SMM conditional probability

Chanwoo Lee, April 20, 2020

1 Simulation of SMM Conditional Probability

P(X|y=-1) = N(0, I_4)   simplest case: rank (D) = 1
P(X|y=1) = N(D; I_4)

I generate feature data matrix with the following rule.

$$\begin{aligned}
&\mathbb{P}(X_{\cdot 1}|y=1) \sim N((1,1)^T, I_2), \quad && \mathbb{P}(X_{\cdot 2}|y=1) \sim N((-1,-1)^T, I_2),\\
&\mathbb{P}(X_{\cdot 1}|y=-1) \sim N((0,0)^T, I_2), \quad && \mathbb{P}(X_{\cdot 2}|y=-1) \sim N((0,0)^T, I_2),\\
&X = (X_{\cdot 1}, X_{\cdot 2}) \in \mathbb{R}^{2\times 2}.
\end{aligned}$$

D = [1, -1; 1, -1]

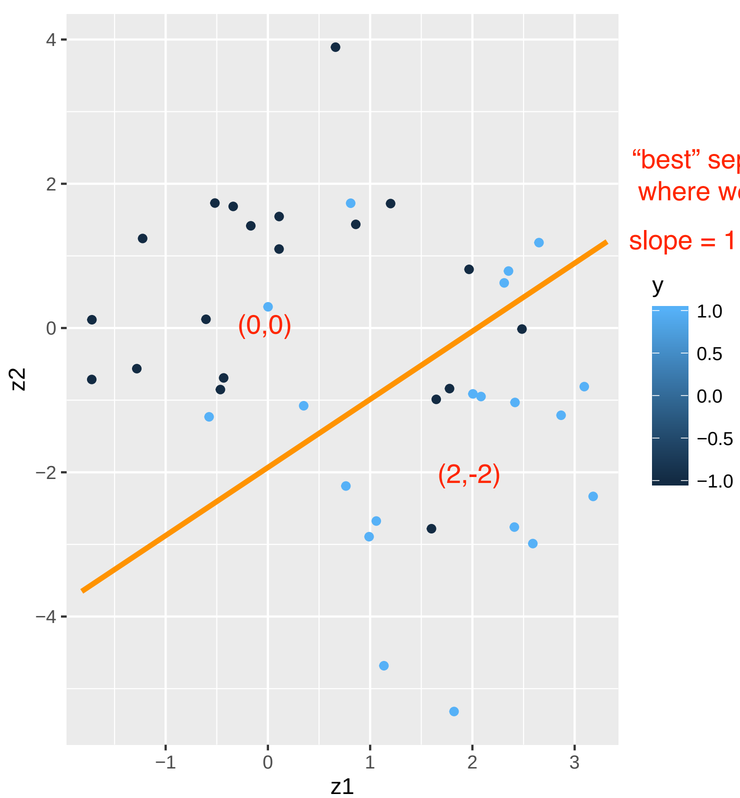
left singular vector: (1,1); right singular vector: (1, -1)

With this rule, we have a test data set $(X^1, 1), \ldots, (X^{20}, 1), (X^{21}, -1), \ldots, (X^{40}, -1)$. Define

$$Z_1 = X_{11} + X_{21} \text{ and } Z_2 = X_{12} + X_{22}.$$

<X, D> = (x11+x21)-(x12+x22)

We can plot the those feature matrices into two dimension transforming the matrices as $\left((Z_1^1, Z_2^1)^T, 1\right), \ldots, \left((Z_1^{20}, Z_2^{20})^T, 1\right), \left((Z_1^{21}, Z_2^{21})^T, -1\right), \ldots, \left((Z_1^{40}, Z_2^{40})^T, -1\right)$. Figure 1 shows the data distribution.



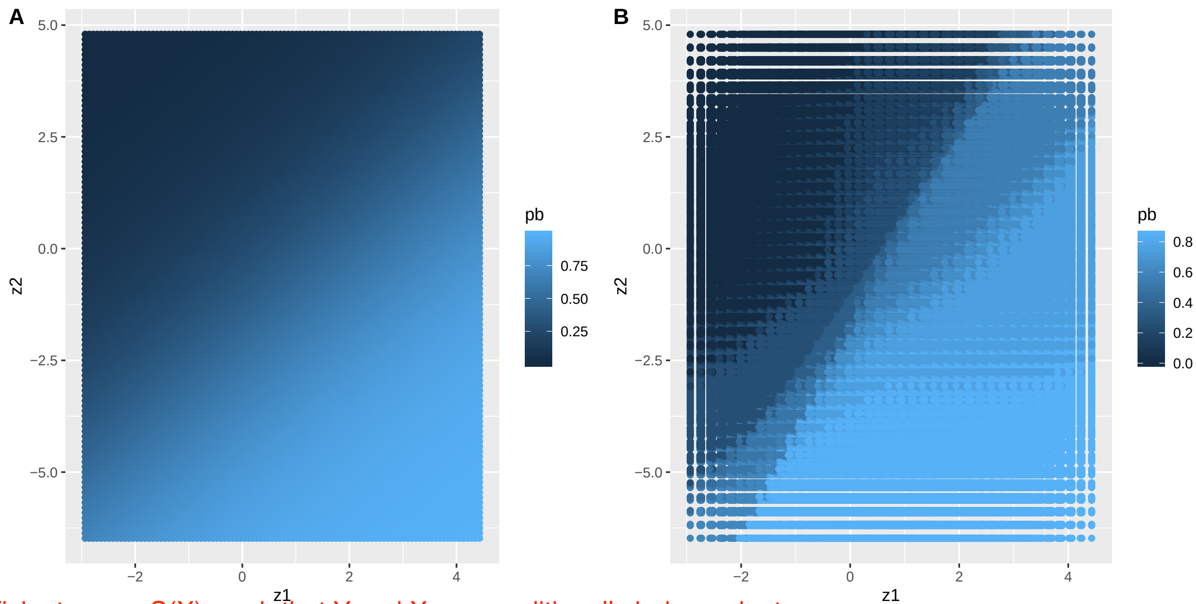
"best" separation: Z1-Z2 = <B, X>
where we define B = [1, -1; 1, -1]

slope = 1

Figure 1: Visualization of the feature matrices. $Z1$ is the sum of the first column and $Z1$ is of the second one.

