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

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

- 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 ($L = 3$)

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 $g$)

$$Y = \sum_{k=1}^K (1_{x \in A_k}) A_k X + b_k + \epsilon_k$$

with $E(\epsilon_k^2) \propto \Sigma_k$ and $Z$ multinomial latent variable

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

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

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

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

$$S_U(y; \mu, \Sigma, \alpha, \gamma) = \int_0^\infty S_U(y; \mu, \Sigma, u) \nu(u; \alpha, \gamma) du$$

→ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

- A mixture of Student distributions encodes the piecewise linear regressions

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

with

$$m_k = \begin{bmatrix} c_k \\ A_k c_k + b_k \end{bmatrix} \quad \text{and} \quad V_k = \begin{bmatrix} \Gamma_k & \Gamma_k A_k^T \\ A_k & A_k A_k^T + \Sigma_k + A_k \Gamma_k A_k^T \end{bmatrix}$$

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

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

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

$$p(X = x|Y = y, \theta) = \sum_{k=1}^K \pi_k S_{D}(x; c_k, \Gamma_k, \alpha_k, 1)$$

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

→ $D = 500, L = 2, \Gamma_k \text{ diagonal} \rightarrow 126 \text{ 254 parameters}$

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

$$p(Y = y|X = x, \theta) = \sum_{k=1}^K \pi_k S_{D}(y; c_k^i, \Gamma_k^i, \alpha_k, 1)$$

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

with $\theta^* = (c_k^i, \Gamma_k^i, A_k^i, b_k)$ and

$$A_k^i = A_k \Sigma_k + A_k \Gamma_k A_k^T; \quad c_k^i = A_k c_k + b_k$$

→ $D = 500, L = 2, \Gamma_k \text{ diagonal} \rightarrow 203 \text{ parameters}$

→ Our approach reduces the number of parameters to estimate

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

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

5 - Estimation of $\theta$ by EM algorithm

- E-step

- E-U step: Update of weight of each data point $\pi_k = \frac{\int p(x|y, \theta^*) \pi_k S_D(y; c_k^i, \Gamma_k^i, \alpha_k, 1) A_k^i y + b_k^i) dy}{\int p(x|y, \theta^*) \pi_k S_D(y; c_k^i, \Gamma_k^i, \alpha_k, 1) \sum_{k=1}^K A_k^i y + b_k^i) dy}$

- E-Z step: Update posterior probabilities $p(Z = k|X, Y, \theta^*)$

- M-step

- $(\alpha_k, c_k, \Gamma_k) → \text{Estimation is like a standard Student mixture} (A_k, b_k, \Sigma_k)$

- $(A_k^i, b_k^i, \Sigma_k)$ - Estimation is “Linear regression-like”

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

6 - Application to air quality in the subway in Paris

- Prediction of NO ($L=1$) from NO$_2$ ($D=1$) in Châtelain station in Paris during March 2015 ($N = 341$ measures)

- SLLiM achieves better prediction $\tilde{g}$ 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

<table>
<thead>
<tr>
<th>Method</th>
<th>Prop. of CO$_2$ 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 splines</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 (0.016)</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-lesueure-dans-la-station-chatelet/