Advanced Machine Learning

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Assignment 1

Deadline: Friday, 22^{nd} of April 2022

Upload your solutions at: https://tinyurl.com/AML-2022-ASSIGNMENT1

1. **(0.5 points)** Give an example of a finite hypothesis class $\mathcal{H}$ with $\text{VCdim}(\mathcal{H}) = 2022$. Justify your choice.

2. **(0.5 points)** What is the maximum value of the natural even number n, $n = 2m$, such that there exists a hypothesis class $\mathcal{H}$ with n elements that shatters a set C of $m = \frac{n}{2}$ points? Give an example of such an $\mathcal{H}$ and C. Justify your answer.

3. **(0.75 points)** Let $\mathcal{X} = \mathbb{R}^2$ and consider $\mathcal{H}$ the set of axis aligned rectangles with the center in origin O(0, 0). Compute the $VCdim(\mathcal{H})$.

4. **(1 point)** Let $\mathcal{X} = \mathbb{R}^2$ and consider $\mathcal{H}_\alpha$ the set of concepts defined by the area inside a right triangle ABC with two catheti AB and AC parallel to the axes (Ox and Oy), and with the ratio $AB/AC = \alpha$ (fixed constant > 0). Consider the realizability assumption. Show that the class $\mathcal{H}_\alpha$ is (ϵ, δ)-PAC learnable by giving an algorithm A and determining an upper bound on the sample complexity $m_H(\epsilon, \delta)$ such that the definition of PAC-learnability is satisfied.

5. **(1.25 points)** Consider $\mathcal{H} = \mathcal{H}_1 \cup \mathcal{H}_2 \cup \mathcal{H}_3$, where:

$$\mathcal{H}_1 = \{h_{\theta_1} : \mathbb{R} \to \{0,1\} \mid h_{\theta_1}(x) = \mathbf{1}_{[x \geq \theta_1]}(x) = \mathbf{1}_{[\theta_1, +\infty)}(x), \theta_1 \in \mathbb{R}\},$$

$$\mathcal{H}_2 = \{h_{\theta_2} : \mathbb{R} \to \{0,1\} \mid h_{\theta_2}(x) = \mathbf{1}_{[x < \theta_2]}(x) = \mathbf{1}_{(-\infty, \theta_2)}(x), \theta_2 \in \mathbb{R}\},$$

$$\mathcal{H}_3 = \{h_{\theta_1, \theta_2} : \mathbb{R} \to \{0,1\} \mid h_{\theta_1, \theta_2}(x) = \mathbf{1}_{[\theta_1 \leq x \leq \theta_2]}(x) = \mathbf{1}_{[\theta_1, \theta_2]}(x), \theta_1, \theta_2 \in \mathbb{R}\}.$$

Consider the realizability assumption.

a) Compute VCdim($\mathcal{H}$).

b) Show that $\mathcal{H}$ is PAC-learnable.

c) Give an algorithm A and determine an upper bound on the sample complexity $m_{\mathcal{H}}(\epsilon, \delta)$ such that the definition of PAC-learnability is satisfied.

6. **(1 point)** A decision list may be thought of as an ordered sequence of if-then-else statements. The sequence of conditions in the decision list is tested in order, and the answer associated with the first satisfied condition is output.

More formally, a *k-decision list* over the boolean variables $x_1, x_2, \ldots, x_n$ is an ordered sequence $L = \{(c_1, b_1), (c_2, b_2), \ldots, (c_l, b_l)\}$ and a bit b, in which each c_i is a conjunction of at most k literals over $x_1, x_2, \ldots, x_n$ and each $b_i \in \{0,1\}$. For any input $a \in \{0,1\}^n$, the value $L(a)$ is defined to be b_j where j is the smallest index satisfying $c_j(a) = 1$; if no such index exists, then $L(a) = b$. Thus, b is the "default" value in case a falls off the end of the list. We call b_i the bit associated with the condition c_i.

The next figure shows an example of a *2-decision list* along with its evaluation on a particular input.

