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Statistical Learning Theory

CS4780/5780 – Machine Learning
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Reading: Mitchell Chapter 7 (not 7.4.4 and 7.5)

Outline

Questions in Statistical Learning Theory:

- How good is the learned rule after n examples?
- How many examples do I need before the learned rule is accurate?
- What can be learned and what cannot?
- Is there a universally best learning algorithm?

In particular, we will address:

What is the true error of h if we only know the training error of h?

- Finite hypothesis spaces and zero training error
- Finite hypothesis spaces and non-zero training error
- Infinite hypothesis spaces and VC dimension

Can you Convince me of your Psychic Abilities?

- Game
  - I think of n bits
  - |H| players try to guess the bit sequence
  - If somebody in the class guesses my bit sequence, that person clearly has telepathic abilities – right?

- Question:
  - If at least one player guesses the bit sequence correctly, is there any significant evidence that he/she has telepathic abilities?
  - How large would n and |H| have to be?

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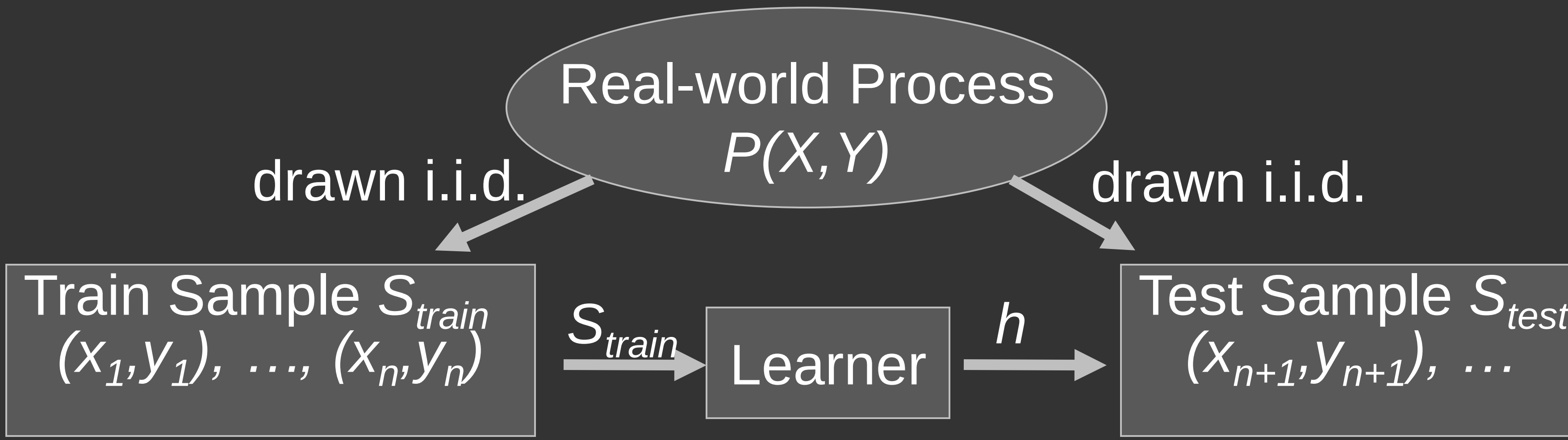
Learning as Prediction Overview



- Goal: Find h with small prediction error $Err_P(h)$ over $P(X,Y)$.
- Strategy: Find (any?) h with small error $Err_{S_{train}}(h)$ on training sample S_{train}.

- Training Error: Error $Err_{S_{train}}(h)$ on training sample.
- Test Error: Error $Err_{S_{test}}(h)$ on test sample is an estimate of $Err_P(h)$.

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Review of Definitions

Definition: *A particular* **instance of a learning problem** *is described by a probability distribution* $P(X,Y)$.

Definition: *A* **sample** $S = ((\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n))$ *is independently identically distributed (i.i.d.) according to* $P(X,Y)$.

Definition: *The* **error on sample** S $Err_S(h)$ *of a hypothesis* h *is* $Err_S(h) = \frac{1}{n}\sum_{i=1}^{n} \Delta(h(\vec{x}_i), y_i)$.

Definition: *The* **prediction/generalization/true error** $Err_P(h)$ *of a hypothesis* h *for a learning task* $P(X,Y)$ *is*

$$Err_P(h) = \sum_{\vec{x} \in X, y \in Y} \Delta(h(\vec{x}), y) P(X = \vec{x}, Y = y).$$

Definition: *The* **hypothesis space H** *is the set of all possible classification rules available to the learner.*

Useful Formulas

- Binomial Distribution: The probability of observing *x* heads in a sample of *n* independent coin tosses, where in each toss the probability of heads is *p*, is

$$P(X = x|p, n) = \frac{n!}{r!(n-x)!}p^x(1-p)^{n-x}$$

- Union Bound:

$$P(X_1 = x_1 \vee X_2 = x_2 \vee ... \vee X_n = x_n) \leq \sum_{i=1}^{n} P(X_i = x_i)$$

