Nonparametric approach for binary matrix completion

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Assumption 1 (GLM tensor). We call the tensor $\mathcal{Y} = [y_{\omega}]$ is exponential family tensor with bounded variance, if the following two assumptions are met.

1. [GLM density] Conditional on canonical parameter tensor $\Theta = [\![\theta_{\omega}]\!]$, the tensor entries y_{ω} 's are independent of each other, and $y_{\omega}|\theta_{\omega}$ follows a generalized linear model (GLM) with density

$$p(y_{\omega}|\theta_{\omega}) = c(y_{\omega}, \phi) \exp\left(\frac{y_{\omega}\theta_{\omega} - b(\theta_{\omega})}{\phi}\right),$$

where $b(\cdot)$ is a known function depending on the distribution family of y_{ω} , $\phi > 0$ is the dispersion parameter, and $c(\cdot)$ is a known normalizing function.

2. [Boundedness] The parameter tensor Θ is bounded, i.e, $\|\Theta\|_{\infty} \leq \alpha$ for some $\alpha > 0$.

Proposition 1 (sub-Gaussian residuals under bounded variance). Let \mathcal{Y} be a GLM data tensor, and $\mathcal{E} = \mathcal{Y} - b'(\Theta)$ be the residual tensor, where $b'(\cdot)$ denotes the first-order derivative. Under Assumption 1, the entries of \mathcal{E} are independent sub-Gaussian entries with parameter (ϕU) , where $U = \max_{|\theta| \le \alpha} b''(\theta) < \infty$ and $\phi > 0$ is the dispersion parameter in the GLM density.

Proof. It is easy to see that the entries of $\mathcal{E} = \llbracket \varepsilon_{\omega} \rrbracket$ are independent conditional on $\Theta = \llbracket \theta_{\omega} \rrbracket$. Furthermore, we show that ε_{ω} is a sub-Gaussian random variable under the boundedness condition on θ_{ω} . For notational convinene, we drop the subscript ω , and simply write ε and θ . By the definition of sub-Gaussian random variable, it suffices to show

$$\mathbb{E}\left[\exp(t\varepsilon|\theta)\right] \le \exp\left(\frac{\phi U t^2}{2}\right), \text{ for all } t \in \mathbb{R}.$$

By the definition of GLM density, we have

$$\mathbb{E}[\exp(t\varepsilon|\theta)] = \int c(y,\phi) \exp\left(\frac{y\theta - b(\theta)}{\phi}\right) \exp\left[t(y - b'(\theta))\right] dy$$

$$= \int c(y,\phi) \exp\left(\frac{y(\theta + \phi t) - b(\theta + \phi t) + b(\theta + \phi t) - b(\theta) - \phi t b'(\theta)}{\phi}\right) dy$$

$$= \exp\left(\frac{b(\theta + \phi t) - b(\theta) - \phi t b'(\theta)}{\phi}\right)$$

$$\leq \exp\left(\frac{\phi U t^2}{2}\right),$$

where the last inequality follows from Taylor expansion and the definition of U. Therefore, ε is sub-Gaussian- (ϕU) .

1 Problem

Suppose that we observe a subset of entries from a binary matrix, $\{y_{ij} \in \{-1,1\}: (i,j) \in \Omega\}$, where $\Omega \subset [d_1] \times [d_2]$ is the index set of observed entries. How to predict the unobserved entries $\{y_{ij} \in \{-1,1\}: (i,j) \in \Omega^c\}$?

$$\begin{bmatrix}
-1 & ? & ? & -1 & ? \\
? & 1 & ? & ? & ? \\
-1 & ? & ? & -1 & ? \\
? & ? & -1 & ? & 1
\end{bmatrix}$$
(1)

2 Earlier solution

First, we perform probability estimation based on parametric models. Assume y_{ij} are independent Bernoulli random variables with success probabilities $P(y_{ij} = 1)$ for all $(i, j) \in [d_1] \times [d_2]$. We model the probability matrix using the GLM logistic model,

$$\mathbb{P}(y_{ij} = 1) = \frac{e^{\theta_{ij}}}{1 + e^{\theta_{ij}}}, \quad \text{where} \quad \Theta = \llbracket \theta_{ij} \rrbracket \in \mathbb{R}^{d_1 \times d_2} \text{ is a rank-} r \text{ matrix.}$$

