A non-asymptotic model selection in mixture of experts models

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Learning nonlinear regression models for heterogeneous data using GLoME models

Random samples: $(\mathbf{X}_i,\mathbf{Y}_i)_{i\in[n]}\in(\mathcal{X}\times\mathcal{Y})^n\subset\left(\mathbb{R}^D\times\mathbb{R}^L\right)^n$ 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 $(\mathbf{x}_i,\mathbf{y}_i)_{i\in[n]}$, $[n]:=\{1,\ldots,n\}$, 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]:

$$s_{\psi_K}(\mathbf{x}|\mathbf{y})=\sum_{k=1}^{K}\underbrace{\mathbf{g}_k(\mathbf{y};\boldsymbol{\omega})}_{\text{Gaussian gating function}}\underbrace{\Phi_D\left(\mathbf{x};\boldsymbol{\upsilon}_k(\mathbf{y}),\boldsymbol{\Sigma}_k\right)}_{\text{Gaussian expert}},\quad \mathbf{g}_k(\mathbf{y};\boldsymbol{\omega})=\frac{\boldsymbol{\pi}_k\Phi_L(\mathbf{y};\mathbf{c}_k,\boldsymbol{\Gamma}_k)}{\sum_{j=1}^{K}\boldsymbol{\pi}_j\Phi_L(\mathbf{y};\mathbf{c}_j,\boldsymbol{\Gamma}_j)},\forall k\in[K],K\in\mathbb{N}^\star,\text{ where:}$$

$\psi_K=(\boldsymbol{\omega},\boldsymbol{\upsilon},\boldsymbol{\Sigma})\in\boldsymbol{\Omega}_K\times\boldsymbol{\Upsilon}_K\times\mathbf{V}_K=:\boldsymbol{\Psi}_K$, $\boldsymbol{\omega}=(\boldsymbol{\pi},\mathbf{c},\boldsymbol{\Gamma})\in(\boldsymbol{\Pi}_{K-1}\times\mathbf{C}_K\times\mathbf{V}'_K)=:\boldsymbol{\Omega}_K$, $\boldsymbol{\Pi}_{K-1}=\left\{(\boldsymbol{\pi}_k)_{k\in[K]}\in(\mathbb{R}^+)^K,\sum_{k=1}^K\boldsymbol{\pi}_k=1\right\}$, $\mathbf{C}_K/\boldsymbol{\Upsilon}_K$: 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).

- **Model selection problem**: estimating the number of mixture components via penalized maximum likelihood estimators.
- **Non-asymptotic oracle inequality**: providing a lower bound on the penalty such that our estimator satisfies an oracle inequality.

Boundedness assumptions

$$S_m=\Big\{\mathcal{X}\times\mathcal{Y}\ni(\mathbf{x},\mathbf{y})\mapsto s_{\psi_K}(\mathbf{x}|\mathbf{y})=:s_m(\mathbf{x}|\mathbf{y}):$$
$$\psi_K=(\boldsymbol{\omega},\boldsymbol{\upsilon},\boldsymbol{\Sigma})\in\widetilde{\boldsymbol{\Omega}}_K\times\boldsymbol{\Upsilon}_K\times\mathbf{V}_K=:\widetilde{\boldsymbol{\Psi}}_K\Big\},$$

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

$m(\mathbf{A})/M(\mathbf{A})$: smallest/largest eigenvalues of matrix $\mathbf{A}$,

$\boldsymbol{\Upsilon}_K=\boldsymbol{\Upsilon}_b^K, d_{\boldsymbol{\Upsilon}}\in\mathbb{N}^\star, T_{\boldsymbol{\Upsilon}}\in\mathbb{R}^+$,

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

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

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

$B_k=|\boldsymbol{\Sigma}_k|^{1/D}$: volume, $B_-\in\mathbb{R}^+,B_+\in\mathbb{R}^+$,

$\mathbf{P}_k$: eigenvectors of $\boldsymbol{\Sigma}_k\in$ special orthogonal $SO(D)$,

$\mathbf{A}_k$: diagonal matrix of normalized eigenvalues of $\boldsymbol{\Sigma}_k$,

such that $|\mathbf{A}_k|=1$ and $0<\forall i\in[D],\lambda_-\le(\mathbf{A}_k)_{i,i}\le\lambda_+$.

