

Consistency of probability estimator

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Lemma 1. Let $\mathcal{B}_r(k) = \{\mathbf{B} \in \mathbb{R}^{d_1 \times d_2} : \text{rank}(\mathbf{B}) \leq r, \|\mathbf{B}\|_F \leq k\}$. Then $N(\epsilon, \mathcal{B}_r(k), \|\cdot\|_F) \leq \mathcal{O}\left(\left(\frac{k}{\epsilon}\right)^{r(d_1+d_2)}\right)$.

Proof. Consider $\mathbf{B} \in \mathcal{B}_r(k)$ in the form of $\mathbf{B} = \mathbf{U}\mathbf{V}^T$ where $\mathbf{U} \in \mathbb{R}^{d_1 \times r}$, $\mathbf{V} \in \mathbb{R}^{d_2 \times r}$ such that $\|\mathbf{U}\|_F \leq \sqrt{k}$ and $\|\mathbf{V}\|_F \leq \sqrt{k}$. We construct set of $\{\mathbf{U}_i\}$ and $\{\mathbf{V}_j\}$ such that for any \mathbf{U}, \mathbf{V} , there exist i, j such that $\|\mathbf{U} - \mathbf{U}_i\|_F \leq \epsilon/2\sqrt{k}$ and $\|\mathbf{V} - \mathbf{V}_j\|_F \leq \epsilon/2\sqrt{k}$. Then, epsilon balls with centers in $\{\mathbf{U}\mathbf{V}^T : \mathbf{U} \in \{\mathbf{U}_i\}, \mathbf{V} \in \{\mathbf{V}_j\}\}$ can cover $\mathcal{B}_r(k)$ because for any $\mathbf{B} = \mathbf{U}\mathbf{V}^T \in \mathcal{B}_r(k)$, we have $\mathbf{U}_i\mathbf{V}_j^T \in \{\mathbf{U}\mathbf{V}^T : \mathbf{U} \in \{\mathbf{U}_i\}, \mathbf{V} \in \{\mathbf{V}_j\}\}$ such that

$$\begin{aligned} \|\mathbf{U}\mathbf{V}^T - \mathbf{U}_i\mathbf{V}_j^T\|_F &\leq \|\mathbf{U}\mathbf{V}^T - \mathbf{U}\mathbf{V}_j^T\|_F + \|\mathbf{U}\mathbf{V}_j^T - \mathbf{U}_i\mathbf{V}_j^T\|_F \\ &\leq \|\mathbf{U}\|_F \|\mathbf{V} - \mathbf{V}_j\|_F + \|\mathbf{V}_j\|_F \|\mathbf{U} - \mathbf{U}_i\|_F \\ &\leq \sqrt{k} \frac{\epsilon}{2\sqrt{k}} + \sqrt{k} \frac{\epsilon}{2\sqrt{k}} \leq \epsilon. \end{aligned}$$

Therefore, the covering number of $N(\epsilon, \mathcal{B}_r(k), \|\cdot\|_F) \leq \mathcal{O}\left(\left(\frac{k}{\epsilon}\right)^{r(d_1+d_2)}\right)$, where $\mathcal{O}\left(\left(\frac{k}{\epsilon}\right)^{r(d_1)}\right)$ comes from $\{\mathbf{U}_i\}$ and $\mathcal{O}\left(\left(\frac{k}{\epsilon}\right)^{r(d_2)}\right)$ from $\{\mathbf{V}_j\}$. \square

Remark 1. This covering number bound is not the sharpest bound. There are several reasons for that. First, there are many representations of $\mathbf{B} = \mathbf{U}\mathbf{V}^T$ i.e. the representation is not unique for given \mathbf{B} , which means there might be redundant centers in the set. In addition, when considered matrices are full rank ($r = \min(d_1, d_2)$), this bound is slightly greater than the covering number bound of coefficient $\mathcal{B}(k)$ only with norm constraint. However, the covering bound in Lemma 1 is small enough to show benefit of low rank structure.

