Model selection by penalization in mixture of experts models with a non-asymptotic approach

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Outline and our contributions

1. Collection of GLoME models
   - Context and motivating example
   - Boundedness conditions
2. Model selection in GLoME and BLoME models
   - Asymptotic approach
   - Non-asymptotic approach with oracle inequalities
3. Main positive messages and perspectives

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   - Non-asymptotic approach with oracle inequalities
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Context

- **We have**: n random samples $(\mathbf{X}_i, \mathbf{Y}_i)_{i \in [n]} \in (\mathcal{X} \times \mathcal{Y})^n$ with observed values $(\mathbf{x}_i, \mathbf{y}_i)_{i \in [n]}$, $[n] = \{1, \ldots, n\}$, arising from an unknown conditional density s_0.
- **Learning**: potentially **nonlinear regression models for high-dimensional heterogeneous data** between output $\mathbf{Y}$ and input $\mathbf{X}$: Regression analysis + Clustering + Model selection (*e.g.*, number of clusters, complexity in each cluster).
- **Our proposal**: using **mixture of experts (MoE[1])** regression models due to their flexibility and effectiveness, *e.g.*, several universal approximation theorems. [2] [3] [4]

[1] Jacobs, R. A., Jordan, M. I., Nowlan, S. J., and Hinton, G. E. (1991). Adaptive mixtures of local experts. Neural computation.

[2] Nguyen, H. D., Chamroukhi, F., and Forbes, F. (2019). Approximation results regarding the multiple-output Gaussian gated mixture of linear experts model. Neurocomputing.

[3] Nguyen, H. D., **Nguyen, T.**, Chamroukhi, F., and McLachlan, G. J. (2021). Approximations of conditional probability density functions in Lebesgue spaces via mixture of experts models. *Journal of Statistical Distributions and Applications.*

[4] **Nguyen, T.**, Chamroukhi, F., Nguyen, H. D., and McLachlan, G. J. (2022). Approximation of probability density functions via location-scale finite mixtures in Lebesgue spaces. *Communications in Statistics - Theory and Methods.*

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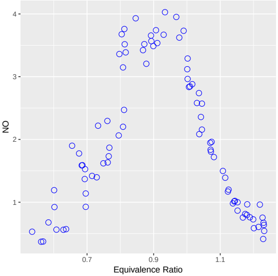
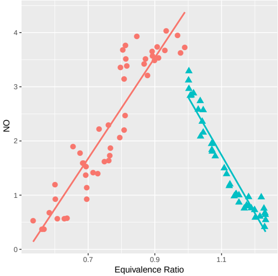
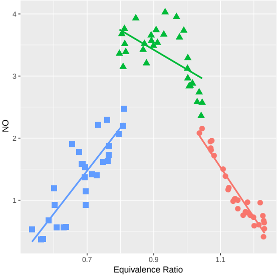
Motivating example: Ethanol data set 88 observations

(a) Raw Ethanol data set

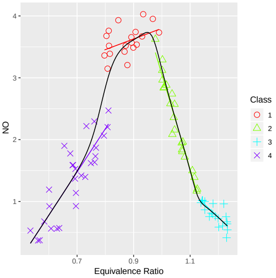


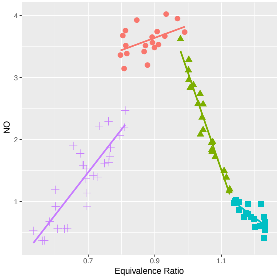
Collection of MoE models with linear mean functions characterized by 2-5 clusters

