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## Non linear robust regression in high dimension

Emeline Perthame, Florence Forbes, Brice Olivier, Antoine Deleforge

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## 1 - Non linear mapping problem

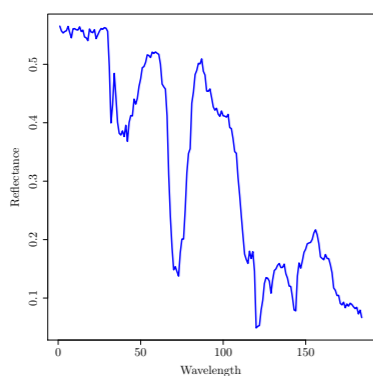
- The goal is to retrieve  $\mathbf{X}$  from  $\mathbf{Y}$  through a **non linear** regression function  $g$

$$\mathbb{E}(\mathbf{X}|\mathbf{Y} = \mathbf{y}) = g(\mathbf{y})$$

with  $Y \in \mathbb{R}^D, X \in \mathbb{R}^L, D \gg L$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_D \end{pmatrix} \xrightarrow{g(\mathbf{y})} \begin{pmatrix} x_1 \\ \vdots \\ x_L \end{pmatrix} = \mathbf{x}$$

- For example,  $\mathbf{Y}$  is a reflectance spectrum ( $D = 184$ ) measured at a specific location of the Mars planet and  $\mathbf{X}$  is the composition of the ground at this location ( $L = 3$ )



prop. of dust  
prop. of CO<sub>2</sub> ice  
prop. of water ice

## 2 - Difficulties

- High dimension ( $D \gg L$ ) → Inverse regression strategy

$$\mathbb{E}(\mathbf{Y}|\mathbf{X} = \mathbf{x}) = f(\mathbf{x})$$

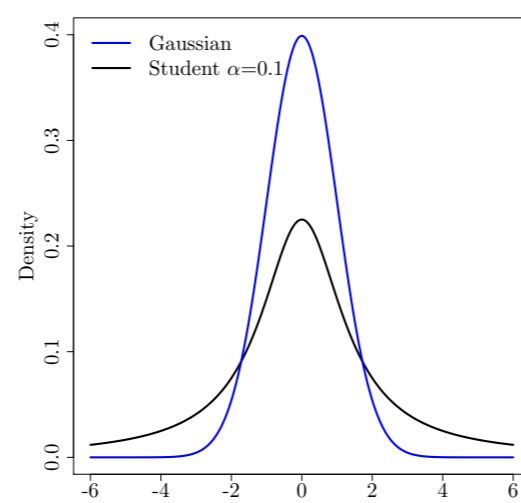
- Non linear mapping → Piecewise linear approximation of  $f$  (and  $g$ )

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

with  $\mathbb{E}(\mathbf{E}_k^2) \propto \Sigma_k$  and  $Z$  multinomial latent variable

$$\mathbb{P}(Z = k) = \pi_k$$

- Dealing with outliers → Heavy tail distribution  
→ Generalized Student distribution



$$\mathcal{S}_M(\mathbf{y}; \boldsymbol{\mu}, \Sigma, \alpha, \gamma) = \frac{\Gamma(\alpha + M/2)}{|\Sigma|^{1/2} \Gamma(\alpha) (2\pi\gamma)^{M/2}} [1 + \delta(\mathbf{y}, \boldsymbol{\mu}, \Sigma)/(2\gamma)]^{-(\alpha + M/2)},$$

→ Gaussian scale mixture representation (using weight variable  $U$  distributed according to a Gamma distribution)

$$\mathcal{S}_M(\mathbf{y}; \boldsymbol{\mu}, \Sigma, \alpha, \gamma) = \int_0^\infty \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu}, \Sigma/u) \mathcal{G}(u; \alpha, \gamma) du$$

→ Parameters estimation is tractable by a general EM algorithm

## 3 - SLLiM model

- A mixture of Student distributions encodes the piecewise linear regressions

$$p(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y} | Z = k) = \mathcal{S}_{L+D}([\mathbf{x}, \mathbf{y}]^T; \mathbf{m}_k, \mathbf{V}_k, \alpha_k, 1)$$

with

$$\mathbf{m}_k = \begin{bmatrix} \mathbf{c}_k \\ \mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k \end{bmatrix} \text{ and } \mathbf{V}_k = \begin{bmatrix} \Gamma_k & \Gamma_k \mathbf{A}_k^T \\ \mathbf{A}_k \Gamma_k & \Sigma_k + \mathbf{A}_k \Gamma_k \mathbf{A}_k^T \end{bmatrix}$$

- Therefore, the joint density  $(\mathbf{X}, \mathbf{Y})$  is a mixture of Student regressions

$$p(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y}) = \sum_{k=1}^K \pi_k \mathcal{S}_{L+D}([\mathbf{x}, \mathbf{y}]^T; \mathbf{m}_k, \mathbf{V}_k, \alpha_k, 1)$$

