Sapienza University of Rome

Master in Engineering in Computer Science

Machine Learning

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Sapienza University of Rome, Italy - Machine Learning (2024/2025)

1. Introduction

Luca Iocchi

Overview

- What is a Machine Learning problem
- Example: learning to play checkers
- Machine Learning problem formulations
- Learning as search in hypothesis space
- Concept learning
- Machine Learning issues

References
T. Mitchell. Machine Learning. Chapters 1, 2

Machine Learning

Machine learning is programming computers to improve a performance criterion using example data or past experience.

Machine learning (or data mining) is the task of producing knowledge from data.

Machine Learning useful when

- Human expertise does not exist
- Humans are unable to explain their expertise
- Solution needs to be adapted to particular cases

Machine Learning

Machine Learning exploits

- Recent progress in algorithms and theory
- Growing flood of on-line data (Big Data)
- Increasing computational power (GPU)

Machine Learning Applications

Almost in any domain

- Computer vision
- Speech interaction
- Document/text analysis
- Data analytics
- Robot control
- Games

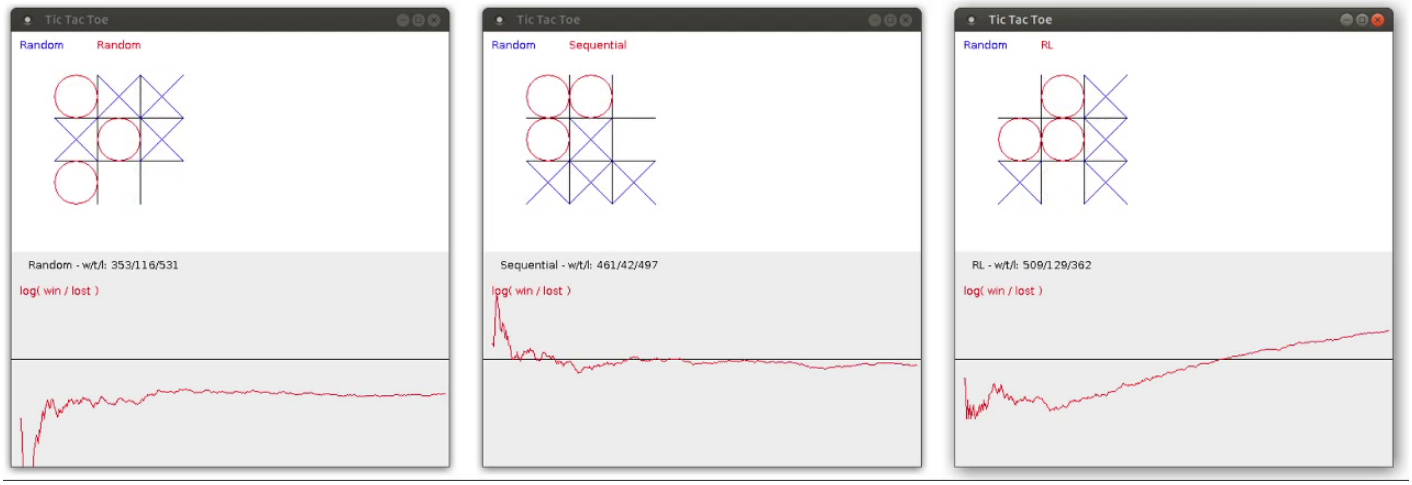
What is a Learning Problem?

Learning = Improving with experience at some task

- Improve over task T,
- with respect to performance measure P,
- based on experience E.

Improving performance over time

Example: Tic Tac Toe (`https://youtu.be/Bpocn3EHYOo`)



Example

Learn to play checkers

- T: Play checkers
- P: % of games won in a tournament
- E: opportunity to play against self

Learning to Play Checkers

- What experience?
- What exactly should be learned?
- How shall it be represented?
- Which algorithm to learn it?

Type of Training Experience

Several options:

- Human expert suggests optimal move for each configuration of the board
- Human expert evaluates each configuration of the board
- Computer plays against a human and automatically detects win/draw/loss configurations
- Computer plays against itself

Problem: is training experience representative of performance goal?

Choose the Target Function

- $ChooseMove : Board \rightarrow Move$
- $V : Board \rightarrow \Re$
- ...

