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:

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

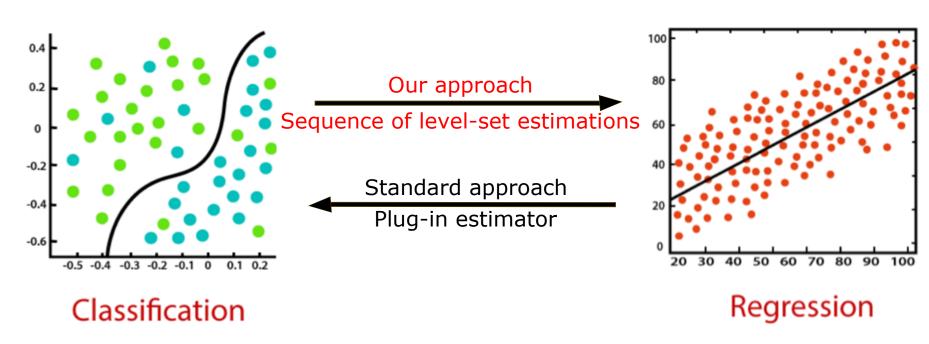
• Regression: How to robustly predict the label probability when little is known to function form of $p(\boldsymbol{X})$:

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

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.

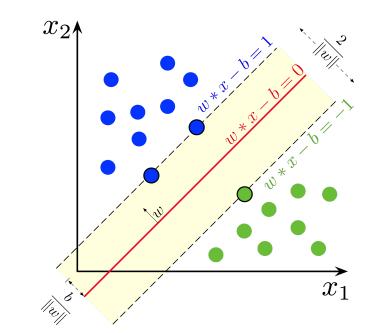


Methods: Classification with matrix predictors

We develop a large-margin classifier for matrix predictors.

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

- We set $\mathcal{F} = \{f: f(\cdot) = \langle \boldsymbol{B}, \cdot \rangle \text{ where } \mathrm{rank}(\boldsymbol{B}) \leq r, \|\boldsymbol{B}\|_F \leq C\}$, $J(f) = \|\boldsymbol{B}\|_F^2$, 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),

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

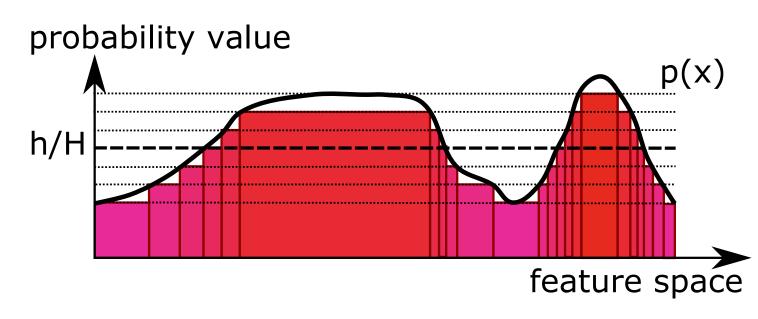
where $\omega_{\pi}(y) = 1 - \pi$ if y = 1 and π if y = -1.

ullet 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.

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

• 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).
- ullet We factor the coefficient matrix $m{B} = m{U}m{V}^T$ where $m{U} \in \mathbb{R}^{d_1 imes r}$ and $m{V} \in \mathbb{R}^{d_2 imes r}$.

Algorithm 1: Classification algorithm with matrix predictors Input: $(X_1, y_1), \dots, (X_n, y_n)$, and prespecified rank rInitialize: $(U^{(0)}, V^{(0)}) \in \mathbb{R}^{d_1 \times r} \times \mathbb{R}^{d_2 \times r}$ Do until converges Update U fixing V: $U = \arg\min_{U} \frac{1}{n} \sum_{i=1}^{n} \left(1 - \langle UV^T, X_i \rangle\right)_+ + \lambda \|UV^T\|_F^2$. Update V fixing U: $V = \arg\min_{V} \frac{1}{n} \sum_{i=1}^{n} \left(1 - \langle UV^T, X_i \rangle\right)_+ + \lambda \|UV^T\|_F^2$. Output: $\hat{f}(X) = \langle UV^T, X \rangle$

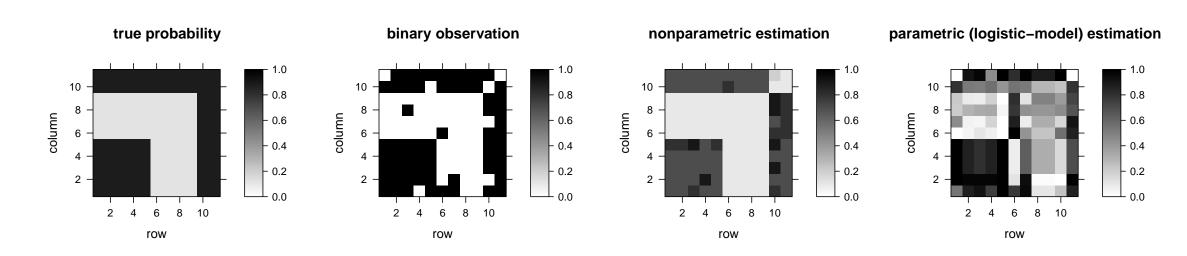
Application: Probability Matrix Estimation

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

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

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 $\{X_i\}_{i=1}^n$ 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

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

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

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

References

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