Notice that we can calculate the distribution of $(Z_1, Z_2)^T$ as,

$$\mathbb{P}((Z_1, Z_2)^T|y=1) \sim N((2,-2), 2I_2), \tag{1}$$



Find sufficient space S(X), such that Y and X are conditionally independent

Figure 2: Figure A shows the true conditional probability of y given (Z_1, Z_2). Figure B shows the estimated probability using SMM weighted hinge loss approach.

Q: Y independent of X | S(X)

A: S(X) = <B, X> in SMM

$$\mathbb{P}((Z_1, Z_2)^T | y = -1) \sim N((0, 0), 2I_2).$$

From the Bayes rule, we calculate the conditional probability $\mathbb{P}(y = 1|(Z_1, Z_2))$ with the assumption $\mathbb{P}(y = 1) = \mathbb{P}(y = -1)$ as

$$\underbrace{\mathbb{P}(y = 1|(Z_1, Z_2)^T)}_{P(y=1|X)} = \frac{\mathbb{P}((Z_1, Z_2)^T|y = 1)\mathbb{P}(y = 1)}{\mathbb{P}((Z_1, Z_2)^T|y = 1)\mathbb{P}(y = 1) + \mathbb{P}((Z_1, Z_2)^T|y = -1)\mathbb{P}(y = -1)} \tag{2}$$
$$= \frac{1}{1 + \exp\left(-\underbrace{(2, -2)((Z_1, Z_2)}_{\text{Sufficient statistics: Z1-Z2=X11+X21-X12-X22}} - (1, -1))^T /4\right)}.$$

In the last equality in (2), we use the distribution in (1).

As a by-product, we learn the dimension reduction from original X-space (dim = 4) to a reduced space (dim = 1)

Using the weighted hinge loss approach, I calculate the conditional probability using SMM method (with modified algorithm for conditional probability). I set the rank as one when fitting SMM model to the data set. Figure 2 shows the true conditional probability $\mathbb{P}(y = 1|(Z_1, Z_2))$ and the estimated one. We can see that SMM conditional probability estimation works well since the true distribution is linear.

SMM achieves two goals simultaneously:
1. estimate the probability
2. find sufficient dimension reduction in X-space.

2 Kernel method

I am suggesting new kernel method which makes optimization easier. Define feature mapping $h : \mathbb{R}^{m\times n} \to \mathbb{R}^{m'\times n}$ where $m < m'$. Kernels for matrix case can be define as

m'=m, n=n

$$K(X, X') = h(X)^T h(X') \in \mathbb{R}^{n\times n}. \quad \text{(column-wise kernel)}$$

(m',n) embedded into the space (m',n,m)

Our objective primal problem is

h: m-by-n —> m-by-n-by-p, where p>>1

$$\min_{U\in\mathbb{R}^{m'\times r}, V\in\mathbb{R}^{n\times r}, \boldsymbol{\xi}} \frac{1}{2}\|UV^T\|^2 + c\sum_{i=1}^{N} \xi_i \tag{3}$$

$$\text{subject to } y_i(\langle UV^T, h(X_i)\rangle + b) \leq 1 - \xi_i$$
$$\xi_i \geq 0, \quad i = 1, \ldots, N.$$

How to update V while fixing U?

Then fixing V we have the dual problem of (3).

(you may want to extend h: m-by-n to m'-by-n', where m'>=m, n'>=n
h induces both row-wise kernel and column-wise kernel)

$$\min_{\boldsymbol{\alpha}} - \sum_{i=1}^{N} \alpha_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j y_i y_j \langle h(X_i)H_V, h(X_j)H_V\rangle$$
$$\text{subject to } \sum_{i=1}^{N} y_i\alpha_i = 0$$
$$0 \leq \alpha_i \leq C, \quad i = 1, \ldots, N.$$

<Uh, Uh> h: m'-by-n hh': m'-by-m'

Kernel: tr(h'U'Uh)=tr(U'Hhh')

Notice $\langle h(X_i)H_V, h(X_j)H_V\rangle = \mathrm{tr}\left(H_V h(X_i)^T h(X_j)\right) = \mathrm{tr}\left(H_V K(X_i, X_j)\right)$. Therefore, we can update U and V without the information of the feature map h. We can define the following kernels.

$$\begin{aligned}
\text{Linear:} &\quad K(X, X') = X^T X' \\
\text{Polynomial:} &\quad K(X, X') = (X^T X' + I_n)^d \\
\text{Radial:} &\quad K(X, X') = \exp\left((X - X')^T (X - X')/\sigma\right),
\end{aligned}$$

where $\exp(A) = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$. Notice that when $X \in \mathbb{R}^{m\times 1}$ i.e. X is a vector, all those definitions are reduced to SVM case. From this way, we can generalize linear SMM method to Kernel SMM with tractable algorithm.

Let SVD of A = PCQ' exp(C)=diag(exp(c_11)…,exp(C_nn))

exp(A) = P exp(C) Q'