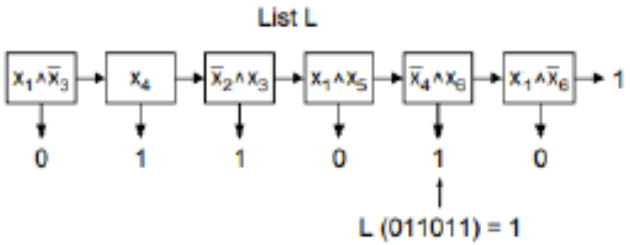


Figure 1: *A 2-decision list and the path followed by an input. Evaluation starts at the leftmost item and continues to the right until the first condition is satisfied, at which point the binary value below becomes the final result of the evaluation.*

Show that the VC dimension of 1-decision lists over $\{0,1\}^n$ is lower and upper bounded by linear functions, by showing that there exists $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that:

$$\alpha \cdot n + \beta \leq VCdim(\mathcal{H}_{1-decision\ list}) \leq \gamma \cdot n + \delta$$

Hint: Show that 1-decision lists over $\{0,1\}^n$ compute linearly separable functions (halfspaces).

Recap: The fundamental theorem of statistical learning

Theorem (The Fundamental Theorem of Statistical Learning).

Let $\mathcal{H}$ be a hypothesis class of functions from a domain $\mathcal{X}$ to $\{0,1\}$ and let the loss function be the $0-1$ loss. Then, the following are equivalent:

1. $\mathcal{H}$ has the uniform convergence property.
2. Any ERM rule is a successful agnostic PAC learner for $\mathcal{H}$.
3. $\mathcal{H}$ is agnostic PAC learnable.
4. $\mathcal{H}$ is PAC learnable.
5. Any ERM rule is a successful PAC learner for $\mathcal{H}$.
6. $\mathcal{H}$ has a finite VC-dimension.

A finite VC- dimension guarantees learnability. Hence, the VC-dimension characterizes PAC learnability.

The Growth function

Definition

Let $\mathcal{H}$ be a hypothesis class. Then the growth function of $\mathcal{H}$, denoted by τ_H, where $\tau_{\mathcal{H}}$: **N**→**N**, is defined as:

$$\tau_H(m) = \max_{C \subseteq X : |C| = m} |H_C|$$

In other words, $\tau_H(m)$ is the maximum number of different functions from a set C of size m to {0,1} that can be obtained by restricting $\mathcal{H}$ to C.

Observation: if VCdim($\mathcal{H}$) = d then for any m ≤ d we have $\tau_{\mathcal{H}}(m) = 2^m$. In such cases, $\mathcal{H}$ induces all possible functions from C to {0,1}.

What happens when m becomes larger than the VC-dimension?

Answer given by the Sauer's lemma: the growth function $\tau_{\mathcal{H}}$ increases polynomially rather than exponentially with m.

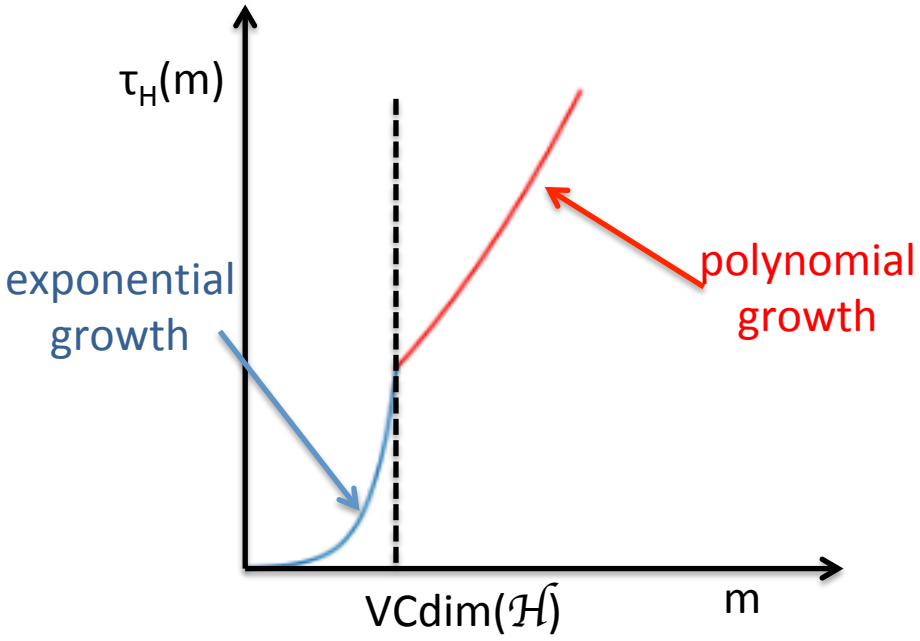
The Sauer's lemma

Lemma (Sauer – Shelah – Perles)

