\[ \mathcal{Y}_p = \left\{ y \mapsto (v_j(y))_{j \in [D]} : = \left( \sum_{|r|=0}^{d_Y} \alpha_r^{(j)} y^r \right)_{j \in [D]} : \| \alpha \|_\infty \leq T_Y \right\}. \]
For the covariances of Gaussian experts, we follow the classical covariance matrix sets described by Celeux & Govaert (1995). In general situation, sets $V_K$ depend on the noise model chosen. Formally, we consider the set

$$V_K = \left\{ \left( B_k P_k A_k P_k^T \right)_{k \in [K]} : \forall k \in [K], B_\cdot \leq B_k \leq B_\cdot, P_k \in SO(D), A_k \in A(\lambda_-, \lambda_+) \right\},$$

where any covariance matrix $\Sigma_k$ can be decomposed into the form $B_k P_k A_k P_k^T$, such that $B_k = |\Sigma_k|^{1/D}$ is a positive scalar corresponding to the volume, $P_k$ is the matrix of eigenvectors of $\Sigma_k$ and $A_k$ the diagonal matrix of normalized eigenvalues of $\Sigma_k$; $B_\cdot \in \mathbb{R}^+$, $B_\cdot \in \mathbb{R}^+$, $A(\lambda_-, \lambda_+)$ is a set of diagonal matrices $A$, such that $|A_k| = 1$ and $\forall i \in [D], \lambda_- \leq (A_k)_{ii} \leq \lambda_+$; and $SO(D)$ is the special orthogonal group of dimension $D$. For example, in the most general case, we can assume that the matrices $V_K$ are different for all Gaussian experts. Alternatively, they can share the same volume or diagonalization matrix.

Next, a characterization of GLLiM model, an affine instance of GLoME model, is described in Section 2.2 and is especially useful for high-dimensional regression data.

### 2.2 High-dimensional regression via GLLiM models

A GLLiM model, as originally introduced in Deleforge et al. (2015), is used to capture the nonlinear relationship between the response and the set of covariates from a high-dimensional regression data, typically in the case when $D \gg L$, by the following $K$ locally affine mappings:

$$Y = \sum_{k=1}^{K} \mathbb{I}(Z = k) (A_k^* x + b_k^* + E_k^*).$$

Here, $\mathbb{I}$ is an indicator function, $Z$ is a latent variable capturing a cluster relationship such that $Z = k$ if $Y$ originates from cluster $k \in [K]$, and cluster specific affine transformations are defined by matrices $A_k^* \in \mathbb{R}^{L \times D}$ and vectors $b_k^* \in \mathbb{R}^L$. Furthermore, $E_k^*$ is an error term capturing both the reconstruction error due to the local affine approximation and the observation noise in $\mathbb{R}^L$.

Following the common assumption that $E_k^*$ is a zero-mean Gaussian variable with covariance matrix $\Sigma_k^* \in \mathbb{R}^{L \times L}$, it holds that

$$p(Y = y | X = x, Z = k; \psi_K^*) = \Phi_L(y; A_k^* x + b_k^*, \Sigma_k^*),$$

where we denote by $\psi_K^*$ the vector of model parameters and $\Phi_L$ is the probability density function (PDF) of a Gaussian distribution of dimension $L$. In order to enforce the affine transformations to be local, $X$ is defined as a mixture of $K$ Gaussian components as follows:

$$p(X = x | Z = k; \psi_K^*) = \Phi_D(x; c_k^*, \Gamma_k^*), p(Z = k; \psi_K^*) = \pi_k^*,$$

where $c_k^* \in \mathbb{R}^D, \Gamma_k^* \in \mathbb{R}^{D \times D},$ and $\pi^* = (\pi_k^*)_{k \in [K]} \in \Pi_{K-1}$, where $\Pi_{K-1}$ is the $K - 1$ dimensional probability simplex. Then, according to formulas for conditional multivariate Gaussian variables and the following hierarchical decomposition

$$p(Y = y, X = x; \psi_K^*) = \sum_{k=1}^{K} p(Y = y | X = x, Z = k; \psi_K^*) p(X = x | Z = k; \psi_K^*) p(Z = k; \psi_K^*),$$

$$= \sum_{k=1}^{K} \pi_k^* \Phi_D(x; c_k^*, \Gamma_k^*) \Phi_L(y; A_k^* x + b_k^*, \Sigma_k^*),$$

we obtain the following forward conditional density (Deleforge et al., 2015):

$$p(Y = y | X = x; \psi_K^*) = \sum_{k=1}^{K} \frac{\pi_k^* \Phi_D(x; c_k^*, \Gamma_k^*)}{\sum_{j=1}^{K} \pi_j^* \Phi_D(x; c_j^*, \Gamma_j^*)} \Phi_L(y; A_k^* x + b_k^*, \Sigma_k^*),$$

(2.10)
where \( \psi_K = (\pi^*, \theta_K^*) \in \Pi_{K-1} \times \Theta_K =: \Psi_K \), \( \theta_K^* = (c_k^*, \Gamma_k^*, A_k^*, b_k^*, \Sigma_k^*)_{k \in [K]} \) and

\[
\Theta_K^* = (\mathbb{R}^D \times S_{D+}^+ \times \mathbb{R}^{L \times D} \times \mathbb{R}^L \times S_{L+}^+ (\mathbb{R}))^K.
\]

Without assuming anything on the structure on of parameters, the dimension of the model (denoted by \( \text{dim}(\cdot) \)), is defined as the total parameters have to be estimated as follows:

\[
\text{dim}(\Psi_K^*) = K \left( 1 + D(L + 1) + \frac{D(D + 1)}{2} + \frac{L(L + 1)}{2} + L \right) - 1.
\]

It is worth mentioning that \( \text{dim}(\Psi_K) \) is very large compared to the sample size (see, e.g., Deleforge et al., 2015, Devijver et al., 2017, Perthame et al., 2018 for more details in their real data sets) whenever \( D \) is large and \( D \gg L \). Furthermore, it is more realistic to make assumption on the residual covariance matrices \( \Sigma_k^* \) of error vectors \( E_k^* \) rather than \( \Gamma_k^* \) (cf. Deleforge et al., 2015, Section 3). This justifies the use of the inverse regression trick from Deleforge et al. (2015), which leads a drastic reduction in the number of parameters to estimate.

More specifically, in (2.10), the role of input and response variables should be exchanged such that \( Y \) becomes the covariates and \( X \) plays the role of a multivariate response. Therefore, its corresponding inverse conditional density is defined as a Gaussian locally-linear mapping (GLLiM), based on the previous hierarchical Gaussian mixture model:

\[
\begin{align*}
    p(X = x | Y = y, Z = k; \psi_K) &= \Phi_D(x; A_k y + b_k, \Sigma_k), \\
    p(Y = y | Z = k; \psi_K) &= \Phi_L(y; c_k, \Gamma_k), \\
    p(Z = k; \psi_k) &= \pi_k,
\end{align*}
\]

(2.11)

\[
\begin{align*}
    p(X = x | Y = y; \psi_K) &= \sum_{k=1}^{K} \pi_k \Phi_L(y; c_k, \Gamma_k) \Phi_D(x; A_k y + b_k, \Sigma_k) \Phi_L(y; c_k, \Gamma_k).
\end{align*}
\]

(2.12)

(2.13)

where \( \Sigma_k \) is a \( D \times D \) covariance structure (usually diagonal, chosen to reduce the number of parameters) automatically learnt from data and \( \psi_K \) is the set of parameters, denoted by \( \psi_K = (\pi, \theta_K) \in \Pi_{K-1} \times \Theta_K =: \Psi_K \). An intriguing feature of GLLiM models is described in the following Lemma 2.1, which is proved in Appendix A.1.

**Lemma 2.1.** The parameter \( \psi_K \) in the forward conditional PDF, defined in (2.10), can then be deduced from \( \psi_K \) in (2.13) via the following one-to-one correspondence:

\[
\theta_K = \begin{pmatrix}
    c_k \\
    \Gamma_k \\
    A_k \\
    b_k \\
    \Sigma_k
\end{pmatrix}_{k \in [K]} \mapsto \begin{pmatrix}
    c_k^* \\
    \Gamma_k^* \\
    A_k^* \\
    b_k^* \\
    \Sigma_k^*
\end{pmatrix}_{k \in [K]} = \begin{pmatrix}
    A_k^* c_k + b_k \\
    \Sigma_k^* + A_k^* \Gamma_k A_k^\top \\
    \Sigma_k^* A_k^\top \Sigma_k^{-1} \Sigma_k^* \\
    \Sigma_k^* (\Gamma_k^\top c_k - A_k^\top \Sigma_k^{-1} b_k) \\
    (\Gamma_k^\top + A_k^\top \Sigma_k^{-1} A_k)^{-1}
\end{pmatrix} \in \Theta_K^*,
\]

(2.14)

with the note that \( \pi^* \equiv \pi \).

### 2.3 Collection of GLoME models

In this paper, we should choose the number of components \( K \) among a finite set \( K = [K_{\text{max}}] \), where \( K_{\text{max}} \in \mathbb{N}^+ \) may depend on the sample size \( n \). We wish to estimate the unknown inverse conditional density \( s_0 \) by conditional densities belonging to the following collection of inverse models \( S = (S_m)_{m \in M} \), with \( M = K \), and

\[
S_m = \{ (x, y) \mapsto s_m(x | y) = s_{\psi_K}(x | y) : \psi_K = (\omega, v, \Sigma) \in \tilde{\Omega}_K \times \Upsilon_K \times V_K =: \tilde{\Psi}_K \},
\]

(2.15)

where \( \tilde{\Omega}_K, \Upsilon_K \) and \( V_K \) are defined previously in (2.3), (2.5) (or more general (2.4)) and (2.6), respectively.
Remark 2.2. It is worth mentioning that we can also define the collection of the forward models in the same framework as in (2.15). More precisely, the unknown forward conditional density $s_0^\ast$ is estimated via the following collection of forward model $S^\ast = (S^\ast_m)_{m \in M}$, with $M = K$, and

$$S^\ast_m = \{ (x, y) \mapsto s_0^\ast (y|x) = s_{\psi^\ast_K} (y|x) : \psi^\ast_K = (\omega^\ast, v^\ast, \Sigma^\ast) \in \tilde{\Omega}^\ast_K \times \tilde{Y}^\ast_K \times \tilde{V}^\ast_K =: \tilde{\Psi}^\ast_K \},$$

where $\tilde{\Omega}^\ast_K$, $\tilde{Y}^\ast_K$, and $\tilde{V}^\ast_K$ are defined similar to (2.3), (2.5) (or more general (2.4)) and (2.6), respectively.

Note that for sake of simplicity of notation via avoiding the utilization of “$s$” on the parameters, we focus on the collection of inverse models, $S$, which is defined in (2.15), as we are motivated by the inverse conditional densities (2.13) of the GLLiM models. However, our finite-sample oracle inequality, Theorem 3.1, holds for any collection of GLoME models satisfying the required regularity conditions. In particular, Theorem 3.1 can be applied to the forward model $S^\ast = (S^\ast_m)_{m \in M}$, established in (2.16), if we consider $y$ and $x$ as realizations of predictors and response variables, respectively.

### 2.4 Penalized maximum likelihood estimator and losses

In the context of PMLE, given the collection of conditional density $S_m$, we aim to estimate $s_0$ by the $\eta$-minimizer $s_m$ of the negative log-likelihood (NLL):

$$\hat{s}_m = \arg\min_{s_m \in S_m} \sum_{i=1}^n -\ln (s_m (x_i|y_i)) + \eta,$$

where the error term $\eta$ is necessary when the infimum may not be unique or even not be reached.

As always, using the NLL of the estimate in each model as a criterion is not sufficient. It is an underestimation of the risk of the estimate and this leads to choose models that are too complex. By adding an adapted penalty $\text{pen}(m)$, one hopes to compensate between the variance term, $\frac{1}{n} \sum_{i=1}^n -\ln (\hat{s}_m (x_i|y_i))$, and the bias, $\inf_{s_m \in S_m} \text{KL}^\otimes (s_0, s_m)$. For a given choice of $\text{pen}(m)$, the best model $\hat{s}_m$ is chosen as the one whose index is an $\eta'$-almost minimizer of the sum of the NLL and this penalty:

$$\hat{m} = \arg\min_{m \in M} \left( \sum_{i=1}^n -\ln (\hat{s}_m (x_i|y_i)) + \text{pen}(m) \right) + \eta'.$$

Note that $\hat{s}_m$ is then called the $\eta'$-penalized likelihood estimate and depends on both the error terms $\eta$ and $\eta'$. From herein, the term best model or estimate is used to indicate that it satisfies the definition in (2.18).

