Mathematics Theory of Neural Network Models

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Lecture 3: Concentration Inequalities Rademacher Complexity

Lecturer: Chao Ma Scribe: Zehao Wang, Haoran Wang

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1 Some backgrounds in Concentration Inequalities

3.1 Markov Inequality

Theorem 3.1 (Markov Inequality) Let X be a random variable that is non-negative with expectation E(X). Then, for every constant a > 0,

$$\Pr(X \ge a) \le \frac{\mathrm{E}(X)}{a}$$
.

This inequality gives a tight upper bound of the tail probability of X when we only know the first order moment of X.

Proof:

$$\Pr(X \geq a) = \mathrm{E}(\mathbf{1}_{[X \geq a]}), \mathbf{1}_{[X \geq a]} \leq \frac{X}{a} \Rightarrow \Pr(X \geq a) \leq \frac{\mathrm{E}(X)}{a}$$

3.2 Chebyshev Inequality

When we know the first order moment and the second order moment of X, we can give a more specific bound of tail probability using Chebyshev Inequality.

Theorem 3.2 (Chebyshev Inequality) For every constant a > 0,

$$\Pr(|X - E(X)| \ge a) \le \frac{\operatorname{var}(X)}{a^2}.$$

This inequality can be derived from the Markov inequality easily.

Go a step further, think about the case when $E(X), E(X^2), ..., E(X^r)$ is known, the straight forward upper bound will become:

$$\Pr(X \ge a) \le \min_{k \in \{1, \dots, r\}} \frac{\mathrm{E}(X^k)}{a^k}.$$

3.3 Chernoff Inequality

The generic Chernoff bound requires all the moments of X, or the Moment Generative Function defined as:

$$M_X(t) = \mathrm{E}(\mathrm{e}^{tX}).$$

In fact these two conditions are equivalent, if we expand the function $M_x(t)$ we can get:

$$M_X(t) = \sum_{k=0}^{\infty} \frac{\mathrm{E}(X^k)}{k!} t^k.$$

Which means by expanding the Moment Generative Function we can get all the moments of X as the parameters in the series.¹

Theorem 3.3 (Chernoff Inequality) Based on Markov's inequality, for every t > 0:

$$\Pr(X \ge a) \le \frac{\mathrm{E}(\mathrm{e}^{tX})}{\mathrm{e}^{ta}}.$$

Proof: $\forall t > 0$

$$\Pr(X \ge a) = \Pr(e^{tX} \ge e^{ta}) \le \frac{E(e^{tX})}{e^{ta}}$$

The last step is exactly Markov's inequality.

3.4 Chernoff Bound

Theorem 3.4 Let $X_1, ..., X_n$ be a set of n i.i.d. Bernoulli random variables, EX = p, then for all $\epsilon > 0$, the following inequality holds:

$$P(\frac{1}{n}\sum_{i=1}^{n}X_i - p \ge \epsilon) \le e^{-nD_e^{(B)}(p+\epsilon||p)}$$

Theorem 3.5 Let X_1, \ldots, X_n be a set of n random variables satisfying $X_i \in [0,1]$ and $EX_i = p$ for $i = 1, \ldots, n$, then for all $\epsilon > 0$, the following inequality holds:

$$P(\frac{1}{n}\sum_{i=1}^{n}X_i - p \ge \epsilon) \le e^{-nD_e^{(B)}(p+\epsilon||p)}$$

Proof: Exponent function is convex and use Jensen's inequality, for all t and $x \in (0,1)$ we can write:

$$Ee^{tx} \le E(xe^t) + E((1-x)e^0) = pe^t + 1 - p$$

Using this inequality, we can prove the theorem like Chernoff Bound.

Theorem 3.6 Let X_1, \ldots, X_n be a set of n random variables satisfying $X_i \in [0,1]$ and $EX_i = p_i$ for $i = 1, \ldots, n$, then for all $\epsilon > 0$, the following inequality holds for $p = \frac{1}{n} \sum_{i=1}^{n} p_i$:

$$P(\frac{1}{n}\sum_{i=1}^{n}X_{i}-p\geq\epsilon)\leq e^{-nD_{e}^{(B)}(p+\epsilon||p)}$$

¹We should notice that the moment-generating function of a real-valued distribution does not always exist, while the characteristic function does. And most distributions' moment-generating function is just to replace the it in the characteristic function with t. For example we consider $X \sim \mathrm{U}(a,b)$, it's characteristic function is $\frac{\mathrm{e}^{itb} - \mathrm{e}^{ita}}{it(b-a)}$ while the moment-generating function is $\frac{\mathrm{e}^{tb} - \mathrm{e}^{ta}}{t(b-a)}$

Proof: Logarithmic function is concave and use Jensen's inequality, for all t we can write:

$$\frac{\sum_{i=1}^{n} \ln(1 - p_i + p_i e^t)}{n} \le \ln(1 - p + p e^t)$$

then

$$\prod_{i=1}^{n} (1 - p_i + p_i e^t) \le (1 - p + p e^t)^n$$

Using this inequality, we can prove the theorem like Chernoff Bound.