Possible Definition for Target Function V

- if b is a final board state that is won, then $V(b) = 100$
- if b is a final board state that is lost, then $V(b) = -100$
- if b is a final board state that is drawn, then $V(b) = 0$
- if b is a not a final state in the game, then $V(b) = V(b')$, where b' is the best final board state that can be achieved starting from b and playing optimally until the end of the game.

Is it a correct function to learn the task?

Can we compute this function?

Possible Definition for Target Function V

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Is it a correct function to learn the task? **YES**

Can we compute this function? **NO**

this is problem (how we can do it?)

Choose Representation for Target Function

- collection of rules
- neural network
- polynomial function of board features
- ...

A Representation for Function to Learn

$$\hat{V}(b) = w_0 + w_1 \cdot bp(b) + w_2 \cdot rp(b) + w_3 \cdot bk(b) + w_4 \cdot rk(b) + w_5 \cdot bt(b) + w_6 \cdot rt(b)$$

(BLACK PIECE) (RED PIECE) (BLACK KING) (RED KING) (THREATENED BLACK) (THREATENED RED)

- $bp(b)$: number of black pieces on board b
- $rp(b)$: number of red pieces on b
- $bk(b)$: number of black kings on b
- $rk(b)$: number of red kings on b
- $bt(b)$: number of red pieces threatened ("MINACCIATO") by black (i.e., which can be taken on black's next turn)
- $rt(b)$: number of black pieces threatened by red

Is it a correct function to learn the task?

Can we compute this function?

A Representation for Function to Learn

$$\hat{V}(b) = w_0 + w_1 \cdot bp(b) + w_2 \cdot rp(b) + w_3 \cdot bk(b) + w_4 \cdot rk(b) + w_5 \cdot bt(b) + w_6 \cdot rt(b)$$

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Is it a correct function to learn the task? **MAYBE**

Can we compute this function? **YES**

A Representation for Function to Learn

$$\hat{V}(b) = w_0 + w_1 \cdot bp(b) + w_2 \cdot rp(b) + w_3 \cdot bk(b) + w_4 \cdot rk(b) + w_5 \cdot bt(b) + w_6 \cdot rt(b)$$

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Note: Features $f_i(b)$ known, Coefficients w_i unknown

Learning $\hat{V} \equiv$ estimating w_i

Obtaining Training Examples

Notation:

- $V(b)$: the true target function (always unknown)
- $\hat{V}(b)$: the learned function (approximation of $V(b)$ computed by the learning algorithm)
- $V_{train}(b)$: the training value obtained at $b \in$ training data

Dataset $D = \{(b_i, V_{train}(b_i))_{i=1}^{n}\}$

Estimating training values:

- $V_{train}(b_i) \leftarrow$ human expert
- $V_{train}(b_i) \leftarrow$ set of games
- ...

Learning algorithm

LMS Weight update rule:

Initialize w_i (e.g., small random value)
Do repeatedly:

- Select a training example b at random
  1. Compute $error(b)$:

$$error(b) = V_{train}(b) - \hat{V}(b)$$

  2. For each board feature $f_i(b)$, update weight w_i:

$$w_i \leftarrow w_i + c \cdot f_i \cdot error(b)$$

c is some small constant, say 0.1, to moderate the rate of learning

Testing and Evaluation

Learned function (after training)

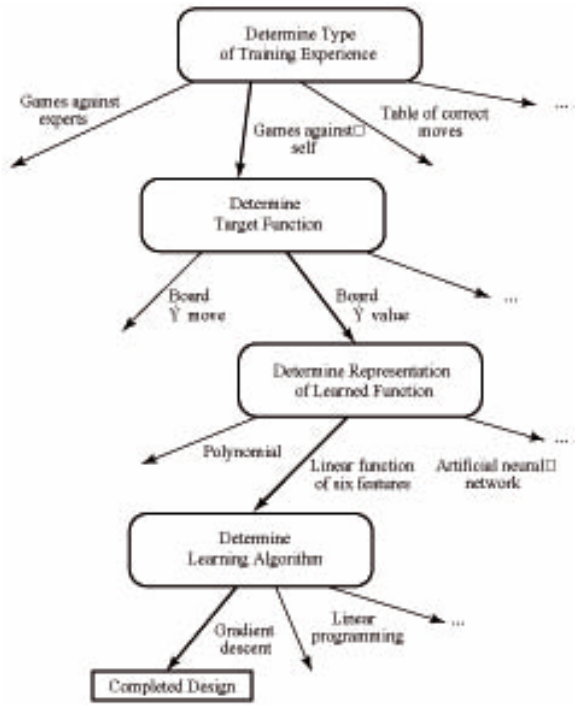
$$\hat{V}(b) = \hat{w}_0 + \hat{w}_1 \cdot bp(b) + \hat{w}_2 \cdot rp(b) + \hat{w}_3 \cdot bk(b) + \hat{w}_4 \cdot rk(b) + \hat{w}_5 \cdot bt(b) + \hat{w}_6 \cdot rt(b)$$

