

Statistical Machine Learning Theory

(Introduction to) **Statistical Learning Theory**

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Statistical learning theory:

Theoretical guarantee for learning from limited data

- We have seen how to estimate the performance of a prediction model *empirically* (using cross validation.)
- Today, we will see theoretical ways:
 - What is the test performance of a classifier with a particular training performance?
 - How far is a classifier from the best performance model?
 - How many training instances are needed to ensure a certain accuracy of the estimate?

REFERENCE:

Bousquet, Boucheron, and Lugosi. "Introduction to statistical learning theory."
Advanced lectures on machine learning. pp. 169-207, 2004.

Error Bounds

True risk and empirical risk: We are interested in true risk but can access only to empirical risk

- Training dataset $\{ (x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)}) \}$ is sampled from probability distribution P in an i.i.d manner

- $y^{(i)} \in \{+1, -1\}$: Binary classification
- We want to estimate $f: \mathcal{X} \rightarrow \{+1, -1\}$

Indicator function
(0 – 1 loss)

- (True) risk: $R(f) = \Pr(f(x) \neq y) = E_{(x,y) \sim P} [1_{f(x) \neq y}]$
 - We cannot directly evaluate this since we do not know P
- Empirical risk: $R_N(f) = \frac{1}{N} \sum_{i=1}^N 1_{f(x^{(i)}) \neq y^{(i)}}$
 - Usually we estimate a classifier that minimizes this

Our goal: How good is the classifier learned by empirical risk minimization?

- Ultimate goal: find the best f in function class \mathcal{F}
 - Best function: $f^* = \operatorname{argmin}_{f \in \mathcal{F}} R(f)$ True risk
- Instead, empirical risk minimization: $f_N = \operatorname{argmin}_{f \in \mathcal{F}} R_N(f)$
 - When using regularization, $f_N = \operatorname{argmin}_{f \in \mathcal{F}} R_N(f) + \lambda \|f\|^2$
- Our goal is to know how good f_N is (in terms of N and \mathcal{F})
 1. $R(f_N) - R_N(f_N) \leq B(N, \mathcal{F})$: Estimate of the true risk of a trained classifier from its empirical risk
 2. $R(f_N) - R(f^*) \leq B(N, \mathcal{F})$: Estimate how far the true risk of a trained classifier is from the best one

Error bound:

We want to give an error bound for a *finite* dataset

- Let us consider to find a bound $R(f_N) - R_N(f_N) \leq B(N, \mathcal{F})$
 - We want a bound depending on N (and \mathcal{F})
- $R(f) - R_N(f) = E_{(x,y) \sim P} [1_{f(x) \neq y}] - \frac{1}{N} \sum_{i=1}^N 1_{f(x^{(i)}) \neq y^{(i)}}$
 - By the law of large numbers, this will converge to 0
 - Empirical risk is a good estimate of the true risk
 - But we want to know $B(N, \mathcal{F})$ depending on a finite N

The bound is a
function of N

\Rightarrow PAC (probably approximately correct) learning framework

Hoeffding's inequality: A tool to analyze difference of expectation and empirical mean for small sample

- Hoeffding's inequality: Let $Z^{(1)}, \dots, Z^{(N)}$ be N i.i.d. random variables with $Z^{(i)} \in [a, b]$. Then, for any $\epsilon > 0$,

$$\Pr \left[\left| E[Z] - \frac{1}{N} \sum_{i=1}^N Z^{(i)} \right| > \epsilon \right] \leq 2 \exp \left(-\frac{2N\epsilon^2}{(b-a)^2} \right)$$

- Gives the bound of probability of difference between expected value and empirical estimate exceeding ϵ
- As N gets larger, the upper bound will get smaller and converge to zero (= the law of large number)
 - But now we have more elaborated bound depending on N
- As ϵ gets smaller, the upper bound will get larger

Applying Hoeffding's inequality:

Bound of true risk for a fixed classifier

- Now we apply the Hoeffding's inequality to our case:

$$\Pr \left[\left| E[Z] - \frac{1}{N} \sum_{i=1}^N Z^{(i)} \right| > \epsilon \right] \leq 2 \exp \left(- \frac{2N\epsilon^2}{(b-a)^2} \right)$$