3.5 Hoeffding Inequality

Lemma 3.7 (Hoeffding's Lemma)Let $X_1,...,X_m$ be independent random variables with E[X] = 0 and $a \le X \le b$. Then for any t > 0, the following inequality holds:

$$E[e^{tX}] \le e^{\frac{t^2(b-a)^2}{8}}$$

Proof: Since $f(x) = e^{tx}$ is a convex function of x, the following holds:

$$e^{tx} \le \frac{b-x}{b-a}e^{ta} + \frac{x-a}{b-a}e^{tb}$$

Then, using E[X] = 0,

$$E[e^{tX}] \le E[\frac{b - X}{b - a}e^{ta} + \frac{X - a}{b - a}e^{tb}] = \frac{b}{b - a}e^{ta} + \frac{-a}{b - a}e^{tb} = e^{\phi(t)}$$

where,

$$\phi(t) = \ln(\frac{b}{b-a}e^{ta} + \frac{-a}{b-a}e^{tb})$$

Taking derivative of $\phi(t)$, note that $\phi(0) = \phi'(0) = 0$, and that $\phi''(t) \leq \frac{(b-a)^2}{4}$. Thus by the second order expansion of function ϕ , there exists $\theta \in [0, t]$, such that:

$$\phi(t) = \phi(0) + t\phi'(0) + \frac{t^2}{2}\phi''(\theta) \le t^2 \frac{(b-a)^2}{8},$$

which completes the proof.

Theorem 3.8 (Hoeffding's inequality) Let $X_1, X_2, ... X_n$ be independent random variables where $X_i \in [a_i, b_i]$, and Let $\mu = \frac{\sum_{i=1}^n E[X_i]}{n}$, the following inequality holds:

$$P(\frac{1}{n}\sum_{i=1}^{n}X_{i} - \mu \ge \epsilon) \le \exp(\frac{-2n^{2}\epsilon^{2}}{\sum_{i=1}^{n}(b_{i} - a_{i})^{2}})$$

Proof: Let $S_n = \sum_{i=1}^n X_i$, Then for any $t \ge 0$,

$$P(S_{n} - E[S_{n}] \ge n\epsilon) \le e^{(-tn\epsilon)} E[e^{t(S_{n} - E[S_{n}])}]$$

$$= \prod_{i=1}^{n} e^{-t\epsilon} E[e^{t(X_{i} - E[X_{i}])}]$$

$$\le \prod_{i=1}^{n} e^{-t\epsilon} e^{\frac{t^{2}(b_{i} - a_{i})^{2}}{8}} \qquad (Lemma 2.6)$$

$$= e^{-tn\epsilon} e^{t^{2} \sum_{i=1}^{n} \frac{(b_{i} - a_{i})^{2}}{8}}$$

$$\le e^{(\sum_{i=1}^{n} (b_{i} - a_{i})^{2}})$$

Where we chose $t = 4n\epsilon/\sum_{i=1}^{n}(b_i - a_i)^2$ to minimize the upper bound. And so,

$$P(\frac{1}{n}\sum_{i=1}^{n}X_{i} - \mu \ge \epsilon) \le \exp(\frac{-2n^{2}\epsilon^{2}}{\sum_{i=1}^{n}(b_{i} - a_{i})^{2}})$$

3.6 McDiarmid Lemma

Theorem 3.9 Assume $\forall i, \forall x_1, x_2, ..., x_n, x_i^{'}, | f(x_1, ..., x_i, ..., x_n) - f(x_1, ..., x_i^{'}, ..., x_n) | \leq c_i$ if $x_1, x_2, ..., x_n$ are independent random variables, then

$$P(|f(x_1,...,x_n) - E[f(x_1,...,x_n])| \ge \epsilon) \le \exp(\frac{-2\epsilon^2}{\sum_{i=1}^n c_i^2})$$

