Report on Single Index Model

Ergan Shang

USTC

June 7, 2022

Overview

- Single Index Model
 - Under Gaussian Space
 - Least Squares on Monotone Functions
 - Score Estimation on Monotone Functions
- Sample Complexity of One-Hidden-Layer Neural Networks
- What am I thinking about

Overview

- Single Index Model
 - Under Gaussian Space
 - Least Squares on Monotone Functions
 - Score Estimation on Monotone Functions
- Sample Complexity of One-Hidden-Layer Neural Networks
- What am I thinking about

Background and Introduction

Suppose our link function has the form

$$f(\mathbf{x}) = g(\langle \mathbf{u}^*, \mathbf{x} \rangle) = \sum_{\ell=0}^{\infty} a_{\ell}^* H_{\ell}(\langle \mathbf{x}, \mathbf{u}^* \rangle)$$

with the function class defined as $\mathcal{F} = \{g : \mathbb{R} \to \mathbb{R} : g(z) = \sum_{i=0}^{L} a_i H_i(z)\}.$

Associated Population Loss

$$R_L(\boldsymbol{u}) = \min_{\boldsymbol{a} \in \mathbb{R}^{L+1}} \mathbb{E}\left[\left(y - \sum_{\ell=0}^{L} a_{\ell} H_{\ell}(\langle \boldsymbol{u}, \boldsymbol{x} \rangle)\right)^2\right] = \sigma^2 + \sum_{\ell=1}^{L} a_{\ell}^{*2} \left(1 - \langle \boldsymbol{u}, \boldsymbol{u}^* \rangle^{2\ell}\right)$$

$$F_{\ell}(\mathbf{u}) = \mathbb{E}[f(\mathbf{x})H_{\ell}(\langle \mathbf{u}, \mathbf{x} \rangle)] = a_{\ell}^* \langle \mathbf{u}, \mathbf{u}^* \rangle^{\ell}$$

Therefore, we can define the goodness-of-fit statistic as

$$\hat{F}_{\ell}(\boldsymbol{u}) = \frac{1}{n} \sum_{i=1}^{n} y_i H_{\ell}(\langle \boldsymbol{x}_i, \boldsymbol{u} \rangle)$$
 $\hat{\boldsymbol{u}} = arg \max_{\boldsymbol{u} \in \mathbb{S}^{p-1}} \hat{F}_{\ell}(\boldsymbol{u})$ for some value ℓ

Ergan Shang (USTC) Single Index Model June 7, 2022

3/28

Concentration Results

In the algorithms to come, we have to analyze $\nabla \hat{F}_{\ell}(\boldsymbol{u}; data) = \frac{1}{n} \sum_{i=1}^{n} \sqrt{\ell} y_{i} H_{\ell-1}(\langle \boldsymbol{x}_{i}, \boldsymbol{u} \rangle) \boldsymbol{x}_{i}$ which can be further decomposed into the form like $\propto \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{x}_{i}) H_{\ell}(\langle \boldsymbol{x}_{i}, \boldsymbol{u} \rangle) \boldsymbol{x}_{i}$ and $\frac{1}{n} \sum_{i=1}^{n} \epsilon_{i} H_{\ell}(\langle \boldsymbol{u}, \boldsymbol{x}_{i} \rangle) \boldsymbol{x}_{i}$

Main Concentration Results

With probability at least $1 - 2\delta - \frac{4}{n}$,

$$\left\|\frac{1}{n}\sum_{i=1}^{n}y_{i}H_{\ell}(\langle \mathbf{x}_{i},\mathbf{u}\rangle)\mathbf{x}_{i}-\mathbb{E}[yH_{\ell}(\langle \mathbf{u},\mathbf{x}\rangle)\mathbf{x}]\right\|$$

$$\leq 100(\|h\|_{\infty} + 4\sigma)2^{\ell}\sqrt{\frac{\textit{max}(\textit{p}, \textit{log}\frac{1}{\delta})(\textit{logn})^{\ell}}{\textit{n}}}$$

Assumptions and a good ℓ

Let $Z \sim \mathcal{N}(0,1)$

- $\hspace{-0.8cm} \bullet \hspace{-0.8cm} \hspace{-0.8cm} \text{(Normalization)} \,\, \mathbb{E}[g^2(z)] = 1 \,\, \text{i.e.} \,\, 1 = \sum_{\ell=1}^{\infty} a_{\ell}^{*2}$
- ② (Smoothness) $\mathbb{E}\left[\left(\frac{d^2g(z)}{dz^2}\right)\right] \leq R^2$ i.e. $\sum_{i=2}^{\infty}i(i-1)a_i^{*2} \leq R^2$
- $\ \, \textbf{(Bounded Link Function)} \,\, \|\textbf{\textit{g}}\| < \infty$

