Trustworthy Machine Learning

Machine Learning Theory

Sangdon Park

POSTECH

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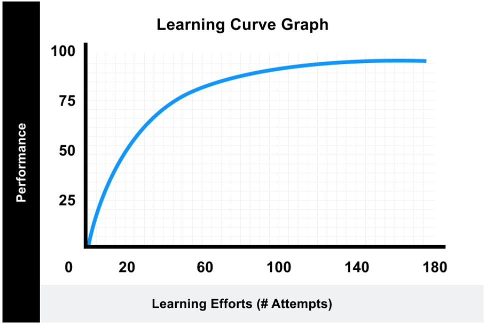
What is Learning Theory?

Theory on exploring conditions (or assumptions) when machines can learn from data.



https://www.valamis.com/hub/learning-curve

- Statistical learning theory
- Online learning theory

Historical Figure: Vladimir Vapnik

vapnik

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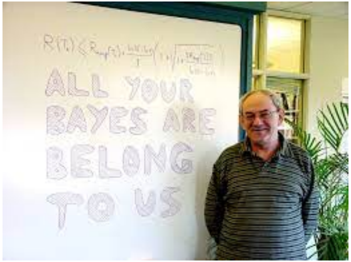
Professor of Columbia, Fellow of NEC Labs America,
Verified email at nec-labs.com

machine learning statistics computer science

TITLE	CITED BY	YEAR
The Nature of Statistical Learning Theory V Vapnik Data mining and knowledge discovery	104201 *	1995
Support-vector networks C Cortes, V Vapnik Machine learning 20, 273-297	62445	1995
A training algorithm for optimal margin classifiers BE Boser, IM Guyon, VN Vapnik Proceedings of the fifth annual workshop on Computational learning theory …	16380	1992
Backpropagation applied to handwritten zip code recognition Y LeCun, B Boser, JS Denker, D Henderson, RE Howard, W Hubbard, ... Neural computation 1 (4), 541-551	15122	1989
Gene selection for cancer classification using support vector machines I Guyon, J Weston, S Barnhill, V Vapnik Machine learning 46, 389-422	11033	2002
Support vector regression machines H Drucker, CJ Burges, L Kaufman, A Smola, V Vapnik Advances in neural information processing systems 9	6005	1996



- "The Nature of Statistical Learning Theory": summary of his papers up to 1995.
- VC dimension, SVM, ...

Historical Figure: Leslie Valiant

Leslie Valiant
Unknown affiliation
No verified email

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TITLE	CITED BY	YEAR
A theory of the learnable LG Valiant Communications of the ACM 27 (11), 1134-1142	7939	1984
A bridging model for parallel computation LG Valiant Communications of the ACM 33 (8), 103-111	5399	1990
The complexity of computing the permanent LG Valiant Theoretical computer science 8 (2), 189-201	3413	1979
The complexity of enumeration and reliability problems LG Valiant siam Journal on Computing 8 (3), 410-421	2579	1979
Cryptographic limitations on learning boolean formulae and finite automata M Kearns, L Valiant Journal of the ACM (JACM) 41 (1), 67-95	1318	1994
Random generation of combinatorial structures from a uniform distribution MR Jerrum, LG Valiant, VV Vazirani Theoretical computer science 43, 169-188	1218	1986

- “PAC Learning Theory” in 1984
- Turing Award winner in 2010

Four Key Ingredients of Learning Theory

The simplified objective of *statistical* learning theory:

$$\begin{aligned} \text{find} \quad & f \\ \text{subj. to} \quad & f \in \mathcal{F} \\ & \mathbb{E}_{(x,y)\sim D}\, \ell(x, y, f) \leq \varepsilon \end{aligned}$$

or

$$\min_{f \in \mathcal{F}} \mathop{\mathbb{E}}_{(x,y)\sim D} \ell(x, y, f)$$

- **Ingredient 1**: A distribution D (*e.g.*, a distribution over labeled images)
- **Ingredient 2**: Hypothesis space $\mathcal{F}$ (*e.g.*, linear functions, a set of resnet)
- **Ingredient 3**: A loss function ℓ (*e.g.*, 0-1 loss, L1 loss, cross-entropy loss)
- **Ingredient 4**: A learning algorithm (*e.g.*, GD)

Main Goal: Finding Conditions for Learnability

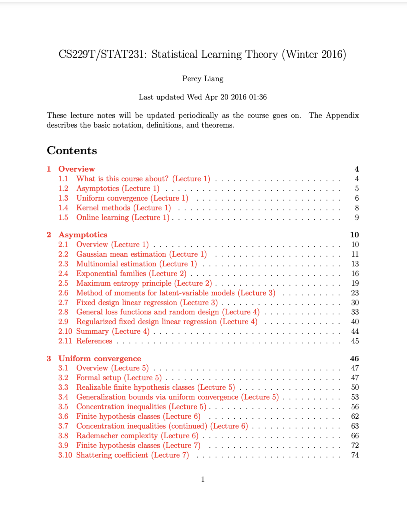
An Example

Conditions:

- D: *linearly separable* dog and cat image distribution
- $\mathcal{F}$: linear functions – encode prior of a data distribution
- ℓ: 0-1 loss for classification – represent task
- a learning algorithm: a gradient descent (GD) algorithm

Checking Learnability:
If we prove that the GD algorithm can find the true linear function with a "desired level" of loss, we say $\mathcal{F}$ is learnable. In this case, we say the GD algorithm is a "good" algorithm.