Proof: Let f(S) denote $f(x_1,...,x_n)$

Define a sequence of random variables V_k , $k \in [1, m]$, as follows: V = f(S) - E[f(S)], $V1 = E[V|x_1] - E[V]$, and for k < 1,

$$V_k = E[V|x_1,...,x_k] - E[V|x_1,...,x_{k-1}].$$

Note that $V = \sum_{k=1}^{m} V_k$. Furthermore, the random variable $E[V|x_1,...,x_k]$ is a function of $x_1,...x_k$. Conditioning on $x_1,...,x_k$ and taking its expectation is therefore:

$$E[E[V|x_1,...,x_k]|x_1,...,x_{k-1}] = E[V|x_1,...,x_{k-1}],$$

which implies $E[V|x_1,...,x_k] = 0$. Thus, the sequence $(V_k)_{k \in [1,m]}$ is a martingale difference sequence. Next, observe that, since E[f(S)] is a scalar, V_k can be expressed as follows:

$$V_k = E[f(S)|x_1,...,x_k] - E[f(S)|x_1,...,x_{k-1}]$$

Thus, we can define an upper bound W_k and lower bound U_k for V_k by:

$$W_k = \sup_x E[f(S)|x_1,...,x_{k-1},x] - E[f(S)|x_1,...,x_{k-1}]$$

$$U_k = inf_x E[f(S)|x_1,...,x_{k-1},x] - E[f(S)|x_1,...,x_{k-1}]$$

Now, $\forall k \in [1, m]$, the following holds:

$$W_k - U_k = \sup_{x,x'} E[f(S)|x_1,...,x_{k-1},x] - E[f(S)|x_1,...,x_{k-1},x'] \le c_k,$$

thus, $U_k \leq V_k \leq U_k + c_k$. In the view of these inequalities, we can apply Azuma's inequality to

$$V = \sum_{k=1}^{m} V_k,$$

which yields the desired inequality.

2 Rademacher complexity and its estimations

3.1 Definition

Definition 3.10 (Rademacher Complexity) Let \mathcal{F} be a collection of functions on $X,S = \{x_i\}_{i=1}^n$ be a sample of distribution D on X. Then we write

$$Rad_n(\mathcal{F}) = E_{\tau} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \tau_i f(x_i)$$

where τ_i takes the value ± 1 with probability $\frac{1}{2}$ for each.

Theorem 3.11 For each $f \in \mathcal{F}$ we have $f \in [0,1]$, then, w.p. $1 - \delta$ over the choice of S, we have

$$\sup_{f \in \mathcal{F}} \left[E_D f(x) - \hat{E}_S f(x) \right] \le 2Rad_n(\mathcal{F}) + 3\sqrt{\frac{\log \frac{1}{\delta}}{n}}$$

Proof: Let

$$\varphi(x_1, \dots, x_n) = \sup_{f \in \mathcal{F}} \left[E_D f(x) - \frac{1}{n} \sum_{i=1}^n f(x_i) \right]$$

Then,

$$\begin{aligned} &|\varphi(x_1, \cdots, x_n) - \varphi(x_1', \cdots, x_n)| \\ &= \left| \sup_{f \in \mathcal{F}} \left[E_D f(x) - \frac{1}{n} \sum_{i=1}^n f(x_i) \right] - \sup_{f \in \mathcal{F}} \left[E_D f(x) - \frac{1}{n} f(x_1') - \frac{1}{n} \sum_{i=2}^n f(x_i) \right] \right| \\ &\leq \left| \sup_{f \in \mathcal{F}} \frac{1}{n} \left(f(x_1) - f(x_1') \right) \right| \\ &\leq \frac{1}{n} \end{aligned}$$

That is φ satisfies the condition of McDiarmid lemma with $c_i = \frac{1}{n}$, then we have

$$P(\varphi(x_1,\dots,x_n)-E\varphi(x_1,\dots,x_n)\geq t)\leq \exp(-2nt^2)$$

that is, w.p. $\geq 1 - \delta$,

$$\varphi(x_1, \dots, x_n) \le E\varphi(x_1, \dots, x_n) + \sqrt{\frac{\log \frac{1}{\delta}}{n}}$$

Then we estimate $E\varphi(x_1,\dots,x_n)$. By definition we have

$$E\varphi(x_1,\dots,x_n) = E_S \sup_{f\in\mathcal{F}} \left[E_D f(x) - \frac{1}{n} \sum_{i=1}^n f(x_i) \right]$$