In the maximum likelihood approach, the Kullback-Leibler divergence is the most natural loss function, which is defined for two densities $s$ and $t$ by

$$\text{KL}(s, t) = \begin{cases} \int_{\mathbb{R}^D} \ln \frac{s(y)}{t(y)} s(y)dy & \text{if } sdy \text{ is absolutely continuous w.r.t. } tdy, \\ +\infty & \text{otherwise.} \end{cases}$$

However, to take into account the structure of conditional densities and the random covariates $(Y_i)_{i \in [n]}$, we consider the tensorized Kullback-Leibler divergence $\text{KL}^\otimes$, defined as:

$$\text{KL}^\otimes (s, t) = \mathbb{E}_Y \left[ \frac{1}{n} \sum_{i=1}^n \text{KL} (s (\cdot|Y_i), t (\cdot|Y_i)) \right],$$

if $sdy$ is absolutely continuous w.r.t. $tdy$, and $+\infty$ otherwise. Note that if the predictors are fixed, this divergence is the classical fixed design type divergence in which there is no expectation. We refer to our result as a weak oracle inequality, because its statement is based on a smaller divergence, when compared to $\text{KL}^\otimes$, namely the tensorized Jensen-Kullback-Leibler divergence,

$$\text{JKL}^\otimes (s, t) = \mathbb{E}_Y \left[ \frac{1}{n} \sum_{i=1}^n \frac{1}{\rho} \text{KL} (s (\cdot|Y_i), (1-\rho) s (\cdot|Y_i) + \rho t (\cdot|Y_i)) \right],$$

if $sdy$ is absolutely continuous w.r.t. $tdy$, and $+\infty$ otherwise.
with \( \rho \in (0, 1) \). We note that JKL\( _\rho^{\otimes n} \) was first used in Cohen & Pennec (2011). However, a version of this divergence appears explicitly with \( \rho = \frac{1}{2} \) in Massart (2007), and it is also found implicitly in Birgé et al. (1998). This loss is always bounded by \( \frac{1}{\rho} \ln \frac{1}{1-\rho} \) but behaves like KL\( _\rho^{\otimes n} \), when \( t \) is close to \( s \). The main tools in the proof of such a weak oracle inequality are deviation inequalities for sums of random variables and their suprema. Those tools require a boundedness assumption on the controlled functions that is not satisfied by \( -\ln \frac{s_m}{s_0} \), and thus also not satisfied by KL\( _\rho^{\otimes n} \). Therefore, we consider instead the use of JKL\( _\rho^{\otimes n} \). In particular, in general, it holds that \( C_\rho d^{2\otimes n} \leq \text{JKL}_{\rho}^{\otimes n} \leq \text{KL}_{\rho}^{\otimes n} \), where \( C_\rho = \frac{1}{\rho} \min \left( \frac{1-\rho}{\rho}, 1 \right) \left( \ln \left( 1 + \frac{1}{1-\rho} \right) - \rho \right) \) (see Cohen & Pennec 2011, Prop. 1), where d\( _{2\otimes n} \) is a tensorized extension of the squared Hellinger distance \( d^{2\otimes n} \), defined by

\[
d^{2\otimes n}(s,t) = \mathbb{E}_Y \left[ \frac{1}{n} \sum_{i=1}^{n} d^2(s(\cdot|Y_i), t(\cdot|Y_i)) \right].
\]

Moreover, if we assume that for any \( m \in \mathcal{M} \) and any \( s_m \in S_m, s_0 d\lambda \ll s_m d\lambda \), then (see Montuelle & Pennec, 2014, Cohen & Pennec, 2011)

\[
\frac{C_\rho}{2 + \ln \|s_0/s_m\|_\infty} \text{KL}_{\rho}^{\otimes n}(s_0, s_m) \leq \text{JKL}_{\rho}^{\otimes n}(s_0, s_m). \tag{2.20}
\]

### 3 Weak oracle inequality

The following result provides a lower bound on the penalty function, \( \text{pen}(m) \), which guarantees that the PMLE selects a model that performs almost as well as the best model.

**Theorem 3.1** (Weak oracle inequality). Assume that we observe \( ((x_i,y_i))_{i\in[n]} \), arising from an unknown conditional density \( s_0 \). Given a collection of GLoME models, \( S = (S_m)_{m\in\mathcal{M}} \), there is a constant \( C \) such that for any \( \rho \in (0, 1) \), for any \( m \in \mathcal{M} \), \( z_m \in \mathbb{R}^+ \), \( \Xi = \sum_{m\in\mathcal{M}} e^{-z_m} < \infty \) and any \( C_1 > 1 \), there is a constant \( \kappa_0 \) depending only on \( \rho \) and \( C_1 \), such that if for every index \( m \in \mathcal{M} \), \( \text{pen}(m) \geq \kappa [(C + \ln n) \dim(S_m) + z_m] \) with \( \kappa > \kappa_0 \), then the \( \eta' \)-penalized likelihood estimate \( \hat{s}_m \), defined in (2.17) and (2.18), satisfies

\[
\mathbb{E} \left[ \text{JKL}_{\rho}^{\otimes n}(s_0, \hat{s}_m) \right] \leq C_1 \inf_{m\in\mathcal{M}} \left( \inf_{s_m \in S_m} \text{KL}_{\rho}^{\otimes n}(s_0, s_m) + \frac{\text{pen}(m)}{n} \right) + \frac{\kappa_0 C_1 \Xi}{n} + \frac{\eta + \eta'}{n}. \tag{3.1}
\]

**Remark 3.2.** As per the SGaME models from Montuelle & Pennec (2014), we also have to deal with three potential issues: the differences of divergence on the left (JKL\( _\rho^{\otimes n} \)) and the right (KL\( _\rho^{\otimes n} \)) hand side, \( C_1 > 1 \), and the relationship between \( \frac{\text{pen}(m)}{n} \) and the variance.

The first issue is important as in general we have JKL\( _\rho^{\otimes n}(s_0, s_m) \leq \text{KL}_{\rho}^{\otimes n}(s_0, s_m) \). However, \( (2.20) \) ensures that the two divergences are equivalent under regularity conditions. Namely, when

\[
\sup_{m\in\mathcal{M}} \sup_{s_m \in S_m} \|s_0/s_m\|_\infty < \infty.
\]

Such a strong assumption is satisfied as long as \( \mathcal{X} \) is compact, \( s_0 \) is compactly supported, and the regression functions are uniformly bounded, and under the condition that there is a uniform lower bound on the eigenvalues of the covariance matrices.

When \( s_0 \notin S \), the error bound converge to \( C_1 \inf_{s_m \in S_m} \text{KL}_{\rho}^{\otimes n}(s_0, s_m) \), which may be large. Nevertheless, as we consider GLoME models, some recent results from Nguyen et al. (2019, 2020a) imply that if we take a sufficiently large number of mixture components, we can approximate a broad class of densities, and thus the term on the right hand side is small for \( K \) sufficiently large. This improves the error bound even when \( s_0 \) does not belong to \( S_m \) for any \( m \in \mathcal{M} \). We aim to provide an oracle inequality with \( C_1 = 1 \) in future work.

For the last issue, we claim that \( \frac{\text{pen}(m)}{n} \) is approximately proportional to the asymptotic variance in the parametric case: \( \frac{\dim(S_m)}{n} \). We shall consider the condition (3.2) for GLoME models. As shown
in the proof of Theorem 3.1, in fact we can replace the assumption on \( \text{pen}(m) \) by a milder one. More precisely, given a constant \( C \), which we specify later, there is a constant \( \kappa_0 \) depending only on \( \rho \) and \( C_1 \), such that with \( \kappa > \kappa_0 \), for every index \( m \in \mathcal{M} \), we may set

\[
\text{pen}(m) \geq \kappa \left( \text{dim}(S_m) \left( 2 \left( \sqrt{\mathcal{C}} + \sqrt{\pi} \right)^2 + \left( \ln \frac{n}{\sqrt{\mathcal{C} + \sqrt{\pi}} \text{dim}(S_m)} \right) \right) + z_m \right). \tag{3.2}
\]

Furthermore, based on the Appendix B.4 from Cohen & Pennec (2011), we can make explicit the dependence of the constant \( \kappa_0 \), with respect to \( \rho \) and \( C_1 \) as follows. For any \( \rho \in (0, 1) \) and \( C_1 > 1 \), define \( \epsilon_{\text{pen}} = 1 - \frac{1}{C_1^3} \). Then \( \kappa_0 \) is determined by

\[
\kappa_0 = \frac{\kappa_0' \left( \kappa_1' + \kappa_2' \right)^2}{2C \rho \epsilon_{\text{pen}}} \left( \sqrt{\frac{1 + \frac{72C \rho \epsilon_{\text{pen}}}{\rho C_1' \left( \kappa_1' + \kappa_2' \right)^2} + 1} \right) + \frac{18}{\rho},
\]

where \( \epsilon_d \) is a given positive constant and

\[
\kappa_0' = \frac{2 (2 + \epsilon_d)}{1 + \epsilon_d}, \kappa_1' = \frac{1}{\sqrt{\rho (1 - \rho)}} \left( 3 \kappa \sqrt{2} + 12 + 16 \sqrt{\frac{1 - \rho}{\rho}} \right), \kappa \leq 27, \kappa_2' = \frac{1}{\sqrt{\rho (1 - \rho)}} \left( 42 + \frac{3}{4 \sqrt{\kappa_0'}} \right).
\]

Note that we only aim to construct an upper bound and do not focus on the important question of the existence of a corresponding lower bound. To the best of our knowledge, providing a minimax analysis of our proposed estimator is still an open question. Furthermore, it is not trivial to extend the lower bound result regarding Gaussian mixtures, as presented in Maugis-Rabusseau & Michel (2013, Theorem 2.8), to the context of GLoME models. However, we wish to provide such minimax analysis in future research.

**Remark 3.3.** The main drawback of the previous weak oracle inequality is using different divergences and requiring some strong assumptions for the inequality to be considered a proper oracle inequality. To illustrate the strictness of the compactness assumption for \( s_0 \), we only need to consider \( s_0 \) as a univariate Gaussian PDF, which obviously does not satisfy such a hypothesis. This motivates us to investigate more an \( l_1 \)-oracle inequality of GLoME with the LASSO estimator, which is an extension of Nguyen et al. (2020c, Theorem 3.1) for SGaME and is considered as a complementary to the Theorem 3.1. In particular, the most intriguing property of the \( l_1 \)-oracle inequality is that it requires only the boundedness assumption of the parameters of the model, which is also required in Theorem 3.1, as well as in Stadler et al. (2010), Meynet (2013), Devijver (2015a), Nguyen et al. (2020c). Note that such a mild assumption is quite common when working with MLE (cf. Baudry 2009, Maugis & Michel 2011), to tackle the problem of the unboundedness of the likelihood at the boundary of the parameter space McLachlan & Peel 2000, Redner & Walker 1984, and to prevent it from diverging. Nevertheless, by using the smaller divergence: JKL\( ^\rho \) (or more strict assumptions on \( s_0 \) and \( s_m \), with the same divergence KLD\( ^n \) as ours), Theorem 3.1 obtain a faster rate of convergence of order \( 1/n \), while in the \( l_1 \)-oracle inequality, we can only obtain a rate of convergence of order \( 1/\sqrt{n} \). Therefore, in the case where there is no guarantee of a compact support of \( s_0 \) or uniformly bounded regression functions, the \( l_1 \)-oracle inequality gives a theoretical foundation for the \( l_1 \)-ball model selection procedure, with the order of convergence of \( 1/\sqrt{n} \), with only the boundedness assumption on the parameter space. However, we leave such nontrivial developments for future work.

**Remark 3.4** (From soft-max to Gaussian gating class). It should be stressed that Theorem 3.1 is a generalization of Theorem 1 from Montuelle & Pennec (2014), when using the linear functions in their logistic scheme. More precisely, such properties can be proved via the following relationship between the soft-max and Gaussian gating classes.
Lemma 3.5 (Lemma 1 from Nguyen et al. 2020a). We denote the space of soft-max and Gaussian gating functions, respectively, as follows

\[ \mathcal{P}_S = \left\{ \mathbf{g} = (g_k(:;\gamma))_{k \in [K]} : \forall k \in [K], \mathbf{g}_k(x;\gamma) = \frac{\exp(a_k + b_k^\top y)}{\sum_{l=1}^K \exp(a_l + b_l^\top y)}, \gamma \in \Gamma_S \right\}, \]

\[ \mathcal{P}_G = \left\{ \mathbf{g} = (g_k(:;\omega))_{k \in [K]} : \forall k \in [K], \mathbf{g}_k(y;\omega) = \frac{\pi_k \Phi_L(y;c_k;\Gamma_k)}{\sum_{j=1}^K \pi_j \Phi_L(y;c_j;\Gamma_j)}, \omega \in \Omega_K \right\}, \]

where \( \Gamma_S = \left\{ \gamma = (a_k)_{k \in [K]}, (b_k)_{k \in [K]} \in \mathbb{R}^K \times (\mathbb{R}^L)^K \right\} \) and \( \Omega_K \) is defined in (2.2). Then, it follows that \( \mathcal{P}_S \subset \mathcal{P}_G \). Furthermore, if we assume that all \( \Gamma_k, k \in [K] \), are identical, then \( \mathcal{P}_G = \mathcal{P}_S \).