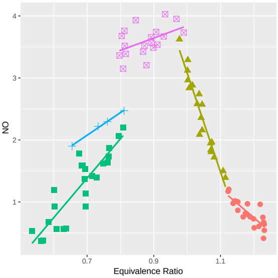




(b) Our best data-driven MoE model







Definition: GLLiM and GLoME models

$$s_{\psi_{K,d}}(\mathbf{x}|\mathbf{y}) = \sum_{k=1}^{K} \underbrace{\frac{\pi_k \mathcal{N}_L(\mathbf{y}; \mathbf{c}_k, \boldsymbol{\Gamma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}_L(\mathbf{y}; \mathbf{c}_j, \boldsymbol{\Gamma}_j)}}_{\text{Gaussian gating network}} \underbrace{\mathcal{N}_D(\mathbf{x}; \boldsymbol{\upsilon}_{k,d}(\mathbf{y}), \boldsymbol{\Sigma}_k)}_{\text{Gaussian expert}}.$$

- $\boldsymbol{\omega} = (\boldsymbol{\pi}, \boldsymbol{c}, \boldsymbol{\Gamma}) \in (\boldsymbol{\Pi}_{K-1} \times \mathbf{C}_K \times \boldsymbol{V}'_K) = \boldsymbol{\Omega}_K$, $\boldsymbol{\Pi}_{K-1}$: probability simplex, $K \in \mathbb{N}^\star$: number of mixture components.
- $d \in \mathbb{N}^\star$: mean functions' hyperparameter *e.g.*, degree of polynomial.
- $\psi_{K,d} = (\boldsymbol{\omega}, \boldsymbol{\upsilon}, \boldsymbol{\Sigma}) \in \boldsymbol{\Omega}_K \times \boldsymbol{\Upsilon}_{K,d} \times \mathbf{V}_K$: model parameter.

High-dimensional data using inverse regression frameworks (GLLiM models[5]): $\mathbf{Y} \equiv$ input, $\mathbf{X} \equiv$ output, $\mathcal{X} \subset \mathbb{R}^D$, $\mathcal{Y} \subset \mathbb{R}^L$, with $D \gg L$ and $D, L \in \mathbb{N}^\star$.

[5] Deleforge, A., Forbes, F., and Horaud, R. (2015). High-dimensional regression with gaussian mixtures and partially-latent response variables. Statistics and Computing.

Definition: Gaussian gating networks

$$\mathbf{g}_k(\mathbf{y};\omega) = \frac{\pi_k \mathcal{N}_L(\mathbf{y};\mathbf{c}_k,\boldsymbol{\Gamma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}_L(\mathbf{y};\mathbf{c}_j,\boldsymbol{\Gamma}_j)}, \text{ for every } k \in [K],$$

- $\omega = (\boldsymbol{\pi}, \boldsymbol{c}, \boldsymbol{\Gamma}) \in (\boldsymbol{\Pi}_{K-1} \times \mathbf{C}_K \times \boldsymbol{V}'_K) = \boldsymbol{\Omega}_K$,
- $\boldsymbol{\Pi}_{K-1} = \left\{ (\pi_k)_{k\in[K]} \in (\mathbb{R}^+)^K, \sum_{k=1}^{K} \pi_k = 1 \right\}$,
- $\mathbf{C}_K$: K-tuples of mean vectors of size $L \times 1$,
- $\boldsymbol{V}'_K$: K-tuples of elements in $\mathcal{S}_L^{++}$,
- $\mathcal{S}_L^{++}$: collection of symmetric positive definite matrices on $\mathbb{R}^L$.

Outline

Mild assumption: Boundedness conditions

- Gaussian gating parameters: there exist positive constants $a_{\pi}, A_{\mathbf{c}}, a_{\mathbf{\Gamma}}, A_{\mathbf{\Gamma}}$ s.t.

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

- Gaussian experts linear combination of bounded functions means: $\boldsymbol{\upsilon} = (\upsilon_{k,d})_{k\in[K]} \in \mathbf{\Upsilon}_{K,d} = \otimes_{k\in[K]} \mathbf{\Upsilon}_{k,d} = \mathbf{\Upsilon}_{k,d}^K$, where $\forall k \in [K]$,

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

Collection of bounded basis functions: $\mathbf{y} \mapsto (\boldsymbol{\theta}_{\mathbf{\Upsilon},i}(\mathbf{y}))_{i\in[d_{\mathbf{\Upsilon}}]}$, $d \in \mathbb{N}^\star$, $T_{\mathbf{\Upsilon}} \in \mathbb{R}^+$.