Use this function to play against human players or other computer programs.

How many games won against other players?

If we keep training (i.e., collecting more samples in the dataset), do we increase performance?

Design Choices



Machine Learning Problems

- Supervised Learning
  - Classification
  - Regression
- Unsupervised Learning
- Reinforcement Learning

Machine Learning Problems

General machine learning problem:

Learning a function $f : X \rightarrow Y$, *given a training set* D *containing information about* f

we want $\hat{f}$ closest to target function

Learning a function f means computing an approximated function $\hat{f}$ that returns values as close as possible to f, specially for samples x not present in the training set D.

|sample dataset| < |samples space|
cardinality

$$\hat{f}(x) \approx f(x) \text{ for } x \in X \setminus X_D$$

Note: $X_D = \{x | x \text{ in } D\} \subset X$ with $|X_D| \lll |X|$

Machine Learning Problems

Different types of ML problems depending on
- type of input dataset

Learning a function $f : X \to Y$, given ...

- $D = \{(x_i, y_i)_{i=1}^n\}$ **(Supervised Learning)**
- $D = \{(x_i)_{i=1}^n\}$ **(Unsupervised Learning)**

Learning a behavior function $\pi : S \to A$, given ...

- $D = \{(< s_0, a_1, r_1, s_1, \ldots, a_n, r_n, s_n >_i)_{i=1}^n\}$ **(Reinforcement Learning)**

how the dataset is form
SL → Input and Output (labeled)
UL → only Input without label (NO label)
RL → representation dataset (temporaly execution)

there are intermediate methods "SEMI SUPERVISED" → we don't see them

Supervised Learning

Different types of ML problems depending on
- type of function to be learned

a vector in real domain
↑
vect attribute with certain values
↑

$$X \equiv \begin{cases} A_1 \times \ldots \times A_m, \ A_i \text{ finite sets } \textbf{(Discrete)} \\ \Re^n \textbf{ (Continuous)} \end{cases}$$

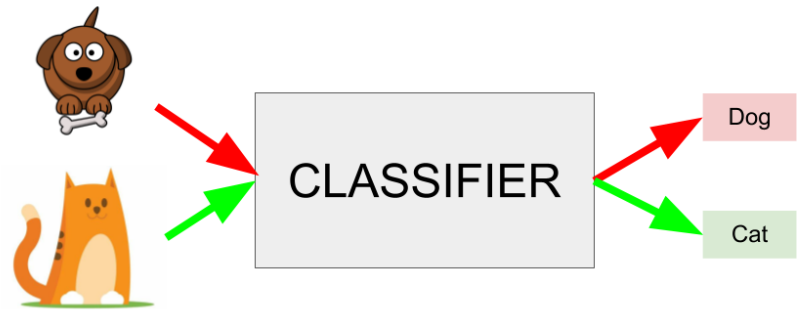
$$Y \equiv \begin{cases} \Re^k \textbf{ (Regression)} \\ \{C_1, \ldots, C_k\}, \textbf{ (Classification)} \end{cases}$$

Special case:
$X \equiv A_1 \times \ldots A_m$ (A_i finite) and $Y \equiv \{0, 1\}$ **(Concept Learning)**

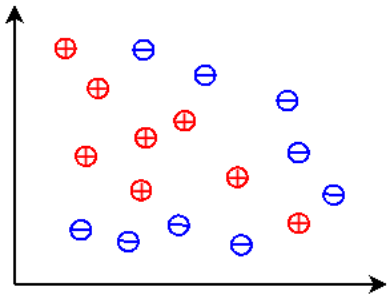
set of attribute
binary set {FALSE, TRUE}

Classification (aka Pattern Recognition)

Return the class to which a specific instance belong.