Proposition 1 (Thm 9.23 in [1]). Suppose the class of functions $\mathcal{F} = \{f_t : t \in T\}$ satisfies,

$$|f_s(x) - f_t(x)| \leq d(s, t)F(x),$$

for some metric d on T , some real function F on the sample space \mathcal{X} . Then, for any norm $\|\cdot\|$,

$$N_{[]} (2\epsilon\|F\|, \mathcal{F}, \|\cdot\|) \leq N(\epsilon, T, d).$$

Lemma 2. Let $\mathcal{F}_r(k) = \{f : \mathbb{R}^{d_1 \times d_2} \rightarrow \mathbb{R} : f(\mathbf{X}) = \langle \mathbf{B}, \mathbf{X} \rangle \text{ for } \mathbf{B} \in \mathcal{B}_r(k)\}$ where $\mathcal{B}_r(k) = \{\mathbf{B} \in \mathbb{R}^{d_1 \times d_2} : \text{rank}(\mathbf{B}) \leq r, \|\mathbf{B}\|_F \leq k\}$. Suppose that there exists $G > 0$ such that $\sqrt{\mathbb{E}\|\mathbf{X}\|_F^2} \leq G$. Then the bracketing number $N_{[]}(\epsilon, \mathcal{F}_r^V(k), \|\cdot\|_2)$ is bounded by

$$\log N_{[]}(\epsilon, \mathcal{F}_r^V(k), \|\cdot\|_2) \leq \mathcal{O}\left(r(d_1 + d_2) \log\left(\frac{Gk}{\epsilon}\right)\right).$$

Proof. Let $f_{\mathbf{B}}(\mathbf{X}) = \langle \mathbf{B}, \mathbf{X} \rangle$. Notice that for any $\mathbf{B}_1, \mathbf{B}_2 \in \mathcal{B}_r(k)$,

$$|f_{\mathbf{B}_1}(\mathbf{X}) - f_{\mathbf{B}_2}(\mathbf{X})| = |\langle \mathbf{B}_1 - \mathbf{B}_2, \mathbf{X} \rangle| \leq \|\mathbf{B}_1 - \mathbf{B}_2\|_F \|\mathbf{X}\|_F.$$

Applying Proposition 1 with $F(\mathbf{X}) = \|\mathbf{X}\|_F$, $d(\mathbf{B}_1, \mathbf{B}_2) = \|\mathbf{B}_1 - \mathbf{B}_2\|_F$ and $\|\cdot\| = \|\cdot\|_2$, we have

$$N_{[]}(\epsilon, \mathcal{F}_r(k), \|\cdot\|_2) \leq N\left(\frac{\epsilon}{2\|F\|_2}, \mathcal{B}_r(k), \|\cdot\|_F\right) \leq N\left(\frac{\epsilon}{2G}, \mathcal{B}_r(k), \|\cdot\|_F\right).$$

From Lemma 1, we have the covering number $N(\epsilon, \mathcal{B}_r(k), \|\cdot\|_F) \leq \mathcal{O}\left(\left(\frac{k}{\epsilon}\right)^{r(d_1+d_2)}\right)$. Note that, for functions f_ℓ and f_u ,

$$\|V^T(f_\ell, \cdot) - V^T(f_u, \cdot)\|_2^2 \leq \|f_\ell - f_u\|_2^2$$

implying that $N_{[]}(\epsilon, \mathcal{F}^V(k), \|\cdot\|_2) \leq N_{[]}(\epsilon, \mathcal{F}(k), \|\cdot\|_2) \leq N\left(\frac{\epsilon}{2G}, \mathcal{B}_r(k), \|\cdot\|_F\right) \leq \mathcal{O}\left(r(d_1 + d_2) \log\left(\frac{Gk}{\epsilon}\right)\right)$. \square

Lemma 3. Let $k > 0$ be a given constant. If $\frac{1}{Ke} > L > 0$, we have

$$\int_{\mathcal{O}(L)}^{\mathcal{O}(L^{\beta/2})} \sqrt{\log\left(\frac{k}{\omega}\right)} d\omega \leq \mathcal{O}\left(\sqrt{L^\beta \log\left(\frac{k}{\sqrt{L}^\beta}\right)}\right),$$

where $\beta = 1 \wedge \alpha$ and $\alpha > 0$.