Classical covariance matrix parameterization[6]

Boundedness conditions on Gaussian expert covariance matrices

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

- $B_k = |\boldsymbol{\Sigma}_k|^{1/D}$: volume, $B_- \in \mathbb{R}^+, B_+ \in \mathbb{R}^+$,
- $\mathbf{P}_k$: eigenvectors of $\boldsymbol{\Sigma}_k$, $SO(D)$: special orthogonal group of dimension D,
- $\mathbf{A}_k$: diagonal matrix of normalized eigenvalues of $\boldsymbol{\Sigma}_k$, $\mathcal{A}(\lambda_-, \lambda_+)$: diagonal matrices $\mathbf{A}_k$, such that $|\mathbf{A}_k| = 1$ and $\forall i \in [D], \lambda_- \leq (\mathbf{A}_k)_{i,i} \leq \lambda_+$, where $\lambda_-, \lambda_+ \in \mathbb{R}$.

[6] Celeux, G. and Govaert, G. (1995). Gaussian parsimonious clustering models. Pattern Recognition.

Definition: Collection of GLLiM and GLoME models

$$S_{\mathbf{m}} = \Big\{ (\mathbf{x}, \mathbf{y}) \mapsto s_{\psi_{K,d}}(\mathbf{x}|\mathbf{y}) = s_{\mathbf{m}}(\mathbf{x}|\mathbf{y}) : \mathbf{m} = (K, d)\,,$$

$$\psi_{K,d} = (\boldsymbol{\omega}, \boldsymbol{\upsilon}, \boldsymbol{\Sigma}) \in \widetilde{\boldsymbol{\Omega}}_K \times \boldsymbol{\Upsilon}_{K,d} \times \mathbf{V}_K = \widetilde{\boldsymbol{\Psi}}_{K,d} \Big\}.$$

- $\mathbf{m} \in \mathcal{M} = [K_{\max}] \times [d_{\max}]\,, K_{\max}, d_{\max} \in \mathbb{N}^{\star}$.

Outline

Model selection in standard MoE regression models

- **Best data-driven model**: selecting from a collection of MoE models characterized by hyperparameters $\mathbf{m} = (K, d)$.

→ **Penalized maximum likelihood estimator (PMLE)**:

  - **MLE is not sufficient**: underestimation of the risk of the estimate $\Rightarrow$ choosing models too complex.
  - **PMLE via adding $\mathbf{pen}(\mathbf{m})$**: compensate bias (too simple model) and variance (too complex model).

- **Our contributions**: establishing **non-asymptotic risk bounds** that take the form of **weak oracle inequalities**, provided that **lower bounds on the penalties** hold true.

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Definition: Penalized maximum likelihood estimator (PMLE)

An η'-**PMLE** $\widehat{s}_{\widehat{\mathbf{m}}}$ (corresponding **the selected model or best data-driven model** $S_{\widehat{\mathbf{m}}}$ among $(S_{\mathbf{m}})_{\mathbf{m}\in\mathcal{M}}$), defined by

$$\sum_{i=1}^{n} -\ln\left(\widehat{s}_{\widehat{\mathbf{m}}}\left(\mathbf{x}_i|\mathbf{y}_i\right)\right) + \mathrm{pen}\left(\widehat{\mathbf{m}}\right) \leq \inf_{\mathbf{m}\in\mathcal{M}}\left(\sum_{i=1}^{n} -\ln\left(\widehat{s}_{\mathbf{m}}\left(\mathbf{x}_i|\mathbf{y}_i\right)\right) + \mathrm{pen}(\mathbf{m})\right) + \eta',$$

- $\widehat{s}_{\mathbf{m}}$ is an η-minimizer of the negative log-likelihood (infimum may not be unique or reached) is defined by

$$\sum_{i=1}^{n} -\ln\left(\widehat{s}_{\mathbf{m}}\left(\mathbf{x}_i|\mathbf{y}_i\right)\right) \leq \inf_{s_{\mathbf{m}}\in S_{\mathbf{m}}} \sum_{i=1}^{n} -\ln\left(s_{\mathbf{m}}\left(\mathbf{x}_i|\mathbf{y}_i\right)\right) + \eta,$$

- $\mathrm{pen}(\mathbf{m})$: penalty function $\leftarrow$ choosing it is tricky but obviously necessary to compensate variance and bias.