A good $\ell_{\#}$

There exists a $\ell_{\#} \leq \frac{2R^2}{\mu}$ such that $\ell_{\#} |a_{\ell_{\#}}^*|^2 \geq \frac{\mu^2}{4R^2}$

Algorithms and Conclusions

Algorithm 1 Estimate-Index-Vector-From-Harmonic(S, ℓ)

input Data $S = \{x_i, y_i\} \subset \mathbb{R}^p \times \mathbb{R}$; Degree of Harmonic $\ell \in \mathbb{N}$ **output** Index Estimate $\hat{\boldsymbol{u}}_{\ell} \in \mathbb{R}^{p}$

1:Split S into two equal parts:

$$S_1 = \{(\mathbf{x}_i, y_i), i = 1, 2, \cdots, \frac{n}{2}\}, S_2 = \{(\mathbf{x}_i, y_i), i = \frac{n}{2} + 1, \cdots, n\}$$

2:Define $\hat{F}_{\ell}(\mathbf{u}; S_1) = \frac{2}{n} \sum_{i=1}^{\frac{n}{2}} y_i H_{\ell}(\langle \mathbf{x}_i, \mathbf{u} \rangle)$ and

2:Define
$$\hat{F}_{\ell}(\boldsymbol{u}; S_1) = \frac{2}{n} \sum_{i=1}^{\frac{n}{2}} y_i H_{\ell}(\langle \boldsymbol{x}_i, \boldsymbol{u} \rangle)$$
 and

$$\hat{F}_{\ell}(\boldsymbol{u}; S_2) = \frac{2}{n} \sum_{i=\frac{n}{2}+1}^{n} y_i H_{\ell}(\langle \boldsymbol{x}_i, \boldsymbol{u} \rangle)$$

3:Random Initialization: $\mathbf{u}_0 \sim Uniform(\mathbb{S}^{p-1})$

4:Compute two steps of iterative process: $u_1 = \frac{\nabla F_{\ell}(u_0; S_1)}{\|\nabla F_{\ell}(u_0; S_1)\|}$ and

$$\mathbf{u}_2 = \frac{\nabla \hat{F}_{\ell}(\mathbf{u}_1; S_2)}{\|\nabla \hat{F}_{\ell}(\mathbf{u}_1; S_2)\|}$$

5:return $\hat{\boldsymbol{u}}_{\ell} := \boldsymbol{u}_2$

Algorithms and Conclusions

Algorithm 2 Learn-single-index-Model $(S, R^2, \mu, \sigma^2, ||f||_{\infty}, \delta)$

Input Data: $S = \{(x_i, y_i)\}_{i=1}^n \subset \mathbb{R}^p \times \mathbb{R};$

Output Index Estimate $\hat{\boldsymbol{u}} \in \mathbb{R}^p$

1:Split S into S_{train} and S_{test} such that

$$m := |S_{test}| = 256 \cdot 2^{\frac{4R^2}{\mu}} R^4 (\sigma^2 + ||f||_{\infty}^2) / (\delta \mu^3)$$

2:Let $L = \frac{2R^2}{4}$

3:Let $\hat{u}_{\ell} := \text{Estimate-Index-Vector-From-Harmonic}(S_{train}, \ell)$ for each

$$\ell \in \{1, 2, \cdots, L\}$$

4:Compute the good-of-fitness $T_{\ell} = \sum_{i \in S_{test}} y_i H_{\ell}(\langle \mathbf{x}_i, \hat{\mathbf{u}}_{\ell} \rangle) / m$ for each $\ell \in \{1, 2, \cdots, L\}.$

5: Let
$$\ell_{host} := arg \max_{\ell \in \mathcal{U}} |T|$$

5:Let $\ell_{best} := arg \max_{\ell \in [I]} |T_{\ell}|$.

6: **return** $\hat{\boldsymbol{u}} := \boldsymbol{u}_{\ell_{hest}}$.