Let $\mathcal{H}$ be a hypothesis class with $\text{VCdim}(\mathcal{H}) \leq d < \infty$. Then, for all m , we have that:

$$\tau_H(m) \leq \sum_{i=0}^{d} C_m^i$$

In particular, if $m > d+1$ then $\tau_{\mathcal{H}}(m) \leq (em/d)^d = O(m^d)$



Proof for 6 → 1

We want to prove that finite VC-dimension → *uniform convergence property*

Two steps:

1. (Sauer's lemma) If $\text{VCdim}(\mathcal{H}) \leq d < \infty$, then even though $\mathcal{H}$ might be infinite, when restricting it to a finite set $C \subseteq \mathcal{X}$, its "effective" size, $|\mathcal{H}_C|$, is only $O(|C|^d)$. That is, the size of $\mathcal{H}_C$ grows polynomially rather than exponentially with $|C|$.

2. we have shown in lecture 4 that finite hypothesis classes enjoy the uniform convergence property. We generalize this result and show that uniform convergence holds whenever the hypothesis class has a "small effective size." By "small effective size" we mean classes for which $|\mathcal{H}_C|$ grows polynomially with $|C|$.

The fundamental theorem of statistical learning – quantitative version

Theorem

Let $\mathcal{H}$ be a hypothesis class of functions from a domain $\mathcal{X}$ to $\{0,1\}$ and let the loss function be the 0−1 loss. Assume that VCdim($\mathcal{H}$) = d <∞. Then, there are absolute constants C_1, C_2 such that:

1. $\mathcal{H}$ has the uniform convergence property with sample complexity:

$$C_1 \frac{d+\log(1/\delta)}{\epsilon^2} \leq m_{\mathcal{H}}^{UC}(\epsilon,\delta) \leq C_2 \frac{d+\log(1/\delta)}{\epsilon^2}$$

2. $\mathcal{H}$ is agnostic PAC learnable with sample complexity:

$$C_1 \frac{d+\log(1/\delta)}{\epsilon^2} \leq m_{\mathcal{H}}(\epsilon,\delta) \leq C_2 \frac{d+\log(1/\delta)}{\epsilon^2}$$

3. $\mathcal{H}$ is PAC learnable with sample complexity:

$$C_1 \frac{d+\log(1/\delta)}{\epsilon} \leq m_{\mathcal{H}}(\epsilon,\delta) \leq C_2 \frac{d\log(1/\epsilon)+\log(1/\delta)}{\epsilon}$$

The VC dimension determines (along with ε, δ) the samples complexities of learning a class. It gives us a lower and an upper bound.

Computational complexity of learning

Computational resources of learning

For learning we need 2 type of resources:

1. *Information = training data*
   - so far we analyzed how much training data (sample size) we need in order to learn
   - *sample complexity*

2. *Computation = runtime*
   - for how much time an algorithm (that implements learning) will run, once we have sufficiently many training examples
   - *computational complexity*
   - crucial when we need fast ML applications (driver surveillance, stock exchange trading, etc)
   - runtime = number of elementary instructions executed - arithmetic operations over real numbers - in an asymptotic sense (with respect to input size) of the algorithm, e.g. *O(n) – where n is the size of the input size*

Input size parameter of learning

What should play the role of the input size parameter in learning?

- size of the training set that the algorithm receives?
  - for a very large number of examples, much larger than the sample complexity of learning, the algorithm can ignore the extra samples
  - a larger training set does not make the problem more difficult

- size of the hypothesis class?
  - might be infinite: $|\mathcal{H}_{\text{thresholds}}| = \infty$

- accuracy ε, confidence δ and another parameter n related to the size/ complexity of $\mathcal{X}$, $\mathcal{H}$
  - how much computation we need in order to get accuracy ε with confidence δ
  - want to have *efficient learning* (give a formal definition later): polynomial in $1/\varepsilon$, $1/\delta$ and n (some parameter related to the size/complexity of domain/hypothesis class: more complex hypothesis needs more computation time)

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- parameter n can be the embedding dimension
  - if we decide to use n features to describe objects, how will that increase runtime?

