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

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Learning nonlinear regression models from complex data using GLoME models

Random sample: $(\mathbf{X}_i, \mathbf{Y}_i)_{i\in[n]} \in (\mathcal{X}\times\mathcal{Y})^n \subset \left(\mathbb{R}^D \times \mathbb{R}^L\right)^n$ of the multivariate response $\mathbf{Y} = (\mathbf{Y}_j)_{j\in[L]}$ and the set of covariates $\mathbf{X} = (\mathbf{X}_j)_{j\in[D]}$ with the corresponding observed values $(\mathbf{x}_i, \mathbf{y}_i)_{i\in[n]}$, $[n] := \{1,\ldots,n\}$ (potentially $D \gg L$), arising from an unknown conditional density s_0.

Our proposal: approximating s_0 by a **Gaussian-gated Localized Mixture of Experts (GLoME)** model due to its flexibility and effectiveness [3, 4, 5]:

$$s_{\psi_{K,d}}(\mathbf{x}|\mathbf{y}) = \sum_{k=1}^{K} \underbrace{\mathbf{g}_k(\mathbf{y};\boldsymbol{\omega})}_{\text{Gaussian-gated network}} \times \underbrace{\mathcal{N}_D\left(\mathbf{x}; \boldsymbol{\upsilon}_{k,d}(\mathbf{y}), \boldsymbol{\Sigma}_k\right)}_{\text{Gaussian expert}}, \quad \mathbf{g}_k(\mathbf{y};\boldsymbol{\omega}) = \frac{\boldsymbol{\pi}_k \mathcal{N}_L(\mathbf{y}; \mathbf{c}_k, \boldsymbol{\Gamma}_k)}{\sum_{l=1}^{K} \boldsymbol{\pi}_l \mathcal{N}_L(\mathbf{y}; \mathbf{c}_l, \boldsymbol{\Gamma}_l)}, \forall k \in [K], K \in \mathbb{N}^\star, \text{where:}$$

$\boldsymbol{\psi}_{K,d} = (\boldsymbol{\omega}, \boldsymbol{\upsilon}, \boldsymbol{\Sigma}) \in \boldsymbol{\Omega}_K \times \boldsymbol{\Upsilon}_{K,d} \times \mathbf{V}_K =: \boldsymbol{\Psi}_{K,d}$, $\boldsymbol{\omega} = (\boldsymbol{\pi}, \boldsymbol{c}, \boldsymbol{\Gamma}) \in (\boldsymbol{\Pi}_{K-1} \times \mathbf{C}_K \times \mathbf{V}'_K) =: \boldsymbol{\Omega}_K$, $\boldsymbol{\Pi}_{K-1} = \left\{(\boldsymbol{\pi}_k)_{k\in[K]} \in (\mathbb{R}^+)^K, \sum_{k=1}^K \boldsymbol{\pi}_k = 1\right\}$, $\mathbf{C}_K/\boldsymbol{\Upsilon}_{K,d}$: K-tuples of mean vectors/functions of size $L\times 1/D\times 1$, $\mathbf{V}'_K/\mathbf{V}_K$: K-tuples of elements in $\mathcal{S}_L^{++}/\mathcal{S}_D^{++}$ (space of symmetric positive-definite matrices).

Main contributions:

- **Model selection criterion**: choosing number of mixture components and mean functions' degree via a penalized maximum likelihood estimator.
- **Finite-sample oracle inequality**: establishing non-asymptotic risk bounds provided a lower bound on the penalty holds.