Define the rank-r maximum log-likelihood estimator $\hat{\Theta}^{\text{MLE}} = [\hat{\theta}_{ij}^{\text{MLE}}] = \arg\min_{\Theta \in \mathcal{P}(r,\alpha)} L(\Theta)$, where

$$L(\Theta) = -\sum_{(i,j)\in\Omega} \log(e^{y_{ij}\theta_{ij}} + 1), \text{ and}$$

$$P(r,\alpha) = \{\Theta \in \mathbb{R}^{d_1 \times d_2} : \text{rank}(\Theta) \le r \text{ and } \|\Theta\|_{\infty} \le \alpha\}.$$
(2)

Second, we perform prediction using plug-in estimates,

$$\hat{y}_{ij} = \text{sign } \hat{\theta}_{ij}^{\text{MLE}}, \quad \text{for all } (i,j) \in \Omega^c.$$

3 New proposal

If our goal is to predict the unobserved entries by two labels $\{-1,1\}$, there is no need to estimate the probability. We could directly perform the prediction in a nonparametric fashion. This scenario reduces to a special case of our matrix-valued classification problem.

1. Feature space:

$$\mathcal{X} = \{ \boldsymbol{X} \in \{0, 1\}^{d_1 \times d_2} | \text{only one entry of } \boldsymbol{X} \text{ is one, and others are zero} \}$$

= $\{ \boldsymbol{e}_i \otimes \boldsymbol{e}_j : (i, j) \in [d_1] \times [d_2] \}.$

- 2. Outcome space: $\mathcal{Y} \in \{0,1\}$.
- 3. Uniform marginal distribution $\mathcal{P}(\boldsymbol{X})$ over \mathcal{X} . No other joint distribution assumptions on $P(\boldsymbol{X}, y)$;
- 4. i.i.d. training set: $\{(\boldsymbol{X}_{ij}, y_{ij}) : (i, j) \in \Omega\}$, where $\boldsymbol{X}_{ij} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j \in \{0, 1\}^{d_1 \times d_2}$ is an indicator matrix specifying the observed index, and $y_{ij} \in \{-1, 1\}$ is the observed label at index (i, j). For example, the features in the training sample for problem (1) are

$$X_1 = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 0 & \cdots & 1 & 0 \\ 0 & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \end{bmatrix}, \quad \cdots, \quad X_7 = \begin{bmatrix} 0 & \cdots & 0 & 0 \\ 0 & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 1 \end{bmatrix}.$$

5. Define the rank-r large-margin estimator $\hat{\Theta}^{\mathrm{margin}} = [\hat{\theta}_{ij}^{\mathrm{margin}}] = \arg\min_{\Theta \in \mathcal{P}(r,\alpha)} L(\Theta)$, where

$$L(\Theta) = \sum_{(i,j)\in\Omega} [1 - y_{ij} \langle \mathbf{X}_{ij}, \Theta \rangle]_{+}, \text{ and}$$

$$\mathcal{P}(r,\alpha) = \{\Theta \in \mathbb{R}^{d_1 \times d_2} : \operatorname{rank}(\Theta) \leq r \text{ and } \|\Theta\|_{\infty} \leq \alpha\}.$$
(3)

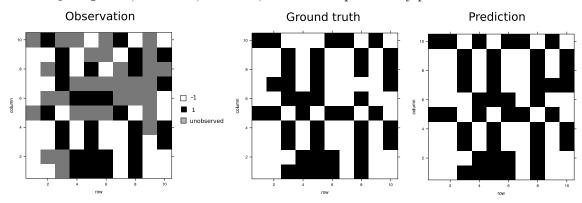
Here, we have omitted the intercept for simplicity.

- 6. Predict unobserved entries using $\hat{y}_{ij} = \text{sign } \hat{\theta}_{ij}^{\text{margin}}$.
- 7. Nonparametric probability estimation $\widehat{\mathbb{P}}(y_{ij} = 1 | \mathbf{X}_{ij})$ is also possible using a sequence of weighted low-rank classifications (3).