- Unnamed: $(1 - \epsilon) \leq e^{-\epsilon}$

Generalization Error Bound: Finite H, Zero Training Error

- Setting
  - Sample of n labeled instances S_{train}
  - Learning Algorithm L with a finite hypothesis space H
  - At least one $h \in H$ has zero training error $Err_{S_{train}}(h)$
  - Learning Algorithm L returns zero training error hypothesis $\hat{h}$
- What is the probability that the prediction error of $\hat{h}$ is larger than ε?

$$P(Err_P(\hat{h}) \geq \epsilon) \leq |H| e^{-\epsilon n}$$

Training Sample S_{train}
$(x_1,y_1), \ldots, (x_n,y_n)$

$\xrightarrow{S_{train}}$ Learner $\xrightarrow{\hat{h}}$

Test Sample S_{test}
$(x_{n+1},y_{n+1}), \ldots$

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Sample Complexity: Finite H, Zero Training Error

- Setting
  - Sample of n labeled instances S_{train}
  - Learning Algorithm *L* with a finite hypothesis space *H*
  - At least one $h \in H$ has zero training error $Err_{S_{train}}(h)$
  - Learning Algorithm *L* returns zero training error hypothesis $\hat{h}$
- How many training examples does L need so that with probability at least (1-δ) it learns an $\hat{h}$ with prediction error less than ε?

$$n \geq \frac{1}{\epsilon}\left(\log(|H|) - \log(\delta)\right)$$

Training Sample S_{train}: $(x_1,y_1), \ldots, (x_n,y_n)$ $\xrightarrow{S_{train}}$ Learner $\xrightarrow{\hat{h}}$ Test Sample S_{test}: $(x_{n+1},y_{n+1}), \ldots$

Probably Approximately Correct Learning

Definition: C *is* **PAC-learnable** *by learning algorithm* $\mathcal{L}$ *using* H *and a sample* S *of* n *examples drawn i.i.d. from some fixed distribution* $P(X)$ *and labeled by a concept* $c \in C$, *if for sufficiently large* n

$$P(Err_P(h_{\mathcal{L}(S)}) \leq \epsilon) \geq (1 - \delta)$$

for all $c \in C, \epsilon > 0, \delta > 0$, *and* $P(X)$. $\mathcal{L}$ *is required to run in polynomial time dependent on* $1/\epsilon, 1/\delta, n$, *the size of the training examples, and the size of* c.

Example: Smart Investing

- **Task:** Pick stock analyst based on past performance.
- **Experiment:**

  Review analyst prediction “next day up/down” for past 10 days. Pick analyst that makes the fewest errors.
  - Situation 1:
    - 1 stock analyst {A1}, A1 makes 5 errors
  - Situation 2:
    - 3 stock analysts {A1,B1,B2}, B2 best with 1 error
  - Situation 3:
    - 1003 stock analysts {A1,B1,B2,C1,…,C1000}, C543 best with 0 errors
- **Question:** Which analysts are you most confident in, A1, B2, or C543?

Useful Formula

Hoeffding/Chernoff Bound:

For any distribution P(X) where X can take the values 0 and 1, the probability that an average of an i.i.d. sample deviates from its mean p by more than ε is bounded as

$$P\left(\left|\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right) - p\right| > \epsilon\right) \leq 2e^{-2n\epsilon^2}$$

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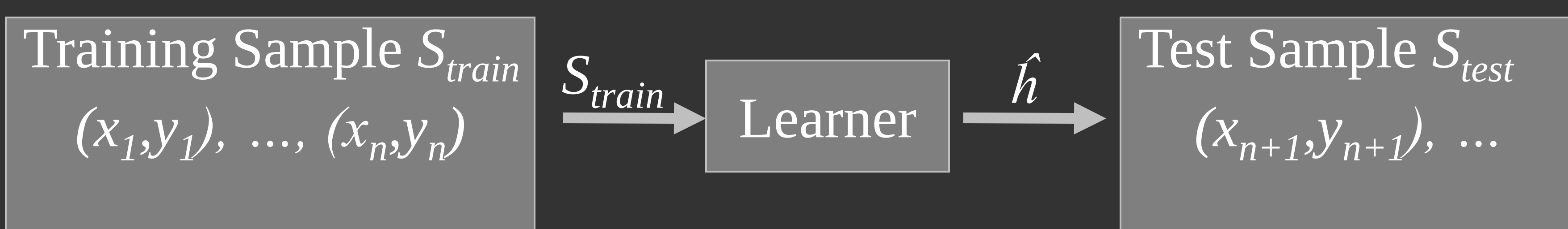
Generalization Error Bound: Finite H, Non-Zero Train Err

- Setting
  - Sample of n labeled instances *S*
  - Learning Algorithm *L* with a finite hypothesis space *H*
  - *L* returns hypothesis $\hat{h}=L(S)$ with lowest training error
- What is the probability that the prediction error of $\hat{h}$ exceeds the fraction of training errors by more than ε?