Proof.

$$\begin{aligned} \int_{\mathcal{O}(L)}^{\mathcal{O}(L^{\beta/2})} \sqrt{\log\left(\frac{k}{\omega}\right)} - \frac{1}{2\sqrt{\log\left(\frac{k}{\omega}\right)}} d\omega &= k \left[\omega \sqrt{\log\left(\frac{1}{\omega}\right)} \right]_{\mathcal{O}(L/k)}^{\mathcal{O}(L^{\beta/2}/k)} \\ &= \mathcal{O}\left(\sqrt{L^\beta \log\left(\frac{k}{\sqrt{L}^\beta}\right)}\right) \end{aligned} \quad (1)$$

The first equality in (1) is from changing variable. Notice that

$$\int_{\mathcal{O}(L)}^{\mathcal{O}(L^{\beta/2})} \sqrt{\log\left(\frac{k}{\omega}\right)} - \frac{1}{2\sqrt{\log\left(\frac{k}{\omega}\right)}} d\omega \geq \int_{\mathcal{O}(L)}^{\mathcal{O}(L^{\beta/2})} \sqrt{\log\left(\frac{k}{\omega}\right)} - \mathcal{O}(1) d\omega, \quad (2)$$

from the condition on L . Combining Equation (1) and Equation (2) completes the proof. \square

Lemma 4. $\sqrt{\frac{d}{L^{2-\beta}} \log\left(\frac{k}{\sqrt{L}^\beta}\right)} \leq \sqrt{n}$ holds if $L \leq \frac{\log(n/d)^{1/(2-\beta)} + 2\log(k)}{(n/d)^{1/(2-\beta)}}$ where $\beta \leq 1$.

Proof. Suppose $L \leq \frac{\log(n/d)^{1/(2-\beta)} + 2\log(k)}{(n/d)^{1/(2-\beta)}}$. By plugging in, we have

$$\begin{aligned} \sqrt{\frac{d}{L^{2-\beta}} \log\left(\frac{k}{\sqrt{L}^\beta}\right)} &\leq \sqrt{\frac{n}{(2-\beta) \log((n/d)^{1/(2-\beta)} k^2)} \left(\frac{\log((n/d)^{1/(2-\beta)} k^2) - \log \log((n/d)^{1/(2-\beta)} k^2)}{2} \right)} \\ &\leq \sqrt{n}. \end{aligned}$$

\square

Theorem 0.1. Assume that

A.1 For some positive sequence such that $s_n \rightarrow 0$ as $n \rightarrow \infty$, there exists $f_\pi^* \in \mathcal{F}_r(M)$ such that $e_V(f_\pi^*, \bar{f}_\pi) \leq s_n$. 0<=alpha<=1

A.2 There exist constant $0 \leq \alpha < \infty$, $a_1 > 0$ such that, for any sufficiently small $\delta > 0$.

$$\sup_{\{f \in \mathcal{F}: e_{VT}(f, \bar{f}_\pi) \leq \delta\}} \| \text{sign}(f) - \text{sign}(\bar{f}_\pi) \|_1 \leq a_1 \delta^\alpha.$$

alpha <=1 <== sign difference <= hinge-loss difference (\delta)

A.3 Considered feature space is uniformly bounded such that there exists $0 < G < \infty$ satisfying $\sqrt{\mathbb{E} \|\mathbf{X}\|_F^2} \leq G$

Then, for the estimator \hat{p} obtained from our algorithm with function class $\mathcal{F}_r(M)$, there exists a constant a_2 such that

E{...}: expectation is taken with respect to test data.

