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

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

• 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](image)

2 - Difficulties
• High dimension (\( D \gg L \)) → Inverse regression strategy

\[ E(Y | X = x) = f(x) \]
• Non linear mapping → Piecewise linear approximation of \( f(x) \) and \( g(y) \)

\[ Y = \sum_{c=1}^{C} \sum_{k=1}^{K} T, \pi, A, \gamma \]
with \( E(Y) \propto \Sigma_d \) and \( Z \) multinomial latent variable

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

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

\[ S_{H}(y; \mu, \Sigma, \alpha, \gamma) = \frac{1}{\sqrt{\Gamma(N/2)}} \left| \frac{1}{\Sigma} \right|^{1/2} \left[ 1 + \frac{|y - \mu|}{\alpha \Sigma} \right]^{-(N+M/2)} \]
→ Gaussian scale mixture representation (using weight variable U distributed according to a Gamma distribution)

\[ S_{H}(y; \mu, \Sigma, \alpha, \gamma) = \int_{0}^{\infty} S_{U}(y; \mu, \Sigma, \alpha, \gamma) u \]  

→ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model
• A mixture of Student distributions encodes the piecewise linear regressions

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

\[ m_k = \left[ \begin{array}{c} c_k \\ A_k c_k + b_k \end{array} \right] \quad \text{and} \quad \Sigma_k = \left[ \begin{array}{cc} \Gamma_k & \Gamma_k^T \Sigma_k + A_k \Gamma_k A_k^T \end{array} \right] \]

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

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

• We denote by \( \theta = (c_1, \Gamma_1, A_1, b_1, \Sigma_1, \alpha_1, \beta_1)_{1 \leq k \leq K} \) the set of parameters

• Extension to partially observed responses

\[ X = [T, W]^T \]
with 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

\[ p(X = x | Y = y; \theta) \]
\[ p(Y = y | X = x; \theta) \]

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

• Inverse strategy \( (y = f(x)) \)

\[ p(Y = y | X = x; \theta^*) \]

\[ p(X = x | Y = y; \theta) = \sum_{k=1}^{K} \pi_k S_{L+D}(y; A_k x + b_k, \Sigma_k, \alpha_k, 1) \]
with \( \theta^* = (c_k^*, \Gamma_k^*, A_k^*, b_k^*, \Sigma_k^*, \alpha_k^*, \beta_k^*)_{1 \leq k \leq K} \) and

\[ c_k^* = A_k c_k + b_k, \Gamma_k^* = \Sigma_k + A_k \Gamma_k A_k^T, \]

\[ A_k^* = \Sigma_k^T \Sigma_k^{-1}, b_k^* = \Sigma_k^T (\Gamma_k^T A_k - A_k \Gamma_k), \Sigma_k^* = (\Gamma_k^T + A_k \Gamma_k A_k^T)^{-1} \]

\[ D = 500, L = 2, \Gamma_k \rightarrow 200 \ \text{parameters} \]
→ Our approach reduces the number of parameters to estimate

• Prediction : The regression function of interest \( g \) is approached by \( \tilde{y} \)

\[ \tilde{y} = E(X | Y = y; \theta^*') = \sum_{k=1}^{K} \pi_k S_{L+D}(y; c_k^*, \Gamma_k^*, A_k^*, b_k^*, \Sigma_k^*, \alpha_k^*, 1) \]

\[ (A_k^* y + b_k^*) \]

5 - Estimation of \( \theta \) by EM algorithm
• E-step
→ E-U step: Update of weight of each data point \( E[U (x, y, Z = k; \theta^*)] \)
→ E-Z step: Update posterior probabilities \( E[Z = k | x, y, \theta^*) \)

• M-step
→ \( (\pi_k, c_k, \Gamma_k) \rightarrow \) 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 NO2 (D=1) in Châtelain 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 CO2 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 CO2 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 splines</td>
<td>0.173 (0.016)</td>
<td>0.180 (0.021)</td>
</tr>
<tr>
<td>SIR</td>
<td>0.243 (0.025)</td>
<td>0.157 (0.066)</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-lair-mesuree-dans-la-station-chatelet