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

$$y = \left( \begin{array}{c} y_1 \\ . \\ . \\ y_D \end{array} \right) \rightarrow g(Y) = \left( \begin{array}{c} x_1 \\ . \\ . \\ x_L \end{array} \right) = X$$

- 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 CO2 ice prop. of water ice]

2 - Difficulties

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

$$E(Y|X = x) = f(x)$$

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

$$Y = \sum_{k=1}^{K} \pi_k A_k X + b_k + E_k$$

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

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

- Dealing with outliers → Heavy tail distribution

- Generalized Student distribution

$$S_{ST}(y; \mu, \Sigma, \alpha, \gamma) = \frac{\Gamma(\alpha + M/2)}{\Gamma(\alpha/2) \Gamma(M/2)} (1 + \frac{d(y; \mu, \Sigma)}{2\gamma})^{-(\alpha + M/2)}$$

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

$$S_{ST}(y; \mu, \Sigma, \alpha, \gamma) = \int_0^\infty S_{ST}(y; \mu, \Sigma/u) \mathcal{G}(u; \alpha, \gamma) \, du$$

$\rightarrow$ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

- A mixture of Student distributions encodes the piecewise linear regressions

$$p(X = x, Y = y|Z = k) = S_{ST}(x, y^T; m_k, V_k, \alpha_k, 1)$$

with

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

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

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

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

- Extension to partially observed responses

$$X = [T, W]^T$$

with $T$ observed and $W$ hidden variables

- 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

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

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

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

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

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

$\rightarrow$ $D = 500$, $L = 2$, $\Sigma_k$ diagonal $\rightarrow 203$ parameters

- Our approach reduces the number of parameters to estimate

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

$$\tilde{g}(y) = E(X|Y = y; \theta^*) = \sum_{k=1}^{K} \pi_k \mathcal{N}((y, c_k \Gamma_k (y, c_k, \Gamma_k, \alpha_k, 1))$$

5 - Estimation of $\theta$ by EM algorithm

- E-step

- E-U step: Update of weight of each data point $E[U|x, y, Z; \theta^{(0)}]$

- E-Z step: Update posterior probabilities $P(Z = k|x, y; \theta^{(0)})$

- M-step

- $$(\alpha_k, \mathbf{c}_k, \mathbf{G}_k) \rightarrow \text{Estimation is like a standard Student mixture}$$

- $$(A_k, b_k, \Sigma_k) \rightarrow \text{Estimation is “Linear regression-like”}$$

- $\alpha_k \rightarrow \text{Not in closed-form but standard}$

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 $^4$ 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 RMSE (standard deviations) for proportions of CO$_2$ ice and dust over 100 cross validation runs

<table>
<thead>
<tr>
<th>Method</th>
<th>Prop. of CO2 ice</th>
<th>Prop. of dust</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLLiM (K=10)</td>
<td>0.168 (0.019)</td>
<td>0.145 (0.020)</td>
</tr>
<tr>
<td>GLLiM (K=10)</td>
<td>0.180 (0.023)</td>
<td>0.155 (0.023)</td>
</tr>
<tr>
<td>Regression s.</td>
<td>0.173 (0.016)</td>
<td>0.160 (0.021)</td>
</tr>
<tr>
<td>SIR</td>
<td>0.243 (0.025)</td>
<td>0.157 (0.064)</td>
</tr>
<tr>
<td>RVM</td>
<td>0.299 (0.021)</td>
<td>0.275 (0.034)</td>
</tr>
</tbody>
</table>

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