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The Bias-Complexity Trade-Off

Machine Learning 2022-23
UML Book Chapter 5
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Recall: Agnostic PAC Learnability

- Idea: We drop the requirement of finding the best predictor
  - but we do not want to be too far from it

- Recall definition of *Agnostic PAC Learnability*:

A hypothesis class $\mathcal{H}$ is agnostic PAC learnable if there exist a function $m_{\mathcal{H}}: (0,1)^2 \rightarrow \mathbb{N}$ and a learning algorithm such that for every $\delta, \epsilon \in (0,1)$ and for every distribution D over $\mathcal{X} x \mathcal{Y}$, when running the algorithm on $m \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d. examples generated by D the algorithm returns a hypothesis h such that, with probability $\geq 1 - \delta$ (over the choice of the m training examples):

$$L_D(h) \leq \min_{h' \in \mathcal{H}} L_D(h') + \epsilon$$

A Universal Learner ?

Given a training set S and a loss function we'd like to find a function $\hat{h}$ for which $\mathrm{L_d}(\hat{h})$ is small

Pick a learning algorithm A that given S produces function $\hat{h}$

It depends on two components:

1. the hypothesis set $\mathcal{H}$
2. the procedure to pick $\hat{h}$ from $\mathcal{H}$

Is there a universal learner, i.e., an algorithm A that predicts the best $\hat{h}$ for any distribution D ?

What about using the set of all functions from $\mathcal{X}$ to $\mathcal{Y}$ as the hypothesis class ?

No Free Lunch Theorem

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 X. Let m be any number smaller than $\frac{|X|}{2}$, representing a training set size. Then there exist a distribution D over $X \times \{0,1\}$ such that:

1. There exist a function $f : X \to \{0,1\}$ with $L_D(f) = 0$
2. With probability of at least 1/7 over the choice of $S \sim D^m$ we have that $L_D(A(S)) \geq \frac{1}{8}$

Corollary (No-Free Lunch)

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

No Free Lunch: Notes

- *Key message*: for every ML algorithm there exist a task on which it fails even if another ML algorithm is able to solve it

- *Idea of the proof*: our training set is smaller than half of the domain → no information on what happens on the other half → there exist some target function f that works on the other half in a way that contradicts our estimated labels
  - *Full demonstration not part of the course*

- Class $\mathcal{H}$ of all possible functions from $\mathcal{X}$ to {0,1} (i.e., assuming *no prior knowledge*) is not a good idea

Corollary: Demonstration

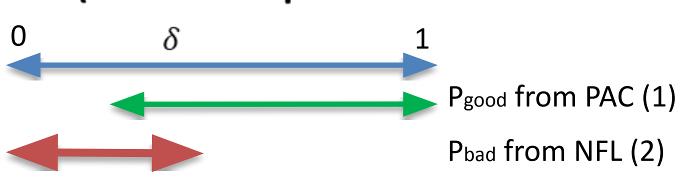
> ***Corollary (No-Free Lunch)***
> Let *X* be an infinite domain set and let *H* be the set of all functions from *X* to $\{0,1\}$. Then, *H* is not PAC learnable

Proceed *by contradiction*

1. Assume PAC Learnable
   - Choose $\epsilon < \frac{1}{8}$, $\delta < \frac{1}{7}$, and recall that $\mathcal{H}$ includes all functions (*)
   - By definition of PAC: it exists an algorithm A and such that for every distribution D, if realizable*, when running the algorithm on m i.i.d. examples generated by D the algorithm returns a hypothesis *h* such that, with probability $\geq 1 - \delta$, $L_D(A(S)) \leq \epsilon$