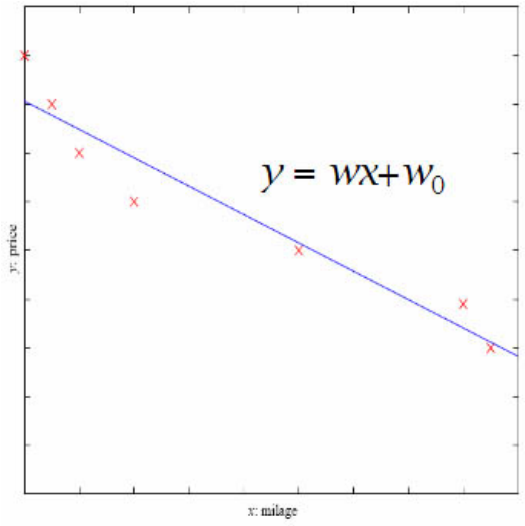
- Face/object/character recognition
- Speech/sound recognition
- Medical diagnosis
- Document classification



Regression

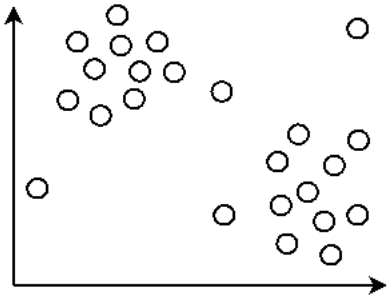
Approximate real-valued functions

Example



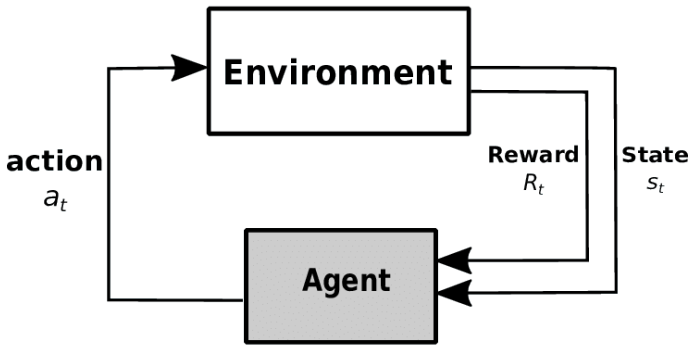
Unsupervised Learning

- Learning what normally happens
- No output available
- Clustering: grouping similar instances
- Example applications
  - Customer segmentation in CRM
  - Image compression: color quantization
  - Bioinformatics: learning motifs



Reinforcement Learning

- Learning a policy (state-action function)
- No supervised output available, only sparse and time-delayed rewards
- Example applications
  - Game playing
  - Robotic tasks
  - ... any dynamic system with unknown or partially known model



Open questions in Machine Learning

- What algorithms can approximate functions well (and when)?
- How does number of training examples influence performance?
- How does complexity of hypothesis representation impact performance?
- How does noisy data influence performance?
- What are the theoretical limits of learnability?
- How can prior knowledge of learner help?
- How can systems alter their own representations?
- How can systems learn continuously?
- What clues can we get from biological learning systems?
- ...

Concept Learning (aka Binary Classification)

Data set:

- Input: X (any kind)
- Output (labels): two classes (Yes/No, True/False, 0/1, +/-)

Target function: $c : X \rightarrow \{0, 1\}$

Example: *PlayTennis* - good time to play tennis

- Input: weather features X
- Output: $\{Yes, No\}$

PlayTennis Data Samples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

PlayTennis Prediction

Prediction on new samples (not in the training data)

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
Today	Sunny	Hot	Normal	Strong	**?**

A model trained with training data can predict a value of *PlayTennis* for Today, for example as Yes.

