Nonparametric learning with matrix-valued predictors in high dimensions

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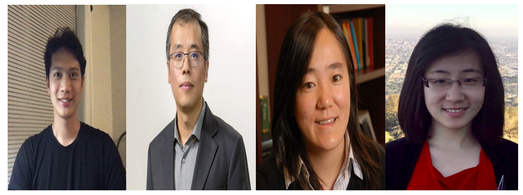


Problems & Existing methods

Problems : Let $\{(\boldsymbol{X}_i, y_i) \in \mathbb{R}^{d_1 \times d_2} \times \{-1, 1\} : i = 1, \ldots, n\}$ denote an i.i.d. sample from unknown distribution $\mathcal{X} \times \mathcal{Y}$.

- Classification: How to efficiently classify high-dimensional matrices with limited sample size:

$$n \ll d_1 d_2 = \text{dimension of feature space?}$$

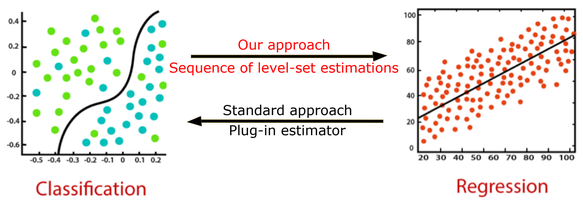
- Regression: How to robustly predict the label probability when little is known to function form of $p(\boldsymbol{X})$:

$$p(\boldsymbol{X}) \overset{\text{def}}{=} \mathbb{P}(y = 1|\boldsymbol{X})?$$

Existing methods :

- Classification: Decision tree, nearest neighbor, neural network, and support vector machine. However, most methods have focused on vector valued features.
- Regression: Logistic regression and linear discriminant analysis. However, it is often difficult to justify the assumptions on the function form, especially when the feature space is high-dimensional.

Goal : We propose nonparametric learning approach with matrix-valued predictors. Unlike classical approaches, our approaches find classification rule first and address regression problem.

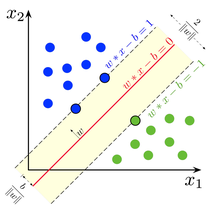


Methods: Classification with matrix predictors

- We develop a large-margin classifier for matrix predictors.

$$\hat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(y_i f(\boldsymbol{X}_i)) + \lambda J(f), \qquad (1)$$

- We set $\mathcal{F} = \{f : f(\cdot) = \langle \boldsymbol{B}, \cdot \rangle \text{ where } \text{rank}(\boldsymbol{B}) \leq r, \|\boldsymbol{B}\|_F \leq C\}$, $J(f) = \|\boldsymbol{B}\|_F^2$, and we choose $L(t)$ to be a large-margin loss, such as hinge loss, logistic loss, etc.
- We also develop nonlinear classifiers for matrix predictors using a new family of matrix-input kernels.



Large margin classifier for vector predictors (Picture source: Wiki).

Methods: Regression function estimation with matrix predictors

- We propose a nonparametric functional estimation using a sequence of weighted classifiers from (1),

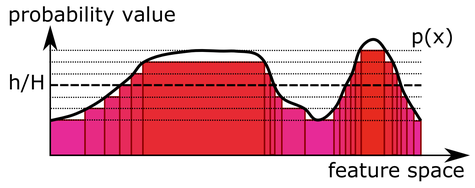
$$\hat{f}_\pi = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \omega_\pi(y_i) L(y_i f(\boldsymbol{X}_i)) + \lambda J(f),$$

where $\omega_\pi(y) = 1 - \pi$ if $y = 1$ and π if $y = -1$.

- The main idea is to estimate $p(\boldsymbol{X})$ through two steps of approximations:

$$p(\boldsymbol{X}) \overset{\text{Step 1}}{\approx} \frac{1}{H} \sum_{h \in [H]} \mathbb{1}\left\{\boldsymbol{X} : p(\boldsymbol{X}) \leq \frac{h}{H}\right\}$$
$$\overset{\text{Step 2}}{\approx} \frac{1}{H} \sum_{h \in [H]} \mathbb{1}\left\{\boldsymbol{X} : \text{sign}\left[\hat{f}_{\frac{h}{H}}(\boldsymbol{X})\right] = -1\right\}.$$

- Step 1 is discretization of target function by level sets.



- Step 2 is to estimate decision region using a sequence of weighted classifiers.

$$\mathbb{1}\left\{\boldsymbol{X} : \underbrace{\text{sign}\left[\hat{f}_\pi(\boldsymbol{X})\right] = -1}_{\text{estimated decision region from classification}}\right\} \xrightarrow{\text{in } p} \mathbb{1}\left\{\boldsymbol{X} : \underbrace{\mathbb{P}(Y = 1|\boldsymbol{X}) \leq \pi}_{\text{targeted level set}}\right\},$$

- We provide accuracy guarantees for the above two steps by extending theories in [2] from vectors to high-dimensional matrix predictors.

