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

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Outline

1. Collection of GLoME and BLoME models
   - Context and motivating example
   - Conditional density estimation
   - Graphical model representation of MoE models
   - Gaussian gating networks
2. Model selection in GLoME amd BLoME models
   - Model selection in standard MoE regression models
   - Penalized maximum likelihood estimator
   - Asymptotic approach
   - Non-asymptotic approach with oracle inequalities
3. Numerical experiments
4. Main positive messages and perspectives

Outline

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**: Regression analysis + Clustering + Model selection (*e.g.*, number of clusters, complexity in each cluster).
- **Our proposal**: using **mixture of experts**[1] **(MoE)** models due to their flexibility and effectiveness (several universal approximation theorems [2] [3] [4] [5] with good convergence rates).

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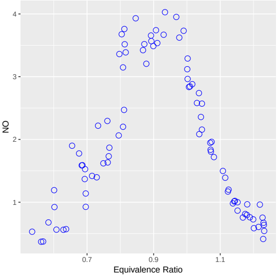
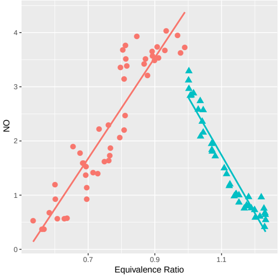
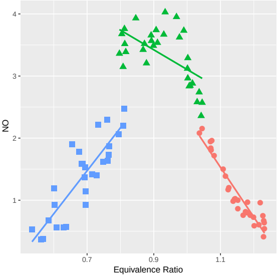
Motivating example: Ethanol data set 88 observations

(a) Raw Ethanol data set

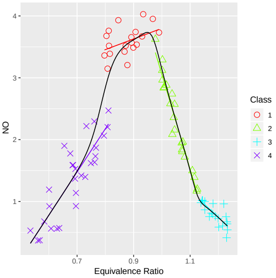


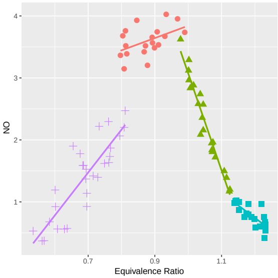
Collection of MoE models with linear mean functions characterized by 2-5 clusters

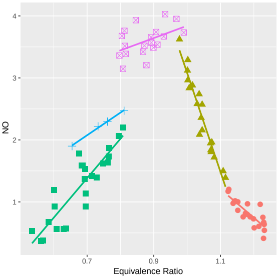




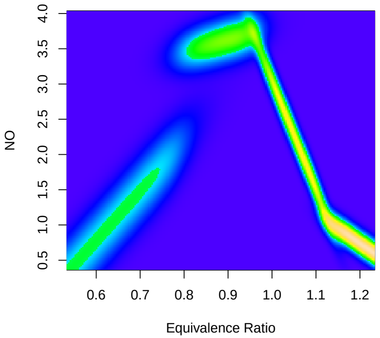
(b) Our best data-driven MoE model



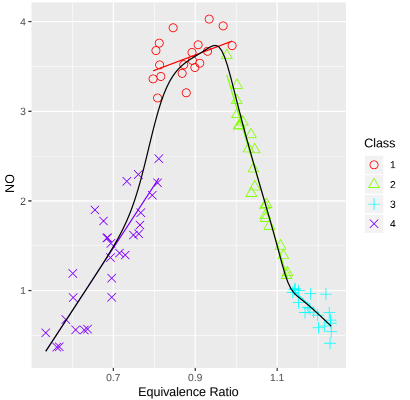




Outline



(a) 2D view of our estimate conditional density with 4 clusters.



(b) Our nonlinear regression and clustering using MoE models.

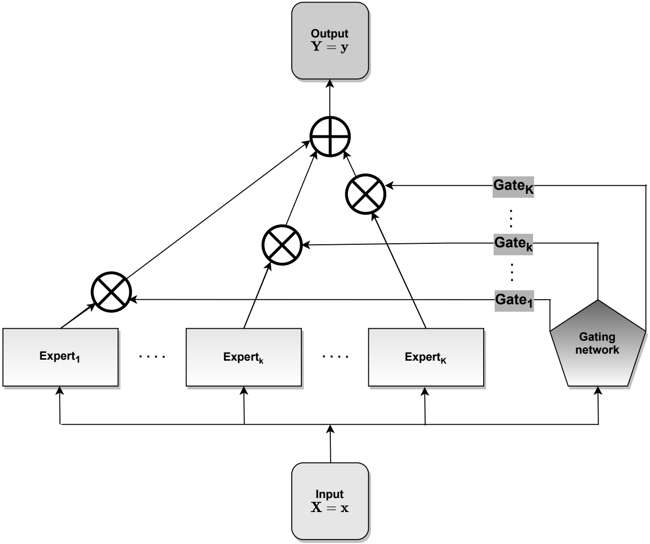
Regression and clustering have been recasted as a task of estimating the true but unknown conditional density estimation s_0 using MoE distribution

$\Rightarrow$ It makes sense to select models from the conditional density point of view.

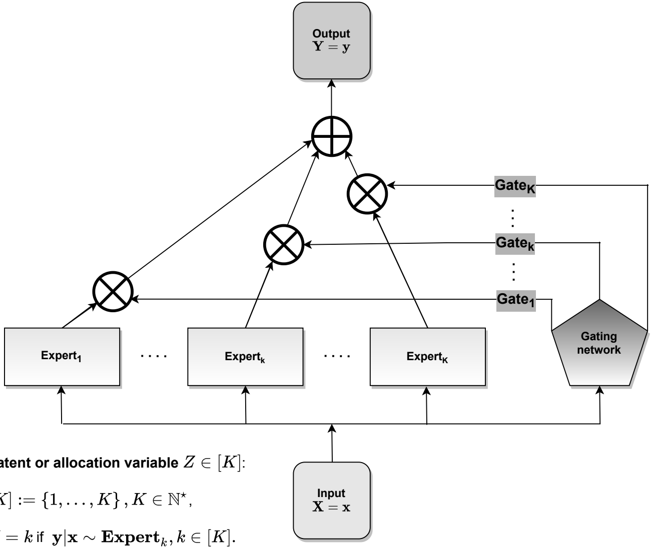
Flexibility and effectiveness of MoE models

Originally introduced as neural network architectures in [Jacobs et al., 1991, Jordan and Jacobs, 1994]:

- Modeling more complex data generating processes than classical finite mixtures or finite mixtures of regression models [McLachlan and Peel, 2000].
- Universal approximation properties with good convergence rates [Mendes and Jiang, 2012, Norets, 2010, Ho et al., 2022, Nguyen et al., 2019, **Nguyen et al., 2020b**, **Nguyen et al., 2021a**, **Nguyen et al., 2020a**].
- Applied to numerous areas of business, science, and technology for the tasks: clustering, regression analysis, conditional density estimation and classification [Yuksel et al., 2012, Masoudnia and Ebrahimpour, 2014, Nguyen and Chamroukhi, 2018, Chamroukhi & Huynh, 2019].



Schematic diagram of the neural network architecture of a K-component MoE model.



Latent or allocation variable $Z \in [K]$:

$[K] := \{1, \dots, K\}, K \in \mathbb{N}^\star$,

$Z = k$ if $\mathbf{y}|\mathbf{x} \sim \mathbf{Expert}_k, k \in [K]$.

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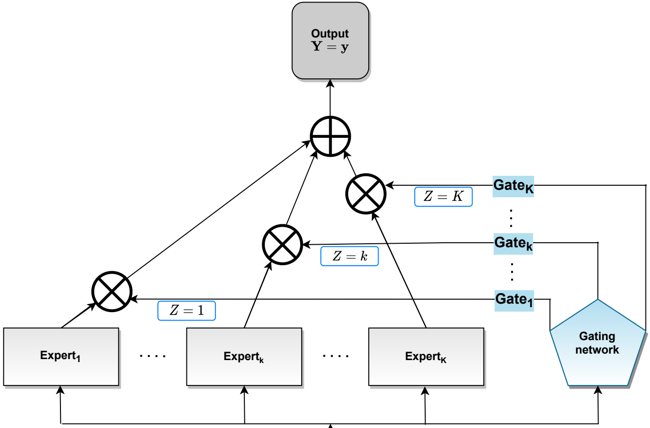

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"Generative" view: two-stage sampling

Step 1: Sample $Z \sim \mathbf{Mult}\left(1, \mathbf{g}\left(\mathbf{x}, \boldsymbol{\omega}\right)\right)$,

$$g_k\left(\mathbf{x}; \boldsymbol{\omega}\right) = p\left(Z = k | \mathbf{X} = \mathbf{x}\right) =: \mathbf{Gate}_k, k \in [K].$$

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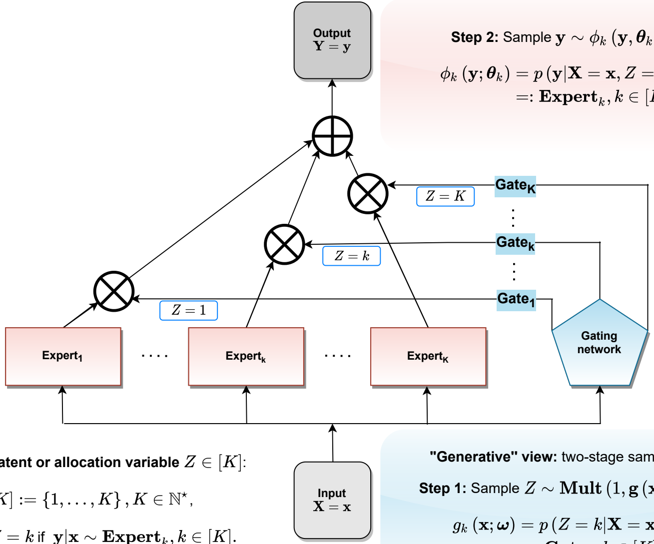

Step 2: Sample $\mathbf{y} \sim \phi_k\left(\mathbf{y}, \boldsymbol{\theta}_k\right)$,

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Schematic diagram of the neural network architecture of a K-component MoE model.