Model selection procedure

Goal: find the best model among $(S_m^*)_{m\in\mathcal{M}}$, $\mathcal{M}=[K_{\max}]$ based one $(\mathbf{x}_i,\mathbf{y}_i)_{i\in[n]}$ arising from an forward conditional density s_0^*.

1. Each $m\in\mathcal{M}$: estimate the forward MLE $(\widehat{s}_m^*(\mathbf{y}_i|\mathbf{x}_i))_{i\in[N]}$ by inverse MLE $\widehat{s}_m$ via an inverse regression trick by GLLiM-EM algorithm (xLLiM package [2]).
2. Calculate η'-PMLE $\widehat{m}$ with $\mathrm{pen}(m)=\kappa\dim(S_m^*)$.
3. **Large enough but not explicit value for κ!** Asymptotic criteria: AIC ($\kappa=1$) and BIC ($\kappa=\frac{\ln n}{2}$). Non-asymptotic criterion: strong justification for slope heuristic approach (capushe package [1]) 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.

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[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 McLachlan. Approximations of conditional probability density functions in Lebesgue spaces via mixture of experts models. *arXiv preprint arXiv:2012.02385*, 2020.

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Non-asymptotic oracle inequality [5]

Given a collection $(S_m)_{m\in\mathcal{M}}$ of GLoME models, $\rho\in(0,1)$, $C_1>1$, assume that $\Xi=\sum_{m\in\mathcal{M}}e^{-z_m}<\infty, z_m\in\mathbb{R}^+,\forall m\in\mathcal{M}$, and there exist constants C and $\kappa(\rho,C_1)>0$ s.t. $\forall m\in\mathcal{M}$, $\mathrm{pen}(m)\ge\kappa(\rho,C_1)\left[(C+\ln n)\dim(S_m)+z_m\right]$. Then, the η'-PMLE $\widehat{s}_{\widehat{m}}$, defined by $\widehat{m}=\operatorname{argmin}_{m\in\mathcal{M}}\left(\sum_{i=1}^n-\ln(\widehat{s}_m(\mathbf{x}_i|\mathbf{y}_i))+\mathrm{pen}(m)\right)+\eta'$, $\widehat{s}_m=\operatorname{argmin}_{s_m\in S_m}\sum_{i=1}^n-\ln(s_m(\mathbf{x}_i|\mathbf{y}_i))$, satisfies, for any $\rho\in(0,1)$, $\mathrm{JKL}_\rho^{\otimes n}(s,t)=\mathbb{E}_{\mathbf{Y}}\left[\frac{1}{n}\sum_{i=1}^n\frac{1}{\rho}\mathrm{KL}\left(s(\cdot|\mathbf{Y}_i),(1-\rho)s(\cdot|\mathbf{Y}_i)+\rho t(\cdot|\mathbf{Y}_i)\right)\right]$,

$$\mathbb{E}\left[\mathrm{JKL}_\rho^{\otimes n}(s_0,\widehat{s}_{\widehat{m}})\right]\le C_1\inf_{m\in\mathcal{M}}\left(\inf_{s_m\in S_m}\mathrm{KL}^{\otimes n}(s_0,s_m)+\frac{\mathrm{pen}(m)}{n}\right)+\frac{\kappa(\rho,C_1)C_1\Xi}{n}+\frac{\eta+\eta'}{n}.$$

Numerical experiment

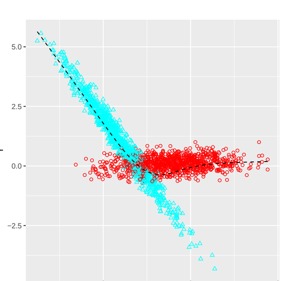
➠**Well-Specified (WS)** : $s_0^*\in S_m^*$,