Algorithms and Conclusions

Convergence Rate

Given any $\epsilon, \delta \in (0,1)$; with probability at least $1-\frac{4R^2}{\mu}e^{-\frac{P}{32}}-\frac{12R^2}{\mu}\delta-\frac{16R^2}{n\mu}$, the estimate returned by Algorithm 2, $\hat{\pmb{u}}$ satisfies

$$|\langle \textbf{\textit{u}}^*, \hat{\textbf{\textit{u}}} \rangle| \geq 1 - \frac{3200 \cdot 2^{\frac{4R^2}{\mu}} (\|\textbf{\textit{f}}\|_{\infty} + 4\sigma) R^4}{\mu^2 \sqrt{\mu}} \sqrt{\frac{\max(\textbf{\textit{p}}, \log(\frac{1}{\delta})) (\log n)^{\frac{2R^2}{\mu}}}{n}}$$

provided that n satisfies

$$n \geq \frac{1024 \cdot 10^4 (\|f\|_{\infty} + 4\sigma)^2 R^4}{\mu^3} \frac{2^{\frac{4R^2}{\mu}}}{\delta^{\frac{4R^2}{\mu} - 2}} max(p, log(\frac{1}{\delta})) p^{\frac{2R^2}{\mu} - 1} (logn)^{\frac{2R^2}{\mu}}$$

◆ロト ◆御 ト ◆ 恵 ト ◆ 恵 ・ 夕 Q (*)

8/28

Ergan Shang (USTC) Single Index Model June 7, 2022

Least Squares under Monotonicity

Suppose the link function is monotone and data are not from Guassian space, we have the problem

$$h_n(\psi, \alpha) = \sum_{i=1}^n (Y_i - \psi(\alpha^T \mathbf{X}_i))^2 \quad (\psi, \alpha) \in \mathcal{M} \times \mathcal{S}_{d-1}$$

where ${\cal M}$ denotes function class of non-decreasing functions. Using the knowledge of isotonic regression, we define

$$n_k = \sum_{i=1}^n \mathbb{I}\{\alpha^T X_i = Z_k\}, t_k = \frac{1}{n_k} \sum_{i=1}^n Y_i \mathbb{I}\{\alpha^T X_i = Z_k\}, \text{ we have } h_n(\psi, \alpha) = \sum_{k=1}^m n_k (t_k - \psi(Z_k))^2 + \sum_{i=1}^n Y_i^2 - \sum_{k=1}^m n_k t_k^2.$$
 Thus, we set $\eta_k = \psi(Z_k)$ leading to

$$min \sum_{k=1}^{m} n_k (t_k - \eta_k)^2 \text{ over } \eta_1 \leq \cdots \leq \eta_m$$

◆ロト ◆母ト ◆差ト ◆差ト 差 めなぐ

Solution for Least Squares

Let P^X be the set of all permutations π on $\{1, \cdots, m\}$ such that $\exists \alpha \in \mathcal{S}_{d-1}$ that linearly induces π in the sense that $\alpha^T x_{\pi(1)} < \cdots < \alpha^T x_{\pi(m)}$ which is available for $\alpha \in \mathcal{S}^X = \{\alpha \in \mathcal{S}_{d-1} : \alpha^T \mathbf{X}_i \neq \alpha^T \mathbf{X}_j \text{ for all } i \neq j \text{ such that } \mathbf{X}_i \neq \mathbf{X}_j\}$

Definition

$$\tilde{n}_k = \sum_{i=1}^n \mathbb{I}\{\boldsymbol{X}_i = \boldsymbol{x}_k\}$$
 $\tilde{y}_k = \frac{1}{\tilde{n}_k} \sum_{i=1}^n Y_i \mathbb{I}\{\boldsymbol{X}_i = \boldsymbol{x}_k\}$

We denote by $d_1^{\pi} \leq \cdots \leq d_m^{\pi}$ the left derivatives of the greatest convex minorant of the cumulative sum diagram define by the set of points

$$\left\{(0,0), \left(\sum_{j=1}^{k} \tilde{n}_{\pi(j)}, \sum_{j=1}^{k} \tilde{n}_{\pi(j)} \tilde{y}_{\pi(j)}\right), k = 1, \cdots, m\right\}$$

10 / 28

Ergan Shang (USTC) Single Index Model June 7, 2022

Solutions for Least Squares

Theoretical Solution

The infimum of $(\psi, \alpha) \mapsto h_n(\psi, \alpha)$ over $\mathcal{M} \times \mathcal{S}_{d-1}$ is achieved. Moreover if $(\hat{\psi}_n, \hat{\alpha}_n)$ satisfies the following conditions, then it is a minimzer:

- $\hat{\alpha}_n \in S^X$ linearly induces $\hat{\pi}_n$ that minimizes $\pi \mapsto \tilde{h}_n(\pi) = \sum_{k=1}^m \tilde{n}_{\pi(k)} (\tilde{y}_{\pi(k)} d_k^{\pi})^2$ over P^X
- $\hat{\psi}_n$ is monotone ,non-decreasing with $\hat{\psi}_n(\hat{\alpha}^T \mathbf{x}_{\hat{\pi}_{n(k)}}) = d_k^{\hat{\pi}_n}$