Boundedness assumptions

$\widetilde{\boldsymbol{\Omega}}_K = \{\boldsymbol{\omega} \in \boldsymbol{\Omega}_K : \forall k \in [K], \ \|\mathbf{c}_k\|_\infty \leq A_{\mathbf{c}},$
$0 < a_{\boldsymbol{\Gamma}} \leq m(\boldsymbol{\Gamma}_k) \leq M(\boldsymbol{\Gamma}_k) \leq A_{\boldsymbol{\Gamma}}, 0 < a_{\boldsymbol{\pi}} \leq \boldsymbol{\pi}_k\}$,

$m(\boldsymbol{\Gamma}_k)/M(\boldsymbol{\Gamma}_k)$: the smallest/largest eigenvalues of $\boldsymbol{\Gamma}_k$,

$$\boldsymbol{\Upsilon}_{b,d} = \left\{\mathbf{y} \mapsto \left(\sum_{i=1}^{d} \boldsymbol{\alpha}_i^{(j)} \varphi_{\boldsymbol{\Upsilon},i}(\mathbf{y})\right)_{j\in[D]} : \|\boldsymbol{\alpha}\|_\infty \leq T_{\boldsymbol{\Upsilon}}\right\},$$

$\boldsymbol{\Upsilon}_{K,d} = \otimes_{k\in[K]} \boldsymbol{\Upsilon}_{k,d} = \boldsymbol{\Upsilon}_{b,d}^K$, $T_{\boldsymbol{\Upsilon}} \in \mathbb{R}^+$,

$(\varphi_{\boldsymbol{\Upsilon},i})_{i\in[d]}$: collection of bounded functions on $\mathcal{Y}$,

$$\mathbf{V}_K = \left\{(\boldsymbol{\Sigma}_k)_{k\in[K]} = \left(B_k \mathbf{P}_k \mathbf{A}_k \mathbf{P}_k^\top\right)_{k\in[K]} : 0 < B_- \leq B_k \leq B_+, \ \mathbf{P}_k \in SO(D), \ \mathbf{A}_k \in \mathcal{A}(\lambda_-, \lambda_+)\right\},$$

$B_k = |\boldsymbol{\Sigma}_k|^{1/D}$: volume, $SO(D)$: eigenvectors of $\boldsymbol{\Sigma}_k$, $\mathcal{A}(\lambda_-, \lambda_+)$: set of diagonal matrices of normalized eigenvalues of $\boldsymbol{\Sigma}_k$ s.t. $\forall i \in [D], 0 < \lambda_- \leq (\mathbf{A}_k)_{i,i} \leq \lambda_+$,

$\mathbf{m} \in \mathcal{M} = \{(K, d) : K \in [K_{\max}], d \in [d_{\max}]\}$,

$$S_{\mathbf{m}} = \left\{(\mathbf{x}, \mathbf{y}) \mapsto s_{\boldsymbol{\psi}_{K,d}}(\mathbf{x}|\mathbf{y}) =: s_{\mathbf{m}}(\mathbf{x}|\mathbf{y}) : \boldsymbol{\psi}_{K,d} \in \widetilde{\boldsymbol{\Omega}}_K \times \boldsymbol{\Upsilon}_{K,d} \times \mathbf{V}_K =: \widetilde{\boldsymbol{\Psi}}_K\right\}.$$

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

References

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Non-asymptotic oracle inequality [5]

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

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

Numerical experiments

➠**Well-Specified (WS)** : $s^*_0 \in S^*_{\mathbf{m}}$,

$$s^*_0(y|x) = \frac{\mathcal{N}(x; 0.2, 0.1)\mathcal{N}(y; \mathbf{-5x+2}, 0.09) + \mathcal{N}(x; 0.8, 0.15)\mathcal{N}(y; \mathbf{0.1x}, 0.09)}{\mathcal{N}(x; 0.2, 0.1) + \mathcal{N}(x; 0.8, 0.15)},$$

➠**Misspecified (MS)** : $s^*_0 \notin S^*_{\mathbf{m}}$,

$$s^*_0(y|x) = \frac{\mathcal{N}(x; 0.2, 0.1)\mathcal{N}(y; \mathbf{x^2 - 6x + 1}, 0.09) + \mathcal{N}(x; 0.8, 0.15)\mathcal{N}(y; \mathbf{-0.4x^2}, 0.09)}{\mathcal{N}(x; 0.2, 0.1) + \mathcal{N}(x; 0.8, 0.15)}.$$

Estimation by EM (xLLiM package [2]) and model selection via the slope heuristic (capushe package [1]).