"Analytic" view:

$$
\begin{aligned}
&p(\mathbf{y}|\mathbf{X}=\mathbf{x}) \text{ (law of total probability)}\\
&= \sum_{k=1}^{K} p(Z=k|\mathbf{X}=\mathbf{x})\, p(\mathbf{y}|\mathbf{X}=\mathbf{x}, Z=k)\\
&= \sum_{k=1}^{K} \mathbf{Gate}_k \times \mathbf{Expert}_k\\
&= \sum_{k=1}^{K} g_k(\mathbf{x};\boldsymbol{\omega})\, \phi_k(\mathbf{y};\boldsymbol{\theta}_k)\\
&=: s_{\boldsymbol{\psi}}(\mathbf{y}|\mathbf{x}), \boldsymbol{\psi} =: (\boldsymbol{\omega}, \boldsymbol{\theta}).
\end{aligned}
$$

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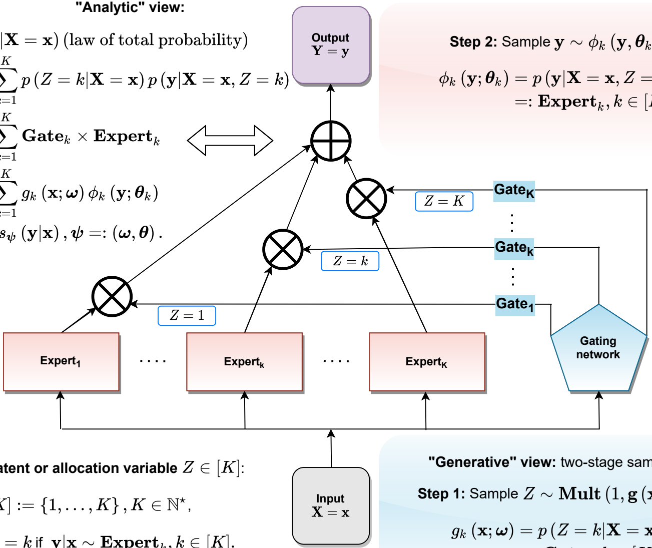

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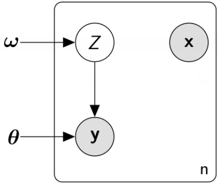
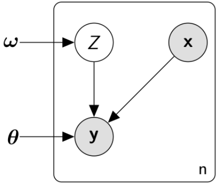
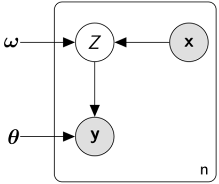


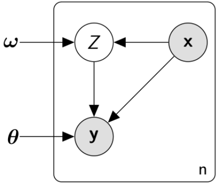
(a) Mixture model



(b) MoE regression model

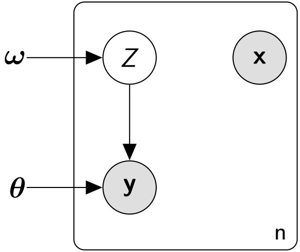


(c) Simple MoE regression model



(d) Standard MoE regression model

Presence or absence of edges between the inputs $\mathbf{x}$, the latent variable Z and the output $\mathbf{y}$ $\implies$ four special cases of MoE regression models.



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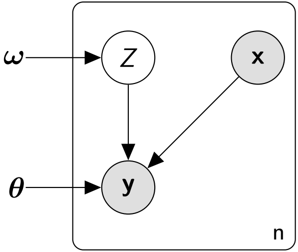

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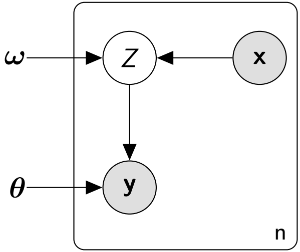

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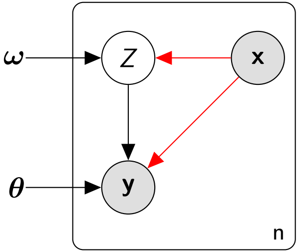
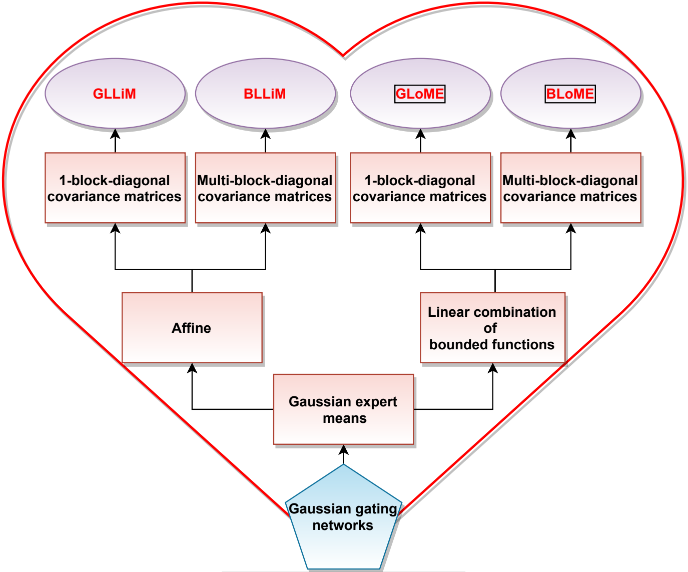


(d) **Standard MoE regression model**

Model selection and approximation for **standard MoE regression models**.

Outline



GLoME: Gaussian-gated Localized MoE

GLLiM: Gaussian Locally-Linear Mapping

BLoME: Block-diagonal covariance Gaussian-gated Localized MoE

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Definition: GLLiM, BLLiM, GLoME and BLoME models

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

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

High-dimensional data using inverse regression frameworks (GLLiM models [Deleforge et al., 2015]): $\mathbf{Y} \equiv$ input, $\mathbf{X} \equiv$ output, $\mathcal{X} \subset \mathbb{R}^D$, $\mathcal{Y} \subset \mathbb{R}^L$, with $D \gg L$.

Establishing non-asymptotic oracle inequalities $\leftarrow$ Boundedness conditions on model parameters $\psi_{K,d,\mathbf{B}}$.

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↑

[Devijver et al., 2017, Devijver et al., 2018] BLLiM procedure: trade-off complexity and sparsity ← Prediction on gene expression data with heterogeneous observations and hidden graph-structured interactions between small modules of correlated genes.

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$\uparrow$

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$\Uparrow$

[Devijver et al., 2017, Devijver et al., 2018] BLLiM procedure: trade-off complexity and sparsity $\leftarrow$ Prediction on gene expression data with heterogeneous observations and hidden graph-structured interactions between small modules of correlated genes.

Outline

Outline

Model selection in standard MoE regression models

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

→ **Penalized maximum likelihood estimator (PMLE)**:
  - **MLE is not sufficient**: underestimation of the risk of the estimate $\Rightarrow$ choosing models too complex.
  - **PMLE via adding pen(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.
  1. Deterministic collection of MoE models characterized by $\mathcal{M}$: GLLiM, GLoME.
  2. **Random** collection of MoE models characterized by $\widetilde{\mathcal{M}}$: **BLLiM, BLoME**.

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Outline

Definition: Penalized maximum likelihood estimator (PMLE)

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

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

- $\widehat{s}_{\mathbf{m}}$: an η-minimizer of the negative log-likelihood (infimum may not be 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 $\leftarrow$ trade-off between good data fit and model complexity.

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.

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

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Fixed predictors $\Rightarrow$ no $\mathbb{E}_{\mathbf{Y}_{[n]}}[\cdot]$.

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Outline

Some asymptotic approaches for model selection in MoE models

- Akaike information criterion (AIC), Bayesian information criterion[6] (BIC) and BIC-like approximation of integrated classification likelihood (ICL-BIC) [Biernacki et al., 2000] criteria:

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

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

- 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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Theorem (Non-asymptotic oracle inequality for deterministic collection of MoE models[a])

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- **Assumptions**: *We are given:* $(S_{\mathbf{m}})_{\mathbf{m}\in\mathcal{M}}$, $\rho \in (0,1)$, $C_1 > 1$, $\Xi = \sum_{\mathbf{m}\in\mathcal{M}} e^{-z_m} < \infty, z_m \in \mathbb{R}^+, \forall m \in \mathcal{M}$.