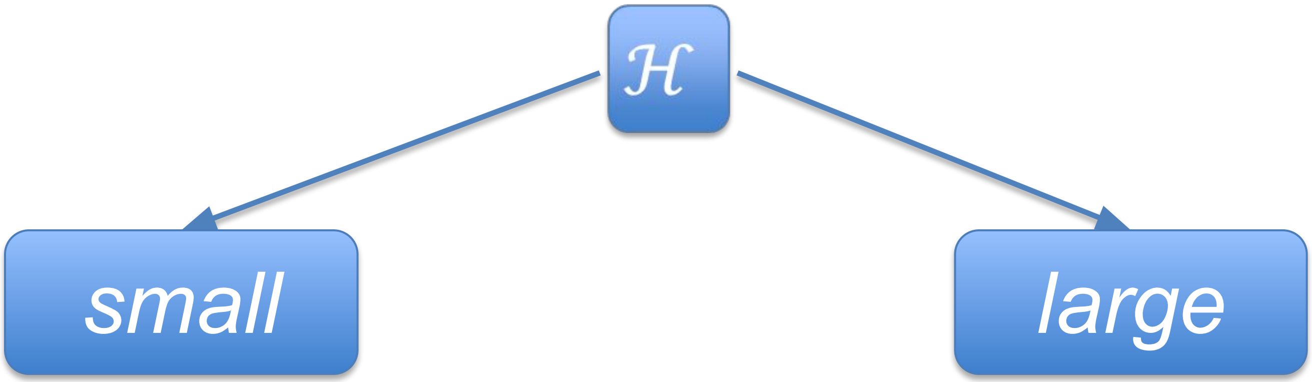
2. Apply No-Free Lunch theorem to A
   - $|\mathcal{X}| > 2m$ (it is ∞) : for any ML algorithm (including A!) there exist a distribution D for which with probability $\geq \frac{1}{7} > \delta$, $L_D(A_S) \geq \frac{1}{8} > \epsilon$

3. The two blue results are in contradiction (sum of probabilities is bigger than one!)



Proof: not part of the course

Choose a Good Hypothesis Set



Low approximation capabilities (large L_S)
Good generalization properties ($L_D \sim L_S$)

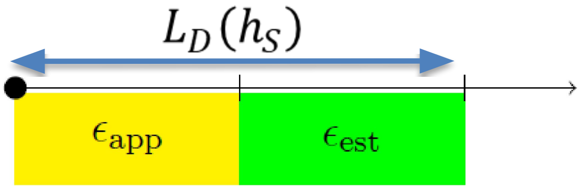
Good approximation capabilities (small L_S)
Risk of overfitting ($L_D \gg L_S$)

- We need to use our prior knowledge about D to pick a good hypothesis set
- We would like $\mathcal{H}$ to be large, so that it may contain a function *h* with small $L_S(h)$ and hopefully a small $L_D(h)$
- No free lunch: $\mathcal{H}$ cannot be too large!

  → A Too large $\mathcal{H}$ leads to the risk of overfitting

Error Decomposition (1)

Consider an $ERM_{\mathcal{H}}$ hypothesis h_s :



The true error of $ERM_{\mathcal{H}}$ can be decomposed as:

$$L_D(h_S) = \epsilon_{app} + \epsilon_{est}$$

$$\epsilon_{app} = \min_{h \in \mathcal{H}} L_D(h)$$

Approximation error

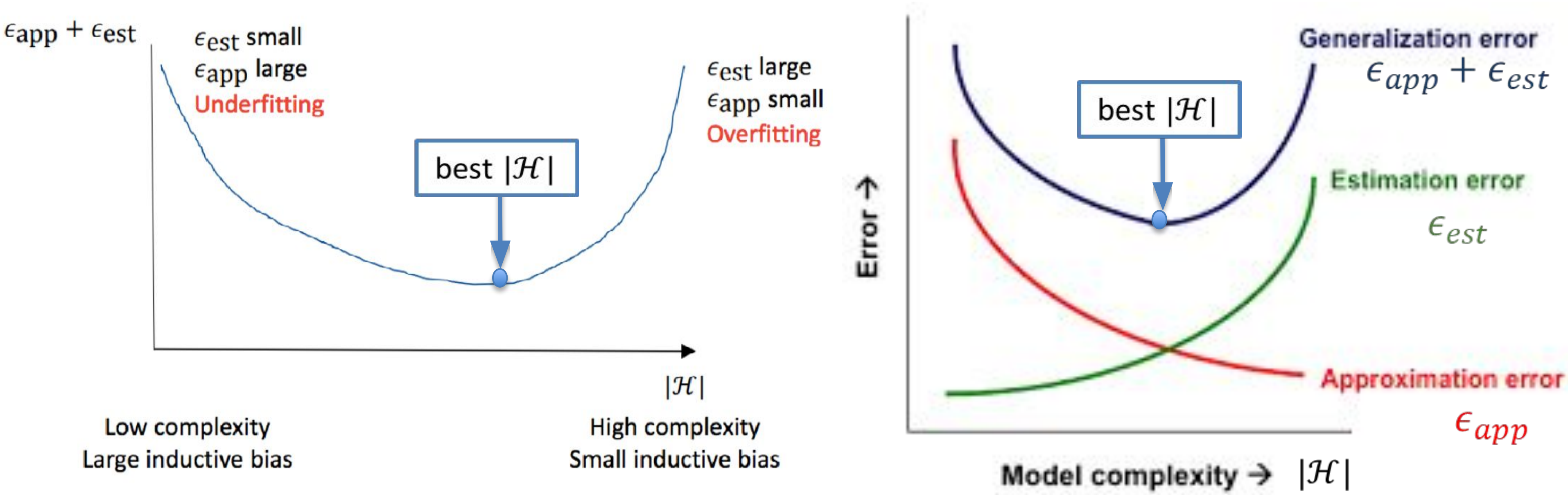
- Minimum true risk achievable by a predictor in $\mathcal{H}$
- Depends on the choice of $\mathcal{H}$ (*but not on S*)
- Once $\mathcal{H}$ is selected it is fixed
- Larger $\mathcal{H}$ → smaller ϵ_{app}
- ϵ_{app} = 0 if realizability holds
- Otherwise bounded by Bayes predictor