4 Numerical experiments

4.1 The procedure

We illustrate our theoretical results in settings similar to those considered by Chamroukhi et al. (2010) and Montuelle & Pennec (2014), regarding simulated as well as real data sets. We first observe \( n \) random samples \((\mathbf{x}_i, y_i)_{i \in [n]}\) from an forward conditional density \( s_0^m \), and look for the best estimate among \( \hat{s}_m \in S_m, m \in M \), defined in (2.16). We considered the simple case where the mean experts are linear functions, which leads to GLoME and supervised GLLiM are identical models and \( \dim(S_m) = \dim(S_m^*) \). Our aim is to estimate the best number of components \( K \), as well as the model parameters. As described in more detail in Deleforge et al. (2015), we use a GLLiM-EM algorithm to estimate the model parameters for each \( K \), and select the optimal model using the penalized approach that was described earlier. More precisely, in the following numerical experiments, the GLoME model is learned using functions from the \( \mathbf{R} \) (R Core Team, 2020) package \texttt{xLLiM}, available on CRAN. It targets to solve the inverse regression problem, defined in (2.13), and obtain the inverse maximum likelihood estimates (MLE) \( (\hat{s}_m^*(\mathbf{x}_i|y_i))_{i \in [N]}, m \in M \), then via (2.14), we obtain the forward MLE \( (\hat{s}_m^*(\mathbf{y}_i|\mathbf{x}_i))_{i \in [N]}, m \in M \).

According to the general procedure for model selection, we first compute the forward MLE for each number of components \( K \). Then, we select the model that satisfies the definition (2.18) with \( \text{pen}(m) = \kappa \dim(S_m^*) \), where \( \kappa \) is a positive hyperparameter. In particularly, we need a data-driven method to choose \( \kappa \), even though our Theorem 3.1 and Remark 2.2 guarantee that there exists a \( \kappa \) large enough for which the estimate has the desired properties. According to the AIC or the BIC, we can select \( \kappa = 1 \) or \( \kappa = \frac{L \cdot n}{2} \). An important limitation of these criteria, however, is that they are asymptotic. To overcome this difficulty, the slope heuristic was proposed by Birgé & Massart (2007) (see, also Baudry et al. 2012). Furthermore, our Theorem 3.1 provides support for the slope heuristic approach in a finite sample setting. Thus, we shall concentrate our attention on the slope heuristic for choosing the number of mixture components in our numerical experiments.

4.2 Simulated data sets

Note that our main objective here is to investigate how well the empirical tensorized Kullback-Leibler divergence between the true model \( (s_m^*) \) and the selected model \( \hat{s}_m^* \) follows the finite-sample oracle inequality of Theorem 3.1, as well as the rate of convergence of the error term. Therefore, we focus on 1-dimensional data sets, that is, with \( L = D = 1 \). Beyond the statistical estimation and model selection objectives considered here, the dimensionality reduction capability of GLLiM in high-dimensional regression data, typically \( D \gg L \), can be found in (Deleforge et al., 2015, Section 6).

We construct simulated data sets following two scenarios: a well-specified (WS) case in which the
4.2 Simulated data sets

true forward conditional density belongs to the class of proposed models:

\[ s^*_0(y|x) = \frac{\Phi(x; 0.2, 0.1)}{\Phi(x; 0.2, 0.1) + \Phi(x; 0.8, 0.15)} \Phi(y; -5x + 2, 0.09) \]

\[ + \frac{\Phi(x; 0.8, 0.15)}{\Phi(x; 0.2, 0.1) + \Phi(x; 0.8, 0.15)} \Phi(y; 0.1x, 0.09), \]

and a misspecified (MS) case, whereupon such an assumption is not true:

\[ s^*_0(y|x) = \frac{\Phi(x; 0.2, 0.1)}{\Phi(x; 0.2, 0.1) + \Phi(x; 0.8, 0.15)} \Phi(y; x^2 - 6x + 1, 0.09) \]

\[ + \frac{\Phi(x; 0.8, 0.15)}{\Phi(x; 0.2, 0.1) + \Phi(x; 0.8, 0.15)} \Phi(y; -0.4x^2, 0.09). \]

Figures 1a and 1e show some typical realizations of 2000 data points arising from the WS and MS scenarios. Note that by using GLoME, our estimator performs well in the WS setting (Figures 1b to 1d). In the MS case, we expect our algorithm to automatically balance the model bias and its variance (Figures 1f to 1h), which leads to the choice of a complex model, with 4 mixture components. This observation will be elaborated upon in the subsequent experiments.

Firstly, by using the capushe (CAlibrating Penalities Using Slope HEuristics) package in R (Baudry et al., 2012), we can select the penalty coefficient, along with the number of mixture components \( K \). This heuristic comprises two possible criteria: the slope criterion and the jump criterion. The first criterion consists of computing the asymptotic slope of the log-likelihood (Figure 2), drawn according to the model dimension, and then penalizing the log-likelihood by twice the slope times the model dimension. Regarding the second criterion, one aims to represent the dimension of the selected model according to \( \kappa \) (Figure 3), and find \( \hat{\kappa} \), such that if \( \kappa < \hat{\kappa} \), then the dimension of the selected model is large, and of reasonable size, otherwise. The slope heuristic prescribes then the use of \( \kappa = 2\hat{\kappa} \). In our simulated data sets, Figure 4 shows that the jump criterion appears to work better. The slope criterion sometimes chooses very highly complex models in the WS case, with the problem exacerbated in the MS case.

Next, a close inspection shows that the bias-variance trade-off differs between the two examples. We run our experiment over 100 trials with \( K \in [20] \), using both the jump and slope criteria. The first remark is that the best choice of \( K = 2 \) appears to be selected with very high probability, even for large \( n = 10000 \) in the WS case. This can be observed in Figures 4a, 4b, 4e and 4f. In the MS case, the best choice for \( K \) should balance between the model approximation error term and the variance one, which is observed in Figures 4c, 4d, 4g and 4h. Here, the larger the number of samples \( n \), the larger the value of \( K \) that is selected as optimal.

From hereon in, we focus on the jump instead of slope criterion, due to its stability regarding the choice of \( K \). We wish to measure the performances of our chosen GLoME models in terms of tensorized Kullback-Leibler divergence, \( \text{KL}^\otimes \), which can not be calculated exactly in the case of Gaussian mixtures. Therefore, we evaluate the divergence using a Monte Carlo simulation, since we know the true density. We should note that the variability of this randomized approximation has been verified to be negligible in practice, which is also supported in the numerical experiments by Montuelle & Pennec (2014). More precisely, we compute the Monte Carlo approximation for the tensorized Kullback-Leibler divergence as follows. First, note that the Monte Carlo approximation for tensorized Kullback-Leibler divergence between the true model \( (s^*_0) \) and the selected model \( \hat{s}^*_m \) can be approximated as

\[ \text{KL}^\otimes (s^*_0, \hat{s}^*_m) = \mathbb{E}_X \left[ \frac{1}{n} \sum_{i=1}^{n} \text{KL} (s^*_0 (\cdot | x_i), \hat{s}^*_m (\cdot | x_i)) \right] \]

\[ \approx \frac{1}{n} \sum_{i=1}^{n} \text{KL} (s^*_0 (\cdot | x_i), \hat{s}^*_m (\cdot | x_i)) \text{ (using 1 data point to approximate } \mathbb{E}_X [\cdot]) \]

\[ = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_y} \sum_{j=1}^{n_y} \ln \left( \frac{s^*_0 (y_{i,j} | x_i)}{\hat{s}^*_m (y_{i,j} | x_i)} \right), \]
4.2 Simulated data sets

Figure 1: Clustering deduced from the estimated conditional density of GLoME by a MAP principle with 2000 data points of example WS and MS. The dash and solid black curves present the true and estimated mean functions.
4.2 Simulated data sets

where the data $x_i, i \in [n]$, and $(y_{ij})_{j \in [n]}$ are drawn from $s_0^* (\cdot | x_i)$. Then, $\mathbb{E} [\text{KL}^{\otimes n} (s_0^*, \hat{s}_m^*)]$ is approximated again by averaging over $N_t = 100$ Monte Carlo trials. Therefore, the simulated data used for approximation can be written as $(x_i, y_{ij})$ with $i \in [n], j \in [n_y], t \in [N_t]$

Based on the approximation, Figure 5 shows the box plots and the mean of the tensorized Kullback-Leibler divergence over 100 trials, based on the jump criterion. Our box-plots confirm that the mean tensorized Kullback-Leibler divergence between $\hat{s}_K^*$ and $s_0^*$, over $K \in \{1, \ldots, 20\}$ number of mixture components, is always larger than the mean of tensorized Kullback-Leibler divergence between the penalized estimator $\hat{s}_K^*$ and $s_0^*$, which is consistent with Theorem 3.1. In particularly, if the true model belongs to our nested collection, the mean tensorized Kullback-Leibler divergence seems to behave like $\frac{\dim(S_m^*)}{2n}$ (shown by a dotted line), which can be explained by the AIC heuristic. More precisely, we firstly assume that

$$S_m^* = \{ \mathcal{X} \times \mathcal{Y} \ni (x, y) \mapsto s_m^* := s_{\psi_m^*}^* (y | x) : \psi_m^* \in \Psi_m \subset \mathbb{R}^{\dim(S_m^*)} \}$$

is identifiable and make some strong regularity assumptions on $\psi_m^* \mapsto s_{\psi_m^*}$. Further, we assume the existence of $\dim(S_m^*) \times \dim(S_m^*)$ matrices $\mathbf{A} (\psi_m^*)$ and $\mathbf{B} (\psi_m^*)$, which are defined as follows:

$$[\mathbf{A} (\psi_m^*)]_{k,l} = \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \int -\frac{\partial^2}{\partial \psi_{m,k}^* \partial \psi_{m,l}^*} s_{\psi_m^*}^* (y | x_i) s_0^* (y | x_i) dy \right],$$

$$[\mathbf{B} (\psi_m^*)]_{k,l} = \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \int \frac{\partial}{\partial \psi_{m,k}^*} s_{\psi_m^*}^* (y | x_i) \frac{\partial}{\partial \psi_{m,l}^*} s_{\psi_m^*}^* (y | x_i) s_0^* (y | x_i) dy \right].$$

Then, the results from White (1982) and Cohen & Pennec (2011) imply that $\mathbb{E} [\text{KL}^{\otimes n} (s_0^*, \hat{s}_m^*)]$ is asymptotically equivalent to

$$\text{KL}^{\otimes n} (s_0^*, s_{\psi_m^*}) + \frac{1}{2n} tr \left( \mathbf{B} (\psi_m^*) \mathbf{A} (\psi_m^*)^{-1} \right),$$

where we defined $\psi_m^* = \text{argmin}_{s_{\psi_m} \in S_m^*} \text{KL}^{\otimes n} (s_{\psi_m}, s_{\psi_m^*})$.

In particular, $\mathbb{E} [\text{KL}^{\otimes n} (s_0^*, \hat{s}_m^*)]$ becomes asymptotically equivalent to $\frac{1}{2n} \dim(S_m^*)$, whenever $s_0^*$ belongs to the model collection $S_m^*$. Furthermore, even though there is no theoretical guarantee, the
4.2 Simulated data sets

| Values of the penalty constant $\kappa$ | Selected Complexity (Model) |
|---------------------------------------|-----------------------------|
| 11 (2)                                | $\kappa^d_j$ $\kappa_{opt}$ 0 0.14 0.84 1.4 1.7 |
| 17 (3)                                |                             |
| 59 (10)                               |                             |
| 113 (19)                              |                             |
| 119 (20)                              |                             |

Maximal Jump

(a) Example WS with 2000 data points

(b) Example MS with 2000 data points

(c) Example WS with 10000 data points

(d) Example MS with 10000 data points

Figure 3: Plot of the selected model dimension using the jump criterion.
4.2 Simulated data sets

Figure 4: Comparison histograms of selected $K$ between WS and MS cases using jump and slope criteria over 100 trials.
2.3.5 Example WS with 2000 data points

Figure 5: Box-plot of the tensorized Kullback-Leibler divergence according to the number of mixture components using the jump criterion over 100 trials. The tensorized Kullback-Leibler divergence of the penalized estimator $\tilde{s}_K$ is shown in the right-most box-plot of each graph.

The slope of the mean error in the misspecified case seems also to grow at the same rate as $\frac{\dim(S_m)}{2n}$, for large enough number of mixture components ($K \geq 6$ in the WS case and $K \geq 9$ in the MS case).