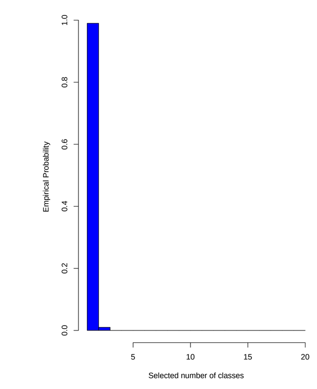
$$s_0^*(y|x)s_0^*(y|x)=\frac{\Phi(x;0.2,0.1)\Phi(y;-5x+2,0.09)+\Phi(x;0.8,0.15)\Phi(y;0.1x,0.09)}{\Phi(x;0.2,0.1)+\Phi(x;0.8,0.15)},$$

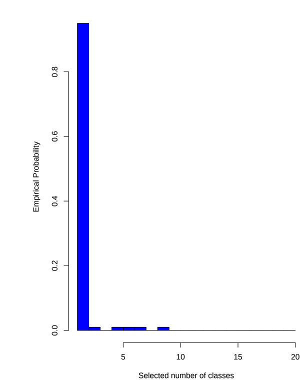
➠**Misspecified (MS)** : $s_0^*\notin S_m^*$,

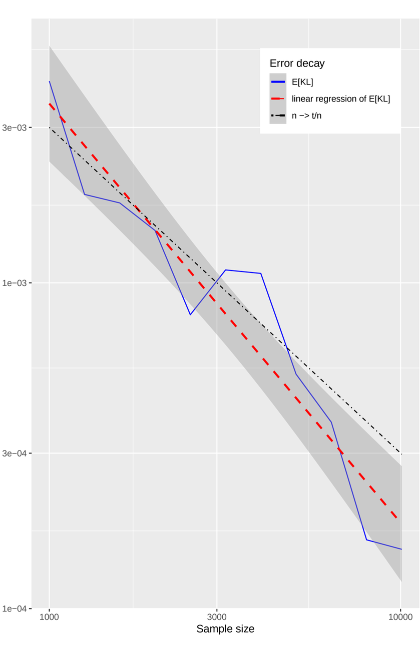
$$s_0^*(y|x)=\frac{\Phi(x;0.2,0.1)\Phi(y;x^2-6x+1,0.09)+\Phi(x;0.8,0.15)\Phi(y;-0.4x^2,0.09)}{\Phi(x;0.2,0.1)+\Phi(x;0.8,0.15)}.$$

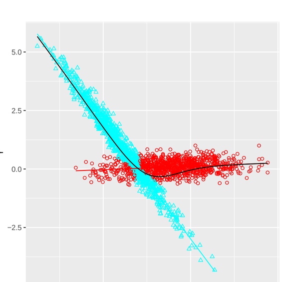
1. Clustering deduced from the estimated conditional density of GLoME by a MAP principle with 2000 data points. The dash and solid black curves present the true and estimated mean functions.
2. Histogram of selected K using slope heuristic over 100 trials.
3. Box-plot of the Kullback-Leibler divergence over 100 trials.
4. Rate of error decay in a log-log scale, using 30 trials.

