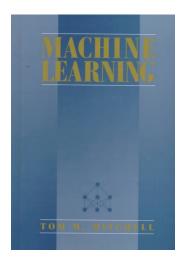
# Introductory Course: Machine Learning (WWI15B4)

Concept Learning and the Hypothesis Space

Fabio Ferreira, David Bethge

DHBW Karlsruhe

## Recommended Literature



- 1 Motivation
- 2 Concept Learning
  - Concept Learning Task
    - Algorithms
  - Learning as Search in the Hypothesis Space
  - Inductive Learning and Biases
- 3 Learning Theory
  - VC-Dimension

## Questions and more questions...

Some questions we will be answering (from a theoretical perspective) in this lecture:

- What does "a model generalizes well" mean?
- Why classification cannot work without making a-priori assumptions?
- What is a bias and what different types do we usually consider?
- Why can we only learn so much what's in the data we provide to a learning algorithm?
- Why are models with lots of parameters usually not a blessing but a curse? (curse of dimensionality)

#### Motivation

#### Statements like

- "Dogs bark."
- "Cars drive."
- "I enjoy going to the theater."

require the knowledge of *concepts* (having learned about larger sets like animals, transportation, entertainment, ...)

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- lacktriangle "I enjoy going to the theater." ightarrow entertainment

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#### Motivation

#### Statements like

- "Dogs bark." → animals
- "Cars drive." → transportation
- "I enjoy going to the theater." → entertainment

require the knowledge of *concepts* (having learned about larger sets like animals, transportation, entertainment, ...)

#### Concept

Description of a subset of objects/events which are defined over a larger set.

#### Why are concepts important?

- Learning often involves inducing general functions from specific (training) examples
- building block for:
  - classification, events
  - inferring possible consequences
  - creating more complex knowledge (relations etc.)
- concept learning: "searching through a predefined space of potential hypotheses for the hypothesis that best fits the training examples" [Mitchell, 1997] ⇒ many machine learning algorithms perform hypothesis space search (e.g. ID3, SVM)

## Concept Learning

#### Concept Learning

Automatic inference of a boolean-valued function based on training examples that yields **true** if an object (e.g. dog) is member of its larger (e.g. animals), **false** if not a member.

- Input: training samples (either member or non-member)
- Goal: automatic inference of definition of the underlying concept

## Concept Learning

```
Example: foo(lion) \rightarrow true foo(giraffe) \rightarrow true foo(jackal) \rightarrow true foo(elephant) \rightarrow true foo(cougar) \rightarrow false foo(snowleopard) \rightarrow false
```

## Concept Learning

```
Example: foo(lion) \rightarrow true foo(giraffe) \rightarrow true foo(jackal) \rightarrow true foo(elephant) \rightarrow true foo(cougar) \rightarrow false foo(snowleopard) \rightarrow false Concept: animals inhabiting Africa
```

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(The following examples are taken from [Mitchell, 1997])

- goal: learn the concept "days on which my friend Aldo enjoys his favorite water sport."
- i.e.:  $c : EnjoySport : X \rightarrow \{true, false\}$
- set of instances X: possible days described by 6 attributes:
  - Sky (Sunny, Cloudy, Rainy)
  - AirTemp (Warm, Cold)
  - Humidity (Normal, High))
  - Wind (Strong, Weak))
  - Water (Warm, Cool)
  - Forecoast (Same, Change)
- e.g. <Sunny, Warm, Normal, Strong, Warm, Same>

- set of hypotheses H specified as a vector of six constraints, which can be evaluated as:
  - attribute value (e.g. "Warm")
  - "?" (any value is acceptable)
  - "∅" (no value acceptable)
- e.g. <Sunny, Warm, Normal, Strong, ?, Same>
- most general hypothesis: <?,?,?,?,?,>
- most specific hypothesis:  $\langle \emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset \rangle$

