



From Complexity to Intelligence

Machine Learning and Complexity









Reminder

What is Machine Learning?

Types of Learning

The no-free-lunch theorem

Analysis of the ERM principle

Basic MDL in i.i.d. setting





What is the difference between deduction and induction?



What is the difference between deduction and induction?

Deductive reasoning is an approach where a set of logic rules are applied to general axioms in order to find (or more precisely *to infer*) conclusions of no greater generality than the premises. Inductive

reasoning is an approach in which the premises provide **a strong evidence** for the truth of the conclusion.





What is the idea of Solomonoff's induction?







■ ※ I Solomonoff's induction

What is the idea of Solomonoff's induction?

Combining the Principle of Multiple Explanations, the Principle of Occam's Razor, Bayes Rule, using Turing Machines to represent hypotheses and Algorithmic Information Theory to calculate their probability.

$$H^* = \arg \max_{H_i} \left\{ 2^{-K(H_i)} \times Pr(D|H_i) \right\}$$



一選家 Proportional analogy

What is the problem of Proportional Analogy?





What is the problem of Proportional Analogy?

Definition (Analogy reasoning)

Analogy reasoning is a form of reasoning in which one entity is inferred to be similar to another entity in a certain respect, on the basis of the known similarity between the entities in other respects.

Proportional Analogy concerns any situation of the form "A is to B as C is to D"







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Three inductive principles

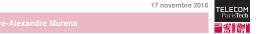
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A basic approach of learning

A definition (T. Mitchell, 1997)

A computer program is said to learn from experience \mathcal{E} with respect to some class of tasks \mathcal{T} and performance measure \mathcal{P} , if its performance at tasks in \mathcal{T} , as measured by \mathcal{P} , improves with experience \mathcal{E} .



Examples

Handwriting recognition



- Task: recognize and label handwritten words in images
- Performance measure : percentage of words successfully labeled
- Experience : database of manually labeled handwritten words



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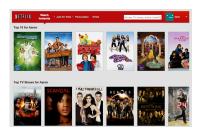


- Task: play checkers
- Performance measure : percentage of victories
- Experience : practice games against itself









- Task: recommend to any user videos he might like
- Performance measure : percentage of recommendation success
- Experience : list of videos liked by a set of users







■選択 A formal model

- Input space : a set X
- **Output space**: a set \mathcal{Y}
- Training data : $\mathcal{D}_{S} = \{(x_1, y_1), \dots, (x_n, y_n)\}$
- **Decision function :** a function $h: \mathcal{X} \mapsto \mathcal{Y}$

Knowing the data \mathcal{D}_S , the system aims at learning the function h.







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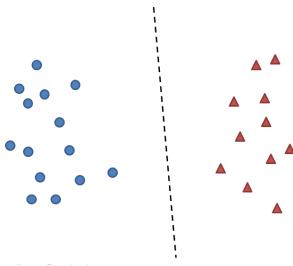


- In **Supervised Learning**, the labels $y \in \mathcal{Y}$ are given. The goal is to estimate a correct labelling function $h: \mathcal{X} \mapsto \mathcal{Y}$.
- In **Unsupervised Learning**, the labels are unknown. The purpose is to group *similar* points.
- In **Semi-Supervised Learning**, some labels are unknown. The purpose is to estimate a correct labelling function h, exploiting information brought by non labelled points.





Supervised Learning



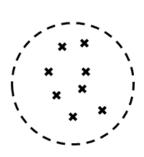








Unsupervised Learning





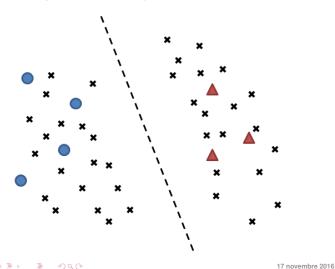








Semi-Supervised Learning









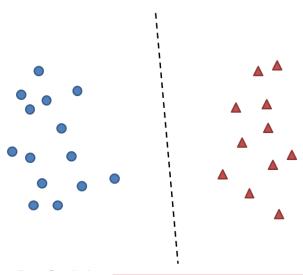
- In **classification**, the output set \mathcal{Y} is discrete (and finite).
- In **regression**, the output set \mathcal{Y} is continuous.