Figure 6 shows that the error decays when the sample size $n$ grows, when using the penalty based on the jump criterion. The first remark is that we observed the error decay is of order $t/n$, as predicted in by the theory, where $t$ is some constant, as expected in the well-specified case. The rate of convergence for the misspecified case seems to be slower.

4.3 Ethanol data set

We now consider the use of GLoME models for performing clustering and regression tasks on a real data set. Following the numerical experiments from Young (2014) and Montuelle & Pennec (2014), we demonstrate our model on the ethanol data set of Brinkman (1981). The data comprises of 88 observations, which represent the relationship between the engine’s concentration of nitrogen oxide (NO) emissions and the equivalence ratio (ER), a measure of the air-ethanol mix, used as a spark-ignition engine fuel in a single-cylinder automobile test (Figures 8a and 8e). Our goal is then to estimate the parameters of a GLoME model, as well as the number of mixture components.

More precisely, we first use the EM algorithm from the xLLiM package to compute the forward PMLE of (2.1), for each $K \in [12]$, on the Ethanol data set. Then, based on the slope heuristic (Figure 7), we select the best model. Given the estimators of the model chosen, we obtain the estimated conditional density and clustering by applying the maximum a posteriori probability (MAP) rule (Figures 8 and 9).

Because we only have 88 data points and roughly 6 parameters per class, the EM algorithm is strongly dependent on the random initialization of the parameters. One solution is that we can modify slightly that procedure in order to guarantee that at least 10 points are assigned to each
(a) WS Example: The slope of the free regression line is ≈ −1.287 and \( t = 3 \).

(b) MS Example: The slope of the free regression line is ≈ −0.6120 and \( t = 20 \).

Figure 6: Tensorized Kullback-Leibler divergence between the true and selected densities based on the jump criterion, represented in a log-log scale, using 30 trials. A free least-square regression with standard error and a regression with slope \(-1\) were added to stress the two different behavior for each graph.

class so that the estimated parameters are more stable (cf. Montuelle & Pennec 2014). In this work, we wish to investigate how well our proposed PMLE performs for detecting the best number of mixture components for the GLoME model. Thus, we run our experiment over 100 trials with different initializations for the EM algorithm. Histograms of selected values of \( K \) are presented in Figures 7a to 7d. Notice that it is quite unlikely that the true conditional PDF of Ethanol data set belongs to our hypothesised collection of GLoME models. In fact, this phenomenon has been observed in the MS case, Figure 4, on the simulated data set. We think this is due to the simplistic affine models used in our experiments. Furthermore, it seems that the jump criterion outperformed the slope criterion in the stability of order selection for GLoME models, as previously observed.

Based on the highest empirical probabilities in all situations, our procedure selects \( K = 4 \) components, which is consistent with the results from Montuelle & Pennec (2014). It is worth noting that if we consider the regression of NO with respect to ER, our proposed PMLE of GLoME performs very well for both the clustering and regression tasks (Figure 9). Here, instead of considering the variable NO as the covariate, we use it as the response variable. Then, the resulting clustering, the estimated mean function (black curve) and mixing probabilities are more easily interpretable. This is very similar to the results obtained in Montuelle & Pennec (2014).

### 5 Proofs of the weak oracle inequality

To work with conditional density estimation in the GLoME regression models, in Section 5.1, we need to present a general theorem for model selection, Theorem 5.1, a generalization of Theorem 7.11 from Massart (2007), from Cohen & Pennec (2011, Theorem 2) and Montuelle & Pennec (2014, Theorem 2). Then, we explain how we can use Theorem 5.1 to obtain the oracle inequality Theorem 3.1 in Section 5.2. To this end, our model collection has to satisfy some regularity assumptions, which is proved in Appendix A.2 and Appendix A.3. The main difficulty to proving our weak oracle inequality lies in bounding the bracketing entropy of the Gaussian gating functions of the GLoME model. To overcome this difficulty, we propose a reparameterization trick to bound the metric entropy of the
Figure 7: Histogram of selected $K$ of GLoME on Ethanol data set based on NO and ER using slope heuristic. We plot the jump and slope criteria corresponding to the models chosen with highest empirical probabilities.
Figure 8: Estimated conditional density with 4 components based upon on the covariate NO or ER from the Ethanol data set.
5.1 General model selection for conditional density

Before stating a general model selection for conditional density, we have to present some regularity assumptions.

First, we need an information theory type assumption to control the complexity of our collection. We assume the existence of a Kraft-type inequality for the collection (Massart, 2007, Barron et al., 2008).

**Assumption 5.1 (K).** There is a family \( (z_m)_{m \in M} \) of non-negative numbers and a real number \( \Xi \) such that

\[
\Xi = \sum_{m \in M} e^{-z_m} < +\infty.
\]

For technical reasons, a seperability assumption always satisfied in the setting of this paper, is also required. It is a mild condition which is classical in empirical process theory (Van Der Vaart & Wellner, 1996). This assumption allows us to work with a countable subset.

**Assumption 5.2 (Sep).** For every model \( S_m \) in the collection \( S \), there exists some countable subset \( S'_m \) of \( S_m \) and a set \( \mathcal{X}'_m \) with \( \iota(\mathcal{X} \setminus \mathcal{X}'_m) = 0 \), here \( \iota \) denotes Lebesgue measure, such that for every \( t \in S_m \), there exists some sequence \( (t_k)_{k \geq 1} \) of elements of \( S'_m \), such that for every \( y \in \mathcal{Y} \) and every \( x \in \mathcal{X}'_m \),

\[
\ln(t_k(x|y)) \xrightarrow{k \to +\infty} \ln(t(x|y)).
\]

Next, recall that the bracketing entropy of a set \( S \) with respect to any distance \( d \), denoted by \( H_{[\cdot],d}((\delta, S)) \), is defined as the logarithm of the minimal number \( N_{[\cdot],d}((\delta, S)) \) of brackets \([t^-, t^+]\) covering \( S \), such that \( d(t^-, t^+) \leq \delta \). That is,

\[
N_{[\cdot],d}((\delta, S)) := \min \left\{ n \in \mathbb{N}^* : \exists t_k^-, t_k^+, \ldots, t_n^-, t_n^+ \text{ s.t. } d(t_k^-, t_k^+) \leq \delta, S \subset \bigcup_{k=1}^n [t_k^-, t_k^+] \right\}, \tag{5.1}
\]
where the bracket \( s \in [t_k^-, t_k^+] \) is defined by \( t_k^-(x, y) \leq s(x, y) \leq t_k^+(x, y) \), \( \forall (x, y) \in \mathcal{X} \times \mathcal{Y} \).

We also need the following important assumption on Dudley-type integral of these bracketing entropies, which is utilized often in empirical process theory (Van Der Vaart & Wellner, 1996; Kosorok, 2007).

**Assumption 5.3 (H).** For every model \( S_m \) in the collection \( \mathcal{S} \), there is a non-decreasing function \( \phi_m \) such that \( \delta \mapsto \frac{1}{\sigma} \phi_m(\delta) \) is non-increasing on \((0, \infty)\) and for every \( \sigma \in \mathbb{R}^+ \),

\[
\int_0^\sigma \sqrt{\mathcal{H}_{\|\cdot\|_{\delta^n}}(\delta, S_m(\tilde{s}, \sigma))} d\delta \leq \phi_m(\sigma),
\]

where \( S_m(\tilde{s}, \sigma) = \{s_m \in S_m : d^n(\tilde{s}, s_m) \leq \sigma\} \). The complexity of \( S_m \) is then defined as \( n \sigma_m^2 \), where \( \sigma_m \) is the unique root of \( \frac{1}{\sigma} \phi_m(\sigma) = \sqrt{n} \sigma \).

Observe that the model complexity does not depend on the bracketing entropies of the global models \( S_m \), but rather on those of smaller localized sets \( S_m(\tilde{s}, \sigma) \). Now we are able to state an important weak oracle inequality from Cohen & Pennec (2011).

**Theorem 5.1** (Theorem 2 from Cohen & Pennec 2011). Assume that we observe \((x_i, y_i)\)\(i \in [n]\), arising from an unknown conditional density \(s_0\). Let \( S = (S_m)_{m \in M} \) be an at most countable conditional density model collection. Assume that Assumption 5.1 (K), Assumption 5.2 (Sep), and Assumption 5.3 (H) hold for every model \( S_m \in S \). Then, for any \( p \in (0, 1) \) and any \( C_1 > 1 \), there is a constant \( \kappa_0 \) depending only on \( p \) and \( C_1 \), such that for every index \( m \in M \),

\[
\text{pen}(m) \geq \kappa (n \sigma_m^2 + z_m)
\]

with \( \kappa > \kappa_0 \) and \( \sigma_m \) is the unique root of \( \frac{1}{\sigma} \phi_m(\sigma) = \sqrt{n} \sigma \), such that the \( \eta' \)-penalized likelihood estimate \( \hat{s}_m \) satisfies

\[
\mathbb{E} [\text{JKL}^\infty_p (s_0, \hat{s}_m)] \leq C_1 \inf_{m \in M} \left( \inf_{s_m \in S_m} \text{KL}^\infty_n (s_0, s_m) + \frac{\text{pen}(m)}{n} \right) + \frac{\kappa_0 C_1 \Xi}{n} + \frac{\eta + \eta'}{n}. \tag{5.2}
\]

### 5.2 Proof of the Theorem 3.1

**Sketch of the proof of the Theorem 3.1** To prove Theorem 3.1, we need to apply Theorem 5.1. Then, our model collection has to satisfy Assumption 5.1 (K), Assumption 5.2 (Sep), and Assumption 5.3 (H). Since our model is defined by \( m = K \in K = [K_{\text{max}}] \), the Assumption 5.1 (K) is always satisfied. It is interesting to find the best family \((z_m)_{m \in M}\) satisfying Assumption 5.1 (K), but that is beyond the scope of this paper. The Assumption 5.2 (Sep) is true when we consider Gaussian densities. Therefore, our model has only to satisfy the remaining Assumption 5.3 (H). Here, we only present the main steps to prove the Assumption 5.3 (H). All the technical details are deferred to Appendix A.2 and Appendix A.3. It is worth noting that a similar procedure has been proposed by Montuelle & Pennec (2014) in the context of SGaME models.

Firstly, we require the following distance over conditional densities:

\[
\sup_y d_x(s, t) = \sup_{y \in Y} \left( \int_{\mathcal{X}} \left( \sqrt{s(x|y)} - \sqrt{t(x|y)} \right)^2 dx \right)^{1/2}.
\]

This leads straightforwardly to \( d^{2\infty}(s, t) \leq \sup_y d_x^2(s, t) \). Then, we also define

\[
\sup_{y \in Y} d_k(g, g') = \sup_{y \in Y} \left( \frac{1}{K} \sum_{k=1}^K \left( \sqrt{g_k(y)} - \sqrt{g'_k(y)} \right)^2 \right)^{1/2},
\]

for any gating functions \( g \) and \( g' \). To this end, given any densities \( s \) and \( t \) over \( \mathcal{X} \), the following distance, depending on \( y \), is constructed as follows:

\[
\sup_{y \in Y} d_k(s, t) = \sup_{k \in [K]} d_k(s_k(\cdot, y), t_k(\cdot, y)) = \sup_{y \in Y} \left( \int_{\mathcal{X}} \left( \sqrt{s_k(x, y)} - \sqrt{t_k(x, y)} \right)^2 dx \right)^{1/2}.
\]

Note that definition of complexity of model \( S_m \) in Assumption 5.3 (H) is related to an classical entropy dimension with respect to a Hellinger type divergence \( d^{\infty} \), due to Proposition 5.2.
Proposition 5.2 (Proposition 2 from Cohen & Pennec 2011). For any $\delta \in (0, \sqrt{2}]$, such that $\mathcal{H}_{\|.,d\|_\infty} (\delta, S_m) \leq \dim(S_m) \left( C_m + \ln \left( \frac{1}{\eta} \right) \right)$, the function
\[
\phi_m (\sigma) = \sigma \sqrt{\dim(S_m)} \left( \sqrt{C_m + \sqrt{\pi} + \sqrt{\ln \left( \frac{1}{\min(\sigma, 1)} \right)} } \right)
\]
satisfies Assumption 5.3 (H). Furthermore, the unique solution $\sigma_m$ of $\frac{1}{\sigma} \phi_m (\sigma) = \sqrt{m} \sigma$, satisfies
\[
ns_m^2 \leq \dim(S_m) \left( 2 \left( \sqrt{C_m + \sqrt{\pi}} \right)^2 + \left( \ln \frac{n}{\sqrt{C_m + \sqrt{\pi}}} \right)^2 \dim(S_m) \right).
\]
Therefore, Proposition 5.2 implies that Assumption 5.3 (H) is proved via Lemma 5.3.