- set of hypotheses H specified as a vector of six constraints, which can be evaluated as:
  - attribute value (e.g. "Warm")
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- most general hypothesis: <?,?,?,?,?,</p>
- most specific hypothesis:  $\langle \emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset \rangle$
- "x satisfies h" if h(x) = 1,  $\exists x \in X$
- a hypothesis is consistent if it correctly classifies all samples
- **goal**: determine  $h \in H$  s.t.  $h(x) = c(x), \forall x \in X$

#### Positive and negative examples of EnjoySport

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

from [Mitchell, 1997]

## Hypothesis Space

## How is the hypotheses space shaped?

- the space of hypotheses is implicitly shaped by selecting the hypothesis representation
- number of instances<sup>1</sup> in X: 3 \* 2 \* 2 \* 2 \* 2 \* 2 \* 2 = 96
- number of hypotheses<sup>2</sup> in H: 5 \* 4 \* 4 \* 4 \* 4 \* 4 = 5120

Many algorithms address learning by viewing it as *searching the hypothesis space* in order to find hypotheses that best fit the data.

<sup>&</sup>lt;sup>1</sup>distinct

<sup>&</sup>lt;sup>2</sup>syntactically distinct

#### Example:

- h1 = <Sunny, ?, ?, Strong, ?, ?>
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

## More general than or equal to: $(\geq)$

Let  $h_j$  and  $h_k$  be defined over X. Then  $h_j \ge h_k$  iff:  $h_k(x) = 1 \Rightarrow h_j(x) = 1, \forall x \in X$ 

#### Example:

- $h1 = \langle Sunny, ?, ?, Strong, ?, ? \rangle$
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

## More general than or equal to: $(\geq)$

Let  $h_j$  and  $h_k$  be defined over X. Then  $h_j \ge h_k$  iff:  $h_k(x) = 1 \Rightarrow h_j(x) = 1, \forall x \in X$ 

#### More general than: (>)

Let  $h_j$  and  $h_k$  be defined over X. Then  $h_j > h_k$  iff:  $h_i \ge h_k \wedge h_k \not \ge h_i$ 

- h1 = <Sunny, ?, ?, Strong, ?, ?>
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

Evaluate the following expressions:

- h2 > h1?
- h3 > h2?

- h1 = <Sunny, ?, ?, Strong, ?, ?>
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

#### Evaluate the following expressions:

- h2 > h1? true, since  $h1 \Rightarrow h2$  AND it is NOT  $h2 \Rightarrow h1$  ( $\forall x$ )
- h3 > h2? false, since NOT  $h2 \Rightarrow h3$  ( $\exists x$ )

- h1 = <Sunny, ?, ?, Strong, ?, ?>
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

Verify the following expressions:

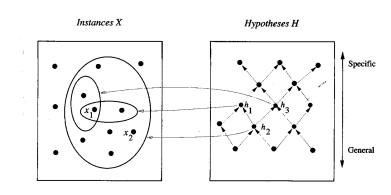
- h2 > h1? true, since  $h1 \Rightarrow h2$  AND it is NOT  $h2 \Rightarrow h1$  ( $\forall x$ )
- h3 > h2? false, since NOT  $h2 \Rightarrow h3$  ( $\exists x$ )
- $h3 \ge h1$ ?

- h1 = <Sunny, ?, ?, Strong, ?, ?>
- h2 = <Sunny, ?, ?, ?, ?, ?>
- h3 = <Sunny, ?, ?, ?, Cool, ?>

Verify the following expressions:

- h2 > h1? true, since  $h1 \Rightarrow h2$  AND it is NOT  $h2 \Rightarrow h1$  ( $\forall x$ )
- h3 > h2? false, since  $h2 \text{ NOT} \Rightarrow h3 (\exists x)$
- $h3 \ge h1$ ? false, x=<Sunny, Warm, High, Strong, Warm, Same>  $\Rightarrow h1(x) = 1 \Rightarrow h3(x) = 1$

## Visualization of X and H



 $x_1$  = <Sunny, Warm, High, Strong, Cool, Same>  $x_2$  = <Sunny, Warm, High, Light, Warm, Same>  $h_1 = \langle Sunny, ?, ?, Strong, ?, ? \rangle$   $h_2 = \langle Sunny, ?, ?, ?, ?, ? \rangle$  $h_3 = \langle Sunny, ?, ?, ?, Cool, ? \rangle$ 

from [Mitchell, 1997]