- we study the runtime in an asymptotic sense by defining a sequence of pairs $(\mathcal{X}_n, \mathcal{H}_n)_{n=1,2,\ldots}$ and studying asymptotic complexity of learning $\mathcal{X}_n$, $\mathcal{H}_n$ as n grows to ∞

Prevent "cheating"

The output of the learning algorithm L is a hypothesis h from $\mathcal{H}$.

- a learning algorithm L can "cheat" by transferring the computational burden to the output hypothesis
  - define the output hypothesis to be the function that stores the training set in memory and computes the ERM hypothesis on the training set and applies it to a test example x

- the runtime of a learning algorithm A defined as the maximum of:
  - the time it takes A to output some h
  - the time it takes h to output a label on any given x from $\mathcal{X}$

Example 1: Conjunctions of Boolean literals

- $\mathcal{H}_{\text{conj}}^{\text{d}}$ = class of conjunctions of at most d Boolean literals $x_1, \ldots, x_{\text{d}}$
  - a Boolean literal is either x_{i} or its negation $\overline{x_i}$ (or 1 = missing literal)
  - can interpret x_{i} as feature i
  - example: $h = x_1 \wedge \overline{x_2} \wedge x_4$ where $\overline{x_2}$ denotes the negation of the Boolean literal x_2
  - $\mathcal{X} = \{0,1\}^{\text{d}}$
- consider the realizable case
  - there is a conjunction h^* in $\mathcal{H}_{\text{conj}}^{\text{d}}$ that labels the examples

- $|\mathcal{H}_{\text{conj}}^{\text{d}}| = 3^{\text{d}} + 1 < \infty$ so it has finite VC dimension (less than $\log_2(3^{\text{d}}+1)$), so it's PAC learnable. In seminar class 3 we shown that $\text{VCdim}(\mathcal{H}_{\text{conj}}^{\text{d}}) = \text{d}$ so the sample complexity $m_{\mathcal{H}}(\varepsilon,\delta)$ is bounded by:

$$C_1 \frac{d + \log(1/\delta)}{\epsilon} \leq m_{\mathcal{H}}(\epsilon, \delta) \leq C_2 \frac{d \log(1/\epsilon) + \log(1/\delta)}{\epsilon}$$

- So, $m_{\mathcal{H}}(\varepsilon,\delta)$ is polynomial in $1/\varepsilon$, $1/\delta$, d (measures the complexity of the hypothesis class $\mathcal{H}_{\text{conj}}^{\text{d}}$)

Example 1: Conjunctions of Boolean literals

- $\mathcal{H}_{\text{conj}}^{d}$ = class of conjunctions of at most d Boolean literals $x_1, \ldots, x_d$
- a simple algorithm for finding an ERM hypothesis is based on positive examples and consists of the following:
  - for each positive example $(b_1, \ldots b_d)$,
    - if $b_i = 1$ then $\overline{x_i}$ is ruled out as a possible literal in the concept class
    - if $b_i = 0$ then x_i is ruled out.
  - the conjunction of all the literals not ruled out is thus a hypothesis consistent with the target

0	1	1	0	1	1	+
0	1	1	1	1	1	+
0	0	1	1	0	1	-
0	1	1	1	1	1	+
1	0	0	1	1	0	-
0	1	0	0	1	1	+

$x_1\ \overline{x_1}\ x_2\ \overline{x_2}\ x_3\ \overline{x_3}\ x_4\ \overline{x_4}\ x_5\ \overline{x_5}\ x_6\ \overline{x_6}$

$\overline{x}_1 \wedge x_2 \wedge x_5 \wedge x_6$

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  - the conjunction of all the literals not ruled out is thus a hypothesis consistent with the target

- runtime of the algorithm is $O(m_{\mathcal{H}}(\varepsilon,\delta)*\text{d})$, so is polynomial in $1/\varepsilon$, $1/\delta$, d

- in the agnostic (unrealizable) case: unless P = NP, there is no algorithm whose running time is polynomial in $m_{\mathcal{H}}(\varepsilon,\delta)$ and d that is guaranteed to find an ERM hypothesis for the class of Boolean conjunctions.