Hypothesis space

Could be also on one possible solution

Hypothesis h: *representation of the learned function (an approximation of the target function)* ~~all~~ possible solutions /

↳ !! error !! (one possible solution)

Hypothesis space H: *set of all the functions that can be learnt (all possible approximations of the target function)*

Learning: *search in the hypothesis space* using dataset D

$$h^* = \text{argmax}_{h \in H} \, Performance(h, D)$$

Example

Target function $f : \mathbb{N} \to \{P, \neg P\}$

Dataset $D = \{(1, P), (3, P), (5, P), (6, \neg P), (8, \neg P), (10, \neg P)\}$

Hypothesis: $P \subseteq \mathbb{N}$

Hypothesis space: $2^{\mathbb{N}}$ (set of subsets of $\mathbb{N}$)

Examples of hypotheses:

1. $h_1 =$ "$P = \{n \in \mathbb{N} \mid \ldots\}$"
2. $h_2 =$ "$P = \{n \in \mathbb{N} \mid \ldots\}$"
3. $h_3 =$ "$P = \{n \in \mathbb{N} \mid \ldots\}$"
4. $h_4 =$ "$P = \{n \in \mathbb{N} \mid \ldots\}$"

$h_4 = \{1, 3, 5\}$

$h_1 =$ {n odd number} } are consist

$h_2 =$ {n < 6}

$h_3 =$ {n prime}

$h_x =$ {n < 3} => D is not consist because there is not ¬P

Example

Target function $f : \mathbb{N} \to \{P, \neg P\}$

Dataset $D = \{(1, P), (3, P), (5, P), (6, \neg P), (8, \neg P), (10, \neg P)\}$

Hypothesis space: $2^{\mathbb{N}}$ (set of subsets of $\mathbb{N}$)

Prediction for new samples $n \notin D$ (e.g., $n = 11$)

1. $h_1(11) = ?$ P
2. $h_2(11) = ?$ $\neg$P
3. $h_3(11) = ?$ P
4. $h_4(11) = ?$ $\neg$P

based on our h_1 h_2 h_3 h_4

Example

Target function $f : \mathbb{N} \to \{P, \neg P\}$

Dataset $D = \{(1, P), (3, P), (5, P), (6, \neg P), (8, \neg P), (10, \neg P)\}$

Representation power vs. Generalization power

Hypothesis space: $2^H = 2^{2^{\mathbb{N}}}$ (set of hypotheses / set of sets of subsets of $\mathbb{N}$)

Solution: $\theta = \{h_1, h_2, h_3, h_4\} \subset H$ set of hypotesis (set of subsets of $\mathbb{N}$) using majority voting
Prediction $\theta(11) = ?$

$h_1 \in H$ has higher generalization power than $\theta \in 2^H$, since
$h_1(11) = P$, $\theta(11) = ?$

Example

in machine learning to impart GENERALIZATION POWER is it ideato always is not always good

Target function $f : \mathbb{N} \to \{P, \neg P\}$

Dataset $D = \{(1, P), (3, P), (5, P), (6, \neg P), (8, \neg P), (10, \neg P)\}$

Hypothesis space: $2^{2^{\mathbb{N}}}$

Useless solution (no generalization power)

$\theta_0 \in 2^H$, s.t.

$\theta_0(1) = P$, $\theta_0(3) = P$, $\theta_0(5) = P$, $\theta_0(6) = \neg P$, $\theta_0(8) = \neg P$, $\theta_0(10) = \neg P$
$\theta_0(n) = ?$, $\forall n \notin D$

Note: not possible for hypothesis space H

Concept Learning: Notation

OVVERO NON CONOSCO LA FUNZIONE CHE MI DETERMINA IL GIUSTO VALORE ($f(x) : x_i \to c(x_i)$) → ALTRIMENTI MI AVREI RISOLTO IL TASK → CONOSCO SOLO DATO x_i IL CORRISPETTIVO $c(x_i)$

c: target function $c : X \to \{0, 1\}$

X: instance space

$x \in X$: one instance

$D = \{(x_i, c(x_i))_{i=1}^n\}$: training set

I only know general value for x_i !NO! for all dataset

$c(x)$: value of the target function over x (*true value* known only for instances in D)

H: hypothesis space

$h \in H$: one hypothesis (an approximation of c)

$h(x)$: estimation of h over x (*predicted or estimated value*)