$$\epsilon_{est} = L_D(h_s) - \min_{h \in \mathcal{H}} L_D(h)$$

Estimation error

- Difference between true error of ERM predictor and approximation error
- Due to the not-optimal ML algorithm not able to find the best h^* using ERM
- Depends on S (typically smaller for larger S)
- To decrease we need a smaller $\mathcal{H}$ so the training error is a good estimate of true error

Error Decomposition (2)



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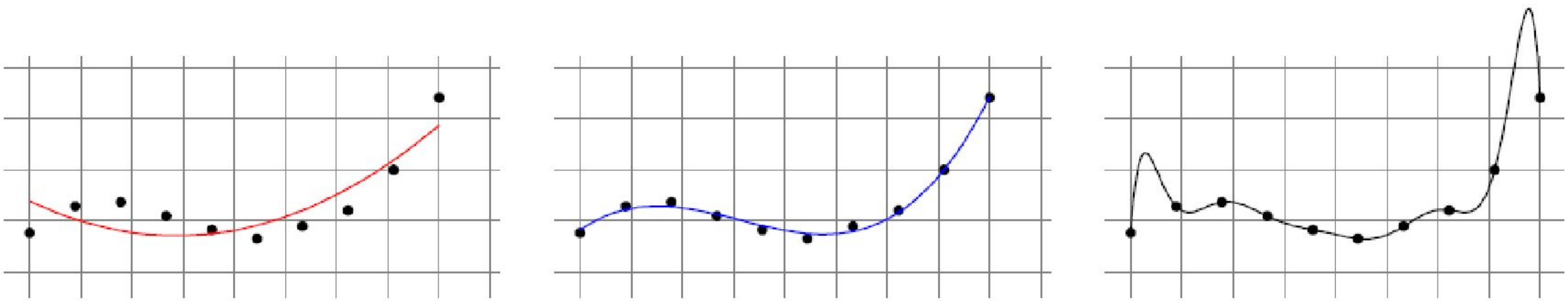
Example: Polynomial Fitting

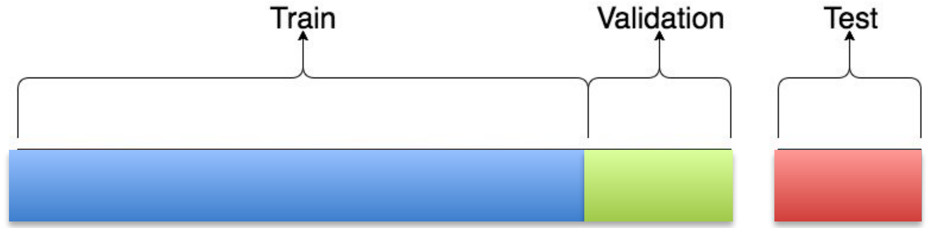
A) degree 2 *B)* degree 3 *C)* degree 10



