Chapter 5 No Free Lunch



• There are many No-Free-Lunch theorems.

• The one we prove in this chapter only says that there is no universal learner.

 If the hypothesis class is not restricted then there is ALWAYS a distribution that causes the algorithm to overfit (not only ERM!)

- (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 X. Let m be any number smaller than |X|/2, representing a training set size. Then, there exists a distribution D over X ×{0,1} such that:
- There exists a function f:X \rightarrow {0,1} with $L_D(f) = 0$. (i.e. task can be learned)
- With probability of at least $\frac{1}{7}$ over the choice of $S \sim D^m$ we have that $L_D(A(S)) \ge \frac{1}{8}$. (i.e at least 1/7 chance to have true error > 1/8)

• Lemma:

Z r.v. in [0,1] with E[Z]=m. Then $\forall a \in (0,1)$ $P[Z > 1 - a] \ge \frac{m - (1 - a)}{a}$

• Proof:

Y=1-Z. Applying Markov we have $P[Z > 1 - a] = 1 - P[\Upsilon \ge a] \ge 1 - \frac{1 - m}{a}$

The above shows that

$$E_{S\sim D}m[L_D(A(S))] \ge \frac{1}{4} \to \boldsymbol{P}[L_D(A(S)) \ge \frac{1}{8}] \ge \frac{1}{7}$$

- It suffices to prove the below (by Markov)
- $\forall A \exists D \text{ such that } E_{S \sim D^m}[L_D(A(S))] \geq \frac{1}{4}$

- In other words every algorithm has a distribution on which it fails ¼ of the time in expectation.
- Intuition:

• Equivalently we want to show

$$\max_{i\in[T]} E_{S\sim D_i}^m [L_{D_i}(A(S))] \ge \frac{1}{4}$$

- Denote S_jⁱ the training sequence of size m labeled by the function f_i corresponding to distribution D_i. There are m^{2m} possible training sets that can be sampled at equal probability.
- Therefore expected loss for a fixed i is equal to k

$$\frac{1}{k}\sum_{j=1}^{\kappa}L_{D_i}\left(A\left(S_j^i\right)\right)$$

where k = m^{2m}

•
$$\max_{i \in [T]} \frac{1}{k} \sum_{j=1}^{k} L_{D_{i}}(A(S_{j}^{i})) \geq \frac{1}{T} \sum_{i=1}^{T} \frac{1}{k} \sum_{j=1}^{k} L_{D_{i}}(A(S_{j}^{i})) = \frac{1}{K} \sum_{j=1}^{k} \frac{1}{T} \sum_{i=1}^{T} L_{D_{i}}(A(S_{j}^{i})) \geq \frac{1}{K} \sum_{j=1}^{k} \frac{1}{T} \sum_{i=1}^{T} L_{D_{i}}(A(S_{j}^{i})) \leq \frac{1}{K} \sum_{j\in [k]}^{T} \frac{1}{T} \sum_{i=1}^{T} L_{D_{i}}(A(S_{j}^{i}))$$

(I)

Let u₁, u₂,..., u_n be the examples not in the training set (so p≥m). The true loss is at least half as much as the loss on the unknown examples.

•
$$L_{D_i}(h) = \frac{1}{2m} \sum_{x \in C} \mathbf{1}_{[h(u_r) \neq f_i(u_r)]} \ge \frac{1}{2m} \sum_{r=1}^p \mathbf{1}_{[h(u_r) \neq f_i(u_r)]} \ge \frac{1}{2p} \sum_{r=1}^p \mathbf{1}_{[h(u_r) \neq f_i(u_r)]}$$

 Bounding true loss from below and changing summation order

•
$$\frac{1}{T} \sum_{i=1}^{T} L_{D_i}(A(S_j^i)) \geq \frac{1}{T} \sum_{i=1}^{T} \frac{1}{2p} \sum_{r=1}^{p} \mathbf{1}_{[A(S_j^i)(u_r) \neq f_i(u_r)]} = \frac{1}{2p} \sum_{r=1}^{p} \frac{1}{T} \sum_{i=1}^{T} \mathbf{1}_{[A(S_j^i)(u_r) \neq f_i(u_r)]} \geq \frac{1}{2} * \min_{r \in [p]} \frac{1}{T} \sum_{i=1}^{T} \mathbf{1}_{[A(S_j^i)(u_r) \neq f_i(u_r)]}$$
(II)

• For a fixed r, all functions f_i , $f_{i'}$ can be paired according to their classification of u_r

•
$$\mathbf{1}_{[A(S_{j}^{i})(u_{r})\neq f_{i}(u_{r})]} + \mathbf{1}_{[A(S_{j}^{i'})(u_{r})\neq f_{i'}(u_{r})]} = 1$$

 $\rightarrow \frac{1}{T} \sum_{i=1}^{T} \mathbf{1}_{[A(S_{j}^{i})(u_{r})\neq f_{i}(u_{r})]} = \frac{1}{2}$ (III)

$$(I),(II),(III) \to \max_{i \in [T]} E_{S \sim D_i} m [L_{D_i} \left(A \left(S_j^i \right) \right)] \ge \frac{1}{4}$$

• Corollary:

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

• Proof:

Assume that H is learnable, choosing $\varepsilon < 1/8$ and $\delta < 1/7$. By PAC definition $\exists A,m=m(\varepsilon,\delta)$ such that A given training size $\geq m$, with P>1- δ , $L_{D_i}(A(S)) \leq \varepsilon$.

However, by No-Free-Lunch theorem since X>2m (i.e learner knows at most half of universe) \exists D such that $P[L_D(A(S)) \ge \frac{1}{8}] \ge \frac{1}{7}$. Contradiction.

- To prevent this we must avoid distributions that can deceive us. (i.e increase our bias about the underlying model).
- On the other hand, we need to keep our hypothesis class rich enough to contain the zero error f (or smallest in APAC setting).

• Bias vs Variance.

• In particular, we can decompose the error of an ERM hypothesis $L_D(h_s) = \varepsilon_{app} + \varepsilon_{est}$

•
$$\varepsilon_{app} = \min_{h \in H} L_D(h)$$

(bias, price of restricting our class, sample size cant reduce this)

•
$$\varepsilon_{est} = L_D(h_s) - \min_{h \in H} L_D(h)$$

(variance, needing more data to train our model)

 The less we restrict the class the more data we need (no restriction=all the data) Therefore we need to restrict our class somewhat with educated guesses. Less sacrifices => need more data to counteract estimation error.

- Example:
- Basic Euclidean classification can generalize better (81%) than more sophisticated Naïve Bayes (75%)