

# A non-asymptotic approach for mixture of

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## Learning nonlinear regression models from

**Random sample:**  $(\mathbf{X}_i, \mathbf{Y}_i)_{i \in [n]} \in (\mathcal{X} \times \mathcal{Y})^n \subset (\mathbb{R}^D \times \mathbb{R}^L)^n$  of the multivariate data, the corresponding observed values  $(\mathbf{x}_i, \mathbf{y}_i)_{i \in [n]}$ ,  $[n] := \{1, \dots, n\}$  (potentially

**Our proposal:** approximating  $s_0$  by a **Gaussian-gated Localized Mixture** [3, 4, 5]:

$$s_{\psi_{K,d}}(\mathbf{x}|\mathbf{y}) = \sum_{k=1}^K \underbrace{g_k(\mathbf{y}; \boldsymbol{\omega})}_{\text{Gaussian-gated network}} \times \underbrace{\mathcal{N}_D(\mathbf{x}; \mathbf{v}_{k,d}(\mathbf{y}), \boldsymbol{\Sigma}_k)}_{\text{Gaussian expert}}$$

$\psi_{K,d} = (\boldsymbol{\omega}, \mathbf{v}, \boldsymbol{\Sigma}) \in \boldsymbol{\Omega}_K \times \boldsymbol{\Upsilon}_{K,d} \times \mathbf{V}_K =: \boldsymbol{\Psi}_{K,d}$ ,  $\boldsymbol{\omega} = (\boldsymbol{\pi}, \mathbf{c}, \boldsymbol{\Gamma}) \in (\boldsymbol{\Pi}_{K-1} \times \mathcal{C})$

$K$ -tuples of mean **vectors/functions** of size  $L \times 1 / D \times 1$ ,  $\mathbf{V}'_K / \mathbf{V}_K$ :  $K$ -tuples

**Main contributions:**

- **Model selection criterion:** choosing number of mixture component
- **Finite-sample oracle inequality:** establishing non-asymptotic risk

## Boundedness assumptions

$$\begin{aligned} \tilde{\boldsymbol{\Omega}}_K &= \{ \boldsymbol{\omega} \in \boldsymbol{\Omega}_K : \forall k \in [K], \|\mathbf{c}_k\|_\infty \leq A_{\mathbf{c}}, \\ &\quad 0 < a_{\boldsymbol{\Gamma}} \leq m(\boldsymbol{\Gamma}_k) \leq M(\boldsymbol{\Gamma}_k) \leq A_{\boldsymbol{\Gamma}}, 0 < a_{\boldsymbol{\pi}} \leq \pi_k \}, \\ m(\boldsymbol{\Gamma}_k)/M(\boldsymbol{\Gamma}_k) &: \text{the smallest/largest eigenvalues of } \boldsymbol{\Gamma}_k, \\ \boldsymbol{\Upsilon}_{b,d} &= \left\{ \mathbf{y} \mapsto \left( \sum_{i=1}^d \alpha_i^{(j)} \varphi_{\boldsymbol{\Upsilon},i}(\mathbf{y}) \right)_{j \in [D]} : \|\boldsymbol{\alpha}\|_\infty \leq T_{\boldsymbol{\Upsilon}} \right\}, \\ \boldsymbol{\Upsilon}_{K,d} &= \otimes_{k \in [K]} \boldsymbol{\Upsilon}_{k,d} = \boldsymbol{\Upsilon}_{b,d}^K, \quad T_{\boldsymbol{\Upsilon}} \in \mathbb{R}^+, \\ (\varphi_{\boldsymbol{\Upsilon},i})_{i \in [d]} &: \text{collection of bounded functions on } \mathcal{Y}, \\ \mathbf{V}_K &= \left\{ (\boldsymbol{\Sigma}_k)_{k \in [K]} = \left( B_k \mathbf{P}_k \mathbf{A}_k \mathbf{P}_k^\top \right)_{k \in [K]} : \right. \\ &\quad \left. 0 < B_- \leq B_k \leq B_+, \mathbf{P}_k \in SO(D), \mathbf{A}_k \in \mathcal{A}(\lambda_-, \lambda_+) \right\}, \\ B_k &= |\boldsymbol{\Sigma}_k|^{1/D}: \text{volume, } SO(D): \text{eigenvectors of } \boldsymbol{\Sigma}_k, \\ \mathcal{A}(\lambda_-, \lambda_+) &: \text{set of linear transformations } \mathbf{A} \text{ satisfying } \lambda_- \mathbf{I} \preceq \mathbf{A} \preceq \lambda_+ \mathbf{I} \end{aligned}$$