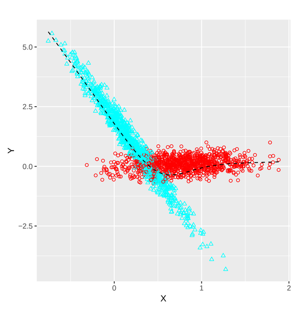
Numerical results:

Fig.1: Clustering deduced from the estimated conditional density of GLoME via the Bayes' optimal allocation rule with 2000 data points. The dash and solid black curves present the true and estimated mean functions.

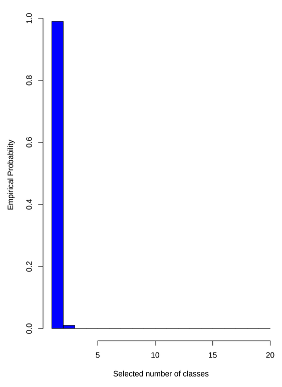
Fig.2: Histogram of selected K using slope heuristic over 100 trials.

Fig.3: Box-plot of the Kullback–Leibler divergence over 100 trials.

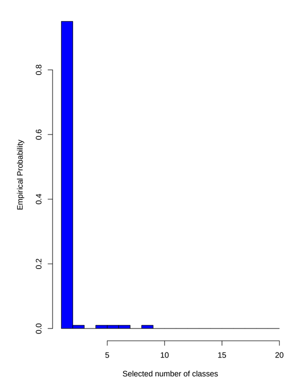
Fig.4: Rate of error upper bound decay in a log-log scale, using 30 trials.



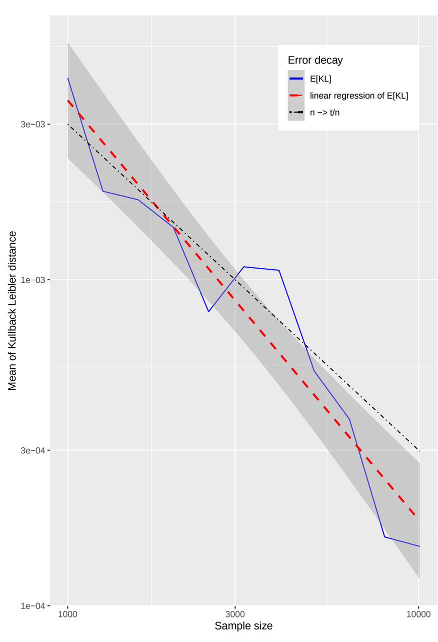
1.1 WS realization



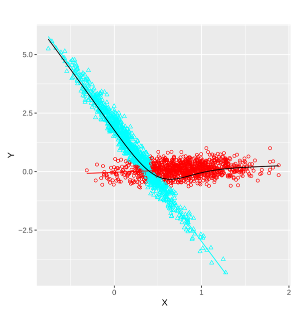
2.1 WS with $n = 2000$



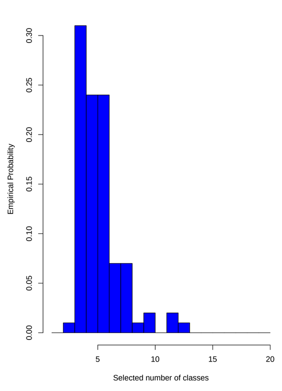
2.2 WS with $n = 10000$



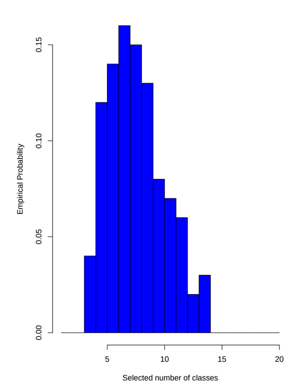
4.1 WS: free regression's slope ≈ -1.287 and $t = 3$.