4 Numerical experiments

4.1 Missing data imputation

dimension $d_1 = d_2 = 10$; rank = 2; cost = 1; observation probability p = 0.6.

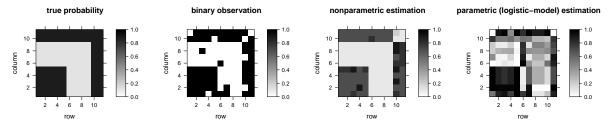


	Unobserved		Observed	
	pred = 1	pred = -1	pred = 1	pred = -1
true = 1	16	3	36	1
true = -1	1	12	1	30

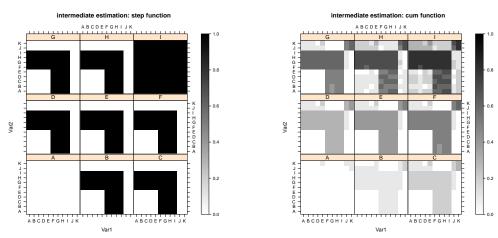
4.2 Probability estimation

dimension $d_1 = d_2 = 11$; cost = 1; observation probability p = 1 (no missing data).

Goal: estimate probability matrix $P \in [0,1]^{d_1 \times d_2}$ from binary observations $\mathbf{Y} = \{0,1\}^{d_1 \times d_2}$.



Intermediate steps.



Define a sequence of cumulative probability matrices $\frac{1}{10} \sum_{h \leq 1} F_h$ (Panel A), $\frac{1}{10} \sum_{h \leq 2} F_h$ (Panel B), $\dots, \frac{1}{10} \sum_{h \leq 9} F_h$ (Panel I), where $F_h = \mathbb{1}(P \leq \frac{h}{10}) \in \{0,1\}^{d_1 \times d_2}$ is the indicator function.

For each matrix entry (i, j), estimate the probability using estimated cumulative probability

$$\hat{P}(i,j) = \frac{1}{10} \underset{H \in [10]}{\arg \max} \sum_{h \le H} \widehat{F}_h(i,j), \text{ for } (i,j) \in [d_1] \times [d_2],$$

where $\widehat{F_h}(i,j)$ is the predicted class indicator for (i,j)-th entry, based on weighted classifiers.

5 Theory

Definition 1 (Misclassification error). Let $Y = [y_{ij}], Z = [z_{ij}] \in \{0,1\}^{d_1 \times d_2}$ be two binary matrices. We define the misclassification error (MCE),

$$MCE(\boldsymbol{Y}, \boldsymbol{Z}) = \frac{1}{d_1 d_2} \sum_{(i,j) \in [d_1] \times [d_2]} \mathbb{1} \{ y_{ij} \neq z_{ij} \}.$$

Theorem 5.1 (Generalization error bounds). Consider a binary target matrix $\mathbf{Y} = \llbracket y_{ij} \rrbracket \in \{-1,1\}^{d_1 \times d_2}$ whose entires are independent realizations from some unknown distributions $Ber(p_{ij})$, for all $(i,j) \in [d_1] \times [d_2]$. Suppose that we observe a subset of entries, $\mathbf{Y}_{\Omega} := \{y_{ij}\}_{(i,j)\in\Omega}$, where $\Omega \subset [d_1] \times [d_2]$ is a random set with $|\Omega|$ entries, and each entry in Ω is an i.i.d. drawn uniformly from $[d_1] \times [d_2]$. Let $\hat{\Theta} = \llbracket \hat{\theta}_{ij} \rrbracket \in \mathcal{P}(r,\alpha)$ denote any estimator based on the observations \mathbf{Y}_{Ω} , where r is the rank bound and α is the infinity norm bound. Then, with probability at least $1 - \delta$ over \mathbf{Y} and the sample selection Ω , the following bound holds uniformly for all $\hat{\Theta} \in \mathcal{P}(r,\alpha)$,