Classification vs Regression

Classification





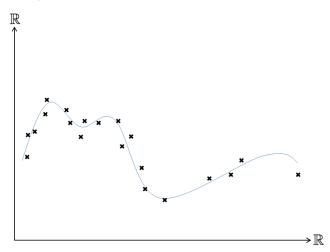






Classification vs Regression

Regression





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We will:

- Focus on classification problems (mainly binary : $\mathcal{Y} = \{0, 1\}$)
- Consider Unsupervised Leaning as a separate problem
- Examine what the statistics have to say
- Try to see a link with Analogy Reasoning





We will:

- Focus on classification problems (mainly binary : $\mathcal{Y} = \{0, 1\}$)
- Consider Unsupervised Leaning as a separate problem
- Examine what the statistics have to say
- Try to see a link with Analogy Reasoning

We won't:

- Focus on methods
- Consider the problems of ranking and recommendation
- Consider "real-time processes"
- Pronounce the words neural network and deep learning







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What is Unsupervised Learning?

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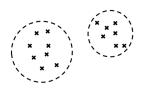
In Unsupervised Learning, the learner receives unlabeled input data and aims at *finding a structure* for these data.

Tasks in Unsupervised Learning

- Clustering : grouping a set of objects such that similar objects end up in the same group and dissimilar objects are separated into different groups.
- Anomaly detection: identifying objects which do not conform to the global behavior.



直接扩 Clustering



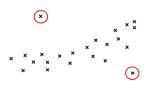
Basic idea : Points which are close are similar; Points which are far are dissimilar.

Applications:

- Marketing : detect groups of users with similar behaviors
- Medicine: detect mutations of a virus
- Visualization : find similar land-use on a satellite picture







Basic idea : Find a general rule describing data and isolate points which do not obey this rule.

Applications:

- Fraud detection
- Networks: intrusion detection, event detection...





■選択 Unsupervised learning = Compression

Idea

In both Clustering and Anomaly Detection, the problem is to find regularities / structure.

Finding structure = Compressing the description of data

Hence, Unsupervised Learning = Compression

Besides, unsupervised learning is just a redescription of data, so is not directly a problem of induction.







K-Means algorithm

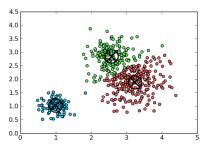
Inputs : Dataset $X = \{X_1, \dots, X_n\}$; Number of clusters k**Initialization :** Randomly choose initial centroids μ_1, \ldots, μ_k Repeat until convergence:

- For all $i \le k$, set $C_i = \{x \in X; i = \operatorname{argmin}_i ||x \mu_i||\}$
- For all $i \le k$, update $\mu_i = \frac{1}{|G_i|} \sum_{x \in G_i} x$









The data points are not described by their **absolute position** but by their **relative position to the closest prototype**.

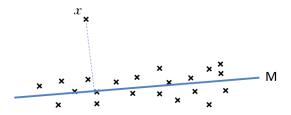




■選載WII Compression in Anomaly Detection

Applying MDL principle : find a model M minimizing C(M) + C(D|M)

x is an anomaly if $C(x|M) \approx C(x)$





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- Suppose that data $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ are generated according to a probability distribution $\mathbb{P}_{X\times Y}$.
- **Consider** a *loss function I* : $\mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}$ which quantifies the "cost" of misclassification
- We define the risk of a classifier $h: \mathcal{X} \mapsto \mathcal{Y}$ as :

$$R(h) = \int_{\mathcal{X} \times \mathcal{Y}} I(h(x), y) d\mathbb{P}_{X \times Y}(x, y)$$

Question: can we find an algorithm which will *always* infer good hypotheses?







The no-free-lunch theorem Wolpert's answer



No!