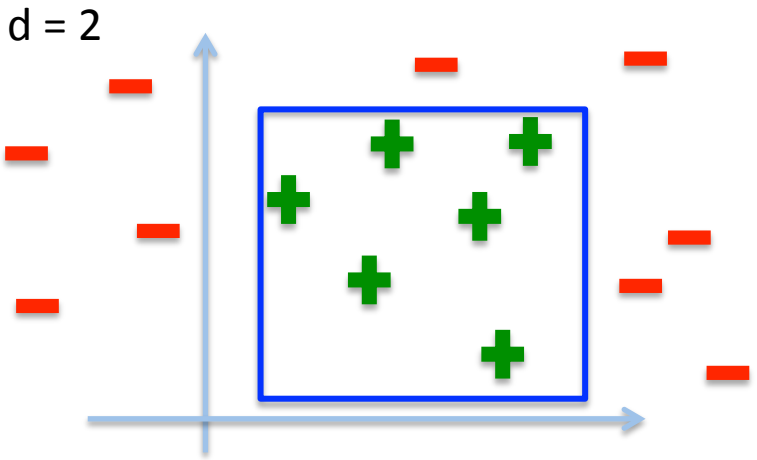
Example 2: Learning axis aligned rectangles in $\mathbf{R}^d$

- $\mathcal{H}_{\text{rec}}^d$ = the class of axis aligned rectangles in $\mathbf{R}^d$

$$H_{rec}^d = \{h_{a_1,b_1,a_2,b_2,\ldots,a_d,b_d} : R^d \to \{0,1\} \mid a_1 \le b_1, a_2 \le b_2, \ldots, a_d \le b_d, a_i \in R, b_i \in R\}$$

$$h_{a_1,b_1,a_2,b_2,\ldots,a_d,b_d}(x_1,x_2\ldots,x_d) = \begin{cases} 1, if\, a_1 \le x_1 \le b_1, a_2 \le x_2 \le b_2, \ldots, a_d \le x_d \le b_d \\ 0, otherwise \end{cases}$$

- consider the realizable case:
  - there exists a rectangle h* in $\mathcal{H}_{\text{rec}}^d$ with real risk = 0



We have shown in the seminar class that:

- the algorithm that returns the rectangle enclosing all positive examples is ERM
- $\mathcal{H}_{\text{rec}}^d$ is PAC learnable with sample size

$$m_{H_{rec}^d}(\varepsilon,\delta) \le \left\lceil \frac{2d \log(\frac{2d}{\delta})}{\varepsilon} \right\rceil$$

- the runtime is O($m_H d$) as for each dimension, the algorithm has to find the minimal and the maximal values among the positive instances in the training sequence. So it is polynomial in $1/\varepsilon$, $1/\delta$, d.

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- consider the agnostic case:
  - distribution $\mathcal{D}$ over $\mathcal{Z} = \mathbf{R}^d \times \{0,1\}$ (a sample could get both labels)
  - if there exist a labeling function f this might not be in $\mathcal{H}_{\text{rec}}^{\text{d}}$

- VCdim($\mathcal{H}_{\text{rec}}^{\text{d}}$) = 2d (see seminar class), so we have that:

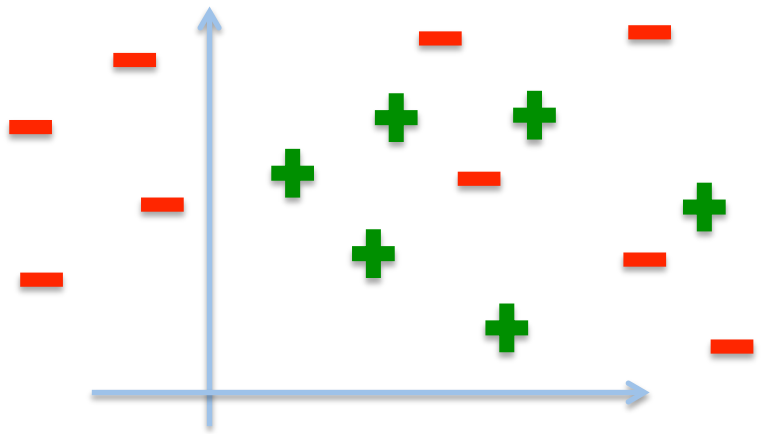
$$C_1 \frac{2d + \log(\frac{1}{\delta})}{\varepsilon^2} \le m_{H_{rec}^d}(\varepsilon, \delta) \le C_2 \frac{2d + \log(\frac{1}{\delta})}{\varepsilon^2}$$