$$\underbrace{\operatorname{MCE}(\boldsymbol{Y},\operatorname{sign}\;\hat{\boldsymbol{\Theta}})}_{misclassification\;error\;in\;targeted\;matrix} \leq \underbrace{\frac{L}{|\Omega|}}_{(i,j)\in\Omega} \underbrace{\operatorname{surrogate-loss}(y_{ij}\hat{\boldsymbol{\theta}}_{ij})}_{surrogate\;loss\;in\;sample} + C_1\alpha\sqrt{\frac{(d_1+d_2)r}{|\Omega|}} + C_2\sqrt{\frac{\log(3/\delta)}{2|\Omega|}},$$

where where $C_1, C_2 > 0$ are two universal constants, and L > 0 is the Lipschitz constant of the surrogate loss,

$$L = \begin{cases} 1, & \text{for hinge loss } S(t) = (1-t)_+, \\ \frac{1}{\log 2}, & \text{for logistic loss } S(t) = \log_2(e^t + 1), \end{cases}$$

In particular, the generalization error of $\hat{\Theta}$ converges to zero as long as the sample size $|\Omega| \geq \tilde{\mathcal{O}}(d_{\max}r)$.

Corollary 1 (Large-margin estimator). Consider the same set-up as in Theorem 5.1. Let $\Theta^* \in \mathbb{R}^{d_1 \times d_2}$ be the optimal estimator in $\mathcal{P}(r, \alpha)$ that minimizes the MCE, i.e.,

$$\Theta^* = \underset{\Theta \in \mathcal{P}(r,\alpha)}{\arg \min} MCE(\boldsymbol{Y}, \operatorname{sign} \Theta).$$

Then, for the constrained MLE defined in (2) and large-margin estimator defined in (3), we have

$$MCE(\boldsymbol{Y}, \text{sign } \hat{\Theta}^{\text{margin}}) - MCE(\boldsymbol{Y}, \text{sign } \Theta^*) \leq C_1 \alpha \sqrt{\frac{(d_1 + d_2)r}{|\Omega|}} + C_2 \sqrt{\frac{\log(1/\delta)}{2|\Omega|}},
MCE(\boldsymbol{Y}, \text{sign } \hat{\Theta}^{\text{MLE}}) - MCE(\boldsymbol{Y}, \text{sign } \Theta^*) \leq C_1 \alpha \sqrt{\frac{(d_1 + d_2)r}{|\Omega|}} + C_2 \sqrt{\frac{\log(1/\delta)}{2|\Omega|}},$$

with probability at least $1 - \delta$ over Y and the sample selection Ω .

Remark 1 (Approximation error). What is the total estimation error of sign $\hat{\Theta}$ from the bayes rule? Two sources of error: generalization error + approximation error. The approximation error reaches zero when the "bayes rule" binary matrix is included in the set of candidate sign matrices. Namely, there exists a low-rank, entrywise bounded matrix $\Theta^* \in \mathcal{P}(r, \alpha)$ such that

$$\Theta^* \stackrel{\text{equal in sign}}{=} [p_{ij} - 0.5], \text{ or equivalently, } \text{MCE}(\Theta^*, \underbrace{\text{sign}(p_{ij} - 0.5)}_{\text{"bayes rule" binary matrix}}) = 0.$$

Remark 2. Given a bayes rule binary matrix, how can we tell whether it is the sign matrix for some low-rank matrix in $\mathbb{P}(r,\alpha)$? For matrix completion problem, the sample size $|\Omega|$ is always smaller than the feature dimension d_1d_2 . What does "decision boundary" mean when the feature space is discrete?

Remark 3. If full rank, then $\theta_{ss'}$ = intercept = sample average = $\frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} y_{ij}^{\text{test}}$ for all $(s,s') \in \Omega^c$. Non-vanishing MCE unless $|\Omega| \approx d_1 d_2$.

Remark 4. MCE vs. MSE. sharpness compared to earlier paper?

Remark 5 (Nonlinear extension).

6 Proofs

Proof of Theorem 5.1. Because the desired conclusion is a uniform bound over all $\hat{\Theta} \in \mathcal{P}(r, \alpha)$, we write Θ in place of $\hat{\Theta}$ for notational convenience. One should note that Θ is a random variable depending on the realizations of the training set $\{y_{ij}\}_{(i,j)\in\Omega}$.

