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

\[ E(Y|X = y) = g(y) \]

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

\[
y = \begin{pmatrix} y_1 \\ \vdots \\ y_D \\ \vdots \\ y_D \\ \end{pmatrix} \sim g(Y) = \begin{pmatrix} x_1 \\ \vdots \\ x_L \end{pmatrix} = x
\]

- 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 \( g \)

\[ Y = \sum_{k=1}^{K} z_2 \cdot Ax + b_k + E_k \]

with \( E(\sum_k) \propto \Sigma_a \) and \( Z \) multinomial latent variable

\[ P(Z = k) = \pi_k \]

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

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

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

\[ S_{\mu}(y; \mu, \Sigma, \alpha, \gamma) = \int_0^\infty S_{\mu}(y; \mu, \Sigma, \alpha, \gamma) \cdot U \cdot \alpha \cdot \gamma \cdot du \]

→ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

- A mixture of Student distributions encodes the piecewise linear regressions

\[ p(X = x, Y = y|Z = k) = S_{\mu,k} \left( [x, y]^T; m_k, V_k, \alpha_k, 1 \right) \]

with

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

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

\[ p(X = x, Y = y) = \sum_{k=1}^{K} \pi_k S_{\mu,k} \left( [x, y]^T; m_k, V_k, \alpha_k, 1 \right) \]

- We denote by \( \theta = (\alpha_k, \Gamma_k, A_k, c_k, \Sigma_k, \pi_k, \alpha_k, 1) \) 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

\[ p(x|y = x; \theta) = \sum_{k=1}^{K} \pi_k S_{\mu,k}(x; \theta) \]

with \( \theta = (\alpha_k, \Gamma_k, A_k, c_k, \Sigma_k, \pi_k, \alpha_k, 1) \)

\[ D = 500, L = 2, \Gamma \rightarrow 126 254 \text{ parameters} \]

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

\[ p(y|X = x; \theta) = \sum_{k=1}^{K} \pi_k S_{\mu,k}(y; \theta) \]

with \( \theta = (\alpha_k, \Gamma_k, A_k, c_k, \Sigma_k, \pi_k, \alpha_k, 1) \)

\[ D = 500, L = 2, \Sigma \rightarrow 2 03 0 \text{ parameters} \]

Our approach reduces the number of parameters to estimate

- Prediction : The regression function of interest \( g \) is approached by \( \hat{y}(x) = E(Y|X = x; \theta) \)

\[ \hat{y}(x) = \sum_{k=1}^{K} \pi_k S_{\mu,k}(y; \theta) \]

5 - Estimation of \( \theta \) by EM algorithm

- E-step

- E-U step: Update of weight of each data point \( P(U|X = x, Y = y, Z = k; \theta) \)

- \( Z \) step: Update posterior probabilities \( P(Z = k|X = x, Y = y, \theta) \)

- M-step

\[ (\alpha_k, c_k, \Gamma_k) \rightarrow \text{Estimation like a standard Student mixture} \]

\[ (A_k, b_k, \Sigma_k) \rightarrow \text{Estimation is "Linear regression-like"} \]

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

6 - Application to air quality in the subway in Paris

- Prediction of NO \((L=1)\) from NO, CO \((D=1)\) in Châtelet station in Paris during March 2015 \((N = 341 \text{ measures})\)

- 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

\[ \hat{\theta}(x) = \sum_{k=1}^{K} \pi_k S_{\mu,k}(y; \theta) \]

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 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>NIR</td>
<td>0.243 (0.025)</td>
<td>0.157 (0.026)</td>
</tr>
<tr>
<td>SVM</td>
<td>0.299 (0.021)</td>
<td>0.275 (0.034)</td>
</tr>
</tbody>
</table>


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