11/28

Ergan Shang (USTC) Single Index Model June 7, 2022

Solutions for Least Squares

Algorithm: Stochastic Search: Find optimal $(\hat{\alpha}_n, \hat{\psi}_n)$

- 1:Choose the total number(maximal iterations) N of stochastic searches to perform and set k=1
- 2:Let $Z_k \sim \mathcal{N}(0, I_d)$ and $\alpha = \frac{Z_k}{\|Z_L\|}$ which is uniform on the sphere
- 3:Compute distinct values $t_1 \leq \cdots \leq t_L$ of $\alpha_{\iota}^T \mathbf{X}_i$ for $i \in [n]$ and also $n_{\ell} = \sum_{i=1}^{n} \mathbb{I}\{\alpha_{k}^{T} \mathbf{X}_{i} = t_{\ell}\}, y_{\ell} = \frac{1}{n} \sum_{i=1}^{n} Y_{i} \mathbb{I}\{\alpha_{k}^{T} \mathbf{X}_{i} = t_{\ell}\}$
- 4:Compute $d_1 < \cdots < d_l$, the left derivatives of the greatest convex minorant of

$$\left\{(0,0),\left(\sum_{j=1}^{\ell}n_j,\sum_{j=1}^{\ell}n_jy_j\right),\ell=1,\cdots,L\right\}$$
 using **PAVA**

- 5:Compute $A_k := \sum_{\ell=1}^L n_\ell (y_\ell d_\ell)^2$ and set k = k+1 and return to 2 when k < N
- 6:Compute \hat{k} that minimizes A_k over $k \in [N]$
- **Return:** $(\hat{\alpha}_n, \hat{\psi}_n) = (\alpha_{\hat{\iota}}, \psi_{\hat{\iota}})$ where $\psi_{\hat{\iota}}$ is piecewise constant: $\psi_{\hat{\iota}}(t_\ell) = d_\ell$

Ergan Shang (USTC) Single Index Model June 7, 2022 12/28

Entropy Results

Observing that $\frac{1}{n}\sum_{i=1}^{n}(Y_{i}-g(\boldsymbol{X}_{i}))^{2}\propto-\frac{1}{n}\sum_{i=1}^{n}\left(Y_{i}g(\boldsymbol{X}_{i})-\frac{g^{2}(\boldsymbol{X}_{i})}{2}\right)$ and \hat{g}_{n} maximizes $\mathbb{M}_{n}g:=\frac{1}{n}\left(Y_{i}g(\boldsymbol{X}_{i})-\frac{g^{2}(\boldsymbol{X}_{i})}{2}\right)$ of form $g(\boldsymbol{x})=\psi(\alpha^{T}\boldsymbol{x})$. Similarly we define $\mathbb{M}g:=\int_{\mathcal{X}\times\mathbb{R}}(yg(\boldsymbol{x})-\frac{1}{2}g^{2}(\boldsymbol{x}))d\mathbb{P}(\boldsymbol{x},y), \mathbb{Q}g:=\int gd\mathbb{Q}$. Also, we denote $\hat{f}_{n}(\boldsymbol{x},y)=y\hat{g}_{n}(\boldsymbol{x})-\frac{1}{2}\hat{g}_{n}^{2}(\boldsymbol{x}), f(\boldsymbol{x},y)=yg(\boldsymbol{x})-\frac{1}{2}g^{2}(\boldsymbol{x})$ and $\mathbb{M}_{n}g=\mathbb{P}_{n}f$ where \mathbb{P}_{n} denotes empirical distribution.

Lemma 3.4.3

Let \mathcal{F} be a class of measurable functions such that $\|f\|_{\mathbb{P}.B} = \left(2\mathbb{P}(e^{|f|}-1-|f|)\right)^{\frac{1}{2}} \leq \delta$ for every $f \in \mathcal{F}$. Then

$$\mathbb{E}[\|G_n\|_{\mathcal{F}}] \lesssim J(\delta, \mathcal{F}, \|\cdot\|_{\mathbb{P}, \mathcal{B}}) \left(1 + \frac{J(\delta, \mathcal{F}, \|\cdot\|_{\mathbb{P}, \mathcal{B}})}{\delta^2 \sqrt{n}}\right) \tag{1}$$

where $J(\eta) = \int_0^{\eta} \sqrt{1 + H_B(\epsilon, \mathcal{F}, \|\cdot\|_{B,\mathbb{P}})} d\epsilon$ and $G_n = \sqrt{n}(\mathbb{P}_n - \mathbb{P}), \|G_n\|_{\mathcal{F}} = \sup_{g \in \mathcal{F}} |G_n g|$ and \mathbb{P}_n denotes the empirical process.