Define the function class $\mathcal{F} = \{f(\mathbf{X}) : \mathbf{X} \mapsto \langle \mathbf{X}, \Theta \rangle \mid \Theta \in \mathcal{P}(r, M)\}$. Given the features in the training set, $\{\mathbf{X}_{ij} = \mathbf{e}_i \otimes \mathbf{e}_j : (i, j) \in \Omega\}$, we consider the empirical Rademacher complexity of \mathcal{F} conditional on Ω and the training set. Let $\{\xi_{ij}\}$ a set of i.i.d. Rademacher random variables with equal probability on ± 1 , then

$$\mathcal{R}_{\Omega}(\mathcal{F}) = \frac{2}{|\Omega|} \mathbb{E}_{\xi_{ij}} \left\{ \sup_{\Theta \in \mathcal{P}(r,\alpha)} \sum_{(i,j) \in \Omega} \xi_{ij} \Theta_{ij} \right\}. \tag{4}$$

Note that $\Theta \in \mathcal{P}(r, M)$ implies that $\|\Theta\|_{\max} \leq \sqrt{r}\alpha$, where $\|\Theta\|_{\max} = \min_{\Theta = \mathbf{U}^T \mathbf{V}} \{\|\mathbf{U}\|_{2,\infty} \|\mathbf{V}\|_{2,\infty} \}$ denotes the matrix max-qnorm. Therefore, the inequality (4) is upper bounded,

$$\frac{2}{|\Omega|} \mathbb{E}_{\xi_{ij}} \left\{ \sup_{\Theta \in \mathcal{P}(r,M)} \sum_{(i,j) \in \Omega} \xi_{ij} \Theta_{ij} \right\} \leq \frac{2}{|\Omega|} \mathbb{E}_{\xi_{ij}} \left\{ \sup_{\|\Theta\|_{\max} \leq \sqrt{r\alpha}} \sum_{(i,j) \in \Omega} \xi_{ij} \Theta_{ij} \right\} \\
\leq c\alpha \sqrt{\frac{r(d_1 + d_2)}{|\Omega|}},$$

where the last inequality follows from Ghadermarzy et al. [2019, Lemma 31].

Using the generalization error inequality in the earlier notes, we have that, with probability at least $1 - \delta$ over the sample selection Ω and training data $\{y_{ij}^{\text{train}}\}_{(i,j)\in\Omega}$, the following bound holds uniformly over $\Theta = [\![\theta_{ij}]\!] \in \mathcal{P}(r,M)$,

$$\mathbb{P}\left[y^{\text{test}} \neq \text{sign } \langle \boldsymbol{X}^{\text{test}}, \Theta \rangle\right] \leq \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} \text{hinge-loss}(y_{ij}^{\text{train}}, \theta_{ij}) + C_1 \alpha \sqrt{\frac{r(d_1 + d_2)}{|\Omega|}} + \sqrt{\frac{\log(1/\delta)}{2|\Omega|}}, (5)$$

for some constant $C_1 > 0$, where the probability at the left hand side is taken with respect to $(\boldsymbol{X}^{\text{test}}, y^{\text{test}}) \in \{\boldsymbol{e}_s \otimes \boldsymbol{e}_s' \colon (s, s') \in [d_1] \times [d_2]\} \times \{0, 1\}$, independent of training data $\{y_{ij}^{\text{train}}\}_{(i,j) \in \Omega}$.

Now, the i.i.d. uniform sampling assumption implies the mutual independence of the events $\mathbb{1}\{y_{ss'} \neq \text{sign } \theta_{ss'}\}$ and marginal uniform distribution $\mathbb{P}(\boldsymbol{X}^{\text{test}} = \boldsymbol{e}_s \otimes \boldsymbol{e}_{s'}) = \frac{1}{d_1 d_2}$ for all $(s, s') \in [d_1] \times [d_2]$. By properties of conditional expectation and concentration inequality, we have, for any $\alpha > 0$,