N

**Theorem.** Given a c  
 $\Xi = \sum_{\mathbf{m} \in \mathcal{M}} e^{-z_{\mathbf{m}}} < \infty$   
 $\forall \mathbf{m} \in \mathcal{M}, \text{pen}(\mathbf{m}) \geq$   
 $\arg \min_{\mathbf{m} \in \mathcal{M}} (\sum_{i=1}^n -\log p(\mathbf{y}_i | \mathbf{m}))$   
the loss  $\text{JKL}_\rho^{\otimes n}(s, t) = 1$

$$\mathbb{E}_{\mathbf{Y}_{[n]}} [\text{JKL}_\rho^{\otimes n}(s_0, t)]$$

Well-Speci

$$s_o^*(y|x) = \frac{\mathcal{N}(y|x)}{\sum_{i=1}^K \mathcal{N}(y|x; \mu_i, \Sigma_i)}$$

# or model selection f experts models

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## om complex data using GLoME models

ariate response  $\mathbf{Y} = (\mathbf{Y}_j)_{j \in [L]}$  and the set of covariates  $\mathbf{X} = (\mathbf{X}_j)_{j \in [D]}$  with  
( $D \gg L$ ), arising from an unknown conditional density  $s_0$ .

cture of Experts (GLoME) model due to its flexibility and effectiveness

$$), \quad \mathbf{g}_k(\mathbf{y}; \boldsymbol{\omega}) = \frac{\pi_k \mathcal{N}_L(\mathbf{y}; \mathbf{c}_k, \boldsymbol{\Gamma}_k)}{\sum_{l=1}^K \pi_l \mathcal{N}_L(\mathbf{y}; \mathbf{c}_l, \boldsymbol{\Gamma}_l)}, \forall k \in [K], K \in \mathbb{N}^*, \text{ where:}$$

$\mathbf{C}_K \times \mathbf{V}'_K) =: \boldsymbol{\Omega}_K, \boldsymbol{\Pi}_{K-1} = \left\{ (\pi_k)_{k \in [K]} \in (\mathbb{R}^+)^K, \sum_{k=1}^K \pi_k = 1 \right\}, \mathbf{C}_K / \boldsymbol{\Upsilon}_{K,d}:$   
es of elements in  $\mathcal{S}_L^{++} / \mathcal{S}_D^{++}$  (space of symmetric positive-definite matrices).

s and mean functions' degree via a penalized maximum likelihood estimator.  
bounds provided a lower bound on the penalty holds.