- $m_{H_{rec}^d}(\varepsilon, \delta)$ is polynomial in 1/ε, 1/δ , d (measures the complexity of the $\mathcal{H}_{\text{rec}}^{\text{d}}$)

Example 2: Learning axis aligned rectangles in $\mathbf{R}^d$

- $\mathcal{H}_{rec}^{d}$ = the class of axis aligned rectangles in $\mathbf{R}^d$
- consider that we have a sample S of size: $m_{H_{rec}^{d}}(\varepsilon,\delta) \approx C\frac{2d+\log(\frac{1}{\delta})}{\varepsilon^2}$
- what is the runtime of the ERM algorithm?
  - how long it will take to find the best rectangle in R^d?
  - go over all axis aligned rectangles in R^d and choose the best one (based on minimizing the error on the training data)

d = 2



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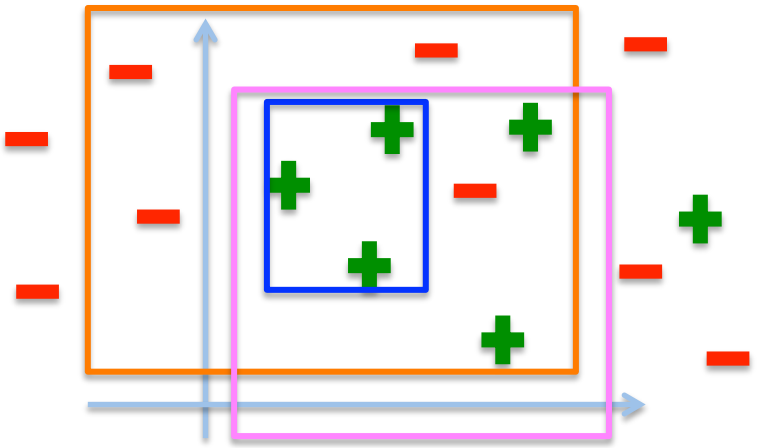

error: (1 + 4)/ (6 + 9) = 5/15

error: (3 + 0)/ (6 + 9) = 3/15

error: (1 + 1)/ (6 + 9) = 2/15

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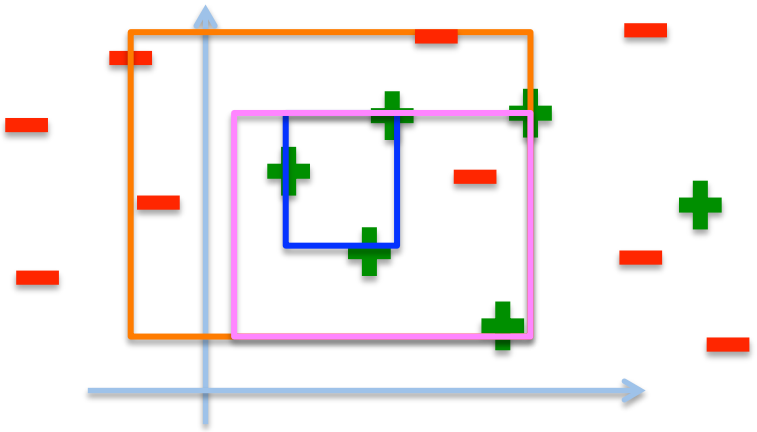

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- the number of all possible rectangles can be reduces to all possible rectangles that have points of S on every boundary edge (very efficient algorithm)

