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Non linear robust regression in high dimension
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1 - Non linear mapping problem

- The goal is to retrieve $X$ from $Y$ through a non linear regression function $g$
  $$E(X|Y = y) = g(y)$$
  with $Y \in \mathbb{R}^D, X \in \mathbb{R}^L, D \gg L$
  $$y = \begin{bmatrix} y_1 \\ \vdots \\ y_D \end{bmatrix}, g(Y) = \begin{bmatrix} x_1 \\ \vdots \\ x_L \end{bmatrix} = x$$

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

  ![prop. of dust prop. of CO$_2$ incice](Image)

2 - Difficulties

- High dimension ($D \gg L$) \rightarrow Inverse regression strategy
  $$E(Y | X = x) = f(x)$$
- Non linear mapping \rightarrow Piecewise linear approximation of $f$ (and $g$)
  $$Y = \sum_{k=1}^{K} f_k(x) x + b_k + \varepsilon_k$$
  with $E(\varepsilon_k) \propto \Sigma_k$ and $Z$ multinomial latent variable
  $$P(Z = k) = \pi_k$$

- Dealing with outliers \rightarrow Heavy tail distribution
- Generalized Student distribution
  $$S_i(y; \mu, \Sigma, \alpha, \gamma) = \frac{\Gamma(\alpha + M/2)}{\Gamma(\alpha) (2\pi)^{M/2} [1 + d(y; \mu, \Sigma)/(2\gamma)]^{(\alpha+M/2)}}$$
  \rightarrow Gaussian scale mixture representation (using weight variable $U$ distributed according to a Gamma distribution)
  $$S_i(y; \mu, \Sigma, \alpha, \gamma) = \int_0^\infty S_i(y; \mu, \Sigma, u) \mathcal{G}(u; \alpha, \gamma) \, du$$

- Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

- A mixture of Student distributions encodes the piecewise linear regressions
  $$p(X = x, Y = y | Z = k) = S_k + D \left( [x, y]^T; m_k, \nu_k, \alpha_k, 1 \right)$$
  with $m_k = [c_k, A_k c_k + b_k]$ and $\nu_k = \left[ \Gamma_k, \Gamma_k A_k \Sigma_k + A_k \Gamma_k A_k^T \right]$

- Therefore, the joint density $(X, Y)$ is a mixture of Student regressions
  $$p(X = x, Y = y) = \sum_{k=1}^{K} \pi_k S_k + D \left( [x, y]^T; m_k, \nu_k, \alpha_k, 1 \right)$$

- We denote by $\theta = (\alpha_k, \Gamma_k, A_k, b_k, \Sigma_k, \pi_k, \alpha_k)_{1 \leq k \leq K}$ the set of parameters

- Extension to partially observed responses
  $$X = [T, W]^T$$
  with $T$ observed and $W$ hidden variables

- To allow to account for dependence among covariates and reduce the sensitivity of the method to model misspecification

4 - Inverse regression strategy

- Forward strategy ($x = g(y)$), conditionals are
  $$p(X = x; \theta) = \sum_{k=1}^{K} \pi_k S_k(x; c_k, \Gamma_k, \alpha_k, 1)$$
  $$p(Y = y | X = x; \theta) = \sum_{k=1}^{K} \pi_k S_k(y; A_k x + b_k, \Sigma_k, \alpha_k, 1)$$
  $$\rightarrow D = 500, L = 2, \Gamma_k \text{ diagonal} \rightarrow 126 \text{ 254 parameters}$$

- Inverse strategy ($y = f(x)$)
  $$p(Y = y; \theta^0) = \sum_{k=1}^{K} \pi_k S_k(d(y; c_k^*, \Gamma_k^*, \alpha_k^*, 1)$$
  $$\left( \Gamma_k^* x + b_k^* \right)$$
  with $\theta^0 = (c_k^*, \Gamma_k^*, A_k^*, b_k^*, \Sigma_k^*, \alpha_k^*, 1)$ and $\pi_k = \pi_k^*$
  $$A_k^* = A_k^* \Sigma_k^* + b_k^*$$
  $$\Gamma_k^* = \Sigma_k + A_k^* \Gamma_k^* \Sigma_k^*$$
  $$\Gamma_k^* = (\Gamma_k^* + A_k^* \Sigma_k^* A_k^*)^{-1}$$
  $$\rightarrow D = 500, L = 2, \Gamma_k \text{ diagonal} \rightarrow 2 \text{ 03 parameters}$$

- Our approach reduces the number of parameters to estimate

- Prediction: The regression function of interest $g$ is approached by $\hat{y}$
  $$\hat{y}(y) = E(X | Y = y; \theta^0) = \sum_{k=1}^{K} \pi_k S_k(y; c_k^*, \Gamma_k^*, \alpha_k^*, 1)$$

5 - Estimation of $\theta$ by EM algorithm

- E-step
  - E-U step: Update of weight of each data point $E[U | x, y, Z = k; \theta^0]$  
  - E-Z step: Update posterior probabilities $P(Z = k | x, y; \theta^0)$

- M-step
  - $(\pi_k, c_k, \Gamma_k)$ \rightarrow Estimation like a standard Student mixture
  - $(A_k, b_k, \Sigma_k)$ \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$_2$ (D=1) in Châtelet station in Paris during March 2015 ($N = 341$ measures)
- SLLiM achieves better prediction $\delta$ 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)

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 $W$ estimated by BIC
    - Prediction of proportion of CO$_2$ 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$_2$ ice and dust over 100 cross validation runs

References

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