Entropy Results

Lemma 3.4.2

Let $\mathcal F$ be a class of measurable functions such that $\|f\|_{\mathbb P} \leq \delta$ and $\|f\|_{\infty} \leq M$ for every f in $\mathcal F$. Then

$$\mathbb{E}_{\mathbb{P}}[\|G_n\|_{\mathcal{F}}] \lesssim J_n(\delta, \mathcal{F}, \|\cdot\|_{\mathbb{P}}) \left(1 + \frac{J_n(\delta, \mathcal{F}, \|\cdot\|_{\mathbb{P}})}{\sqrt{n}\delta^2}M\right)$$

where
$$G_n = \sqrt{n}(\mathbb{P}_n - \mathbb{P})$$
 and $J_n(\delta, \mathcal{F}, \|\cdot\|) = \int_0^\delta \sqrt{1 + H_B(\epsilon, \mathcal{F}, \|\cdot\|)} d\epsilon$.

Before using Lemma 3.4.2 and Lemma 3.4.3, there is a useful little trick: whenever we have a bound for $H_B \leq \frac{c}{\epsilon}$, we will write

$$J_n(e)=\int_0^e \left(1+rac{\mathcal{C}}{\epsilon}
ight)^{rac{1}{2}} \leq e+2\sqrt{c\epsilon},$$
 thus bounds for $\mathbb{E}[\|\mathit{G}_n\|]$

$$H_B \Rightarrow J_n \Rightarrow \mathbb{E} \stackrel{Markov}{\Rightarrow} \text{consistency}$$

◆ロト ◆問ト ◆恵ト ◆恵ト ・恵 ・ 夕久で

Theorem for deriving Convergence Rates

Theorem 3.2.5

If for every θ in a neighborhood of θ_0

$$\mathbb{M}(\theta) - \mathbb{M}(\theta_0) \lesssim -d^2(\theta, \theta_0)$$

Suppose that, for every n and sufficiently small δ , the centered process $\mathbb{M}_n - \mathbb{M}$ satisfies

$$\mathbb{E}\left[\sup_{d(\theta,\theta_0)<\delta}|(\mathbb{M}_n-\mathbb{M})(\theta)-(\mathbb{M}_n-\mathbb{M})(\theta_0)|\right]\lesssim \frac{\phi_n(\delta)}{\sqrt{n}}$$

for functions $\phi_n(\delta)$ such that $\delta \mapsto \phi_n(\delta)/\delta^{\alpha}$ is decreasing for some $\alpha < 2$. Let $r_n^2 \phi_n\left(\frac{1}{r_n}\right) \leq \sqrt{n}$ hold and $\mathbb{M}_n(\hat{\theta}_n) \geq \mathbb{M}_n(\theta_0) - O_p(r_n^{-2})$. Then

$$r_n d(\hat{\theta}_n, \theta_0) = O_p(1) \tag{2}$$

Entropy for function class

Two useful conclusions

Under the assumption: $\exists a_0 > 0, M > 0$ such that $\forall s \geq 2, x \in \mathcal{X}, \int |y|^s \mathbb{P}_x(y) \leq a_0 s! M^{s-2}$, we have

$$\sup_{\boldsymbol{x}\in\mathcal{X}}|\hat{g}_n(\boldsymbol{x})|\leq O_p(\log n)\qquad D(\hat{g}_n,g_0)=O_p(n^{-\frac{1}{3}}(\log n)^{\frac{5}{3}})$$

where
$$D(g,g_0)=\left(\int_{\mathcal{X}}(g_0(extbf{\emph{x}})-g(extbf{\emph{x}}))^2d\mathbb{Q}(extbf{\emph{x}})\right)^{rac{1}{2}}$$

By setting K = Clogn, $v = Cn^{-\frac{1}{3}}(logn)^2$ with proper constant C. We derive entropy bounds for these function class:

- $G_{\kappa} = \{ g(\mathbf{x}) = \psi(\alpha^T \mathbf{x}) : \alpha \in \mathcal{S}_{d-1}, \psi \in \mathcal{M}_{\kappa} \}$ $\mathcal{F}_{K} = \{ f(\mathbf{x}, y) = yg(\mathbf{x}) - \frac{1}{2}g^{2}(\mathbf{x}) : g \in G_{K} \}$
- $G_{\kappa_{\nu}} = \{ g \in G_{\kappa} : D(g, g_0) \leq \nu \}$ $\mathcal{F}_{K_V} = \left\{ f(\mathbf{x}, y) = yg(\mathbf{x}) - \frac{1}{2}g^2(\mathbf{x}) : g \in G_{K_V} \right\}$