The no-free-lunch theorem

[Wolpert, 1996]

For any two learning algorithms \mathcal{A}_1 and \mathcal{A}_2 with posterior distributions $p_1(h|\mathcal{S})$ and $p_2(h|\mathcal{S})$ (where \mathcal{S} is a data set), for any distribution $\mathbb{P}_{\mathcal{X}}$ of data and for any number m of data, the following propositions are true :

- 1. In uniform average over all target functions $f \in \mathcal{F}$: $\mathbb{E}_1[R|f,m] \mathbb{E}_2[R|f,m] = 0$
- 2. For any given learning set S, in uniform average over all target functions $f \in \mathcal{F} : \mathbb{E}_1[R|f,S] \mathbb{E}_2[R|f,S] = 0$
- 3. In uniform average over all possible distributions P(f): $\mathbb{E}_1[R|f] \mathbb{E}_2[R|f] = 0$
- 4. For any given learning set S, in uniform average over all possible distributions P(f): $\mathbb{E}_1[R|S] \mathbb{E}_2[R|S] = 0$







The no-free-lunch theorem [Wolpert, 1996]

Consequences of the no-free-lunch theorem

- A "good" classification algorithm will have **in average** the same performance as a "bad" classification algorithm (*average over the space of problems*) if all target functions *f* are equiprobable.
- For any region of the space of problems where an algorithm \mathcal{A} is good, there exists a region where \mathcal{A} is bad.























Conclusions of the no-free-lunch theorem

- 1. A learning algorithm is **biased** to a certain class of problems.
- 2. The performance of an algorithm is **necessarily** relative to a class of problems.
- 3. Induction does not create information: it only *transforms* a prior information contained in the algorithm.

There exists two types of biases:

- 1. Representation bias: a bias on the form of concept
- 2. Research bias: a bias on how the concept is searched







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First principle : Empirical Risk **Minimization**

Given a loss function $I: \mathcal{Y} \times \mathcal{Y} \mapsto \mathbb{R}$ and a classifier h, we can define :

The risk of h:

$$R(h) = \int_{\mathcal{X} \times \mathcal{Y}} I(h(x), y) d\mathbb{P}_{X,Y}(x, y)$$

The empirical risk of h:

$$\widehat{R}_n(h) = \frac{1}{n} \sum_{i=1}^n I(h(x_i), y_i)$$

ERM principle : $\widehat{h} = \arg \min_{h} \widehat{R_n}(h)$







Second Principle : Bayesianism

Bayesianism is based on Bayes rule:

$$P(M|D) = \frac{P(M) \times P(D|M)}{P(D)}$$

Maximum A Posteriori (MAP) :

$$\widehat{h}_{MAP} = \operatorname{argmax}_h \{P(h|D) \times P(h)\}$$

Maximum Likelihood (ML):

$$\hat{h}_{ML} = \operatorname{argmax}_h P(D|h)$$







Third Principle : Minimum Description Length

One more time!

MDL Principle

The best theory to describe observed data is the one which minimizes the sum of the description length (in bits) of :

- the theory description
- the data encoded from the theory

$$\hat{h} = \operatorname{argmin}_h K(h) + K(D|h)$$

or

$$\widehat{h} = \operatorname{argmin}_h \quad C(h) + C(D|h)$$







Using the prefix complexity K, MDL principle is equivalent to Bayes rule :

$$K(h) + K(D|h) = -\log P(h) - \log P(D|h)$$

Thus:

$$\operatorname{argmin}_h\{K(h)+K(D|h)\}=\operatorname{argmax}_h\{\log P(h)+\log P(D|h)\}$$



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Reminder : the ERM principle

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The risk of h:

$$R(h) = \int_{\mathcal{X} \times \mathcal{Y}} I(h(x), y) d\mathbb{P}_{X,Y}(x, y)$$

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ERM principle : $\widehat{h} = \arg \min_{h} \widehat{R_n}(h)$



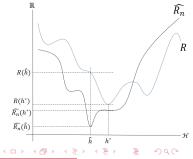
■選擇 Is ERM legit?

1. Is the hypothesis \hat{h} good in the real risk?

$$\widehat{R_n}(\widehat{h}) \stackrel{?}{\longleftrightarrow} R(\widehat{h})$$

2. Am I far from the real optimum $(h^* = \arg \min_h R(h))$?

$$R(\widehat{h}) \stackrel{?}{\longleftrightarrow} R(h^*)$$



Probabilities help us answer these questions.

PAC learning



Leslie Valiant (1949-...)

The purpose of PAC learning is to select with high probability (*probably*) a hypothesis with low generalization error (*approximately correct*).

PAC = Probably Approximately Correct





Let's choose a classifier h with empirical risk $\widehat{R_n}(h) = 0$. What is the probability to have $R(h) > \epsilon$?