- **Non-asymptotic upper bound:** *There exist constants* C *and* $\kappa(\rho, C_1) > 0$ *such that whenever for all* $m \in \mathcal{M}$,

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Theorem: Oracle inequality for random collection [Nguyen et al., 2022]

- Given random (defined on datasets) subcollection $(S_{\mathbf{m}})_{\mathbf{m}\in\widetilde{\mathcal{M}}}$, $\widetilde{\mathcal{M}} \subset \mathcal{M}$, $\rho \in (0,1)$, $C_1 > 1$, we define $\Xi = \sum_{\mathbf{m}\in\mathcal{M}} e^{-z_m} < \infty, z_m \in \mathbb{R}^+, \forall m \in \mathcal{M}$. Assume that there exists $\tau > 0$ and $\epsilon_{KL} > 0$ such that, for all $\mathbf{m} \in \mathcal{M}$, one can find $\bar{s}_{\mathbf{m}} \in S_{\mathbf{m}}$, such that $\bar{s}_{\mathbf{m}} \geq e^{-\tau} s_0$, and

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Outline

Procedure for deterministic collection of GLLiM models

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

1. Each $m \in \mathcal{M}$: estimate the forward MLE $\widehat{s}_{\mathbf{m}}^*(\mathbf{y}_i|\mathbf{x}_i)$ by inverse MLE $\widehat{s}_{\mathbf{m}}$ via an inverse regression trick by GLLiM-EM algorithm (xLLiM package).
2. Calculate η'-PMLE $\widehat{s}_{\widehat{\mathbf{m}}}$ with a "simplified" $\mathrm{pen}(\mathbf{m}) = \kappa \dim(S_m^*)$.

➞ Data-driven non-asymptotic approach for choosing κ.

- ➞ Our oracle inequality partially suggests **shape of penalty function** in a finite sample setting.
- ➞ Slope heuristic approach (capushe package) works well with our simplified $\mathrm{pen}(\mathbf{m}) = \kappa \dim(S_m^*)$ [Birgé and Massart, 2007, Baudry et al., 2012, Arlot et al., 2016, Arlot, 2019].

Numerical protocols

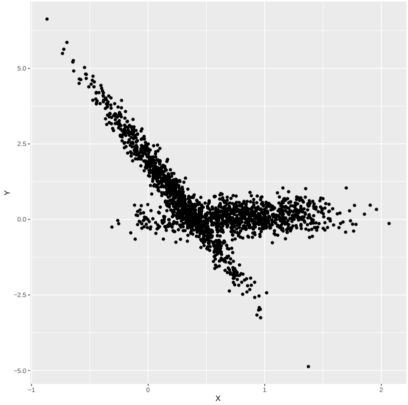
- $L = D = 1$: behavior of $\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0^*, \widehat{s}_{\widehat{\mathbf{m}}}^*\right)$ and convergence rates of error terms $\frac{1}{n}$.
- $D \gg L$: dimensionality reduction capability of GLLiM in high-dimensional regression data [Deleforge et al., 2015].

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

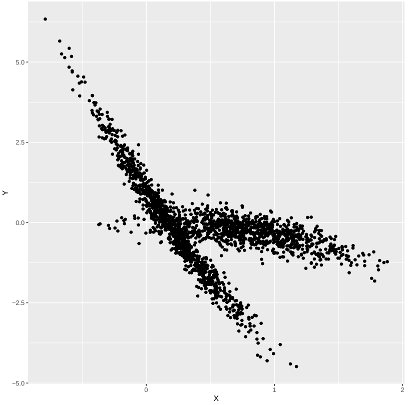
$$s_0^*(y|x) = \frac{\Phi(x; 0.2, 0.1)\Phi(y; -5x + 2, 0.09) + \Phi(x; 0.8, 0.15)\Phi(y; 0.1x, 0.09)}{\Phi(x; 0.2, 0.1) + \Phi(x; 0.8, 0.15)}.$$

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

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



(a) WS case

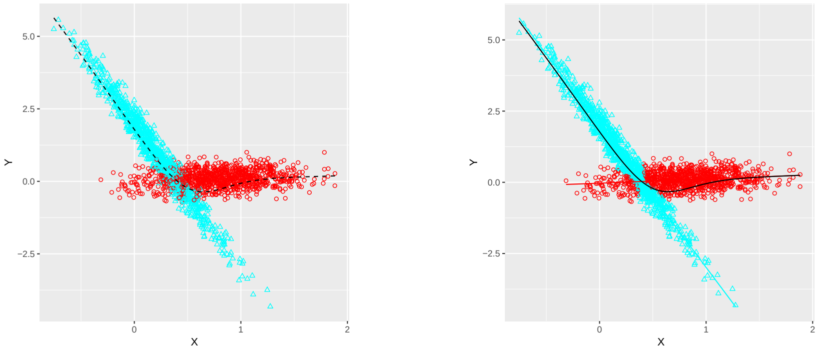


(b) MS case

Typical realizations of heterogeneous data from nonlinear regression models.

Perform multiple tasks simultaneously: regression analysis, clustering, conditional density estimation and model selection (*e.g.*, number of clusters, degree of polynomials).

Typical realization and regression clustering results



(a) Typical realization: WS case

(b) Regression clustering by GLLiM

Regression and clustering deduced from the estimated conditional density of GLLiM with $n = 2000$ in example WS. The dash and solid black curves present the true and estimated mean functions.

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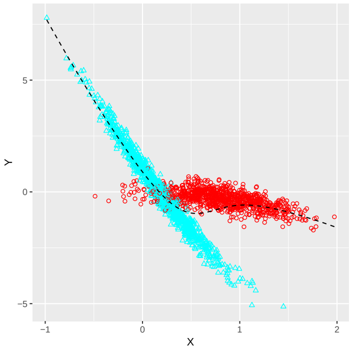

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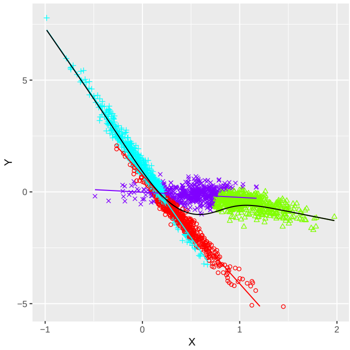

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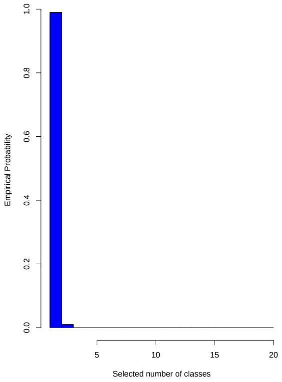
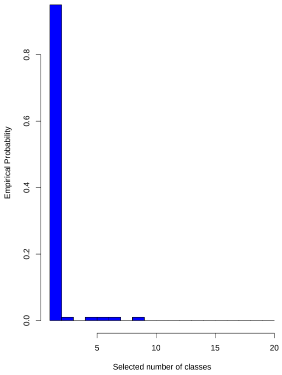
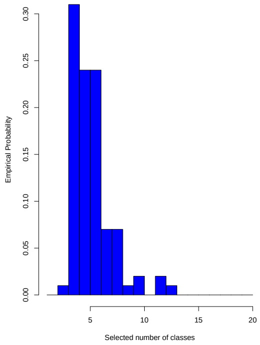


(a) $n = 2000$

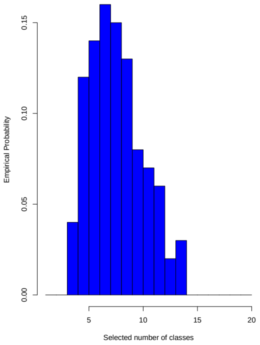


(b) $n = 10000$

Comparison histograms of selected K in WS case using jump criterion over 100 trials between $n = 2000$ and $n = 10000$.



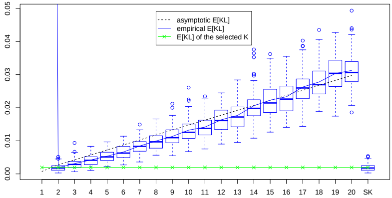
(a) 2000 data points



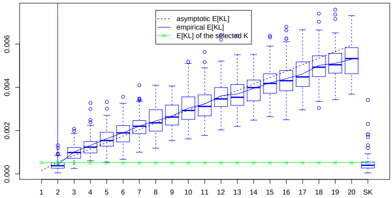
(b) 10000 data points

Comparison histograms of selected K in MS case using jump criterion over 100 trials between $n = 2000$ and $n = 10000$.

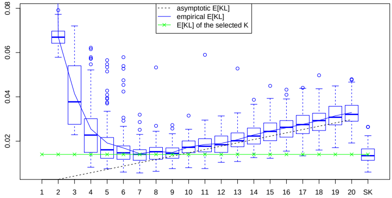
Box-plot of Kullback-Leibler divergence over 100 trials



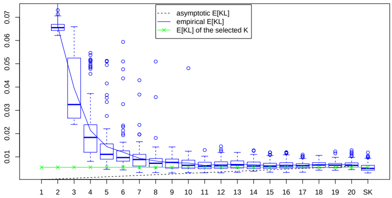
(a) WS with $n = 2000$



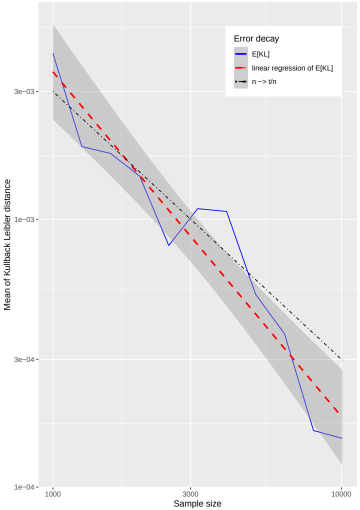
(b) WS with $n = 10000$



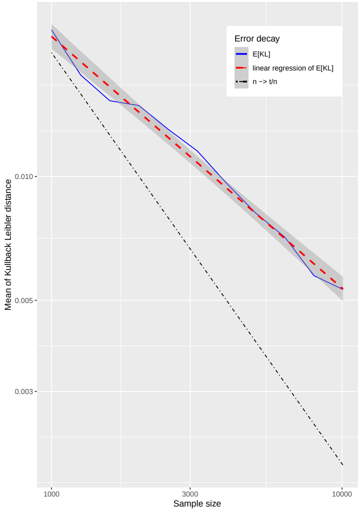
(c) MS with $n = 2000$



(d) MS with $n = 10000$



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



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

Rate of error decay, $\mathbb{E}\left[\mathrm{KL}^{\otimes n}\left(s_0, \widehat{s_{\mathbf{m}}}\right)\right]$, is represented in a log-log scale, using 30 trials. A free least-square regression (black dashed line) with standard error and a regression with slope -1 were added for presenting rate of convergence $1/n$.