16 / 28

Main Results: $O_p(n^{-\frac{1}{3}})$

With the entropy bounds at hand, combining with 15, we have

Consistency and Convergence

- $\left(\int_{\mathcal{X}} (\hat{g}_n(\mathbf{x}) g_0(\mathbf{x}))^2 d\mathbb{Q}(\mathbf{x})\right)^{\frac{1}{2}} = O_p(n^{-\frac{1}{3}})$
- $\hat{\alpha}_n = \alpha_0 + o_p(1)$, particularly, $\|\hat{\alpha}_n \alpha_0\| = O_p(n^{-\frac{1}{3}})$
- For all fixed continuity points t of ψ_0 in the interior of $C_{\alpha_0} = \{\alpha_0^T \mathbf{X} : \mathbf{X} \in \mathcal{X}\}, \ \psi_n(t) \overset{P}{\to} \psi_0(t); \ \text{if} \ \psi_0 \ \text{is continuous, then} \ \sup_{t \in I} |\hat{\psi}_n(t) \psi_0(t)| = o_p(1)$
- If moreover, ψ_0 has a derivative bounded from above on C_{α_0} , then $\left(\int_{\underline{c}+v_n}^{\overline{c}-v_n}(\hat{\psi}_n(t)-\psi_0(t))^2dt\right)^{\frac{1}{2}}=O_p\left(n^{-\frac{1}{3}}\right) \text{ for all sequence } v_n \text{ such that } n^{\frac{1}{3}}v_n\to\infty \text{ and } \underline{c}+v_n<\overline{c}-v_n \text{ with } \overline{c}=\sup C_{\alpha_0}, \underline{c}=\inf C_{\alpha_0}.$

◆□▶◆圖▶◆臺▶◆臺▶ 臺 釣۹○

Score Estimator

We define $S_n(\psi,\alpha) = \frac{1}{n}(Y_i - \psi(\alpha^T \boldsymbol{X}_i))^2$. For a fixed α , by the conclusion obtained via the left derivative of the greatest convex minorant of the cumulative sum diagram $\left\{(0,0), (\sum_{j=1}^i n_j^\alpha, \sum_{j=1}^i n_j^\alpha Y_j^\alpha), i=1,\cdots,m\right\}$, the minimizer for a fixed α is denoted by $\hat{\psi}_{n\alpha}$. Now we consider the estimation for α :

$$\min_{\alpha} \frac{1}{n} \left(Y_i - \hat{\psi}_{n\alpha} (\alpha^T \mathbf{X}_i) \right)^2$$

Let $\mathbb{S}: \mathbb{R}^{d-1} \to \mathcal{S}_{d-1} \subset \mathbb{R}^d$; $\beta \to \alpha = \mathbb{S}(\beta)$ be a local parametrization, obtaining

$$\min_{\alpha} \frac{1}{n} \sum_{i=1}^{n} \left(Y_i - \hat{\psi}_{n\alpha}(\mathbb{S}(\beta)^T \mathbf{X}_i) \right)^2$$

Zero-Crossing Solution

By derivative, we get

$$\frac{1}{n}\sum_{i=1}^{n} 2\left(Y_{i} - \hat{\psi}_{n\alpha}(\mathbb{S}(\beta)^{T}\boldsymbol{X}_{i})\right) \cdot (-1)\frac{d\hat{\psi}_{n\alpha}(x)}{dx} \cdot (J_{\mathbb{S}}(\beta))^{T}\boldsymbol{X}_{i} = 0, \text{ i.e.}$$

$$\frac{1}{n} \sum_{i=1}^{n} (J_{\mathbb{S}}(\beta))^{T} \boldsymbol{X}_{i} \left(Y_{i} - \hat{\psi}_{n\alpha} (\mathbb{S}(\beta)^{T} \boldsymbol{X}_{i}) \right)$$

where
$$J_{\mathbb{S}}(\beta) = \left(rac{\partial \mathbb{S}_i(\beta)}{\partial \beta_j}
ight) \in \mathbb{R}^{d imes (d-1)}$$

We cannot hope to find the exact solution for the equations, instead we can derive the zero-crossing of

$$\phi_n(\beta) = \int (J_{\mathbb{S}}(\beta))^T \mathbf{x} (y - \hat{\psi}_{n\alpha} \left(y - \hat{\psi}_{n\alpha} (\mathbb{S}(\beta)^T \mathbf{x}) \right) d\mathbb{P}_n(\mathbf{x}, y)$$

and with population version

$$\phi(\beta) = \int (J_{\mathcal{S}}(\beta))^{\mathsf{T}} \mathbf{x} (\mathbf{y} - \psi_{\alpha}(\mathcal{S}(\beta)^{\mathsf{T}} \mathbf{x})) dP_{0}(\mathbf{x}, \mathbf{y})$$

where $\psi_{\alpha}(u) = \mathbb{E}[\psi_0(\alpha_0^T \mathbf{X}) | \alpha^T \mathbf{X} = u]$