Let $S' = \{x_i'\}_{i=1}^n$ be a sample i.i.d of S, then

$$E\varphi(x_1, \dots, x_n) = E_S \sup_{f \in \mathcal{F}} S' \left[\hat{E}_{S'} f(x) - \hat{E}_S f(x) \right]$$

$$\leq E_{S,S'} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \left(f(x_i) - f(x_i') \right)$$

$$= E_{\tau,S,S'} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \tau_i \left(f(x_i') - f(x_i) \right)$$

$$\leq E_{\tau,S,S'} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \tau_i f(x_i) + E_{\tau,S,S'} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \tau_i f(x_i')$$

$$= 2E_S Rad_n(\mathcal{F})$$

Similarly, let

$$\psi(x_1, \dots, x_n) = E_{\tau} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \tau_i f(x_i)$$

and we can verify that

$$|\psi(x_1,\dots,x_n)-\psi(x_1',\dots,x_n)|\leq \frac{1}{n}$$

Then, according to Mcdiarmid lemma we have, w.p $\geq 1 - \delta$

$$E_S Rad_n(\mathcal{F}) \le Rad_n(\mathcal{F}) + \sqrt{\frac{\log \frac{1}{\delta}}{n}}$$

Then we finish the proof.

As an example, we estimate the Rademacher complexity of the set

$$\mathcal{F} = \{ w^T x : ||w||_2 \le W \}, ||x_i||_2 \le X$$

$$Rad_{n}(\mathcal{F}) = \frac{1}{n} E_{\tau} \sup_{\|w\|_{2} \leq W} \sum_{i=1}^{n} \tau_{i} w^{T} x_{i}$$

$$= \frac{1}{n} E_{\tau} \sup_{\|w\|_{2} \leq W} w^{T} \sum_{i=1}^{n} \tau_{i} x_{i}$$

$$= \frac{1}{n} W E_{\tau} \left\| \sum_{i=1}^{n} \tau_{i} x_{i} \right\|_{2}$$

$$\leq \frac{W}{n} \sqrt{E_{\tau} \left\| \sum_{i=1}^{n} \tau_{i} x_{i} \right\|_{2}^{2}}$$

$$= \frac{W}{n} \sqrt{\sum_{i=1}^{n} \|x_{i}\|_{2}^{2}} \leq \frac{WX}{\sqrt{n}}$$

3.2 Properties of Rademacher Complexity

The following two properties are trivial

$$Rad(\mathcal{F} + f_0) = Rad(\mathcal{F})$$

$$Rad(\lambda \mathcal{F}) = \lambda Rad(\mathcal{F})$$

Theorem 3.12 Let φ be a Lipschitz-continuous function with Lipschitz-constant L, and

$$\varphi \circ \mathcal{F} = \{ \varphi \circ f : f \in \mathcal{F} \}$$

then,

$$Rad(\varphi \circ \mathcal{F}) \leq LRad(\mathcal{F})$$

Proof:

$$Rad(\varphi \circ \mathcal{F}) = E \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \tau_{i} \varphi \circ f(x_{i})$$

$$= \frac{1}{n} E \left[\sup_{f \in \mathcal{F}} \left[\varphi \circ f(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) \right] + \sup_{f \in \mathcal{F}} \left[-\varphi \circ f(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) \right] \right]$$

$$= \frac{1}{n} E \sup_{f, f' \in \mathcal{F}} \left[\varphi \circ f(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) - \varphi \circ f'(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f'(x_{i}) \right]$$

$$\leq \frac{1}{n} E \sup_{f, f' \in \mathcal{F}} \left[L|f(x_{1}) - f'(x_{1})| + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f'(x_{i}) \right]$$

$$= \frac{1}{n} E \sup_{f, f' \in \mathcal{F}} \left[L(f(x_{1}) - f'(x_{1})) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f'(x_{i}) \right]$$

$$= \frac{1}{n} E \sup_{f \in \mathcal{F}} \left[Lf(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) \right] + \sup_{f \in \mathcal{F}} \left[-Lf(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) \right]$$

$$= \frac{1}{n} E \sup_{f \in \mathcal{F}} \left[\tau_{1} Lf(x_{1}) + \sum_{i=2}^{n} \tau_{i} \varphi \circ f(x_{i}) \right]$$

Repeat this process for index $i = 2, \dots, n$, and we have

$$Rad(\varphi \circ \mathcal{F}) \leq E \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \tau_i Lf(x_i) = LRad(\mathcal{F})$$

3.3 Generalization to Subset of \mathbb{R}^n

For a subset A of \mathbb{R}^n , we write

$$Rad_n(A) = \frac{1}{n} E \sup_{a \in A} \tau^T a$$

Definition 3.13 (Covering number) Let (S, ρ) be a metric space, $T \subset S$, $\alpha > 0$. $T' \subset T$ is an α -cover of T, if $\forall x \in T$, $\exists x' \in T'$, s.t. $\rho(x, x') \leq \alpha$. We let the covering number be

$$N(\alpha, T, \rho) = \min |T'|$$

where the minimum is taken over all α -covering T'.

