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

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

- 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 ($L = 3$)

![prop. of dust prop. of CO2 ice prop. of water 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 $f$ (and $g$)

$$Y = \sum_{k=1}^K (\Sigma_k x + b_k + E_k)$$

with $E_i \sim \Sigma_k$ and $Z$ multinomial latent variable

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

- Dealing with outliers → Heavy tail distribution

→ Generalized Student distribution

$$S_U(y; \mu, \Sigma, \alpha, \gamma) = \frac{\Gamma(\alpha + M/2)}{\Gamma(\alpha)\pi^{M/2} \Gamma((\alpha+1)/2)|\Sigma|^{1/2}(1 + \delta(y, \mu, \Sigma)/(2\gamma)^{(\alpha+M/2)})^{-\alpha-M/2}}$$

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

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

→ 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

$$m_k = [c_k, A_k c_k + b_k]$$

and

$$V_k = \begin{bmatrix} \Gamma_k & \Gamma_k A_k^T \\ A_k \Gamma_k & \Sigma_k + A_k \Gamma_k A_k^T \end{bmatrix}$$

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 $\theta = (\alpha, \Gamma_k, A_k, b_k, \Sigma_k, \pi_k, \alpha_k)_{1 \leq k \leq K}$ the set of parameters

- Extension to partially observed responses

$$X = [T, W]^T$$

with $T$ observed and $W$ hidden variables

→ 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

$$p(X = x; \theta) = \sum_{k=1}^K \pi_k S_i(x; c_k, \Gamma_k, \alpha_k, 1)$$

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

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

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

$$p(Y = y; \theta) = \sum_{k=1}^K \pi_k S_i(y; c_k^T, \Gamma_k, \alpha_k, 1)$$

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

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

$$c_k^T = A_k c_k + b_k$$

$$\Gamma_k = \Sigma_k + A_k \Gamma_k A_k^T$$

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

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

→ Our approach reduces the number of parameters to estimate

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

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

5 - Estimation of $\theta$ by EM algorithm

- E-step

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

  - 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

6 - Application to air quality in the subway in Paris

- Prediction of NO (L=1) from NO2 (D=1) in Châtelet station in Paris during March 2015 ($N = 341$ measures)

- SLLiM achieves better prediction $d$ 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 for Mars data: average NRMSE (standard deviations) for proportions of CO

- 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

7 - Other applications

References


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