## on-asymptotic oracle inequality [5]

ollection  $(S_{\mathbf{m}})_{\mathbf{m} \in \mathcal{M}}$  of GLoME models,  $\rho \in (0, 1)$ ,  $C_1 > 1$ , assume that  
 $\infty, z_{\mathbf{m}} \in \mathbb{R}^+, \forall \mathbf{m} \in \mathcal{M}$ , and there exist constants  $C$  and  $\kappa(\rho, C_1) > 0$  s.t.  
 $\kappa(\rho, C_1) [(C + \ln n) \dim(S_{\mathbf{m}}) + z_{\mathbf{m}}]$ . Then, a PMLE- $\hat{s}_{\hat{\mathbf{m}}}$ , defined by  $\hat{\mathbf{m}} =$   
 $\arg \min_{\mathbf{m} \in \mathcal{M}} (\hat{s}_{\mathbf{m}}(\mathbf{x}_i | \mathbf{y}_i) + \text{pen}(\mathbf{m}))$ ,  $\hat{s}_{\mathbf{m}} = \arg \min_{s_{\mathbf{m}} \in S_{\mathbf{m}}} \sum_{i=1}^n -\ln(s_{\mathbf{m}}(\mathbf{x}_i | \mathbf{y}_i))$ , with  
 $\mathbb{E}_{\mathbf{Y}_{[n]}} \left[ \frac{1}{n} \sum_{i=1}^n \frac{1}{\rho} \text{KL}(s(\cdot | \mathbf{Y}_i), (1 - \rho)s(\cdot | \mathbf{Y}_i) + \rho t(\cdot | \mathbf{Y}_i)) \right]$ , satisfies

$$), \hat{s}_{\hat{\mathbf{m}}})] \leq C_1 \inf_{\mathbf{m} \in \mathcal{M}} \left( \inf_{s_{\mathbf{m}} \in S_{\mathbf{m}}} \text{KL}^{\otimes n}(s_0, s_{\mathbf{m}}) + \frac{\text{pen}(\mathbf{m})}{n} \right) + \frac{\kappa(\rho, C_1) C_1 \mathbb{E}}{n}.$$

## Numerical experiments

fied (WS) :  $s_0^* \in S_{\mathbf{m}}^*$ ,

$$r; 0.2, 0.1) \mathcal{N}(y; -5\mathbf{x} + 2, 0.09) + \mathcal{N}(x; 0.8, 0.15) \mathcal{N}(y; 0.1\mathbf{x}, 0.09)$$

$\mathcal{A}(\lambda_-, \lambda_+)$ : set of diagonal matrices of normalized eigenvalues of  $\Sigma_k$  s.t.  $\forall i \in [D], 0 < \lambda_- \leq (\mathbf{A}_k)_{i,i} \leq \lambda_+$ ,  
 $\mathbf{m} \in \mathcal{M} = \{(K, d) : K \in [K_{\max}], d \in [d_{\max}]\}$ ,  
 $S_{\mathbf{m}} = \left\{(\mathbf{x}, \mathbf{y}) \mapsto s_{\psi_{K,d}}(\mathbf{x}|\mathbf{y}) =: s_{\mathbf{m}}(\mathbf{x}|\mathbf{y}) : \right.$   
 $\left. \psi_{K,d} \in \tilde{\Omega}_K \times \Upsilon_{K,d} \times \mathbf{V}_K =: \tilde{\Psi}_K \right\}.$

## Model selection procedure

**GLLiM model:** finding the best data-driven model among  $(S_{\mathbf{m}}^*)_{\mathbf{m} \in \mathcal{M}}$ ,  $\mathcal{M} = [K_{\max}] \times \{1\}$ , based on  $(\mathbf{x}_i, \mathbf{y}_i)_{i \in [n]}$  arising from a forward conditional density  $s_0^*$ .

1. For each  $\mathbf{m} \in \mathcal{M}$ : estimate the forward MLE  $(\hat{s}_{\mathbf{m}}^*(\mathbf{y}_i|\mathbf{x}_i))_{i \in [N]}$  by inverse MLE  $\hat{s}_{\mathbf{m}}$  via an **inverse regression trick** by GLLiM-EM algorithm.
2. Calculate PMLE  $\hat{\mathbf{m}}$  with  $\text{pen}(\mathbf{m}) = \kappa \dim(S_{\mathbf{m}}^*)$ .  
**Large enough but not explicit value for  $\kappa$ !** Asymptotic: AIC:  $\kappa = 1$ ; BIC:  $\kappa = \frac{\ln n}{2}$ .  
**Non-asymptotic:** partially justification for **slope heuristic criterion** in a finite-sample setting.