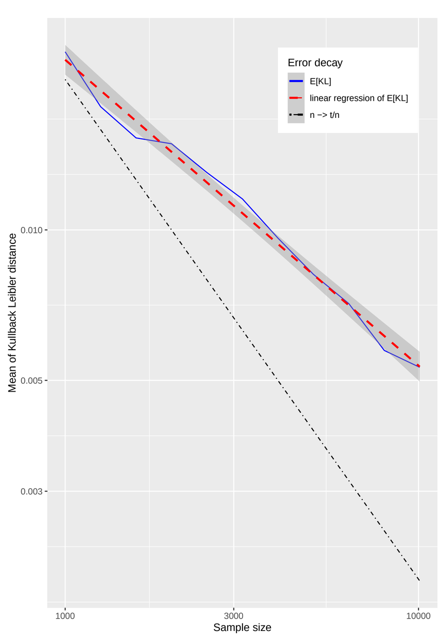
1.2 GLoME clustering



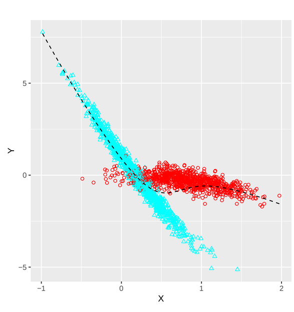
2.3 MS with $n = 2000$



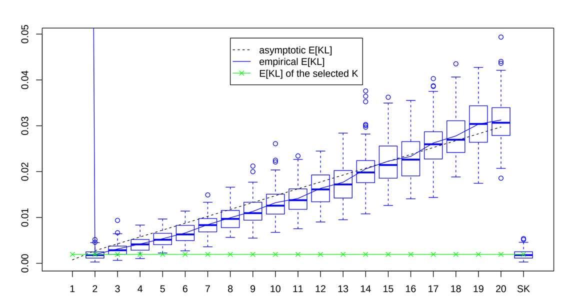
2.4 MS with $n = 10000$



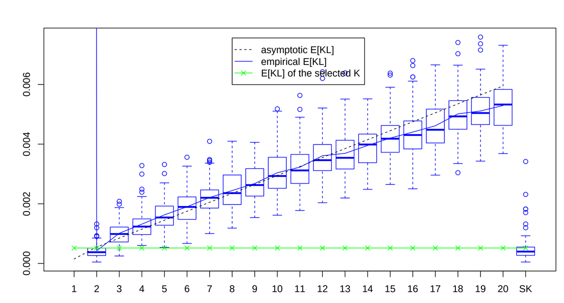
4.2 MS: free regression's slope ≈ -0.6120, $t = 20$.



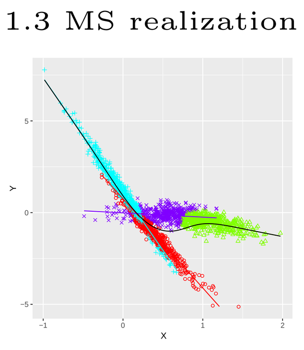
1.3 MS realization



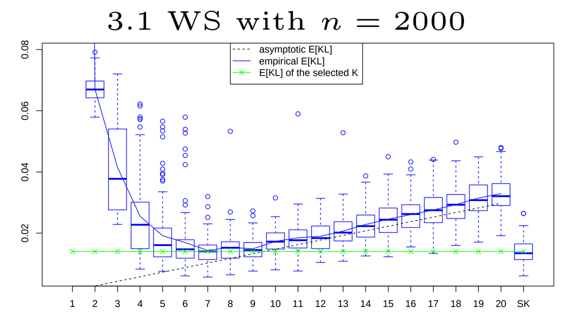
3.1 WS with $n = 2000$



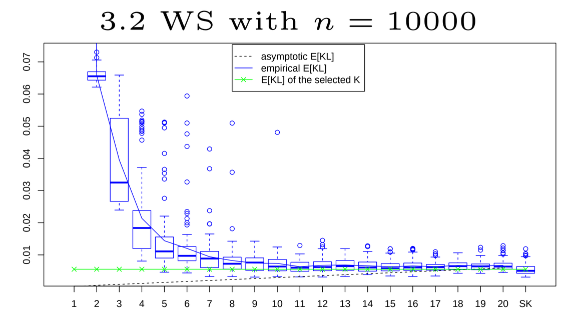
3.2 WS with $n = 10000$



1.4 GLoME clustering



3.3 MS with $n = 2000$



3.4 MS with $n = 10000$