Learning task

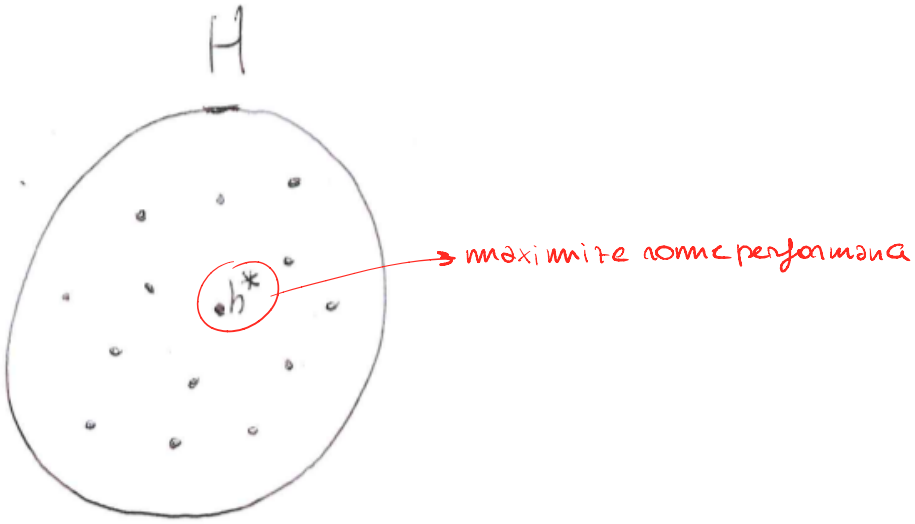
Given a training set $D = \{(x_i, c(x_i))\}$, find the *best* approximation $h^* \in H$ of the target function $c : X \to \{0, 1\}$.

Steps:

1. Define the hypothesis space H (i.e., a representation of the hypotheses)
2. Define a performance metric to determine the *best* approximation
3. Define an appropriate algorithm

Learning as a search problem

Given a representation of the hypothesis space H, search for the *best* hypothesis $h^* \in H$, according to a given performance measure.



Evaluating instances on hypotheses

$h(x)$ can be computed for every $x \in X$

$h(x_i) = c(x_i)$ can be verified only for instances x_i appearing in the data set D ($x_i \in D$), for which we know $c(x_i)$

> *A hypothesis h is* **consistent** *with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $(x, c(x))$ in D.*

Projection of X over D

$$Consistent(h, D) \equiv (\forall x \in D)\ h(x) = c(x)$$

this is FORMAL definition

$X_D = \{x_i \in X : (x_i, c(x_i)) \in D\}$

↳ because is not precise notation

The *real goal* of a machine learning system is to find the *best* hypothesis h that predicts correct values of $h(x')$ for instances $x' \notin D$ with respect to the unknown values $c(x')$.

Performance measure

Given a training set $D = \{(x_i, c(x_i))\}$ and a hypothesis $h \in H$, a performance measure is based on evaluating $c(x_i) = h(x_i)$ for all $x_i \in D$.

Inductive learning hypothesis: Any hypothesis that approximates the target function well over a sufficiently large set of training examples will also approximate the target function well over other unobserved examples.

VERSUS-SPACE and HYPOTHESIS-SPACE

VERSUS SPACE → si riferisce allo "spazio delle caratteristiche" ossia allo spazio in cui ogni punto rappresenta una combinazione delle variabili dei dati

HYPOTHESIS SPACE → è l'insieme di tutte le possibili funzioni o modelli che l'algoritmo può adottare per fare previsioni o classificazioni all'interno del VERSUS SPACE

Prototypical Concept Learning Task

Given:

- Instances X (e.g., possible days, each described by the attributes *Outlook, Temperature, Humidity, Wind*)
- Target function $c : X \to \{0, 1\}$ (e.g., $c = \mathit{PlayTennis} : X \to \{\mathit{No}, \mathit{Yes}\}$)
- Hypotheses H
- Training examples $D = \{(x_1, c(x_1)), \ldots, (x_n, c(x_n))\}$, positive and negative examples of the target function

Determine:

- A consistent hypothesis (i.e., $h \in H$ such that $h(x) = c(x)$, $\forall x \in D$).