Approximation error and variance term

The bias-variance trade-off differs between the two examples:

- **WS case:** since the true density belongs to the model, the best data-driven choice is $K = 2$ even for large n.
- **MS case:** best data-driven choice K should balance a model **approximation error term** and a **variance** one, *i.e.*, the larger n the more complex the model and thus K.

Empirical behavior of weak oracle inequality

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

- No closed form formula for $\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right)$ ➠ Monte Carlo method.
- Empirical mean $\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right) \leq$ Empirical mean $\mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_{\mathbf{m}}\right)$, $m \in \mathcal{M} = [20]$ over 55 trials.
- Empirical mean $\mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_{\mathbf{m}}\right) \sim \frac{\dim(S_{\mathbf{m}})}{2n}$ (shown by a dotted line): **expected behavior in asymptotic theory in WS case!**

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- Empirical mean $\mathrm{JKL}_{\rho}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right) \leq$ Empirical mean $\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\mathbf{m}}\right)$, $m \in \mathcal{M} = [20]$ over 55 trials.
- Empirical mean $\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\mathbf{m}}\right) \sim \frac{\dim(S_{\mathrm{m}})}{2n}$ (shown by a dotted line): **expected behavior in asymptotic theory in WS case!**

Empirical behavior of weak oracle inequality

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

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Outline

Main positive messages and perspectives

- **Our contributions**: establishing **non-asymptotic risk bounds** that take the form of **weak oracle inequalities**, provided that **lower bounds on the penalties** hold true.
- Partially answering important questions on model selection:
  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.
- **Numerical experiment** for **high-dimensional data**.
- **Minimax lower bounds**: only known for mixture models[7].
- **Mathematically justifying the slope heuristic** in MoE models as in least-squares regression on a random (or fixed) design with regressogram (projection) estimators, respectively, [Birgé and Massart, 2007, Arlot and Massart, 2009, Arlot and Bach, 2009, Arlot, 2019].

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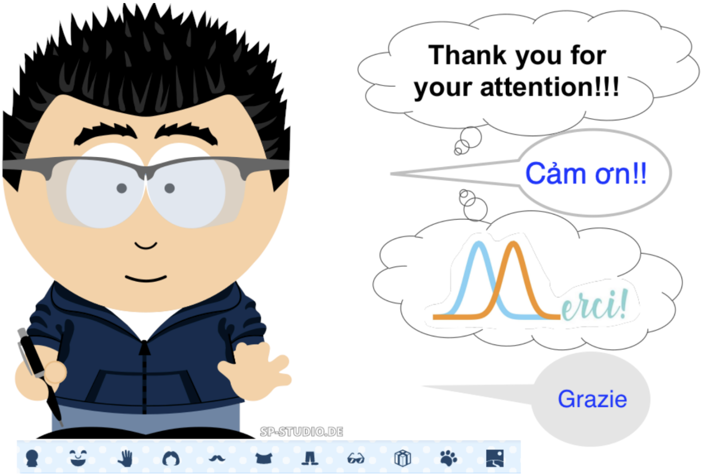
My Coauthors ∈ Mixture of French and Australian Experts

Hien Duy Nguyen

Faicel Chamroukhi

Florence Forbes

“Essentially, all models are wrong, but some are useful”.[8]



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

[8] Box, G. E.P. (1979). “Robustness in the strategy of scientific model building”. In Robustness in Statistics (pp. 201-236). Academic Press.

Supplementary material

Outline

Mild assumption: Boundedness conditions

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

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

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

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

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

Classical covariance matrix parameterization[9]

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 $\lambda_-, \lambda_+ \in \mathbb{R}$.

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

Mild assumption: Boundedness conditions on eigenvalues of Gaussian expert block-diagonal covariance matrices

$$0 < \lambda_m \leq m\left(\boldsymbol{\Sigma}_k\left(\mathbf{B}_k\right)\right) \leq M\left(\boldsymbol{\Sigma}_k\left(\mathbf{B}_k\right)\right) \leq \lambda_M, \text{ for every } k \in [K].$$

↑ constant ↑ smallest ↑ largest eigenvalue

$$\left\{ \boldsymbol{\Sigma}_k\left(\mathbf{B}_k\right) \in \mathcal{S}_q^{++} \;\middle|\; \begin{array}{l} \boldsymbol{\Sigma}_k\left(\mathbf{B}_k\right) = \mathbf{P}_k \begin{pmatrix} \boldsymbol{\Sigma}_k^{[1]} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_k^{[2]} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \dots & \boldsymbol{\Sigma}_k^{[G_k]} \end{pmatrix} \mathbf{P}_k^{-1}, \\ \boldsymbol{\Sigma}_k^{[g]} \in \mathcal{S}^{++}_{\text{card}\left(d_k^{[g]}\right)}, \forall g \in [G_k] \end{array} \right\}$$

$\mathbf{V}_K\left(\mathbf{B}\right) = \left(\mathbf{V}_k\left(\mathbf{B}_k\right)\right)_{k\in[K]}$, $\mathbf{P}_k$: permutation, $\mathbf{B}_k = \left(d_k^{[g]}\right)_{g\in[G_k]}$: block structure, $d_k^{[g]}$: set of variables in gth group, $\mathbf{B} = \left(\mathbf{B}_k\right)_{k\in[K]}$.

Outline

Solution for different divergences

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

- In general: $\mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right) \leq \mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right)$.
- If $\sup_{\mathbf{m}\in\mathcal{M}} \sup_{s_{\mathbf{m}}\in S_{\mathbf{m}}} \left\|s_0/s_{\mathbf{m}}\right\|_{\infty} < \infty \Leftarrow \mathcal{Y}$ is compact, s_0 is compactly supported, the regression functions are uniformly bounded, and a uniform lower bound on the eigenvalues of the covariance matrices, Proposition 1 from [Cohen and Le Pennec, 2011] implies that

$$\frac{C_{\rho}}{2+\ln\left\|s_0/\widehat{s}_{\widehat{\mathbf{m}}}\right\|_{\infty}} \mathrm{KL}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right) \leq \mathrm{JKL}_{\rho}^{\otimes n}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right).$$

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- $C_1 = 1$ with $\mathrm{KL}^{\otimes n}$ loss: still an open question, only known for aggregation of a finite number of densities as [Dalalyan & Sebbar, 2018, Rigollet, 2012].
- Bias $\inf_{s_{\mathbf{m}}\in S_{\mathbf{m}}} \mathrm{KL}^{\otimes n}\left(s_0, s_{\mathbf{m}}\right)$: small for $\mathcal{M}$ well-chosen via approximation capabilities of MoE and GMM models [Nguyen et al., 2019, **Nguyen et al., 2020b**, **Nguyen et al., 2020a**, **Nguyen et al., 2021a**].

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Lemma: Relationship between linear-weight softmax and Gaussian gating networks [Nguyen et al., 2021a]

In general, $\mathcal{P}_G \supset \mathcal{P}_S$.
Furthermore, if all $\boldsymbol{\Gamma}_k$, $k \in [K]$, are identical, then $\mathcal{P}_G = \mathcal{P}_S$.

$$\mathcal{P}_S = \left\{ \mathbf{y} \mapsto \left(\mathbf{g}_k\left(\mathbf{y};\gamma\right)\right)_{k\in[K]} = \left(\frac{\exp\left(\mathbf{a}_k + \mathbf{b}_k^\top \mathbf{y}\right)}{\sum_{l=1}^K \exp\left(\mathbf{a}_l + \mathbf{b}_l^\top \mathbf{y}\right)} \right)_{k\in[K]}, \gamma \in \boldsymbol{\Gamma}_S \right\}.$$

$$\boldsymbol{\Gamma}_S = \left\{ \gamma = \left(\left(\mathbf{a}_k\right)_{k\in[K]}, \left(\mathbf{b}_k\right)_{k\in[K]} \right) \in \mathbb{R}^K \times \left(\mathbb{R}^L\right)^K \right\}.$$

$$\mathcal{P}_G = \left\{ \mathbf{y} \mapsto \left(\mathbf{g}_k\left(\mathbf{y};\boldsymbol{\omega}\right)\right)_{k\in[K]} = \left(\frac{\boldsymbol{\pi}_k \Phi_L\left(\mathbf{y}; \mathbf{c}_k, \boldsymbol{\Gamma}_k\right)}{\sum_{j=1}^K \boldsymbol{\pi}_j \Phi_L\left(\mathbf{y}; \mathbf{c}_j, \boldsymbol{\Gamma}_j\right)} \right)_{k\in[K]}, \boldsymbol{\omega} \in \boldsymbol{\Omega} \right\}.$$