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## Learning as Search in the Hypothesis Space

- 1 Search from general to specific
  - initial point is the most general hypothesis <?,...,?>
  - positive samples are omitted
  - negative samples are used for specialization
- Search from specific to general
  - initial point is the most specific hypothesis  $\langle \emptyset, ..., \emptyset \rangle$
  - negative samples are omitted
  - positive samples are used for generalization
- 3 Combination of both: Candidate Elimination algorithm (later)

## Learning as Search in the Hypothesis Space

- 1 Search from general to specific
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- Search from specific to general
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  - negative samples are omitted
  - positive samples are used for generalization
- 3 Combination of both: Candidate Elimination algorithm (later)

## Specific-to-General Algorithm

- 1 initialize h as most specific hypothesis in H
- 2 for each positive training sample
  - for each attribute constraint  $a_i$  in  $h < a_0,...,a_n >$ 
    - $\blacksquare$  if  $a_i$  is satisfied by x: do nothing
    - else replace a<sub>i</sub> in h by the next more general constraint that is satisfied by x
- 3 return hypothesis h

# Specific-to-General Algorithm (2)

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

- initialization:  $h=<\emptyset,\emptyset,\emptyset,\emptyset,\emptyset,\emptyset>$
- first sample is positive (EnjoySport( $x_1$ ) = true)
- However,  $h(x_1)$ =false  $\rightarrow$  generalize
- h=<Sunny, Warm, Normal, Strong, Warm, Same>

# Specific-to-General Algorithm (3)

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
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4	Sunny	Warm	High	Strong	Cool	Change	Yes

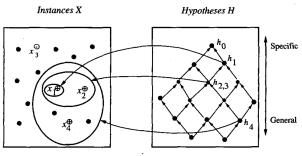
- h=<Sunny, Warm, Normal, Strong, Warm, Same>
- second sample is positive
- However,  $h(x_2)$ =false  $\rightarrow$  generalize (minimally)
- h=<Sunny, Warm, ?, Strong, Warm, Same>

# Specific-to-General Algorithm (4)

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

- h=<Sunny, Warm, ?, Strong, Warm, Same>
- third sample is negative (EnjoySport( $x_3$ ) = false)  $\rightarrow$  ignored
- forth sample is positive
- However,  $h(x_2)$ =false  $\rightarrow$  generalize (minimally)
- h=<Sunny, Warm, ?, Strong, ?, ?>
- termination, return h

## Specific-to-General Algorithm (5)



 $x_1$  = <Sunny Warm Normal Strong Warm Same>, +  $x_2$  = <Sunny Warm High Strong Warm Same>, +  $x_3$  = <Rainy Cold High Strong Warm Change>, -

Same War High Same Carl Character

 $x_4 = \langle Sunny | Warm | High | Strong | Cool | Change \rangle$ , +

 $h_0 = \langle \emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset \rangle$ 

 $h_1 = \langle Sunny | Warm | Normal | Strong | Warm | Same \rangle$ 

 $h_2 = \langle Sunny \ Warm \ ? \ Strong \ Warm \ Same \rangle$ 

h<sub>3</sub> = <Sunny Warm? Strong Warm Same>

 $h_4 = \langle Sunny \ Warm \ ? \ Strong \ ? \ ? \rangle$ 

# Specific-to-general Algorithm (5)

#### Properties of the Specific-to-General Algorithm

- algorithm is guaranteed to output the most specific hypothesis within H that is consistent with the positive training samples
- final hypothesis is also consistent with negative samples provided
  - the correct target concept is in H
  - the examples are correct

## Specific-to-general Algorithm (5)

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- algorithm is guaranteed to output the most specific hypothesis within H that is consistent with the positive training samples
- final hypothesis is also consistent with negative samples provided
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#### BUT:

- is the found h the only one consistent with the data?
- why prefer the most specific  $h_{specific}$ ? Unclear whether we should prefer it over the most general  $h_{general}$ .
- data-inefficient (negative samples ignored) ... and more

## Version Space and Candidate Elimination Algorithm

#### Candidate Elimination algorithm

The Candidate Elimination algorithm finds all describable hypotheses that are consistent with the observed training examples.