Lemma 5.3. For any $\delta \in (0, \sqrt{2}]$, the collection of GLoME models, $S = (S_m)_{m \in \mathcal{M}}$, satisfies
\[
\mathcal{H}_{\|.,d\|_\infty} (\delta, S_m) \leq \dim(S_m) \left( C_m + \ln \left( \frac{1}{\delta} \right) \right).
\]

Lemma 5.3 is then obtained by decomposing the entropy terms between the Gaussian gating functions and the Gaussian experts. For the Gaussian gating parameters, the technique for handling the logistic weights of Montuelle & Pennec (2014) is not directly applicable to the GLoME setting. Therefore, we propose the following reparameterization trick of the Gaussian gating space $\mathcal{P}_K$:
\[
\mathcal{W}_K = \left\{ Y \ni y \mapsto (\ln (\pi_k \Phi_L (y; c_k, \Gamma_k)))_{k \in [K]} =: (w_k(y; \omega))_{k \in [K]} = w(y; \omega) : \omega \in \Omega_K \right\}, \quad \mathcal{P}_K = \left\{ Y \ni y \mapsto \left( \frac{e^{w_k(y)}}{\sum_{l=1}^K e^{w_l(y)}} \right)_{k \in [K]} =: (g_{w,k}(y))_{k \in [K]} , w \in \mathcal{W}_K \right\}.
\]
We also require the definition of metric entropy of the set $\mathcal{W}_K$: $\mathcal{H}_{\|.,d\|_\infty} (\delta, \mathcal{W}_K)$, and of the set $\mathcal{Y}_K$: $\mathcal{H}_{\|.,d\|_\infty} (\delta, \mathcal{Y}_K)$, which measure the logarithm of the minimal number of balls of radius at most $\delta$, according to a distance $d_{\|,sup\|_\infty}$, needed to cover $\mathcal{W}_K$ and $\mathcal{Y}_K$, respectively, where
\[
d_{\|,sup\|_\infty} \left( (s_k)_{k \in [K]} , (t_k)_{k \in [K]} \right) = \sup_{k \in [K]} \|s_k(y) - t_k(y)\|_2, \quad \text{for any } K\text{-tuples of functions } (s_k)_{k \in [K]}\text{ and } (t_k)_{k \in [K]).
\]
Here, $s_k, t_k : Y \ni y \mapsto s_k(y), t_k(y) \in \mathbb{R}^L, \forall k \in [K]$, and given $y \in X, k \in [K]$, $\|s_k(y) - t_k(y)\|_2$ is the Euclidean distance in $\mathbb{R}^L$.

Since $\sum_{k=1}^K g_{w,k}(y) = 1, \forall y \in Y, \forall w \in \mathcal{W}_K$, Lemma 5.3 is proved due to the following Lemma 5.4 by using the fact that $H_{\|.,d\|_\infty} (\delta, S_m) \leq \mathcal{H}_{\|.,sup\|_\infty} (\delta, S_m)$, which is obtained by definition of bracketing entropy and $d_{\|,sup\|_\infty}(s,t) \leq \max_{\mathcal{Y}} d_K(s,t)$.

Lemma 5.4 (Lemma 5 from Montuelle & Pennec 2014). Let
\[
\mathcal{W}_K = \left\{ Y \ni y \mapsto (\ln (\pi_k \Phi_L (y; c_k, \Gamma_k)))_{k \in [K]} =: (w_k(y; \omega))_{k \in [K]} = w(y; \omega) : \omega \in \Omega_K \right\}, \quad \mathcal{P}_K = \left\{ Y \ni y \mapsto \left( \frac{e^{w_k(y)}}{\sum_{l=1}^K e^{w_l(y)}} \right)_{k \in [K]} =: (g_{w,k}(y))_{k \in [K]} , w \in \mathcal{W}_K \right\}, \quad \text{and}
\]
\[
\mathcal{G}_K = \left\{ X \ni (x,y) \mapsto (\Phi_D (x; v_k(y), \Sigma_k))_{k \in [K]} : v \in \mathcal{Y}_K, \Sigma \in \mathcal{V}_K \right\}.
\]
For all $\delta \in (0, \sqrt{2}]$ and $m \in \mathcal{M}$,
\[
\mathcal{H}_{\|.,sup\|_\infty} (\delta, S_m) \leq \mathcal{H}_{\|.,sup\|_\infty} \left( \frac{\delta}{5}, \mathcal{P}_K \right) + \mathcal{H}_{\|.,sup\|_\infty} \left( \frac{\delta}{5}, \mathcal{G}_K \right).
\]
By making use of the Lemma 5.4, the remaining task is to control the bracketing entropy of the Gaussian gating functions and experts separately via Lemmas 5.5 and 5.6, which are proved in Appendices A.2 and A.3, respectively.

**Lemma 5.5.** For all $\delta \in (0, \sqrt{2}]$, there exists a constant $C_W^K$ such that

$$H[\cdot, \sup_y d_k \left( \frac{\delta}{5}, P^K \right)] \leq H\left[ d_{\sup y, \infty} \left( \frac{3\sqrt{3}\delta}{20\sqrt{K}}, W^K \right) \right] \leq \dim(W^K) \left( C_W^K + \ln \left( \frac{20\sqrt{K}}{3\sqrt{3}\delta} \right) \right).$$

**Lemma 5.6.** For all $\delta \in (0, \sqrt{2}]$, there exists a constant $C_G^K$ such that

$$H[\cdot, \sup_y \max_k d_x \left( \frac{\delta}{5}, G^K \right)] \leq \dim(G^K) \left( C_G^K + \ln \left( \frac{1}{\delta} \right) \right).$$

(5.5)

To this end, Lemma 5.4 allows us to conclude that given $C = C_W^K + \ln \left( \frac{5K_{\max} \sqrt{K_{\max}}}{4\sqrt{\pi}} \right) + C_G^K$,

$$H[\cdot, \sup_y d_k \left( \frac{\delta}{5}, P^K \right)] + H[\cdot, \sup_y \max_k d_x \left( \frac{\delta}{5}, G^K \right)] \leq \dim(S_m) \left( C + \ln \left( \frac{1}{\delta} \right) \right).$$

Then, Proposition 5.2 leads to

$$n \sigma_m^2 \leq \dim(S_m) \left( 2 \left( \sqrt{C} + \sqrt{\pi} \right)^2 + \left( \ln \frac{n}{\left( \sqrt{C} + \sqrt{\pi} \right)^2 \dim(S_m)} \right)^+ \right).$$

Finally, Theorem 5.1 implies that for any given collection of GLoME models $S = (S_m)_{m \in \mathcal{M}}$, the oracle inequality of Theorem 3.1 is satisfied when

$$\text{pen}(m) \geq \kappa \left( \dim(S_m) \left( 2 \left( \sqrt{C} + \sqrt{\pi} \right)^2 + \left( \ln \frac{n}{\left( \sqrt{C} + \sqrt{\pi} \right)^2 \dim(S_m)} \right)^+ \right) + z_m \right).$$

### 6 Conclusion and perspectives

We have studied the PMLE for GLoME regression models. Our main contribution is the proof of a weak oracle inequality that provides lower bounds on the penalty that ensures non-asymptotic control of the Kullback-Leibler loss. Furthermore, aside from important theoretical issues regarding the tightness of the bounds of the PMLE, we hope that our contribution helps to popularize GLoME models, as well as GLLiM models and and slope heuristics, by giving some theoretical foundations for model selection technique in this area and demonstrating some interesting numerical schemes and experiments. In particular, we aim to provide an extension of the finite-sample oracle inequality, Theorem 3.1, to a more general framework where Gaussian experts are replaced by the elliptical distributions in the future work.

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Appendix: Lemma proofs

A.1 Proof of Lemma 2.1

In Appendix A.1, we aim to provide the proof of one-to-one correspondence defines the link between the inverse and forward conditional distributions not only for the special case of Gaussian distribution in (2.14) but also for elliptical distributions (cf. Cambanis et al., 1981, Fang et al., 1990). It is worth mentioning that the multivariate normal distribution, multivariate \( \text{in} (2.14) \) but also for elliptical distributions (cf. Cambanis et al., 1981, Fang et al., 1990). It is worth the inverse and forward conditional distributions not only for the special case of Gaussian distribution

In Appendix A.1, we aim to provide the proof of one-to-one correspondence defines the link between

A.1 Proof of Lemma 2.1

A Appendix: Lemma proofs

A.1.1 Elliptically symmetric distributions

Note that we will provide the proof of Lemma 2.1 by using some general results regarding elliptical distributions.

Definition A.1. Let \( X \) be a \( D \)-dimensional random vector. Then \( X \) is said to be elliptically distributed (or simply elliptical) if and only if there exist a vector \( \mu \in \mathbb{R}^D \), a positive semidefinite matrix \( \Sigma \in \mathbb{R}^{D \times D} \) and a function \( \phi : \mathbb{R}^+ \to \mathbb{R} \) such that the characteristic function \( t \mapsto \phi_{X - \mu}(t) \) of \( X - \mu \) corresponds to \( t \mapsto \phi(t^\top \Sigma t) \), \( t \in \mathbb{R}^D \). We write \( X \sim \mathcal{E}_D(\mu, \Sigma, \phi) \) to denote that \( X \) is elliptical.

The function \( \phi \) is referred to as the characteristic generator of \( X \). When \( D = 1 \) the class of elliptical distributions coincides with the class of univariate symmetric distributions. Thanks to Proposition 1 from Frahm (2004), it holds that every affinely transformed elliptical random vector is elliptically distributed. Moreover, the following stochastic representation theorem, Theorem A.2, shows that the converse is true if the transformation matrix has full rank.

Theorem A.2 (Theorem 1 from Cambanis et al., 1981). Let \( X \) be a \( D \)-dimensional random vector. Then \( X \sim \mathcal{E}_D(\mu, \Sigma, \phi) \) with \( \text{rank}(\Sigma) = k \) if and only if

\[
X = \mu + \mathcal{R} \Lambda U^{(k)},
\]

where \( U^{(k)} \) is a \( k \)-dimensional random vector uniformly distributed on the unit hypersphere with \( k - 1 \) dimensions \( S^{k-1} = \{ x \in \mathbb{R}^D : \|x\|_2 = 1 \} \), \( \mathcal{R} \) is a non-negative random variable with distribution function \( F \) related to \( \phi \) being stochastically independent of \( U^{(k)} \), \( \mu \in \mathbb{R}^D \) and \( \Sigma = \Lambda \Lambda^\top \) is a rank factorization of \( \Sigma \) where \( \Lambda \in \mathbb{R}^{D \times k} \) with \( \text{rank}(\Lambda) = k \).

Note that via the transformation matrix \( \Lambda \), the spherical random vector \( U^{(k)} \) produces elliptically contoured density surfaces, whereas the generating random variable \( \mathcal{R} \) determines the distribution’s shape, in particular the heaviness of the distribution’s tails. Further, \( \mu \) determines the location of the random vector \( X \). The matrix \( \Sigma \) is called the dispersion matrix or scatter matrix of \( X \). Therefore, it holds that every elliptical distribution belongs to a location-scale-family (Kelker, 1970) defined by an underlying spherical standard distribution.

Example A.3 (Multivariate normal distribution). Let \( \mu \in \mathbb{R}^D \) and \( \Lambda \in \mathbb{R}^{D \times k} \) such that \( \Sigma := \Lambda \Lambda^\top \in \mathbb{R}^{D \times D} \) is positive definite. The random vector \( X \sim \mathcal{F}_D(\mu, \Sigma) \) is elliptically distributed since \( X \) is representable as \( X = \mu + \sqrt{\chi_k^2/\lambda_k} \Lambda U^{(k)} \). The underlying spherical standard distribution is the standard normal distribution. Further, since \( s \mapsto \exp(-s/2) \) is the characteristic generator for the class of normal distributions, the characteristic function of \( X - \mu \) corresponds to \( t \mapsto \phi_{X - \mu}(t) = \exp(-t^\top \Sigma t) \), \( t \in \mathbb{R}^D \).

We next describe some important results on the conditional distributions of elliptical random vectors (cf. Cambanis et al., 1981, Corollary 5, Frahm, 2004, Chapter 1).

Theorem A.4. Let \( X \sim \mathcal{E}_D(\mu, \Sigma, \phi) \) with \( \text{rank}(\Sigma) = k \). It holds that:
(a) \( \mathbb{E}(X) = \mu. \)

(b) \( \text{var}(X) = \frac{\mathbb{E}(X^2)}{k} - \mathbb{E}(X)^2 = -2\phi'(0)\Sigma, \) if \( \phi \) is differentiable at 0.

