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

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

* 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$_2$ ice](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 $g$)

$$Y = \sum_{k=1}^K \alpha_k x + b_k + E_k$$

with $E_k \sim \Sigma_k$ and $Z$ multinomial latent variable

$$P(Z = k) = \pi_k$$

* Dealing with outliers \rightarrow Heavy tail distribution \rightarrow Generalized Student distribution

$$S_U(y; \mu, \Sigma, \alpha, \gamma) = \frac{\Gamma(\alpha + M/2)}{\Gamma(\alpha)} \frac{1}{\left|\Sigma\right|^{1/2} \Gamma(\alpha) (2\pi)^{M/2}} \left[1 + \frac{d(y; \mu, \Sigma)}{(2\gamma)^{1/2}}\right]^{-\alpha - M/2},$$

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

$$S_U(y; \mu, \Sigma, \alpha, \gamma) = \int_{0}^{\infty} S_U(y; \mu, \Sigma, \alpha, \gamma) dU$$

\rightarrow Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

* A mixture of Student distributions encodes the piecewise linear regressions

$$p(X = x, Y = y|Z = k) = S_{L_D}(x, y; m_k, \Sigma_k, \alpha_k, 1)$$

with

$$m_k = \begin{bmatrix} \alpha_k \\ A_k \alpha_k + b_k \end{bmatrix}$$

and $V_k = \begin{bmatrix} \Gamma_k & \Gamma_k A_k^T \\ A_k \Gamma_k & \Sigma_k + A_k \Gamma_k A_k^T \end{bmatrix}$

* Therefore, the joint density $(X, Y)$ is a mixture of Student regressions

$$p(X = x, Y = y) = \sum_{k=1}^K \pi_k S_{L_D}(x, y; m_k, \Sigma_k, \alpha_k, 1)$$

* 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

\rightarrow 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

$$p(X = x; \theta) = \sum_{k=1}^K \pi_k S_U(x; c_k, \Gamma_k, \alpha_k, 1)$$

$$p(Y = y|X = x; \theta) = \sum_{k=1}^K \pi_k S_U(y; A_k x + b_k, \Sigma_k, \alpha_k, \gamma_k)$$

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

* Inverse strategy ($y = f(x)$)

$$p(Y = y; \theta) = \sum_{k=1}^K \pi_k S_U(y; c_k, \Gamma_k, \alpha_k, 1)$$

$$p(X = x|Y = y; \theta) = \sum_{k=1}^K \pi_k S_U(x; A_k y + b_k, \Sigma_k, \alpha_k, \gamma_k)$$

with $\theta' = (c_k, \Gamma_k, A_k, b_k, \Sigma_k, \pi_k, \alpha_k)_{1 \leq k \leq K}$ and $c_k = A_k c_k + b_k$, $\Gamma_k = \Sigma_k + A_k \Gamma_k A_k^T$

$A_k^* = \Sigma_k^{1/2} A_k^{1/2}$, $b_k^* = \Sigma_k^{1/2} (\Gamma_k^{1/2} c_k - A_k^{1/2} b_k)$, $\Sigma_k^* = (\Gamma_k^{1/2} + A_k^{1/2} A_k^{1/2})^{-1}$

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

* Our approach reduces the number of parameters to estimate

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

$$\tilde{g}(y) = E(X|Y = y; \theta') = \sum_{k=1}^K \pi_k S_U(y; c_k, \Gamma_k, \alpha_k, 1) (A_k^* y + b_k^*)$$

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

  * $(\alpha_k, c_k, \Gamma_k) \rightarrow$ Estimation is 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 $\hat{d}$ 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

References


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