Reparameterization of the space of Gaussian gating networks

☼ Reparameterization trick:

$$\mathbf{W}_K = \left\{ \mathbf{w} : \mathbf{y} \mapsto \left(\underbrace{\ln\left(\pi_k \Phi_L\left(\mathbf{y}; \mathbf{c}_k, \boldsymbol{\Gamma}_k\right)\right)}_{\text{Nonlinear}} \right)_{k \in [K]} = \mathbf{w}\left(\mathbf{y}; \boldsymbol{\omega}\right) : \boldsymbol{\omega} \in \boldsymbol{\Omega} \right\}.$$

$$\mathcal{P}_G = \left\{ \mathbf{y} \mapsto \left(\frac{\exp\left(w_k(\mathbf{y})\right)}{\sum_{l=1}^{K} \exp\left(w_l(\mathbf{y})\right)} \right)_{k \in [K]}, \mathbf{w} \in \mathbf{W}_K \right\}.$$

- We obtain non-asymptotic oracle inequality for BLoME models, which is much more challenging compared to LinBoSGaME models [?] since we controlled several difficult bracketing entropies from:
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Asymptotic theory of a single parametric model

Misspecified case: $s_0 \notin S_{\mathbf{m}}$, $\psi^{\star}_m = \operatorname{argmin}_{\psi_{\mathbf{m}} \in \boldsymbol{\Psi}_{\mathbf{m}}} \mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\psi_{\mathbf{m}}}\right)$,

$$S_{\mathbf{m}} = \left\{ (\mathbf{x}, \mathbf{y}) \mapsto s_{\psi_{\mathbf{m}}}(\mathbf{x}|\mathbf{y}) = s_{\mathbf{m}}(\mathbf{x}|\mathbf{y}) : \psi_{\mathbf{m}} \in \boldsymbol{\Psi}_{\mathbf{m}} \subset \mathbb{R}^{\dim(S_{\mathbf{m}})} \right\}.$$

Theorem: [White, 1982, Cohen and Le Pennec, 2011]

- Assumptions: $S_{\mathbf{m}}$ is identifiable and there are some strong regularity assumptions on $\psi_{\mathbf{m}} \mapsto s_{\psi_{\mathbf{m}}}$, $\exists$ $\mathbf{A}\left(\psi_{\mathbf{m}}\right)$ and $\mathbf{B}\left(\psi_{\mathbf{m}}\right)$:
  $\left[\mathbf{A}\left(\psi_{\mathbf{m}}\right)\right]_{k,l} = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\int \frac{-\partial^2 \ln s_{\psi_{\mathbf{m}}}}{\partial \psi_{m,k} \partial \psi_{m,l}}\left(\mathbf{x}|\mathbf{Y}_i\right) s_0\left(\mathbf{x}|\mathbf{Y}_i\right) d\lambda\right]$,
  $\left[\mathbf{B}\left(\psi_{\mathbf{m}}\right)\right]_{k,l} = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\int \frac{\partial \ln s_{\psi_{\mathbf{m}}}}{\partial \psi_{m,k}}\left(\mathbf{x}|\mathbf{Y}_i\right) \frac{\partial \ln s_{\psi_{\mathbf{m}}}}{\partial \psi_{m,l}}\left(\mathbf{x}|\mathbf{Y}_i\right) s_0\left(\mathbf{x}|\mathbf{Y}_i\right) d\lambda\right]$.
- Conclusion: $\mathbb{E}\left[\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\mathbf{m}}\right)\right]$ is asymptotically equivalent to

$$\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\psi^{\star}_m}\right) + \frac{1}{2n} tr\left(\mathbf{B}\left(\psi^{\star}_m\right) \mathbf{A}\left(\psi^{\star}_m\right)^{-1}\right).$$

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Asymptotic theory of a single parametric model

Well-specified case: $s_0 \in S_{\mathbf{m}}$, $\psi_m^\star = \operatorname{argmin}_{\psi_{\mathbf{m}} \in \Psi_{\mathbf{m}}} \mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\psi_{\mathbf{m}}}\right)$.

Theorem: [White, 1982, Cohen and Le Pennec, 2011]

- It holds that

$$s_0 = s_{\psi_m^\star}, \mathbf{A}\left(\psi_m^\star\right) = \mathbf{B}\left(\psi_m^\star\right).$$

- The same assumption in misspecified case: $\mathbb{E}\left[\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\mathbf{m}}\right)\right]$ is asymptotically equivalent to

$$\underbrace{\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\psi_m^\star}\right)}_{=0} + \frac{1}{2n} \dim\left(S_{\mathbf{m}}\right).$$

Asymptotic theory of a single parametric model

Well-specified case: $s_0 \in S_{\mathbf{m}}$, $\psi^\star_m = \operatorname{argmin}_{\psi_{\mathbf{m}} \in \boldsymbol{\Psi}_{\mathbf{m}}} \mathrm{KL}^{\otimes \mathrm{n}} \left(s_0, s_{\psi_{\mathbf{m}}}\right)$.

Theorem: [White, 1982, Cohen and Le Pennec, 2011]

- It holds that

$$s_0 = s_{\psi^\star_m}, \mathbf{A}\left(\psi^\star_m\right) = \mathbf{B}\left(\psi^\star_m\right).$$

- The same assumption in misspecified case: $\mathbb{E}\left[\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\mathbf{m}}\right)\right]$ is asymptotically equivalent to

$$\underbrace{\mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\psi^\star_m}\right)}_{=0} + \frac{1}{2n} \dim\left(S_{\mathbf{m}}\right).$$

Drawbacks of asymptotic theory

Drawbacks: **asymptotic normality** of $\sqrt{n}\left(\widehat{\psi}_m - \psi_m^\star\right)$ is required!

➡ Some previous ideas to handle **non-asymptotic normality**:

- Extension in non parametric case or non-identifiable model, Wilk's phenomenon, [Wilks, 1938].
- Generalization of the corresponding Chi-Square goodness-of-fit test [Fan et al., 2001].
- Finite sample deviation of the corresponding empirical quantity in a bounded loss setting [Boucheron and Massart, 2011].

Our targets: Obtain an upper bound on similar expected loss:

✔ Holds for finite sample.

✖ Strong regularity assumptions of [White, 1982].

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Weak oracle inequalities

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

Potential issues

1. Different divergences: $\mathrm{JKL}_{\rho}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right) \leq \mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, \widehat{s}_{\widehat{\mathbf{m}}}\right)$.
2. $C_1 > 1$ and misspecified case: Given fixed collection $\mathcal{M}$, as $n \to \infty$, the error bound $\to C_1 \inf_{s_{\mathbf{m}}\in S_{\mathbf{m}}} \mathrm{KL}^{\otimes \mathrm{n}}\left(s_0, s_{\mathbf{m}}\right)$ (potentially large!).

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Outline

Universal approximation of finite location-scale mixtures

Given a PDF φ (*e.g.*, standard multivariate normal distribution (MND)),

$$\mathcal{S}^{\varphi} = \bigcup_{K\in\mathbb{N}^\star} \mathcal{S}_K^{\varphi}, \text{ where } \mathcal{S}_K^{\varphi} = \Big\{\mathcal{Y} \ni \mathbf{y} \mapsto s_K^{\varphi}(\mathbf{y}) = \sum_{k=1}^{K} \frac{\boldsymbol{\pi}_k}{\sigma_k^L} \varphi\left(\frac{\mathbf{y}-\boldsymbol{\upsilon}_k}{\sigma_k}\right),$$
$$\boldsymbol{\upsilon}_k \in \mathbb{R}^L, \sigma_k \in \mathbb{R}^+, \boldsymbol{\pi} \in \boldsymbol{\Pi}_{K-1}\Big\}.$$

$\mathcal{L}_\infty$: essentially bounded function, $\mathcal{L}_p$: Lebesgue PDF.

Theorem: [Nguyen et al., 2020b, Nguyen et al., 2020a]

- Given any PDFs $s_0, \varphi \in \mathcal{C}$ and a compact set $\mathcal{Y} \subset \mathbb{R}^L$, there exists $\{s_K^{\varphi}\}_{K\in\mathbb{N}^\star} \subset \mathcal{S}^{\varphi}$, $\lim_{K\to\infty} \sup_{\mathbf{y}\in\mathcal{Y}} |s_0(\mathbf{y}) - s_K^{\varphi}(\mathbf{y})| = 0$.
- For $p \in [1,\infty)$, if $s_0 \in \mathcal{L}_p$ and $\varphi \in \mathcal{L}_\infty$, there exists $\{s_K^{\varphi}\}_{K\in\mathbb{N}^\star} \subset \mathcal{S}^{\varphi}$, $\lim_{K\to\infty} \|s_0 - s_K^{\varphi}\|_{\mathcal{L}_p} = 0$.

✸ $\mathcal{S}_K^{\varphi} \not\subseteq S_{\mathbf{m}}$!