P{...}: probability is taken with respect to training data.

$$\mathbb{P} \left\{ \|\hat{p} - p\|_1 \geq \frac{1}{2m} + \frac{a_1}{2} (m+1) \delta_n^{2\alpha} \right\} \leq 15 \exp\{-a_2 n (\lambda J_\pi^*)^{2-\alpha \wedge 1}\}, \quad (3)$$

provided that $\lambda^{-1} \geq \max\left(\frac{MJ_\pi^*}{2\delta_n^2}, \frac{4J_\pi^*}{\delta_n^2}\right)$ where $J_\pi^* = \max(J(f_\pi^*), 1)$, $\delta_n = \max\left(\mathcal{O}\left(\frac{\log(n/r(d_1+d_2))^{1/(2-\beta)} + 2\log(GM)}{(n/r(d_1+d_2))^{1/(2-\beta)}}\right), s_n\right)$ and $\beta = \alpha \wedge 1$.

Remark 2. From the definition of δ_n , we can check the larger α we obtain, the sharper bound we can have. In addition, the sharpest δ_n we can obtain is $\mathcal{O}\left(\frac{\log n}{n}\right)$ when $\alpha \geq 1$.

Proof. We apply Theorem 3 in [2] to our case.

The second condition of the assumption is

$$\sup_{\{f \in \mathcal{F}: e_{VT}(f, \bar{f}_\pi) \leq \delta\}} \text{var}\{V(f, \mathbf{X}, y) - V(\bar{f}_\pi, \mathbf{X}, y)\} \leq a_2 \delta^\beta.$$

Notice that

$$\begin{aligned} \text{var}\{V^T(f, \mathbf{X}, y) - V(\bar{f}_\pi, \mathbf{X}, y)\} &\leq \mathbb{E}|V^T(f, \mathbf{X}, y) - V(\bar{f}_\pi, \mathbf{X}, y)|^2 \\ &\leq T \mathbb{E}|V^T(f, \mathbf{X}, y) - V(\bar{f}_\pi, \mathbf{X}, y)| \\ &= T(\lambda_1 + \lambda_2). \end{aligned}$$

where

$$\begin{aligned} \lambda_1 &= \mathbb{E}|S(y)(1 - \text{sign}(yf(\mathbf{X})) - V(\bar{f}_\pi, \mathbf{X}, y)| = \mathbb{E}|S(y)| |\text{sign}(f) - \text{sign}(\bar{f}_\pi)| \\ &\leq \|\text{sign}(f) - \text{sign}(\bar{f}_\pi)\|_1 \leq a_1 \delta^\alpha \quad \text{from A.2.} \end{aligned}$$

and

$$\begin{aligned} \lambda_2 &= \mathbb{E}[V^T(f, \mathbf{X}, y) - S(y)(1 - \text{sign}(yf(\mathbf{X})))] \\ &\leq e_{VT}(f, \bar{f}_\pi) + \mathbb{E}\{V(\bar{f}_\pi, \mathbf{X}, y) - S(y)(1 - \text{sign}(yf(\mathbf{X}))\} \\ &\leq 2e_{VT}(f, \bar{f}_\pi) \leq 2\delta \end{aligned}$$

Therefore, β in [2] can be replaced by $1 \wedge \alpha$.

Now we check Assumption 3 in [2]. From Lemma 2, we have

$$H_B(\epsilon, \mathcal{F}^V(k)) \leq \mathcal{O} \left(r(d_1 + d_2) \log \left(\frac{Gk}{\epsilon} \right) \right).$$

Therefore, we have the following equation from Lemma 3.

$$\phi(\epsilon, k) \approx \int_{\mathcal{O}(L)}^{\mathcal{O}(L^{\beta/2})} \sqrt{r(d_1 + d_2) \log \left(\frac{kG}{\omega} \right)} d\omega / L \lesssim \mathcal{O} \left(\sqrt{r(d_1 + d_2)} \left(\log \left(\frac{kG}{\sqrt{L}^\beta} \right) / L^{2-\beta} \right)^{1/2} \right),$$

where $L = \min\{\epsilon^2 + \lambda(k/2 - 1)J_\pi^*, 1\}$. Solving Assumption 3 in [2] gives us $\epsilon_n^2 = \mathcal{O} \left(\frac{\log(n/r(d_1 + d_2))^{1/(2-\beta)} + 2\log(GM)}{(n/r(d_1 + d_2))^{1/(2-\beta)}} \right)$ by Lemma 4 when $\epsilon_n^2 \geq \frac{\lambda M J_\pi^*}{2}$. Plugging each variable into Theorem 3 proves the theorem. \square

Remark 3. We show that the Assumption 2 is satisfied when there exists $\eta > 0$ such that $|\mathbb{P}(y = 1|\mathbf{X}) - \pi| \geq \eta$ almost surely with respect to distribution \mathbf{X} . Smooth parameter is $a_1 = \frac{1}{\eta}$ and $\alpha = 1$ in this case.

