Machine Learning

Bias-Complexity Trade-off

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Our Goal in Learning

Given:

- training set: $S = ((x_1, y_1), \dots, (x_m, y_m))$
- loss function: $\ell(h, (x, y))$

Want: a function $\hat{h}$ such that $L_{\mathcal{D}}(\hat{h})$ *is small*

We can pick: the learning algorithm A, that given S will produce $\hat{h} = A(S)$

for example with perceptron algorithm we are also implying we use linear models (we implicitly specify H)

Note: A comprises:

- the hypothesis set $\mathcal{H}$
- the procedure to pick $\hat{h} = A(S)$ from $\mathcal{H}$

Question: is there a *universal learner*, i.e., an (implementable) algorithm A that predicts the best $\hat{h}$ for any distribution $\mathcal{D}$?

The No Free Lunch Theorem

The following answers the previous question for some specific settings.

Theorem (No-Free Lunch)

Let A be any learning algorithm for the task of binary classification with respect to the 0-1 loss over a domain $\mathcal{X}$. Let m be any number smaller than $|\mathcal{X}|/2$, representing a training set size. Then, there exists a distribution $\mathcal{D}$ over $\mathcal{X} \times \{0,1\}$ such that:

- *there exists a function $f\colon \mathcal{X} \to \{0,1\}$ with $L_{\mathcal{D}}(f) = 0$*
- *with probability of at least $1/7$ over the choice of $S \sim \mathcal{D}^m$ we have that $L_{\mathcal{D}}(A(S)) \geq 1/8$.*

Note: there are similar results for other learning tasks.

No Free Lunch and Prior Knowledge

Corollary

Let $\mathcal{X}$ be an infinite domain set and let $\mathcal{H}$ be the set of all functions from $\mathcal{X}$ to $\{0, 1\}$. Then, $\mathcal{H}$ is not PAC learnable.

What's the implication?

We need to use our prior knowledge about $\mathcal{D}$ to pick a *good* hypothesis set.

How do we choose $\mathcal{H}$?

- we would like $\mathcal{H}$ to be *large*, so that it may contain a function h with small $L_{\mathcal{D}}(h)$
- no free lunch $\Rightarrow$ $\mathcal{H}$ cannot be too large!

Error Decomposition

Let h_S be an $\mathrm{ERM}_{\mathcal{H}}$ hypothesis.

Then

$$L_{\mathcal{D}}(h_S) = \epsilon_{\text{app}} + \epsilon_{\text{est}}$$

where

- $\epsilon_{\text{app}} = \min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$ (approximation error)
- $\epsilon_{\text{est}} = L_{\mathcal{D}}(h_S) - \min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$ (estimation error)

for example if I just have one hypotesis we will have big approx. err. and estimation error

if I have H all functions to {0,1} I will have big estimation error (best h hard to find) but small approx error, there probably is a good h in H

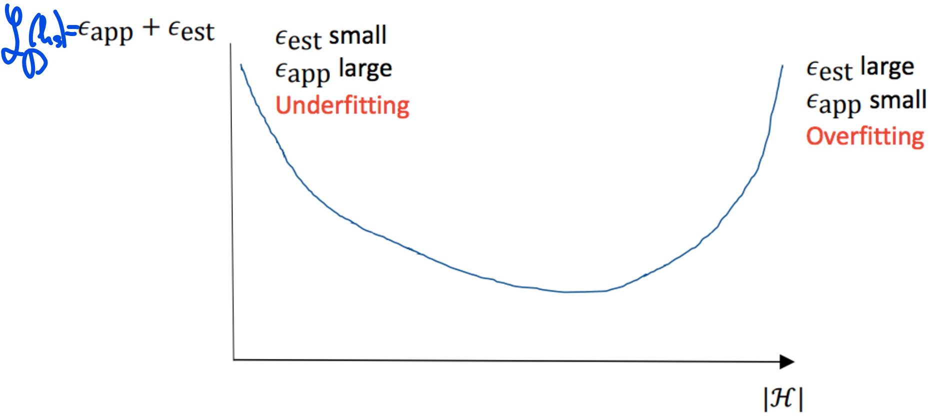
Approximation error: $\epsilon_{\text{app}} = \min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$

- derives from our choice of $\mathcal{H}$
- once we have chosen $\mathcal{H} \Rightarrow \epsilon_{\text{app}}$ is unavoidable!
- to decrease it, chose a "larger" $\mathcal{H}$

Estimation error: $\epsilon_{\text{est}} = L_{\mathcal{D}}(h_S) - \min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$

- derives from our inability to choose (with ERM) the best hypothesis
- could be avoided if had chosen the best hypothesis!
- to decrease, we need a low number of hypotheses in $\mathcal{H}$ so that training error is good estimate of generalization error for all of them $\Rightarrow$ need a "small" $\mathcal{H}$

Complexity of $\mathcal{H}$ and Error Decomposition



Low complexity
Large inductive bias

High complexity
Small inductive bias

Estimating $L_{\mathcal{D}}(h_S)$

How can we estimate the generalization error $L_{\mathcal{D}}(h)$ for a function h, for example $h_S \in \text{ERM}_{\mathcal{H}}$?

We can use a **test set**: new set of samples not used for picking h_S (=the training set).

Notes:

- the test must not be looked at until we have picked our **final** hypothesis!
- in practice: we have 1 set of samples and we split it in *training set* and *test set*.

Bibliography

[UML] Chapter 5