- For a classifier $f \in \mathcal{F}$, setting $Z = \overset{\text{zero-one loss}}{1_{f(x) \neq y}}$ gives

$$\Pr[|R(f) - R_N(f)| > \epsilon] \leq 2 \exp(-2N\epsilon^2) \equiv \delta$$

- Note that $(b-a)^2 \leq 1$
- With probability at least $1 - \delta$,

$$R(f) - R_N(f) \leq \sqrt{\frac{\log \frac{2}{\delta}}{2N}}$$

A bad news: Simple application of Hoeffding's inequality does not give the error bound we want

- For a fixed classifier f , its true risk is bounded using Hoeffding's inequality
 - With a fixed f , we can draw a sample with the bounded error with high probability
- But, this is not the estimate of the true risk of the algorithm
 - For a fixed sample, there can be many classifiers in the pool that violate the error bound
 - We do not know which classifier the algorithm will be chosen before seeing the data
 - So, we want a bound which holds for all classifier $f \in \mathcal{F}$

Error bound:

Depends on the log number of possible classifiers

- Theorem: With probability at least $1 - \delta$, $\forall f \in \mathcal{F}$

$$R(f) - R_N(f) \leq \sqrt{\frac{\log|\mathcal{F}| + \log \frac{2}{\delta}}{2N}}$$

- This also implies: for $f_N = \operatorname{argmin}_{f \in \mathcal{F}} R_N(f)$,

$$R(f_N) - R_N(f_N) \leq \sqrt{\frac{\log|\mathcal{F}| + \log \frac{2}{\delta}}{2N}}$$

- The bound depends on the log number of functions in \mathcal{F}
 - $|\mathcal{F}|$: The size of the hypothesis space

Slow increase

Error bound:

Proof using the union bound

- We apply the Hoeffding's inequality to all classifiers in \mathcal{F} simultaneously
- We use the union bound:
 - For two events A_1, A_2 , $\Pr[A_1 \cup A_2] \leq \Pr[A_1] + \Pr[A_2]$
 - For K events, $\Pr[A_1 \cup \dots \cup A_K] \leq \sum_{i=1}^K \Pr[A_K]$
- Combining Hoeffding bound + union bound gives:
 - $\Pr[\exists f \in \mathcal{F}: |R(f) - R_N(f)| > \epsilon] \leq 2|\mathcal{F}| \exp(-2N\epsilon^2)$
 - Equate the right hand side to δ to obtain the upper bound

Sample complexity: Number of examples required to ensure a certain accuracy

- Theorem: With probability at least $1 - \delta$, $\forall f \in \mathcal{F}$

$$R(f) - R_N(f) \leq \sqrt{\frac{\log|\mathcal{F}| + \log\frac{2}{\delta}}{2N}} \equiv \epsilon$$

- This theorem means, in other words, for any $\epsilon > 0$

if we take $N \geq \frac{\log|\mathcal{F}| + \log\frac{2}{\delta}}{2\epsilon^2}$ examples, with probability at least $1 - \delta$, we have

$$R(f) - R_N(f) \leq \epsilon$$

- This tells us how many examples are required to (probabilistically) ensure a certain accuracy ϵ

Error bound against the optimal classifier:

Similar bound holds

- We are also interested in how far the true risk of a **trained** classifier from the **best** one in \mathcal{F}
 - $R(f_N) - R(f^*) \leq B(N, \mathcal{F})$
- Similar analysis gives a bound depending on $\log|\mathcal{F}|$
- Theorem: With probability at least $1 - \delta$,

$$R(f_N) - R(f^*) \leq 2 \sqrt{\frac{\log|\mathcal{F}| + \log \frac{2}{\delta}}{2N}}$$

Summary: How good is the classifier learned by empirical risk minimization?

- Empirical risk minimization: $f_N = \operatorname{argmin}_{f \in \mathcal{F}} R_N(f)$
- Unknown best function: $f^* = \operatorname{argmin}_{f \in \mathcal{F}} R(f)$ R: true risk
- We can know how good f_N is in two ways:

1. $R(f_N) \leq R_N(f_N) + \sqrt{\frac{\log|\mathcal{F}| + \log\frac{2}{\delta}}{2N}}$: Estimate of the true risk of a trained classifier from its empirical risk
2. $R(f_N) - R(f^*) \leq 2\sqrt{\frac{\log|\mathcal{F}| + \log\frac{2}{\delta}}{2N}}$: How far is the true risk of a trained classifier from the best one?