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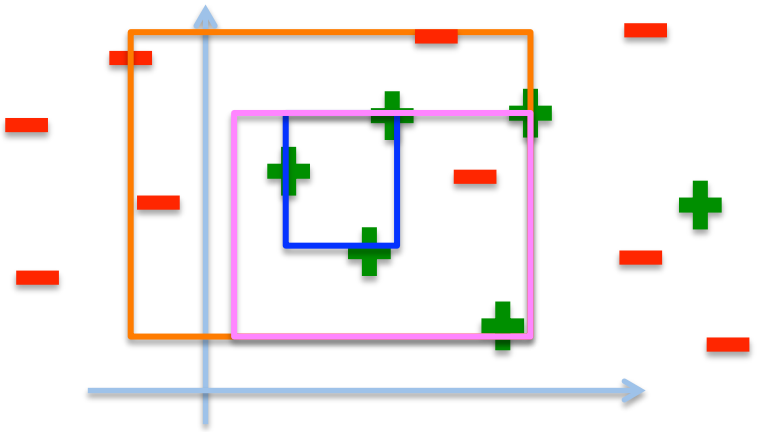
- what is the runtime of the ERM algorithm?
  - how long it will take to find the best rectangle in R^d?
  - Step 1: generate all the rectangles based on the sample points in R^d
  - Step 2: for each such rectangle compute the training error
  - Step 3: choose the rectangle with the smallest training error



error: (1 + 4)/ (6 + 9) = 5/15

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error: (1 + 1)/ (6 + 9) = 2/15

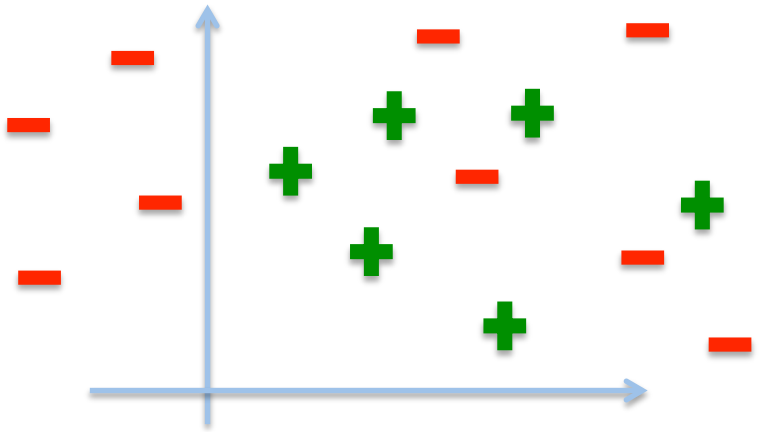
- how many possible rectangles can we construct based on the points in the sample S?

Example 2: Learning axis aligned rectangles in $\mathbf{R}^d$

- $\mathcal{H}_{rec}^{d}$ = the class of axis aligned rectangles in $\mathbf{R}^d$
- how many possible rectangles can we construct based on the points in the sample S?

d = 1

d = 2



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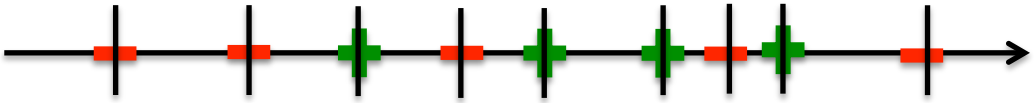
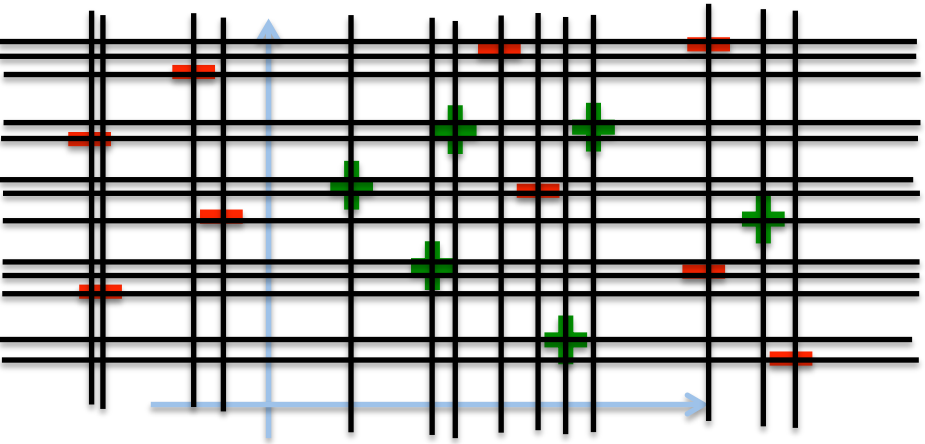


d = 2



Every such rectangle is determined by at most 2d points from S

So there are at most $|S|^{2d}$ such rectangles.