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Outline

5 Boundedness conditions

6 Non-asymptotic approach for model selection in MoE models

7 Universal approximation theorems of MoE models
- Finite location-scale MoE models
- Inverse regression trick

8 Softmax gating networks

Definition: Isotropic SGaME and GLLiM models

- Location-scale family: given a PDF φ, $\boldsymbol{\upsilon} \in \mathcal{X}$, $\sigma \in R^{+}$,

$$\mathcal{E}_{\varphi} = \left\{ \mathbf{x} \mapsto \frac{1}{\sigma^{D}} \varphi \left(\frac{\mathbf{x} - \boldsymbol{\upsilon}}{\sigma} \right) = \Phi_{D}(\mathbf{x}; \boldsymbol{\upsilon}, \sigma) \right\}.$$

- Isotropic SGaME models ($\subset S_{\mathbf{m}}$):

$$\mathcal{S}_{S}^{\varphi} = \Big\{ (\mathbf{x}, \mathbf{y}) \mapsto s_{K}^{\varphi}(\mathbf{x}|\mathbf{y}) = \sum_{k=1}^{K} \mathbf{g}_{k} \left(\mathbf{y}; \gamma \right) \Phi_{D} \left(\mathbf{x}; \boldsymbol{\upsilon}_{k}, \sigma_{k} \right),$$
$$\Phi_{D} \in \mathcal{E}_{\varphi} \cap \mathcal{L}_{\infty}, \mathbf{g}_{k} \left(\cdot ; \gamma \right) \in \mathcal{P}_{S}^{K}, \in \mathbb{N}^{\star} \Big\}.$$

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$$\mathcal{S}_{G}^{\varphi} = \Big\{ (\mathbf{x}, \mathbf{y}) \mapsto s_{K}^{\varphi}(\mathbf{x}|\mathbf{y}) = \sum_{k=1}^{K} \mathbf{g}_{k} \left(\mathbf{y}; \omega \right) \Phi_{D} \left(\mathbf{x}; \boldsymbol{\upsilon}_{k}, \sigma_{k} \right),$$
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Theorem: Approximation capabilities of isotropic SGaME and GLLiM models [Nguyen et al., 2021a]

(a) Given $p \in [1, \infty)$, a compact set $\mathcal{Y} \subset \mathbb{R}^L$, $\varphi \in \mathcal{F} \cap \mathcal{C}$, for target $s_0 \in \mathcal{F}_p \cap \mathcal{C}_b^u$, there exist sequences $\{s_K^{\varphi}\}_{K \in \mathbb{N}^\star} \subset \mathcal{S}_S^{\varphi}$ and $\{s_K'^{\varphi}\}_{K \in \mathbb{N}^\star} \subset \mathcal{S}_G^{\varphi}$ such that

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$$\lim_{K \to \infty} \left\|s_0 - s_K'^{\varphi}\right\|_{\mathcal{L}_p} = 0.$$

(b) Given $L = 1$, and $0 < \lambda(\mathcal{X}) < \infty$, $\varphi \in \mathcal{F} \cap \mathcal{C}_b^u$, for any target $s_0 \in \mathcal{F} \cap \mathcal{C}_b^u$, there exist sequences $\{s_K^{\varphi}\}_{K \in \mathbb{N}^\star} \subset \mathcal{S}_S^{\varphi}$ and $\{s_K'^{\varphi}\}_{K \in \mathbb{N}^\star} \subset \mathcal{S}_G^{\varphi}$ such that

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Mild assumption: Linear combination of bounded functions whose coefficients belong to a compact set

- Weights: $\mathbf{W}_{K,d_{\mathbf{W}}} = \{0\} \otimes \mathbf{W}_{Bo,d_{\mathbf{W}}}^{K-1}$ (identifiability condition),

$$\mathbf{W}_{Bo,d_{\mathbf{W}}} = \left\{ \mathbf{x} \mapsto \sum_{d=1}^{d_{\mathbf{W}}} \omega_d \theta_{\mathbf{W},d}(\mathbf{x}) : \max_{d \in [d_{\mathbf{W}}]} |\omega_d| \leq T_{\mathbf{W}} \right\}.$$

- Gaussian expert means: $\Upsilon_{K,d_\Upsilon} = \Upsilon_{Bo,d_\Upsilon}^{K}$,

$$\Upsilon_{Bo,d_\Upsilon} = \left\{ \mathbf{x} \mapsto \left(\sum_{d=1}^{d_\Upsilon} \beta_d^{(z)} \theta_{\Upsilon,d}(\mathbf{x}) \right)_{z \in [q]} : \max_{d \in [d_\Upsilon], z \in [q]} \left| \beta_d^{(z)} \right| \leq T_\Upsilon \right\}.$$

- Collections of bounded basis functions: $\mathbf{x} \mapsto \left(\theta_{\mathbf{W},d}(\mathbf{x}), \theta_{\Upsilon,d}(\mathbf{x}) \right)$, $T_{\mathbf{W}} \in \mathbb{R}^+$, $T_\Upsilon \in \mathbb{R}^+$.

Mild assumption: Polynomials on compact sets to **simplify the interpretation of sparsity in high-dimensional data**

- Weights: $\mathbf{W}_{K,d_{\mathbf{W}}} = \{0\} \otimes \mathbf{W}_{Po,d_{\mathbf{W}}}^{K-1}$ (identifiability condition), $T_{\mathbf{W}} \in \mathbb{R}^{+}$,

$$\mathbf{W}_{Po,d_{\mathbf{W}}} = \left\{ \mathbf{x} \mapsto \sum_{|\boldsymbol{\alpha}|=0}^{d_{\mathbf{W}}} \omega_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}} \in \mathbb{R} : \max_{\boldsymbol{\alpha} \in \mathcal{A}} |\omega_{\boldsymbol{\alpha}}| \leq T_{\mathbf{W}} \right\}.$$

- Gaussian expert means: $|||\mathbf{A}|||_{\infty} = \max_{i \in [q], j \in [p]} \left| [\mathbf{A}]_{i,j} \right|$, $T_{\boldsymbol{\Upsilon}} \in \mathbb{R}^{+}$,

$$\boldsymbol{\Upsilon}_{K,d_{\boldsymbol{\Upsilon}}} = \Bigg\{ \mathbf{x} \mapsto \left(\beta_{k0} + \sum_{d=1}^{d_{\boldsymbol{\Upsilon}}} \beta_{kd} \mathbf{x}^{d} \right)_{k \in [K]} : \max \left\{ |||\beta_{kd}|||_{\infty} : k \in [K], d \in (\{0\} \cup [d_{\boldsymbol{\Upsilon}}]) \right\} \leq T_{\boldsymbol{\Upsilon}} \Bigg\},$$

High-dimensional regression data: $\mathcal{X} = [0,1]^{p}$, $\mathcal{Y} \subset \mathbb{R}^{q}$, with $p, q \gg n$, see [Nguyen et al., 2020c] for example.

Mild assumption: Boundedness conditions on eigenvalues of Gaussian expert block-diagonal covariance matrices

$$0 < \lambda_m \leq m\left(\Sigma_k\left(\mathbf{B}_k\right)\right) \leq M\left(\Sigma_k\left(\mathbf{B}_k\right)\right) \leq \lambda_M, \text{ for every } k \in [K].$$

↑ constant ↑ smallest ↑ largest eigenvalue

$$\left\{ \Sigma_k\left(\mathbf{B}_k\right) \in \mathcal{S}_q^{++} \;\middle|\; \begin{array}{l} \Sigma_k\left(\mathbf{B}_k\right) = \mathbf{P}_k \begin{pmatrix} \Sigma_k^{[1]} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \Sigma_k^{[2]} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \dots & \Sigma_k^{[G_k]} \end{pmatrix} \mathbf{P}_k^{-1}, \\ \Sigma_k^{[g]} \in \mathcal{S}^{++}_{\mathrm{card}\left(d_k^{[g]}\right)}, \forall g \in [G_k] \end{array} \right\}$$

↑

$\mathbf{V}_K\left(\mathbf{B}\right) = \left(\mathbf{V}_k\left(\mathbf{B}_k\right)\right)_{k \in [K]}$, $\mathbf{P}_k$: permutation, $\mathbf{B}_k = \left(d_k^{[g]}\right)_{g \in [G_k]}$: block structure, $d_k^{[g]}$: set of variables in gth group, $\mathbf{B} = \left(\mathbf{B}_k\right)_{k \in [K]}$.

Definition: Variable selection via selecting relevant variables

- A couple $(\mathbf{Y}_z, \mathbf{X}_j)$ and its corresponding indices $(z, j) \in [q] \times [p]$:
  - irrelevant if $\mathbf{X}_j$ does not explain the variable $\mathbf{Y}_z$, *i.e.*,

$$[\beta_{kd}]_{z,j} = 0,\ \omega_k^{[j,l]} = \mathbf{0}, \text{ for all } k \in [K],\ d \in [d_{\Upsilon}],\ l \in [d_{\mathbf{W}}]:$$

    - β_{kd}, $k \in [K]$, $d \in [d_{\Upsilon}]$: matrices of d-th term regression coefficients of k-th mixture component.
    - $\omega_k^{[j,l]} = \{\omega_{k\boldsymbol{\alpha}} \in \mathbb{R} : \boldsymbol{\alpha} \in \mathcal{A}_l, \boldsymbol{\alpha}_j > 0\}$, $\forall l \in [d_{\mathbf{W}}]$, $j \in [p]$: vector of monomial coefficients of l-th degree involving $\mathbf{x}_j$,
    - $\mathcal{A}_l = \left\{\boldsymbol{\alpha} = (\alpha_t)_{t \in [p]} \in \mathbb{N}^p, |\boldsymbol{\alpha}| = l\right\}$, $|\boldsymbol{\alpha}|$ degree of monomials $\mathbf{x}^{\boldsymbol{\alpha}}$.
  - relevant if they are not irrelevant.
- Sparse model: few of relevant variables.
- $\mathbf{J} = \{(z, j) \in [q] \times [p] : (\mathbf{Y}_z, \mathbf{X}_j) \text{ are relevant couples}\}$.
- The set of **relevant variables (columns)**:
  $\mathbf{J}_\omega = \{j \in [p] : \exists z \in [q], (z, j) \in \mathbf{J}\}$.

