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 $g$

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

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

\[
y(k) = \begin{pmatrix}
g(y) \\ 
\vdots \\ 
g(y)
\end{pmatrix} = \begin{pmatrix}
x(1) \\ 
\vdots \\ 
x(L)
\end{pmatrix} = x
\]

- 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 CO₂ ice](image)

2 - Difficulties

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

\[
\mathbb{E}(Y|X=x) = f(x)
\]

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

\[
Y = \sum_{i=1}^{m} (z_i x_i + b_i + E_i)
\]

with $E_i \propto \Sigma_z$ and $Z$ multinomial latent variable

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

- Dealing with outliers → Heavy tail distribution

→ Generalized Student distribution

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

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

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

→ 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

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

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

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

- 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

→ Allow to account for dependence among covariates and reduce the sensitivity of the method to model misspecification

References


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

4 - Inverse regression strategy

- Forward strategy ($x = g(y)$), conditionals are

\[
p(X=x; \theta) = \sum_{k=1}^{K} \pi_k S_{L}(x; c_k, \Gamma_k, \alpha_k, 1)
\]

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

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

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

\[
p(Y=y; \theta) = \sum_{k=1}^{K} \pi_k S_{D}(y; c_k, \Gamma_k, \alpha_k, 1)
\]

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

with $\theta = (c_k, \Gamma_k, A_k, b_k, \Sigma_k, \pi_k, \alpha_k)_{1 \leq k \leq K}$ and

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

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

→ Our approach reduces the number of parameters to estimate

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

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

5 - Estimation of $\theta$ by EM algorithm

- E-step

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

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

- M-step

- $(\pi_k, c_k, \Gamma_k)$ → Estimation is like a standard Student mixture

- $(A_k, b_k, \Sigma_k)$ → Estimation is “linear regression-like”

- $\alpha_k$ → 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

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 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>0.160 (0.021)</td>
</tr>
<tr>
<td>SIR</td>
<td>0.243 (0.025)</td>
<td>0.157 (0.026)</td>
</tr>
<tr>
<td>RVM</td>
<td>0.299 (0.021)</td>
<td>0.275 (0.034)</td>
</tr>
</tbody>
</table>