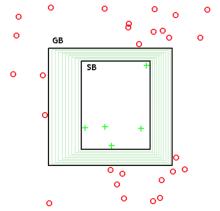
ightarrow represents the set of *all* hypotheses consistent with the observed data. This set is called *Version Space* 

#### Version Space?

The version space, denoted  $VS_{H,D}$ , with respect to hypothesis space H and training examples D, is the subset of hypotheses from H *consistent* with the training examples in D.

[Russell and Norvig, 2003, Mitchell, 1997]

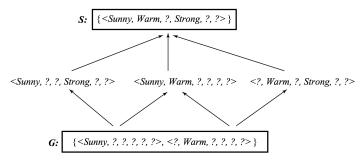
## Example of the Version Space (2)



 $\mathsf{GB} = \mathsf{maximally}$  general positive boundary,  $\mathsf{SB} = \mathsf{maximally}$  specific positive boundary

[Wikipedia: The Free Encyclopedia, 2006]

# Example of the Version Space (2)



The version space for the <code>EnjoySports</code> concept learning task with the previously shown samples. The VS includes all six hypotheses. However, it can simply represented by  ${\sf G}$  and  ${\sf S}$ .

### Candidate Elimination Algorithm

#### Preliminary:

- $S = \{s \mid s \text{ being a hypothesis consistent with the observed samples } \land \text{ there exists no hypothesis which is more specific than } s \text{ that is also consistent with all samples} \}$
- initialize S with < ∅ >
- $G = \{g \mid g \text{ being a hypothesis consistent with the observed samples } \land \text{ there exists no hypothesis which is more general than } g \text{ that is also consistent with all samples} \}$
- initialize G with <? >

# Candidate Elimination Algorithm (2)

### x is a negative sample:

- remove from S any hypothesis inconsistent with x
- for each hypothesis g in G inconsistent with x:
  - remove g from G
  - add to G all minimal specializations h s.t. h is consistent with x, and some member of S is more specific than h
- remove from G any hypothesis less general than another hypothesis in G

# Candidate Elimination Algorithm (2)

#### x is a negative sample:

- remove from S any hypothesis inconsistent with x
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#### x is a positive sample:

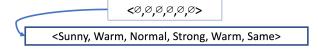
- remove from G any hypothesis inconsistent with x
- for each hypothesis s in S inconsistent with x:
  - remove s from S
  - add to S all minimal generalizations h of S s.t. h is consistent with x, and some member of G is more general than h
- remove from S any hypothesis less general than other hypothesis in S

#### i=1

- S0 = {<Ø,Ø,Ø,Ø,Ø,Ø,Ø>}
- G0 = {<?,?,?,?,?,?>}

#### i=2

- x1= <Sunny, Warm, Normal, Strong, Warm, Same>, c(x1)=true
- · G consistent with x1
- S too specific → generalize until consistent



Learning as Search in the Hypothesis Space

## Candidate Elimination Algorithm Example

#### i=3

- x2= <Sunny, Warm, High, Strong, Warm, Same>, c(x2)=true
- G consistent with x2
- S too specific → generalize until consistent

<Sunny, Warm, Normal, Strong, Warm, Same>

<Sunny, Warm, ?, Strong, Warm, Same>

#### i=4

- x3= <Rainy, Cold, High, Strong, Warm, Change>, c(x3)=false
- S consistent with x3

<Sunny, Warm, Normal, Strong, Warm, Same>

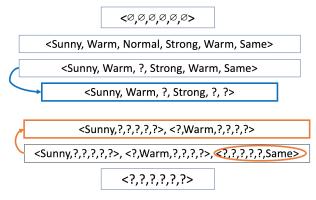
<Sunny, Warm, ?, Strong, Warm, Same>

#### i=4

- x3= <Rainy, Cold, High, Strong, Warm, Change>, c(x3)=false
- S consistent with x3 (no hypotheses in S classify x3 positive)
- G too general→ search minimal specializations, sort out inconsistencies, at least one s∈S must be more specific