(c) The sum of independent elliptically distributed random vector with the same dispersion matrix \( \Sigma \) is elliptically too. Furthermore, the sum of two dependent elliptical random vectors with the same dispersion matrix, which are dependent only through their radial parts \( R \), is also elliptical (Hult & Lindskog, 2002, Theorem 4.1). More precisely, let \( R \) and \( \tilde{R} \) be nonnegative random variables and let \( X := \mu + RZ \sim \mathcal{E}_D(\mu, \Sigma, \phi) \) and \( \tilde{X} := \mu + \tilde{R}\tilde{Z} \sim \mathcal{E}_D(\mu, \Sigma, \phi) \), where \( (R, \tilde{R}), Z, \) and \( \tilde{Z} \) are independent. Then \( X + \tilde{X} \sim \mathcal{E}_D(\mu + \mu, \Sigma, \phi^*). \)

(d) Affine transformation: every affinely transformed and particularly every linearly combined elliptically distributed random vector is elliptical, too. More formally, for any \( b \in \mathbb{R}^L, A \in \mathbb{R}^{L \times D} \), and \( Y = b + AX \) where \( X = \mu + \mathcal{E}_{D}^{(k)}(\mu, \Sigma, \phi) \) with \( \Sigma \in \mathbb{R}^{D \times k} \), it follows that \( Y \sim \mathcal{E}_{\Lambda}^{(k)}(b + A\mu, A\Lambda \Lambda^\top A^\top, \phi) = \mathcal{E}_{\Lambda}(b + A\mu, A\Sigma A^\top, \phi) \) since

\[
Y = b + A \left( \mu + \mathcal{E}_{D}^{(k)}(\mu) \right) = (A\mu + b) + \mathcal{E}_{\Lambda}^{(k)}. \tag{A.1}
\]

(e) Marginal distribution: let \( \mathcal{P}_m \in \{0, 1\}^{m \times D} \) be a permutation and deletion matrix, i.e., \( \mathcal{P}_m \) has only binary entries of 0’s and 1’s and \( \mathcal{P}_m \mathcal{P}_m^\top = \mathbb{I}_m \). So the transformation \( \mathcal{P}_m X := Y \) permutes and deletes certain components of \( X \) such that \( Y \) is a \( k \)-dimensional random vector containing the remaining components of \( X \) and having a (multivariate) marginal distribution with respect to the joint distribution of \( X \). Then by (A.1), we obtain \( Y \sim \mathcal{E}_m(\mathcal{P}_m \mu, \mathcal{P}_m \Sigma \mathcal{P}_m^\top, \phi) \) since

\[
Y = \mathcal{P}_m \left( \mu + \mathcal{E}_{\Lambda}^{(k)}(\mu) \right) = \mathcal{P}_m \mu + \mathcal{E}_{\Lambda}^{(k)}. \tag{A.2}
\]

(f) Conditional distribution: let \( X = (X_1, X_2) \), where \( X_1 \) is a \( k \)-dimensional sub-vector of \( X \), and let \( \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \in \mathbb{R}^{D \times D} \). Provided the conditional random vector \( X_2 | X_1 = x_1 \) exists, it is also elliptically distributed: \( X_2 | (X_1 = x_1) \sim \mathcal{E}_{D-k}^{(D-k)}(\mu^*, \Sigma^*, \phi^*) \). Moreover, it can be presented stochastically by

\[
X_2 | (X_1 = x_1) = \mu^* + \mathcal{R}^* U^{(D-k)} \Gamma^*,
\]

and \( U^{(D-k)} \) is uniformly distributed on \( S^{(D-k-1)} \), and

\[
\begin{align*}
\mathcal{R}^* &= \mathcal{R} \sqrt{1 - \beta} \left( \mathcal{R} \sqrt{\beta} U^{(k)} = \Sigma_{11}^{-1} (x_1 - \mu_1) \right), \\
\mu^* &= \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (x_1 - \mu_1), \\
\Sigma^* &= \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12},
\end{align*}
\]

where \( \beta \sim \text{Beta}(k/2, (D-k)/2) \) and \( \mathcal{R}, \beta, U^{(k)} \) and \( U^{(D-k)} \) are mutually independent, and \( \Sigma^* = (\Gamma^*)^\top \Gamma^* \).

### A.1.2 Relation between forward and inverse regression

Proposition 1 from Deleforge et al. (2015), a multivariate extension of Ingrassia et al. (2012), leads to a link between GLLiM, defined in (2.13) models, and a Gaussian mixture model on the joint variable \([X; Y]\). This result motivates us to establish the general proof for the relationship between forward and inverse mixture of elliptical regression models. More precisely, we consider the following generative model, conditionally on the cluster label:

\[
[X; Y] | (Z = k) \sim \mathcal{E}_{L+D}(m_k, V_k, \phi), \tag{A.3}
\]
where \( \mathcal{E}_{L+D} \) denotes an elliptical distribution of dimension \( D + L \), and are \( \mathbf{m}_k \) and \( \mathbf{V}_k \) its location and scale parameters, respectively.

When applying the inverse regression strategy in the context of mixture of elliptical locally-linear mapping, the key point is to account for (A.4):

\[
\mathbf{X} = \sum_{k=1}^{K} \mathbb{I}(Z = k) (\mathbf{A}_k \mathbf{Y} + \mathbf{b}_k + \mathbf{E}_k),
\]

(A.4)

where \( \mathbf{A}_k \in \mathbb{R}^{D \times L} \) and vector \( \mathbf{b}_k \in \mathbb{R}^D \), and \( \mathbf{E}_k \) is an error term capturing both the reconstruction error due to the local affine approximation and the observation noise in \( \mathbb{R}^D \), into the parameterization of \( \mathbf{m}_k \) and \( \mathbf{V}_k \). Given \( Z = k \), it follows from (A.3) that \( \mathbf{Y} \) is also elliptical distribution by using Theorem A.4 (e) and \( \mathbf{Y} \) can be assumed to have a location \( \mathbf{c}_k \in \mathbb{R}^L \) and a scale matrix \( \mathbf{\Gamma}_k \in \mathbb{R}^{L \times L} \).

We assume further that the error term \( \mathbf{E}_k \sim \mathcal{E}(0, \phi_{\varepsilon_k}, \Sigma_k) \) is an unobserved centered elliptical random noise with residual covariance matrix \( \Sigma_k \) of type \( \phi_{\varepsilon_k} \), and is independent of \( \mathbf{Y} \). Then, using (A.4) and Theorem A.4, we have

\[
\begin{align*}
\mathbb{E} (\mathbf{X} | (Z = k)) &= \mathbb{E} (\mathbf{A}_k \mathbf{Y} + \mathbf{b}_k + \mathbf{E}_k) = \mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k, \\ 
\text{var} (\mathbf{X} | (Z = k)) &= \text{var} (\mathbf{A}_k \mathbf{Y} + \mathbf{b}_k + \mathbf{E}_k) = \text{var} (\mathbf{A}_k \mathbf{Y}) + \text{var} (\mathbf{E}_k) = \mathbf{A}_k \mathbf{\Gamma}_k \mathbf{A}_k^\top + \Sigma_k, \\ 
\text{cov} (\mathbf{X}, \mathbf{Y} | (Z = k)) &= \text{cov} (\mathbf{A}_k \mathbf{Y} + \mathbf{b}_k + \mathbf{E}_k, \mathbf{Y}) = \mathbf{A}_k \mathbf{\Gamma}_k, \text{cov} (\mathbf{Y}, \mathbf{X}) = \text{cov} (\mathbf{Y}, \mathbf{A}_k \mathbf{Y}) = \mathbf{\Gamma}_k \mathbf{A}_k^\top, \\ 
\mathbf{m}_k &= \begin{bmatrix} \mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k \\ \mathbf{c}_k \end{bmatrix}, \\ 
\mathbf{V}_k &= \begin{bmatrix} \Sigma_k + \mathbf{A}_k \mathbf{\Gamma}_k \mathbf{A}_k^\top & \mathbf{A}_k \mathbf{\Gamma}_k \\ \mathbf{A}_k \mathbf{\Gamma}_k^\top & \mathbf{\Gamma}_k \end{bmatrix}.
\end{align*}
\]

(A.5)

Note that in the forward and inverse regression problems of elliptical locally-linear mapping (containing the Gaussian case (2.8), (2.9), (2.11) and (2.12)), by using Theorem A.4, the joint distribution defined in (A.3) allows us to consider a mixture of linear regression problem, characterized by the following marginal and conditional distributions:

\[
\begin{align*}
\mathbf{X} | (Z = k) &\sim \mathcal{E}_D (\mathbf{c}_k, \mathbf{\Gamma}_k, \phi), \\
\mathbf{Y} | (\mathbf{X}, Z = k) &\sim \mathcal{E}_n (\mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k), \\
\mathbf{Y} | (Z = k) &\sim \mathcal{E}_D (\mathbf{c}_k, \mathbf{\Gamma}_k, \phi), \\
\mathbf{X} | (\mathbf{Y}, Z = k) &\sim \mathcal{E}_n (\mathbf{A}_k \mathbf{Y} + \mathbf{b}_k).
\end{align*}
\]

(A.6) to (A.9)

where \( \mathbf{E}_k \sim \mathcal{E}(0, \phi_{\varepsilon_k}, \Sigma_k) \) and \( \mathbf{E}_k^* \sim \mathcal{E} (0, \phi_{\varepsilon_k}, \Sigma_k^*) \).

Then, we claim that the joint distribution, defined in (A.3) and (A.5), leads to the marginal and the conditional distributions of Equations (A.6) to (A.9) and to a mapping between their mean and variance parameters. Indeed, by using conditioning properties of elliptical distributions, see more in Theorem A.4, implies the following marginal for \( \mathbf{X} \) and conditional distribution for \( \mathbf{Y} \) given \( \mathbf{X} \) as follows:

\[
\begin{align*}
\mathbf{X} | (Z = k) &\sim \mathcal{E}_D (\mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k, \Sigma_k + \mathbf{A}_k \mathbf{\Gamma}_k \mathbf{A}_k^\top, \phi), \\
\mathbf{Y} | (\mathbf{X}, Z = k) &\sim \mathcal{E}_L (\mathcal{m}_{L}^{xx}, \Sigma_{L}^{xx}, \tilde{\phi}),
\end{align*}
\]

(A.10) to (A.11)

where the explicit expression of the characteristic function \( \tilde{\phi} \) can be found in Cambanis et al. (1981, Corollary 5), and

\[
\begin{align*}
\mathcal{m}_{L}^{xx} &= \mathbf{c}_k + \mathbf{\Gamma}_k^\top \left( \Sigma_k + \mathbf{A}_k \mathbf{\Gamma}_k \mathbf{A}_k^\top \right)^{-1} (\mathbf{X} - \mathbf{A}_k \mathbf{c}_k - \mathbf{b}_k), \\
\Sigma_{L}^{xx} &= \mathbf{\Gamma}_k - \mathbf{\Gamma}_k^\top \left( \Sigma_k + \mathbf{A}_k \mathbf{\Gamma}_k \mathbf{A}_k^\top \right)^{-1} \mathbf{A}_k \mathbf{\Gamma}_k = \left( \mathbf{\Gamma}_k^{-1} + \mathbf{A}_k^\top \Sigma_k^{-1} \mathbf{A}_k \right)^{-1},
\end{align*}
\]

with the fact that the last equality is the Woodbury matrix identity. Note that the locations and scale matrices of the conditional distribution do not depend upon the third parameter of the joint
distribution, and consequently, we do not describe the explicit expression for $\tilde{\varphi}$. We then utilize again the Woodbury matrix identity and the symmetric property of $\Gamma$ to identify (A.6) and (A.7) with (A.10) and (A.11), respectively, which implies the following important connections:

\[
c_k^* = A_k c_k + b_k, \quad \Gamma_k^* = \Sigma_k + A_k \Gamma_k A_k^T, \quad \Sigma_k^* = \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1},
\]

\[
A_k^* = \Gamma_k^* A_k^T \left( \Sigma_k + A_k \Gamma_k A_k^T \right)^{-1}
\]

\[
= \Gamma_k^* A_k^T \Sigma_k^{-1} - \Gamma_k^* A_k^T \Sigma_k^{-1} A_k \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1} A_k^T \Sigma_k^{-1}
\]

\[
= \left[ \Gamma_k \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right) - \Gamma_k A_k^T \Sigma_k^{-1} A_k \right] \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1} A_k^T \Sigma_k^{-1}
\]

\[
= \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1} A_k^T \Sigma_k^{-1} = \Sigma_k^* A_k^T \Sigma_k^{-1},
\]

\[
b_k^* = c_k + \Gamma_k^* A_k^T \left( \Sigma_k + A_k \Gamma_k A_k^T \right)^{-1} (-A_k c_k - b_k)
\]

\[
= c_k + \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1} A_k^T \Sigma_k^{-1} (-A_k c_k - b_k)
\]

\[
= \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right)^{-1} \left[ \left( \Gamma_k^{-1} + A_k^T \Sigma_k^{-1} A_k \right) c_k + A_k^T \Sigma_k^{-1} (-A_k c_k - b_k) \right]
\]

\[
= \Sigma_k^* (\Gamma_k^{-1} c_k - A_k^T \Sigma_k^{-1} b_k).
\]

Therefore, the desired results then are obtained by using the fact that the multivariate normal distribution not only has the property of having Gaussian marginal and conditional distributions (Bishop, 2006, Sections 2.3.1 and 2.3.2) but also belongs to elliptical distributions (detailed in Example A.3). Furthermore, it should be stressed that several versions of multivariate $t$-distributions (e.g., Section 5.5, page 94 of Kotz & Nadarajah (2004), Ding (2016)) have the previous property. This leads to the inverse regression model based on the multivariate $t$-distributions (Perthame et al., 2018). It will be interesting to find other sub-classes of elliptically contoured distributions that have the closedness property on marginal and conditional distribution so that the previous inverse regression trick can be applied.