Proof.

$$\begin{aligned} e_{VT}(f, \bar{f}_\pi) &= \mathbb{E} [S(y)L(yf(\mathbf{X})) \wedge T - S(y)L(y\bar{f}_\pi(\mathbf{X}))] \\ &\geq \mathbb{E} [S(y)(1 - \text{sign}(yf(\mathbf{X}))) - S(y)(1 - \text{sign}(y\bar{f}_\pi(\mathbf{X})))] \\ &= \mathbb{E} [yS(y) (\text{sign}(\bar{f}_\pi) - \text{sign}(f))] \\ &= \mathbb{E} [\mathbb{E}(yS(y)|\mathbf{X}) (\text{sign}(\bar{f}_\pi) - \text{sign}(f))] \\ &= \mathbb{E} [|\mathbb{P}(y = 1|\mathbf{X}) - \pi| |\text{sign}(\bar{f}_\pi) - \text{sign}(f)|] \\ &\geq \eta \mathbb{E} |\text{sign}(\bar{f}_\pi) - \text{sign}(f)| = \eta \|\text{sign}(\bar{f}_\pi) - \text{sign}(f)\|_1. \end{aligned}$$

\square

The main part of the proof is the following inequality

$$\mathbb{E} [|f_\pi| |\text{sign}(f) - \text{sign}(\bar{f}_\pi)|] \geq \eta \mathbb{E} [|\text{sign}(f) - \text{sign}(\bar{f}_\pi)|]. \quad (4)$$

Therefore, we can replace the condition by

$$\text{For a given } \pi, \text{ there exists } \eta > 0 \text{ such that } \mathbb{E} [|f_\pi| \mathbf{1}_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}}] \geq \eta \mathbb{E} [\mathbf{1}_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}}].$$

Example 1. When ground truth $p(\mathbf{X})$ is step function such that $p(\mathbf{X}) = \sum_{k=1}^K c_k \mathbf{1}_{\{\mathbf{X} \in A_k\}}$, then $\eta = \min_k \{|c_k - \pi|\}$.

Example 2. Assume that ground truth $p(x) = x$ and x is a random variable from $\text{Unif}(0, 1)$. If considered function class is a set of functions with only one sign change, we show Assumption 2 holds with $\alpha = 1/2, a_1 = 2$.

Proof. We check two terms of Equation (4) in this case. If $f^{-1}(0) = \pi$, then the conclusion trivially holds. So we consider $f^{-1}(0) \neq \pi$ case. Let $f^{-1}(0) = \pi'$. Notice that right side of Equation (4) is

$$\mathbb{E}|\text{sign}(f) - \text{sign}(\bar{f}_\pi)| = 2|\pi - \pi'|.$$

The left side of the equation is

$$\mathbb{E} [|f_\pi| |\text{sign}(f) - \text{sign}(\bar{f}_\pi)|] = \mathbb{E} [2|x - \pi| \mathbb{1}_{\{\pi \wedge \pi' < x < \pi \vee \pi'\}}] = \int_{\pi \wedge \pi'}^{\pi \vee \pi'} 2|x - \pi| dx = |\pi - \pi'|^2.$$

Therefore, $e_{VT}(f, \bar{f}_\pi) \geq \mathbb{E} [|f_\pi| |\text{sign}(f) - \text{sign}(\bar{f}_\pi)|] = \frac{1}{4} (\mathbb{E} [|\text{sign}(f) - \text{sign}(\bar{f}_\pi)|])^2$, which implies $\alpha = 1/2, a_1 = 2$