Algorithms

- We develop an alternating optimization to solve non-convex problem (1).
- We factor the coefficient matrix $\boldsymbol{B} = \boldsymbol{U}\boldsymbol{V}^T$ where $\boldsymbol{U} \in \mathbb{R}^{d_1 \times r}$ and $\boldsymbol{V} \in \mathbb{R}^{d_2 \times r}$.

Algorithm 1: Classification algorithm with matrix predictors

Input: $(\boldsymbol{X}_1, y_1), \cdots, (\boldsymbol{X}_n, y_n)$, and prespecified rank r

Initialize: $(\boldsymbol{U}^{(0)}, \boldsymbol{V}^{(0)}) \in \mathbb{R}^{d_1 \times r} \times \mathbb{R}^{d_2 \times r}$

Do until converges

Update $\boldsymbol{U}$ fixing $\boldsymbol{V}$:

$\boldsymbol{U} = \arg\min_{\boldsymbol{U}} \frac{1}{n} \sum_{i=1}^{n} \left(1 - \langle \boldsymbol{U}\boldsymbol{V}^T, \boldsymbol{X}_i \rangle\right)_+ + \lambda \|\boldsymbol{U}\boldsymbol{V}^T\|_F^2.$

Update $\boldsymbol{V}$ fixing $\boldsymbol{U}$:

$\boldsymbol{V} = \arg\min_{\boldsymbol{V}} \frac{1}{n} \sum_{i=1}^{n} \left(1 - \langle \boldsymbol{U}\boldsymbol{V}^T, \boldsymbol{X}_i \rangle\right)_+ + \lambda \|\boldsymbol{U}\boldsymbol{V}^T\|_F^2.$

Output: $\hat{f}(\boldsymbol{X}) = \langle \boldsymbol{U}\boldsymbol{V}^T, \boldsymbol{X} \rangle$

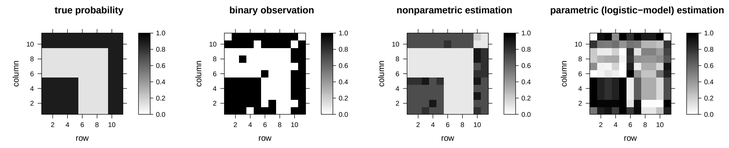
Application: Probability Matrix Estimation

- Our method leads itself well to nonparametric matrix estimation problems.
- Goal: Estimate the probability matrix $\boldsymbol{P} = [\![p_{ij}]\!] \in [0, 1]$ from binary observations $\boldsymbol{Y} = [\![y_{ij}]\!] \in \{0, 1\}$ where $y_{ij} \overset{\text{ind.}}{\sim} \text{Ber}(p_{ij})$ for $(i, j) \in [d_1] \times [d_2]$.
- Training set: $\{(\boldsymbol{X}_{ij}, y_{ij}) : (i, j) \in [d_1] \times [d_2]\}$ where

$$[\boldsymbol{X}_{ij}]_{pq} = \begin{cases} 1 & \text{if } (p, q) = (i, j) \\ 0 & \text{otherwise} \end{cases}.$$

is an indicator matrix with 1 in $(i, j)-$th position and 0's everywhere.

- We apply our developed methods to estimate $p_{ij} = \mathbb{P}(y_{ij} = 1|\boldsymbol{X}_{ij})$.



- Our nonparametric approach provides more robust matrix estimation than parametric approaches [1],[3]

Theoretical results

Theorem 1. *Assume that $\{\boldsymbol{X}_i\}_{i=1}^n$ be set of i.i.d. Gaussian distribution with bounded variation. Then with high probability,*

$$\mathbb{P}[Y \neq \textit{sign}(\hat{f}(\boldsymbol{X}))] - \mathbb{P}[Y \neq \textit{sign}(f^*(\boldsymbol{X}))] \leq \frac{4C\sqrt{r(d_1 + d_2)}}{\sqrt{n}},$$

where f^* is the best predictor in $\mathcal{F}$.

Theorem 2. *Let $\hat{p}$ be an estimated probability function from our method. Under some assumptions, we have*

$$\mathbb{E}\|\hat{p} - p\|_1 = \mathcal{O}\left(\left(\frac{\log\left(n/r(d_1 + d_2)\right)}{(n/r(d_1 + d_2))}\right)^{1/(2-\alpha\wedge 1)}\right),$$

where α is a regularity parameter determined by the true probability. If $\alpha > 1$ and $d_1 = d_2 = d$, we have

$$\mathbb{E}\|\hat{p} - p\|_1 = \mathcal{O}\left(\frac{\log\left(n/rd\right)}{(n/rd)}\right).$$

References

[1] Chanwoo Lee and Miaoyan Wang. "Tensor denoising and completion based on ordinal observations". In: *International conference on machine learning* (2020).

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[3] Miaoyan Wang and Lexin Li. "Learning from binary multiway data: Probabilistic tensor decomposition and its statistical optimality". In: *The Journal of Machine Learning Research* In press (2020).