### A.2 Proof of Lemma 5.5

Note that the first inequality of Lemma 5.5 comes from Montuelle & Pennec (2014, Lemma 4) and describes relationship between the bracketing entropy of $P_K$ and the entropy of $W_K$. Therefore, Lemma 5.5 is obtained by proving that there exists a constant $C_{W_K}$ such that $\forall \delta \in (0, 2]$,

\[
\mathcal{H}_{d_{\sup}}(\delta, W_K) \leq \dim(W_K) \left( C_{W_K} + \ln \left( \frac{1}{\delta} \right) \right), \quad (A.12)
\]

where $\dim(W_K) = K - 1 + KL + K \frac{L(L+1)}{2}$.

In order to establish the proof for A.12, we have to construct firstly the $\delta_\pi$-covering $\Pi_{K-1}$ of $\Pi_{K-1}$ via Lemma A.5, which is proved in Appendix A.2.1.

**Lemma A.5** (Covering number of probability simplex with maximum norm). Given any $\delta_\pi > 0$, any $\pi \in \Pi_{K-1}$, we can choose $\hat{\pi} \in \Pi_{K-1, \omega}$, an $\delta_\pi$-covering of $\Pi_{K-1}$, so that $\max_{k \in |K|} |\pi_k - \hat{\pi}_k| \leq \delta_\pi$. Furthermore, it holds that

\[
\mathcal{N}(\delta_\pi, \Pi_{K-1}, \|\cdot\|_\infty) \leq \frac{K (2\pi e)^{K/2}}{\delta_\pi^{K-1}}. \quad (A.13)
\]

Then, by definition of the covering number, (A.12) is obtained immediately via Lemma A.6, which controls the covering number of $W_K$ and is proved in Appendix A.2.2.

**Lemma A.6**. Given a bounded set $\mathcal{Y}$ in $\mathbb{R}^K$ such that $\mathcal{Y} = \{ y \in \mathbb{R}^K : \|y\|_\infty \leq C \}$, it holds that $W_K$ has a covering number satisfied $\mathcal{N}(\delta, W_K, d_{\sup}) \leq C \delta^{-\dim(W_K)}$, for some constant $C$. 

27
Indeed, Lemma A.6 implies the desired result by noting that
\[
\mathcal{H}_{d_{\sup}, \infty} (\delta, W_K) = \ln \mathcal{N} (\delta, W_K, d_{\sup, \infty}) \leq \ln \left( \frac{C}{\delta^{\dim(W_K)}} \right) = \dim(W_K) \left( \frac{1}{\dim(W_K)} \ln C + \ln \left( \frac{1}{\delta} \right) \right) = \dim(W_K) \left( C W_K + \ln \left( \frac{1}{\delta} \right) \right).
\]

### A.2.1 Proof of Lemma A.5

We mimic the proof of Lemma 2 from Genovese et al. (2000), which constructs a \( \delta \)-\( \pi \)-Hellinger bracketing of \( \Pi_{K-1} \). Given any \( \pi = (\pi_k)_{k \in [K]} \in \Pi_{K-1} \), let \( \xi = (\xi_k)_{k \in [K]} \) where \( \xi_k = \sqrt{\pi_k} \), \( \forall k \in [K] \). Then \( \pi \in \Pi_{K-1} \) if and only if \( \xi \in Q^+ \cap U \), where \( U \) is the surface of the unit sphere and \( Q^+ \) is the positive quadrant of \( \mathbb{R}^K \). Next, we divide the unit cube in \( \mathbb{R}^K \) into disjoint cubes with sides parallel to the axes and sides of length \( \delta \pi / \sqrt{K} \). Let \( (C_j)_{j \in [N]} \) is the subset of these cubes that have non-empty intersection with \( Q^+ \cap U \). For any \( j \in [N] \), let \( \nu_j = (\nu_{j,k})_{k \in [K]} \) be the center of the cube \( C_j \) and
\[

nu_j^2 = \left( \nu_{j,k}^2 \right)_{k \in [K]}.
\]

Then \( \{\nu_j\}_{j \in [N]} \) is a \( \delta \pi / (2 \sqrt{K}) \)-covering of \( Q^+ \cap U \), since we have for any \( \xi = (\xi_k)_{k \in [K]} \in Q^+ \cap U \), there exists \( j_0 \in [N] \) such that \( \xi \in C_{j_0} \), and
\[
||\xi - \nu_{j_0}||_\infty = \max_{k \in [K]} |\xi_k - \nu_{j_0,k}| \leq \frac{\delta \pi}{2 \sqrt{K}}.
\]

Therefore, it follows that \( \Pi_{K-1, \omega} := \{\nu_j^2\}_{j \in [N]} \) is a \( \delta \pi \)-covering of \( \Pi_{K-1} \), since for any \( \pi = (\pi_k)_{k \in [K]} \in \Pi_{K-1} \), (A.14) leads to the existence of \( j_0 \in [N] \), such that
\[
||\pi - \nu_{j_0}^2||_\infty = \max_{k \in [K]} |\xi_k^2 - \nu_{j_0,k}^2| = \max_{k \in [K]} \left( |\xi_k - \nu_{j_0,k}| |\xi_k + \nu_{j_0,k}| \right) \leq \frac{\delta \pi}{2 \sqrt{K}} \max_{k \in [K]} |\xi_k + \nu_{j_0,k}| \leq \frac{\delta \pi}{\sqrt{K}} \leq \delta \pi,
\]
where we used the fact that \( \max_{k \in [K]} |\xi_k + \nu_{j_0,k}| \leq 2 \). Now, it remains to count the number of cubes \( N \). Let \( T_a = \{z \in Q^+: ||z||_2 \leq a\} \) and let \( C = \bigcup_{j \in [N]} C_j \). Note that \( C \subset T_{1+\delta \pi} - T_{1-\delta \pi} \equiv T \), and so
\[
\text{Volume}(T) \geq \text{Volume}(C) = N \left( \frac{\delta \pi}{\sqrt{K}} \right)^K.
\]

Note that here we use the notation \( \pi \) for the Archimedean’s constant, which differs from \( \pi = (\pi_k)_{k \in [K]} \) for the mixing proportion of the GLOME model. Then, we define \( \mathcal{V}_K(a) = a^{K} \pi^{K/2} \) as the volume of a sphere of radius \( a \). Since \( z! \geq z^{z} e^{-z} \) and \( (1 + \delta \pi)^K - (1 - \delta \pi)^K = K \int_{1-\delta \pi}^{1+\delta \pi} z^{K-1} d z \leq 2 \delta \pi K (1 + \delta \pi)^{K-1} \), it follows that
\[
\mathcal{N} (\delta \pi, \Pi_{K-1}, ||\cdot||_\infty) \leq N \leq \frac{\text{Volume}(C)}{\left( \frac{\delta \pi}{\sqrt{K}} \right)^K} = \frac{1}{2^K} \frac{\mathcal{V}_K(1 + \delta \pi) - \mathcal{V}_K(1 - \delta \pi)}{\left( \frac{\pi}{\sqrt{K}} \right)^K} \leq \frac{1}{2^K} \left[ \left( 1 + \delta \pi \right)^{K/2} - \left( 1 - \delta \pi \right)^{K/2} \right] \leq \frac{K}{\delta \pi} \frac{K/2}{\delta \pi^{K/2}} \leq \frac{K}{\delta \pi^{K/2}}.
\]

### A.2.2 Proof of Lemma A.6

In order to find an upper bound for a covering number of \( W_K \), we wish to construct a finite \( \delta \)-covering \( W_{K,\omega} \) of \( W_K \), with respect to the distance \( d_{\sup, \infty} \). That is, given any \( \delta > 0 \), \( w(\cdot; \omega) \in W_K \), we aim to prove that there exists \( w(\cdot; \tilde{\omega}) \in W_{K,\omega} \) such that
\[
d_{\sup, \infty} (w(\cdot; \omega), w(\cdot; \tilde{\omega})) = \max_{k \in [K]} \sup_{y \in Y} |w_k(y; \omega) - w_k(y; \tilde{\omega})| \leq \delta.
\]

(A.15)
In order to accomplish such task, given any positive constants $\delta_c, \delta_\Gamma, \delta_\pi$, and any $k \in [K]$, let us define

$$
\mathcal{F} = \{ \mathcal{Y} \ni y \mapsto \ln (\Phi_L (y; c, \Gamma)) : \|c\|_\infty \leq A_c, a_\Gamma \leq m (\Gamma) \leq M (\Gamma) \leq A_\Gamma \},
$$

$$
\mathcal{F}_{c_k} = \{ \ln (\Phi_L (c_k, \Gamma_k)) : \ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F},
\quad c_{k,j} \in \{-C_Y + b \delta_c / L : l = 0, \ldots, 2C_Y L / \delta_c \}, j \in [L] \},
$$

$$
\mathcal{F}_{c_k, r_k} = \{ \ln (\Phi_L (c_k, \Gamma_k)) : \ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F}_{c_k},
\quad [\text{vec} (\Gamma_k)]_{i,j} = \gamma_{i,j} \frac{\delta \Gamma}{L^2} : \gamma_{i,j} = \gamma_{j,i} \in \mathbb{Z} \cap \left[ -\frac{L^2 A_\Gamma}{\delta_\Gamma}, \frac{L^2 A_\Gamma}{\delta_\Gamma} \right], i \in [L], j \in [L] \},
$$

$$
\mathcal{W}_{K, \omega} = \{ w (\cdot; \omega) : w (\cdot; \omega) \in \mathcal{W}_K, \forall k \in [K], \ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F}_{c_k, r_k}, \pi \in \Pi_{K-1, \omega} \}.
$$

Here, \([-\cdot] \text{ and } \lceil \cdot \rceil \text{ are ceiling and floor functions, respectively, and vec(\cdot) is an operator that stacks matrix columns into a column vector. In particular, we denote } \Pi_{K-1, \omega} \text{ as a } \delta_\pi\text{-covering of } \Pi_{K-1}, \text{ which is defined in Lemma A.5. By the previous definition, it holds that } \forall k \in [K], \mathcal{F}_{c_k, r_k} \subset \mathcal{F}_{c_k} \subset \mathcal{F}, \text{ and } \mathcal{W}_{K, \omega} \subset \mathcal{W}_K.