## References

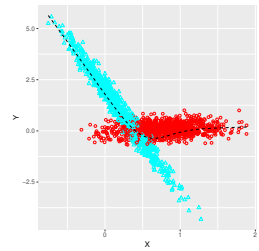
- [1] Jean-Patrick Baudry, Cathy Maugis, and Bertrand Michel. Slope heuristics: overview and implementation. *Statistics and Computing*, 22(2):455–470, 2012.
- [2] Antoine Deleforge, Florence Forbes, and Radu Horaud. High-dimensional regression with gaussian mixtures and partially-latent response variables. *Statistics and Computing*, 25(5):893–911, 2015.
- [3] Nhat Ho, Chiao-Yu Yang, and Michael I Jordan. Convergence Rates for Gaussian Mixtures of Experts. *arXiv preprint arXiv:1907.04377*, 2019.
- [4] Hien Duy Nguyen, TrungTin Nguyen, Faicel Chamroukhi, and Geoffrey John McLachlan. Approximations of conditional probability density functions in Lebesgue spaces via mixture of experts models. *Journal of Statistical Distributions and Applications*, 8(1):13, 2021.
- [5] Trung Tin Nguyen, Hien Duy Nguyen, Faicel Chamroukhi, and Florence Forbes. A non-asymptotic penalization criterion for model selection in mixture of experts models. *arXiv preprint arXiv:2104.02640*, 2021.

Misspecified

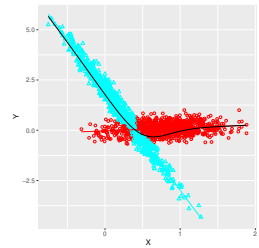
$$s_0^*(y|x) = \frac{\mathcal{N}(y|x)}{\sum_{k=1}^K \mathcal{N}(y|x; \mu_k, \Sigma_k)}$$

Estimation by EM (xLLiM)  
**Numerical results:**

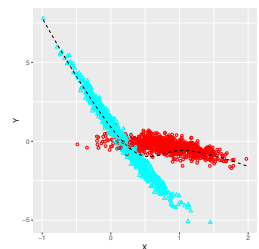
Fig.1: Clustering deduced by EM rule with 2000 data point  
Fig.2: Histogram of selected models  
Fig.3: Box-plot of the Kullback-Leibler divergence  
Fig.4: Rate of error upper bound



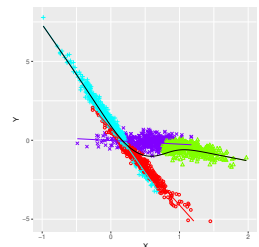
1.1 WS realization



1.2 GLoME clustering



1.3 MS realization



1.4 GLoME clustering

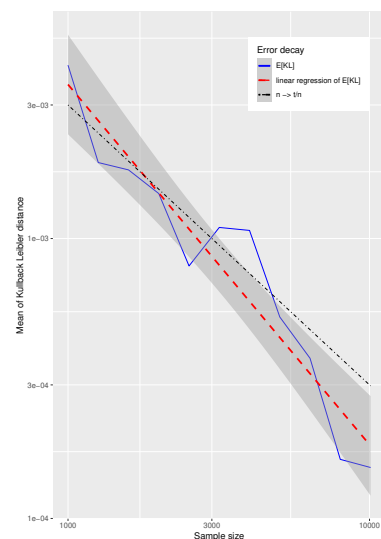
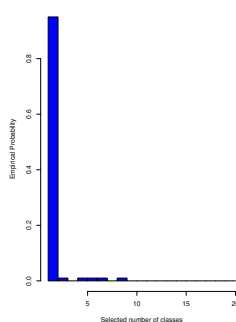
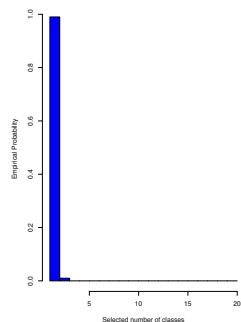
$$\mathcal{N}(x; 0.2, 0.1) + \mathcal{N}(x; 0.8, 0.15)$$

ed (MS) :  $s_0^* \notin S_m^*$ ,

$$\frac{\mathcal{N}(y; \mathbf{x}^2 - 6\mathbf{x} + 1, 0.09) + \mathcal{N}(y; -0.4\mathbf{x}^2, 0.09)}{\mathcal{N}(x; 0.2, 0.1) + \mathcal{N}(x; 0.8, 0.15)}.$$

M package [2]) and model selection via the slope heuristic (capushe package [1]).