A) underfitting *B) good approximation* *C) overfitting*

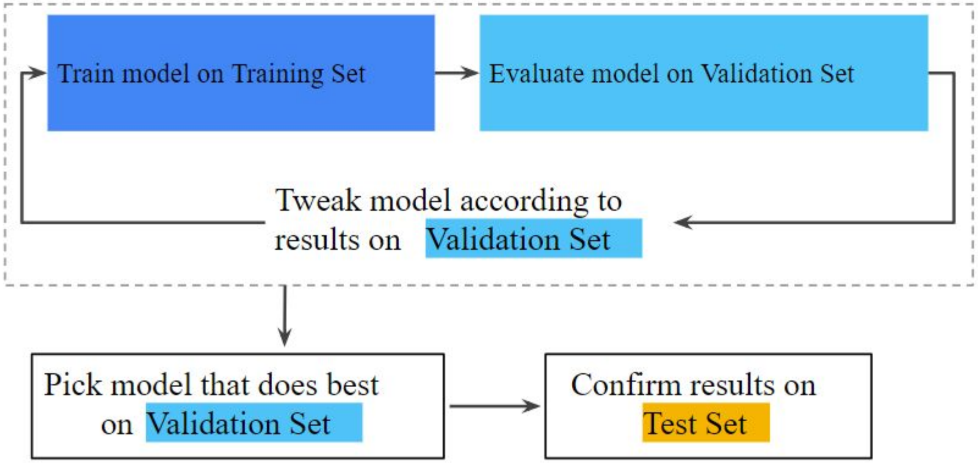
A. Degree 2: large ϵ_{app} , small ϵ_{est} (underfitting)
B. Degree 10: $\epsilon_{app} = 0$, large ϵ_{est} (overfitting)
C. Degree 3: good compromise *(best solution ?)*

Train, Test and Validation Sets



- We need to estimate the generalization error $L_D(h)$ for a function *h* (e.g., the one we selected with ERM)
- Use a test set: a new set of samples not used for picking *h*
  - It must be different (disjoint) from the training set
  - More reliable estimation of $L_D(h)$ (***but still an estimation!!***)
  - 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
- Sometimes the training set is further divided into a training set and a validation set
  - The validation set is used for selecting the hyper-parameters of the algorithm
  - Can be used to evaluate error while iterative training procedures are running

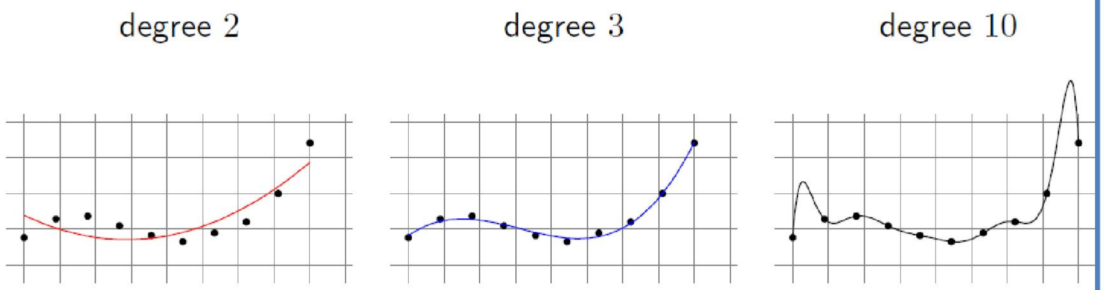
Iterative Training Procedure with Validation Set



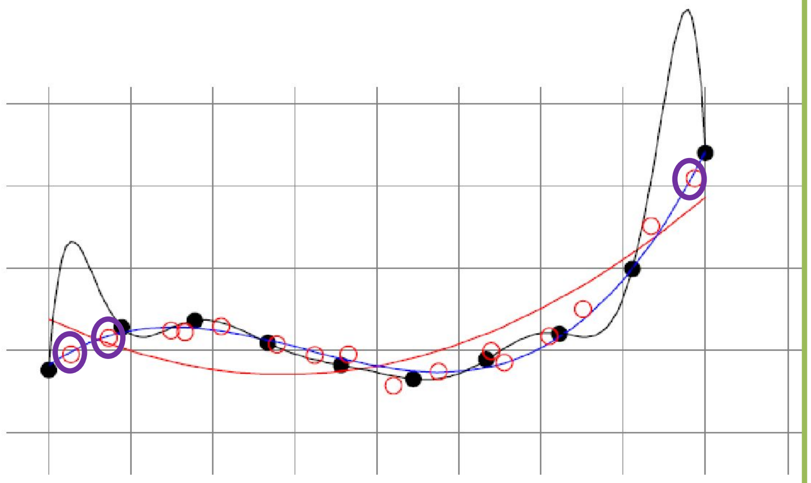
Train a ML algorithm parametrized by some Hyper-Parameters (HP):

1. Select Hyper-Parameters values
2. Train on the training set
3. Evaluate performances on the validation set
4. Go back to 1 (select new HP values)
5. Select HP leading to smallest validation error
6. Compute error estimation on the test set

Example (with validation set)



- Training set S : black circles
- Hyper-parameter = degree of the model (2, 3 or 10)
- Perform ERM minimization over **training** set S:
  - Degree 10 is the best solution ($L_S(h_S) = 0$) !