■ Suppose that $R(h) \ge \epsilon$. The probability that **one** point is drawn with an empirical risk $\widehat{R_1}(h) = 0$ is :

$$p(\widehat{R_1}(h)=0)\leq 1-\epsilon$$

After m independent and identically distributed draws :

$$p^m(\widehat{R_n}(h)=0) \leq (1-\epsilon)^m$$



For any $\epsilon, \delta \in [0, 1]$,

$$p^{m}(R(h) \ge \epsilon) \le \delta \Leftrightarrow m \ge \frac{\ln\left(\frac{1}{\delta}\right)}{\epsilon}$$



Let's choose our hypothesis in a finite set \mathcal{H} . Then for all $h \in \mathcal{H}, \delta \in [0,1]$:

$$P^{m}\left[R(h) \leq \widehat{R_{m}}(h) + \frac{\ln|\mathcal{H}| + \ln\frac{1}{\delta}}{m}\right] > 1 - \delta$$

Oracle inequality:

For any $\delta \in [0, 1]$:

$$P^m \left\lceil R(\widehat{h_m}) \leq R(h^*) + \sqrt{\frac{2}{n} \ln \left(\frac{2|\mathcal{H}|}{\delta}\right)} \right\rceil > 1 - \delta$$





Is ERM legit?

Step 3: What if the hypothesis space is infinite?



Vladimir Vapnik (1936-...)

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Alexei Chervonenkis (1938-2014)

17 novembre 2016



Is ERM legit?

Step 3: What if the hypothesis space is infinite?

Vapnik-Chervonenkis theory

Let \mathcal{H} be a Vapnik-Chervonenkis class. Then for any $\delta \in [0, 1]$:

$$P\left[R(\widehat{h_m}) \leq R(h^*) + 4\sqrt{\frac{2(V_{\mathcal{H}}\ln(m+1) + \ln 2)}{m}} + \sqrt{\frac{2\ln\frac{1}{\delta}}{m}}\right] > 1 - \delta$$

and:

$$P\left[|R(\widehat{h_m})-\widehat{R_n}(\widehat{h})|\leq 2\sqrt{\frac{2(V_{\mathcal{H}}\ln(m+1)+\ln 2)}{m}}+\sqrt{\frac{\ln\frac{1}{\delta}}{2m}}\right]>1-\delta$$





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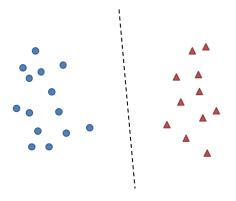
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Classification problem



Goal : find a *classifier* which "separates" the two classes.





17 novembre 2016



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Independent and Identically Distributed

In **statistical learning**, it is often assumed that data are i.i.d. This assumption is **very strong and limiting** (but has really nice properties...!)

- Independent : $P(X_i, X_i) = P(X_i)P(X_i)$
- **Identically distributed**: The data X_i are drawn from a same distribution





Notations

- Data $\mathcal{D} = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$
- Input space ${\mathcal X}$ and output space ${\mathcal Y}$
- \blacksquare Hypothesis space \mathcal{H}
- A classifier is a function $h: \mathcal{X} \mapsto \mathcal{Y}$
- \blacksquare $h \in \mathcal{H}$





Basic MDL in i.i.d. setting

minimize_M
$$K(M) + K(X, Y|M)$$

minimize_M $C(M) + C(X, Y|M)$

Generative approach:

- Aims at discovering the joint distribution of X and Y
- Gives a procedure to *generate* data from the same distribution.
- The model describes the data

Discriminative approach:

- Aims at discovering the conditional distribution of Y|X
- Gives a procedure to determine the classes
- The model does not describe the input data





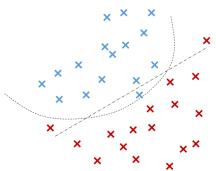




i ※劉祉 ■ MDL and model selection

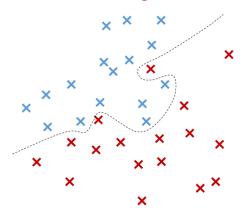
Main (admitted) use of MDL principle in Machine Learning!

If several models can explain the data, choose the model with the lowest Kolmogorov complexity.