Infinite Case

Infinite case:

Previous results assume finite number of classifiers

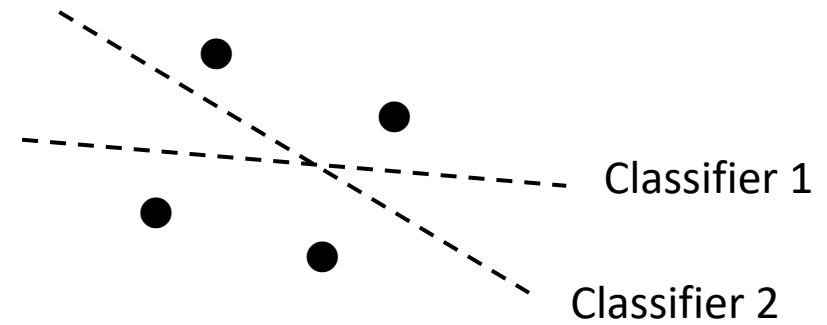
- We assumed the number of classifiers is finite
 - The bound depends on the number of classifiers in the pool

$$\mathcal{F}: R(f_N) - R_N(f_N) \leq \sqrt{\frac{\log |\mathcal{F}| + \log \frac{2}{\delta}}{2N}}$$

- $\log |\mathcal{F}|$ is considered as the “complexity” of class \mathcal{F}
 - So far we measure the complexity of the model using the number of possible classifiers (= size of hypothesis space)
- What if it is infinite? (E.g. linear classifiers $f = \mathbf{w}^\top \mathbf{x}$)
 - The upper bound goes to infinity 😞
- Do we have another complexity measure for the infinite case?

Growth function: Infinite number of functions can be grouped into finite number of function groups

- Use “growth function” as a complexity measure of infinite numbers of classifiers
- Idea: group the infinite number of classifiers into a finite number of equivalent sets
 - Two classifiers make same predictions for the 4 data points
 - They can be considered equivalent for the purpose of classifying the 4 data points



Growth function:

Error bound using growth function

- Growth function $\mathcal{S}_{\mathcal{F}}(N)$: The maximum number of ways into which N points can be classified by the function class \mathcal{F}
 - Apparently, $\mathcal{S}_{\mathcal{F}}(N) \leq 2^N$
 - For two-dimensional linear classifiers, $\mathcal{S}_{\mathcal{F}}(4) = 14 \leq 2^4$



only the two cases
cannot be classified

- Theorem: With probability at least $1 - \delta$, $\forall f \in \mathcal{F}$

$$R(f) - R_N(f) \leq 2 \sqrt{2 \frac{\log \mathcal{S}_{\mathcal{F}}(2N) + \log \frac{2}{\delta}}{N}}$$

VC dimension:

Intrinsic dimension of function class

- When $\mathcal{S}_{\mathcal{F}}(N) = 2^N$, any classification of N points is possible (we say that \mathcal{F} shatters the set)
- Vapnik-Chervonenkis (VC) dimension h of class \mathcal{F} :
The largest N such that $\mathcal{S}_{\mathcal{F}}(N) = 2^N$
- For two-dimensional linear classifiers, $h = 3$
 - It can realize 2^3 ways of dividing 3 points, but cannot for 2^4 ways
- Generally, for d -dimensional linear classifiers, $h = d + 1$

VC dimension and growth function:

Intrinsic dimension of function class

- Relation between VC-dim. and growth function:

- Apparently, for $N < h$, $\mathcal{S}_{\mathcal{F}}(N) = 2^N$;
otherwise, $\mathcal{S}_{\mathcal{F}}(N) < 2^N$ 😞

- Actually, a more tight upper bound exists:

For $N \geq h$, $\mathcal{S}_{\mathcal{F}}(N) < \left(\frac{eN}{h}\right)^h$

- Theorem: With probability at least $1 - \delta$, $\forall f \in \mathcal{F}$

$$R(f) - R_N(f) \leq 2 \sqrt{2 \frac{\textcolor{red}{h} \log \frac{2eN}{\textcolor{red}{h}} + \log \frac{2}{\delta}}{N}}$$

Statistical learning theory:

Theoretical guarantee for learning from limited data

- Questions about the generalization performance:
 - What is the test performance of a classifier with a particular training performance?
 - How far is a classifier from the best performance model?
 - How many training instances are needed to ensure a certain accuracy of the estimate?
- Probably Approximately Correct (PAC) learning framework:
 - Bounds for finite hypothesis space: Hoeffding's inequality
 - Infinite case: Growth function and VC-dimension