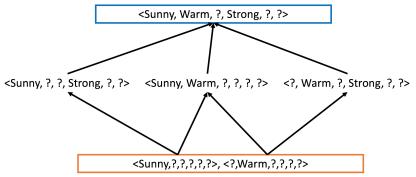
#### i=5

- x4= <Sunny, Warm, High, Strong, Cool, Change>, c(x4)=true
- · One hypothesis inconsistent in G with x4
- S inconsistent with x4 → generalize until consistent



### Resulting Version Space

· all consistent hypotheses



# Candidate Elimination Algorithm Summary

#### Summary:

- the version space learned by the algorithm converges toward the hypothesis correctly describing the target concept given:
  - there are no errors in the training samples
  - there is some hypothesis in H that correctly describes the target concept

# Candidate Elimination Algorithm Summary(2)

#### Advantages:

- instances don't have to be stored (lazy-learning)
- convergence is determinable (S=G)
- data-efficient

#### Disadvantages:

- consistent samples required
- noisy data problematic
- target concept must be represented by hypothesis space

In semi-supervised learning: optimal query strategy is to request instances that satisfy half the hypotheses in the current VS

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Inductive Learning and Biases

### Inductive Learning

What has been shown is associated with inductive learning

#### Induction

Plausible conclusion to the general given an input (specific).

#### Deduction

Logical reasoning from given knowledge (e.g. rules).

### Inductive Learning Hypothesis

Inductive learning makes one fundamental assumption:

#### Induction Learning Hypothesis

Any hypothesis found to approximate a target function well over a sufficiently large set of training examples will also approximate a target function well over unknown samples.

- ⇒ The success of learning an inductive learning machine is heavily dependent on the provided data
- $\Rightarrow$  it can at best guarantee that the output hypothesis fits the target concept over the training data.

## Inductive Learning Hypothesis

- problem: target concept might not be contained in the hypothesis space
- solution(?): use hypothesis space that includes all possible hypotheses

## Inductive Learning Hypothesis

- problem: target concept might not be contained in the hypothesis space
- solution(?): use hypothesis space that includes all possible hypotheses

#### Fundamental Property of Inductive Inference:

An inductive learning machine that makes no a-priori assumptions about the identity of the target concept has no rational basis for classifying unseen instances.

See [Mitchell, 1997] for an example of the futility of bias-free learning.

Inductive Learning and Biases

# Inductive Learning Hypothesis(2)

#### Inductive bias of the Candidate Elimination algorithm

The target concept is contained in the hypothesis space and the concept could be represented by a conjunction of attribute values.

Inductive Learning and Biases

### Biases

#### General Bias

Specification after which hypotheses are constructed. For example: classification accuracy, costs for storing hypotheses, human readability etc.

### Hypothesis Space Bias

What could this be?

#### Preference Bias

What could this be?

### Biases

#### General Bias

Specification after which hypotheses are constructed. For example: classification accuracy, costs for storing hypotheses or human readability

#### Hypothesis Space Bias

An hypothesis belongs to a restricted space of hypotheses, e.g. boolean conjunctions, linear threshold functions or 3-nearest neighbor

#### Preference Bias

There exists an order within the hypothesis space, e.g. prefer hypotheses with fewer disjunctions or prefer smaller decision trees

# Biases (2)

### Adjusting for the Hypothesis Space Bias:

- good classification might require complex hypothesis
- might result in overfitting

#### Adjusting for the Preference Bias:

- choose an hypothesis that correctly classifies as many samples as possible
- misclassification might be taken into account

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### Two central questions

- Recap: inductive learning hypothesis states that any hypothesis that approx. a target function well over train data will also approx it well over unknown examples
- Now: is there a way
  - to quantify a (classification) model's test error over unseen data?
  - that yields the amount of data necessary to learn?
- Vapnik-Chervonenkis (VC) theory can help us here [Vapnik, 1971]
- PAC (probably approximately correct) not addressed here

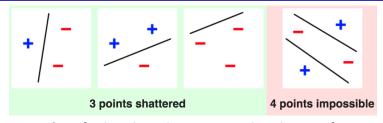
### Definition

A measure of the **capacity** of the hypothesis space that can be learned by a classification model.