Definition: Loss functions for conditional densities

- Tensorized Kullback-Leibler divergence $\mathrm{KL}^{\otimes n}$ **(conditional densities and random covariate variables)**:

$$\mathrm{KL}^{\otimes n}(s,t) = \mathbb{E}_{\mathbf{Y}_{[n]}}\left[\frac{1}{n}\sum_{i=1}^{n}\mathrm{KL}\left(s\left(\cdot|\mathbf{Y}_i\right), t\left(\cdot|\mathbf{Y}_i\right)\right)\right],$$

if $sdy \ll tdy$, $+\infty$ otherwise. Fixed predictors $\Rightarrow$ no $\mathbb{E}_{\mathbf{Y}_{[n]}}[\cdot]$.

- Tensorized Jensen-Kullback-Leibler divergence $\mathrm{JKL}_{\rho}^{\otimes n}$ **(technical difficulties with conditional densities)**, given $\rho \in (0,1)$,

$$\mathrm{JKL}_{\rho}^{\otimes n}(s,t) = \mathbb{E}_{\mathbf{Y}_{[n]}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{\rho}\mathrm{KL}\left(s\left(\cdot|\mathbf{Y}_i\right), (1-\rho)s\left(\cdot|\mathbf{Y}_i\right)+\rho t\left(\cdot|\mathbf{Y}_i\right)\right)\right].$$

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Outline

- Akaike information criterion (AIC) [Akaike, 1974], Bayesian information criterion (BIC) [Schwarz et al., 1978] and BIC-like approximation of integrated classification likelihood (ICL-BIC) [Biernacki et al., 2000] criteria:

$$\mathrm{pen}_{\mathrm{AIC}}(\mathbf{m}) = \dim(S_{\mathbf{m}}), \quad \mathrm{pen}_{\mathrm{BIC}}(\mathbf{m}) = \frac{\ln(n)\dim(S_{\mathbf{m}})}{2}.$$

$$\mathrm{pen}_{\text{ICL-BIC}}(\mathbf{m}) = \mathrm{pen}_{\mathrm{BIC}}(\mathbf{m}) + \mathrm{ENT}(\mathbf{m}) \longleftarrow \text{ estimated mean entropy.}$$

AIC (based on asymptotic theory), BIC, ICL-BIC (based on Bayesian approach):

- May be wrong in a non-asymptotic context: $\dim(S_{\mathbf{m}})$ and $\mathrm{card}(\mathcal{M})$ depend on and can be much larger than n.
- No finite sample guarantees.

Obtain an upper bound on $\mathbb{E}\left[\mathrm{KL}^{\otimes n}(s_0, \widehat{s}_{\mathbf{m}})\right]$:

✔ Finite sample guarantee.

✖ Strong regularity assumptions of [White, 1982].