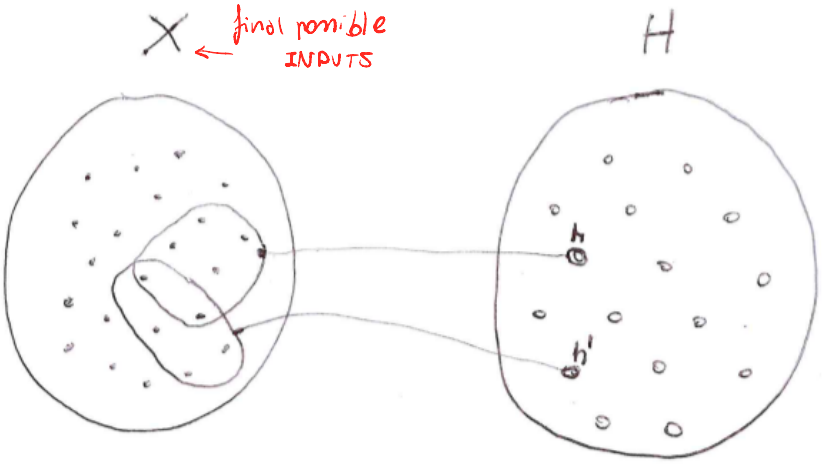
Representation of hypothesis space

... let's skip this part for the moment ...

Representation of hypothesis space

In concept learning (i.e., binary classification), every hypothesis is associated to a set of instances (i.e., all the instances that are classified as positive by such hypothesis).

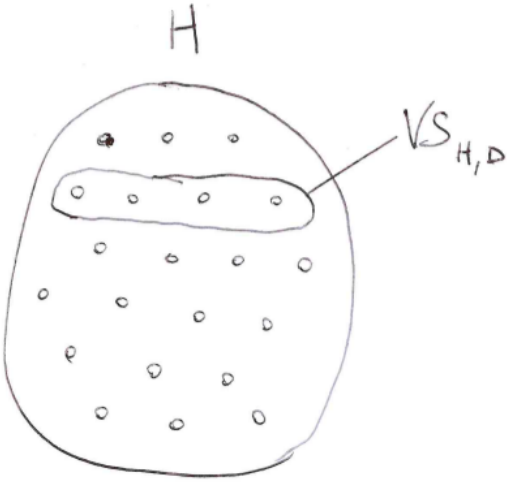
$$h \leftrightarrow S = \{x \in X | h(x) = 1\} \subseteq X \qquad H \leftrightarrow 2^X$$



Version Spaces

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

$$VS_{H,D} \equiv \{h \in H | Consistent(h, D)\}$$



List-Then-Eliminate Algorithm

1. *VersionSpace* $\leftarrow$ a list containing every hypothesis in H
2. For each training example, $(x, c(x))$
   remove from *VersionSpace* any hypothesis h for which $h(x) \neq c(x)$
3. Output the list of hypotheses in *VersionSpace*

Note: enumerating all the hypotheses!

Example 1

Instance space X: integer points in a 2D plane

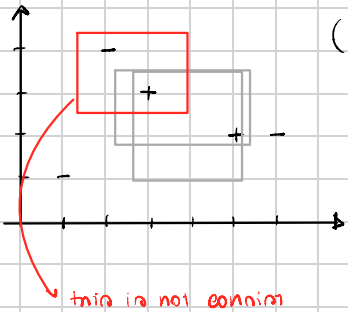
Output classes: $\{+, -\}$

Data set D: positive and negative examples in 2D plane

Hypotheses H: rectangles in the 2D plane with edges parallel to the axes ($h(x) = +$ iff x inside the rectangle)

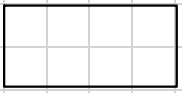
Exercises:
1) Determine the version space of data set
$D = \{((3,3),+),((4,2),+),((2,4),-),((1,1),-),((5,2),-)\}$
2) Draw a dataset for which the version space is empty (i.e., no consistent hypothesis can be determined)

EXAMPLE



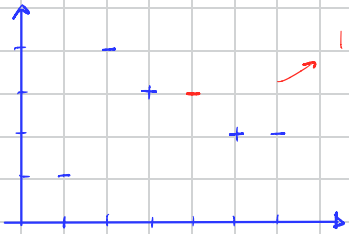
x_i $c(x_i)$

$((3,3), +)$

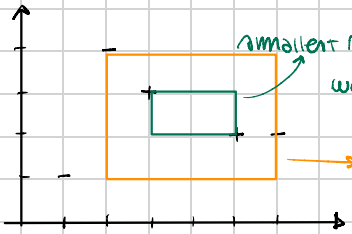
our hypothesis space →  → + for all points inside and − for all points that are outside

will be empty in this case (mean there isn't a coming hypothesis)