MDL and overfitting

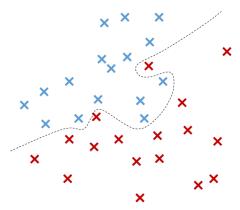












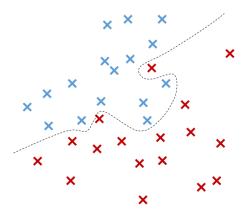
MDL naturally prevents overfitting!

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図版 MDL and overfitting



MDL naturally prevents overfitting! But was it intended ... ?







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Back to Analogy Reasoning

 $ABC \Longrightarrow ABD$ $IJK \Longrightarrow ?$









$$\mathbf{ABC} \Longrightarrow \mathbf{ABD}$$
$$\mathbf{IJK} \Longrightarrow ?$$

The problem can be formulated with the machine learning notations:

$$X_{learn} \Longrightarrow Y_{learn}$$

 $X_{test} \Longrightarrow ?$

This problem has a name: transfer learning





Transductive Learning

Statistics Professors HATE Him!



Doctor's discovery revealed the secret to learning any problem with just 10 training samples. Watch this shocking video and learn how rapidly you can find a solution to your learning problems using this one sneaky kernel trick! Free from overfitting!

http://www.oneweirdkerneltrick.com





Transductive Learning

Solving a problem of interest, do not solve a more general (and therefore worse-posed) problem as an intermediate step. Try to get the answer that you really need but not a more general one.

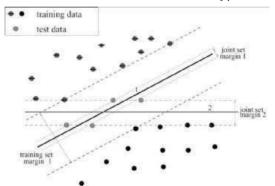
- Do not estimate a density if you need to estimate a function. (Do not use classical generative models; use ML predictive models.)
- Do not estimate a function if you need to estimate values at given points. (Try to perform transduction, not induction)
- Do not estimate predictive values if your goal is to act well. (A good strategy of action can rely just on good selective inference.)





Transductive Learning

Transduction = Transfer with i.i.d. hypothesis









An equation (with familiar terms...)

$$C(M_S) + C(X_S|M_S) + C(\beta_S|M_S, X_S) + C(Y_S|M_S, X_S, \beta_S) + C(M_T|M_S) + C(X_T|M_T)$$







An equation (with familiar terms...)

$$C(M_{S}) + C(X_{S}|M_{S}) + C(\beta_{S}|M_{S}, X_{S}) + C(Y_{S}|M_{S}, X_{S}, \beta_{S}) + C(M_{T}|M_{S}) + C(X_{T}|M_{T})$$

- lacksquare C(M): prior
- C(X|M) : likelihood
- lacksquare C(Y|M,X,eta) : risk
- lacksquare $C(M_T|M_S)$: transfer term (related to a prior?)







In many problems, I don't know the future test data! Transduction is not possible... And our equation is not valid anymore...

- What does it mean to generalize well from a complexity point of view?
- Is it enough to write that $X_T = \langle \rangle$?
- Our equation seems still valid (the individual terms are used in classical inductive principles.)





Isn't this question of generalization already answered by PAC learning, VC theory etc...?

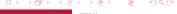


Isn't this question of generalization already answered by PAC learning, VC theory etc...?

Yes and no!

These theories are valid only for the limit case of i.i.d. data **and i.i.d. questions**









- 1. The learner is not indifferent to the future question : the *priors* over the future are my only guarantee of generalization?
- 2. All previously encountered data, problems and knowledge have a maximal pertinence : Asymptotic results in statistical learning and Solomonoff's induction theories? Creation of knowledge by one-shot learning?







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- Induction is **definitely not** a simple problem!
- Compression is closely related to learning
- The no-free-lunch theorem : no miracle classifier!
- MDL is hidden everywhere in Machine Learning
- New principles are necessary to formalize the transition from the particular to the general





- Induction is definitely not a simple problem!
- Compression is closely related to learning
- The no-free-lunch theorem : no miracle classifier!
- MDL is hidden everywhere in Machine Learning
- New principles are necessary to formalize the transition from the particular to the general

But...

- Most of these questions are never addressed in ML courses
- Most people prefer focusing on algorithms
- Most people ignore that such problems exist









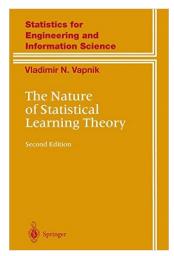








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