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

$$y = \left[ \begin{array}{c} y_1 \\ \vdots \\ y_D \end{array} \right] \xrightarrow{g} \left[ \begin{array}{c} x_1 \\ \vdots \\ x_L \end{array} \right] = x$$

- 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 CO$_2$ ice](prop_of_dust_prop_of_co2_ice)

![Prop. of water 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 $g$)

$$Y = \sum_{i=1}^{N_t} \mathbb{1}(x < x_i) A_i x + b_i + \varepsilon_i$$

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

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

- Dealing with outliers → Heavy tail distribution

- Generalized Student distribution

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

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

$$S_{U} (y; \mu, \Sigma, \alpha, \gamma) = \int_0^\infty S_{U}(y; \mu, \Sigma, \alpha) \varphi(u; \alpha) \, du$$

→ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

A mixture of Student distributions encodes the piecewise linear regressions

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

with

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

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 $\theta = (c_1, \Gamma_1, A_1, b_1, \Sigma_1, \pi_1, \alpha_1)_{1 \leq k \leq K}$ 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:

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

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

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

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

$$\rightarrow D = 500, L = 2, \Sigma_k \text{ diagonal } \rightarrow 2 \, 003 \text{ parameters}$$

- Our approach reduces the number of parameters to estimate

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

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

5 - Estimation of $\theta$ by EM algorithm

- E-step

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

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

- 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

Estimated regression functions with 7 outliers (left panel) and no outliers (center panel) and prediction error rates (right panel)

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 $^*$ 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)](estimated_regression_functions)

- Prediction error rates for Mars data: average RMSE (standard deviations) for proportions of CO$_2$ ice and dust over 100 cross validation runs

- Comparison with other non linear regression methods

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

References


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