this is not coming

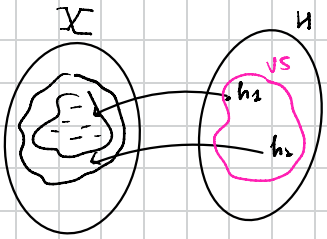


I can't create a rectangular



smallest rectangular we can have → the biggest

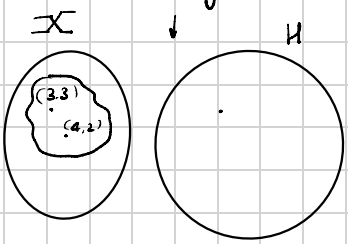
are called "BOUNDARIES OF VERSION SPACE"



$\theta_1 = \langle h_1, h_2 \rangle \in H'$

$H' = 2^H$ $H \to 2^X$ ⇒ much powerfull

meaning that



no hp can be mapped in X

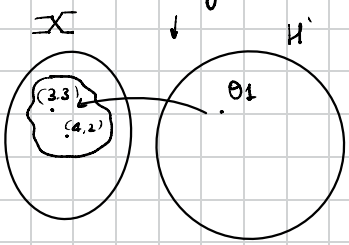
such that $(2, +)$

very bad for ML

$\exists \theta_1, \theta_2 \in H'$ s.t. $\theta_1(x) = +$ $\theta_2(x) = -$

because represent every subset ... (min 1:00:00)

meaning that



!! with H' yes !!

↳ we have to restrict the power of language in H we don't have this problem :

H → must have 2 features
- representation language BIAS
- search algorithm BIAS

GENERALIZATION POWER

we can combine hypothesis → example $H_1 = \square$ $H_2 = \square$ $H_3 = \diamond$ $H_4 = \bigcirc$ $H_5 = H_1 \cup H_4$

usually more powerfull less generalization

Example 2

Now let's consider a different hypothesis space.

Hypotheses H': sets of rectangles in the 2D plane with edges parallel to the axes

Note: H' can represent any possible subset of X

$$\forall S \in 2^X, \exists h \in H', \textit{such that } S = \{x \in X | h(x) = +\}$$

(while this property is not true for the hypothesis space H)

Output of a learning system

1. $VS_{H',D}$ (H' can represent all the subsets of X)
2. $VS_{H,D}$ (H can not represent all the subsets of X)
3. $h^* \in VS_{H,D}$ (h^* is one hypothesis chosen within the VS)

Classify new instances

Given $x' \notin D$, predict class $+$ or $-$.

1. $VS_{H',D} \Rightarrow \forall x' \notin D$, for some $h' \in VS_{H',D}, h'(x') = +$, for some other $h' \in VS_{H',D}, h'(x') = -$
2. $VS_{H,D} \Rightarrow \exists x' \notin D$, for some $h \in VS_{H,D}, h(x') = +$, for some other $h \in VS_{H,D}, h(x') = -$
3. $h^* \in VS_{H,D} \Rightarrow \forall x' \notin D$, $h^*(x')$ is either $+$ or $-$.

Machine Learning representation issue

1. $VS_{H',D} \Rightarrow$ cannot predict instances not in D (for all $x' \notin D$, it will answer *unknown*)
2. $VS_{H,D} \Rightarrow$ limited prediction instances not in D (for some $x' \notin D$, it will answer *unknown*)
3. $h^* \in VS_{H,D} \Rightarrow$ maximum prediction power on values not in D (for all $x' \notin D$, it will always return a predicted value)

If hypothesis space is too powerful (any subset of the instances can be represented in it), and the search is complete (all the solutions are computed), then the system is not able to classify new instances (no generalization power).

↳ !! OVERFITTING !!

Machine Learning noisy data issue

Data set may contain noisy data (a typical case in real applications) $D = \{(x_i, y_i)\}$ with $y_i \neq c(x_i)$ for some i

There may be no consistent hypotheses, i.e., $VS_{H,D} = \emptyset$

In case of noisy data set, statistical methods must be used to implement robust algorithms.

Summary

- Machine Learning can be seen as learning a function from samples.
- Learning as search requires definition of a hypothesis space and an algorithm to search solutions in this space
- Performance are based on consistency
- Two main issues: 1) representation vs. generalization power, 2) noisy data
- **Statistical methods are needed!!!**