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Definition: Low-rank regression matrices

- **Low-rank matrices**: Regression coefficients β_{kd}, $k \in [K]$, $d \in [L]$: can be **well approximated by low-rank matrices**.
  - β_{kd} is fully determined by $R_{kd}\left(p+q-R_{kd}\right)$ coefficients if $\operatorname{rank}\left(\beta_{kd}\right) = R_{kd}$.
  - The total parameters to be estimate **may be smaller** than the sample size nq.
- **Vector of ranks**: **Combining rank and column sparsity**. $\mathbf{R} = \left(R_{kd}\right)_{k\in[K],d\in[d_\Upsilon]} \in \left[\operatorname{card}\left(\mathbf{J}_\omega\right) \wedge q\right]^{d_\Upsilon K}$, where $\operatorname{rank}\left(\beta_{kd}\right) = R_{kd}$, $a \wedge b = \min\left(a, b\right)$.

- $\mathbf{J} \subset \mathcal{P}\left([q] \times [p]\right)$ and $\mathbf{J}_\omega \subset \mathcal{P}\left([q]\right)$, where $\mathcal{P}\left([q] \times [p]\right)$ contains all subsets of $[q] \times [p]$.
- If for all $k \in [K]$, $d \in [d_\Upsilon]$, a matrix β_{kd} has $\operatorname{card}\left(\mathbf{J}_\omega\right)$ relevant columns ➔ there are $q \operatorname{card}\left(\mathbf{J}_\omega\right)$ coefficients $\ll qp$ per clusters if when $\operatorname{card}\left(\mathbf{J}_\omega\right) \ll p$.

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Definition: Essentially bounded and Lebesgue conditional PDF

- Essentially bounded function on $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$:

$$\mathcal{L}_\infty(\mathcal{Z}) = \left\{ f : \underbrace{\inf \{ a \geq 0 : \lambda (\{ \mathbf{z} \in \mathcal{Z} : |f(\mathbf{z})| > a \}) = 0 \}}_{= \|f\|_{\infty, \mathcal{Z}}} < \infty \right\}.$$

- Lebesgue conditional PDF: $\mathcal{F}_p = \mathcal{F} \cap \mathcal{L}_p$, $p \in [1, \infty)$,

$$\mathcal{F} = \left\{ f : \mathcal{Z} \to [0, \infty), \int_{\mathcal{Y}} f(\mathbf{x}|\mathbf{y}) d\lambda(\mathbf{x}) = 1 \right\},$$

$$\mathcal{L}_p(\mathcal{Z}) = \left\{ f := \underbrace{\left(\int_{\mathcal{Z}} |f(\mathbf{z})|^p \, d\lambda(\mathbf{z}) \right)^{1/p}}_{= \|f\|_{p, \mathcal{Z}}} < \infty \right\}.$$

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Definition: softmax gating networks

$$g_{\mathbf{w},k,d_W}(\mathbf{x}) = \underbrace{\frac{\exp\left(w_{k,d_W}(\mathbf{x})\right)}{\sum_{l=1}^{K}\exp\left(w_{l,d_W}(\mathbf{x})\right)}}_{\text{normalized exponential function}}, \text{ for every } k \in [K],$$

- $\mathbf{w} = \left(w_{k,d_W}\right)_{k\in[K]} \in \mathbf{W}_{K,d_W}$: functions defined in logistic schemes (weights),
- For every $\mathbf{x} \in \mathcal{X}$, $\left(g_{\mathbf{w},k,d_W}(\mathbf{x})\right)_{k\in[K]} \in \mathbf{\Pi}_{K-1}$,
- $\mathbf{\Pi}_{K-1} = \left\{\left(\pi_k\right)_{k\in[K]} \in \left(\mathbb{R}^+\right)^K, \sum_{k=1}^{K}\pi_k = 1\right\}$.

Appendix: GLLiM model hierarchical definition

$$\mathbf{Y} = \sum_{k=1}^{K} \mathbb{I}\left(Z = k\right)\left(\mathbf{A}_k^*\mathbf{X} + \mathbf{b}_k^* + \mathbf{E}_k^*\right),$$

$\mathbf{Y} \in \mathbb{R}^L$, $\mathbf{X}$(or $\boldsymbol{\theta}$) $\in \mathbb{R}^D$ with $D \gg L$, $\mathbb{I}$ Indicator function, $\mathbf{A}_k^* \in \mathbb{R}^{L\times D}$, $\mathbf{b}_k^* \in \mathbb{R}^L$.
$\boldsymbol{E}_k'$: capturing both observation noise in $\mathbb{R}^L$ and reconstruction error due to the local affine approximations, Gaussian, centered:

$$p\left(\mathbf{Y} = \mathbf{y}|\mathbf{X} = \mathbf{x}, Z = k; \psi_K^*\right) = \mathcal{N}_L\left(\mathbf{y}; \mathbf{A}_k^*\mathbf{x} + \mathbf{b}_k^*, \boldsymbol{\Sigma}_k^*\right),$$

- Affine transformations are local: mixture of K Gaussians

$$p\left(\mathbf{X} = \mathbf{x}|Z = k; \psi_K^*\right) = \mathcal{N}_D\left(\mathbf{x}; \mathbf{c}_k^*, \boldsymbol{\Gamma}_k^*\right), p\left(Z = k; \psi_K^*\right) = \boldsymbol{\pi}_k^*,$$

  where $\mathbf{c}_k^* \in \mathbb{R}^D, \boldsymbol{\Gamma}_k^* \in \mathbb{R}^{D\times D}$, $\boldsymbol{\pi}^* = \left(\boldsymbol{\pi}_k^*\right)_{k\in[K]} \in \boldsymbol{\Pi}_{K-1}$.
- The set of all model parameters is:

$$\psi_K^* = \left(\boldsymbol{\pi}_k^*, \mathbf{c}_k^*, \boldsymbol{\Gamma}_k^*, \mathbf{A}_k^*, \mathbf{b}_k^*, \boldsymbol{\Sigma}_k^*\right)_{k\in[K]}$$

  Usually $\boldsymbol{\Sigma}_k^* = \sigma^2\boldsymbol{I}_L$ for $k = 1\ldots K$ (isotropic reconstruction error).

Outline

Appendix : GLLiM link between ϕ and ϕ'

Idea: $\mathbf{Y} \equiv$ input, $\mathbf{X} \equiv$ output, $\mathbf{X} \subset \mathbb{R}^D$, $\mathbf{Y} \subset \mathbb{R}^L$:

$$p\left(\mathbf{X}=\mathbf{x} | \mathbf{Y}=\mathbf{y}, Z=k ; \psi_K\right)=\phi_D\left(\mathbf{x} ; \mathbf{A}_k \mathbf{y}+\mathbf{b}_k, \boldsymbol{\Sigma}_k\right),$$

$$p\left(\mathbf{Y}=\mathbf{y} | Z=k ; \psi_K\right)=\phi_L\left(\mathbf{y} ; \mathbf{c}_k, \boldsymbol{\Gamma}_k\right), p\left(Z=k ; \psi_k\right)=\pi_k,$$

$$p\left(\mathbf{X}=\mathbf{x} | \mathbf{Y}=\mathbf{y} ; \psi_K\right)=\sum_{k=1}^K \frac{\pi_k \phi_L\left(\mathbf{y} ; \mathbf{c}_k, \boldsymbol{\Gamma}_k\right)}{\sum_{j=1}^K \pi_j \phi_L\left(\mathbf{y} ; \mathbf{c}_j, \boldsymbol{\Gamma}_j\right)} \phi_D\left(\mathbf{x} ; \mathbf{A}_k \mathbf{y}+\mathbf{b}_k, \boldsymbol{\Sigma}_k\right).$$

Link function:

$$\theta_K=\begin{pmatrix}\mathbf{c}_k \\ \boldsymbol{\Gamma}_k \\ \mathbf{A}_k \\ \mathbf{b}_k \\ \boldsymbol{\Sigma}_k\end{pmatrix}_{k \in[K]} \mapsto\begin{pmatrix}\mathbf{c}_k^* \\ \boldsymbol{\Gamma}_k^* \\ \mathbf{A}_k^* \\ \mathbf{b}_k^* \\ \boldsymbol{\Sigma}_k^*\end{pmatrix}_{k \in[K]}=\begin{pmatrix}\mathbf{A}_k \mathbf{c}_k+\mathbf{b}_k \\ \boldsymbol{\Sigma}_k+\mathbf{A}_k \boldsymbol{\Gamma}_k \mathbf{A}_k^{\top} \\ \boldsymbol{\Sigma}_k^* \mathbf{A}_k^{\top} \boldsymbol{\Sigma}_k^{-1} \\ \boldsymbol{\Sigma}_k^*\left(\boldsymbol{\Gamma}_k^{-1} \mathbf{c}_k-\mathbf{A}_k^{\top} \boldsymbol{\Sigma}_k^{-1} \mathbf{b}_k\right) \\ \left(\boldsymbol{\Gamma}_k^{-1}+\mathbf{A}_k^{\top} \boldsymbol{\Sigma}_k^{-1} \mathbf{A}_k\right)^{-1}\end{pmatrix}_{k \in[K]} \in \boldsymbol{\Theta}_K^*,$$

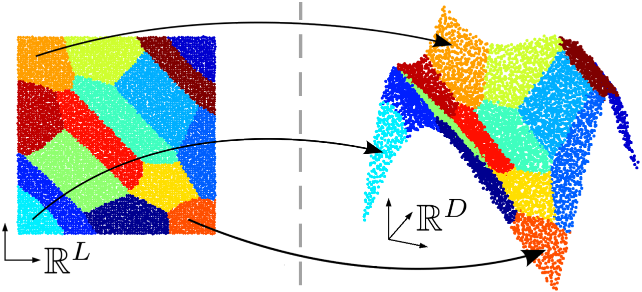
with the note that $\boldsymbol{\pi}^* \equiv \boldsymbol{\pi}$.

