Learning Theory

Lecture 2

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SUMMER OF MACHINE LEARNING AT SKOLTECH

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Course on Machine Learning Theory

Lecture 1, Monday Introduction to learning theory, notation, warm-up exercises

Lecture 2, Tuesday Small historical tour of ML theory, basic concepts and techniques in statistical learning theory: VC-theory and and No Free Lunch

Lecture 3, Wednesday Research topics

Lecture 4, Thursday Fireside chat

A Historical Tour of Learning Theory

Basic question:

How well does the error of predictor h that we observe on the data S represent the error it will make on unseen data/on the underlying process P?

We know:

$$\mathcal{L}_P(h) \ \leq \ \mathcal{L}_S(h) + |\mathcal{L}_P(h) - \mathcal{L}_S(h)|$$

We want:

$$|\mathcal{L}_S(h) - \mathcal{L}_P(h)| \leq \epsilon(|S|)$$

70's: Vapnik and Chervonenkis

If (and only if) a class H of binary predictors $h : X \to \{0, 1\}$ has finite VC-dimension, then we get uniform convergence of empirical to true losses:

$$|\mathcal{L}_S(h) - \mathcal{L}_P(h)| \leq \sqrt{\frac{VC(H)}{|S|}}$$

for all functions $h \in H$ simultaneously.

80's: PAC Learning

Computational complexity is an emerging topic...

PAC Learning

A class H of binary predictors $h : \mathcal{X} \to \{0, 1\}$ is PAC (Probably Approximately Correct) learnable, if there exists an algorithm $\mathcal{A}$ such that for all $\epsilon, \delta > 0$, there exists a sample size n such that, for all data generating distributions P, algorithm $\mathcal{A}$ computes a predictor $\mathcal{A}(S)$ in time polynomial in $\frac{1}{\epsilon}$ and $\frac{1}{\delta}$ and we have

$$\Pr_{S \sim P^n}[\mathcal{L}_P(\mathcal{A}(S)) \leq \inf_{h \in H} \mathcal{L}_P(h) + \epsilon] \geq 1 - \delta$$

Valiant '84: A Theory of the Learnable

80's: PAC Learning

Statistical aspects of PAC learnability satisfied if:

Finite VC-dimension

Bounded compression sizes

$$\mathcal{L}_P(h) \;\leq\; \mathcal{L}_S(h) + \sqrt{\frac{d}{|S|}}$$

$\Rightarrow$ For a good trade-off, the class needs to have bounded capacity.

However, for many classes empirical risk minimization (ERM) is NP-hard...

90's: Boosting and Support Vector Machines

Emergence of efficient, practical learning algorithms..

Freund, Shapire

Weak learning (returning a classifier that is slightly better than random guessing) is as difficult as strong learning.

This was turned into a practical tool ("boosting")

Vapnik, Cortes, Schölkopf, Smola

The concept of large margin classifiers lead to development of Support Vector Machines.

Theory of kernels turned this into a highly successful tool.

2000's: More bounds, better understanding

Various concepts formalize that, as long as a learner will not be allowed enough flexibility to fit to random noise, it will generalize.

- Rademacher complexities
- Data dependent generalization bounds
- PAC Bayes bounds
- Compression bounds
- Algorithmic Stability

2010's: Deep Learning Taking over...

Very large neural networks solve complex learning tasks.

Issues:

- Classes of networks have huge capacity... they "shouldn't" generalize.
- Loss minimization is computationally hard...

Belief:
There still must be some inherent property in either learning method or the predictors that leads to generalization.

2017: Understanding deep learning requires rethinking generalization (Zhang, Bengio, Hardt, Recht, Vinyals)

$$\mathcal{L}_P(h) \;\leq\; \mathcal{L}_S(h) + |\mathcal{L}_P(h) - \mathcal{L}_S(h)|$$

1.) Training deep nets on image data with correct labels

- Training error 0
- Small test error
- Generalizes well

2.) Training deep nets on image data with randomly permuted labels

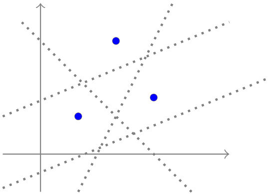
- Training error 0
- Large test error
- Does not generalize!