- We denote by  $\boldsymbol{\theta} = (\mathbf{c}_k, \Gamma_k, \mathbf{A}_k, \mathbf{b}_k, \Sigma_k, \pi_k, \alpha_k)_{1 \leq k \leq K}$  the set of parameters
- Extension to partially observed responses

$$\mathbf{X} = [\mathbf{T}, \mathbf{W}]^T$$

with  $\mathbf{T}$  observed and  $\mathbf{W}$  hidden variables

→ Allow to account for dependence among covariates and reduce the sensitivity of the method to model misspecification

## References

[1] A. Deleforge, F. Forbes, and R. Horaud. High-dimensional regression with Gaussian mixtures and partially-latent response variables. *Statistics and Computing*, 2015.

[2] E. Perthame, F. Forbes, and A. Deleforge. Inverse regression approach to robust non-linear high-to-low dimensional mapping. *Submitted*, 2016.

[3] Link to RATP (subway) data: <http://data.ratp.fr/explore/dataset/qualite-de-lair-mesuree-dans-la-station-chatelet>

## 4 - Inverse regression strategy

- Forward strategy ( $\mathbf{x} = g(\mathbf{y})$ ), conditionals are

$$p(\mathbf{X} = \mathbf{x}; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{S}_L(\mathbf{x}; \mathbf{c}_k, \Gamma_k, \alpha_k, 1)$$

$$p(\mathbf{Y} = \mathbf{y} | \mathbf{X} = \mathbf{x}; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{S}_D(\mathbf{y}; \mathbf{A}_k \mathbf{x} + \mathbf{b}_k, \Sigma_k, \alpha_k^y, \gamma_k^y)$$

→  $D = 500, L = 2, \Gamma_k$  diagonal → 126 254 parameters

- Inverse strategy ( $\mathbf{y} = f(\mathbf{x})$ )

$$p(\mathbf{Y} = \mathbf{y}; \boldsymbol{\theta}^*) = \sum_{k=1}^K \pi_k \mathcal{S}_D(\mathbf{y}; \mathbf{c}_k^*, \Gamma_k^*, \alpha_k, 1)$$

$$p(\mathbf{X} = \mathbf{x} | \mathbf{Y} = \mathbf{y}; \boldsymbol{\theta}^*) = \sum_{k=1}^K \pi_k \mathcal{S}_L(\mathbf{x}; \mathbf{A}_k^* \mathbf{y} + \mathbf{b}_k^*, \Sigma_k^*, \alpha_k^x, \gamma_k^x)$$

with  $\boldsymbol{\theta}^* = (\mathbf{c}_k^*, \Gamma_k^*, \mathbf{A}_k^*, \mathbf{b}_k^*, \Sigma_k^*, \pi_k, \alpha_k)_{1 \leq k \leq K}$  and

$$\mathbf{c}_k^* = \mathbf{A}_k \mathbf{c}_k + \mathbf{b}_k; \quad \Gamma_k^* = \Sigma_k + \mathbf{A}_k \Gamma_k \mathbf{A}_k^T;$$

$$\mathbf{A}_k^* = \Sigma_k^* \mathbf{A}_k^T \Sigma_k^{-1}; \quad \mathbf{b}_k^* = \Sigma_k^* (\Gamma_k^{-1} \mathbf{c}_k - \mathbf{A}_k^T \Sigma_k^{-1} \mathbf{b}_k); \quad \Sigma_k^* = (\Gamma_k^{-1} + \mathbf{A}_k^T \Sigma_k^{-1} \mathbf{A}_k)^{-1}$$

→  $D = 500, L = 2, \Sigma_k$  diagonal → 2 003 parameters

→ Our approach reduces the number of parameters to estimate

- Prediction : The regression function of interest  $g$  is approached by  $\tilde{g}$

$$\tilde{g}(\mathbf{y}) = \mathbb{E}(\mathbf{X} | \mathbf{Y} = \mathbf{y}; \boldsymbol{\theta}^*) = \sum_{k=1}^K \frac{\pi_k \mathcal{S}_D(\mathbf{y}; \mathbf{c}_k^*, \Gamma_k^*, \alpha_k, 1)}{\sum_{j=1}^K \pi_j \mathcal{S}_D(\mathbf{y}; \mathbf{c}_j^*, \Gamma_j^*, \alpha_j, 1)} (\mathbf{A}_k^* \mathbf{y} + \mathbf{b}_k^*)$$

## 5 - Estimation of $\boldsymbol{\theta}$ by EM algorithm

- E-step

- E-U step: Update of weight of each data point  $\mathbb{E}[U | \mathbf{x}, \mathbf{y}, Z = k; \boldsymbol{\theta}^{(i)}]$
- E-Z step: Update posterior probabilities  $\mathbb{P}(Z = k | \mathbf{x}, \mathbf{y}, \boldsymbol{\theta}^{(i)})$