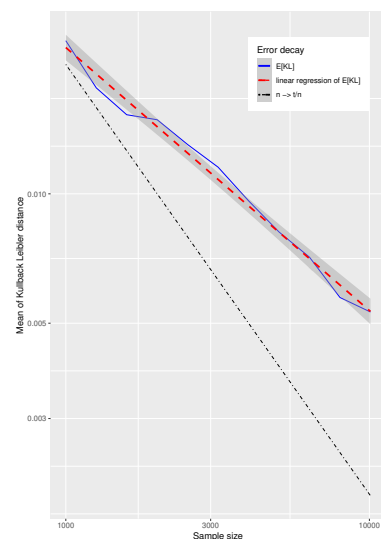
l from the estimated conditional density of GLoME via the Bayes' optimal allocation  
s. The dash and solid black curves present the true and estimated mean functions.  
ted  $K$  using slope heuristic over 100 trials.  
illback–Leibler divergence over 100 trials.  
r bound decay in a log-log scale, using 30 trials.



4.1 WS:

free regression's slope

$\approx -1.287$  and  $t = 3$ .



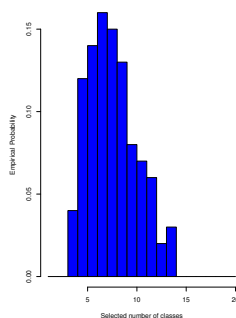
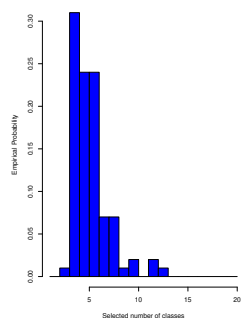
4.2 MS:

free regression's slope

$\approx -0.6120$ ,  $t = 20$ .

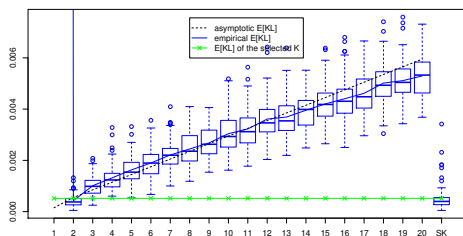
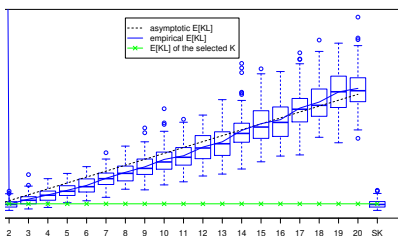
2.1 WS with  $n = 2000$

2.2 WS with  $n = 10000$



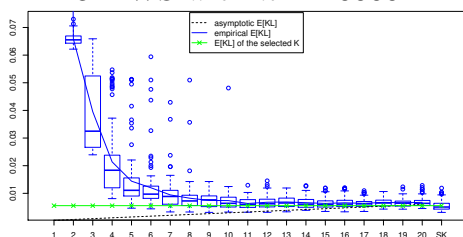
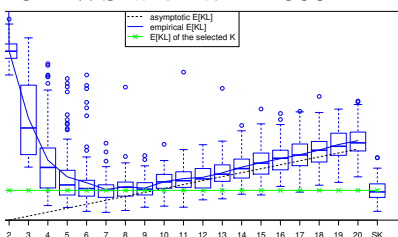
2.3 MS with  $n = 2000$

2.4 MS with  $n = 10000$



3.1 WS with  $n = 2000$

3.2 WS with  $n = 10000$



3.3 MS with  $n = 2000$

3.4 MS with  $n = 10000$