Both the class of predictors and the training method were identical in the two experiments!

...

The VC-dimension–Shattering

Instance space: $\mathcal{X} \subseteq \mathbb{R}^d$
Label set: $\mathcal{Y} = \{0, 1\}$
Hypothesis class: $H \subseteq \{0, 1\}^{\mathcal{X}}$



Definition: Shattering
We say that class H shatters a set of points $U \subseteq \mathcal{X}$ if

$$H|_U = \{0, 1\}^U$$

The restriction of the function class H to the set U contains all binary functions over U.

The VC-dimension–Definition

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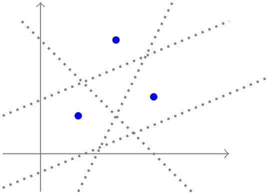
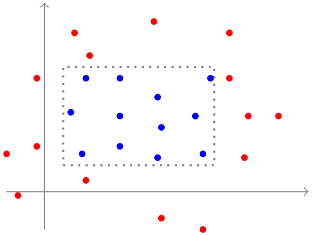


Definition: VC-Dimension
The VC-dimension of H is the maximal size of a set $U \subseteq \mathcal{X}$ that is shattered by H (or ∞ if H can shatter sets of arbitrarily large size).

Quiz 1: What does the above illustration tell us about the VC-dimension of halfspace classifiers in $\mathbb{R}^2$? $\Rightarrow$ It is at least 3!

Quiz 2

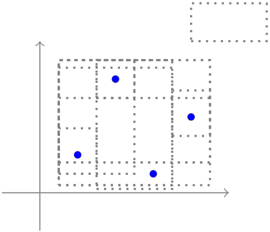
What is the VC-dimension of (axis-aligned) rectangle classifiers in $\mathbb{R}^2$?



H = classifiers that are defined by a fixed range in each feature.

Quiz 2–Solution

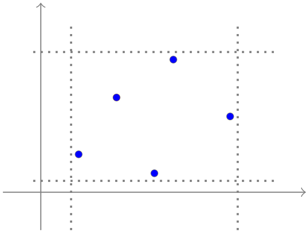
The VC-dimension of rectangle classifiers in $\mathbb{R}^2$ is 4!



Proof step 1: There exist 4 points that are shattered.

Quiz 2–Solution

The VC-dimension of rectangle classifiers in $\mathbb{R}^2$ is 4!



Proof step 2: No set of 5 points is shattered!

The VC-dimension–more examples

Consider domain $\mathcal{X} = \mathbb{R}^d$:

The VC-dimension of linear halfspaces in $\mathbb{R}^d$:

$$d + 1$$

The VC-dimension of all predictors h with $|h^{-1}(1)| < \infty$:

$$\infty$$

The VC-dimension of neural networks with fixed architecture and sign activation:

$$O(|E| \log(|E|))$$

Lemma (Sauer-Shelah-Perles)
Let H be a class of VC-dimension d. Then, for every finite domain subset $U \subseteq \mathcal{X}$, we have

$$|H|_U| \leq \sum_{i=1}^{d} \binom{|U|}{i} \leq \left(\frac{\mathrm{e}|U|}{d}\right)^d \simeq |U|^d$$

$\Rightarrow$ The number of "patterns" that the class H can induce on any domain subset U grows polynomially in $|U|$ once $|U| > d$.

Learnability of bounded VC-classes

Theorem

- Let $\mathcal{X}$ be some domain.
- Let $H \subseteq \{0,1\}^{\mathcal{X}}$ be a hypothesis class with $\mathrm{VC}(H) = d < \infty$.
- Let P be a distribution over $\mathcal{X} \times \{0,1\}$.
- Let $\delta > 0$.