For each rectangle we need to iterate over all examples to compute the training error.

So, the runtime is: $O\left(\left[C\frac{2d+\log(\frac{1}{\delta})}{\varepsilon^2}\right]^{2d+1}\right)$

Example 2: Learning axis aligned rectangles in $\mathbf{R}^d$

- $\mathcal{H}_{rec}^d$ = the class of axis aligned rectangles in $\mathbf{R}^d$

- the runtime of the ERM_H is: $O\left(\left\lceil C\frac{2d+\log(\frac{1}{\delta})}{\varepsilon^2}\right\rceil^{2d+1}\right)$

- for every fixed dimension *d,* ERM_H can be implemented in time which is polynomial in $1/\varepsilon$, $1/\delta$, *d* (measures the complexity of the $\mathcal{H}_{rec}^d$) therefore we have efficient learning (see the formal definition later)

- however, as a function of d the runtime of the algorithm implementing the ERM_H presented is exponential in *d.* It can be proved that there is no better algorithm (unless P = NP) than the one proposed.

Formal definition of efficient learning

Definition 1

Given a function $f : (0,1)^2 \rightarrow \mathrm{N}$, a learning task $(\mathcal{Z}, \mathcal{H}, \ell)$, and a learning algorithm A, we say that A solves the learning task in time $O(f)$ if there exists some constant number c, such that for every probability distribution $\mathcal{D}$ over $\mathcal{Z}$, and input $\varepsilon, \delta \in (0,1)$, when A has access to samples generated i.i.d by $\mathcal{D}$, we have that:

- A terminates after performing at most $c * f(\varepsilon, \delta)$ operations;
- the output of A, denoted h_A, can be applied to predict the label of a new example while performing at most $c * f(\varepsilon, \delta)$ operations;
- the output of A is probably approximately correct; namely, with probability of at least $1 - \delta$ (over the random samples A receives):

$$L_{\mathcal{D}}(h_A) \leq \min_h L_{\mathcal{D}}(h) + \varepsilon$$

Formal definition of efficient learning

Definition (for graded hypothesis spaces)

Consider a sequence of learning problems, $(\mathcal{Z}_n, \mathcal{H}_n, \ell_n)_{n=1,2,\ldots}$ where problem n is defined by a domain $\mathcal{Z}_n$, a hypothesis class $\mathcal{H}_n$, and a loss function ℓ_n. Let A be a learning algorithm designed for solving learning problems of this form. Given a function g: $\mathbb{N} \times (0,1)^2 \rightarrow \mathbb{N}$, we say that the runtime of A with respect to the preceding sequence is $O(g)$, if for all n, A solves the problem $(\mathcal{Z}_n, \mathcal{H}_n, \ell_n)$ in time $O(f_n)$, where $f_n : (0,1)^2 \rightarrow \mathbb{N}$ is defined by $f_n(\varepsilon, \delta) = g(n, \varepsilon, \delta)$.

We say that A is an *efficient* PAC algorithm with respect to a sequence $(\mathcal{Z}_n, \mathcal{H}_n, \ell_n)$ if its runtime is $O(p(n, 1/\varepsilon, 1/\delta))$ for some polynomial p.

Formal definition of efficient PAC learning (Valiant 1984)

In 1984, Leslie Valiant defined efficient PAC learning: PAC learnability + require the number of examples and the runtime of the algorithm A (training + testing) to be polynomial in *1/ε, 1/δ, n*.

Example:

- $\mathcal{U}_n = \{h: B^n \rightarrow \{0,1\}\}$ - the concept class formed by all subsets of B^n
- $|\mathcal{U}_n| = 2^{2^n}$ – finite, so is PAC learnable with $m_{\mathcal{H}}(\varepsilon, \delta)$ in the order of m:

$$m \geq \left\lceil \frac{1}{\varepsilon}\left(2^n \log(2) + \log(\frac{1}{\delta})\right)\right\rceil$$

- sample complexity exponential in *n*, number of variables
- it is not efficient PAC-learnable in any practical sense (need polynomial sample complexity)