Contents from



CS229T/STAT231: Statistical Learning Theory (Winter 2016)

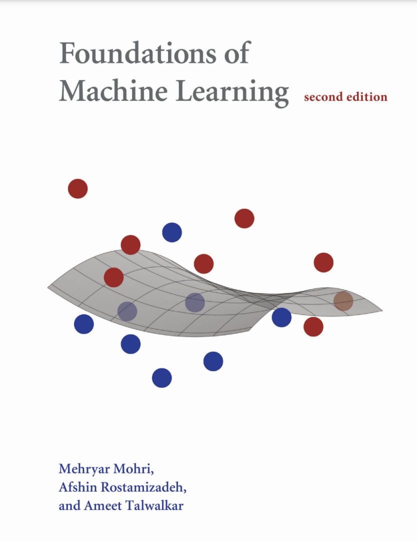
Percy Liang

Last updated Wed Apr 20 2016 01:36

These lecture notes will be updated periodically as the course goes on. The Appendix describes the basic notation, definitions, and theorems.

Contents

1



and various papers.

Why PAC Learning?

The key questions in machine learning:

- When can we learn?
- How many samples do we need to have a good model?

The PAC framework provides partial answers to these key questions.

Recall Four Key Ingredients of Learning Theory

- Distribution – setup / assumption
  - image distribution, language distribution
  - samples are independently drawn from the same distribution
- Loss – a goodness metric for a desired task
  - classification: 0-1 loss
  - regression: L1 loss
- Hypothesis space – prior on the distribution, what we will design!
  - convolution network: good for image classification
  - transformers: good for language modeling
- A learning algorithm – what we will design!
  - convolution network: good for image classification

Assumption

Assumption

We assume that labeled examples are independently drawn from the same (and unknown) distribution $\mathcal{D}$ over labeled examples $\mathcal{X} \times \mathcal{Y}$.

- "independent": not sequential data
- "unknown": yes, we don't the true distribution
- "same": key for success
- A.K.A. the i.i.d. assumption
- The i.i.d. assumption is the standard setup.
- It is easily broken due to distribution shift.
- Online learning relaxes this assumption (under some conditions).

A Goodness Metric: Expected Error for Classification

Definition (expected error)

Given a hypothesis $h \in \mathcal{H}$ and an underlying distribution $\mathcal{D}$, the expected error is defined by

$$L(h) := \mathbb{P}\left\{h(x) \neq y\right\} = \mathbb{E}\left\{\mathbb{1}\left(h(x) \neq y\right)\right\},$$

where the probability is taken over $(x, y) \sim \mathcal{D}$ and $\mathbb{1}$ is the indicator function.

- Suppose the classification task. But, we can use any task-dependent loss.
- This expected error of h is sometimes called the *risk* of h or the *generalization error* of h.
- The indicator function is defined as follows:

$$\mathbb{1}\left(s\right) := \begin{cases} 1 & \text{if } s \text{ is true} \\ 0 & \text{if } s \text{ is false} \end{cases}.$$

A Goodness Metric: Empirical Error

Definition (empirical error)

Given a hypothesis $h \in \mathcal{H}$ and labeled samples $\mathcal{S} := ((x_1, y_1), \cdots, (x_n, y_n))$, the empirical error is defined by

$$\hat{L}(h) := \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(h(x_i) \neq y_i\right),$$

where $\mathbb{1}$ is the indicator function.

- This empirical error of h is sometimes called the *empirical risk* of h.

One More Assumption

Assumption

We assume that a distribution $\mathcal{D}$ is separable by some hypothesis $h^* \in \mathcal{H}$, i.e.,

$$L(h^*) = 0.$$

- *e.g.*, learning a threshold function.
- This assumption is strong but useful in some cases (*e.g.*, PAC conformal prediction).
- This assumption will be removed later (in a more general learning framework).

Approximately Correct

A Goodness Metric for Algorithms

Definition

Given $\varepsilon > 0$, we say that h is approximately correct if

$$L(h) \leq \varepsilon.$$

- ε is a user-defined parameter.
- Recall that L is an expected error.
- We want to find h that achieves a desired error level ε.
- h is learned from data; thus, h is also a random variable.