$$\mathbb{P}\left[y^{\text{test}} \neq \text{sign } \langle \boldsymbol{X}^{\text{test}}, \Theta \rangle\right] = \frac{1}{d_1 d_2} \sum_{(s,s') \in [d_1] \times [d_2]} \mathbb{E}_{y_{ss'}^{\text{test}}} \mathbb{1}\left\{y_{ss'}^{\text{test}} \neq \text{sign } \theta_{ss'}\right\} \\
\geq \frac{1}{d_1 d_2} \sum_{(s,s') \in [d_1] \times [d_2]} \mathbb{1}\left\{y_{ss'}^{\text{test}} \neq \text{sign } \theta_{ss'}\right\} - C\alpha \sqrt{\frac{1}{d_1 d_2}}, \tag{6}$$

where the last statement holds with probability at least $1 - \exp(-\alpha^2)$ over the test matrix $\mathbf{Y}^{\text{test}} = [y_{ss'}^{\text{test}}] \in \{0, 1\}^{d_1 \times d_2}$.

Combining (5) and (6) with $\alpha = \sqrt{\log(1/\delta)}$ yields the uniform bound for all $\Theta \in \mathcal{P}(r,\alpha)$,

$$MCE(\boldsymbol{Y}^{\text{test}}, \text{sign }\Theta) \leq \frac{1}{|\Omega|} \sum_{(i,j)\in\Omega} \text{hinge-loss}(y_{ij}^{\text{train}}, \theta_{ij}) + C_1 \alpha \sqrt{\frac{r(d_1 + d_2)}{|\Omega|}} + C_2 \sqrt{\frac{\log(1/\delta)}{2|\Omega|}}, \quad (7)$$

with probability at least $1 - 2\alpha$ taken jointly over the test data \mathbf{Y}^{test} , sample selection Ω , and training data $\{y_{ij}^{\text{train}}\}_{(i,j)\in\Omega}$. Note that in the bound (7), the test data \mathbf{Y}^{test} at the left hand side and training data $\{y_{ij}^{\text{train}}\}_{(i,j)\in\Omega}$ at the right hand side are independent of each other.

We write the target binary matrix $\mathbf{Y} = [y_{ij}] \in \{0,1\}^{d_1 \times d_2}$ as

$$y_{ij} = \begin{cases} y_{ij}^{\text{train}}, & (i,j) \in \Omega, \\ y_{ij}^{\text{test}}, & (i,j) \in \Omega^c. \end{cases}$$

Then, the classification error satisfies

$$MCE(\boldsymbol{Y}, \text{sign } \Theta) = \frac{1}{d_1 d_2} \left\{ \sum_{(s,s') \in \Omega^c} \mathbb{1} \left\{ y_{ss'}^{\text{test}} \neq \text{sign } \theta_{ss'} \right\} + \sum_{(s,s') \in \Omega} \mathbb{1} \left\{ y_{ss'}^{\text{test}} \neq \text{sign } \theta_{ss'} \right\} \right\}$$

$$\begin{split} & + \frac{1}{d_1 d_2} \left\{ \sum_{(s,s') \in \Omega} \mathbbm{1} \left\{ y_{ss'}^{\text{train}} \neq \text{sign } \theta_{ss'} \right\} - \sum_{(s,s') \in \Omega} \mathbbm{1} \left\{ y_{ss'}^{\text{test}} \neq \text{sign } \theta_{ss'} \right\} \right\} \\ & \leq \frac{1}{|\Omega|} \sum_{(i,j) \in \Omega} \text{hinge-loss}(y_{ij}^{\text{train}}, \theta_{ij}) + C_1 \alpha \sqrt{\frac{r(d_1 + d_2)}{|\Omega|}} + C_2' \sqrt{\frac{\log(1/\delta)}{2|\Omega|}}, \end{split}$$

with probability at least $1-3\delta$, where the last line follows from (7) and the concentration inequality for $\sum_{(s,s')\in\Omega} \left[\mathbbm{1}\left\{y_{ss'}^{\text{train}}\neq \text{sign }\theta_{ss'}\right\}-\mathbbm{1}\left\{y_{ss'}^{\text{test}}\neq \text{sign }\theta_{ss'}\right\}\right]$.

References

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