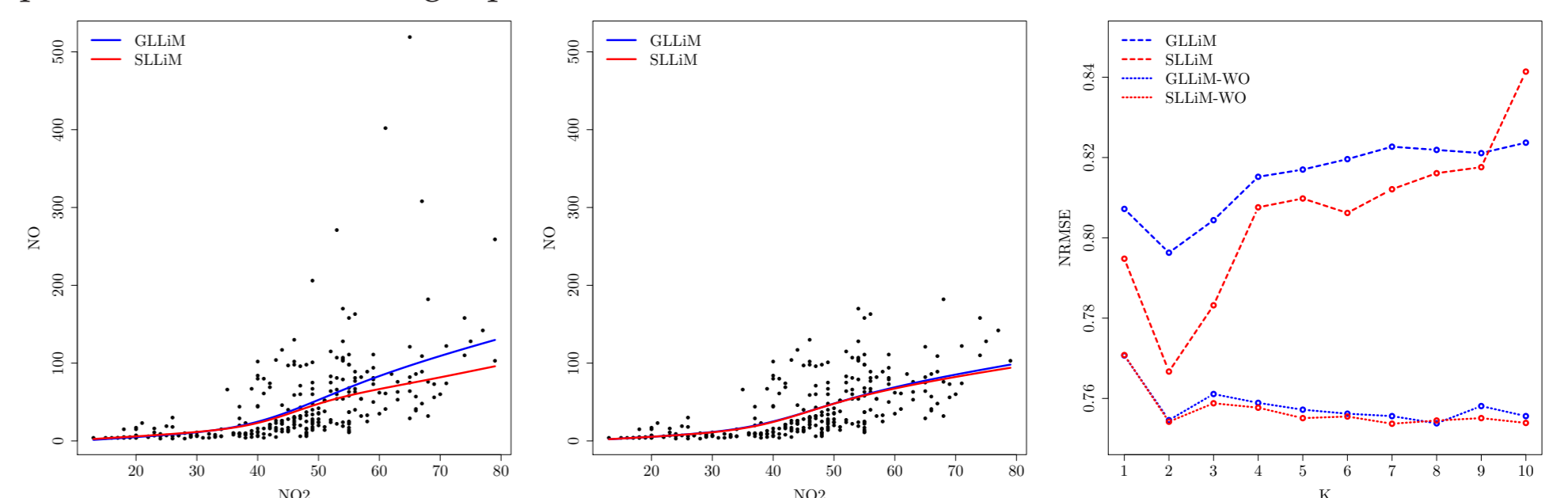
- M-step

- $(\pi_k, \mathbf{c}_k, \Gamma_k) \rightarrow$  Estimation is like a standard Student mixture
- $(\mathbf{A}_k, \mathbf{b}_k, \Sigma_k) \rightarrow$  Estimation is "Linear regression-like"
- $\alpha_k \rightarrow$  Not in closed-form but standard

## 6 - Application to air quality in the subway in Paris

- Prediction of NO (L=1) from NO<sub>2</sub> (D=1) in Châtelet station in Paris during March 2015 ( $N = 341$  measures)
- SLLiM achieves better prediction <sup>a</sup> than its Gaussian counterpart (GLLiM) on complete data
- SLLiM is equivalent to GLLiM when no outliers (removed)

Estimated regression functions with 7 outliers (left panel) and no outliers (center panel) and prediction error rates (right panel)



$$a_{\text{NRMSE}} = \sqrt{\frac{\sum_i (t_i - \hat{t}_i)^2}{\sum_i (t_i - \hat{t}_{\text{train}})^2}}$$

## 7 - Other applications

- Application when  $D \gg L$

- Hyperspectral data on Mars

- \*  $D=184, L=3, N=6983$
- \*  $K$  fixed to 10, number of latent variables  $\mathbf{W}$  estimated by BIC
- \* Prediction of proportion of CO<sub>2</sub> ice and dust from spectra

- Near-infrared spectra on orange juices

- \*  $D=134, L=1, N=218$
- \* Prediction of sucrose level of each orange juice from its spectra

→ Comparison with other non linear regression methods

Prediction error rates for Mars data: average NRMSE (standard deviations) for proportions of CO<sub>2</sub> ice and dust over 100 cross validation runs

Method	Prop. of CO <sub>2</sub> ice	Prop. of dust
SLLiM (K=10)	0.168 (0.019)	0.145 (0.020)
GLLiM (K=10)	0.180 (0.023)	0.155 (0.023)
Regression splines	0.173 (0.016)	0.160 (0.021)
SIR	0.243 (0.025)	0.157 (0.016)
RVM	0.299 (0.021)	0.275 (0.034)