Lemma 3.14 (Massart) Assume that $|A| < \infty, r = \max_{a \in A} ||a||_2$, then $Rad(A) \leq \frac{r\sqrt{2\log|A|}}{n}$.

Proof:

$$\exp\left(\lambda E \max_{a \in A} \tau^T a\right) \leq E \exp\left(\lambda \max_{a \in A} \tau^T a\right)$$

$$\leq E \sum_{a \in A} \exp\left(\lambda \tau^T a\right)$$

$$= \sum_{a \in A} E \exp\left(\lambda \sum_{i=1}^n \tau_i a_i\right)$$

$$= \sum_{a \in A} \prod_{i=1}^n E \exp\left(\lambda \tau_i a_i\right)$$

$$\leq \sum_{a \in A} \prod_{i=1}^n \exp\frac{(2\lambda a_i)^2}{8}$$

$$\leq |A| \exp\frac{\tau^2 \lambda^2}{2}$$

In the 5th line we have adopted Hoeffding inequality. Take the logarithm of both sides, we have

$$\max_{a \in A} \tau^T a \le \frac{r^2 \lambda}{2} + \frac{1}{\lambda} \log|A|$$

As $\lambda > 0$ is chosen arbitrarily, we can choose proper λ to minimize the right side. Then we have

$$Rad(A) \le \frac{r\sqrt{2\log|A|}}{n}$$

Theorem 3.15

$$Rad(A) \le \inf_{\alpha > 0} \left\{ \max_{a \in A} \|a\|_2 \frac{\sqrt{2\log N(\sqrt{n\alpha}, A, l_2)}}{n} + \alpha \right\}$$

Proof: For $\alpha > 0$, let A' be a $\sqrt{n}\alpha$ -cover of A, $|A'| = N(\sqrt{n}\alpha, A, l_2)$.

$$Rad(A) = \frac{1}{n} E \sup_{a \in A} \tau^{T} a$$

$$\leq \frac{1}{n} E \sup_{a' \in A'} \tau^{T} a' + \frac{1}{n} E \sup_{a \in A} \tau^{T} (a - a')$$

$$\leq \max_{a \in A} ||a||_{2} \frac{\sqrt{2 \log |A'|}}{n} + \alpha$$

Theorem 3.16 Let A be a bounded subset of \mathbb{R}^n , then

$$Rad(A) \le 4 \int_0^{+\infty} \frac{\sqrt{2\log N(\alpha, A, l_2)}}{n} d\alpha$$

Proof: Let $r = \max_{a \in A} \|a\|_2$, \hat{A}^j be a $2^{-j}r$ -cover of A which has the least elements, and for fixed $a \in A$, let \hat{a}^j be an element in \hat{A}^j s.t. $\|a - \hat{a}^j\| \le 2^{-j}r$. We can choose \hat{A}^0 to be $\{0\}$. For any sufficiently big integer N, we have

$$\begin{aligned} Rad(A) &= \frac{1}{n} E \sup_{a \in A} \tau^T a \\ &\leq \frac{1}{n} E \sup_{a \in \hat{A}^N} \tau^T a + \frac{1}{n} E \sup_{a \in A} \tau^T (a - \hat{a}^N) \\ &\leq \frac{1}{n} E \sup_{a \in \hat{A}^{N-1}} \tau^T a + \frac{1}{n} E \sup_{a \in \hat{A}^N} \tau^T (a - \hat{a}^{N-1}) + \frac{1}{n} E \sup_{a \in A} \tau^T (a - \hat{a}^N) \\ &\leq \cdots \leq \sum_{j=1}^N \frac{1}{n} E \sup_{a \in \hat{A}^j} \tau^T (a - \hat{a}^{j-1}) + \frac{1}{n} E \sup_{a \in A} \tau^T (a - \hat{a}^N) \\ &\leq \sum_{j=1}^N \frac{2^{-j+1}r}{n} \sqrt{2 \log N(2^{-j}r, A, l_2)} + \frac{2^{-N}r}{\sqrt{n}} \\ &\leq 4 \int_0^{+\infty} \frac{\sqrt{2 \log N(\alpha, A, l_2)}}{n} d\alpha + \frac{2^{-N}r}{\sqrt{n}} \end{aligned}$$

Let $N \to \infty$, we get the inequality to be proved.

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