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Non-asymptotic upper bound of a single model

- **Initial target**:

$$\mathbb{E}\left[\mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_{\mathbf{m}}\right)\right] \leq \left(\inf_{\psi_{\mathbf{m}} \in \boldsymbol{\Psi}_{\mathbf{m}}} \mathrm{KL}^{\otimes n}\left(s_0, s_{\psi_{\mathbf{m}}}\right) + \frac{1}{2n} \dim\left(S_{\mathbf{m}}\right)\right) + C_2 \frac{1}{n}.$$

- **Our contribution**:

$$\mathbb{E}\left[\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_{\mathbf{m}}\right)\right] \leq C_1 \left(\inf_{\psi_{\mathbf{m}} \in \boldsymbol{\Psi}_{\mathbf{m}}} \mathrm{KL}^{\otimes n}\left(s_0, s_{\psi_{\mathbf{m}}}\right) + \frac{\kappa}{n} \mathfrak{D}_m\right) + C_2 \frac{1}{n}.$$

1. Different divergences: $\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_m\right) \leq \mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_m\right)$.
2. $C_1 > 1$, κ is a constant that depends on C_1, $\mathfrak{D}_m \propto \dim\left(S_{\mathbf{m}}\right)$.

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Theorem: Non-asymptotic oracle inequality[7]

- **Assumptions**: given a deterministic collection $(S_{\mathbf{m}})_{\mathbf{m}\in\mathcal{M}}$ of MoE models, $\rho \in (0,1)$, $C_1 > 1$,
$\Xi = \sum_{\mathbf{m}\in\mathcal{M}} e^{-z_m} < \infty, z_m \in \mathbb{R}^+, \forall m \in \mathcal{M}$.
- **Conclusion**: there exist constants C and $\kappa(\rho, C_1) > 0$ such that whenever for all $m \in \mathcal{M}$,

$$\mathrm{pen}(\mathbf{m}) \geq \kappa(\rho, C_1)\left[(C + \ln n)\dim(S_{\mathbf{m}}) + z_m\right],$$

the η'-PMLE $\widehat{s}_{\widehat{\mathbf{m}}}$ satisfies

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[7] **Nguyen, T.**, Nguyen, H.D., Chamroukhi, F., and Forbes, F. (2022). A non-asymptotic approach for model selection via penalization in high-dimensional mixture of experts. arXiv 2104.02640. Under revision, Electronic Journal of Statistics.

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Outline

Main positive messages and perspectives

- **Our risk assessments are non-asymptotic**.
- If pen($\mathbf{m}$) is properly chosen, then our PMLE behaves in a comparable manner compared to **the best (oracle) model $S_{\mathbf{m}^\star}$ in the collection**.
- **Partially answer** the two following important questions raised in the area of MoE regression models:
  1. **Which value of K** should be chosen, given the sample size n,
  2. Whether it is better to use a **few complex experts** or **combine many simple experts**, given the total number of parameters.
- **Minimax lower bounds** for MoE regression models, which is only known for mixture models[8].

[8] Maugis-Rabusseau, C. and Michel, B. (2013). Adaptive density estimation for clustering with Gaussian mixtures. ESAIM: Probability and Statistics.

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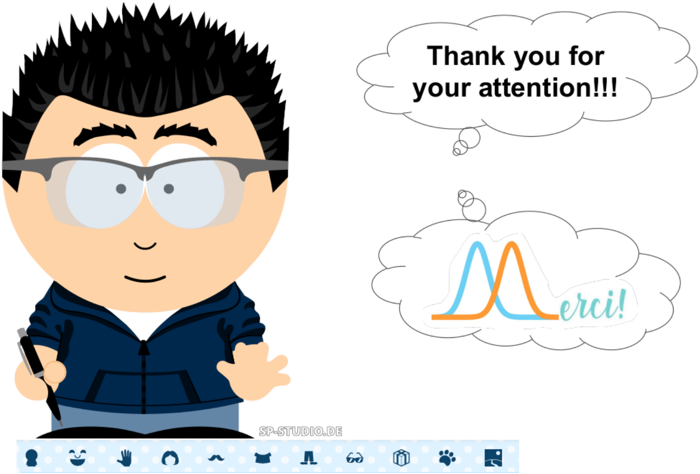
My Coauthors $\in$ Mixture of French and Australian Experts

Faicel Chamroukhi

Hien Duy Nguyen

Florence Forbes

“Essentially, all models are wrong, but some are useful”. George E.P. Box (1987).



↑ This is my best data-driven model to approximate myself.