With probability at least $1 - \delta$ (over the draw of a data-sample $S \sim P$) we have

$$\sup_{h \in H} |\mathcal{L}_S(h) - \mathcal{L}_P(h)| \;\leq\; c \cdot \sqrt{\frac{\mathrm{VC}(H) + \log(1/\delta)}{n}}$$

(where c is a constant that does not depend on P).

Learnability of VC-classes – proof idea

Recall our proof for finite classes:

$$\Pr\left[\max_{h\in H} |\mathcal{L}_P(h) - \mathcal{L}_S(h)| > \epsilon/2\right]$$
$$\leq \Pr\left[\bigvee_{h\in H} |\mathcal{L}_P(h) - \mathcal{L}_S(h)| > \epsilon/2\right]$$
$$\leq |H| \cdot 2\mathrm{e}^{-2n\epsilon^2} = N \cdot 2\mathrm{e}^{-2n\epsilon^2} := \delta$$

Solving for ϵ gave, w.h.P. $> 1-\delta$:

$$|\mathcal{L}_P(h) - \mathcal{L}_S(h)| \leq \sqrt{\frac{2(\log(2N) + \log(1/\delta))}{n}}$$

for all $h \in H$.

For classes of bounded VC (sketch!):

$$\Pr\left[\sup_{h\in H} |\mathcal{L}_P(h) - \mathcal{L}_S(h)| > \epsilon\right]$$
$$\lesssim \Pr\left[\sup_{h\in H} |\mathcal{L}_{S'}(h) - \mathcal{L}_S(h)| > \epsilon/2\right]$$
$$\lesssim \Pr\left[\bigvee_{h\in H|_{S'\cup S}} |\mathcal{L}_{S'}(h) - \mathcal{L}_S(h)| > \epsilon/2\right]$$
$$\lesssim |S' \cup S|^d \cdot 2\mathrm{e}^{-2n\epsilon^2} := \delta$$

We get w.h.P. $> 1-\delta$:

$$|\mathcal{L}_P(h) - \mathcal{L}_S(h)| \leq c \cdot \sqrt{\frac{d + \log(1/\delta))}{n}}$$

for all $h \in H$.

No Free Lunch Theorem

Theorem
Let $\mathcal{X}$ be an infinite domain. For every learning algorithm $\mathcal{A}$, and every sample size $n \in \mathbb{N}$, there exists a distribution P such that

$$\mathop{\mathbb{E}}_{S \sim P^n} [\mathcal{L}_P(\mathcal{A}(S))] \geq \frac{1}{4}$$

The distribution P is rather benign:

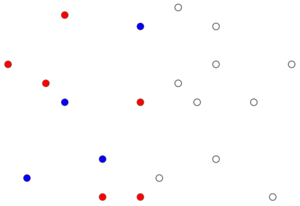
- There is a predictor h with $\mathcal{L}_P(h) = 0$
- The support of P has size $2n$.

No Free Lunch – Proof idea

$$\forall \mathcal{A} \forall n \exists P : \underset{S \sim P^n}{\mathbb{E}} [\mathcal{L}_P(\mathcal{A}(S))] \geq \frac{1}{4}$$

As **possible distributions** P, consider:

- support of $2n$ points
- all possible labelings over these points
- $\mathcal{A}$ gets to "see" labels on half the points
- for each point not in S, $\mathcal{A}$ mis-predicts with probability $1/2$



Implications of the No Free Lunch Theorem

The same proof technique can be used to prove lower bounds for learning VC-classes.

The sample complexity of learning a class H with $\mathrm{VC}(H) = d$, even in the realizable case, is lower bounded by $\Omega(\frac{d}{\epsilon})$.

There is no universally successful learning algorithm.
(Every learner has an "inductive bias", and needs this bias to be successful on some tasks).

Thank You!