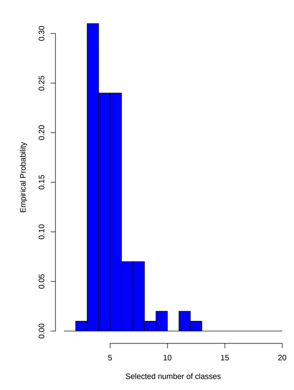

1.1 WS realization

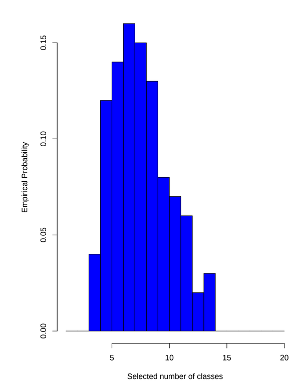

2.1 WS with $n=2000$

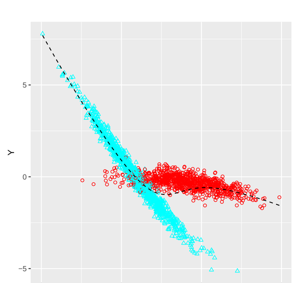

2.2 WS with $n=10000$

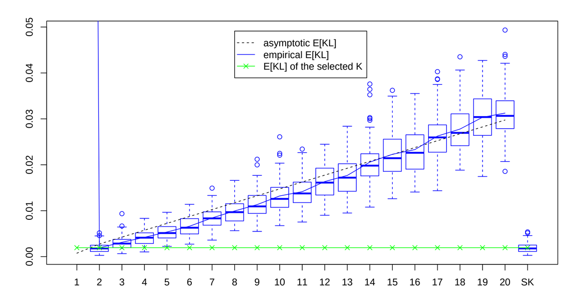

4.1 WS: free regression's slope ≈ -1.287 and $t=3$.

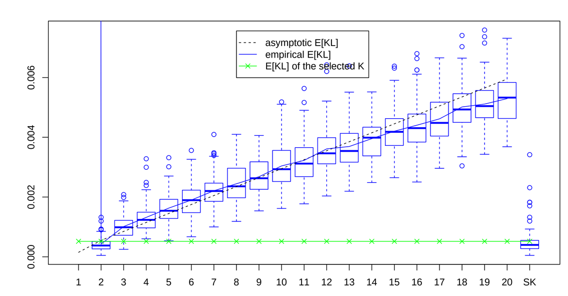

1.2 GLoME clustering

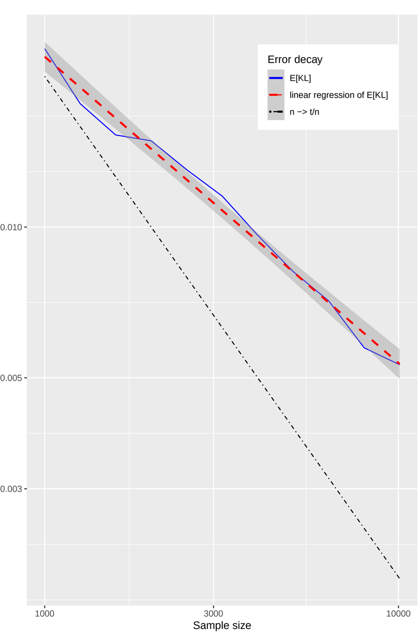

2.3 MS with $n=2000$

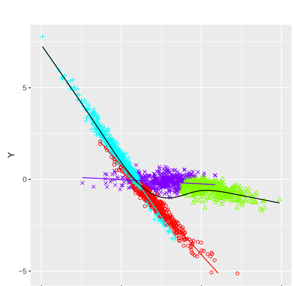

2.4 MS with $n=10000$

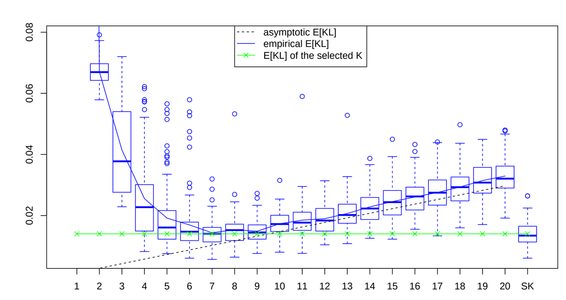

1.3 MS realization

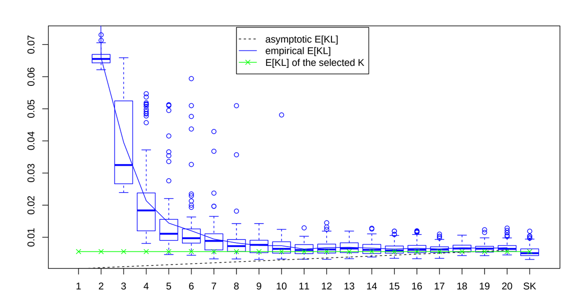

3.1 WS with $n=2000$


3.2 WS with $n=10000$


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


1.4 GLoME clustering


3.3 MS with $n=2000$


3.4 MS with $n=10000$