Next, we claim that $\mathcal{W}_{K, \omega}$ is a finite $\delta_\Gamma$-covering of $\mathcal{W}_K$ with respect to the distance $d_{\|\sup\|_\infty}$. To do this, for any $w (\cdot; \omega) = (\ln (\pi_k \Phi_L (c_k, \Gamma_k)))_{k \in [K]} \in \mathcal{W}_K$, $\ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F}, \pi \in \Pi_{K-1}$, and for any $k \in [K]$, by (A.16), we first choose a function $\ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F}_{c_k}$ so that

$$
\| \hat{c}_k - c_k \|_1 = \sum_{j=1}^L |\hat{c}_{k,j} - c_{k,j}| \leq L \frac{\delta_c}{L} = \delta_c.
$$

Furthermore, by (A.17), we obtain a similar result from Maugis & Michel (2011, Equation B.15) to construct the covariance matrix lattice. That is, any $\ln (\Phi_L (c_k, \Gamma_k)) \in \mathcal{F}_{c_k}$ can be approximated by $\ln (\Phi_L (\hat{c}_k, \hat{\Gamma}_k)) \in \mathcal{F}_{c_k, r_k}$ such that

$$
\left\| \text{vec} (\hat{\Gamma}_k) - \text{vec} (\Gamma_k) \right\|_1 = \left\| \text{vec} (\hat{\Gamma}_k - \Gamma_k) \right\|_1 = \sum_{i=1}^L \sum_{j=1}^L \left| [\text{vec} (\hat{\Gamma}_k - \Gamma_k)]_{i,j} \right| \leq L \frac{\delta_\Gamma}{L} = \delta_\Gamma.
$$

Note that since for any $k \in [K]$, $(y, c_k, \text{vec}(\Gamma_k)) \mapsto \ln (\Phi_L (y; c_k, \Gamma_k))$ is differentiable, it is also continuous w.r.t. $y$ and its parameters $c_k$ and $\Gamma_k$. Thus, for every fixed $y \in \mathcal{Y}$, for every $\hat{c}_k, c_k \in \mathcal{X}$ with $\hat{c}_k \in c_k$, and for every $\hat{\Gamma}_k, \Gamma_k$, where $\text{vec}(\hat{\Gamma}_k) \leq \text{vec}(\Gamma_k)$, we can apply the mean value theorem (see Duistermaat & Kolk 2004, Lemma 2.5.1) to $\ln (\Phi_L (y; \cdot, \Gamma_k))$ and $\ln (\Phi_L (y; \cdot, \hat{\Gamma}_k))$ on the intervals $[c_k, \hat{c}_k]$ and $[\text{vec}(\Gamma_k), \text{vec}(\hat{\Gamma}_k)]$ for some $z_{c_k} \in (c_k, \hat{c}_k)$ and $z_{\Gamma_k} \in (\text{vec}(\Gamma_k), \text{vec}(\hat{\Gamma}_k))$, respectively, to get

$$
\ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) - \ln (\Phi_L (y; c_k, \Gamma_k)) = (\hat{c}_k - c_k)^\top \nabla_{c_k} \ln (\Phi_L (y; z_{c_k}, \Gamma_k)),
$$

$$
\ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) - \ln (\Phi_L (y; \hat{c}_k, \Gamma_k)) = (\text{vec}(\hat{\Gamma}_k) - \text{vec}(\Gamma_k)) \top \nabla_{\text{vec}(\Gamma_k)} \ln (\Phi_L (y; \hat{c}_k, z_{\Gamma_k})).
$$

Moreover, $(y, c_k, \text{vec}(\Gamma_k)) \mapsto \nabla_{c_k} \ln (\Phi_L (y; z_{c_k}, \Gamma_k))$ and $(y, c_k, \text{vec}(\Gamma_k)) \mapsto \nabla_{\text{vec}(\Gamma_k)} \ln (\Phi_L (y; \hat{c}_k, z_{\Gamma_k}))$ are continuous functions on the compact set $U := \mathcal{Y} \times \mathcal{Y} \times [a_\Gamma, A_\Gamma]^L$ leads to them attain minimum and maximum values (see Duistermaat & Kolk 2004, Theorem 1.8.8). That is, we can set that

$$
0 < (C_c)^\top_{1, \ldots, L} := \max_{k \in [K]} \sup_{(y, c_k, \text{vec}(\Gamma_k)) \in U} |\nabla_{c_k} \ln (\Phi_L (y; c_k, \Gamma_k))| < \infty,
$$

$$
0 < (C_\Gamma)^{L, 2} := \max_{k \in [K]} \sup_{(y, c_k, \text{vec}(\Gamma_k)) \in U} |\nabla_{\text{vec}(\Gamma_k)} \ln (\Phi_L (y; c_k, \Gamma_k)) (x)| < \infty.
$$
Therefore, by the Cauchy–Schwarz inequality, we have
\[
\sup_{y \in \mathcal{Y}} |\ln (\Phi_L (y; \hat{c}_k, \Gamma_k)) - \ln (\Phi_L (y; c_k, \Gamma_k))| \leq |\hat{c}_k - c_k|^\top (C_c)^\top L = C_c \|\hat{c}_k - c_k\|_1 \leq C_c \delta, \\
\sup_{y \in \mathcal{Y}} \Big| \ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) - \ln (\Phi_L (y; \hat{c}_k, \Gamma_k)) \Big| \leq C_T \|\vec{\Gamma}_k - \Gamma_k\|_1 \leq C_T \delta, 
\]
and by using the triangle inequality, it follows that
\[
\max_{k \in [K]} \sup_{y \in \mathcal{Y}} \left| \ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) - \ln (\Phi_L (y; c_k, \Gamma_k)) \right| \leq C_c \delta_c + C_T \delta. \tag{A.19} 
\]
Moreover, for every \( \pi \in \Pi_{K-1} \), Lemma A.5 implies that we can choose \( \hat{\pi} \in \Pi_{K-1,\omega} \) so that \( \max_{k \in [K]} |\pi_k - \hat{\pi}_k| \leq \delta_{\pi} \). Notice that \([a_\pi, \infty) \ni t \mapsto \ln(t), a_\pi > 0\) is a Lipschitz continuous function on \([a_\pi, \infty)\). Indeed, by the mean value theorem, it holds that there exists \( c \in (t_1, t_2) \), such that
\[
|\ln (t_1) - \ln (t_2)| = |\ln'(c) (t_1 - t_2)| \leq \frac{1}{a_\pi} |t_1 - t_2|, \text{ for all } t_1, t_2 \in [a_\pi, \infty). \tag{A.20} 
\]
Therefore, (A.15) can be obtained by the following evaluation
\[
d_{\sup, \infty}(w(\cdot; \omega), w(\cdot; \hat{\omega})) = \max_{k \in [K]} \sup_{y \in \mathcal{Y}} \left| \ln (\pi_k \Phi_L (y; c_k, \Gamma_k)) - \ln (\hat{\pi}_k \Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) \right| \\
= \max_{k \in [K]} \sup_{y \in \mathcal{Y}} \left| \ln (\pi_k) - \ln (\hat{\pi}_k) + \ln (\Phi_L (y; c_k, \Gamma_k)) - \ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) \right| \\
\leq \max_{k \in [K]} \left| \ln (\pi_k) - \ln (\hat{\pi}_k) \right| + \max_{k \in [K]} \sup_{y \in \mathcal{Y}} \left| \ln (\Phi_L (y; c_k, \Gamma_k)) - \ln (\Phi_L (y; \hat{c}_k, \hat{\Gamma}_k)) \right| \\
\leq \frac{1}{a_\pi} \max_{k \in [K]} |\pi_k - \hat{\pi}_k| + C_c \delta_c + C_T \delta \tag{using (A.20) and (A.19)} \\
\leq \frac{\delta_{\pi}}{a_\pi} + C_c \delta_c + C_T \delta \tag{using Lemma A.5} \leq \frac{\delta}{3} + \frac{\delta}{3} + \frac{\delta}{3} = \delta, 
\]
where we choose \( \delta_{\pi} = \frac{\delta_{\pi}}{a_\pi}, \delta_c = \frac{\delta}{a_\pi}, \delta_T = \frac{\delta}{C_T} \). Finally, we get the covering number
\[
\mathcal{N}(\delta, W_K, d_{\sup, \infty}) \leq \text{card}(W_{K, \omega}) \leq \left[ \frac{2C_Y L}{\delta_c} \right]^{KL} \left[ \frac{2A_T L^2}{\delta_T} \right]^{\frac{L(L+1)}{2}} \mathcal{N}(\delta_{\pi}, \Pi_{K-1}, \|\cdot\|) \leq \frac{C}{\delta^{\dim(W_K)}} \mathcal{N}(\delta_{\pi}, \Pi_{K-1, \omega}, \|\cdot\|), 
\]
where
\[
C = (6C_c C_Y L)^{KL} (6C_T A_T L^2)^{\frac{L(L+1)}{2}} \left( \frac{3}{a_\pi} \right)^{K-1} K (2\pi e)^{K/2}. 
\]

A.3 Proof of Lemma 5.6

Note that Lemmas 1 and 2 from Montuelle & Pennec (2014) imply that there exists a constant \( C_\mathcal{Y} = \ln \left( \sqrt{2} + \sqrt{D_d T_{\mathcal{Y}}} \right) \) (when \( Y_K = Y_b^K \)) or \( C_\mathcal{Y} = \ln \left( \sqrt{2} + \sqrt{D_{\delta} L^2} T_{\mathcal{Y}} \right) \) (when \( Y_K = Y_\delta^K \)) such that, \( \forall \delta \in (0, \sqrt{2}) \),
\[
\mathcal{H}_{d_{\sup, \infty}}(\delta, Y_K) \leq \dim(Y_K) \left( C_\mathcal{Y} + \ln \frac{1}{\delta} \right). \tag{A.21} 
\]
Next, we rely on Proposition A.7 for constructing of Gaussian brackets to for the Gaussian experts.
Proposition A.7 (Proposition 2 from Montuelle & Pennec 2014). Let \( \kappa \geq \frac{17}{29} \) and \( \gamma_\kappa = \frac{25(\kappa - \frac{1}{2})}{49(1 + \frac{5}{4}\kappa)} \).
For any \( 0 < \delta \leq \sqrt{2} \), any \( D \geq 1 \), and any \( \delta_S \leq \frac{1}{5\sqrt{\kappa^2 \cosh(D/2) + D/2}} \), let \((v, B, A, P) \in \mathcal{Y} \times [B_-, B_+] \times \mathcal{A}(\lambda_-, \lambda_+) \times SO(D) \) and \((\tilde{v}, \tilde{B}, \tilde{A}, \tilde{P}) \in \mathcal{Y} \times [B_-, B_+] \times \mathcal{A}(\lambda_-, +\infty) \times SO(D) \), and define \( \Sigma = B\Pi A P^\top, \tilde{\Sigma} = \tilde{B}\tilde{\Pi} A \tilde{P}^\top \),
\[
t^-(x, y) = (1 + \kappa \delta_S)^{-D} \Phi_D \left( x; \tilde{v}(y), (1 + \delta_S)^{-1} \tilde{\Sigma} \right)
\]
and \( t^+(x, y) = (1 + \kappa \delta_S)^D \Phi_D \left( x; \tilde{v}(y), (1 + \delta_S) \tilde{\Sigma} \right) \).
If
\[
\begin{align*}
&\forall y \in \mathcal{Y}, \|v(y) - \tilde{v}(y)\|^2 \leq D \gamma_\kappa \mathcal{L}_- \lambda_- \frac{\lambda_+}{\lambda_+ - \delta_S} \\
&(1 + \frac{\delta_S}{2\kappa})^{-1} \tilde{B} \leq B \leq \tilde{B} \\
&\forall i \in [D], \|A_{i, i} - \tilde{A}_{i, i}\| \leq \frac{\delta_S}{10 \lambda_+} \\
&\forall x \in \mathbb{R}^D, \|Px - \tilde{P}x\| \leq \frac{\lambda_- \delta_S}{10 \lambda_+} \|x\|
\end{align*}
\]
then \([t^-, t^+]\) is a \( \frac{\delta_S}{5} \) Hellinger bracket such that \( t^-(x, y) \leq \Phi_D (x; v(y), \Sigma) \leq t^+(x, y) \).

Then, following the same argument as in Montuelle & Pennec (2014, Appendix B.2.3), Proposition A.7 allows us to construct nets over the spaces of the means, the volumes, the eigenvector matrices, the normalized eigenvalue matrices and then control the bracketing entropy of \( G_K \). More precisely, three different contexts are considered for the mean, volume and matrix parameters. They can be all known (\(* = 0\)), unknown but common to all classes (\(* = c\)), unknown and possibly different for every class (\(* = K\)). For example, \([v_K, B_0, P_0, A_0]\) denotes a model in which only mean vectors are assumed to be free. Then, we obtain
\[
\mathcal{H}^{[\cdot], \sup_y, \max x} d_x \left( \frac{\delta_S}{5}, G_K \right) \leq \dim \left( \mathcal{G}_K \right) \left( C_{\mathcal{G}_K} + \ln \left( \frac{1}{\delta} \right) \right),
\]
(A.22)
where \( \dim \left( \mathcal{G}_K \right) = Z_{v,*} + Z_{B,*} + \frac{D(D-1)}{2} Z_{P,*} + (D-1)Z_{A,*}, Z_{v,K} = \dim \left( \mathcal{Y}_K \right), Z_{v,c} = \dim \left( \mathcal{Y}_1 \right), Z_{B,0} = 0, Z_{B,0} = Z_{P,0} = Z_{A,0} = 0, Z_{B,c} = Z_{P,c} = Z_{A,c} = 1, Z_{B,K} = Z_{P,K} = Z_{A,K} = K, \) and given a universal constant \( C_U \),
\[
C_{\mathcal{G}_K} = \ln \left( 5D \sqrt{\kappa^2 \cosh \left( \frac{2\kappa}{5} \right) + \frac{1}{2}} \right) + C_\mathcal{Y} + \frac{1}{2} \ln \left( \frac{\lambda_+}{D \gamma_\kappa B_- \lambda_+^2} \right)
\]
\[+ \ln \left( \frac{4 + 129 \ln \left( \frac{B_*}{\pi^2} \right)}{10} \right) + \frac{D(D-1)}{2} \ln (c_U) + \ln \left( \frac{10 \lambda_+}{\lambda_-} \right) + \ln \left( \frac{4}{5} + \frac{52 \lambda_+}{5 \lambda_-} \ln \left( \frac{\lambda_+}{\lambda_-} \right) \right).
\]

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34
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