□▶→□▶→重▶→重→ 9へ◎

19 / 28

Ergan Shang (USTC) Single Index Model June 7, 2022

Technical Lemmas

Link Function under L₂

The functional L_{α} given by $\psi \mapsto L_{\alpha}(\psi) = \int_{\mathcal{X}} (\psi_0(\alpha_0^T \mathbf{x}) - \psi(\alpha^T \mathbf{x}))^2 dG(\mathbf{x})$ admits a minimizer ψ^{α} over the set of non-decreasing functions, such that ψ^{α} is uniquely given by $\psi_{\alpha} = \mathbb{E}[\psi_0(\alpha_0^T \mathbf{X}) | \alpha^T \mathbf{X} = u]$

Distance and Bound

Similar to 16, we have when $\alpha \in B(\alpha_0, \delta_0)$

$$\max_{\alpha} \sup_{\mathbf{x} \in \mathcal{X}} |\hat{\psi}_{n\alpha}(\alpha^T \mathbf{x})| = O_p(\log n) \quad \sup_{\alpha} \int \left(\hat{\psi}_{n\alpha}(\alpha^T \mathbf{x}) - \psi_{\alpha}(\alpha^T \mathbf{x})\right)^2 = O_p\left((\log n) - \sum_{\alpha} \int_{\alpha} \left(\hat{\psi}_{n\alpha}(\alpha^T \mathbf{x}) - \psi_{\alpha}(\alpha^T \mathbf{x})\right)^2 \right) = O_p\left(\log n\right)$$

The estimation
$$\hat{\psi}_{n\alpha} \stackrel{distance}{\longleftrightarrow} \psi_{\alpha}(u)$$
 link function
$$\updownarrow \qquad \qquad \updownarrow \qquad \qquad \downarrow \qquad \downarrow$$

Main Results

Asymptotic Property

- (Existence) A crossing of zero $\hat{\beta}_n$ of $\phi_n(\beta)$ exists with probability tending to 1
- (Consistency) $\hat{\alpha}_n \stackrel{P}{\rightarrow} \alpha_0$
- (Asymptotic normality) Define $A = \mathbb{E}\left[\psi_0'\left(\alpha_0^T\pmb{X}\right)\operatorname{Cov}\left(\pmb{X}|\alpha_0^T\pmb{X}\right)\right]$ and $\Sigma = \mathbb{E}\left[\left(Y \psi_0(\alpha_0^T\pmb{X})\right)^2\left(\pmb{X} \mathbb{E}[\pmb{X}|\alpha_0^T\pmb{X}]\right)\left(\pmb{X} \mathbb{E}[\pmb{X}|\alpha_0^T\pmb{X}]\right)^T\right]$, then $\sqrt{n}(\hat{\alpha}_n \alpha_0) \stackrel{d}{\to} \mathcal{N}_d(0, A^-\Sigma A^-)$

Overview

- Single Index Model
 - Under Gaussian Space
 - Least Squares on Monotone Functions
 - Score Estimation on Monotone Functions
- Sample Complexity of One-Hidden-Layer Neural Networks
- What am I thinking about

Background and Introduction

Definition: Learnable algorithm

Suppose that F is a set of functions mapping from a domain X into the real interval [0,1]. A learning algorithm L for F is a function $L: \bigcup_{m=1}^{\infty} (X \times \mathbb{R})^m \to F$ with the following property:

• given any $\epsilon \in (0,1)$, $\delta \in (0,1)$, $B \ge 1$: there is an integer $m_0(\epsilon,\delta,B)$ such that if $m \ge m_0(\epsilon,\delta,B)$

then, for any probablity distribution P on $X \times [1-B,B]$, if z is a training sample of length m, drawn randomly according to the product probability distribution P^m , then, with probability at least $1-\delta$, the function L(z) output by L is such that

$$er_P(L(z)) < opt_P(F) + \epsilon$$

where $opt_P(F) = \inf_{f \in F} \mathbb{E}[(f(x) - y)^2]$; $er_P(f) = \mathbb{E}[(f(x) - y)^2]$ We say that F is **learnable** if there is a learning algorithm for F.

