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 $g$

$$E(\mathbf{X} | Y = y) = g(y)$$

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 ($L = 3$)

$\sum \propto$ prop. of dust prop. of CO$_2$ 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)

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

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

$P(Z = k) = \pi_k$

• Dealing with outliers → Heavy tail distribution

→ Generalized Student distribution

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

→ Parameters estimation is tractable by a general EM algorithm

3 - SLLiM model

• A mixture of Student distributions encodes the piecewise linear regressions

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

with

$m_k = \begin{bmatrix} c_k \\ A_k c_k + b_k \end{bmatrix}$ and $\Sigma_k = \begin{bmatrix} \Gamma_k & A_k \Gamma_k \\ \Gamma_k \Sigma_k + A_k \Gamma_k A_k^T \end{bmatrix}$

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

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

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

• Extension to partially observed responses

$X = [T, W]^T$

with $T$ observed and $W$ hidden variables

→ 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

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

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

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

• Inverse strategy ($y = f(x)$)

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

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

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

$c_k^* = A_k c_k + b_k$

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

$A_k^* = \Sigma_k^* \Gamma_k^*^{-1}$, $b_k^* = \Sigma_k^* (\Gamma_k^*^{-1} c_k - A_k^* \Sigma_k^* b_k)$

$\Sigma_k^* = (\Gamma_k^*^{-1} + A_k^* \Sigma_k^* A_k^*)^{-1}$

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

→ Our approach reduces the number of parameters to estimate

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

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

5 - Estimation of $\theta$ by EM algorithm

• E-step

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

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

• M-step

→ $(\alpha_k, c_k, \Gamma_k) \rightarrow$ 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 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) 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

Method | Prop. of CO$_2$ ice | Prop. of dust
SLLiM (K=10) | 0.168 (0.019) | 0.145 (0.020)
GLLiM (K=10) | 0.180 (0.023) | 0.155 (0.023)
Regression splines | 0.173 (0.016) | 0.160 (0.021)
SIR | 0.243 (0.025) | 0.157 (0.064)
RVM | 0.299 (0.021) | 0.275 (0.034)

References


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

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