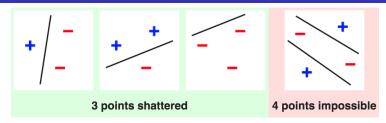
#### **VC-Dimension**

The cardinality of the largest set of points that a classification algorithm can *shatter*.

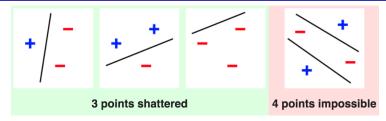
- Assume a binary data separation problem. What does shatter mean?
- Intuitively described:
- $\implies$  all +/- label combinations of a fixed set of points can be separated with the classifier



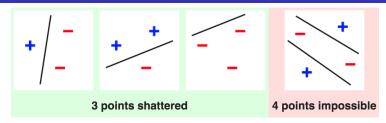
from [Wikipedia: The Free Encyclopedia, 2012]



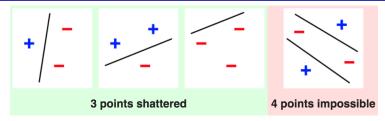
- to show the VC dimension is  $\geq$  a number:
  - ∃data points ∀labelings ∃hypothesis



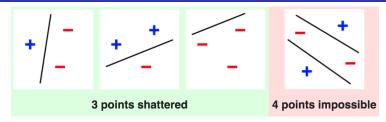
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- to show the VC dimension is **not** > a number:
  - ∀data points ∃labelings ¬(∃hypothesis)



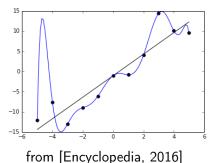
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- showing the lower bound is easier than showing higher bound



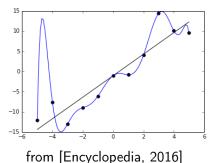
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- Question: which arrangement of 3 points cannot be shattered in a binary classification problem?



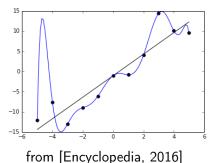
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- showing the lower bound is easier than showing higher bound
- Question: which arrangement of 3 points cannot be shattered in a binary classification problem?
  - $\implies$  3 collinear points



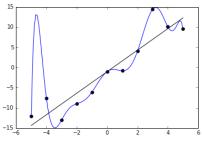
- VC(H) high capacity
- VC(H) low capacity
- assumption: the higher VC(H) the better the classification model



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from [Encyclopedia, 2016]

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- ⇒ wrong

the VC dimension can predict a probabilistic **upper bound** on the test error:

$$Pr\left(testerror \leq trainingerror + \sqrt{...\frac{VC(H)}{N}...}\right) = 1 - \delta$$

while N being the size of the training set, VC(H) the VC dimension of the family of hypotheses H and  $0 \le \delta \le 1$ . What are the implications?

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Without going much into the details, it follows:

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main takeaway: if you use a complex algorithm you will require a lot of data to generalize well

# Curse of Dimensionality

Problems that face the *curse of dimensionality* in inductive learning typically refer to the phenomenon that, when increasing the model dimensionality<sup>3</sup>, the available data becomes sparse

 $\Rightarrow$  the demand for additional data often grows exponentially with the dimensionality

 $<sup>^3</sup>$ e.g. attributes of concepts  $<\times 1, \times 2...>$ , weights/learned parameters in parameterized models

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#### Structural Risk Minimization (SRM)

- the choose a class of functions (e.g. polynomials of degree n)
- 2 divide the class of functions into subsets:  $H_1 \subset H_2 \subset ... \subset H_n$  (e.g. polynomials of increasing degree)
- 3 perform parameter selection (optimize)
- 4 select the model with lowest (empirical) error (and implicitly lowest VC dim)

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for example SVM performs SRM

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VC dimension.