Ergan Shang (USTC) Single Index Model June 7, 2022 22 / 28

Fat shattering and Rademacher complexity

Lower bound for sample complexity through fat-shattering dimension

F is the function class: $X \to [0,1]$. Then for $B \ge 2, \epsilon \in (0,1)$ and $0 < \delta < \frac{1}{100}$, any learning algorithm L for F has sample complexity satisfying

$$m_L(\epsilon, \delta, B) \geq \frac{fat_F(\epsilon/\alpha) - 1}{16\alpha} \quad \forall \alpha \in (0, \frac{1}{4})$$

Rademacher complexity

$$R_m(\mathcal{F}) = \sup_{\{x_i\}_{i=1}^m \subset \mathcal{X}} \mathbb{E}_{\epsilon} \left[\sup_{f \in \mathcal{F}} \frac{1}{m} \sum_{i=1}^m \epsilon_i f(x_i) \right]$$

Frankly speaking, although I read Chapter 13 in Martin's book, I still cannot figure out the relationship between Rademacher complexity and upper bound for sample complexity

Overview

- Single Index Model
 - Under Gaussian Space
 - Least Squares on Monotone Functions
 - Score Estimation on Monotone Functions
- Sample Complexity of One-Hidden-Layer Neural Networks
- What am I thinking about

My idea

For single index model

$$f(\mathbf{x}) = \psi_0(\alpha_0^T \mathbf{x})$$

under i.i.d. observations $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, the problem is how to "test" $\alpha_0 = \mathbf{0}$

In those papers I read, they always assume $\alpha_0 \in \mathcal{S}_{d-1}$, with the condition ψ is monotone or noise ϵ_i and \mathbf{x}_i are normal random variable. $\alpha_0 \in \mathcal{S}_{d-1}$ bypasses the problem of non-identifiability,i.e. if we define $\phi_0(t) = \psi_0(\|\alpha_0\|t)$. With $\beta_0 = \frac{\alpha_0}{\|\alpha_0\|}$, we have $\psi_0(\alpha_0^T \mathbf{x}) = \phi_0(\beta_0^T \mathbf{x})$.

Therefore, it may not work if we apply least squares methods to estimate $\alpha_0 \in \mathcal{S}_{d-1}$. Perhaps we have to solve the problem from a prospective of hypothesis testing.

◄□▶◀圖▶◀불▶◀불▶ 불 ∽Q҈

Estimation or Testing?

- Estimation
 - If we can tackle the problem of non-identifiability, then we can, under the conditions that the link is monotone or in Gaussian space, make an estimation for both ψ_0 and α_0 . It will be clear to see whether $\alpha_0=0$.
- Testing

$$H_0: Y = \psi_0(0) + \epsilon \sim \mathcal{N}(\mu, \sigma^2) \longleftrightarrow H_1: Y = \psi_0(\alpha_0^T \mathbf{x}) + \epsilon \quad \alpha_0 \in \mathcal{S}_{d-1}$$

where $\mu=\psi_0(0)$. If ψ_0 is linear, the testing problem can be done by ANOVA. Similarly, is it possible to derive a testing statistic similar to "RSS₁-RSS₂" and figure it out distribution?

Testing and Estimation

We can define $RSS_1 = \sum_{i=1}^n (Y_i - \bar{Y})^2$ and $RSS_2 = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$, where we can using the algorithm finding $\hat{\psi}_n$, $\hat{\alpha}_n$ and let $\hat{Y}_i = \hat{\psi}_n(\hat{\alpha}_n^T \mathbf{x}_i)$. And we can define F-statistic

$$F = \frac{(RSS_1 - RSS_2)/d.f.1}{RSS_2/d.f.2}$$

And another method is to define the likelihood ratio test and perhaps do minimax hypothesis testing. Observing that $\psi_0(\alpha_0^T \mathbf{x}) - \psi_0(0)$ is still a non-decreasing function, we can test

$$H_0: \theta = 0 \longleftrightarrow H_1: \theta = \psi_0(\alpha_0^T \mathbf{x})$$

where the null and alternative are both simple.



References

- 1 Balabdaoui F, Durot C, Jankowski H. Least squares estimation in the monotone single index model[J]. Bernoulli, 2019, 25(4B): 3276-3310.
- 2 Vardi G, Shamir O, Srebro N. The Sample Complexity of One-Hidden-Layer Neural Networks[J]. arXiv preprint arXiv:2202.06233, 2022.
- 3 Balabdaoui F , Piet Groeneboom. Score estimation in the monotone single index mode.
- 4 Dudeja R , Hsu D . Learning Single-Index Models in Gaussian Space. 2018.
- 5 Wainwright M J. High-dimensional statistics: A non-asymptotic viewpoint[M]. Cambridge University Press, 2019.
- 6 Anthony M, Bartlett P L, Bartlett P L. Neural network learning: Theoretical foundations[M]. Cambridge: cambridge university press, 1999.
- 7 Groeneboom P, Jongbloed G. Nonparametric estimation under shape constraints[M]. Cambridge University Press, 2014.

Thank you!