□

Remark 4. In Example 1, the order of ground truth function is 0 and we obtain the smooth parameter $\alpha = 1$. In Example 2, the order of ground truth function is 1 and we have the smooth parameter $\alpha = \frac{1}{2}$. We can conjecture that the smooth parameter $\alpha = \frac{1}{\text{order}(\bar{f}_\pi)+1}$ because if we consider each term of the condition (4), the left side is calculated as

$$L \stackrel{\text{def}}{=} \mathbb{E} \left[|f_\pi| \mathbb{1}_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}} \right] = \int_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}} |f_\pi| dF(x)$$

where $F(x)$ is distribution of x . The right side is

$$R \stackrel{\text{def}}{=} \mathbb{E} \left[\mathbb{1}_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}} \right] = \int_{\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}} 1 dF(x)$$

If we consider the simple case where $\{\text{sign}(f) \neq \text{sign}(\bar{f}_\pi)\}$ is an interval, we can easily see that $L = \mathcal{O} \left((R)^{\text{order}(\bar{f}_\pi)+1} \right)$ which explains the conjecture. Therefore, Assumption 2 consider features of ground truth probability.

Remark 5. *A.1 measures accuracy of approximation to the ground truth function from considered function class \mathcal{F}_r . A.2 considers the complexity of ground truth function as in Remark 4. A.3 is related to the covering number which measures the complexity of considered function class \mathcal{F}_r .*

Remark 6. Our theorem shows that a higher sample complexity is needed when the ground truth function has a high level of complexity or the candidate function class is either too small or too large. This reflect the trade off between A.1 and A.3.

Remark 7. We can think of our estimation method consisting of two parts.

S.1 Approximation of the target probability function

$$\left\| p(\mathbf{X}) - \sum_{i=1}^m \frac{1}{m} \mathbb{1}_{\{\mathbf{X}: p(\mathbf{X}) < \frac{i}{m}\}} \right\|_1. \quad (5)$$

S.2 For each i , Estimation of sublevel set

$$\left\| \sum_{i=1}^m \frac{1}{m} \mathbb{1}_{\{\mathbf{X}: p(\mathbf{X}) < \frac{i}{m}\}} - \sum_{i=1}^m \frac{1}{m} \mathbb{1}_{\{\mathbf{X}: \text{sign}[\hat{f}_{\pi_i}(\mathbf{X})] = -1\}} \right\|_1. \quad (6)$$

Those estimation procedures are reflected in Theorem 0.1. In the first step, the maximum error of the approximation is $\frac{1}{2m}$ at given \mathbf{X} . Therefore, we have the bound $\frac{1}{2m}$ for Equation (5). In the second step, two functions are m -step functions. Let $f(\mathbf{X}) = \sum_{i=1}^m \frac{1}{m} \mathbb{1}_{\{\mathbf{X}: p(\mathbf{X}) < \frac{i}{m}\}}$ and $g(\mathbf{X}) = \sum_{i=1}^m \frac{1}{m} \mathbb{1}_{\{\mathbf{X}: \text{sign}[\hat{f}_{\pi_i}(\mathbf{X})] = -1\}}$. Define $A_i = \{\mathbf{X} : f(\mathbf{X}) = \frac{i}{m}\} - \{\mathbf{X} : g(\mathbf{X}) = \frac{i}{m}\}$. Then total measure at which f and g disagree is at most $m \max_i \mathbb{P}(A_i)$. Therefore, we have bound $m \max_i \mathbb{P}(A_i)$ bound for Equation (6). This shows why we have two terms $\frac{1}{2m}$ and $\frac{a_1}{2}(m+1)\delta_n^{2\alpha}$ in Equation (3).

References

- [1] Michael R Kosorok. *Introduction to empirical processes and semiparametric inference*. Springer Science & Business Media, 2007.
- [2] Junhui Wang, Xiaotong Shen, and Yufeng Liu. Probability estimation for large-margin classifiers. *Biometrika*, 95(1):149–167, March 2008.