$$P\left(\left|Err_S(h_{\mathcal{L}(S)}) - Err_P(h_{\mathcal{L}(S)})\right| \geq \epsilon\right) \leq 2|H|e^{-2\,\epsilon^2\,n}$$



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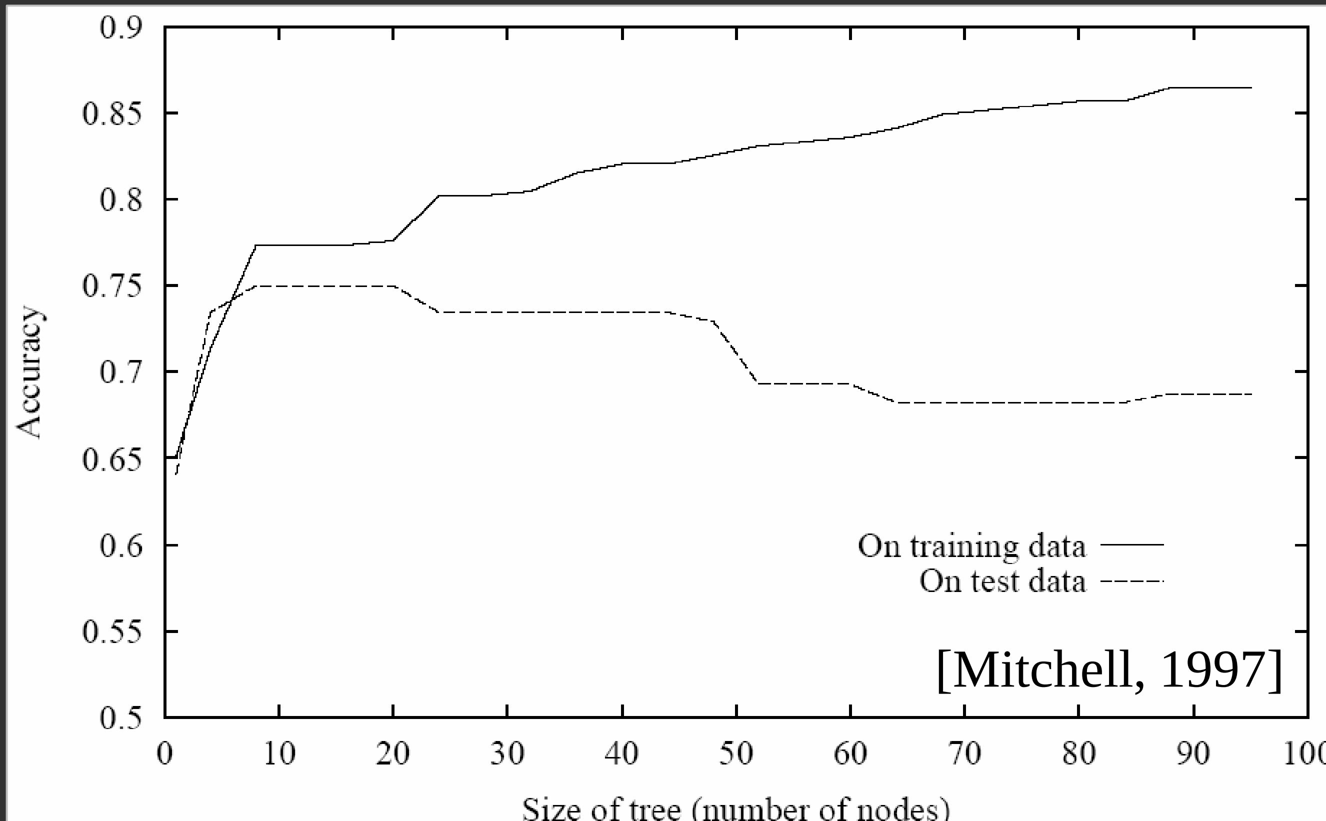
Overfitting vs. Underfitting



With probability at least *(1-δ)*:

$$Err_P(h_{\mathcal{L}(S_{train})}) \leq Err_{S_{train}}(h_{\mathcal{L}(S_{train})}) + \sqrt{\frac{(\ln(2|H|) - \ln(\delta))}{2n}}$$

Generalization Error Bound: Infinite H, Non-Zero Train Err

- Setting
  - Sample of n labeled instances *S*
  - Learning Algorithm *L* using a hyp space *H* with *VCDim(H)=d*
  - *L* returns hypothesis $\hat{h}=L(S)$ with lowest training error
- **Definition:** *The* **VC-Dimension of** H *is equal to the maximum number* d *of examples that can be split into two sets in all* 2^d *ways using functions from* H *(shattering).*
- Given hypothesis space *H* with *VCDim(H)* equal to *d* and an i.i.d. sample *S* of size *n*, with probability (1-δ) it holds that

$$Err_P(h_{\mathcal{L}(S)}) \leq Err_S(h_{\mathcal{L}(S)}) + \sqrt{\frac{d\left(\ln\left(\frac{2n}{d}\right)+1\right)-\ln\left(\frac{\delta}{4}\right)}{n}}$$