- Introduce a validation set (red circles)
- Train on training set for each of the 3 HP values (2,3 and 10)
- Select solution with lower error on **validation** set
  - Degree 3 is the best solution
  - Degree 10 has low error on training set but high on validation set

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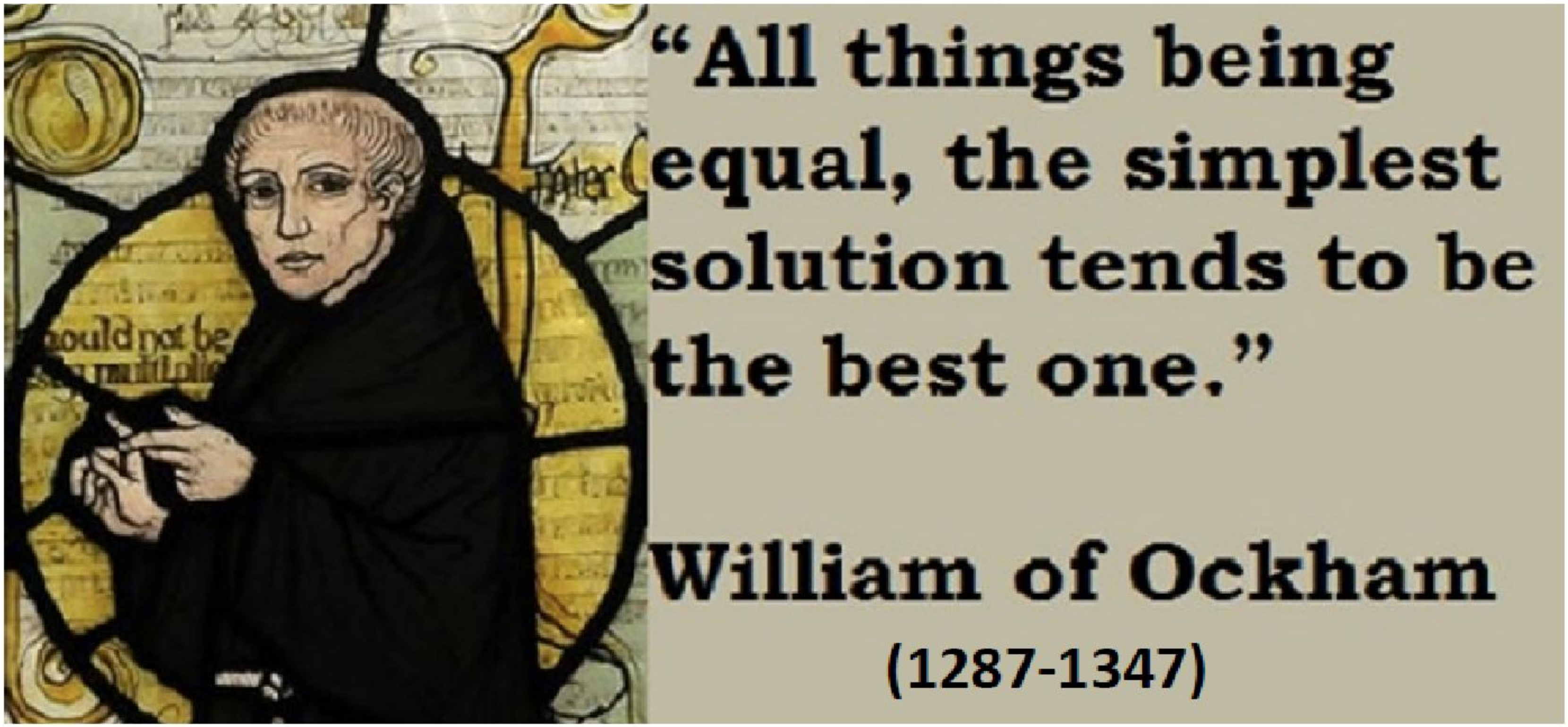
Occam's Razor



A short explanation (that is, a hypothesis that has a short length) tends to be more valid than a long explanation