Probably Approximately Correct (PAC)

A Goodness Metric for Algorithms

Definition

Given $\varepsilon > 0$, $\delta > 0$, and $\mathcal{S} := ((x_1, y_1), \ldots, (x_n, y_n)) \in (\mathcal{X} \times \mathcal{Y})^n$, we say that an algorithm $\mathcal{A}$ is probably approximately correct if

$$\mathbb{P}\left\{L(\mathcal{A}(\mathcal{S})) \leq \varepsilon\right\} \geq 1 - \delta,$$

where $\mathcal{A} : (\mathcal{X} \times \mathcal{Y})^* \to \mathcal{H}$ and the probability is taken over $\mathcal{S} \sim \mathcal{D}^n$.

- $S^* := \bigcup_{i=0}^{\infty} S^i$
- $\mathcal{S} \sim \mathcal{D}^n$: i.i.d. samples
- $\mathcal{A}$: a learning algorithm

PAC Learning Algorithm

Definition (simplified definition)

An algorithm $\mathcal{A}$ is a PAC-learning algorithm for $\mathcal{H}$ if for any $\varepsilon > 0$, $\delta > 0$, $h^* \in \mathcal{H}$, and $\mathcal{D}$ separable by h^*, and for some minimum sample size n^* (which depends on $\varepsilon, \delta, \mathcal{D}$), the following holds with any sample size $n \geq n'$:

$$\mathbb{P}\left\{L(\mathcal{A}(\mathcal{S})) \leq \varepsilon\right\} \geq 1 - \delta,$$

where $\mathcal{S} := ((x_1, y_1), \ldots, (x_n, y_n)) \sim \mathcal{D}^n$.

- Please check out the original PAC learning definition.
- The algorithm should satisfy the PAC guarantee for any $\mathcal{D}$ and h^*.
- If $\mathcal{D}$ is "complex" (thus h^* is complex), we need more samples.
- If ε (or δ) is small, we need more samples.

Example: A Learning Bound for a Finite Hypothesis Set I

Setup:

- $\mathcal{H}$: a *finite* set of functions mapping from $\mathcal{X}$ to $\mathcal{Y}$
  - *e.g.*, a set of experts
- $\mathcal{D}$: a distribution is separable by $h^* \in \mathcal{H}$
- $\mathcal{S}$: labeled examples
- $\mathcal{A}$: an algorithm that satisfies $\hat{L}(\mathcal{A}(\mathcal{S})) = 0$
  - *i.e.*, $\mathcal{A}$ returns a "consistent" hypothesis.
  - Here, the algorithm exploits the fact on separability!

Example: A Learning Bound for a Finite Hypothesis Set II

Theorem

For any $\varepsilon > 0$, $\delta > 0$, $h^* \in \mathcal{H}$, and $\mathcal{D}$ separable by h^*, we have

$$L(\mathcal{A}(\mathcal{S})) \leq \frac{1}{m}\left(\log|\mathcal{H}| + \log\frac{1}{\delta}\right)$$

with probability at least $1 - \delta$.

- $\mathcal{A}$ is a PAC learning algorithm.
- Sample complexity?

$$m \geq \frac{1}{\varepsilon}\left(\log|\mathcal{H}| + \log\frac{1}{\delta}\right)$$

  - See? As $\mathcal{H}$ gets complex and as ε and δ are smaller, we need more samples.
- **key**: A union bound over the events of each hypothesis.

Example: A Learning Bound for a Finite Hypothesis Set III

Lemma (the union bound)

Let $A_1, \ldots, A_K$ be K different events (which might not be independent). Then,

$$\mathbb{P}\left\{\bigcup_{k=1}^{K} A_k\right\} \leq \sum_{k=1}^{K} \mathbb{P}\left\{A_k\right\}.$$

Example: A Learning Bound for a Finite Hypothesis Set IV

Proof Sketch:
Let $\mathcal{H}_\varepsilon := \{h \in \mathcal{H} \mid L(h) > \varepsilon\}$. Then, we have

$$\begin{aligned}
\mathbb{P}\left\{\exists h \in \mathcal{H}_\varepsilon, \hat{L}(h) = 0\right\} &= \mathbb{P}\left\{\bigvee_{h \in \mathcal{H}_\varepsilon} \hat{L}(h) = 0\right\} &(1)\\
&\leq \sum_{h \in \mathcal{H}_\varepsilon} \mathbb{P}\left\{\hat{L}(h) = 0\right\} &(2)\\
&\leq \sum_{h \in \mathcal{H}_\varepsilon} (1-\varepsilon)^m &(3)\\
&\leq |\mathcal{H}|(1-\varepsilon)^m.
\end{aligned}$$

- (1): uniform convergence
- (2): union bound due to the finite hypotheses
- (3): a "point" bound due to the i.i.d. assumption and $\mathbb{1}\{h(x) \neq y\}$ is a Bernoulli r.v.

Next

Relax assumptions:

- What if we have an infinite hypothesis set?
- What if $\mathcal{D}$ is not separable?

We will explore a more general learning bound.