Reduce the number of parameters: The number of parameters depends on the GLLiM variant but is in $\mathcal{O}(DKL)$

If diagonal covariances $\boldsymbol{\Sigma}_k$, the number of parameters is $K-1+K(L+L(L+1)/2+DL+2D)$ $\rightarrow$ for $K=100$, $L=4$ and $D=10$ leads to 7499 parameters and to 61499 parameters if $D=100$.

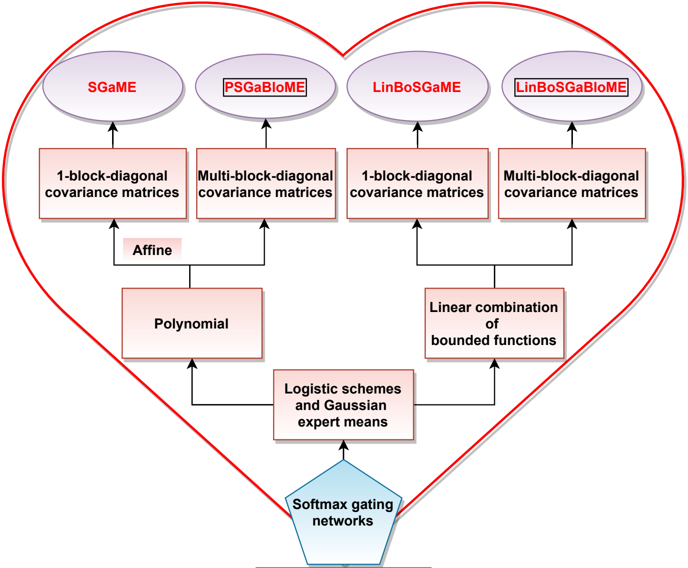
Appendix: GLLiM Geometric Interpretation

Interpretation: This model induces a partition of $\mathbb{R}^L$ into K regions $\mathcal{R}_k$ where the transformation is the most probable. If $|\boldsymbol{\Gamma}_1| = \cdots = |\boldsymbol{\Gamma}_K|$: $\{\mathcal{R}_k, k = 1 \dots K\}$ define a Voronoi diagram of centroids $\{\boldsymbol{c}_k, k = 1 \dots K\}$ (Mahalanobis distance $||.||_{\boldsymbol{\Gamma}^*}$).



$L = 2, D = 3, K = 15$. The low-to-high regression (shown here) may well be interpreted as a parameterization of an L-dimensional manifold embedded in a D-dimensional space.

Outline



SGaME: Softmax-Gated MoE

PSGaBloME: Polynomial Softmax-Gated Block-diagonal MoE

LinBoSGaME: Linear-combination-of-Bounded-functions Softmax-Gated MoE

LinBoSGaBloME: Linear-combination-of-Bounded-functions Softmax-Gated Block-diagonal MoE

Definition: SGaME, PSGaBloME, LinBoSGaME and LinBoSGaBloME

$$s_{\psi_{K,d_{\mathbf{W}},d_{\mathbf{\Upsilon}},\mathbf{B}}}(\mathbf{y}|\mathbf{x}) = \sum_{k=1}^{K} \underbrace{\frac{\exp\left(w_{k,d_{\mathbf{W}}}(\mathbf{x})\right)}{\sum_{l=1}^{K}\exp\left(w_{l,d_{\mathbf{W}}}(\mathbf{x})\right)}}_{\text{Softmax gating network}} \underbrace{\mathcal{N}_q\left(\mathbf{y}; \upsilon_{k,d_{\mathbf{\Upsilon}}}(\mathbf{x}), \mathbf{\Sigma}_k\left(\mathbf{B}_k\right)\right)}_{\text{Gaussian expert}}.$$

- $\mathbf{w} = \left(w_{k,d_{\mathbf{W}}}\right)_{k\in[K]} \in \mathbf{W}_{K,d_{\mathbf{W}}}$: functions defined in logistic schemes (weights),
- $K \in \mathbb{N}^{\star}$: number of mixture components,
- $d_{\mathbf{W}}, d_{\mathbf{\Upsilon}} \in \mathbb{N}^{\star}$: gating networks and mean functions' hyperparameters, *e.g.*, degrees of polynomials,
- $\mathbf{B} = \left(\mathbf{B}_k\right)_{k\in[K]}$: block-diagonal structures for covariance matrices,
- $\psi_{K,d_{\mathbf{W}},d_{\mathbf{\Upsilon}},\mathbf{B}} = \left(\mathbf{w}, \upsilon, \mathbf{\Sigma}\left(\mathbf{B}\right)\right) \in \mathbf{W}_{K,d_{\mathbf{W}}} \times \mathbf{\Upsilon}_{K,d} \times \mathbf{V}_K\left(\mathbf{B}\right) = \psi_{K,d_{\mathbf{W}},d_{\mathbf{\Upsilon}},\mathbf{B}}$: model parameter.

Definition: Collection of models (SGaME, PSGaBloME, LinBoSGaME and LinBoSGaBloME)

$$S_{\mathbf{m}} = \Big\{ (\mathbf{x}, \mathbf{y}) \mapsto s_{\psi_{(K, L_{\mathbf{W}}, d_{\Upsilon}, \mathbf{B}, \mathbf{J}, \mathbf{R})}}(\mathbf{y}|\mathbf{x}) = s_{\mathbf{m}}(\mathbf{y}|\mathbf{x}) : \\ \mathbf{m} = (K, L_{\mathbf{W}}, d_{\Upsilon}, \mathbf{J}, \mathbf{R}), \psi_{(K, L_{\mathbf{W}}, d_{\Upsilon}, \mathbf{B}, \mathbf{J}, \mathbf{R})} \in \boldsymbol{\Psi}_{(K, L_{\mathbf{W}}, d_{\Upsilon}, \mathbf{B}, \mathbf{J}, \mathbf{R})} \Big\}.$$

- $\mathbf{J} = \{(z, j) \in [q] \times [p] : (\mathbf{Y}_z, \mathbf{X}_j) \text{ are relevant couples}\}$.
- $\mathbf{R}$: vector ranks regression matrices.
- $\mathbf{m} \in \mathcal{M}$.
- $\mathcal{M} = [K_{\max}] \times [L_{\max}] \times [D_{\max}] \times (\mathcal{B}_k)_{k \in [K]} \times \mathcal{P}([q] \times [p]) \times [\min(q, p)]^{D_{\max} K}$.
- $K_{\max}, L_{\max}, D_{\max} \in \mathbb{N}^\star$ may depend on n, $\mathcal{P}(\mathbf{A})$ all subsets of $\mathbf{A}$.
- $\mathcal{B}_k$ = all possible partitions of the covariables indexed by $[q]$.

High-dimensional regression data: $\mathcal{X} \subset \mathbb{R}^p$, $\mathcal{Y} \subset \mathbb{R}^q$, with $p, q \gg n$.

Definition: Random subcollection of models ⟵ large number of models

$$S_{\mathbf{m}} = \Big\{(\mathbf{x},\mathbf{y}) \mapsto s_{\psi_{(K,L_{\mathbf{W}},d_{\Upsilon},\mathbf{B},\mathbf{J},\mathbf{R})}}(\mathbf{y}|\mathbf{x}) = s_{\mathbf{m}}(\mathbf{y}|\mathbf{x}) : \mathbf{m} = (K, L_{\mathbf{W}}, d_{\Upsilon}, \mathbf{B}, \mathbf{J}, \mathbf{R}), \psi_{(K,L_{\mathbf{W}},d_{\Upsilon},\mathbf{B},\mathbf{J},\mathbf{R})} \in \boldsymbol{\Psi}_{(K,L_{\mathbf{W}},d_{\Upsilon},\mathbf{B},\mathbf{J},\mathbf{R})}\Big\}.$$

- $\mathbf{m} \in \widetilde{\mathcal{M}} = [K_{\max}] \times [L_{\max}] \times [D_{\max}] \times (\mathcal{B}_{k,\boldsymbol{\Lambda}})_{k\in[K]} \times \mathcal{J} \times \mathcal{R}_{(K,\mathbf{J},D_{\max})} \subset \mathcal{M}$.
- $\mathcal{B}_{k,\boldsymbol{\Lambda}} = (\mathcal{B}_{k,\lambda})_{\lambda\in\boldsymbol{\Lambda}}$ **(potentially random)** $\subset \mathcal{B}_k$: partition of the variables corresponding to the block-diagonal structure of the adjacency matrix $\mathbf{E}_{k,\lambda} = \left[\mathbb{I}\left\{\left|[\mathbf{S}_k]_{z,z'}\right| > \lambda\right\}\right]_{z\in[q],z'\in[q]}$, based on the thresholded absolute value of the sample covariance matrix $\mathbf{S}_k$ in each cluster $k \in [K]$.
- $\mathcal{J}$ (**relevant couples, potentially random**) $\subset \mathcal{P}([q]\times[p])$.
  $\mathbf{J}_\omega$ relevant variable: $\mathbf{J}_\omega = \{j \in [p] : \exists\, z \in [q], (z,j) \in \mathcal{J}\}$.
  $\uparrow\downarrow$ **Our Lasso+l_2-Rank procedure**
- $\mathcal{R}_{(K,\mathbf{J},D_{\max})}$(**vector ranks regression matrices**) $\subset [\min(\mathrm{card}(\mathbf{J}_\omega), q)]^{D_{\max}K}$.

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